Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 08:19 PM EST

PDB ID	:	1VQ4
Title	:	The structure of the transition state analogue "DAA" bound to the large ribosomal subunit of Haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

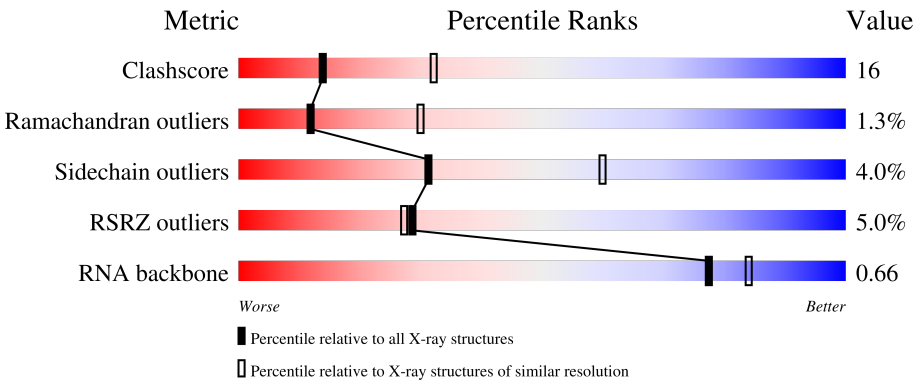
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	%, 59%, 30%, 5%, 6%
2	9	122	3%, 53%, 34%, 11%
3	4	8	38%, 50%, 12%
4	A	240	4%, 56%, 38%
5	B	338	%, 52%, 42%, 6%

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Mol	Chain	Length	Quality of chain
6	C	246	%, 54%, 41%, 5%
7	D	177	35%, 28%, 47%, 21%
8	E	178	8%, 59%, 36%
9	F	120	18%, 55%, 42%
10	G	348	3%, 5%, 92%
11	H	171	4%, 57%, 33%, 6%
12	J	145	%, 68%, 26%
13	K	132	2%, 55%, 42%
14	L	165	13%, 52%, 35%, 12%
15	M	194	%, 66%, 31%
16	N	187	10%, 52%, 43%
17	O	116	69%, 30%
18	P	149	64%, 29%
19	Q	96	%, 72%, 25%
20	R	155	%, 58%, 37%
21	S	85	2%, 65%, 31%, 5%
22	T	120	11%, 51%, 42%, 6%
23	U	66	5%, 48%, 32%, 20%
24	V	71	30%, 46%, 44%, 8%
25	W	154	%, 47%, 49%
26	X	92	8%, 43%, 42%, 11%
27	Y	241	%, 41%, 17%, 41%
28	Z	83	4%, 46%, 37%, 5%, 12%
29	1	57	65%, 33%
30	2	50	10%, 50%, 42%, 8%

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Mol	Chain	Length	Quality of chain
31	3	92	3% 66% 34%
32	I	162	34% 19% 23% 57%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8090	-	-	-	X
33	MG	0	8092	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9182	-	-	-	X
35	NA	R	9186	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 98999 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59021	26350	10878	19048	2745	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	127	61	23	38	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	237	1753	1072	352	324	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	337	2625	1616	493	511	5	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	246	1859	1131	344	383	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	D	140	1094	685	195	210	4	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	E	172	1357	840	224	289	4	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	F	119	890	551	141	197	1	0	0	0

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	G	29	240	149	39	51	1	0	0	0

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	H	160	1266	785	237	238	6	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	J	142	1120	696	199	222	3	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	K	132	992	609	187	192	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	L	145	1118	670	222	226	0	0	0

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	M	194	1560	943	332	284	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	N	186	1445	895	262	286	2	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	O	115	865	529	161	175	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	P	143	1136	683	229	224	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	Q	95	735	450	141	144	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	150	1149	713	209	223	4	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	S	81	641	389	111	138	3	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
22	T	119	950	568	180	202	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	U	53	410	244	75	86	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	V	65	499	304	94	100	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	W	154	1196	737	209	244	6	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	X	82	654	402	129	122	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
27	Y	142	1130	686	228	216	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	Z	73	578	346	116	111	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	1	56	431	258	86	83	4	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	2	46	396	239	89	67	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	3	92	755	458	153	137	7	0	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	I	70	519	323	81	114	1	0	0	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
33	0	108	108	108	0	0
33	9	2	2	2	0	0
33	A	2	2	2	0	0
33	B	1	1	1	0	0
33	K	1	1	1	0	0
33	T	1	1	1	0	0
33	Y	1	1	1	0	0
33	3	1	1	1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
34	0	3	3	3	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
35	0	72	72	72	0	0
35	9	2	2	2	0	0
35	A	1	1	1	0	0
35	C	1	1	1	0	0
35	H	2	2	2	0	0
35	J	1	1	1	0	0
35	L	1	1	1	0	0
35	M	1	1	1	0	0
35	Q	1	1	1	0	0
35	R	3	3	3	0	0
35	S	1	1	1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
36	0	10	10	10	0	0
36	A	1	1	1	0	0
36	B	1	1	1	0	0
36	J	3	3	3	0	0
36	K	1	1	1	0	0
36	L	1	1	1	0	0
36	M	1	1	1	0	0
36	N	1	1	1	0	0
36	O	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	R	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5764	Total O 5764 5764	0	0
38	9	133	Total O 133 133	0	0
38	4	3	Total O 3 3	0	0
38	A	116	Total O 116 116	0	0
38	B	143	Total O 143 143	0	0
38	C	173	Total O 173 173	0	0
38	D	44	Total O 44 44	0	0
38	E	43	Total O 43 43	0	0
38	F	24	Total O 24 24	0	0
38	G	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	H	66	Total O 66 66	0	0
38	J	52	Total O 52 52	0	0
38	K	57	Total O 57 57	0	0
38	L	81	Total O 81 81	0	0
38	M	115	Total O 115 115	0	0
38	N	61	Total O 61 61	0	0
38	O	45	Total O 45 45	0	0
38	P	63	Total O 63 63	0	0
38	Q	52	Total O 52 52	0	0
38	R	89	Total O 89 89	0	0
38	S	31	Total O 31 31	0	0
38	T	36	Total O 36 36	0	0
38	U	26	Total O 26 26	0	0
38	V	13	Total O 13 13	0	0
38	W	70	Total O 70 70	0	0
38	X	31	Total O 31 31	0	0
38	Y	93	Total O 93 93	0	0
38	Z	31	Total O 31 31	0	0
38	1	61	Total O 61 61	0	0
38	2	42	Total O 42 42	0	0
38	3	71	Total O 71 71	0	0

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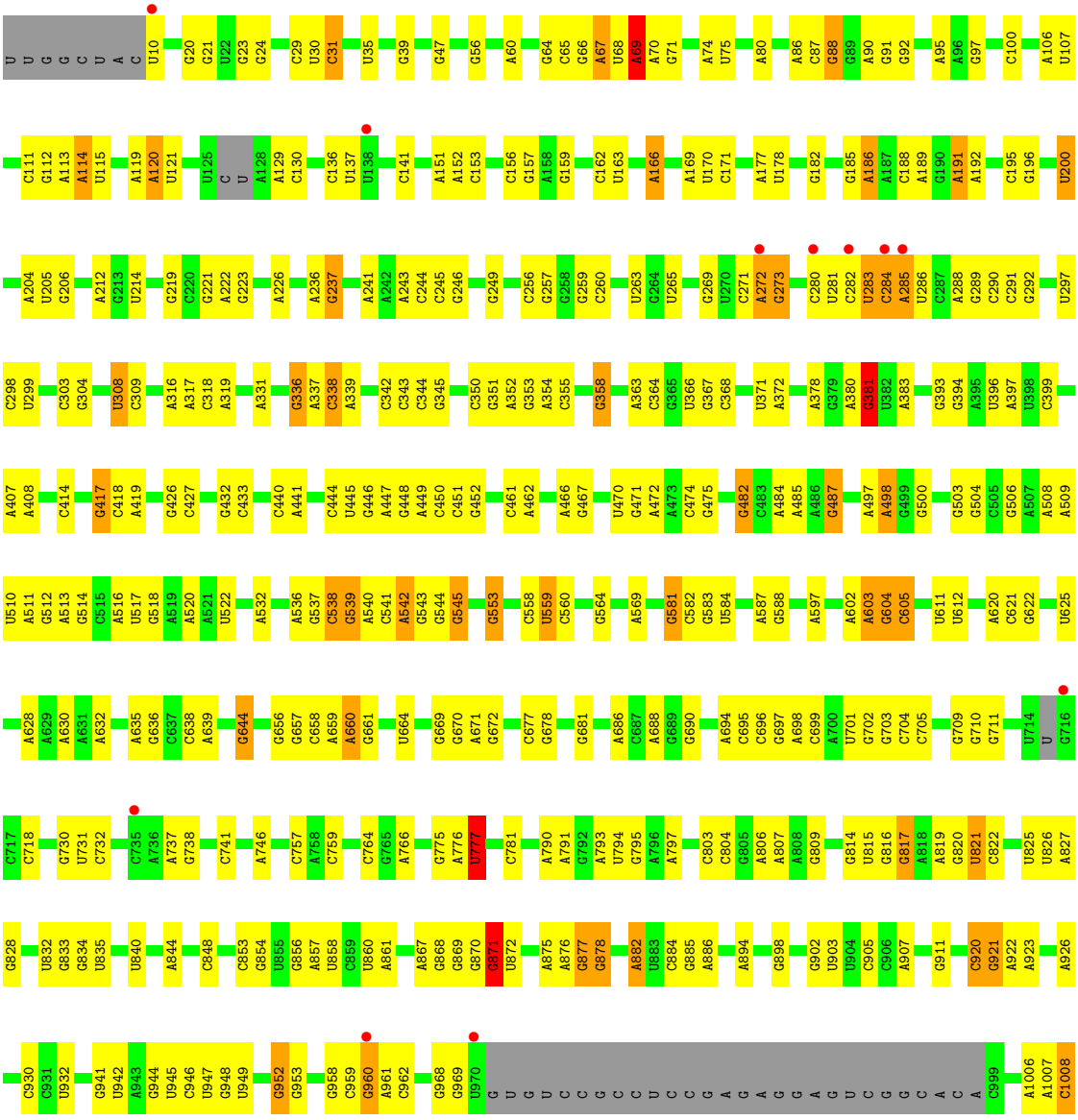
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
38	I	9	9	9	0	0

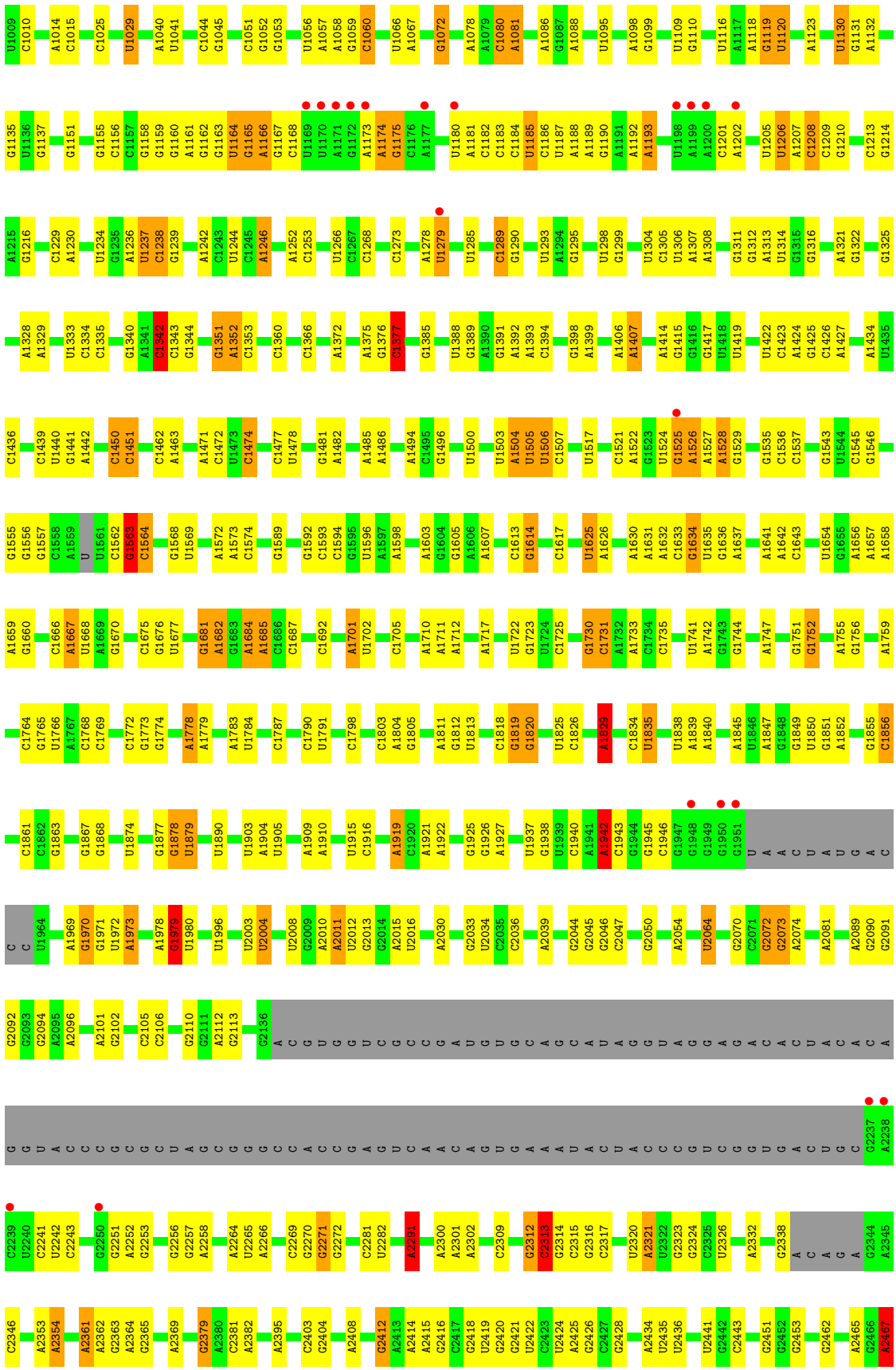
3 Residue-property plots (i)

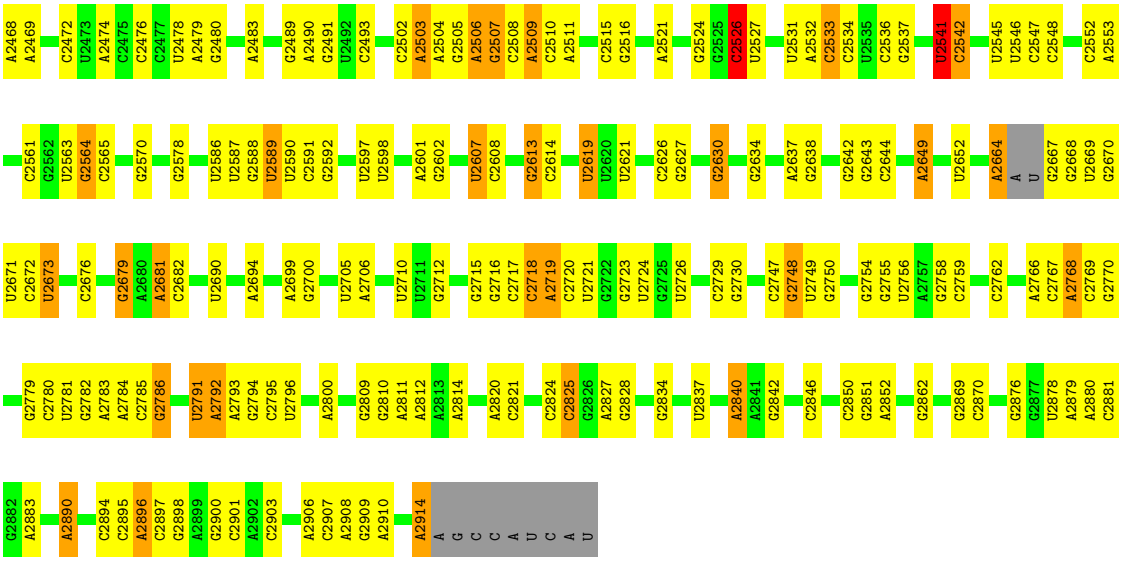
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ribosomal rna

Chain 0:

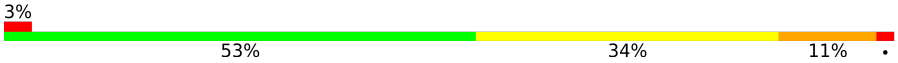


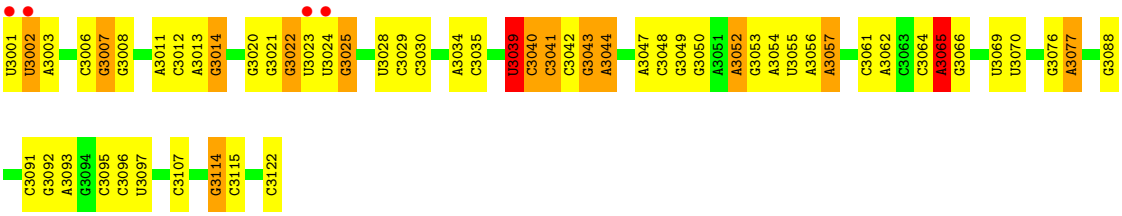

U1009 C1010 A1014 C1015 C1025 U1029 A1040 U1041 C1044 G1045 C1051 G1052 G1053 U1056 A1057 A1058 G1059 C1060 U1066 A1067 G1072 A1078 A1079 C1080 A1081 A1086 G1087 A1088 U1095 A1098 G1099 U1109 G1110 U1116 A1117 A1118 G1119 U1120 A1123 U1130 G1131 A1132
G1135 U1136 G1137 G1151 G1155 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 A1175 C1176 A1177 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 A1190 A1191 A1192 A1193 U1198 A1199 A1200 C1201 A1202 U1205 U1206 A1207 C1208 C1209 G1210 C1213 G1214
A1215 G1216 C1229 A1230 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 A1252 C1253 U1266 C1267 C1268 C1273 A1278 U1279 U1285 C1289 G1290 U1293 A1294 G1295 U1298 G1299 U1304 C1305 U1306 A1307 A1308 G1311 G1312 A1313 U1314 G1315 G1316 A1321 G1322 G1325
A1328 A1329 U1333 C1334 C1335 G1340 A1341 C1342 C1343 G1344 G1351 A1352 C1353 C1360 C1366 A1372 A1375 G1376 C1377 G1385 U1388 G1389 A1390 G1391 A1392 A1393 C1394 G1398 A1399 A1406 A1407 A1414 G1415 G1416 G1417 U1418 U1419 U1422 C1423 A1424 C1425 C1426 A1427 A1434 U1435
C1436 C1439 U1440 G1441 A1442 C1450 C1451 C1462 A1463 A1471 C1472 U1473 C1474 C1477 U1478 G1481 A1482 A1485 A1486 A1494 C1495 G1496 U1500 U1503 A1504 U1505 U1506 C1507 U1517 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1537 G1543 U1544 C1545 G1546
G1555 G1556 G1557 C1558 A1559 U U1561 C1562 G1563 C1564 G1568 U1569 A1572 A1573 C1574 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 A1606 A1607 C1613 G1614 C1617 U1625 A1626 A1630 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 U1654 G1655 A1656 A1657 A1658
A1659 G1660 C1666 A1667 U1668 A1669 G1670 C1675 G1676 U1677 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 A1701 U1702 C1705 A1710 A1711 A1712 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 U1741 A1742 G1743 G1744 A1747 G1751 G1752 A1755 G1756 A1759
C1764 G1765 U1766 A1767 C1768 C1769 C1772 G1773 G1774 A1778 A1779 A1783 U1784 C1787 C1790 U1791 C1798 C1803 A1804 G1805 A1811 G1812 U1813 C1818 G1819 G1820 U1825 C1826 A1829 C1834 U1835 U1838 A1839 A1840 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 G1855 C1856
C1861 C1862 G1863 G1867 G1868 U1874 G1877 G1878 U1879 U1890 U1903 A1904 U1905 A1909 A1910 U1915 C1916 A1919 C1920 A1921 A1922 G1925 G1926 A1927 U1937 G1938 U1939 C1940 A1941 A1942 C1943 G1944 G1945 C1946 G1947 G1948 G1949 G1950 G1951 U A A A C U A U A C U A C A
C C U1964 A1969 G1970 G1971 U1972 A1973 A1978 G1979 U1980 U1996 U2003 U2004 U2008 G2009 A2010 A2011 U2012 G2013 G2014 A2015 U2016 A2030 G2033 U2034 C2035 C2036 A2039 G2044 G2045 G2046 C2047 G2050 A2054 U2064 G2070 C2071 G2072 G2073 A2074 A2081 A2089 G2090 G2091
G2092 G2093 G2094 A2095 A2096 A2101 G2102 C2105 C2106 G2110 G2111 A2112 G2113 G2136 A C G U G G U C G C C G A U G U G C A G C A A U A G G U A C A G G A C A C U A C A C A
G G U A C C C G C G C U G C A C G G A G U C C C G U C A G G A C C A G G U G C G G A C U A A G C A C U A C A G C A
C2239 U2240 C2241 U2242 C2243 G2250 G2251 A2252 G2253 G2256 G2257 A2258 A2264 U2265 A2266 C2269 G2270 G2271 G2272 C2281 U2282 A2291 A2300 A2301 A2302 C2309 G2312 C2313 G2314 C2315 G2316 C2317 U2320 A2321 U2322 G2323 G2324 C2325 U2326 A2332 G2338 A C A G A G2344 A2345
C2346 A2353 A2354 A2361 A2362 G2363 A2364 G2365 A2369 G2379 A2380 C2381 A2382 A2395 C2403 G2404 A2408 G2412 A2413 A2414 A2415 G2416 C2417 G2418 U2419 G2420 G2421 U2422 C2423 U2424 A2425 G2426 C2427 G2428 A2434 U2435 U2436 U2441 G2442 C2443 G2451 G2452 G2453 G2462 A2465 G2466 A2467



- Molecule 2: 5S ribosomal RNA

Chain 9:



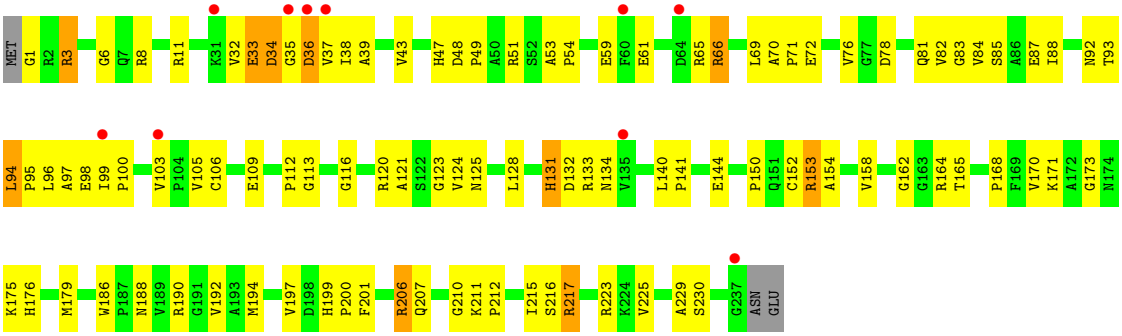


- Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3')

Chain 4:

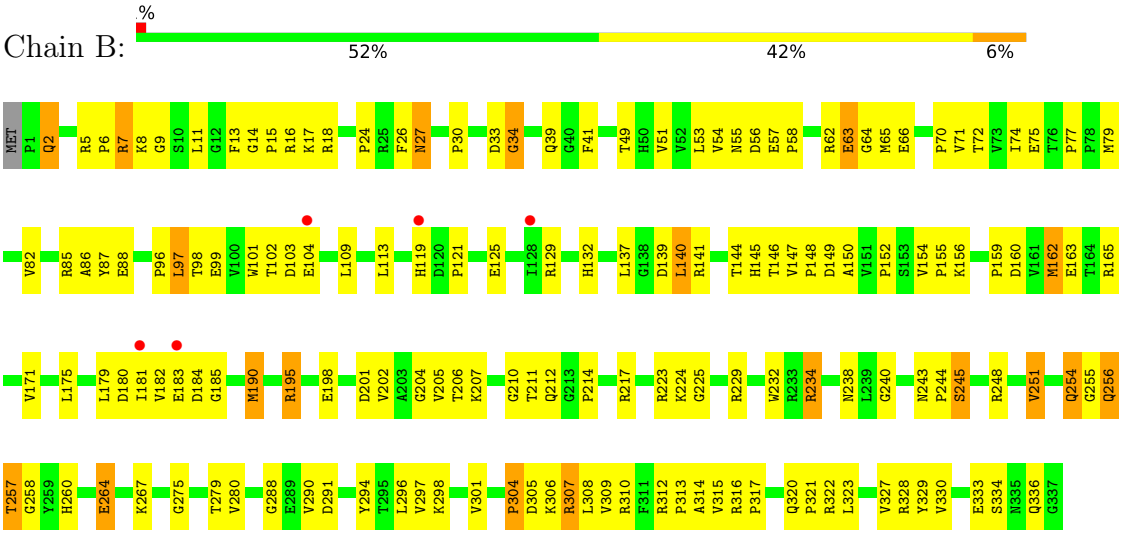
- Molecule 4: 50S ribosomal protein L2P

Chain A:



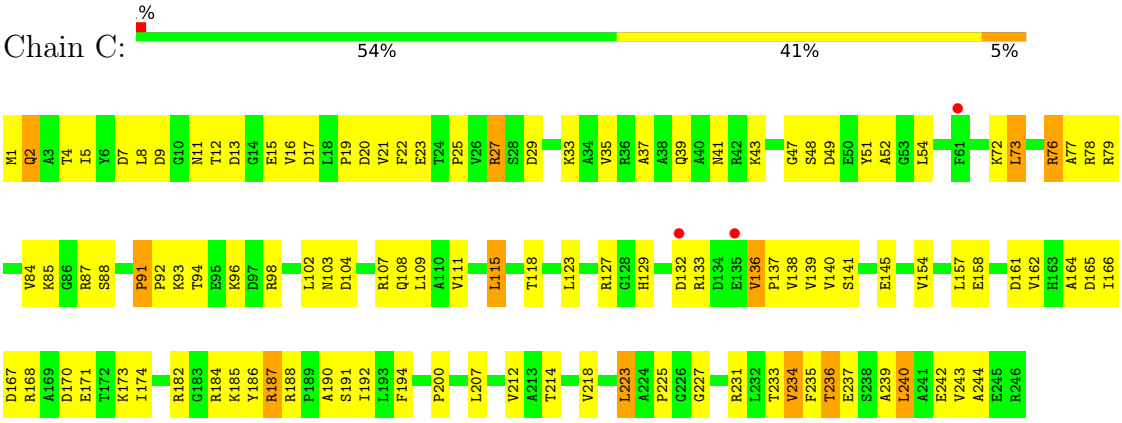
- Molecule 5: 50S ribosomal protein L3P

Chain B:



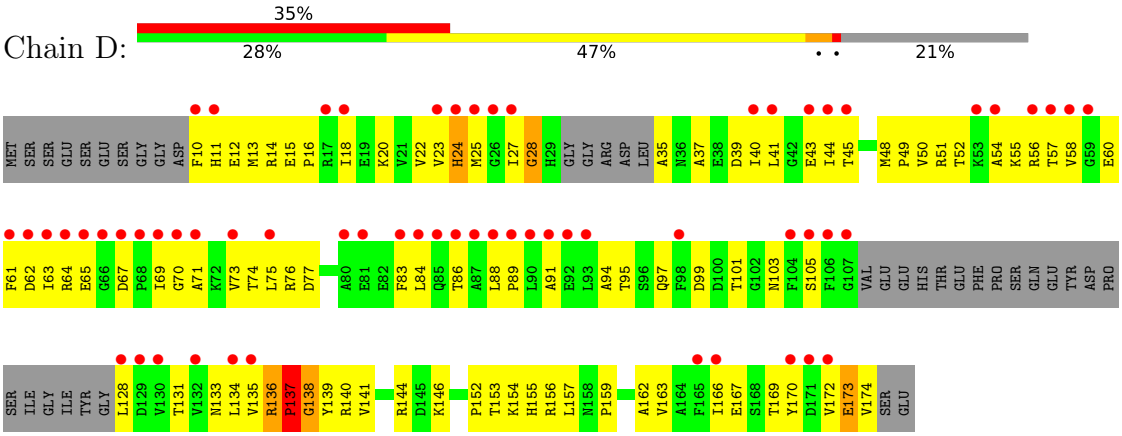
- Molecule 6: 50S ribosomal protein L4E

Chain C:



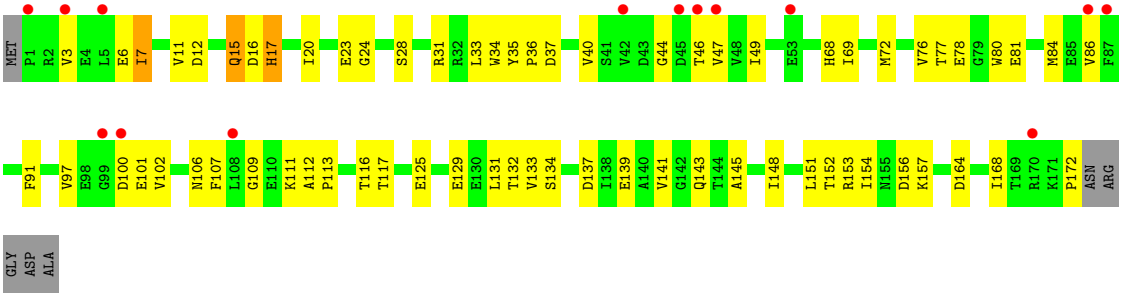
- Molecule 7: 50S ribosomal protein L5P

Chain D:



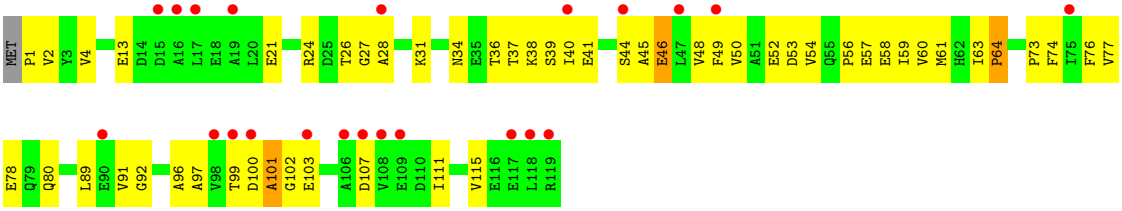
- Molecule 8: 50S ribosomal protein L6P

Chain E:



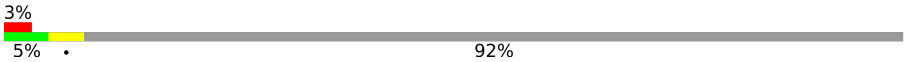
• Molecule 9: 50S ribosomal protein L7AE

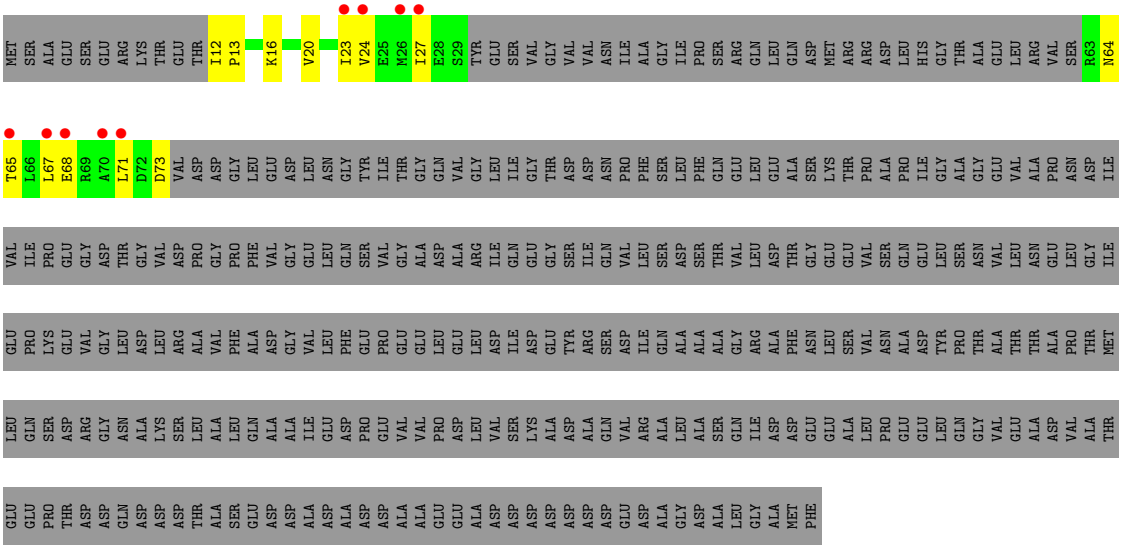
Chain F:



• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

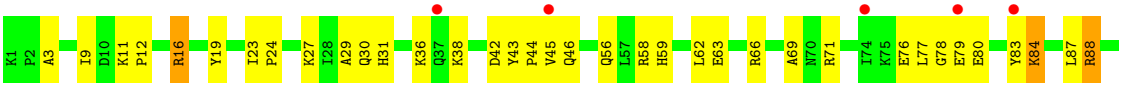
Chain G:

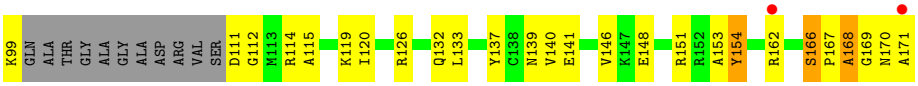




• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

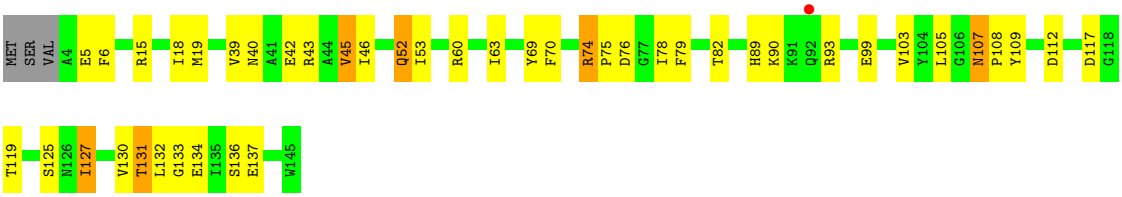
Chain H:





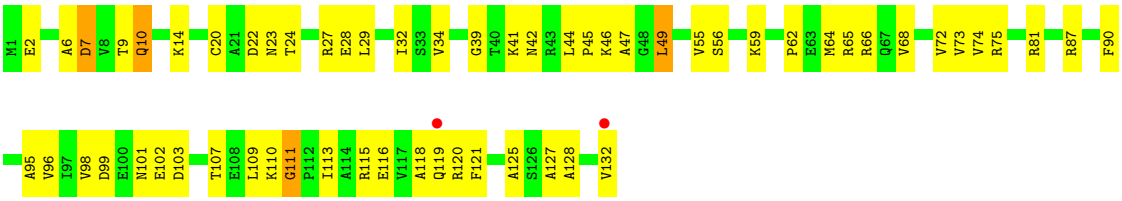
• Molecule 12: 50S ribosomal protein L13P

Chain J:



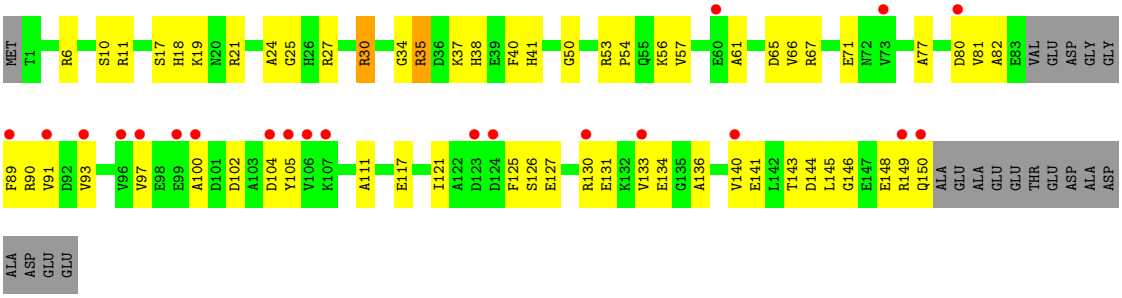
• Molecule 13: 50S ribosomal protein L14P

Chain K:



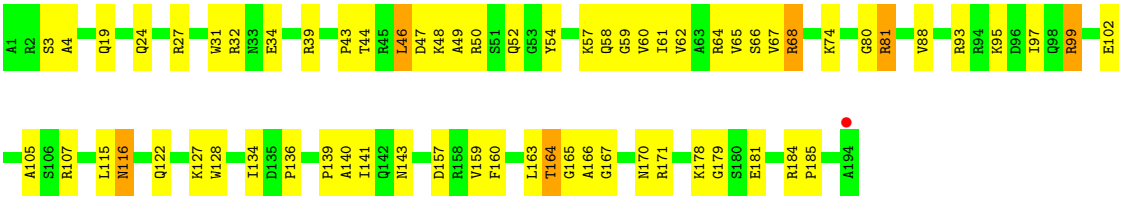
• Molecule 14: 50S ribosomal protein L15P

Chain L:



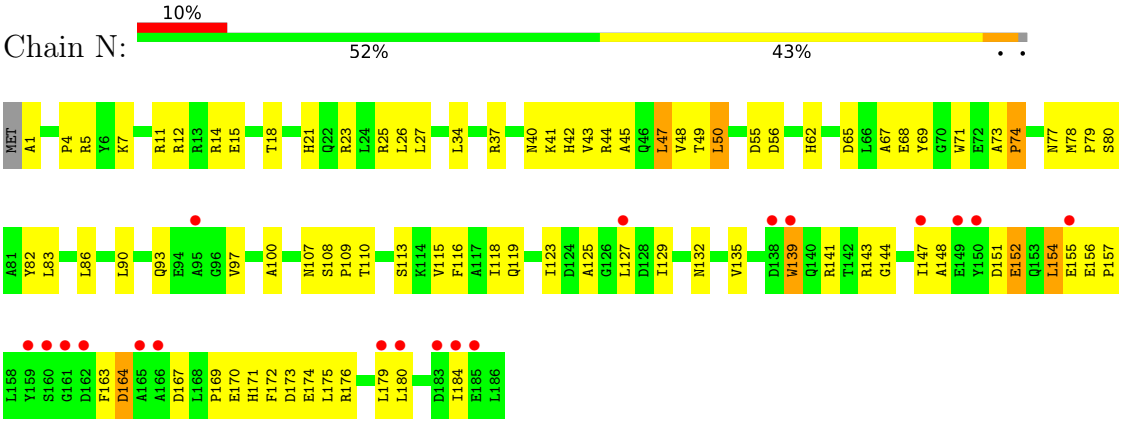
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



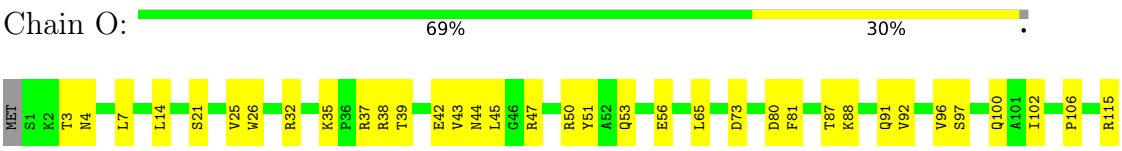
• Molecule 16: 50S ribosomal protein L18P

Chain N:



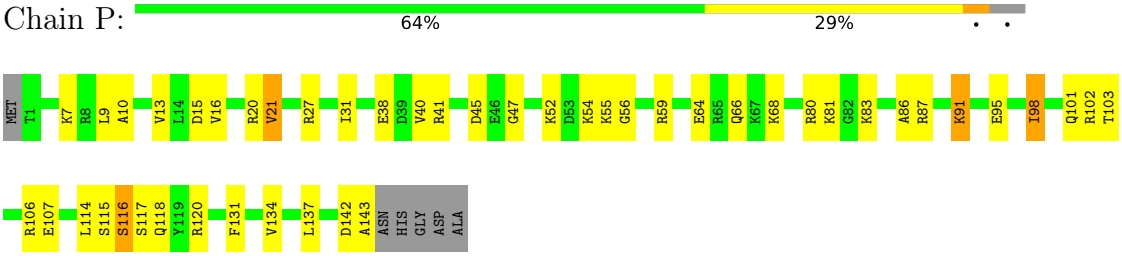
- Molecule 17: 50S ribosomal protein L18e

Chain O:



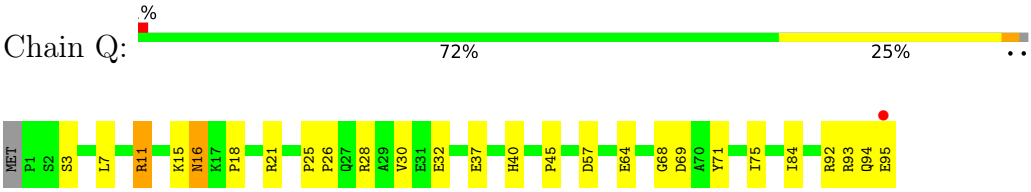
- Molecule 18: 50S ribosomal protein L19E

Chain P:



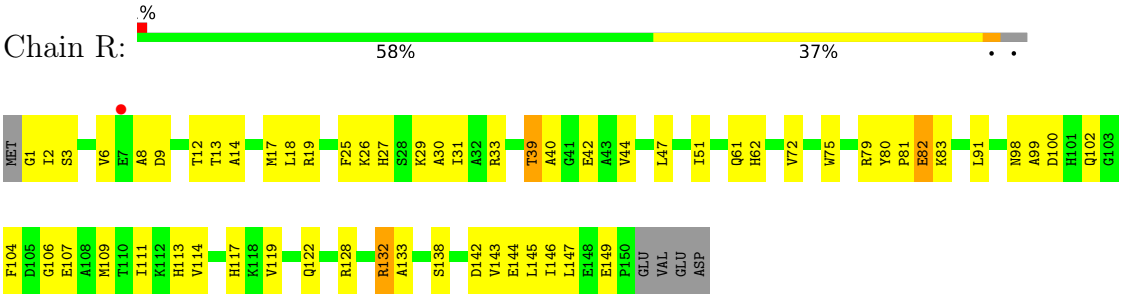
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



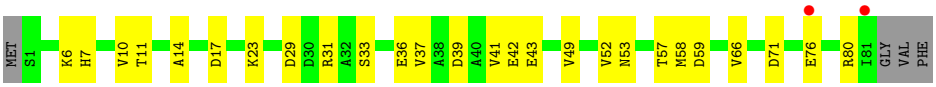
- Molecule 20: 50S ribosomal protein L22P

Chain R:



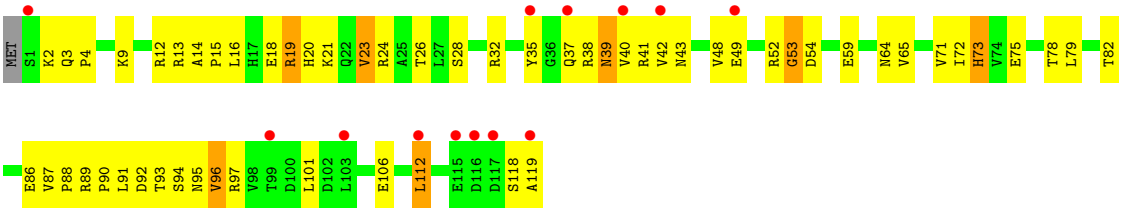
- Molecule 21: 50S ribosomal protein L23P

Chain S: 2% 65% 31% 5%



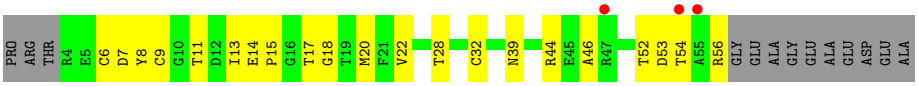
• Molecule 22: 50S ribosomal protein L24P

Chain T: 11% 51% 42% 6%



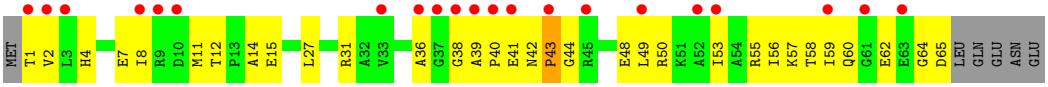
• Molecule 23: 50S ribosomal protein L24E

Chain U: 5% 48% 32% 20%



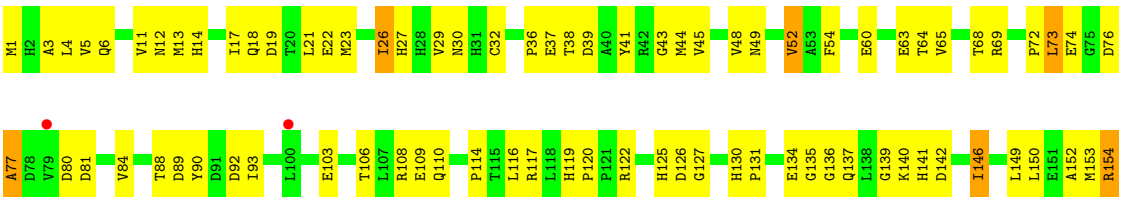
• Molecule 24: 50S ribosomal protein L29P

Chain V: 30% 46% 44% 8%



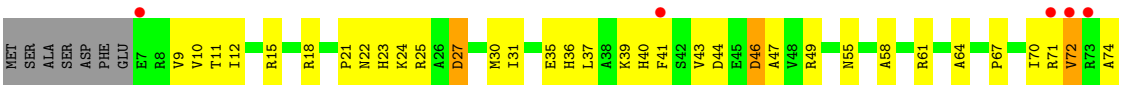
• Molecule 25: 50S ribosomal protein L30P

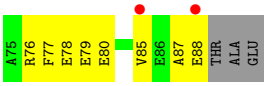
Chain W: % 47% 49%



• Molecule 26: 50S ribosomal protein L31e

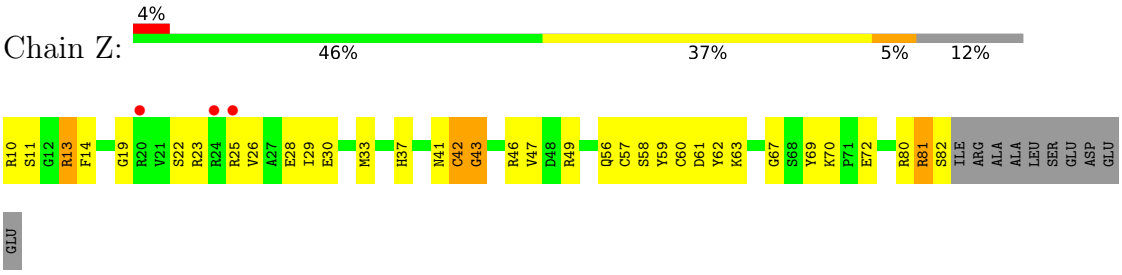
Chain X: 8% 43% 42% 11%



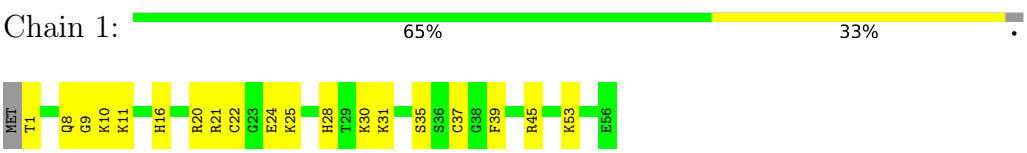


• Molecule 27: 50S ribosomal protein L32E

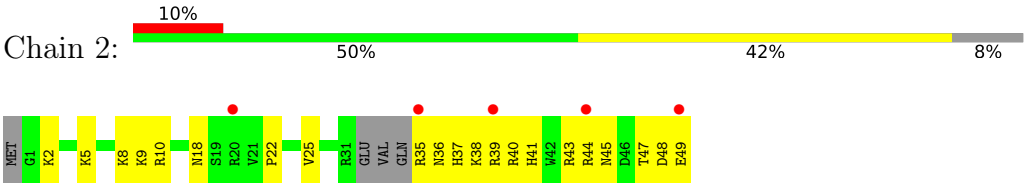
• Molecule 28: 50S ribosomal protein L37Ae



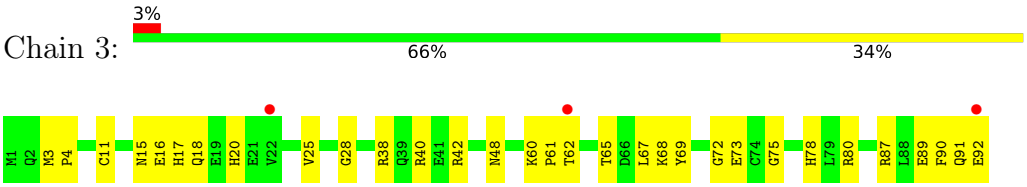
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



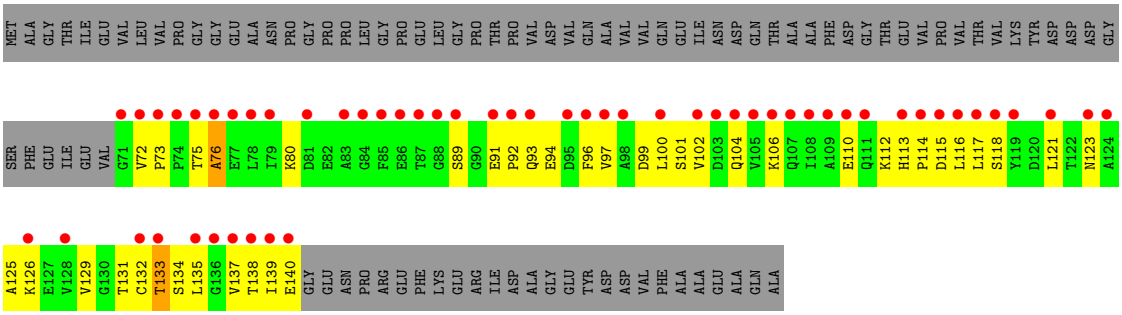
• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:

34%
19%
23%
57%


MET ALA GLY THR ILE GLU VAL LEU VAL PRO GLY GLY GLU ALA ASN PRO GLY PRO PRO LEU GLY PRO GLU LEU GLY PRO THR PRO VAL ASP VAL GLN ALA VAL VAL GLN GLU ILE ASN ASP GLN THR ALA ALA PHE ASP GLY THR GLU VAL PRO VAL THR VAL LYS TYR ASP ASP ASP GLY
SER PHE GLU ILE GLU VAL G71 V72 P73 P74 T75 A76 E77 L78 T79 K80 D81 E82 A83 G84 F85 E86 T87 G88 S89 G90 E91 P92 Q93 E94 D95 F96 V97 A98 D99 L100 S101 V102 D103 Q104 V105 K106 Q107 I108 A109 E110 Q111 K112 H113 P114 D115 L116 L117 S118 Y119 D120 L121 T122 N123 A124
A125 K126 E127 V128 V129 G130 T131 C132 T133 S134 L135 G136 V137 T138 I139 E140 GLY GLU ASN PRO ARG GLU PHE LYS GLU ARG ILE ASP ALA GLY GLU TYR ASP ASP VAL PHE ALA ALA GLU ALA GLN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.00Å 301.03Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.83 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 94.8 (49.83-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.230 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	98999	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5AA, MG, CD, NA, PSU, CL, OMG, 1MA, 2OP, UR3, OMU, PO2, K

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	0	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.35	0/2905	0.71	2/4528 (0.0%)
3	4	0.46	0/102	0.73	0/149
4	A	0.31	0/1786	0.65	0/2408
5	B	0.34	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	1/2551 (0.0%)
7	D	0.30	0/1111	0.53	0/1498
8	E	0.33	0/1382	0.58	0/1880
9	F	0.30	0/901	0.54	0/1224
10	G	0.30	0/241	0.49	0/324
11	H	0.35	0/1287	0.67	0/1725
12	J	0.37	0/1136	0.63	0/1530
13	K	0.36	0/1001	0.69	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.33	0/1584	0.61	0/2119
16	N	0.30	0/1474	0.63	0/1999
17	O	0.31	0/874	0.56	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.36	0/749	0.72	0/1005
20	R	0.36	0/1172	0.65	0/1578
21	S	0.32	0/648	0.57	0/875
22	T	0.32	0/958	0.61	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.27	0/502	0.54	0/675
25	W	0.36	0/1219	0.63	0/1655
26	X	0.36	0/664	0.58	0/895
27	Y	0.37	0/1146	0.64	0/1536
28	Z	0.36	0/589	0.67	0/787
29	1	0.36	0/438	0.62	0/578
30	2	0.33	0/401	0.52	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.30	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.37	0/98794	0.67	23/147726 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	47
2	9	0	2
3	4	0	1
25	W	0	1
All	All	0	51

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	8.54	128.28	109.50
1	0	1942	A	C5'-C4'-C3'	8.16	129.06	116.00
1	0	1979	G	C2'-C3'-O3'	6.72	124.45	113.70
1	0	871	G	C5'-C4'-O4'	-6.61	101.17	109.10
2	9	3039	U	N1-C1'-C2'	6.29	122.18	114.00
1	0	2313	C	C5'-C4'-O4'	6.29	116.65	109.10
1	0	2291	A	N9-C1'-C2'	6.28	122.16	114.00
2	9	3065	A	N9-C1'-C2'	6.26	122.14	114.00
1	0	1504	A	C1'-O4'-C4'	-6.11	105.01	109.90
1	0	2467	A	C1'-O4'-C4'	-5.87	105.21	109.90
1	0	2541	U	C2'-C3'-O3'	5.70	122.83	113.70
1	0	206	G	C5'-C4'-C3'	-5.49	107.22	116.00
1	0	1504	A	N9-C1'-C2'	5.34	120.94	114.00
1	0	1979	G	N9-C1'-C2'	5.28	120.87	114.00
1	0	2526	C	N1-C1'-C2'	5.21	120.77	114.00
1	0	777	U	O4'-C1'-N1	5.16	112.33	108.20
1	0	2313	C	C1'-O4'-C4'	-5.14	105.79	109.90
1	0	2313	C	C5'-C4'-C3'	5.10	124.15	116.00
6	C	73	LEU	CA-CB-CG	-5.09	103.58	115.30
1	0	2607	U	N1-C1'-C2'	5.09	120.62	114.00
1	0	1942	A	C5'-C4'-O4'	5.07	115.19	109.10
1	0	381	G	N9-C1'-C2'	5.07	120.59	114.00
1	0	69	A	C5'-C4'-O4'	-5.07	103.02	109.10

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1614	G	Sidechain
1	0	1681	G	Sidechain
1	0	1744	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	221	G	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2395	A	Sidechain
1	0	24	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2679	G	Sidechain
1	0	2840	A	Sidechain
1	0	2842	G	Sidechain
1	0	417	G	Sidechain
1	0	471	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	781	C	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	882	A	Sidechain
1	0	952	G	Sidechain
3	4	176	DA	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
25	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	849	0
2	9	2600	0	1326	65	0
3	4	127	0	75	4	0
4	A	1753	0	1766	119	0
5	B	2625	0	2533	159	0
6	C	1859	0	1816	127	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	64	0
9	F	890	0	843	56	0
10	G	240	0	231	13	0
11	H	1266	0	1268	70	0
12	J	1120	0	1098	55	0
13	K	992	0	1031	65	0
14	L	1118	0	1076	55	0
15	M	1560	0	1568	70	0
16	N	1445	0	1401	107	0
17	O	865	0	873	39	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	62	0
21	S	641	0	605	21	0
22	T	950	0	923	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U	410	0	364	24	0
24	V	499	0	511	33	0
25	W	1196	0	1137	95	0
26	X	654	0	653	50	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	27	0
29	1	431	0	426	30	0
30	2	396	0	413	27	0
31	3	755	0	728	31	0
32	I	519	0	500	54	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
37	1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5764	0	0	97	0
38	1	61	0	0	3	0
38	2	42	0	0	3	0
38	3	71	0	0	5	0
38	4	3	0	0	0	0
38	9	133	0	0	4	0
38	A	116	0	0	18	0
38	B	143	0	0	23	0
38	C	173	0	0	21	0
38	D	44	0	0	8	0
38	E	43	0	0	5	0
38	F	24	0	0	4	0
38	G	17	0	0	0	0
38	H	66	0	0	9	0
38	I	9	0	0	2	0
38	J	52	0	0	3	0
38	K	57	0	0	8	0
38	L	81	0	0	11	0
38	M	115	0	0	4	0
38	N	61	0	0	10	0
38	O	45	0	0	6	0
38	P	63	0	0	3	0
38	Q	52	0	0	1	0
38	R	89	0	0	5	0
38	S	31	0	0	2	0
38	T	36	0	0	2	0
38	U	26	0	0	0	0
38	V	13	0	0	1	0
38	W	70	0	0	5	0
38	X	31	0	0	5	0
38	Y	93	0	0	7	0
38	Z	31	0	0	1	0
All	All	98999	0	59974	2378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3006:C:H5”	16:N:37:ARG:NH1	1.64	1.13
6:C:236:THR:HG22	6:C:239:ALA:H	1.11	1.13
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.32	1.11
2:9:3006:C:H5”	16:N:37:ARG:HH12	1.08	1.07
1:0:1160:G:H5’	1:0:1161:A:H5’	1.34	1.04
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.71	1.04
1:0:156:C:H5”	15:M:171:ARG:HD3	1.38	1.03
1:0:1242:A:H5’	12:J:82:THR:HG23	1.40	1.03
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.37	1.03
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.39	1.02
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.02	1.01
28:Z:10:ARG:HA	38:Z:9216:HOH:O	1.57	1.01
5:B:238:ASN:HD22	5:B:240:GLY:H	1.06	1.00
13:K:10:GLN:HE21	13:K:10:GLN:H	1.05	1.00
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.43	0.99
1:0:2364:A:H5”	19:Q:15:LYS:HD3	1.45	0.98
1:0:871:G:H5’	1:0:871:G:H8	1.27	0.97
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.44	0.97
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.45	0.96
1:0:871:G:H5’	1:0:871:G:C8	1.99	0.96
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.46	0.96
1:0:56:G:H5”	24:V:50:ARG:HH12	1.31	0.95
1:0:1751:G:H2’	1:0:1752:G:H5”	1.46	0.95
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.47	0.95
1:0:870:G:H2’	1:0:871:G:H5”	1.45	0.94
2:9:3056:A:H2’	2:9:3057:A:H5”	1.48	0.94
18:P:115:SER:H	18:P:118:GLN:HE21	0.96	0.94
9:F:91:VAL:HG12	9:F:92:GLY:H	1.32	0.92
7:D:154:LYS:H	7:D:154:LYS:HD2	1.31	0.92
1:0:1187:U:HO2’	1:0:1189:A:H2	1.10	0.91
1:0:1474:C:H6	1:0:1474:C:H5’	1.36	0.91
20:R:39:THR:HG22	20:R:42:GLU:H	1.35	0.91
13:K:39:GLY:HA2	38:K:4183:HOH:O	1.71	0.91
1:0:1835:U:H5	1:0:1840:A:N7	1.69	0.90
2:9:3076:G:H3’	2:9:3077:A:H5”	1.52	0.90
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.33	0.90
21:S:57:THR:HG22	21:S:59:ASP:H	1.37	0.90
1:0:2717:C:H2’	1:0:2718:C:H5”	1.53	0.90
15:M:164:THR:HG22	15:M:167:GLY:H	1.36	0.89
13:K:10:GLN:H	13:K:10:GLN:NE2	1.70	0.89
1:0:2717:C:C2’	1:0:2718:C:H5”	2.03	0.88
1:0:1116:U:HO2’	1:0:1118:A:H2	0.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.56	0.88
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.55	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.89	0.88
1:0:2812:A:H2	1:0:2814:A:H62	1.22	0.88
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.15	0.88
1:0:2506:A:HO2'	1:0:2507:G:H8	0.89	0.87
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.53	0.87
24:V:1:THR:HG23	24:V:2:VAL:H	1.36	0.87
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.56	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.38	0.87
1:0:506:G:H22	1:0:509:A:H5'	1.40	0.87
1:0:56:G:H5"	24:V:50:ARG:NH1	1.90	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.56	0.86
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.56	0.85
18:P:115:SER:N	18:P:118:GLN:HE21	1.74	0.85
1:0:282:C:H1'	1:0:368:C:N4	1.91	0.85
5:B:179:LEU:O	5:B:183:GLU:HG2	1.75	0.85
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.59	0.85
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.85
1:0:2533:C:H5'	1:0:2533:C:H6	1.42	0.84
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.59	0.84
25:W:88:THR:HG22	25:W:89:ASP:H	1.41	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.90	0.84
1:0:1667:A:H8	1:0:1667:A:H5'	1.42	0.84
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.59	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.42	0.83
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.44	0.83
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.83
1:0:1160:G:C5'	1:0:1161:A:H5'	2.08	0.83
32:I:99:ASP:OD1	32:I:138:THR:HB	1.77	0.83
1:0:545:G:H5'	1:0:545:G:H8	1.44	0.83
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.61	0.82
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.59	0.82
30:2:41:HIS:H	30:2:45:ASN:HD22	1.23	0.82
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.44	0.82
1:0:2506:A:O2'	1:0:2507:G:H8	1.61	0.82
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.94	0.82
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.60	0.82
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.62	0.82
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.62	0.82
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.81
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.79	0.81
13:K:10:GLN:HE21	13:K:10:GLN:N	1.79	0.81
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.46	0.81
1:0:1372:A:H3'	38:0:7376:HOH:O	1.81	0.80
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.44	0.80
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.81	0.80
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.79	0.80
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.45	0.80
1:0:1593:C:H5'	18:P:116:SER:O	1.81	0.80
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.46	0.79
1:0:559:U:H6	1:0:559:U:H5'	1.47	0.79
1:0:870:G:C2'	1:0:871:G:H5"	2.11	0.79
5:B:62:ARG:HA	5:B:65:MET:HE3	1.62	0.79
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.48	0.79
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.63	0.79
9:F:46:GLU:O	9:F:73:PRO:HD2	1.83	0.79
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.64	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.66	0.79
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.64	0.79
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.81	0.78
1:0:506:G:H22	1:0:509:A:C5'	1.95	0.78
1:0:542:A:H5'	1:0:542:A:H8	1.48	0.78
16:N:176:ARG:HE	16:N:180:LEU:HD21	1.48	0.78
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.65	0.78
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.13	0.78
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.49	0.78
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.66	0.78
7:D:99:ASP:HB3	7:D:103:ASN:H	1.47	0.78
1:0:21:G:C5'	20:R:2:ILE:HA	2.14	0.77
1:0:1116:U:H3	1:0:1246:A:H62	1.32	0.77
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.64	0.77
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.77
8:E:6:GLU:HA	8:E:46:THR:HG22	1.67	0.77
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.65	0.77
5:B:238:ASN:HD22	5:B:240:GLY:N	1.83	0.77
1:0:541:C:H2'	1:0:542:A:H5"	1.65	0.77
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.66	0.77
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.66	0.77
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.66	0.76
1:0:541:C:C2'	1:0:542:A:H5"	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.85	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.67	0.76
6:C:182:ARG:HB2	6:C:184:ARG:NH1	1.99	0.76
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.68	0.76
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.66	0.76
1:0:2908:A:H2'	1:0:2909:G:O4'	1.86	0.76
2:9:3014:G:H5'	2:9:3014:G:H8	1.50	0.76
1:0:188:C:H5"	15:M:163:LEU:HD21	1.68	0.76
1:0:1603:A:H5'	1:0:1605:G:O4'	1.86	0.76
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.68	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.50	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.76
1:0:1118:A:C8	1:0:1118:A:H3'	2.21	0.76
1:0:1120:U:H6	1:0:1120:U:H5'	1.51	0.75
1:0:2291:A:C8	1:0:2309:C:H5'	2.21	0.75
1:0:2716:G:H5"	5:B:206:THR:HG21	1.66	0.75
1:0:1474:C:H5'	1:0:1474:C:C6	2.21	0.75
16:N:113:SER:HB2	38:N:9357:HOH:O	1.86	0.75
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.69	0.75
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.52	0.75
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.66	0.75
1:0:236:A:H4'	1:0:237:G:H5'	1.69	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.74
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.16	0.74
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.51	0.74
1:0:1118:A:H3'	1:0:1118:A:H8	1.51	0.74
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.04	0.74
1:0:111:C:O2'	29:1:20:ARG:HG2	1.87	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.17	0.74
1:0:1181:A:H5'	32:I:94:GLU:OE2	1.88	0.74
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.02	0.74
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.52	0.74
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.53	0.74
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.69	0.74
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.03	0.74
6:C:236:THR:H	6:C:239:ALA:HB3	1.53	0.73
1:0:1189:A:H1'	1:0:1209:C:O4'	1.89	0.73
2:9:3056:A:C2'	2:9:3057:A:H5"	2.18	0.73
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.18	0.73
1:0:1160:G:H5'	1:0:1161:A:C5'	2.15	0.73
31:3:17:HIS:O	31:3:18:GLN:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:164:ASP:CG	16:N:167:ASP:HA	2.09	0.73
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.03	0.73
1:0:657:G:OP1	6:C:27:ARG:NH2	2.21	0.73
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.89	0.73
5:B:98:THR:HG22	5:B:99:GLU:H	1.53	0.73
5:B:238:ASN:ND2	5:B:240:GLY:H	1.86	0.73
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.22	0.73
1:0:1234:U:N3	5:B:244:PRO:HB3	2.03	0.72
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.88	0.72
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.04	0.72
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.54	0.72
1:0:396:U:H1'	38:0:7793:HOH:O	1.90	0.72
1:0:289:G:H22	1:0:363:A:H2	1.38	0.72
10:G:16:LYS:O	10:G:20:VAL:HG23	1.90	0.72
1:0:272:A:H5'	1:0:273:G:OP2	1.90	0.72
1:0:877:G:H5'	1:0:878:G:OP1	1.89	0.72
1:0:1206:U:H5'	1:0:1206:U:H6	1.55	0.72
16:N:132:ASN:O	16:N:135:VAL:HG12	1.89	0.72
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.36	0.72
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.72	0.72
1:0:2524:G:H21	1:0:2526:C:N4	1.88	0.72
4:A:36:ASP:HB2	4:A:83:GLY:HA3	1.72	0.72
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.71	0.72
21:S:57:THR:HG22	21:S:59:ASP:N	2.04	0.72
9:F:38:LYS:NZ	15:M:3:SER:HA	2.04	0.72
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.20	0.72
5:B:125:GLU:O	5:B:129:ARG:HG3	1.90	0.71
15:M:164:THR:CG2	15:M:167:GLY:H	2.02	0.71
26:X:78:GLU:HG2	26:X:79:GLU:H	1.55	0.71
1:0:541:C:H2'	1:0:542:A:C5'	2.19	0.71
1:0:2426:G:H1'	38:0:6331:HOH:O	1.89	0.71
8:E:100:ASP:HB2	38:E:2789:HOH:O	1.89	0.71
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.91	0.71
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.18	0.71
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.72	0.71
1:0:2769:C:H2'	1:0:2770:G:O4'	1.90	0.71
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.71
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.90	0.71
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.71
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.71	0.71
1:0:2524:G:H21	1:0:2526:C:H41	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:962:C:H1'	16:N:5:ARG:NH1	2.06	0.71
14:L:133:VAL:HA	38:L:9372:HOH:O	1.91	0.71
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.70	0.71
17:O:73:ASP:HA	17:O:92:VAL:O	1.91	0.71
20:R:39:THR:HG23	20:R:107:GLU:O	1.90	0.71
11:H:169:GLY:HA3	38:H:9187:HOH:O	1.91	0.70
1:0:1058:A:H2'	1:0:1060:C:H5"	1.71	0.70
1:0:2533:C:H5'	1:0:2533:C:C6	2.25	0.70
6:C:139:VAL:HG13	38:C:9249:HOH:O	1.89	0.70
7:D:136:ARG:HD2	7:D:155:HIS:O	1.91	0.70
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.38	0.70
1:0:1751:G:C2'	1:0:1752:G:H5"	2.20	0.70
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.71	0.70
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.72	0.70
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.74	0.70
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.22	0.70
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.21	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.72	0.70
24:V:56:ILE:O	24:V:60:GLN:HG3	1.90	0.70
15:M:164:THR:HG22	15:M:167:GLY:N	2.07	0.70
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.74	0.70
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.90	0.70
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.06	0.70
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.92	0.70
1:0:2586:U:H3	1:0:2592:G:H22	1.38	0.69
1:0:553:G:P	27:Y:204:ARG:HH22	2.16	0.69
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.73	0.69
1:0:1118:A:H62	1:0:1244:U:H3	1.39	0.69
1:0:1201:C:H2'	1:0:1202:A:H5'	1.74	0.69
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.07	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
1:0:544:G:H2'	1:0:545:G:H5"	1.73	0.69
11:H:166:SER:HB2	11:H:167:PRO:CD	2.22	0.69
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.74	0.69
23:U:52:THR:CG2	23:U:54:THR:HB	2.23	0.69
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.93	0.69
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.23	0.69
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.91	0.69
24:V:12:THR:HG22	24:V:15:GLU:CG	2.23	0.69
1:0:1205:U:H2'	1:0:1206:U:C5'	2.23	0.68
27:Y:144:ARG:CZ	38:Y:8197:HOH:O	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.25	0.68
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.75	0.68
24:V:44:GLY:O	24:V:48:GLU:HG2	1.94	0.68
1:0:797:A:H4'	28:Z:10:ARG:N	2.08	0.68
12:J:76:ASP:HA	38:J:9361:HOH:O	1.92	0.68
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.57	0.68
1:0:1205:U:H2'	1:0:1206:U:H5"	1.75	0.68
1:0:2768:A:H2'	1:0:2769:C:O4'	1.93	0.68
1:0:2768:A:H5"	38:0:4707:HOH:O	1.94	0.68
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.09	0.68
12:J:131:THR:HG22	12:J:134:GLU:H	1.57	0.68
20:R:99:ALA:HB1	20:R:109:MET:CE	2.22	0.68
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.75	0.68
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.57	0.68
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.31	0.68
24:V:39:ALA:N	24:V:40:PRO:HD2	2.09	0.68
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.06	0.68
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.58	0.68
32:I:138:THR:HG22	32:I:139:ILE:H	1.58	0.68
2:9:3039:U:H1'	2:9:3044:A:N6	2.08	0.68
14:L:37:LYS:HG2	38:L:9334:HOH:O	1.92	0.68
17:O:32:ARG:O	17:O:32:ARG:HD3	1.94	0.68
2:9:3064:C:H2'	2:9:3065:A:H5'	1.76	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.76	0.68
7:D:37:ALA:O	7:D:40:ILE:HG12	1.94	0.68
1:0:656:G:OP2	17:O:37:ARG:HD2	1.94	0.68
30:2:41:HIS:HD2	30:2:44:ARG:H	1.41	0.68
1:0:2468:A:H61	31:3:48:ASN:HD21	1.41	0.67
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.77	0.67
9:F:58:GLU:HA	9:F:61:MET:HG3	1.75	0.67
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.57	0.67
30:2:36:ASN:O	30:2:39:ARG:HG3	1.93	0.67
7:D:50:VAL:O	7:D:71:ALA:HA	1.95	0.67
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.76	0.67
1:0:157:G:H4'	15:M:95:LYS:HE2	1.77	0.67
1:0:2252:A:C5	1:0:2253:G:H1'	2.30	0.67
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.76	0.67
21:S:33:SER:O	21:S:37:VAL:HG23	1.93	0.67
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.76	0.67
24:V:64:GLY:O	24:V:65:ASP:HB2	1.94	0.67
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.58	0.67
1:0:871:G:C8	1:0:871:G:C5'	2.76	0.67
1:0:1666:C:O2'	1:0:1667:A:H5"	1.95	0.67
1:0:1819:G:H5'	38:0:4985:HOH:O	1.93	0.67
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.75	0.67
1:0:2054:A:N3	20:R:128:ARG:NH2	2.42	0.67
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.29	0.67
1:0:1080:C:H4'	1:0:1081:A:OP1	1.94	0.67
1:0:1701:A:H5'	38:0:6518:HOH:O	1.93	0.67
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.95	0.67
6:C:16:VAL:HG12	6:C:17:ASP:H	1.59	0.66
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.66
6:C:7:ASP:OD2	6:C:9:ASP:HB2	1.95	0.66
10:G:20:VAL:O	10:G:24:VAL:HG23	1.96	0.66
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.95	0.66
15:M:59:GLY:HA3	15:M:141:ILE:HD11	1.77	0.66
29:1:25:LYS:HD2	30:2:49:GLU:H	1.59	0.66
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.75	0.66
38:0:5785:HOH:O	15:M:58:GLN:HG3	1.95	0.66
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.10	0.66
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.59	0.66
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.77	0.66
25:W:88:THR:HG22	25:W:89:ASP:N	2.10	0.66
1:0:1641:A:H2'	1:0:1642:A:H5'	1.76	0.66
1:0:2649:A:H5'	1:0:2649:A:H8	1.60	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.26	0.66
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.78	0.66
20:R:6:VAL:HG21	20:R:113:HIS:CD2	2.31	0.66
25:W:65:VAL:HA	25:W:68:THR:HG22	1.78	0.66
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.66
38:0:7598:HOH:O	22:T:9:LYS:HB2	1.93	0.66
9:F:52:GLU:HG3	9:F:77:VAL:O	1.96	0.66
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.31	0.65
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.31	0.65
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.65
1:0:1130:U:H2'	1:0:1131:G:O4'	1.97	0.65
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.97	0.65
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.78	0.65
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.78	0.65
32:I:125:ALA:O	32:I:129:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1189:A:H1'	1:0:1209:C:C1'	2.27	0.65
1:0:558:C:O2'	1:0:559:U:H5"	1.96	0.65
1:0:870:G:OP2	4:A:3:ARG:HD3	1.97	0.65
2:9:3029:C:H2'	2:9:3030:C:H5'	1.78	0.65
1:0:560:C:H42	1:0:597:A:H61	1.43	0.65
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.78	0.65
11:H:166:SER:CB	11:H:167:PRO:HD3	2.26	0.65
5:B:162:MET:CE	5:B:308:LEU:HD21	2.27	0.65
1:0:820:G:C6	4:A:171:LYS:HB2	2.32	0.65
1:0:1681:G:H5"	1:0:1682:A:H5'	1.78	0.65
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.65
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.26	0.65
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.95	0.65
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.62	0.65
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.78	0.65
12:J:52:GLN:HG3	12:J:53:ILE:N	2.11	0.64
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.12	0.64
1:0:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.32	0.64
1:0:1701:A:H4'	1:0:1702:U:H5"	1.78	0.64
10:G:64:ASN:HD22	10:G:64:ASN:N	1.95	0.64
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.64
19:Q:18:PRO:O	19:Q:21:ARG:HB2	1.97	0.64
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.27	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
16:N:119:GLN:O	16:N:123:ILE:HG13	1.97	0.64
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.79	0.64
1:0:545:G:H5'	1:0:545:G:C8	2.31	0.64
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.12	0.64
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.79	0.64
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.78	0.64
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.81	0.64
8:E:69:ILE:HA	8:E:72:MET:HE3	1.79	0.64
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.80	0.64
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.78	0.64
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.78	0.64
1:0:380:A:H2'	38:0:7412:HOH:O	1.97	0.64
1:0:2690:U:O2'	8:E:111:LYS:HE3	1.98	0.64
2:9:3014:G:H5'	2:9:3014:G:C8	2.32	0.64
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.12	0.64
1:0:558:C:H2'	1:0:559:U:H5'	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1667:A:H5'	1:0:1667:A:C8	2.31	0.64
1:0:2491:G:H1'	38:0:7076:HOH:O	1.98	0.64
1:0:1060:C:H6	1:0:1060:C:H5'	1.63	0.63
1:0:1819:G:H2'	1:0:1820:G:H4'	1.79	0.63
7:D:57:THR:HG23	7:D:63:ILE:HA	1.79	0.63
7:D:105:SER:HB2	7:D:131:THR:HG23	1.80	0.63
8:E:69:ILE:HA	8:E:72:MET:CE	2.28	0.63
11:H:27:LYS:H	11:H:59:HIS:HD2	1.46	0.63
1:0:281:U:H2'	1:0:282:C:O4'	1.98	0.63
1:0:2896:A:H5"	38:0:6338:HOH:O	1.98	0.63
16:N:169:PRO:O	16:N:172:PHE:HB3	1.99	0.63
18:P:134:VAL:O	18:P:137:LEU:HB3	1.98	0.63
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.63
1:0:2570:G:H5"	38:0:5188:HOH:O	1.99	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.14	0.63
14:L:149:ARG:O	14:L:150:GLN:HB2	1.98	0.63
1:0:447:A:OP1	22:T:2:LYS:HG2	1.98	0.63
7:D:99:ASP:HA	38:D:5675:HOH:O	1.97	0.63
8:E:145:ALA:HB1	8:E:168:ILE:HD11	1.81	0.63
18:P:91:LYS:O	18:P:95:GLU:HG3	1.99	0.63
38:0:7629:HOH:O	6:C:188:ARG:HD2	1.96	0.63
25:W:125:HIS:HD2	25:W:127:GLY:H	1.46	0.63
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.28	0.63
1:0:2414:A:H2'	1:0:2415:A:C8	2.34	0.63
7:D:57:THR:HG23	7:D:63:ILE:HG22	1.80	0.63
1:0:1377:C:H5'	1:0:1377:C:H6	1.64	0.63
1:0:1741:U:H5'	1:0:1742:A:OP1	1.98	0.63
38:0:4132:HOH:O	11:H:11:LYS:HE2	1.99	0.63
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.34	0.63
16:N:170:GLU:HA	16:N:173:ASP:OD2	1.98	0.63
32:I:75:THR:HA	32:I:112:LYS:NZ	2.14	0.63
1:0:1184:C:H1'	38:0:7636:HOH:O	1.99	0.63
21:S:11:THR:H	21:S:14:ALA:HB3	1.64	0.63
1:0:1130:U:H5'	38:0:7834:HOH:O	1.98	0.62
1:0:1299:G:O6	14:L:6:ARG:HD3	1.98	0.62
4:A:65:ARG:C	4:A:66:ARG:HG3	2.19	0.62
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.81	0.62
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.62
1:0:1834:C:H2'	1:0:1840:A:N6	2.14	0.62
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.81	0.62
1:0:564:G:H1'	38:0:6543:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2756:U:H3	1:0:2896:A:H2	1.47	0.62
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.81	0.62
26:X:41:PHE:O	26:X:43:VAL:HG23	1.98	0.62
1:0:2320:U:H4'	1:0:2321:A:O4'	1.98	0.62
2:9:3114:G:O6	16:N:11:ARG:HD3	1.98	0.62
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.61	0.62
1:0:1187:U:O2'	1:0:1189:A:H2	1.80	0.62
6:C:145:GLU:HG3	38:C:9175:HOH:O	1.99	0.62
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.82	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.62	0.62
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.82	0.62
26:X:30:MET:HE1	26:X:55:ASN:HA	1.81	0.62
1:0:2251:G:H2'	1:0:2252:A:C8	2.34	0.62
38:0:7228:HOH:O	4:A:211:LYS:HG2	2.00	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.28	0.62
1:0:2004:U:H4'	38:0:5568:HOH:O	1.99	0.62
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.99	0.62
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.62
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.97	0.62
2:9:3002:U:OP2	2:9:3003:A:H5'	1.99	0.62
20:R:9:ASP:O	20:R:13:THR:HB	1.99	0.62
22:T:48:VAL:CG1	22:T:96:VAL:HG13	2.30	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.15	0.62
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.82	0.62
16:N:110:THR:HB	16:N:113:SER:OG	2.00	0.62
32:I:134:SER:O	32:I:135:LEU:HD23	2.00	0.62
1:0:544:G:C2'	1:0:545:G:H5"	2.30	0.61
6:C:127:ARG:HH21	6:C:225:PRO:HG2	1.61	0.61
16:N:23:ARG:HD3	38:N:9346:HOH:O	1.99	0.61
1:0:926:A:O2'	14:L:41:HIS:HD2	1.81	0.61
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.68	0.61
9:F:21:GLU:O	9:F:24:ARG:HG3	2.00	0.61
14:L:143:THR:HG21	38:L:9336:HOH:O	1.99	0.61
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.98	0.61
1:0:1086:A:C6	25:W:11:VAL:HG11	2.35	0.61
1:0:2840:A:OP1	5:B:211:THR:HG23	2.00	0.61
26:X:25:ARG:HD2	38:X:3861:HOH:O	1.99	0.61
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.03	0.61
31:3:62:THR:HB	38:3:9349:HOH:O	2.00	0.61
1:0:399:C:H5'	15:M:179:GLY:O	2.01	0.61
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:11:VAL:HG12	8:E:12:ASP:N	2.16	0.61
1:0:1625:U:H4'	38:0:4940:HOH:O	2.00	0.61
1:0:2256:G:C2'	1:0:2257:G:H5'	2.31	0.61
38:0:7081:HOH:O	15:M:178:LYS:HB2	2.00	0.61
2:9:3055:U:H4'	2:9:3056:A:C8	2.36	0.61
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.82	0.61
22:T:48:VAL:HG13	22:T:97:ARG:O	2.00	0.61
25:W:149:LEU:HG	25:W:153:MET:HE2	1.81	0.61
1:0:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
4:A:88:ILE:O	4:A:88:ILE:HG22	1.99	0.61
5:B:297:VAL:HB	38:B:9406:HOH:O	2.00	0.61
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.83	0.61
15:M:60:VAL:C	15:M:61:ILE:HD12	2.20	0.61
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.36	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
25:W:125:HIS:CD2	25:W:127:GLY:H	2.19	0.61
32:I:131:THR:O	32:I:135:LEU:HG	2.01	0.61
8:E:137:ASP:O	8:E:141:VAL:HG23	2.01	0.61
1:0:1166:A:H1'	1:0:1192:A:C2	2.36	0.61
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.01	0.61
27:Y:235:GLU:CD	27:Y:235:GLU:H	2.03	0.61
1:0:848:C:H5'	38:0:7455:HOH:O	1.99	0.60
1:0:2346:C:H6	1:0:2346:C:O5'	1.84	0.60
38:0:7626:HOH:O	5:B:211:THR:HG21	2.01	0.60
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.66	0.60
5:B:140:LEU:HD23	38:B:9378:HOH:O	1.99	0.60
6:C:16:VAL:HG12	6:C:17:ASP:N	2.16	0.60
15:M:64:ARG:HD2	38:M:9378:HOH:O	2.00	0.60
1:0:1189:A:O2'	1:0:1208:C:H2'	2.00	0.60
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.65	0.60
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.17	0.60
25:W:38:THR:HG22	25:W:39:ASP:H	1.67	0.60
1:0:1266:U:H4'	27:Y:115:ARG:HH21	1.65	0.60
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.83	0.60
11:H:166:SER:CB	11:H:167:PRO:CD	2.78	0.60
12:J:99:GLU:HA	38:J:9371:HOH:O	2.01	0.60
1:0:282:C:O2'	1:0:283:U:H5'	2.01	0.60
1:0:2256:G:H2'	1:0:2257:G:H5'	1.83	0.60
11:H:23:ILE:HA	11:H:120:ILE:HG21	1.82	0.60
16:N:152:GLU:C	16:N:154:LEU:H	2.03	0.60
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:449:A:N7	6:C:43:LYS:HG2	2.16	0.60
1:0:2502:C:C2'	1:0:2503:A:H5'	2.32	0.60
11:H:63:GLU:HA	38:H:9177:HOH:O	2.00	0.60
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.16	0.60
1:0:793:A:H5"	18:P:83:LYS:HG2	1.83	0.60
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.67	0.60
7:D:13:MET:HA	7:D:137:PRO:HG2	1.83	0.60
4:A:194:MET:CE	4:A:199:HIS:HB2	2.31	0.60
4:A:210:GLY:HA3	38:A:9380:HOH:O	2.02	0.60
6:C:33:LYS:HE2	38:C:9160:HOH:O	2.01	0.60
9:F:91:VAL:HG12	9:F:92:GLY:N	2.09	0.60
11:H:45:VAL:HA	11:H:167:PRO:O	2.01	0.60
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.60
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.83	0.60
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.60
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.42	0.60
1:0:338:C:H4'	6:C:174:ILE:CD1	2.32	0.60
1:0:1119:G:H8	12:J:52:GLN:HE22	1.48	0.60
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.67	0.60
6:C:233:THR:HG22	6:C:234:VAL:N	2.17	0.60
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.32	0.60
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.32	0.59
14:L:136:ALA:HB3	38:L:9372:HOH:O	2.01	0.59
16:N:27:LEU:HD13	16:N:50:LEU:HD21	1.82	0.59
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.84	0.59
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.25	0.59
5:B:150:ALA:O	5:B:152:PRO:HD3	2.02	0.59
10:G:64:ASN:O	10:G:68:GLU:HG3	2.02	0.59
1:0:485:A:N3	1:0:487:G:H5"	2.17	0.59
2:9:3055:U:H4'	2:9:3056:A:H8	1.67	0.59
15:M:164:THR:HG23	15:M:165:GLY:N	2.17	0.59
29:1:10:LYS:HG3	38:1:9236:HOH:O	2.01	0.59
1:0:120:A:H5'	29:1:20:ARG:HH21	1.68	0.59
1:0:1441:G:O2'	1:0:1442:A:H5'	2.02	0.59
1:0:1926:G:H2'	1:0:1927:A:C8	2.36	0.59
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.36	0.59
14:L:61:ALA:HA	38:L:9363:HOH:O	2.03	0.59
1:0:1118:A:H2'	1:0:1120:U:H5"	1.84	0.59
1:0:2748:G:H5'	38:0:7705:HOH:O	2.02	0.59
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.84	0.59
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.84	0.59
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.59
1:0:121:U:OP2	30:2:10:ARG:NH2	2.32	0.59
1:0:1299:G:N7	14:L:6:ARG:NH1	2.50	0.59
2:9:3064:C:C2'	2:9:3065:A:H5'	2.33	0.59
21:S:52:VAL:C	21:S:53:ASN:HD22	2.06	0.59
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.59
1:0:65:C:O2'	1:0:66:G:H5'	2.02	0.59
1:0:625:U:H5"	1:0:1044:C:N4	2.17	0.59
1:0:2668:G:H2'	1:0:2669:U:C6	2.38	0.59
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.31	0.59
4:A:94:LEU:HD23	4:A:94:LEU:N	2.18	0.59
4:A:194:MET:HE2	4:A:199:HIS:HB2	1.85	0.59
7:D:10:PHE:CG	7:D:11:HIS:N	2.71	0.59
2:9:3028:U:H5"	16:N:40:ASN:HD21	1.67	0.59
7:D:166:ILE:HB	38:D:6326:HOH:O	2.03	0.59
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.84	0.59
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.13	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.33	0.59
30:2:5:LYS:O	30:2:9:LYS:HG3	2.03	0.59
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.59
1:0:88:G:H8	1:0:88:G:H5'	1.68	0.59
1:0:1213:C:O2'	1:0:1214:G:H5'	2.03	0.59
1:0:1733:A:H4'	5:B:212:GLN:HA	1.84	0.59
1:0:1813:U:O2'	18:P:81:LYS:HE3	2.03	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
14:L:143:THR:HG22	14:L:145:LEU:H	1.66	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.38	0.59
27:Y:212:ARG:HD2	38:Y:8187:HOH:O	2.02	0.59
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.33	0.59
5:B:16:ARG:NH1	38:B:9416:HOH:O	2.36	0.59
26:X:25:ARG:HD3	26:X:64:ALA:O	2.01	0.59
31:3:73:GLU:HB3	38:3:9360:HOH:O	2.02	0.59
38:0:7333:HOH:O	29:1:1:THR:HB	2.01	0.58
5:B:16:ARG:HB3	5:B:217:ARG:NH2	2.18	0.58
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.38	0.58
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.76	0.58
1:0:381:G:H5"	38:0:4603:HOH:O	2.02	0.58
1:0:2502:C:H2'	1:0:2503:A:H5'	1.84	0.58
1:0:2649:A:H5'	1:0:2649:A:C8	2.38	0.58
1:0:2779:G:H21	8:E:143:GLN:NE2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.03	0.58
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.58
4:A:8:ARG:HG2	38:A:9349:HOH:O	2.03	0.58
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.67	0.58
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.84	0.58
1:0:2717:C:H2'	1:0:2718:C:C5'	2.31	0.58
11:H:167:PRO:O	11:H:168:ALA:HB2	2.02	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.58
20:R:40:ALA:O	20:R:44:VAL:HG23	2.03	0.58
1:0:1450:C:O2'	1:0:1494:A:H5'	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C5	2.38	0.58
1:0:2546:U:H5	5:B:2:GLN:HE22	1.50	0.58
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.67	0.58
5:B:41:PHE:HB3	5:B:190:MET:HE3	1.84	0.58
5:B:307:ARG:HH11	5:B:307:ARG:HB2	1.68	0.58
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.84	0.58
20:R:132:ARG:HG2	20:R:133:ALA:N	2.17	0.58
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.38	0.58
1:0:2094:G:H4'	5:B:245:SER:HB3	1.84	0.58
1:0:2365:G:H4'	19:Q:45:PRO:O	2.03	0.58
1:0:2524:G:N2	1:0:2526:C:H41	2.01	0.58
6:C:154:VAL:O	6:C:158:GLU:HG3	2.03	0.58
7:D:25:MET:HE3	7:D:37:ALA:CB	2.31	0.58
1:0:31:C:H4'	38:0:7598:HOH:O	2.03	0.58
1:0:1741:U:O2'	1:0:2723:G:H4'	2.04	0.58
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.51	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.39	0.58
1:0:2578:G:H5'	1:0:2578:G:H8	1.69	0.58
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.37	0.58
22:T:48:VAL:HG12	22:T:49:GLU:N	2.18	0.58
25:W:13:MET:HE1	25:W:18:GLN:HA	1.86	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.34	0.58
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.85	0.58
32:I:139:ILE:HG22	32:I:140:GLU:N	2.19	0.58
1:0:1527:A:H1'	1:0:1528:A:C8	2.38	0.58
6:C:182:ARG:HB2	6:C:184:ARG:HH12	1.68	0.58
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.16	0.58
1:0:447:A:O2'	1:0:448:G:H5'	2.04	0.58
11:H:120:ILE:N	11:H:120:ILE:HD12	2.19	0.58
20:R:145:LEU:HD12	20:R:146:ILE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:O	25:W:32:CYS:HA	2.04	0.58
1:0:182:G:H5'	38:0:5426:HOH:O	2.03	0.58
1:0:962:C:H1'	16:N:5:ARG:HH12	1.68	0.58
1:0:1180:U:H1'	38:0:3528:HOH:O	2.03	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.69	0.58
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.22	0.58
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.84	0.58
17:O:37:ARG:HG3	38:O:3002:HOH:O	2.03	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.57
6:C:168:ARG:NH2	6:C:190:ALA:O	2.37	0.57
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.86	0.57
1:0:644:G:H5'	1:0:644:G:N3	2.18	0.57
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.85	0.57
23:U:17:THR:HG22	23:U:18:GLY:N	2.19	0.57
25:W:84:VAL:HG12	38:W:6679:HOH:O	2.03	0.57
25:W:108:ARG:HE	25:W:114:PRO:CG	2.17	0.57
32:I:138:THR:HG22	32:I:139:ILE:N	2.19	0.57
1:0:2256:G:H2'	1:0:2257:G:C5'	2.35	0.57
5:B:55:ASN:HB3	5:B:63:GLU:HA	1.86	0.57
18:P:9:LEU:O	18:P:13:VAL:HG12	2.03	0.57
20:R:47:LEU:O	20:R:51:ILE:HG13	2.04	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.18	0.57
4:A:121:ALA:O	4:A:124:VAL:HG22	2.04	0.57
7:D:39:ASP:O	7:D:43:GLU:HG3	2.03	0.57
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.70	0.57
1:0:1008:C:H5"	11:H:16:ARG:HH12	1.70	0.57
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.57
15:M:61:ILE:HD12	15:M:61:ILE:N	2.19	0.57
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.87	0.57
27:Y:200:THR:HG22	27:Y:201:GLU:HG2	1.86	0.57
1:0:1182:C:H1'	1:0:1192:A:H8	1.68	0.57
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.57
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.19	0.57
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.68	0.57
1:0:2508:C:H2'	38:0:6966:HOH:O	2.04	0.57
1:0:2679:G:H2'	1:0:2681:A:OP2	2.05	0.57
18:P:64:GLU:HG2	38:P:170:HOH:O	2.05	0.57
1:0:703:G:O2'	1:0:704:C:H5'	2.05	0.57
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.18	0.57
5:B:275:GLY:O	5:B:291:ASP:HA	2.05	0.57
16:N:80:SER:HB2	38:N:9336:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1163:G:H5'	32:I:115:ASP:O	2.05	0.57
8:E:80:TRP:O	8:E:134:SER:HA	2.05	0.57
17:O:87:THR:O	17:O:91:GLN:HG3	2.04	0.57
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.34	0.57
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.57
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.70	0.57
1:0:960:G:N3	1:0:960:G:H2'	2.20	0.57
1:0:1118:A:C8	1:0:1118:A:C3'	2.85	0.57
1:0:1926:G:H2'	1:0:1927:A:H8	1.70	0.57
5:B:280:VAL:CG1	5:B:334:SER:HA	2.35	0.57
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.86	0.57
21:S:17:ASP:HB3	21:S:23:LYS:HB2	1.87	0.57
1:0:256:C:H2'	1:0:257:G:O4'	2.05	0.56
14:L:77:ALA:HB3	38:L:9329:HOH:O	2.05	0.56
20:R:145:LEU:HD12	20:R:146:ILE:H	1.70	0.56
1:0:1189:A:H3'	38:0:7842:HOH:O	2.04	0.56
1:0:1462:C:H2'	1:0:1463:A:C8	2.41	0.56
1:0:2265:U:H2'	1:0:2266:A:C8	2.40	0.56
1:0:2346:C:O2'	7:D:52:THR:HG21	2.04	0.56
2:9:3041:C:H4'	7:D:48:MET:HB2	1.87	0.56
4:A:82:VAL:HG13	4:A:93:THR:HB	1.87	0.56
9:F:38:LYS:HZ1	15:M:3:SER:HA	1.68	0.56
9:F:96:ALA:HA	38:F:3111:HOH:O	2.04	0.56
29:1:25:LYS:O	29:1:25:LYS:HG2	2.05	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.56
1:0:1657:A:H2'	1:0:1658:A:C8	2.40	0.56
1:0:2256:G:O2'	1:0:2257:G:H5'	2.05	0.56
7:D:135:VAL:HG22	7:D:136:ARG:N	2.20	0.56
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.34	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.69	0.56
1:0:2415:A:C2	16:N:25:ARG:HB3	2.41	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
2:9:3054:A:O2'	2:9:3055:U:H5'	2.06	0.56
5:B:305:ASP:O	5:B:306:LYS:HB2	2.06	0.56
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.35	0.56
21:S:33:SER:OG	21:S:36:GLU:HG3	2.06	0.56
23:U:9:CYS:HA	23:U:52:THR:HG23	1.87	0.56
1:0:1314:U:H2'	38:0:6124:HOH:O	2.03	0.56
38:0:4274:HOH:O	22:T:82:THR:HA	2.06	0.56
1:0:602:A:O2'	1:0:605:C:H4'	2.04	0.56
1:0:1535:G:H2'	1:0:1536:C:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1682:A:H5"	38:0:9763:HOH:O	2.06	0.56
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.40	0.56
1:0:119:A:H2'	1:0:120:A:H5"	1.88	0.56
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.04	0.56
23:U:14:GLU:O	23:U:17:THR:HB	2.05	0.56
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.88	0.56
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.19	0.56
1:0:709:G:O2'	17:O:25:VAL:HG12	2.05	0.56
1:0:820:G:OP2	4:A:171:LYS:NZ	2.37	0.56
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.36	0.56
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.52	0.56
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.40	0.56
31:3:87:ARG:HD2	31:3:89:GLU:OE2	2.06	0.56
1:0:136:C:H2'	1:0:137:U:O4'	2.06	0.56
1:0:2271:G:H5'	38:0:5025:HOH:O	2.06	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.05	0.56
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.41	0.56
23:U:52:THR:HG21	23:U:54:THR:HB	1.87	0.56
1:0:1778:A:H2'	1:0:1779:A:H5'	1.88	0.55
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.06	0.55
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.39	0.55
20:R:3:SER:HA	38:R:9348:HOH:O	2.06	0.55
23:U:52:THR:HG22	23:U:54:THR:N	2.21	0.55
24:V:1:THR:HG23	24:V:2:VAL:N	2.15	0.55
1:0:2769:C:C2'	1:0:2770:G:H5'	2.36	0.55
2:9:3013:A:O2'	2:9:3014:G:H5"	2.05	0.55
6:C:109:LEU:HD12	6:C:109:LEU:O	2.05	0.55
8:E:23:GLU:HG2	8:E:28:SER:CB	2.35	0.55
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.06	0.55
18:P:115:SER:O	18:P:117:SER:N	2.36	0.55
1:0:426:G:H2'	1:0:427:C:O4'	2.07	0.55
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.06	0.55
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.88	0.55
1:0:290:C:H1'	38:0:6342:HOH:O	2.05	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.71	0.55
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.39	0.55
4:A:35:GLY:O	4:A:36:ASP:HB3	2.06	0.55
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.87	0.55
5:B:198:GLU:HA	38:B:9454:HOH:O	2.06	0.55
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.88	0.55
1:0:660:A:H4'	1:0:661:G:O5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1766:U:O2	1:0:1778:A:H5'	2.07	0.55
1:0:1909:A:H2'	1:0:1910:A:C8	2.40	0.55
1:0:2755:G:H1'	38:0:4956:HOH:O	2.06	0.55
3:4:176:DA:O4'	3:4:175:C:H2'	2.06	0.55
13:K:115:ARG:HG3	13:K:116:GLU:N	2.20	0.55
7:D:86:THR:C	7:D:89:PRO:HD2	2.27	0.55
25:W:73:LEU:O	25:W:74:GLU:HG3	2.06	0.55
1:0:968:G:O2'	1:0:969:G:H5'	2.07	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.72	0.55
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.20	0.55
6:C:111:VAL:HB	38:C:9123:HOH:O	2.07	0.55
25:W:119:HIS:HD2	25:W:120:PRO:O	1.89	0.55
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.55
1:0:1972:U:H2'	1:0:1973:A:H5'	1.88	0.55
1:0:2505:G:O2'	1:0:2506:A:H5'	2.07	0.55
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.88	0.55
5:B:88:GLU:HB3	5:B:97:LEU:HG	1.89	0.55
20:R:39:THR:HB	20:R:42:GLU:HG3	1.89	0.55
20:R:104:PHE:HB2	20:R:109:MET:HE1	1.88	0.55
1:0:681:G:N3	1:0:681:G:H5'	2.22	0.55
1:0:1242:A:C5'	12:J:82:THR:HG23	2.25	0.55
1:0:1505:U:H6	1:0:1505:U:H5'	1.70	0.55
1:0:2768:A:O2'	1:0:2769:C:H5'	2.07	0.55
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.89	0.55
21:S:37:VAL:O	21:S:41:VAL:HG23	2.06	0.55
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.88	0.55
1:0:2613:G:O2'	1:0:2614:C:H5'	2.07	0.55
9:F:107:ASP:O	9:F:111:ILE:HG13	2.07	0.55
11:H:9:ILE:O	11:H:9:ILE:HG22	2.07	0.55
17:O:21:SER:OG	17:O:106:PRO:HB2	2.07	0.55
18:P:143:ALA:HA	38:P:190:HOH:O	2.07	0.55
25:W:80:ASP:O	25:W:84:VAL:HG23	2.06	0.55
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.75	0.55
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.06	0.55
1:0:2630:G:O6	4:A:206:ARG:NH2	2.41	0.54
38:0:4897:HOH:O	4:A:6:GLY:HA3	2.07	0.54
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.22	0.54
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.86	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.20	0.54
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.37	0.54
1:0:2526:C:O2'	1:0:2527:U:H5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2783:A:H3'	38:0:5494:HOH:O	2.07	0.54
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.72	0.54
25:W:139:GLY:O	25:W:141:HIS:CD2	2.59	0.54
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.36	0.54
1:0:1234:U:C4	5:B:244:PRO:HB3	2.43	0.54
1:0:1289:C:H3'	38:0:6638:HOH:O	2.06	0.54
1:0:2509:A:H2'	1:0:2510:C:O4'	2.08	0.54
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.42	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.54
26:X:22:ASN:O	26:X:25:ARG:HG3	2.07	0.54
1:0:21:G:H4'	20:R:2:ILE:HG22	1.87	0.54
1:0:92:G:H4'	24:V:44:GLY:HA3	1.89	0.54
1:0:282:C:H1'	1:0:368:C:H42	1.68	0.54
1:0:2862:G:H4'	5:B:336:GLN:O	2.07	0.54
2:9:3001:U:H5"	2:9:3003:A:OP1	2.08	0.54
2:9:3028:U:H5"	16:N:40:ASN:ND2	2.22	0.54
2:9:3091:C:H2'	2:9:3092:G:O4'	2.07	0.54
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.20	0.54
5:B:51:VAL:HG13	5:B:53:LEU:HD13	1.89	0.54
5:B:119:HIS:O	5:B:121:PRO:HD3	2.08	0.54
6:C:77:ALA:O	6:C:78:ARG:HG3	2.07	0.54
7:D:25:MET:SD	7:D:40:ILE:HD11	2.48	0.54
8:E:84:MET:HB2	8:E:131:LEU:HB2	1.90	0.54
10:G:64:ASN:N	10:G:64:ASN:ND2	2.54	0.54
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.07	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54
32:I:139:ILE:HG22	32:I:140:GLU:H	1.71	0.54
1:0:2717:C:O2'	1:0:2718:C:H5"	2.06	0.54
12:J:103:VAL:HG12	38:J:9361:HOH:O	2.07	0.54
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.39	0.54
1:0:776:A:OP1	29:1:28:HIS:HE1	1.91	0.54
6:C:1:MET:HG2	6:C:2:GLN:N	2.15	0.54
1:0:583:G:H2'	1:0:584:U:C6	2.42	0.54
6:C:235:PHE:HE2	6:C:243:VAL:HG21	1.72	0.54
9:F:27:GLY:HA3	9:F:101:ALA:O	2.08	0.54
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.07	0.54
16:N:151:ASP:OD1	16:N:154:LEU:HD13	2.08	0.54
20:R:17:MET:CE	20:R:19:ARG:CZ	2.85	0.54
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.07	0.54
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.54
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.54
5:B:146:THR:O	5:B:159:PRO:HB3	2.08	0.54
6:C:140:VAL:HB	38:C:9252:HOH:O	2.07	0.54
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.72	0.54
24:V:38:GLY:C	24:V:40:PRO:HD2	2.27	0.54
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.07	0.54
1:0:1278:A:H4'	1:0:1279:U:C4	2.43	0.54
1:0:1342:C:O2'	1:0:1343:C:H5'	2.08	0.54
23:U:52:THR:HG22	23:U:54:THR:HB	1.90	0.54
25:W:122:ARG:HG3	25:W:152:ALA:O	2.07	0.54
27:Y:133:HIS:HD2	38:Y:8168:HOH:O	1.90	0.54
32:I:92:PRO:C	32:I:94:GLU:H	2.10	0.54
1:0:371:U:H2'	1:0:372:A:H8	1.73	0.54
1:0:1116:U:O2'	1:0:1118:A:C2	2.51	0.54
2:9:3003:A:N6	2:9:3022:G:H1'	2.23	0.54
5:B:162:MET:HG3	5:B:310:ARG:CZ	2.38	0.54
14:L:104:ASP:O	14:L:105:TYR:HB3	2.06	0.54
19:Q:28:ARG:HD2	19:Q:92:ARG:NH1	2.23	0.54
1:0:56:G:C5'	24:V:50:ARG:HH12	2.12	0.53
1:0:2300:A:H4'	1:0:2301:A:O5'	2.09	0.53
1:0:2720:C:O2	13:K:87:ARG:NH2	2.41	0.53
6:C:2:GLN:HB3	38:C:9186:HOH:O	2.07	0.53
16:N:100:ALA:O	16:N:129:ILE:HG23	2.08	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.08	0.53
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.90	0.53
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.90	0.53
32:I:75:THR:CA	32:I:112:LYS:NZ	2.71	0.53
1:0:1942:A:O2'	1:0:1943:C:H5'	2.09	0.53
7:D:25:MET:HE1	7:D:41:LEU:HG	1.91	0.53
16:N:37:ARG:NE	38:N:9334:HOH:O	2.41	0.53
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.73	0.53
27:Y:144:ARG:NH1	38:Y:8163:HOH:O	2.41	0.53
2:9:3042:C:H5'	2:9:3043:G:OP2	2.08	0.53
4:A:36:ASP:HB2	4:A:83:GLY:CA	2.39	0.53
6:C:127:ARG:HG2	6:C:127:ARG:NH1	2.24	0.53
12:J:45:VAL:HG22	12:J:130:VAL:O	2.09	0.53
1:0:407:A:H2'	1:0:408:A:C8	2.43	0.53
1:0:657:G:H2'	1:0:658:C:C6	2.43	0.53
1:0:1164:U:H3	1:0:1192:A:H2	1.56	0.53
1:0:2064:U:H5'	1:0:2652:U:H4'	1.90	0.53
38:0:9668:HOH:O	29:1:1:THR:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:294:TYR:HE2	38:B:9446:HOH:O	1.90	0.53
38:C:9168:HOH:O	22:T:2:LYS:HE2	2.06	0.53
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.37	0.53
16:N:23:ARG:O	16:N:27:LEU:HG	2.08	0.53
1:0:1014:A:H2'	1:0:1015:C:H5'	1.91	0.53
1:0:2597:U:H2'	1:0:2598:U:H5'	1.90	0.53
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.89	0.53
1:0:1667:A:H2'	1:0:1668:U:C6	2.44	0.53
7:D:153:THR:HA	7:D:156:ARG:HG3	1.91	0.53
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.39	0.53
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.91	0.53
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.23	0.53
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.37	0.53
1:0:90:A:H2'	1:0:91:G:O4'	2.09	0.53
1:0:539:G:H2'	1:0:540:A:C8	2.43	0.53
1:0:1377:C:H5'	1:0:1377:C:C6	2.44	0.53
1:0:2769:C:O2'	1:0:2770:G:H5'	2.09	0.53
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.34	0.53
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.23	0.53
9:F:38:LYS:HZ2	15:M:3:SER:HA	1.70	0.53
1:0:289:G:N2	1:0:363:A:H2	2.04	0.53
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.44	0.53
9:F:101:ALA:HA	38:F:5413:HOH:O	2.09	0.53
11:H:76:GLU:C	11:H:77:LEU:HD23	2.29	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.53
38:9:4707:HOH:O	16:N:147:ILE:HB	2.08	0.53
5:B:27:ASN:HD22	5:B:27:ASN:H	1.57	0.53
15:M:46:LEU:HG	38:M:9411:HOH:O	2.09	0.53
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.35	0.53
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.39	0.53
1:0:1175:G:H1'	1:0:1193:A:H2'	1.91	0.52
1:0:2324:G:H4'	1:0:2418:G:O2'	2.09	0.52
5:B:17:LYS:O	5:B:260:HIS:HD2	1.92	0.52
6:C:184:ARG:CZ	38:C:9216:HOH:O	2.57	0.52
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.91	0.52
12:J:19:MET:CE	12:J:132:LEU:HD11	2.38	0.52
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.25	0.52
22:T:78:THR:OG1	22:T:86:GLU:HG2	2.08	0.52
25:W:122:ARG:CZ	38:W:5817:HOH:O	2.57	0.52
26:X:30:MET:CE	26:X:58:ALA:HB3	2.39	0.52
1:0:338:C:H4'	6:C:174:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.38	0.52
16:N:37:ARG:HD3	36:N:9307:CL:CL	2.47	0.52
20:R:114:VAL:HG13	20:R:114:VAL:O	2.09	0.52
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.10	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.90	0.52
1:0:814:G:H4'	38:0:3429:HOH:O	2.09	0.52
1:0:2909:G:H2'	1:0:2910:A:H8	1.74	0.52
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.92	0.52
11:H:24:PRO:HD3	11:H:120:ILE:HG22	1.90	0.52
11:H:31:HIS:HD2	11:H:87:LEU:O	1.93	0.52
16:N:176:ARG:O	16:N:180:LEU:HD13	2.09	0.52
17:O:4:ASN:HB3	17:O:7:LEU:HB3	1.92	0.52
18:P:83:LYS:O	18:P:86:ALA:HB3	2.09	0.52
18:P:114:LEU:HA	18:P:118:GLN:NE2	2.25	0.52
20:R:106:GLY:HA2	20:R:109:MET:CE	2.35	0.52
22:T:28:SER:O	22:T:32:ARG:HG3	2.08	0.52
25:W:139:GLY:O	25:W:141:HIS:HD2	1.92	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
1:0:475:G:H5'	6:C:73:LEU:HD23	1.91	0.52
1:0:1342:C:C2'	1:0:1343:C:H5'	2.40	0.52
38:0:4516:HOH:O	30:2:38:LYS:HE3	2.10	0.52
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.20	0.52
25:W:13:MET:CE	25:W:17:ILE:HG22	2.39	0.52
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.10	0.52
1:0:553:G:O4'	1:0:1325:G:H5'	2.09	0.52
1:0:1634:G:H3'	38:0:4181:HOH:O	2.09	0.52
1:0:2758:G:H2'	1:0:2759:C:C6	2.45	0.52
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.40	0.52
8:E:11:VAL:CG1	8:E:12:ASP:N	2.72	0.52
12:J:107:ASN:C	12:J:107:ASN:HD22	2.13	0.52
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.75	0.52
6:C:132:ASP:HB3	38:C:9162:HOH:O	2.09	0.52
25:W:5:VAL:HG11	25:W:153:MET:CE	2.40	0.52
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.10	0.52
1:0:503:G:H2'	1:0:504:G:H8	1.75	0.52
1:0:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
1:0:1423:C:O2'	1:0:1424:A:H5'	2.10	0.52
1:0:2364:A:OP1	19:Q:11:ARG:NH1	2.42	0.52
26:X:21:PRO:HD3	38:X:6179:HOH:O	2.09	0.52
1:0:542:A:H2'	1:0:543:G:O4'	2.10	0.52
1:0:816:G:H5'	1:0:1598:A:H4'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.75	0.52
38:0:7598:HOH:O	22:T:9:LYS:HD2	2.10	0.52
2:9:3003:A:OP2	2:9:3025:G:N2	2.42	0.52
5:B:54:VAL:HB	38:B:9412:HOH:O	2.09	0.52
22:T:71:VAL:HG13	22:T:91:LEU:O	2.10	0.52
25:W:11:VAL:O	25:W:12:ASN:HB2	2.10	0.52
1:0:69:A:H5'	1:0:69:A:C8	2.45	0.52
1:0:259:G:O2'	1:0:260:C:H5'	2.10	0.52
1:0:1874:U:OP1	4:A:51:ARG:HD2	2.10	0.52
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.22	0.52
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.90	0.52
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.45	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.40	0.52
26:X:25:ARG:HG2	38:X:5356:HOH:O	2.10	0.52
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.56	0.52
8:E:34:TRP:O	12:J:127:ILE:HD11	2.10	0.52
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.45	0.52
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.92	0.52
1:0:960:G:H4'	38:0:7605:HOH:O	2.10	0.51
1:0:1855:G:H8	4:A:144:GLU:OE2	1.93	0.51
5:B:214:PRO:HD2	38:B:9321:HOH:O	2.09	0.51
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.40	0.51
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.57	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.91	0.51
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.51
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.45	0.51
1:0:67:A:H5"	1:0:69:A:C8	2.46	0.51
1:0:1205:U:C2'	1:0:1206:U:H5"	2.40	0.51
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.35	0.51
5:B:162:MET:HG3	5:B:310:ARG:HD3	1.92	0.51
5:B:258:GLY:H	5:B:260:HIS:CE1	2.27	0.51
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.25	0.51
14:L:145:LEU:O	14:L:148:GLU:HG3	2.10	0.51
15:M:65:VAL:HG21	15:M:105:ALA:HB2	1.90	0.51
15:M:107:ARG:HD2	38:M:9370:HOH:O	2.09	0.51
16:N:11:ARG:O	16:N:15:GLU:HG3	2.10	0.51
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.22	0.51
1:0:512:G:O3'	1:0:513:A:H8	1.94	0.51
1:0:1850:U:H2'	1:0:1851:G:H8	1.74	0.51
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.45	0.51
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:62:ARG:CA	5:B:65:MET:HE3	2.35	0.51
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.45	0.51
28:Z:46:ARG:HD3	28:Z:58:SER:OG	2.11	0.51
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.55	0.51
4:A:36:ASP:CB	4:A:83:GLY:HA3	2.41	0.51
4:A:199:HIS:CD2	4:A:201:PHE:H	2.28	0.51
5:B:310:ARG:HD2	38:B:9444:HOH:O	2.08	0.51
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.40	0.51
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.46	0.51
24:V:27:LEU:HA	24:V:49:LEU:HD13	1.92	0.51
1:0:159:G:OP1	15:M:74:LYS:HE3	2.10	0.51
5:B:141:ARG:HD2	5:B:163:GLU:OE2	2.11	0.51
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.10	0.51
30:2:48:ASP:O	30:2:49:GLU:HB2	2.10	0.51
1:0:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.51
1:0:2897:C:H2'	1:0:2898:G:H8	1.74	0.51
10:G:23:ILE:O	10:G:27:ILE:HG13	2.10	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.26	0.51
31:3:40:ARG:HD2	38:3:9357:HOH:O	2.10	0.51
1:0:638:C:H2'	1:0:639:A:C8	2.46	0.51
1:0:1500:U:P	18:P:41:ARG:HH22	2.33	0.51
4:A:179:MET:HG3	4:A:186:TRP:CG	2.46	0.51
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.93	0.51
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.09	0.51
20:R:132:ARG:CZ	38:R:9385:HOH:O	2.59	0.51
21:S:43:GLU:HB3	38:S:9141:HOH:O	2.10	0.51
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.75	0.51
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.46	0.51
32:I:101:SER:OG	32:I:104:GLN:HG3	2.11	0.51
1:0:419:A:H1'	1:0:1921:A:C2	2.45	0.51
1:0:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
1:0:1252:A:H2'	1:0:1253:C:O4'	2.11	0.51
1:0:2036:C:O4'	13:K:44:LEU:HG	2.11	0.51
15:M:59:GLY:CA	15:M:141:ILE:HD11	2.41	0.51
15:M:157:ASP:HB3	15:M:160:PHE:HD1	1.75	0.51
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.57	0.51
1:0:263:U:C4	9:F:54:VAL:HG13	2.45	0.51
1:0:583:G:H2'	1:0:584:U:H6	1.76	0.51
1:0:694:A:H2'	1:0:695:C:H5'	1.93	0.51
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:790:A:H2'	1:0:791:A:O4'	2.10	0.51
1:0:1167:G:H2'	1:0:1168:C:O4'	2.11	0.51
1:0:1422:U:H2'	1:0:1423:C:C6	2.46	0.51
38:0:9863:HOH:O	25:W:119:HIS:HE1	1.93	0.51
6:C:233:THR:HG22	6:C:234:VAL:H	1.76	0.51
11:H:36:LYS:HA	11:H:84:LYS:NZ	2.26	0.51
16:N:151:ASP:O	16:N:154:LEU:HB2	2.10	0.51
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.92	0.51
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.93	0.51
25:W:130:HIS:O	25:W:136:GLY:HA3	2.10	0.51
32:I:91:GLU:HB3	32:I:94:GLU:OE2	2.11	0.51
1:0:1528:A:H2'	1:0:1529:G:O4'	2.11	0.51
1:0:1555:G:H4'	1:0:1630:A:H2	1.75	0.51
1:0:2361:A:H5'	1:0:2361:A:H8	1.76	0.51
4:A:105:VAL:HG12	4:A:106:CYS:N	2.26	0.51
4:A:217:ARG:HG2	4:A:229:ALA:HB2	1.93	0.51
6:C:13:ASP:OD1	6:C:13:ASP:O	2.27	0.51
21:S:53:ASN:HD22	21:S:53:ASN:N	2.09	0.51
24:V:42:ASN:O	24:V:44:GLY:N	2.43	0.51
25:W:36:PRO:HD2	25:W:41:TYR:CE1	2.46	0.51
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.50
1:0:1730:G:H5"	1:0:1731:C:H6	1.76	0.50
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.50
4:A:211:LYS:HB2	38:A:9412:HOH:O	2.10	0.50
13:K:6:ALA:CB	13:K:116:GLU:HG2	2.41	0.50
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.50
1:0:243:A:H61	1:0:269:G:H1'	1.76	0.50
1:0:289:G:O2'	1:0:290:C:H5'	2.11	0.50
1:0:366:U:H2'	1:0:367:G:O4'	2.11	0.50
1:0:1189:A:H1'	1:0:1209:C:H1'	1.92	0.50
6:C:242:GLU:HG3	38:C:9183:HOH:O	2.11	0.50
9:F:56:PRO:HG2	15:M:43:PRO:O	2.11	0.50
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.94	0.50
16:N:170:GLU:O	16:N:174:GLU:HG3	2.10	0.50
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.12	0.50
32:I:106:LYS:O	32:I:110:GLU:HG3	2.12	0.50
1:0:451:C:O2'	1:0:452:G:H5'	2.11	0.50
1:0:1904:A:H2'	1:0:1905:U:O4'	2.12	0.50
1:0:2453:G:H4'	14:L:50:GLY:C	2.31	0.50
38:0:3252:HOH:O	26:X:23:HIS:HD2	1.93	0.50
4:A:164:ARG:CZ	38:A:9383:HOH:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.76	0.50
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.94	0.50
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.92	0.50
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.93	0.50
1:0:241:A:C2	1:0:378:A:H4'	2.46	0.50
1:0:559:U:H2'	1:0:560:C:O4'	2.11	0.50
1:0:657:G:H2'	1:0:658:C:H6	1.75	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.11	0.50
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.11	0.50
1:0:2419:U:H5"	1:0:2420:G:H5'	1.94	0.50
5:B:304:PRO:CG	5:B:307:ARG:NH1	2.74	0.50
7:D:23:VAL:HG11	7:D:83:PHE:CZ	2.46	0.50
11:H:170:ASN:HD22	11:H:170:ASN:N	2.08	0.50
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.10	0.50
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.41	0.50
14:L:148:GLU:HA	38:L:9371:HOH:O	2.10	0.50
1:0:263:U:O4'	9:F:59:ILE:HD13	2.11	0.50
1:0:2507:G:H2'	1:0:2510:C:H42	1.77	0.50
4:A:33:GLU:O	4:A:34:ASP:HB2	2.11	0.50
5:B:145:HIS:HD2	5:B:146:THR:O	1.94	0.50
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.42	0.50
1:0:113:A:OP2	1:0:114:A:H2'	2.11	0.50
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.12	0.50
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.27	0.50
6:C:237:GLU:HB2	38:C:9234:HOH:O	2.11	0.50
9:F:99:THR:HA	38:F:3461:HOH:O	2.11	0.50
17:O:38:ARG:HD3	38:O:7674:HOH:O	2.10	0.50
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.11	0.50
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.92	0.50
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.50
1:0:1563:G:O2'	1:0:1564:C:OP2	2.25	0.50
1:0:1641:A:C2'	1:0:1642:A:H5'	2.42	0.50
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.93	0.50
12:J:117:ASP:O	12:J:119:THR:HG23	2.12	0.50
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.93	0.50
26:X:18:ARG:NH1	38:X:4132:HOH:O	2.41	0.50
1:0:189:A:OP1	15:M:171:ARG:NH2	2.45	0.50
1:0:1205:U:H2'	1:0:1206:U:H5'	1.92	0.50
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.50
1:0:2851:G:C2'	1:0:2852:A:H5'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:74:C:H2'	3:4:75:C:H5'	1.93	0.50
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.94	0.50
6:C:104:ASP:O	6:C:108:GLN:HG3	2.11	0.50
38:K:7438:HOH:O	23:U:20:MET:HE1	2.12	0.50
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.11	0.50
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.93	0.50
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.12	0.50
1:0:1183:C:N4	1:0:1184:C:H41	2.09	0.50
1:0:2509:A:OP2	1:0:2510:C:H5	1.94	0.50
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.94	0.50
7:D:52:THR:N	7:D:70:GLY:O	2.45	0.50
7:D:84:LEU:C	7:D:86:THR:H	2.16	0.50
13:K:72:VAL:HG11	13:K:121:PHE:CD1	2.46	0.50
15:M:99:ARG:HD2	15:M:167:GLY:CA	2.39	0.50
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.94	0.50
25:W:41:TYR:HA	25:W:44:MET:HE3	1.94	0.50
29:1:25:LYS:HD2	30:2:49:GLU:N	2.26	0.50
1:0:475:G:OP1	6:C:73:LEU:HD22	2.12	0.49
5:B:147:VAL:HG12	5:B:150:ALA:H	1.76	0.49
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.95	0.49
9:F:31:LYS:HD3	9:F:89:LEU:HG	1.94	0.49
22:T:65:VAL:HG22	22:T:72:ILE:HG22	1.94	0.49
22:T:106:GLU:HG3	38:T:4913:HOH:O	2.12	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.49
1:0:69:A:H5'	1:0:69:A:H8	1.77	0.49
1:0:396:U:O2'	1:0:418:C:H4'	2.12	0.49
1:0:944:G:H21	25:W:44:MET:CE	2.25	0.49
1:0:1180:U:H2'	1:0:1181:A:O4'	2.12	0.49
1:0:1593:C:OP1	18:P:117:SER:HB3	2.12	0.49
1:0:1730:G:C5'	1:0:1731:C:C6	2.95	0.49
5:B:79:MET:HE3	5:B:144:THR:HG21	1.93	0.49
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.49
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.42	0.49
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.42	0.49
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.11	0.49
1:0:316:A:H5'	22:T:54:ASP:OD2	2.12	0.49
1:0:1406:A:H4'	1:0:1407:A:H5"	1.93	0.49
5:B:75:GLU:C	5:B:77:PRO:HD3	2.33	0.49
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.43	0.49
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.94	0.49
16:N:154:LEU:O	16:N:155:GLU:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.27	0.49
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.94	0.49
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.13	0.49
1:0:500:G:H21	20:R:98:ASN:HD21	1.58	0.49
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.49
1:0:1735:C:OP2	5:B:234:ARG:HG3	2.12	0.49
1:0:2241:C:O2'	1:0:2242:U:H5'	2.12	0.49
1:0:2506:A:O2'	1:0:2507:G:O5'	2.30	0.49
38:0:5245:HOH:O	11:H:58:ARG:HG3	2.12	0.49
4:A:99:ILE:O	4:A:131:HIS:HE1	1.95	0.49
15:M:80:GLY:O	15:M:81:ARG:HD3	2.12	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
16:N:67:ALA:C	16:N:69:TYR:H	2.14	0.49
17:O:25:VAL:HG23	17:O:26:TRP:N	2.26	0.49
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.49
22:T:48:VAL:CG1	22:T:49:GLU:N	2.74	0.49
26:X:30:MET:CE	26:X:55:ASN:HA	2.41	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:0:1537:C:H1'	38:0:6807:HOH:O	2.12	0.49
6:C:170:ASP:O	6:C:171:GLU:HG3	2.12	0.49
8:E:125:GLU:HB2	8:E:132:THR:CG2	2.43	0.49
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.49
18:P:55:LYS:CG	18:P:56:GLY:N	2.75	0.49
27:Y:123:VAL:HG12	27:Y:124:GLY:O	2.12	0.49
1:0:80:A:H3'	22:T:43:ASN:OD1	2.11	0.49
1:0:1166:A:H61	1:0:1180:U:H3	1.61	0.49
1:0:1804:A:H2'	1:0:1805:G:C8	2.48	0.49
1:0:2793:A:H2'	1:0:2794:G:H5'	1.94	0.49
2:9:3008:G:O6	16:N:11:ARG:NH1	2.46	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.45	0.49
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.94	0.49
7:D:159:PRO:O	7:D:163:VAL:HG23	2.13	0.49
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.27	0.49
12:J:107:ASN:ND2	12:J:109:TYR:H	2.11	0.49
13:K:101:ASN:HB2	13:K:103:ASP:OD2	2.13	0.49
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.94	0.49
25:W:60:GLU:O	25:W:63:GLU:HB2	2.13	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
31:3:65:THR:HG23	31:3:67:LEU:HG	1.94	0.49
32:I:123:ASN:HA	32:I:126:LYS:HD2	1.94	0.49
1:0:542:A:H5'	1:0:542:A:C8	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1086:A:N6	25:W:11:VAL:HG11	2.28	0.49
1:0:2834:G:OP1	26:X:39:LYS:HE2	2.12	0.49
2:9:3034:A:H2'	2:9:3035:C:O4'	2.12	0.49
5:B:248:ARG:O	5:B:251:VAL:HG13	2.13	0.49
15:M:134:ILE:O	15:M:136:PRO:HD3	2.13	0.49
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.43	0.49
25:W:126:ASP:HB3	25:W:135:GLY:O	2.12	0.49
1:0:371:U:H2'	1:0:372:A:C8	2.48	0.49
1:0:569:A:H5"	1:0:587:A:N1	2.27	0.49
1:0:894:A:C2	6:C:87:ARG:NH2	2.80	0.49
1:0:1311:G:O6	6:C:173:LYS:HE3	2.13	0.49
1:0:1787:C:H4'	1:0:2883:A:O4'	2.12	0.49
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.13	0.49
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.95	0.49
38:0:9527:HOH:O	4:A:11:ARG:HD3	2.13	0.49
6:C:25:PRO:HG2	38:C:9124:HOH:O	2.11	0.49
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.43	0.49
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.94	0.49
23:U:17:THR:CG2	23:U:18:GLY:N	2.75	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
29:1:22:CYS:SG	29:1:24:GLU:HB2	2.53	0.49
1:0:432:G:O2'	1:0:433:C:H5'	2.12	0.49
1:0:603:A:H5"	1:0:604:G:OP1	2.12	0.49
1:0:1393:A:H2'	1:0:1394:C:C6	2.48	0.49
1:0:2073:G:OP2	1:0:2490:A:H5'	2.13	0.49
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.13	0.49
6:C:39:GLN:O	6:C:43:LYS:HD3	2.13	0.49
7:D:23:VAL:HG23	7:D:23:VAL:O	2.13	0.49
1:0:541:C:H2'	1:0:542:A:H5'	1.95	0.49
1:0:1878:G:H1'	38:0:6359:HOH:O	2.13	0.49
4:A:168:PRO:O	4:A:170:VAL:HG23	2.12	0.49
6:C:118:THR:O	6:C:136:VAL:HG13	2.13	0.49
14:L:81:VAL:HG12	14:L:82:ALA:N	2.28	0.49
1:0:383:A:H4'	38:0:5588:HOH:O	2.13	0.48
1:0:482:G:H4'	1:0:508:A:N1	2.28	0.48
1:0:506:G:N2	1:0:509:A:H5'	2.20	0.48
38:0:6921:HOH:O	27:Y:165:GLU:HB3	2.11	0.48
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.48	0.48
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.94	0.48
8:E:101:GLU:HB2	8:E:116:THR:O	2.13	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:46:GLN:CB	11:H:167:PRO:HD2	2.22	0.48
11:H:80:GLU:HA	38:H:9182:HOH:O	2.13	0.48
20:R:39:THR:HG22	20:R:42:GLU:N	2.16	0.48
1:0:1206:U:H2'	1:0:1207:A:O4'	2.13	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.12	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.94	0.48
1:0:2890:A:C1'	23:U:56:ARG:NH2	2.72	0.48
4:A:211:LYS:CB	4:A:212:PRO:HD2	2.28	0.48
5:B:85:ARG:NH1	38:B:9431:HOH:O	2.45	0.48
11:H:120:ILE:N	11:H:120:ILE:CD1	2.76	0.48
20:R:29:LYS:NZ	38:R:9341:HOH:O	2.47	0.48
30:2:41:HIS:CD2	30:2:44:ARG:H	2.27	0.48
1:0:214:U:H5'	38:0:6378:HOH:O	2.13	0.48
1:0:440:C:H2'	1:0:441:A:C8	2.48	0.48
1:0:926:A:O2'	14:L:41:HIS:CD2	2.65	0.48
1:0:1507:C:H4'	38:0:3891:HOH:O	2.14	0.48
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.95	0.48
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.11	0.48
27:Y:184:GLU:OE2	27:Y:204:ARG:HD2	2.13	0.48
32:I:135:LEU:HB2	32:I:137:VAL:HG23	1.95	0.48
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.12	0.48
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.77	0.48
4:A:164:ARG:HA	28:Z:69:TYR:CE1	2.48	0.48
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.14	0.48
8:E:31:ARG:NH1	38:E:5919:HOH:O	2.46	0.48
18:P:115:SER:OG	18:P:118:GLN:HG3	2.13	0.48
22:T:26:THR:HA	22:T:39:ASN:HB3	1.94	0.48
25:W:14:HIS:HB2	25:W:17:ILE:HG13	1.95	0.48
1:0:920:C:H5"	1:0:921:G:O5'	2.13	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.48
1:0:2428:G:N7	31:3:60:LYS:HE2	2.29	0.48
4:A:53:ALA:HB3	38:A:9401:HOH:O	2.12	0.48
4:A:72:GLU:OE1	28:Z:72:GLU:HA	2.13	0.48
4:A:194:MET:HE2	4:A:199:HIS:CB	2.44	0.48
5:B:98:THR:HG22	5:B:99:GLU:N	2.26	0.48
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.95	0.48
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.49	0.48
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.94	0.48
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.61	0.48
20:R:17:MET:HE3	20:R:19:ARG:CZ	2.43	0.48
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:55:ARG:O	24:V:59:ILE:HG12	2.14	0.48
1:0:152:A:O2'	1:0:153:C:H5'	2.13	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:2561:C:OP1	8:E:153:ARG:NH2	2.46	0.48
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.95	0.48
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.43	0.48
5:B:5:ARG:HD2	5:B:8:LYS:HZ1	1.79	0.48
6:C:236:THR:HG21	38:C:9175:HOH:O	2.13	0.48
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.17	0.48
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.47	0.48
24:V:58:THR:O	24:V:62:GLU:HG3	2.13	0.48
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.42	0.48
1:0:558:C:H2'	1:0:559:U:C5'	2.41	0.48
1:0:1878:G:O2'	1:0:1879:U:C6	2.64	0.48
1:0:2362:A:H2'	1:0:2363:G:C8	2.48	0.48
7:D:163:VAL:HA	38:D:6326:HOH:O	2.13	0.48
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.44	0.48
9:F:99:THR:HG23	9:F:99:THR:O	2.13	0.48
27:Y:155:ARG:NH1	38:Y:8147:HOH:O	2.47	0.48
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.92	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.49	0.48
1:0:1168:C:H4'	38:I:5128:HOH:O	2.13	0.48
1:0:2015:A:H2'	1:0:2016:U:O4'	2.13	0.48
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.48
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.95	0.48
2:9:3012:C:H5'	2:9:3070:U:O4'	2.12	0.48
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.14	0.48
14:L:133:VAL:HB	38:L:9357:HOH:O	2.13	0.48
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.43	0.48
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.13	0.48
22:T:24:ARG:NH2	22:T:39:ASN:HD22	2.12	0.48
1:0:1352:A:N1	6:C:48:SER:HB3	2.28	0.48
1:0:2478:U:O2'	1:0:2479:A:H5'	2.14	0.48
1:0:2783:A:H2'	1:0:2784:A:C8	2.49	0.48
6:C:236:THR:O	6:C:237:GLU:C	2.52	0.48
8:E:16:ASP:O	8:E:17:HIS:HB2	2.13	0.48
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.44	0.48
12:J:52:GLN:HG3	12:J:53:ILE:H	1.77	0.48
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.94	0.48
26:X:12:ILE:HB	26:X:70:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1849:G:H1'	1:0:2011:A:N1	2.28	0.48
1:0:2269:C:C2'	1:0:2270:G:H5'	2.43	0.48
25:W:3:ALA:O	25:W:54:PHE:HA	2.14	0.48
1:0:157:G:H4'	15:M:95:LYS:CE	2.43	0.47
1:0:396:U:OP2	31:3:38:ARG:HD2	2.13	0.47
1:0:832:U:H2'	1:0:833:G:C8	2.49	0.47
1:0:1568:G:O2'	1:0:1569:U:H5'	2.14	0.47
1:0:1942:A:H3'	38:0:7527:HOH:O	2.15	0.47
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.47
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.96	0.47
5:B:72:THR:HB	38:B:9406:HOH:O	2.13	0.47
7:D:153:THR:HA	7:D:156:ARG:CG	2.43	0.47
7:D:159:PRO:O	7:D:162:ALA:HB3	2.14	0.47
17:O:45:LEU:HD12	17:O:88:LYS:HD2	1.95	0.47
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.79	0.47
1:0:1634:G:H2'	1:0:1635:U:C6	2.49	0.47
7:D:128:LEU:C	7:D:128:LEU:HD23	2.35	0.47
8:E:132:THR:HB	38:E:2227:HOH:O	2.15	0.47
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.28	0.47
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.44	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.47
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.47
1:0:1940:C:H4'	38:0:7527:HOH:O	2.13	0.47
20:R:119:VAL:O	20:R:119:VAL:HG12	2.14	0.47
22:T:71:VAL:HG12	22:T:72:ILE:N	2.28	0.47
1:0:343:C:O2'	1:0:344:C:H5'	2.14	0.47
1:0:1120:U:H5'	1:0:1120:U:C6	2.40	0.47
1:0:1613:C:H2'	1:0:1614:G:O4'	2.14	0.47
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.48	0.47
2:9:3028:U:H2'	2:9:3029:C:C6	2.48	0.47
7:D:135:VAL:HG22	7:D:136:ARG:H	1.79	0.47
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.29	0.47
32:I:133:THR:N	38:I:5371:HOH:O	2.47	0.47
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.15	0.47
1:0:1825:U:O2'	1:0:1826:C:H5'	2.14	0.47
2:9:3114:G:H2'	2:9:3115:C:C6	2.50	0.47
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.97	0.47
7:D:138:GLY:N	38:D:7597:HOH:O	2.47	0.47
9:F:26:THR:HG21	9:F:102:GLY:C	2.34	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.47
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.41	0.47
1:0:731:U:H2'	1:0:732:C:C6	2.50	0.47
1:0:1925:G:O2'	1:0:1926:G:H5'	2.15	0.47
1:0:2379:G:H5'	1:0:2381:C:O4'	2.14	0.47
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.47
7:D:25:MET:CE	7:D:41:LEU:HG	2.44	0.47
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.42	0.47
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.96	0.47
8:E:37:ASP:OD1	12:J:125:SER:HB3	2.14	0.47
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.96	0.47
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.47
18:P:103:THR:O	18:P:106:ARG:HB3	2.15	0.47
24:V:39:ALA:C	24:V:41:GLU:H	2.18	0.47
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.15	0.47
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.97	0.47
1:0:1427:A:H61	1:0:1440:U:C1'	2.27	0.47
1:0:2547:C:OP2	5:B:5:ARG:NH1	2.47	0.47
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.80	0.47
38:0:4353:HOH:O	5:B:27:ASN:HB2	2.14	0.47
4:A:192:VAL:HG13	38:A:9354:HOH:O	2.15	0.47
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.27	0.47
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.45	0.47
16:N:37:ARG:CZ	38:N:9334:HOH:O	2.62	0.47
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.95	0.47
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.49	0.47
28:Z:33:MET:SD	28:Z:49:ARG:HD2	2.54	0.47
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.95	0.47
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.49	0.47
32:I:92:PRO:O	32:I:94:GLU:HG3	2.14	0.47
32:I:132:CYS:O	32:I:135:LEU:N	2.47	0.47
1:0:705:C:O2	1:0:705:C:H2'	2.15	0.47
1:0:1118:A:H8	1:0:1119:G:H5"	1.79	0.47
1:0:1462:C:H2'	1:0:1463:A:H8	1.78	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.15	0.47
1:0:1730:G:H5'	1:0:1731:C:H5	1.78	0.47
1:0:1890:U:H4'	1:0:2010:A:C6	2.50	0.47
4:A:36:ASP:HB2	4:A:84:VAL:N	2.30	0.47
4:A:217:ARG:CG	4:A:217:ARG:NH1	2.77	0.47
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.45	0.47
6:C:76:ARG:HH11	6:C:76:ARG:CG	2.28	0.47
13:K:99:ASP:OD1	13:K:101:ASN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:112:LYS:C	32:I:114:PRO:HD2	2.35	0.47
1:0:945:U:O2'	25:W:43:GLY:HA3	2.14	0.47
1:0:1701:A:H5"	1:0:1702:U:H3'	1.97	0.47
1:0:2869:G:H2'	1:0:2870:C:C6	2.50	0.47
2:9:3001:U:O3'	2:9:3003:A:H5'	2.14	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
2:9:3076:G:C3'	2:9:3077:A:H5"	2.36	0.47
5:B:162:MET:HE3	5:B:308:LEU:HD21	1.96	0.47
5:B:279:THR:OG1	5:B:290:VAL:HB	2.14	0.47
6:C:20:ASP:O	6:C:23:GLU:HB2	2.15	0.47
8:E:97:VAL:HG12	38:E:4191:HOH:O	2.15	0.47
9:F:56:PRO:HG2	15:M:44:THR:HA	1.95	0.47
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.76	0.47
25:W:76:ASP:O	25:W:77:ALA:C	2.52	0.47
1:0:284:C:H4'	1:0:285:A:O5'	2.15	0.47
1:0:659:A:N1	17:O:42:GLU:OE2	2.48	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.30	0.47
1:0:2668:G:H2'	1:0:2669:U:H6	1.77	0.47
1:0:2748:G:H2'	38:0:7705:HOH:O	2.15	0.47
2:9:3056:A:H1'	7:D:14:ARG:HG2	1.97	0.47
2:9:3107:C:H5	38:9:3167:HOH:O	1.97	0.47
4:A:48:ASP:HB3	38:A:9401:HOH:O	2.15	0.47
4:A:211:LYS:NZ	38:A:9413:HOH:O	2.46	0.47
5:B:210:GLY:HA2	5:B:256:GLN:HE22	1.80	0.47
7:D:91:ALA:HB1	38:D:5198:HOH:O	2.15	0.47
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.97	0.47
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.45	0.47
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.14	0.47
11:H:154:TYR:CD1	11:H:154:TYR:C	2.87	0.47
16:N:5:ARG:HG3	19:Q:18:PRO:CB	2.44	0.47
1:0:100:C:H4'	22:T:16:LEU:HB2	1.98	0.46
1:0:947:U:H2'	1:0:948:G:C8	2.50	0.46
1:0:1419:U:H2'	1:0:1685:A:C2	2.51	0.46
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.15	0.46
1:0:2545:U:OP2	5:B:2:GLN:HG2	2.14	0.46
2:9:3013:A:N3	16:N:14:ARG:NH2	2.57	0.46
5:B:5:ARG:HD2	5:B:8:LYS:HZ3	1.79	0.46
5:B:41:PHE:HB3	5:B:190:MET:CE	2.45	0.46
9:F:4:VAL:HG13	9:F:76:PHE:CE1	2.50	0.46
9:F:37:THR:O	9:F:41:GLU:HG3	2.14	0.46
15:M:59:GLY:C	15:M:141:ILE:HD11	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:47:ARG:HA	17:O:50:ARG:NH1	2.30	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
21:S:57:THR:CG2	21:S:58:MET:N	2.78	0.46
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.15	0.46
1:0:352:A:H2'	1:0:353:G:C8	2.49	0.46
1:0:1162:G:H1'	32:I:117:LEU:CD1	2.37	0.46
1:0:1285:U:H4'	25:W:74:GLU:OE1	2.15	0.46
11:H:66:ARG:HD3	38:H:9177:HOH:O	2.14	0.46
11:H:162:ARG:HD3	38:H:9180:HOH:O	2.14	0.46
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.45	0.46
20:R:19:ARG:HA	20:R:142:ASP:OD1	2.15	0.46
1:0:669:G:O2'	1:0:670:G:H5'	2.16	0.46
1:0:1434:A:H2'	1:0:1436:C:C5	2.50	0.46
1:0:2534:C:H1'	38:0:3787:HOH:O	2.14	0.46
1:0:2840:A:H3'	38:0:7810:HOH:O	2.14	0.46
4:A:164:ARG:NE	38:A:9383:HOH:O	2.47	0.46
6:C:4:THR:HA	6:C:15:GLU:HB3	1.96	0.46
6:C:76:ARG:HH11	6:C:76:ARG:HG2	1.81	0.46
7:D:18:ILE:HD13	7:D:84:LEU:CD1	2.45	0.46
14:L:146:GLY:C	14:L:148:GLU:H	2.18	0.46
15:M:164:THR:HG23	15:M:166:ALA:N	2.30	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.51	0.46
26:X:10:VAL:HG12	26:X:11:THR:N	2.29	0.46
1:0:466:A:H2'	1:0:467:G:O4'	2.15	0.46
1:0:1187:U:H2'	38:0:7102:HOH:O	2.16	0.46
1:0:1759:A:N3	1:0:1818:C:H2'	2.31	0.46
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.46
1:0:2820:A:H2'	1:0:2821:C:C6	2.51	0.46
5:B:24:PRO:HG2	5:B:204:GLY:HA2	1.98	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.29	0.46
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.15	0.46
6:C:166:ILE:CD1	6:C:207:LEU:HD13	2.45	0.46
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.48	0.46
14:L:35:ARG:O	14:L:40:PHE:HA	2.15	0.46
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.46
17:O:39:THR:O	17:O:115:ARG:NH2	2.48	0.46
17:O:96:VAL:HG12	17:O:97:SER:N	2.30	0.46
18:P:101:GLN:HG3	38:P:164:HOH:O	2.16	0.46
20:R:30:ALA:HA	20:R:33:ARG:HH12	1.81	0.46
31:3:72:GLY:HA2	38:3:9373:HOH:O	2.15	0.46
1:0:20:G:H21	20:R:117:HIS:HD2	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.51	0.46
1:0:506:G:H22	1:0:509:A:H5"	1.79	0.46
1:0:945:U:H2'	1:0:946:C:H6	1.80	0.46
1:0:1521:C:H2'	1:0:1522:A:H8	1.80	0.46
10:G:67:LEU:O	10:G:71:LEU:HG	2.16	0.46
15:M:139:PRO:O	15:M:143:ASN:ND2	2.49	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46
23:U:53:ASP:O	23:U:54:THR:C	2.54	0.46
32:I:132:CYS:O	32:I:134:SER:N	2.49	0.46
1:0:166:A:N7	14:L:25:GLY:HA2	2.30	0.46
1:0:226:A:H1'	1:0:393:G:C5	2.50	0.46
1:0:853:C:H2'	1:0:854:G:O4'	2.15	0.46
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.46
1:0:1185:U:H5'	38:0:7636:HOH:O	2.16	0.46
1:0:1329:A:N1	36:0:9313:CL:CL	2.85	0.46
1:0:1545:C:H2'	1:0:1546:G:O4'	2.16	0.46
1:0:1603:A:H5'	1:0:1605:G:C4'	2.45	0.46
1:0:1919:A:H5'	38:0:6245:HOH:O	2.16	0.46
1:0:2421:G:H4'	38:0:5056:HOH:O	2.15	0.46
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.15	0.46
15:M:49:ALA:C	15:M:54:TYR:HB3	2.35	0.46
15:M:61:ILE:HG22	15:M:62:VAL:N	2.31	0.46
15:M:159:VAL:HG13	15:M:160:PHE:N	2.30	0.46
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.97	0.46
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.45	0.46
27:Y:97:LEU:C	27:Y:98:GLN:HG2	2.36	0.46
29:1:28:HIS:HD2	29:1:30:LYS:H	1.62	0.46
1:0:74:A:H2'	1:0:75:U:C6	2.51	0.46
1:0:522:U:O2'	1:0:1366:C:H5'	2.15	0.46
1:0:820:G:H5'	1:0:821:U:H5'	1.96	0.46
1:0:821:U:H2'	1:0:822:C:H6	1.80	0.46
1:0:1804:A:H2'	1:0:1805:G:H8	1.80	0.46
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.15	0.46
1:0:2715:G:N2	5:B:264:GLU:OE1	2.45	0.46
1:0:2900:G:H2'	1:0:2901:C:O4'	2.16	0.46
38:9:3472:HOH:O	16:N:41:LYS:HD3	2.15	0.46
6:C:88:SER:O	6:C:91:PRO:HD3	2.15	0.46
9:F:56:PRO:CG	15:M:44:THR:HA	2.45	0.46
32:I:123:ASN:HA	32:I:126:LYS:CD	2.46	0.46
1:0:911:G:H5'	1:0:932:U:OP1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1385:G:O3'	26:X:49:ARG:NH1	2.49	0.46
1:0:1517:U:C2	1:0:1670:G:N2	2.84	0.46
6:C:12:THR:HB	38:C:9244:HOH:O	2.15	0.46
6:C:182:ARG:HD2	6:C:184:ARG:HH12	1.81	0.46
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.63	0.46
12:J:131:THR:HB	12:J:134:GLU:OE1	2.15	0.46
13:K:23:ASN:HD21	13:K:107:THR:HB	1.81	0.46
25:W:149:LEU:HG	25:W:153:MET:CE	2.46	0.46
1:0:497:A:H2'	1:0:498:A:C5'	2.46	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.15	0.46
4:A:188:ASN:HA	38:A:9363:HOH:O	2.16	0.46
6:C:93:LYS:O	6:C:98:ARG:NH2	2.49	0.46
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.50	0.46
7:D:67:ASP:O	7:D:69:ILE:HG13	2.16	0.46
8:E:77:THR:OG1	8:E:78:GLU:N	2.48	0.46
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.51	0.46
14:L:17:SER:C	14:L:19:LYS:H	2.18	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
18:P:15:ASP:O	18:P:16:VAL:HG23	2.16	0.46
26:X:27:ASP:OD2	26:X:27:ASP:N	2.48	0.46
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.80	0.46
1:0:671:A:O2'	1:0:672:G:H2'	2.16	0.46
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.46
1:0:1072:G:P	27:Y:154:ARG:HH22	2.39	0.46
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.15	0.46
4:A:96:LEU:HD22	4:A:128:LEU:HD13	1.97	0.46
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.15	0.46
5:B:195:ARG:N	5:B:198:GLU:OE1	2.50	0.46
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.46	0.46
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.97	0.46
11:H:84:LYS:NZ	11:H:84:LYS:HB2	2.31	0.46
12:J:133:GLY:O	12:J:137:GLU:HG3	2.16	0.46
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.49	0.46
14:L:35:ARG:C	14:L:35:ARG:HD3	2.36	0.46
22:T:88:PRO:O	22:T:90:PRO:HD3	2.16	0.46
25:W:64:THR:O	25:W:68:THR:HG22	2.16	0.46
25:W:131:PRO:HD2	25:W:134:GLU:OE1	2.15	0.46
25:W:154:ARG:HE	25:W:154:ARG:HB3	1.53	0.46
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.45	0.46
1:0:1184:C:O2'	1:0:1185:U:OP2	2.24	0.45
1:0:2420:G:O2'	1:0:2421:G:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.80	0.45
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.98	0.45
7:D:35:ALA:C	7:D:37:ALA:H	2.18	0.45
9:F:1:PRO:HB2	38:F:5897:HOH:O	2.16	0.45
11:H:9:ILE:HG12	11:H:56:GLN:HG3	1.98	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.16	0.45
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.45	0.45
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.17	0.45
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.51	0.45
29:1:45:ARG:NH2	38:1:9232:HOH:O	2.43	0.45
1:0:316:A:N3	1:0:336:G:O2'	2.45	0.45
1:0:553:G:O2'	27:Y:179:PRO:HG3	2.16	0.45
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.45
6:C:19:PRO:CB	6:C:244:ALA:HB2	2.45	0.45
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.97	0.45
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.27	0.45
11:H:171:ALA:HA	38:H:9168:HOH:O	2.17	0.45
13:K:66:ARG:HD3	38:K:2777:HOH:O	2.16	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.79	0.45
15:M:122:GLN:HG3	15:M:122:GLN:O	2.15	0.45
16:N:67:ALA:C	16:N:69:TYR:N	2.69	0.45
25:W:38:THR:HG22	38:W:3580:HOH:O	2.16	0.45
1:0:2506:A:H1'	38:0:4035:HOH:O	2.15	0.45
13:K:6:ALA:HB2	13:K:116:GLU:HG2	1.98	0.45
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.16	0.45
19:Q:94:GLN:HG2	19:Q:95:GLU:OE1	2.17	0.45
1:0:86:A:C2	30:2:25:VAL:HG13	2.51	0.45
1:0:285:A:C2	1:0:368:C:H4'	2.51	0.45
1:0:1406:A:H4'	1:0:1407:A:C5'	2.46	0.45
5:B:149:ASP:HB2	38:B:9379:HOH:O	2.15	0.45
6:C:136:VAL:HA	6:C:137:PRO:C	2.37	0.45
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.97	0.45
7:D:101:THR:O	7:D:157:LEU:HB3	2.16	0.45
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.44	0.45
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.83	0.45
22:T:20:HIS:ND1	22:T:41:ARG:NE	2.60	0.45
31:3:3:MET:O	31:3:90:PHE:HA	2.16	0.45
1:0:35:U:H5'	6:C:47:GLY:O	2.17	0.45
1:0:1155:G:H2'	1:0:1156:C:C6	2.52	0.45
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.45
1:0:2404:G:OP1	19:Q:68:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2589:U:H2'	1:0:2590:U:C6	2.51	0.45
2:9:3020:G:O2'	2:9:3021:G:H5'	2.16	0.45
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.45
4:A:109:GLU:CD	4:A:113:GLY:H	2.20	0.45
5:B:7:ARG:HD3	5:B:9:GLY:O	2.16	0.45
6:C:236:THR:O	6:C:239:ALA:N	2.50	0.45
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.51	0.45
16:N:44:ARG:HG3	16:N:45:ALA:N	2.32	0.45
16:N:67:ALA:O	16:N:69:TYR:N	2.50	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.81	0.45
20:R:30:ALA:HA	20:R:33:ARG:NH1	2.31	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.46	0.45
1:0:710:G:O2'	1:0:711:G:H5'	2.16	0.45
5:B:82:VAL:HG12	5:B:101:TRP:CE3	2.51	0.45
5:B:145:HIS:HA	5:B:160:ASP:O	2.17	0.45
5:B:320:GLN:NE2	5:B:321:PRO:CD	2.79	0.45
15:M:32:ARG:NH2	38:M:9391:HOH:O	2.49	0.45
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.05	0.45
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.45	0.45
1:0:1185:U:O2'	1:0:1186:C:H5'	2.17	0.45
1:0:1279:U:O2	1:0:1279:U:H2'	2.17	0.45
1:0:1298:U:H2'	1:0:1299:G:C8	2.51	0.45
1:0:2050:G:H5"	20:R:80:TYR:O	2.17	0.45
2:9:3056:A:C3'	2:9:3057:A:H5"	2.45	0.45
4:A:8:ARG:NH1	38:A:9349:HOH:O	2.45	0.45
4:A:103:VAL:O	4:A:105:VAL:HG23	2.16	0.45
6:C:138:VAL:O	6:C:234:VAL:HA	2.16	0.45
17:O:32:ARG:HG2	38:O:2336:HOH:O	2.16	0.45
17:O:44:ASN:OD1	17:O:65:LEU:HB2	2.17	0.45
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.17	0.45
25:W:4:LEU:HD23	25:W:4:LEU:HA	1.75	0.45
1:0:1573:A:H2'	1:0:1574:C:O4'	2.16	0.45
1:0:1874:U:P	4:A:51:ARG:HD2	2.57	0.45
1:0:2039:A:OP2	5:B:234:ARG:NH2	2.50	0.45
1:0:2045:G:H2'	1:0:2046:G:O4'	2.17	0.45
1:0:2424:U:H1'	19:Q:7:LEU:HD12	1.99	0.45
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.16	0.45
1:0:2812:A:C2	1:0:2814:A:N6	2.72	0.45
5:B:248:ARG:NH2	38:B:9325:HOH:O	2.49	0.45
11:H:36:LYS:HA	11:H:84:LYS:HZ1	1.82	0.45
12:J:75:PRO:HD3	12:J:136:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:89:PHE:CD1	14:L:89:PHE:N	2.84	0.45
14:L:97:VAL:O	14:L:100:ALA:HB2	2.16	0.45
16:N:152:GLU:C	16:N:154:LEU:N	2.70	0.45
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.17	0.45
23:U:6:CYS:C	23:U:8:TYR:H	2.20	0.45
1:0:1666:C:H2'	1:0:1667:A:C5'	2.46	0.45
1:0:1730:G:C5'	1:0:1731:C:H6	2.30	0.45
1:0:1790:C:H2'	1:0:1791:U:C6	2.50	0.45
1:0:1855:G:H4'	1:0:1856:C:O5'	2.16	0.45
6:C:218:VAL:HG12	38:C:9228:HOH:O	2.16	0.45
7:D:15:GLU:HA	7:D:16:PRO:HD3	1.83	0.45
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.17	0.45
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.99	0.45
15:M:61:ILE:CG2	15:M:62:VAL:N	2.80	0.45
16:N:163:PHE:O	16:N:164:ASP:OD1	2.35	0.45
20:R:33:ARG:NH1	38:R:9344:HOH:O	2.49	0.45
21:S:52:VAL:HG22	21:S:66:VAL:HG13	1.98	0.45
26:X:43:VAL:CG1	26:X:44:ASP:N	2.79	0.45
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.32	0.45
1:0:21:G:H5"	20:R:1:GLY:O	2.17	0.45
1:0:222:A:H2'	1:0:223:G:O4'	2.17	0.45
1:0:746:A:C6	17:O:65:LEU:HD13	2.52	0.45
1:0:902:G:N7	14:L:18:HIS:CD2	2.83	0.45
1:0:1185:U:H2'	1:0:1186:C:C6	2.51	0.45
1:0:1293:U:O2'	27:Y:149:GLN:NE2	2.46	0.45
1:0:1425:G:O2'	1:0:1426:C:H5'	2.17	0.45
4:A:53:ALA:HB1	4:A:54:PRO:HD2	1.99	0.45
5:B:62:ARG:HG2	5:B:65:MET:CE	2.47	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45
10:G:64:ASN:ND2	10:G:64:ASN:H	2.15	0.45
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.45
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.44
1:0:2404:G:OP1	19:Q:69:ASP:N	2.46	0.44
38:0:6984:HOH:O	16:N:5:ARG:HB2	2.17	0.44
2:9:3035:C:H5"	38:9:4078:HOH:O	2.16	0.44
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.98	0.44
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.44
6:C:115:LEU:CD2	6:C:243:VAL:HG13	2.45	0.44
6:C:132:ASP:HB2	6:C:161:ASP:HB3	1.98	0.44
9:F:28:ALA:CB	9:F:99:THR:HG23	2.47	0.44
13:K:110:LYS:O	13:K:111:GLY:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:37:GLU:OE1	19:Q:93:ARG:NE	2.49	0.44
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.32	0.44
1:0:170:U:H2'	1:0:171:C:H5'	1.99	0.44
1:0:303:C:H2'	1:0:304:G:O4'	2.17	0.44
1:0:558:C:C2'	1:0:559:U:H5"	2.46	0.44
1:0:694:A:H4'	1:0:2441:U:OP1	2.18	0.44
1:0:877:G:H1'	38:0:9479:HOH:O	2.17	0.44
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.00	0.44
1:0:1209:C:H2'	1:0:1210:G:H8	1.82	0.44
1:0:1486:A:C5	30:2:2:LYS:HG3	2.52	0.44
1:0:2699:A:H2'	1:0:2700:G:O4'	2.16	0.44
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.47	0.44
13:K:68:VAL:O	13:K:68:VAL:HG12	2.17	0.44
22:T:18:GLU:O	22:T:21:LYS:HE2	2.17	0.44
31:3:69:TYR:CE1	31:3:80:ARG:HD2	2.52	0.44
1:0:1205:U:C2'	1:0:1206:U:C5'	2.95	0.44
1:0:1496:G:H5'	1:0:1572:A:H1'	1.98	0.44
1:0:1589:G:N2	1:0:1605:G:H1'	2.33	0.44
1:0:1803:C:H2'	1:0:1804:A:C8	2.52	0.44
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.00	0.44
1:0:2301:A:H5"	1:0:2302:A:H5'	1.98	0.44
38:0:4497:HOH:O	13:K:2:GLU:HA	2.17	0.44
2:9:3002:U:P	2:9:3003:A:H5'	2.58	0.44
4:A:33:GLU:OE1	4:A:33:GLU:N	2.47	0.44
5:B:207:LYS:HG2	5:B:304:PRO:HB3	1.99	0.44
11:H:170:ASN:N	11:H:170:ASN:ND2	2.66	0.44
12:J:42:GLU:O	12:J:131:THR:HG23	2.18	0.44
16:N:115:VAL:HG23	16:N:116:PHE:N	2.31	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.53	0.44
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.44
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.44
1:0:299:U:H5'	38:0:7516:HOH:O	2.16	0.44
1:0:604:G:H2'	38:0:7912:HOH:O	2.17	0.44
1:0:827:A:H2'	1:0:828:G:O4'	2.17	0.44
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.44
1:0:1398:G:O2'	1:0:1399:A:H5'	2.18	0.44
1:0:1477:C:H5'	1:0:1868:G:H5"	2.00	0.44
1:0:2781:U:C2'	1:0:2782:G:H5'	2.47	0.44
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.44
6:C:103:ASN:HB3	38:C:9109:HOH:O	2.18	0.44
13:K:96:VAL:HG21	13:K:109:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.99	0.44
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.87	0.44
22:T:41:ARG:NH1	22:T:42:VAL:O	2.51	0.44
32:I:89:SER:HB3	32:I:97:VAL:HG23	1.98	0.44
1:0:290:C:O2'	1:0:291:C:H5'	2.17	0.44
1:0:794:U:H3	1:0:819:A:H61	1.66	0.44
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.05	0.44
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.99	0.44
4:A:199:HIS:HD2	4:A:201:PHE:H	1.65	0.44
4:A:212:PRO:HB2	38:A:9357:HOH:O	2.17	0.44
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.48	0.44
5:B:125:GLU:OE2	5:B:129:ARG:NH1	2.51	0.44
17:O:32:ARG:HH21	17:O:35:LYS:CD	2.31	0.44
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.82	0.44
31:3:25:VAL:HG13	31:3:68:LYS:HE3	2.00	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.33	0.44
1:0:825:U:H5"	1:0:826:U:OP1	2.18	0.44
1:0:1119:G:C8	12:J:52:GLN:NE2	2.85	0.44
1:0:2092:G:H2'	1:0:2613:G:OP1	2.18	0.44
1:0:2271:G:N3	1:0:2271:G:H2'	2.33	0.44
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.16	0.44
5:B:175:LEU:O	5:B:175:LEU:HD23	2.18	0.44
6:C:19:PRO:HB3	6:C:244:ALA:HB2	2.00	0.44
8:E:7:ILE:HD11	8:E:11:VAL:C	2.37	0.44
13:K:125:ALA:C	13:K:127:ALA:H	2.21	0.44
24:V:31:ARG:NE	38:V:2682:HOH:O	2.51	0.44
25:W:6:GLN:HA	25:W:52:VAL:HG23	1.99	0.44
32:I:99:ASP:O	32:I:100:LEU:HG	2.18	0.44
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.44
1:0:1525:G:H5'	1:0:1526:A:OP2	2.17	0.44
1:0:2670:G:O2'	1:0:2671:U:H5'	2.17	0.44
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.44
38:0:5004:HOH:O	16:N:21:HIS:HD2	2.01	0.44
2:9:3053:G:O2'	2:9:3054:A:H5'	2.18	0.44
4:A:36:ASP:O	4:A:38:ILE:N	2.50	0.44
5:B:62:ARG:HA	5:B:65:MET:CE	2.40	0.44
5:B:180:ASP:O	5:B:181:ILE:C	2.55	0.44
5:B:310:ARG:HB3	38:B:9444:HOH:O	2.16	0.44
15:M:47:ASP:CG	15:M:48:LYS:N	2.71	0.44
15:M:159:VAL:HG12	36:M:9318:CL:CL	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:37:ARG:NH2	38:N:9334:HOH:O	2.51	0.44
20:R:82:GLU:HG3	20:R:83:LYS:N	2.32	0.44
22:T:78:THR:HB	22:T:87:VAL:O	2.18	0.44
24:V:12:THR:HG23	24:V:14:ALA:H	1.83	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.60	0.44
29:1:8:GLN:NE2	29:1:11:LYS:HZ2	2.11	0.44
1:0:64:G:H2'	1:0:65:C:O4'	2.18	0.44
1:0:1135:G:H5'	38:0:6173:HOH:O	2.18	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.53	0.44
1:0:2312:G:H2'	1:0:2313:C:H5'	1.99	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.47	0.44
1:0:2451:G:O2'	31:3:38:ARG:NH2	2.51	0.44
6:C:19:PRO:HG2	6:C:22:PHE:CE1	2.53	0.44
6:C:54:LEU:HD23	6:C:79:ARG:HG3	1.98	0.44
7:D:35:ALA:C	7:D:37:ALA:N	2.71	0.44
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.00	0.44
16:N:147:ILE:HG23	16:N:148:ALA:N	2.33	0.44
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.51	0.44
1:0:820:G:C5	4:A:171:LYS:HB2	2.53	0.44
1:0:1334:C:H2'	1:0:1335:C:H6	1.83	0.44
1:0:1596:U:H2'	1:0:1598:A:OP2	2.17	0.44
1:0:1711:A:O2'	1:0:1712:A:H5'	2.18	0.44
1:0:2467:A:O2'	1:0:2468:A:H2'	2.17	0.44
4:A:165:THR:O	4:A:165:THR:HG22	2.17	0.44
4:A:192:VAL:HB	38:A:9387:HOH:O	2.18	0.44
11:H:83:TYR:CD1	11:H:83:TYR:C	2.91	0.44
14:L:91:VAL:HB	38:L:9358:HOH:O	2.17	0.44
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.43
1:0:794:U:H2'	1:0:795:G:H5'	2.00	0.43
1:0:816:G:C6	1:0:817:G:N1	2.86	0.43
1:0:941:G:C5	1:0:942:U:C4	3.06	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.43
38:0:4890:HOH:O	17:O:35:LYS:HD3	2.18	0.43
6:C:84:VAL:O	6:C:85:LYS:HB2	2.17	0.43
8:E:107:PHE:CE1	8:E:152:THR:HB	2.52	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.47	0.43
14:L:134:GLU:HG3	38:L:9357:HOH:O	2.18	0.43
15:M:68:ARG:O	15:M:68:ARG:HD3	2.17	0.43
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.36	0.43
16:N:62:HIS:O	16:N:65:ASP:OD1	2.35	0.43
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:86:LEU:O	16:N:90:LEU:HG	2.18	0.43
16:N:127:LEU:HB2	38:N:9356:HOH:O	2.17	0.43
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.51	0.43
22:T:23:VAL:C	22:T:93:THR:HG21	2.38	0.43
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.43
26:X:76:ARG:NH1	26:X:76:ARG:CG	2.74	0.43
32:I:132:CYS:C	32:I:134:SER:H	2.21	0.43
1:0:474:C:O3'	6:C:73:LEU:HD21	2.17	0.43
1:0:757:C:OP1	14:L:27:ARG:HD2	2.16	0.43
1:0:2050:G:OP1	20:R:79:ARG:HB3	2.18	0.43
6:C:236:THR:HA	38:C:9252:HOH:O	2.18	0.43
7:D:76:ARG:O	7:D:77:ASP:HB2	2.18	0.43
14:L:93:VAL:HG12	14:L:97:VAL:HG23	2.00	0.43
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.82	0.43
18:P:59:ARG:NH2	18:P:66:GLN:NE2	2.62	0.43
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.99	0.43
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.99	0.43
1:0:1850:U:H2'	1:0:1851:G:C8	2.53	0.43
4:A:128:LEU:HG	38:A:9366:HOH:O	2.18	0.43
5:B:109:LEU:CG	5:B:113:LEU:HD12	2.49	0.43
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.99	0.43
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.00	0.43
11:H:9:ILE:HG23	11:H:126:ARG:NE	2.33	0.43
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.98	0.43
11:H:146:VAL:HG22	38:H:9174:HOH:O	2.19	0.43
11:H:154:TYR:C	11:H:154:TYR:HD1	2.22	0.43
14:L:21:ARG:N	38:L:9330:HOH:O	2.51	0.43
14:L:121:ILE:HA	14:L:141:GLU:O	2.18	0.43
18:P:27:ARG:O	18:P:31:ILE:HG13	2.18	0.43
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.43
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	2.00	0.43
30:2:35:ARG:HB2	38:2:2691:HOH:O	2.18	0.43
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.34	0.43
1:0:136:C:P	15:M:39:ARG:HH22	2.42	0.43
1:0:541:C:O2'	1:0:542:A:H5"	2.19	0.43
1:0:690:G:H4'	1:0:741:C:O2	2.19	0.43
1:0:1375:A:C2'	1:0:1376:G:H5'	2.48	0.43
1:0:1768:C:H2'	1:0:1769:C:H5'	2.00	0.43
6:C:5:ILE:HG23	38:C:9234:HOH:O	2.18	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.17	0.43
6:C:184:ARG:NE	38:C:9216:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:49:PRO:HA	7:D:73:VAL:HG22	2.00	0.43
9:F:36:THR:O	9:F:40:ILE:HG13	2.19	0.43
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.76	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.43
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.99	0.43
31:3:65:THR:CG2	31:3:67:LEU:HG	2.48	0.43
1:0:922:A:N7	1:0:2281:C:H5'	2.33	0.43
1:0:2719:A:C2	5:B:70:PRO:HG3	2.53	0.43
5:B:13:PHE:N	38:B:9416:HOH:O	2.47	0.43
5:B:147:VAL:HG12	5:B:147:VAL:O	2.19	0.43
6:C:19:PRO:HD2	6:C:240:LEU:CD2	2.49	0.43
8:E:47:VAL:HG11	8:E:69:ILE:HD13	2.01	0.43
9:F:34:ASN:HA	15:M:4:ALA:HB2	2.01	0.43
25:W:88:THR:CG2	25:W:89:ASP:H	2.22	0.43
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.48	0.43
1:0:244:C:OP2	9:F:38:LYS:HE3	2.19	0.43
1:0:661:G:C5	1:0:686:A:C2	3.07	0.43
1:0:737:A:H2'	1:0:738:G:O4'	2.18	0.43
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:1772:C:H5'	1:0:1773:G:C5	2.53	0.43
1:0:2754:G:H2'	1:0:2755:G:O4'	2.18	0.43
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.43
1:0:2909:G:H2'	1:0:2910:A:C8	2.52	0.43
5:B:148:PRO:HD2	38:B:9379:HOH:O	2.18	0.43
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.42	0.43
13:K:49:LEU:HA	13:K:73:VAL:HG12	2.00	0.43
14:L:130:ARG:O	14:L:131:GLU:C	2.57	0.43
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.01	0.43
16:N:163:PHE:O	16:N:164:ASP:CG	2.56	0.43
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.99	0.43
1:0:363:A:O2'	1:0:364:C:H5'	2.18	0.43
1:0:1151:G:OP2	10:G:65:THR:HG21	2.19	0.43
5:B:26:PHE:HE1	38:B:9444:HOH:O	2.00	0.43
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.44	0.43
8:E:81:GLU:O	8:E:172:PRO:HD3	2.18	0.43
11:H:84:LYS:HB2	11:H:84:LYS:HZ2	1.84	0.43
13:K:9:THR:O	13:K:10:GLN:C	2.57	0.43
25:W:146:ILE:HG23	25:W:150:LEU:HD12	2.00	0.43
26:X:12:ILE:HB	26:X:70:ILE:CG2	2.48	0.43
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:470:U:O2'	29:1:16:HIS:CD2	2.68	0.43
1:0:635:A:H2'	1:0:636:G:H5"	2.01	0.43
1:0:766:A:H5'	38:0:4926:HOH:O	2.18	0.43
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.54	0.43
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.19	0.43
1:0:1852:A:H4'	4:A:230:SER:HB2	2.00	0.43
1:0:2241:C:H2'	1:0:2242:U:H6	1.81	0.43
1:0:2264:A:H2'	1:0:2265:U:C6	2.54	0.43
1:0:2382:A:H5'	38:0:5017:HOH:O	2.18	0.43
1:0:2531:U:O2'	1:0:2532:A:H5'	2.19	0.43
4:A:35:GLY:O	4:A:36:ASP:CB	2.67	0.43
5:B:41:PHE:CB	5:B:190:MET:HE3	2.48	0.43
6:C:7:ASP:C	6:C:9:ASP:H	2.22	0.43
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.49	0.43
7:D:58:VAL:HB	7:D:62:ASP:HB3	2.01	0.43
8:E:132:THR:HG23	8:E:132:THR:O	2.19	0.43
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.49	0.43
11:H:112:GLY:N	38:H:9185:HOH:O	2.52	0.43
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.43
13:K:72:VAL:O	13:K:95:ALA:HA	2.18	0.43
25:W:1:MET:N	25:W:103:GLU:OE2	2.47	0.43
1:0:677:C:O2'	1:0:678:G:H5'	2.18	0.43
1:0:1943:C:O4'	4:A:212:PRO:HA	2.18	0.43
38:0:3098:HOH:O	13:K:39:GLY:HA3	2.18	0.43
4:A:140:LEU:HB3	4:A:141:PRO:HD2	2.00	0.43
7:D:140:ARG:O	7:D:144:ARG:HG2	2.19	0.43
7:D:169:THR:C	7:D:170:TYR:HD1	2.22	0.43
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.19	0.43
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.32	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.54	0.43
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.84	0.43
28:Z:81:ARG:O	28:Z:82:SER:C	2.56	0.43
32:I:113:HIS:N	32:I:114:PRO:HD2	2.33	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.37	0.43
1:0:553:G:P	27:Y:204:ARG:NH2	2.89	0.43
1:0:1080:C:O5'	1:0:1080:C:H6	2.01	0.43
1:0:1123:A:C6	1:0:1238:C:H5'	2.54	0.43
1:0:2070:G:H2'	1:0:2072:G:OP1	2.18	0.43
1:0:2785:C:H4'	1:0:2786:G:OP2	2.18	0.43
5:B:103:ASP:HB2	38:B:9395:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:ARG:CD	5:B:257:THR:HG22	2.49	0.43
6:C:107:ARG:HB3	6:C:107:ARG:CZ	2.49	0.43
8:E:156:ASP:OD2	8:E:157:LYS:NZ	2.46	0.43
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.76	0.43
28:Z:56:GLN:HG3	28:Z:62:TYR:O	2.19	0.43
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.42
1:0:288:A:H61	1:0:364:C:H42	1.67	0.42
1:0:1095:U:O2	25:W:120:PRO:HG2	2.19	0.42
1:0:1603:A:H5"	1:0:1605:G:H5'	2.00	0.42
1:0:1617:C:C4	1:0:1643:C:H4'	2.54	0.42
1:0:1675:C:H5"	30:2:5:LYS:HD2	2.01	0.42
1:0:2265:U:H2'	1:0:2266:A:H8	1.84	0.42
1:0:2791:U:H1'	1:0:2792:A:H5"	2.00	0.42
4:A:123:GLY:HA3	4:A:162:GLY:HA2	2.01	0.42
5:B:66:GLU:HG2	38:B:9443:HOH:O	2.18	0.42
6:C:5:ILE:HA	6:C:139:VAL:HG12	2.01	0.42
6:C:37:ALA:O	6:C:41:ASN:ND2	2.51	0.42
7:D:11:HIS:CG	7:D:12:GLU:N	2.87	0.42
20:R:114:VAL:HA	20:R:144:GLU:O	2.19	0.42
31:3:75:GLY:HA2	38:3:9358:HOH:O	2.18	0.42
1:0:451:C:C2'	1:0:452:G:H5'	2.49	0.42
1:0:1236:A:C8	12:J:63:ILE:HD11	2.53	0.42
1:0:1829:A:H5"	38:0:3377:HOH:O	2.18	0.42
1:0:2489:G:H1'	38:0:7457:HOH:O	2.19	0.42
5:B:154:VAL:HA	5:B:155:PRO:HD3	1.84	0.42
8:E:84:MET:HE1	8:E:148:ILE:HD12	2.00	0.42
13:K:14:LYS:HD2	13:K:45:PRO:HG3	2.01	0.42
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.32	0.42
28:Z:60:CYS:SG	28:Z:62:TYR:HB2	2.59	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.72	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.42
1:0:907:A:H4'	1:0:1328:A:C2	2.54	0.42
1:0:1051:C:H2'	1:0:1052:G:O4'	2.20	0.42
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.19	0.42
1:0:1903:U:O2'	1:0:1904:A:N7	2.50	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:2869:G:H2'	1:0:2870:C:H6	1.84	0.42
13:K:28:GLU:HB3	13:K:59:LYS:HB2	2.02	0.42
17:O:26:TRP:HB2	38:O:3062:HOH:O	2.18	0.42
20:R:39:THR:HB	20:R:42:GLU:CG	2.48	0.42
1:0:297:U:H2'	1:0:298:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.42
1:0:1299:G:H5'	38:0:4362:HOH:O	2.19	0.42
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.42
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.19	0.42
1:0:2664:A:H8	1:0:2664:A:OP1	2.02	0.42
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.42
2:9:3047:A:C2	2:9:3048:C:C2	3.07	0.42
4:A:65:ARG:O	4:A:66:ARG:HG3	2.18	0.42
4:A:199:HIS:HD2	4:A:201:PHE:HB2	1.85	0.42
7:D:40:ILE:HG23	38:D:5583:HOH:O	2.18	0.42
14:L:57:VAL:O	14:L:57:VAL:HG12	2.19	0.42
16:N:151:ASP:HB3	38:N:9328:HOH:O	2.19	0.42
21:S:58:MET:SD	30:2:8:LYS:HE3	2.59	0.42
21:S:76:GLU:HB3	38:S:9143:HOH:O	2.19	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.19	0.42
1:0:95:A:H5"	1:0:97:G:O4'	2.19	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.34	0.42
1:0:2269:C:H2'	1:0:2270:G:C5'	2.48	0.42
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.42
2:9:3007:G:H5'	38:N:9346:HOH:O	2.18	0.42
3:4:74:C:C2'	3:4:75:C:H5'	2.49	0.42
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.48	0.42
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.88	0.42
9:F:28:ALA:HB3	9:F:99:THR:O	2.19	0.42
11:H:169:GLY:C	11:H:170:ASN:HD22	2.23	0.42
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.20	0.42
21:S:57:THR:C	21:S:59:ASP:H	2.22	0.42
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.33	0.42
1:0:156:C:H5"	15:M:171:ARG:CD	2.27	0.42
1:0:245:C:H2'	1:0:246:G:H5'	2.02	0.42
1:0:1201:C:C2'	1:0:1202:A:H5'	2.46	0.42
1:0:1676:G:O2'	1:0:1677:U:H5'	2.20	0.42
1:0:2323:G:H5'	38:0:7221:HOH:O	2.19	0.42
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.20	0.42
5:B:62:ARG:HG2	5:B:65:MET:HE3	2.02	0.42
5:B:195:ARG:HG2	5:B:323:LEU:HD22	2.02	0.42
6:C:164:ALA:O	6:C:167:ASP:HB2	2.20	0.42
7:D:20:LYS:HA	7:D:75:LEU:O	2.20	0.42
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.48	0.42
7:D:55:LYS:O	7:D:56:ARG:HB2	2.19	0.42
7:D:173:GLU:O	7:D:174:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:139:ASN:O	11:H:141:GLU:N	2.52	0.42
13:K:34:VAL:HG21	13:K:46:LYS:O	2.20	0.42
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.55	0.42
25:W:29:VAL:O	25:W:30:ASN:HB2	2.19	0.42
1:0:111:C:H2'	1:0:112:G:O4'	2.20	0.42
1:0:394:G:H1	15:M:181:GLU:CD	2.23	0.42
1:0:517:U:H1'	38:0:7742:HOH:O	2.17	0.42
1:0:794:U:C2'	1:0:795:G:H5'	2.50	0.42
1:0:1025:C:H5'	25:W:23:MET:O	2.20	0.42
1:0:1166:A:H2'	1:0:1166:A:N3	2.35	0.42
1:0:1314:U:H5"	1:0:1316:G:O4'	2.19	0.42
1:0:1631:A:H2'	1:0:1632:A:C8	2.54	0.42
1:0:1979:G:H2'	38:0:3589:HOH:O	2.19	0.42
1:0:2064:U:H5'	1:0:2652:U:O3'	2.20	0.42
1:0:2541:U:H3'	1:0:2541:U:H6	1.84	0.42
1:0:2638:G:H1'	38:0:4856:HOH:O	2.19	0.42
1:0:2824:C:H5"	1:0:2825:C:H5'	2.00	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.73	0.42
5:B:195:ARG:CG	5:B:323:LEU:HD22	2.50	0.42
5:B:238:ASN:ND2	5:B:240:GLY:N	2.56	0.42
6:C:187:ARG:NH2	38:C:9164:HOH:O	2.51	0.42
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.02	0.42
10:G:12:ILE:N	10:G:13:PRO:HD3	2.34	0.42
20:R:61:GLN:CD	38:R:9341:HOH:O	2.58	0.42
21:S:6:LYS:O	21:S:7:HIS:HB3	2.20	0.42
24:V:42:ASN:N	24:V:43:PRO:HD3	2.34	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.47	0.42
26:X:70:ILE:HG23	26:X:70:ILE:O	2.20	0.42
32:I:112:LYS:HB3	32:I:116:LEU:HG	2.02	0.42
1:0:39:G:N2	1:0:444:C:C2	2.88	0.42
1:0:472:A:H5'	29:1:35:SER:OG	2.19	0.42
1:0:656:G:H3'	17:O:37:ARG:HH12	1.84	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.19	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.42
38:0:6519:HOH:O	27:Y:158:LYS:HD3	2.19	0.42
4:A:51:ARG:HB2	38:A:9401:HOH:O	2.19	0.42
5:B:86:ALA:HA	38:B:9378:HOH:O	2.19	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.02	0.42
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.02	0.42
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.50	0.42
18:P:115:SER:OG	18:P:118:GLN:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.50	0.42
27:Y:187:VAL:HB	38:Y:8158:HOH:O	2.19	0.42
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.42
1:0:2425:A:H5'	1:0:2426:G:OP2	2.20	0.42
5:B:104:GLU:HG3	38:B:9395:HOH:O	2.20	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.02	0.42
30:2:49:GLU:HB2	38:2:719:HOH:O	2.20	0.42
1:0:195:C:H2'	1:0:196:G:H5'	2.02	0.42
1:0:462:A:C8	30:2:37:HIS:CE1	3.08	0.42
1:0:611:U:H2'	1:0:612:U:C6	2.55	0.42
1:0:790:A:H1'	1:0:1710:A:H2'	2.02	0.42
1:0:1562:C:N4	38:0:6115:HOH:O	2.51	0.42
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
38:0:9421:HOH:O	5:B:229:ARG:HD2	2.20	0.42
4:A:95:PRO:HG2	4:A:98:GLU:HG2	2.02	0.42
6:C:115:LEU:HD12	6:C:115:LEU:HA	1.92	0.42
8:E:101:GLU:HB3	8:E:117:THR:HA	2.01	0.42
10:G:71:LEU:C	10:G:73:ASP:N	2.73	0.42
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.35	0.42
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.20	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.88	0.42
22:T:37:GLN:OE1	22:T:118:SER:HA	2.19	0.42
1:0:249:G:H1'	1:0:265:U:O2	2.20	0.41
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.49	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.41
4:A:99:ILE:O	4:A:131:HIS:CE1	2.72	0.41
14:L:143:THR:HG22	14:L:144:ASP:H	1.83	0.41
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.55	0.41
22:T:12:ARG:O	22:T:19:ARG:NH2	2.53	0.41
22:T:49:GLU:HB3	22:T:59:GLU:HG3	2.02	0.41
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.02	0.41
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.41
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.41
1:0:711:G:C2	1:0:718:C:C2	3.08	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.41
1:0:886:A:OP2	1:0:2113:G:H5'	2.20	0.41
1:0:1163:G:H5"	32:I:115:ASP:HB3	2.03	0.41
1:0:1192:A:N6	32:I:134:SER:CB	2.82	0.41
1:0:2003:U:H4'	1:0:2004:U:H5	1.85	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2780:C:H2'	1:0:2781:U:C6	2.56	0.41
2:9:3096:C:O2'	2:9:3097:U:H5'	2.21	0.41
5:B:82:VAL:HG12	5:B:82:VAL:O	2.19	0.41
6:C:51:TYR:CE2	29:1:53:LYS:HB3	2.55	0.41
7:D:22:VAL:HA	7:D:73:VAL:O	2.19	0.41
7:D:169:THR:O	7:D:169:THR:HG22	2.19	0.41
9:F:91:VAL:CG1	9:F:92:GLY:H	2.15	0.41
11:H:76:GLU:O	11:H:77:LEU:HD23	2.20	0.41
13:K:24:THR:HB	13:K:64:MET:HE2	2.01	0.41
16:N:50:LEU:HD12	16:N:55:ASP:OD1	2.20	0.41
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.56	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.53	0.41
24:V:49:LEU:O	24:V:53:ILE:HG13	2.20	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.52	0.41
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.59	0.41
1:0:664:U:O4	1:0:681:G:H5"	2.19	0.41
1:0:1474:C:H6	1:0:1474:C:C5'	2.20	0.41
1:0:1481:G:H2'	1:0:1482:A:O4'	2.21	0.41
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.85	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.20	0.41
4:A:36:ASP:HA	4:A:83:GLY:HA3	2.01	0.41
5:B:51:VAL:HG23	5:B:330:VAL:HG22	2.01	0.41
5:B:205:VAL:O	5:B:307:ARG:NE	2.53	0.41
5:B:280:VAL:HG13	5:B:333:GLU:O	2.19	0.41
6:C:165:ASP:O	6:C:168:ARG:HB3	2.19	0.41
7:D:153:THR:O	7:D:156:ARG:HB2	2.20	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.19	0.41
9:F:58:GLU:HG3	9:F:61:MET:HE1	2.02	0.41
13:K:41:LYS:O	13:K:42:ASN:HB2	2.20	0.41
14:L:66:VAL:HG23	14:L:67:ARG:N	2.35	0.41
20:R:114:VAL:HB	20:R:145:LEU:HD13	2.01	0.41
26:X:44:ASP:HB3	26:X:46:ASP:OD2	2.20	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.45	0.41
1:0:200:U:H2'	38:0:3736:HOH:O	2.20	0.41
1:0:559:U:O2'	1:0:560:C:H5'	2.20	0.41
1:0:815:U:O2'	1:0:1598:A:H4'	2.20	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41
1:0:1343:C:H2'	1:0:1344:G:O5'	2.20	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:1730:G:H5"	1:0:1731:C:C6	2.54	0.41
1:0:1764:C:H2'	1:0:1765:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1945:G:O2'	1:0:1946:C:H5'	2.20	0.41
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.20	0.41
2:9:3049:G:C2'	2:9:3050:G:H5'	2.51	0.41
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.49	0.41
4:A:93:THR:HG23	4:A:154:ALA:O	2.21	0.41
5:B:33:ASP:O	5:B:34:GLY:O	2.38	0.41
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.94	0.41
9:F:58:GLU:HA	9:F:61:MET:HE2	2.00	0.41
22:T:48:VAL:O	22:T:59:GLU:HG2	2.20	0.41
25:W:6:GLN:HG2	25:W:29:VAL:HA	2.01	0.41
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.67	0.41
1:0:88:G:H5'	1:0:88:G:C8	2.53	0.41
1:0:656:G:H5'	17:O:3:THR:HB	2.02	0.41
1:0:1056:U:H2'	1:0:1057:A:O4'	2.20	0.41
1:0:1477:C:H4'	1:0:1868:G:H5"	2.01	0.41
1:0:2252:A:H2'	1:0:2253:G:H5'	2.02	0.41
1:0:2474:A:N6	3:4:176:DA:OP2	2.53	0.41
1:0:2712:G:H5'	38:K:4183:HOH:O	2.21	0.41
1:0:2766:A:O2'	1:0:2767:C:H5'	2.20	0.41
38:0:5775:HOH:O	5:B:298:LYS:HD3	2.19	0.41
4:A:134:ASN:O	4:A:150:PRO:HD3	2.20	0.41
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.41
6:C:140:VAL:HG12	6:C:141:SER:N	2.34	0.41
12:J:70:PHE:CD2	12:J:70:PHE:O	2.74	0.41
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.51	0.41
14:L:17:SER:C	14:L:19:LYS:N	2.74	0.41
15:M:50:ARG:N	15:M:54:TYR:HB3	2.34	0.41
16:N:82:TYR:CD2	16:N:82:TYR:C	2.94	0.41
20:R:122:GLN:HB3	20:R:138:SER:HB2	2.03	0.41
1:0:711:G:H1'	38:0:7290:HOH:O	2.20	0.41
1:0:870:G:C3'	1:0:871:G:H5"	2.50	0.41
1:0:947:U:H2'	1:0:948:G:H8	1.83	0.41
1:0:1188:A:C6	1:0:1189:A:C6	3.09	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1838:U:O2'	1:0:2644:C:H5'	2.21	0.41
1:0:2436:U:H5'	31:3:68:LYS:HE2	2.01	0.41
1:0:2781:U:H2'	1:0:2782:G:C5'	2.51	0.41
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.49	0.41
5:B:5:ARG:HA	5:B:6:PRO:HD3	1.97	0.41
5:B:27:ASN:HB3	38:B:9425:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:224:LYS:HA	5:B:224:LYS:HD3	1.93	0.41
5:B:280:VAL:HG13	5:B:334:SER:HA	2.03	0.41
7:D:41:LEU:CA	7:D:44:ILE:HG22	2.48	0.41
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.48	0.41
9:F:63:ILE:HB	9:F:64:PRO:CD	2.47	0.41
11:H:78:GLY:C	11:H:80:GLU:H	2.24	0.41
16:N:154:LEU:C	16:N:156:GLU:H	2.22	0.41
18:P:45:ASP:C	18:P:47:GLY:H	2.24	0.41
26:X:78:GLU:CG	26:X:79:GLU:H	2.27	0.41
1:0:212:A:O4'	1:0:214:U:C6	2.74	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.41
1:0:844:A:C6	1:0:882:A:C5	3.09	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.36	0.41
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.41
1:0:1717:A:H5"	18:P:54:LYS:HB2	2.03	0.41
1:0:1915:U:O2'	1:0:1916:C:H5'	2.20	0.41
1:0:1937:U:O2'	1:0:1938:G:H5'	2.20	0.41
1:0:2090:G:H2'	1:0:2091:G:C8	2.55	0.41
2:9:3011:A:O2'	2:9:3012:C:H3'	2.21	0.41
2:9:3057:A:C8	7:D:141:VAL:HG21	2.56	0.41
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.84	0.41
4:A:173:GLY:O	4:A:176:HIS:HB3	2.21	0.41
11:H:27:LYS:H	11:H:59:HIS:CD2	2.32	0.41
11:H:114:ARG:O	11:H:115:ALA:C	2.59	0.41
20:R:26:LYS:HB3	20:R:62:HIS:CD2	2.56	0.41
23:U:20:MET:CG	23:U:28:THR:HG23	2.51	0.41
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.51	0.41
28:Z:80:ARG:O	28:Z:81:ARG:O	2.39	0.41
1:0:47:G:N3	1:0:114:A:C2	2.89	0.41
1:0:350:C:O2'	1:0:351:G:H5'	2.21	0.41
1:0:903:U:O4	14:L:18:HIS:HB2	2.21	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.86	0.41
1:0:1439:C:H6	1:0:1439:C:O5'	2.04	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.20	0.41
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.21	0.41
4:A:200:PRO:HD3	38:A:9319:HOH:O	2.21	0.41
6:C:76:ARG:CG	6:C:76:ARG:NH1	2.81	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.84	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.02	0.41
22:T:40:VAL:HG23	22:T:119:ALA:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:61:ARG:HH12	26:X:67:PRO:HD3	1.84	0.41
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.51	0.41
1:0:318:C:H5'	1:0:339:A:C4	2.55	0.41
1:0:638:C:H2'	1:0:639:A:H8	1.85	0.41
1:0:697:G:H4'	1:0:730:G:O3'	2.21	0.41
1:0:764:C:OP1	6:C:87:ARG:NH1	2.54	0.41
1:0:930:C:N3	1:0:1040:A:N6	2.68	0.41
1:0:1313:A:H5'	27:Y:208:LYS:O	2.21	0.41
1:0:1321:A:H2'	1:0:1322:G:C8	2.56	0.41
1:0:1406:A:H5'	1:0:1407:A:C8	2.56	0.41
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
1:0:1543:G:N1	1:0:1641:A:OP2	2.39	0.41
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.54	0.41
1:0:1747:A:C8	13:K:44:LEU:HD13	2.56	0.41
1:0:1811:A:H2'	1:0:1812:G:H5'	2.01	0.41
1:0:1820:G:C6	1:0:2030:A:C2	3.09	0.41
1:0:1839:A:H5'	1:0:2643:G:H4'	2.02	0.41
1:0:2403:C:H2'	1:0:2404:G:O5'	2.20	0.41
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.41
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:2724:U:O5'	1:0:2724:U:H6	2.03	0.41
2:9:3003:A:H2	2:9:3021:G:N3	2.19	0.41
2:9:3039:U:H3'	2:9:3040:C:H5"	2.02	0.41
5:B:7:ARG:HH11	5:B:7:ARG:CG	2.33	0.41
5:B:33:ASP:HB3	5:B:34:GLY:H	1.76	0.41
5:B:225:GLY:HA3	38:B:9367:HOH:O	2.21	0.41
7:D:172:VAL:HG12	7:D:173:GLU:N	2.35	0.41
8:E:12:ASP:HA	38:E:1750:HOH:O	2.19	0.41
8:E:81:GLU:HA	8:E:133:VAL:O	2.21	0.41
11:H:88:ARG:HG2	11:H:133:LEU:O	2.20	0.41
13:K:90:PHE:CD1	13:K:90:PHE:N	2.89	0.41
16:N:47:LEU:HD13	16:N:97:VAL:HG11	2.02	0.41
16:N:93:GLN:HG2	38:N:9356:HOH:O	2.21	0.41
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.21	0.41
20:R:27:HIS:O	20:R:31:ILE:HG13	2.21	0.41
22:T:48:VAL:CG1	22:T:96:VAL:HG22	2.50	0.41
23:U:9:CYS:O	23:U:52:THR:HG23	2.20	0.41
24:V:1:THR:O	24:V:4:HIS:CE1	2.74	0.41
24:V:4:HIS:O	24:V:8:ILE:HG13	2.20	0.41
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.20	0.41
26:X:61:ARG:NH1	26:X:67:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HE2	38:1:9262:HOH:O	2.20	0.41
1:0:29:C:O2'	1:0:30:U:H5'	2.21	0.41
1:0:185:G:H4'	1:0:186:A:H4'	2.03	0.41
1:0:396:U:P	31:3:38:ARG:HH11	2.44	0.41
1:0:414:C:H5'	38:0:9961:HOH:O	2.20	0.41
1:0:1130:U:H4'	38:0:6364:HOH:O	2.20	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
1:0:1471:A:H2'	1:0:1472:C:C6	2.55	0.41
1:0:2705:U:O2'	1:0:2706:A:H5'	2.20	0.41
1:0:2880:A:H2'	1:0:2881:C:H5'	2.03	0.41
2:9:3061:C:H2'	2:9:3062:A:H8	1.85	0.41
4:A:215:ILE:HG13	4:A:216:SER:N	2.36	0.41
5:B:55:ASN:HB3	5:B:64:GLY:H	1.85	0.41
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.03	0.41
7:D:24:HIS:HB2	7:D:71:ALA:O	2.21	0.41
7:D:154:LYS:H	7:D:154:LYS:CD	2.09	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.89	0.41
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.19	0.41
17:O:50:ARG:HD2	17:O:51:TYR:CE1	2.56	0.41
20:R:39:THR:O	20:R:40:ALA:C	2.59	0.41
25:W:1:MET:N	25:W:37:GLU:HG3	2.36	0.41
25:W:92:ASP:N	25:W:92:ASP:OD1	2.54	0.41
26:X:76:ARG:O	26:X:77:PHE:HB3	2.20	0.41
1:0:1705:C:C5'	18:P:59:ARG:HH12	2.34	0.40
1:0:1969:A:N7	1:0:1970:G:C6	2.89	0.40
1:0:2408:A:H4'	31:3:15:ASN:O	2.21	0.40
4:A:1:GLY:HA2	4:A:197:VAL:HG23	2.02	0.40
4:A:36:ASP:HB2	4:A:83:GLY:C	2.41	0.40
4:A:211:LYS:CB	38:A:9412:HOH:O	2.68	0.40
5:B:57:GLU:HA	5:B:58:PRO:HD2	1.96	0.40
6:C:21:VAL:HG23	6:C:22:PHE:CD1	2.56	0.40
9:F:102:GLY:O	9:F:103:GLU:HB2	2.21	0.40
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.41	0.40
19:Q:16:ASN:HD22	19:Q:16:ASN:HA	1.70	0.40
1:0:354:A:H2'	1:0:355:C:C6	2.56	0.40
1:0:450:C:OP1	6:C:184:ARG:NH2	2.55	0.40
1:0:803:C:O2'	1:0:804:C:H5'	2.21	0.40
1:0:1160:G:O2'	1:0:1190:G:H1'	2.21	0.40
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.22	0.40
1:0:1477:C:H5'	1:0:1868:G:C5'	2.51	0.40
1:0:1634:G:H2'	1:0:1635:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2047:C:H5'	38:0:3119:HOH:O	2.20	0.40
1:0:2072:G:N2	38:0:7076:HOH:O	2.46	0.40
1:0:2072:G:C6	1:0:2533:C:H1'	2.57	0.40
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.50	0.40
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.61	0.40
5:B:51:VAL:HG23	5:B:329:TYR:O	2.21	0.40
5:B:132:HIS:CE1	5:B:171:VAL:CG2	3.05	0.40
5:B:321:PRO:HA	38:B:9454:HOH:O	2.21	0.40
6:C:191:SER:OG	6:C:192:ILE:N	2.54	0.40
7:D:94:ALA:HB3	7:D:97:GLN:NE2	2.35	0.40
7:D:146:LYS:HZ1	16:N:107:ASN:ND2	2.19	0.40
8:E:154:ILE:HD11	8:E:157:LYS:HE2	2.03	0.40
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.21	0.40
11:H:66:ARG:HB3	38:H:9177:HOH:O	2.21	0.40
11:H:167:PRO:O	11:H:168:ALA:CB	2.67	0.40
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.69	0.40
18:P:103:THR:O	18:P:107:GLU:HG3	2.21	0.40
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.40
24:V:12:THR:H	24:V:15:GLU:HB2	1.86	0.40
25:W:69:ARG:HD2	25:W:117:ARG:O	2.21	0.40
27:Y:141:THR:HG23	38:Y:8175:HOH:O	2.19	0.40
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.37	0.40
32:I:92:PRO:C	32:I:94:GLU:N	2.74	0.40
1:0:308:U:H5'	22:T:97:ARG:NH2	2.37	0.40
1:0:622:G:P	27:Y:148:GLY:HA3	2.60	0.40
1:0:860:U:H2'	1:0:861:A:C8	2.56	0.40
1:0:1118:A:C8	1:0:1119:G:H5"	2.56	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.48	0.40
1:0:2105:C:H2'	1:0:2106:C:C6	2.56	0.40
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.40
1:0:2710:U:H1'	38:0:7786:HOH:O	2.21	0.40
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.40
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.82	0.40
8:E:69:ILE:HA	8:E:72:MET:HE2	2.00	0.40
13:K:98:VAL:CG1	13:K:99:ASP:N	2.85	0.40
13:K:118:ALA:O	13:K:120:ARG:N	2.54	0.40
14:L:126:SER:O	14:L:127:GLU:C	2.57	0.40
15:M:67:VAL:HB	15:M:97:ILE:HG23	2.04	0.40
16:N:108:SER:HA	16:N:109:PRO:HD3	1.79	0.40
17:O:80:ASP:OD1	17:O:81:PHE:N	2.54	0.40
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:41:PHE:CZ	26:X:74:ALA:HB3	2.57	0.40
31:3:91:GLN:O	31:3:92:GLU:HB2	2.21	0.40
1:0:318:C:H5'	1:0:339:A:C2	2.57	0.40
1:0:475:G:C5'	6:C:73:LEU:HD23	2.52	0.40
1:0:536:A:H3'	38:0:5321:HOH:O	2.21	0.40
1:0:581:G:O2'	1:0:582:C:H5'	2.21	0.40
1:0:694:A:C2'	1:0:695:C:H5'	2.51	0.40
1:0:1375:A:H2'	1:0:1376:G:H5'	2.03	0.40
1:0:1556:G:O2'	1:0:1557:G:H5'	2.21	0.40
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.21	0.40
1:0:2729:C:O2'	1:0:2730:G:H5'	2.22	0.40
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.51	0.40
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.56	0.40
5:B:223:ARG:HG3	5:B:232:TRP:O	2.22	0.40
5:B:313:PRO:O	5:B:314:ALA:C	2.59	0.40
7:D:13:MET:CA	7:D:137:PRO:HG2	2.51	0.40
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.21	0.40
9:F:39:SER:HB3	9:F:45:ALA:HB2	2.04	0.40
9:F:57:GLU:O	9:F:61:MET:HG3	2.22	0.40
11:H:27:LYS:N	11:H:59:HIS:HD2	2.14	0.40
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.34	0.40
15:M:164:THR:HG23	15:M:166:ALA:H	1.85	0.40
1:0:68:U:O2'	1:0:69:A:H5"	2.22	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.57	0.40
1:0:1311:G:C2	1:0:1312:G:C8	3.09	0.40
1:0:1388:U:H2'	1:0:1389:G:O4'	2.22	0.40
1:0:1391:G:H2'	1:0:1392:A:H5'	2.03	0.40
1:0:2667:G:H1'	1:0:2914:A:N3	2.36	0.40
4:A:109:GLU:HG2	4:A:116:GLY:H	1.85	0.40
4:A:125:ASN:HB3	4:A:158:VAL:HG12	2.03	0.40
5:B:162:MET:HE1	5:B:308:LEU:HD21	2.03	0.40
6:C:157:LEU:HD11	6:C:194:PHE:HZ	1.85	0.40
7:D:57:THR:CG2	7:D:63:ILE:HG22	2.49	0.40
9:F:26:THR:CG2	9:F:102:GLY:HA3	2.52	0.40
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.67	0.40
16:N:139:TRP:CZ2	16:N:176:ARG:NH1	2.90	0.40
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.37	0.40
20:R:100:ASP:C	20:R:102:GLN:N	2.74	0.40
26:X:12:ILE:HD13	26:X:36:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	A	235/240 (98%)	205 (87%)	28 (12%)	2 (1%)	17	40
5	B	335/338 (99%)	303 (90%)	27 (8%)	5 (2%)	10	26
6	C	244/246 (99%)	223 (91%)	20 (8%)	1 (0%)	34	60
7	D	134/177 (76%)	94 (70%)	34 (25%)	6 (4%)	2	5
8	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	13	32
9	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	5	13
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	144 (92%)	7 (4%)	5 (3%)	4	9
12	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	11	28
13	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	10	26
14	L	141/165 (86%)	118 (84%)	23 (16%)	0	100	100
15	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	29	54
16	N	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	5	12
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	131 (93%)	9 (6%)	1 (1%)	22	46
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	22	46
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	17	40
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	7	19
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	9	24
25	W	152/154 (99%)	144 (95%)	6 (4%)	2 (1%)	12	30
26	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	12	30
27	Y	140/241 (58%)	134 (96%)	6 (4%)	0	100	100
28	Z	71/83 (86%)	57 (80%)	9 (13%)	5 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
32	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	4	10
All	All	3705/4430 (84%)	3348 (90%)	308 (8%)	49 (1%)	12	30

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	D	27	ILE
7	D	137	PRO
7	D	173	GLU
9	F	101	ALA
11	H	140	VAL
11	H	166	SER
11	H	168	ALA
16	N	154	LEU
28	Z	42	CYS
28	Z	81	ARG
5	B	34	GLY
6	C	8	LEU
7	D	65	GLU
7	D	138	GLY
12	J	5	GLU
13	K	111	GLY
16	N	139	TRP
24	V	43	PRO
4	A	34	ASP
5	B	139	ASP
5	B	184	ASP
11	H	16	ARG
12	J	89	HIS
16	N	68	GLU
16	N	164	ASP
18	P	116	SER
25	W	49	ASN
25	W	77	ALA
26	X	87	ALA
28	Z	41	ASN
32	I	76	ALA
32	I	133	THR

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Mol	Chain	Res	Type
5	B	185	GLY
8	E	17	HIS
9	F	44	SER
13	K	119	GLN
28	Z	43	GLY
4	A	37	VAL
7	D	28	GLY
23	U	7	ASP
28	Z	28	GLU
8	E	44	GLY
9	F	64	PRO
11	H	79	GLU
22	T	53	GLY
5	B	2	GLN
15	M	88	VAL
20	R	81	PRO
16	N	74	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	A	179/182 (98%)	167 (93%)	12 (7%)	16	37
5	B	282/283 (100%)	263 (93%)	19 (7%)	16	37
6	C	193/193 (100%)	180 (93%)	13 (7%)	16	37
7	D	117/148 (79%)	112 (96%)	5 (4%)	29	57
8	E	152/156 (97%)	148 (97%)	4 (3%)	46	75
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	90
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	27	55
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	30
13	K	106/106 (100%)	103 (97%)	3 (3%)	43	73
14	L	113/127 (89%)	108 (96%)	5 (4%)	28	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	M	158/158 (100%)	151 (96%)	7 (4%)	28	56
16	N	149/150 (99%)	145 (97%)	4 (3%)	44	74
17	O	93/94 (99%)	92 (99%)	1 (1%)	73	90
18	P	113/117 (97%)	109 (96%)	4 (4%)	36	65
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	62
20	R	117/122 (96%)	114 (97%)	3 (3%)	46	75
21	S	71/74 (96%)	69 (97%)	2 (3%)	43	73
22	T	105/106 (99%)	98 (93%)	7 (7%)	16	37
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	51 (100%)	0	100	100
25	W	130/130 (100%)	123 (95%)	7 (5%)	22	47
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	41
27	Y	120/196 (61%)	116 (97%)	4 (3%)	38	67
28	Z	60/68 (88%)	59 (98%)	1 (2%)	60	84
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	77
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2968 (96%)	125 (4%)	31	60

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	66	ARG
4	A	69	LEU
4	A	78	ASP
4	A	94	LEU
4	A	120	ARG
4	A	131	HIS
4	A	153	ARG
4	A	206	ARG
4	A	217	ARG
5	B	7	ARG

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Mol	Chain	Res	Type
5	B	11	LEU
5	B	27	ASN
5	B	49	THR
5	B	63	GLU
5	B	97	LEU
5	B	140	LEU
5	B	162	MET
5	B	190	MET
5	B	195	ARG
5	B	234	ARG
5	B	245	SER
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	257	THR
5	B	264	GLU
5	B	304	PRO
5	B	307	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	61	PHE
7	D	133	ASN
7	D	136	ARG
7	D	137	PRO
8	E	7	ILE
8	E	15	GLN
8	E	102	VAL
8	E	164	ASP
9	F	46	GLU
11	H	30	GLN

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Mol	Chain	Res	Type
11	H	84	LYS
11	H	88	ARG
11	H	111	ASP
11	H	132	GLN
11	H	154	TYR
12	J	45	VAL
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP
12	J	127	ILE
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP
14	L	102	ASP
14	L	117	GLU
15	M	46	LEU
15	M	68	ARG
15	M	81	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	26	LEU
16	N	47	LEU
16	N	50	LEU
16	N	152	GLU
17	O	43	VAL
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	57	ASP
20	R	39	THR

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Mol	Chain	Res	Type
20	R	82	GLU
20	R	132	ARG
21	S	71	ASP
21	S	80	ARG
22	T	19	ARG
22	T	23	VAL
22	T	39	ASN
22	T	73	HIS
22	T	75	GLU
22	T	96	VAL
22	T	112	LEU
25	W	26	ILE
25	W	45	VAL
25	W	52	VAL
25	W	73	LEU
25	W	142	ASP
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	72	VAL
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	203	VAL
28	Z	13	ARG
30	2	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	47	HIS
4	A	92	ASN
4	A	125	ASN
4	A	127	GLN
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	238	ASN
5	B	256	GLN

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Mol	Chain	Res	Type
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
6	C	163	HIS
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	74	HIS
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	132	GLN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	58	GLN
15	M	24	GLN
15	M	58	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN

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Mol	Chain	Res	Type
20	R	113	HIS
20	R	117	HIS
20	R	123	GLN
21	S	25	GLN
21	S	53	ASN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	27	HIS
25	W	28	HIS
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	237 (8%)	34 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
3	4	1/8 (12%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2867/3052 (93%)	254 (8%)	35 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G

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Mol	Chain	Res	Type
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	630	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C

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Mol	Chain	Res	Type
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1120	U
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C

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Mol	Chain	Res	Type
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1563	G
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A

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Mol	Chain	Res	Type
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2332	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U

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Mol	Chain	Res	Type
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3040	C
2	9	3041	C
2	9	3043	G

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Mol	Chain	Res	Type
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	604	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1563	G
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U

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Mol	Chain	Res	Type
1	0	2649	A
1	0	2718	C
1	0	2791	U
2	9	3065	A

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	0	2588	1,3	18,26,27	1.04	2 (11%)	19,38,41	0.71	1 (5%)
1	UR3	0	2619	1	19,22,23	0.37	0	26,32,35	0.62	1 (3%)
1	PSU	0	2621	1	18,21,22	1.57	2 (11%)	22,30,33	1.27	3 (13%)
3	5AA	4	76	1,3	18,26,27	0.76	0	15,38,41	0.80	1 (6%)
1	OMU	0	2587	1	19,22,23	0.28	0	26,31,34	0.38	0
1	1MA	0	628	1	16,25,26	1.37	2 (12%)	18,37,40	1.18	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1,3	-	1/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.10	1.43	1.36
1	0	628	1MA	C2-N3	3.74	1.33	1.29
1	0	2621	PSU	C6-C5	3.23	1.39	1.35
1	0	628	1MA	C6-N6	2.62	1.34	1.27
1	0	2588	OMG	C5-C6	-2.52	1.42	1.47
1	0	2588	OMG	C8-N7	-2.48	1.30	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.24	120.47	118.20
1	0	2621	PSU	C6-N1-C2	-3.05	119.57	122.68
1	0	628	1MA	N1-C2-N3	2.92	129.42	126.02
1	0	2621	PSU	O2-C2-N1	2.62	125.68	122.79
1	0	628	1MA	C5-C6-N1	2.44	117.53	113.90
1	0	2619	UR3	C4-N3-C2	2.28	126.71	124.56
3	4	76	5AA	C9-N6-C6	2.21	126.20	119.51
1	0	628	1MA	CM1-N1-C6	2.20	123.60	120.27
1	0	2588	OMG	O6-C6-C5	2.06	128.40	124.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2619	UR3	1	0
1	0	2587	OMU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 233 ligands modelled in this entry, 233 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	0	2749/2922 (94%)	-0.58	31 (1%) 80 82	29, 51, 94, 161	0
2	9	122/122 (100%)	-0.55	4 (3%) 46 46	39, 62, 91, 152	0
3	4	5/8 (62%)	-0.53	0 100 100	41, 43, 47, 47	0
4	A	237/240 (98%)	0.15	10 (4%) 36 35	33, 57, 95, 119	0
5	B	337/338 (99%)	0.01	5 (1%) 73 76	29, 57, 80, 94	0
6	C	246/246 (100%)	-0.10	3 (1%) 79 80	27, 53, 75, 84	0
7	D	140/177 (79%)	2.15	62 (44%) 0 0	58, 101, 127, 137	0
8	E	172/178 (96%)	0.62	14 (8%) 12 10	47, 67, 87, 93	0
9	F	119/120 (99%)	0.92	22 (18%) 1 1	60, 82, 104, 119	0
10	G	29/348 (8%)	1.77	9 (31%) 0 0	65, 90, 102, 105	0
11	H	160/171 (93%)	0.26	7 (4%) 34 33	41, 59, 90, 99	0
12	J	142/145 (97%)	-0.04	1 (0%) 87 89	37, 52, 72, 90	0
13	K	132/132 (100%)	0.01	2 (1%) 73 76	34, 56, 77, 87	0
14	L	145/165 (87%)	0.63	21 (14%) 2 1	30, 72, 118, 132	0
15	M	194/194 (100%)	-0.11	1 (0%) 91 92	34, 50, 67, 74	0
16	N	186/187 (99%)	0.58	19 (10%) 6 5	38, 66, 115, 121	0
17	O	115/116 (99%)	0.10	0 100 100	45, 61, 77, 85	0
18	P	143/149 (95%)	0.26	0 100 100	45, 60, 77, 85	0
19	Q	95/96 (98%)	-0.07	1 (1%) 80 82	40, 48, 60, 75	0
20	R	150/155 (96%)	-0.18	1 (0%) 87 89	37, 48, 68, 75	0
21	S	81/85 (95%)	0.25	2 (2%) 57 59	49, 67, 85, 94	0
22	T	119/120 (99%)	0.70	13 (10%) 5 4	46, 63, 91, 110	0
23	U	53/66 (80%)	0.21	3 (5%) 23 22	43, 57, 74, 84	0
24	V	65/71 (91%)	1.73	21 (32%) 0 0	63, 86, 117, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	-0.07	2 (1%) 77 78	39, 50, 67, 76	0
26	X	82/92 (89%)	0.44	7 (8%) 10 9	45, 59, 77, 94	0
27	Y	142/241 (58%)	-0.00	3 (2%) 63 65	30, 49, 71, 86	0
28	Z	73/83 (87%)	0.17	3 (4%) 37 36	44, 63, 77, 97	0
29	1	56/57 (98%)	-0.43	0 100 100	33, 40, 46, 54	0
30	2	46/50 (92%)	0.52	5 (10%) 5 4	41, 65, 97, 109	0
31	3	92/92 (100%)	0.29	3 (3%) 46 46	37, 59, 73, 84	0
32	I	70/162 (43%)	3.59	55 (78%) 0 0	99, 121, 143, 145	0
All	All	6651/7482 (88%)	-0.05	330 (4%) 28 27	27, 56, 102, 161	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	11.9
32	I	133	THR	10.3
32	I	71	GLY	9.6
7	D	63	ILE	9.4
32	I	93	GLN	8.5
32	I	96	PHE	8.1
7	D	88	LEU	7.9
32	I	88	GLY	7.6
32	I	113	HIS	7.3
7	D	90	LEU	7.2
32	I	79	ILE	6.9
7	D	57	THR	6.8
24	V	40	PRO	6.7
32	I	76	ALA	6.7
16	N	166	ALA	6.7
24	V	39	ALA	6.5
32	I	137	VAL	6.5
22	T	119	ALA	6.4
7	D	128	LEU	6.4
7	D	69	ILE	6.4
32	I	117	LEU	6.2
2	9	3023	U	6.1
30	2	49	GLU	6.1
24	V	38	GLY	6.1
1	0	1173	A	6.1
32	I	109	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
32	I	97	VAL	5.9
32	I	102	VAL	5.8
7	D	130	VAL	5.7
32	I	91	GLU	5.7
7	D	106	PHE	5.5
24	V	43	PRO	5.5
7	D	93	LEU	5.4
2	9	3024	U	5.3
7	D	66	GLY	5.3
16	N	183	ASP	5.3
7	D	18	ILE	5.3
7	D	85	GLN	5.2
21	S	81	ILE	5.2
7	D	87	ALA	5.2
26	X	88	GLU	5.2
9	F	119	ARG	5.1
22	T	112	LEU	5.1
32	I	98	ALA	5.1
7	D	84	LEU	5.0
32	I	111	GLN	4.9
7	D	89	PRO	4.9
1	0	2237	G	4.9
7	D	64	ARG	4.9
30	2	35	ARG	4.8
10	G	27	ILE	4.8
7	D	65	GLU	4.8
32	I	118	SER	4.7
32	I	116	LEU	4.7
32	I	87	THR	4.7
7	D	44	ILE	4.7
4	A	37	VAL	4.6
14	L	105	TYR	4.6
7	D	56	ARG	4.5
14	L	60	GLU	4.5
1	0	1199	A	4.5
7	D	25	MET	4.4
7	D	170	TYR	4.4
8	E	45	ASP	4.4
7	D	62	ASP	4.3
14	L	80	ASP	4.3
1	0	1198	U	4.3
1	0	282	C	4.2

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Mol	Chain	Res	Type	RSRZ
24	V	41	GLU	4.2
7	D	26	GLY	4.2
7	D	83	PHE	4.2
7	D	58	VAL	4.2
32	I	77	GLU	4.2
7	D	68	PRO	4.2
1	0	1171	A	4.2
32	I	85	PHE	4.1
2	9	3001	U	4.1
7	D	41	LEU	4.0
24	V	8	ILE	4.0
10	G	23	ILE	4.0
8	E	170	ARG	3.9
32	I	107	GLN	3.9
1	0	1172	G	3.9
27	Y	235	GLU	3.8
31	3	22	VAL	3.8
16	N	179	LEU	3.8
14	L	106	VAL	3.8
7	D	10	PHE	3.8
7	D	165	PHE	3.8
30	2	39	ARG	3.7
7	D	27	ILE	3.7
1	0	1177	A	3.7
32	I	110	GLU	3.7
7	D	61	PHE	3.7
7	D	104	PHE	3.7
23	U	47	ARG	3.7
7	D	86	THR	3.7
9	F	47	LEU	3.6
32	I	135	LEU	3.6
7	D	92	GLU	3.6
32	I	114	PRO	3.6
32	I	95	ASP	3.6
32	I	89	SER	3.6
1	0	2238	A	3.6
16	N	147	ILE	3.6
32	I	75	THR	3.6
9	F	107	ASP	3.5
7	D	23	VAL	3.5
7	D	172	VAL	3.5
24	V	52	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
32	I	128	VAL	3.5
16	N	165	ALA	3.5
24	V	3	LEU	3.5
7	D	129	ASP	3.5
1	0	284	C	3.4
22	T	42	VAL	3.4
22	T	40	VAL	3.4
32	I	121	LEU	3.4
14	L	104	ASP	3.3
1	0	1279	U	3.3
14	L	96	VAL	3.3
32	I	139	ILE	3.3
9	F	106	ALA	3.3
1	0	960	G	3.3
1	0	1951	G	3.3
7	D	134	LEU	3.3
1	0	970	U	3.3
32	I	103	ASP	3.3
7	D	17	ARG	3.3
32	I	81	ASP	3.2
7	D	45	THR	3.2
14	L	124	ASP	3.2
1	0	735	C	3.2
9	F	17	LEU	3.2
7	D	166	ILE	3.2
8	E	5	LEU	3.2
11	H	45	VAL	3.2
26	X	85	VAL	3.2
16	N	138	ASP	3.2
8	E	100	ASP	3.2
9	F	28	ALA	3.2
23	U	55	ALA	3.2
9	F	117	GLU	3.1
26	X	41	PHE	3.1
27	Y	108	ASP	3.1
32	I	106	LYS	3.1
9	F	16	ALA	3.1
10	G	24	VAL	3.1
9	F	90	GLU	3.1
14	L	130	ARG	3.0
19	Q	95	GLU	3.0
1	0	1202	A	3.0

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Mol	Chain	Res	Type	RSRZ
11	H	171	ALA	3.0
7	D	98	PHE	3.0
14	L	150	GLN	3.0
22	T	49	GLU	3.0
24	V	49	LEU	3.0
9	F	108	VAL	2.9
6	C	132	ASP	2.9
16	N	127	LEU	2.9
14	L	100	ALA	2.9
7	D	171	ASP	2.9
9	F	49	PHE	2.9
4	A	135	VAL	2.9
28	Z	20	ARG	2.9
32	I	105	VAL	2.9
24	V	37	GLY	2.9
22	T	1	SER	2.9
32	I	83	ALA	2.9
15	M	194	ALA	2.8
32	I	104	GLN	2.8
8	E	42	VAL	2.8
7	D	40	ILE	2.8
32	I	78	LEU	2.8
14	L	91	VAL	2.8
32	I	124	ALA	2.8
24	V	45	ARG	2.8
22	T	116	ASP	2.8
6	C	135	GLU	2.8
7	D	24	HIS	2.8
9	F	103	GLU	2.8
16	N	159	TYR	2.8
24	V	59	ILE	2.8
1	0	2239	C	2.8
1	0	1170	U	2.7
5	B	128	ILE	2.7
9	F	98	VAL	2.7
7	D	54	ALA	2.7
8	E	3	VAL	2.7
9	F	100	ASP	2.7
10	G	71	LEU	2.7
31	3	62	THR	2.7
14	L	89	PHE	2.7
32	I	72	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
11	H	37	GLN	2.7
16	N	161	GLY	2.7
7	D	75	LEU	2.7
9	F	109	GLU	2.6
28	Z	24	ARG	2.6
32	I	123	ASN	2.6
4	A	237	GLY	2.6
23	U	54	THR	2.6
1	0	1950	G	2.6
4	A	64	ASP	2.6
5	B	104	GLU	2.6
14	L	107	LYS	2.6
24	V	36	ALA	2.6
32	I	132	CYS	2.6
32	I	108	ILE	2.6
5	B	119	HIS	2.6
4	A	35	GLY	2.6
1	0	1525	G	2.6
32	I	73	PRO	2.6
7	D	70	GLY	2.6
26	X	73	ARG	2.6
26	X	71	ARG	2.5
1	0	138	U	2.5
7	D	43	GLU	2.5
32	I	140	GLU	2.5
24	V	63	GLU	2.5
4	A	36	ASP	2.5
32	I	138	THR	2.5
9	F	118	LEU	2.5
14	L	73	VAL	2.5
9	F	15	ASP	2.5
7	D	107	GLY	2.5
14	L	123	ASP	2.5
10	G	65	THR	2.5
16	N	95	ALA	2.5
22	T	99	THR	2.5
9	F	99	THR	2.4
32	I	119	TYR	2.4
32	I	115	ASP	2.4
13	K	119	GLN	2.4
8	E	46	THR	2.4
9	F	19	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
7	D	132	VAL	2.4
16	N	149	GLU	2.4
2	9	3002	U	2.4
11	H	79	GLU	2.4
22	T	37	GLN	2.4
32	I	126	LYS	2.4
32	I	86	GLU	2.4
10	G	67	LEU	2.4
4	A	99	ILE	2.4
13	K	132	VAL	2.4
20	R	7	GLU	2.4
25	W	79	VAL	2.4
32	I	92	PRO	2.3
7	D	80	ALA	2.3
16	N	185	GLU	2.3
24	V	9	ARG	2.3
16	N	139	TRP	2.3
16	N	155	GLU	2.3
7	D	11	HIS	2.3
7	D	59	GLY	2.3
11	H	74	ILE	2.3
14	L	140	VAL	2.3
21	S	76	GLU	2.3
1	0	1180	U	2.3
12	J	92	GLN	2.3
24	V	33	VAL	2.3
32	I	84	GLY	2.2
8	E	1	PRO	2.2
5	B	181	ILE	2.2
9	F	75	ILE	2.2
7	D	53	LYS	2.2
30	2	20	ARG	2.2
24	V	61	GLY	2.2
1	0	2250	G	2.2
22	T	115	GLU	2.2
7	D	135	VAL	2.2
1	0	716	G	2.2
26	X	72	VAL	2.2
7	D	105	SER	2.2
7	D	91	ALA	2.2
1	0	1948	G	2.2
5	B	183	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
24	V	10	ASP	2.2
1	0	1200	A	2.2
8	E	87	PHE	2.2
30	2	44	ARG	2.2
9	F	44	SER	2.2
22	T	117	ASP	2.2
9	F	40	ILE	2.2
24	V	53	ILE	2.2
1	0	280	C	2.2
7	D	73	VAL	2.1
27	Y	96	GLU	2.1
1	0	10	U	2.1
8	E	108	LEU	2.1
14	L	149	ARG	2.1
28	Z	25	ARG	2.1
4	A	31	LYS	2.1
1	0	272	A	2.1
8	E	53	GLU	2.1
6	C	61	PHE	2.1
7	D	67	ASP	2.1
10	G	68	GLU	2.1
31	3	92	GLU	2.1
16	N	160	SER	2.1
16	N	162	ASP	2.1
22	T	35	TYR	2.1
24	V	2	VAL	2.1
7	D	81	GLU	2.1
14	L	99	GLU	2.1
26	X	7	GLU	2.1
10	G	70	ALA	2.1
10	G	26	MET	2.1
8	E	99	GLY	2.1
14	L	97	VAL	2.1
11	H	83	TYR	2.1
16	N	150	TYR	2.1
16	N	180	LEU	2.1
25	W	100	LEU	2.1
7	D	71	ALA	2.1
16	N	184	ILE	2.1
32	I	74	PRO	2.1
1	0	1169	U	2.1
32	I	136	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
22	T	103	LEU	2.0
32	I	100	LEU	2.0
14	L	93	VAL	2.0
14	L	133	VAL	2.0
8	E	47	VAL	2.0
11	H	162	ARG	2.0
4	A	60	PHE	2.0
4	A	103	VAL	2.0
1	0	285	A	2.0
8	E	86	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMG	0	2588	24/25	0.98	0.13	32,36,39,40	0
3	5AA	4	76	24/25	0.98	0.14	38,44,48,48	0
1	1MA	0	628	23/24	0.99	0.15	29,32,34,36	0
1	UR3	0	2619	21/22	0.99	0.16	32,39,41,42	0
1	PSU	0	2621	20/21	0.99	0.13	30,33,37,38	0
1	OMU	0	2587	21/22	0.99	0.13	35,37,39,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	CD	O	9205	1/1	0.04	0.30	200,200,200,200	0
35	NA	R	9186	1/1	0.30	0.75	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	9	9151	1/1	0.65	0.35	87,87,87,87	0
35	NA	0	9129	1/1	0.68	0.17	65,65,65,65	0
33	MG	0	8092	1/1	0.72	0.70	115,115,115,115	0
35	NA	0	9171	1/1	0.73	0.40	64,64,64,64	0
35	NA	0	9182	1/1	0.74	0.45	84,84,84,84	0
33	MG	0	8090	1/1	0.76	0.60	69,69,69,69	0
33	MG	0	8085	1/1	0.80	0.24	74,74,74,74	0
35	NA	0	9177	1/1	0.80	0.41	73,73,73,73	0
33	MG	K	8069	1/1	0.84	0.14	49,49,49,49	0
35	NA	0	9126	1/1	0.84	0.19	44,44,44,44	0
33	MG	0	8024	1/1	0.84	0.64	83,83,83,83	0
35	NA	0	9168	1/1	0.84	0.15	56,56,56,56	0
36	CL	0	9322	1/1	0.84	0.53	92,92,92,92	0
33	MG	0	8093	1/1	0.84	0.11	52,52,52,52	0
35	NA	R	9137	1/1	0.85	0.12	50,50,50,50	0
33	MG	9	8095	1/1	0.85	0.14	75,75,75,75	0
36	CL	0	9305	1/1	0.85	0.18	71,71,71,71	0
35	NA	0	9170	1/1	0.85	0.47	97,97,97,97	0
35	NA	0	9166	1/1	0.85	0.11	68,68,68,68	0
35	NA	0	9152	1/1	0.86	0.41	65,65,65,65	0
35	NA	0	9124	1/1	0.86	0.17	67,67,67,67	0
35	NA	S	9112	1/1	0.86	0.52	75,75,75,75	0
33	MG	0	8049	1/1	0.87	0.29	80,80,80,80	0
33	MG	0	8082	1/1	0.87	0.20	65,65,65,65	0
35	NA	0	9174	1/1	0.87	0.90	64,64,64,64	0
35	NA	0	9150	1/1	0.88	0.30	48,48,48,48	0
35	NA	9	9183	1/1	0.89	0.14	49,49,49,49	0
36	CL	A	9309	1/1	0.89	0.19	77,77,77,77	0
35	NA	C	9104	1/1	0.89	0.15	41,41,41,41	0
33	MG	T	8073	1/1	0.90	0.09	66,66,66,66	0
35	NA	0	9149	1/1	0.90	0.14	42,42,42,42	0
34	K	0	9003	1/1	0.90	0.13	66,66,66,66	0
35	NA	0	9173	1/1	0.90	0.24	58,58,58,58	0
33	MG	0	8054	1/1	0.90	0.15	39,39,39,39	0
35	NA	0	9158	1/1	0.90	0.58	84,84,84,84	0
35	NA	0	9161	1/1	0.90	0.30	56,56,56,56	0
35	NA	0	9185	1/1	0.90	0.65	54,54,54,54	0
33	MG	0	8041	1/1	0.90	0.22	72,72,72,72	0
33	MG	0	8043	1/1	0.91	0.08	53,53,53,53	0
35	NA	0	9163	1/1	0.91	0.41	63,63,63,63	0
33	MG	0	8106	1/1	0.91	0.08	63,63,63,63	0
35	NA	0	9107	1/1	0.91	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9142	1/1	0.91	0.16	53,53,53,53	0
35	NA	R	9138	1/1	0.91	0.06	61,61,61,61	0
35	NA	0	9111	1/1	0.92	0.11	59,59,59,59	0
35	NA	0	9117	1/1	0.92	0.11	46,46,46,46	0
33	MG	A	8066	1/1	0.92	0.05	66,66,66,66	0
35	NA	0	9164	1/1	0.92	0.24	55,55,55,55	0
33	MG	0	8089	1/1	0.92	0.09	60,60,60,60	0
33	MG	0	8101	1/1	0.92	0.11	74,74,74,74	0
35	NA	0	9133	1/1	0.92	0.11	32,32,32,32	0
33	MG	0	8050	1/1	0.92	0.08	61,61,61,61	0
35	NA	0	9101	1/1	0.92	0.22	47,47,47,47	0
33	MG	0	8047	1/1	0.92	0.17	78,78,78,78	0
35	NA	0	9110	1/1	0.92	0.16	38,38,38,38	0
35	NA	0	9155	1/1	0.92	0.52	78,78,78,78	0
35	NA	0	9167	1/1	0.93	0.08	47,47,47,47	0
33	MG	0	8076	1/1	0.93	0.07	70,70,70,70	0
35	NA	0	9169	1/1	0.93	0.38	79,79,79,79	0
35	NA	L	9180	1/1	0.93	0.52	72,72,72,72	0
35	NA	Q	9148	1/1	0.93	0.29	43,43,43,43	0
33	MG	0	8088	1/1	0.93	0.06	36,36,36,36	0
33	MG	3	8078	1/1	0.93	0.05	55,55,55,55	0
35	NA	0	9172	1/1	0.93	0.37	61,61,61,61	0
35	NA	0	9135	1/1	0.93	0.28	50,50,50,50	0
33	MG	0	8039	1/1	0.93	0.06	51,51,51,51	0
36	CL	0	9315	1/1	0.93	0.40	84,84,84,84	0
33	MG	0	8098	1/1	0.93	0.24	40,40,40,40	0
35	NA	0	9165	1/1	0.93	0.21	42,42,42,42	0
36	CL	3	9304	1/1	0.93	0.15	70,70,70,70	0
35	NA	0	9125	1/1	0.93	0.25	69,69,69,69	0
33	MG	0	8044	1/1	0.94	0.12	49,49,49,49	0
35	NA	0	9113	1/1	0.94	0.16	66,66,66,66	0
35	NA	0	9140	1/1	0.94	0.20	45,45,45,45	0
33	MG	0	8083	1/1	0.94	0.08	42,42,42,42	0
33	MG	0	8114	1/1	0.94	0.18	56,56,56,56	0
36	CL	0	9303	1/1	0.94	0.14	64,64,64,64	0
35	NA	0	9184	1/1	0.94	0.54	96,96,96,96	0
33	MG	0	8084	1/1	0.94	0.10	51,51,51,51	0
33	MG	0	8071	1/1	0.94	0.13	72,72,72,72	0
33	MG	0	8042	1/1	0.94	0.08	39,39,39,39	0
36	CL	J	9302	1/1	0.94	0.06	61,61,61,61	0
36	CL	N	9307	1/1	0.94	0.19	66,66,66,66	0
35	NA	0	9132	1/1	0.94	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9159	1/1	0.94	0.23	56,56,56,56	0
33	MG	0	8094	1/1	0.95	0.12	86,86,86,86	0
35	NA	0	9160	1/1	0.95	0.33	49,49,49,49	0
33	MG	0	8097	1/1	0.95	0.14	40,40,40,40	0
35	NA	0	9162	1/1	0.95	0.23	72,72,72,72	0
35	NA	0	9127	1/1	0.95	0.10	35,35,35,35	0
35	NA	H	9109	1/1	0.95	0.13	36,36,36,36	0
33	MG	0	8087	1/1	0.95	0.14	54,54,54,54	0
33	MG	0	8099	1/1	0.95	0.10	63,63,63,63	0
33	MG	0	8080	1/1	0.95	0.15	46,46,46,46	0
35	NA	0	9106	1/1	0.95	0.81	51,51,51,51	0
33	MG	0	8057	1/1	0.95	0.14	45,45,45,45	0
33	MG	0	8111	1/1	0.95	0.14	77,77,77,77	0
33	MG	0	8112	1/1	0.95	0.11	47,47,47,47	0
33	MG	0	8063	1/1	0.95	0.15	84,84,84,84	0
35	NA	0	9116	1/1	0.95	0.11	36,36,36,36	0
33	MG	0	8027	1/1	0.95	0.13	55,55,55,55	0
35	NA	0	9156	1/1	0.95	0.44	51,51,51,51	0
35	NA	0	9157	1/1	0.95	0.10	69,69,69,69	0
35	NA	0	9179	1/1	0.95	0.19	57,57,57,57	0
35	NA	0	9181	1/1	0.95	0.12	48,48,48,48	0
33	MG	0	8014	1/1	0.95	0.11	41,41,41,41	0
37	CD	3	9204	1/1	0.95	0.09	66,66,66,66	0
33	MG	0	8075	1/1	0.96	0.06	43,43,43,43	0
33	MG	0	8059	1/1	0.96	0.07	44,44,44,44	0
35	NA	A	9145	1/1	0.96	0.16	45,45,45,45	0
33	MG	0	8062	1/1	0.96	0.10	57,57,57,57	0
34	K	0	9001	1/1	0.96	0.24	74,74,74,74	0
35	NA	H	9122	1/1	0.96	0.13	59,59,59,59	0
33	MG	0	8104	1/1	0.96	0.22	73,73,73,73	0
33	MG	0	8081	1/1	0.96	0.18	54,54,54,54	0
35	NA	0	9102	1/1	0.96	0.16	44,44,44,44	0
35	NA	0	9105	1/1	0.96	0.08	39,39,39,39	0
33	MG	0	8046	1/1	0.96	0.10	54,54,54,54	0
35	NA	0	9141	1/1	0.96	0.07	47,47,47,47	0
33	MG	0	8064	1/1	0.96	0.12	33,33,33,33	0
33	MG	0	8113	1/1	0.96	0.12	45,45,45,45	0
33	MG	0	8068	1/1	0.96	0.08	59,59,59,59	0
36	CL	0	9316	1/1	0.96	0.16	61,61,61,61	0
36	CL	0	9320	1/1	0.96	0.11	48,48,48,48	0
33	MG	0	8115	1/1	0.96	0.12	49,49,49,49	0
35	NA	0	9114	1/1	0.96	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9115	1/1	0.96	0.15	39,39,39,39	0
33	MG	0	8096	1/1	0.96	0.07	51,51,51,51	0
36	CL	R	9306	1/1	0.96	0.12	48,48,48,48	0
33	MG	0	8051	1/1	0.96	0.07	61,61,61,61	0
35	NA	0	9121	1/1	0.96	0.33	58,58,58,58	0
35	NA	0	9123	1/1	0.96	0.17	43,43,43,43	0
35	NA	0	9103	1/1	0.97	0.15	39,39,39,39	0
33	MG	0	8028	1/1	0.97	0.11	44,44,44,44	0
35	NA	0	9154	1/1	0.97	0.19	38,38,38,38	0
33	MG	0	8116	1/1	0.97	0.06	47,47,47,47	0
33	MG	0	8102	1/1	0.97	0.13	67,67,67,67	0
35	NA	0	9108	1/1	0.97	0.09	61,61,61,61	0
35	NA	0	9175	1/1	0.97	0.43	56,56,56,56	0
35	NA	0	9176	1/1	0.97	0.18	42,42,42,42	0
35	NA	0	9128	1/1	0.97	0.07	35,35,35,35	0
36	CL	0	9314	1/1	0.97	0.07	53,53,53,53	0
35	NA	0	9178	1/1	0.97	0.21	57,57,57,57	0
33	MG	0	8103	1/1	0.97	0.11	81,81,81,81	0
36	CL	0	9317	1/1	0.97	0.08	64,64,64,64	0
35	NA	0	9131	1/1	0.97	0.08	36,36,36,36	0
33	MG	0	8045	1/1	0.97	0.11	62,62,62,62	0
33	MG	0	8086	1/1	0.97	0.06	47,47,47,47	0
33	MG	0	8108	1/1	0.97	0.10	75,75,75,75	0
36	CL	J	9321	1/1	0.97	0.13	54,54,54,54	0
36	CL	K	9312	1/1	0.97	0.10	55,55,55,55	0
33	MG	0	8012	1/1	0.97	0.16	32,32,32,32	0
36	CL	O	9308	1/1	0.97	0.21	81,81,81,81	0
33	MG	0	8040	1/1	0.97	0.18	52,52,52,52	0
33	MG	0	8056	1/1	0.97	0.12	51,51,51,51	0
35	NA	0	9144	1/1	0.97	0.10	27,27,27,27	0
33	MG	0	8048	1/1	0.97	0.16	62,62,62,62	0
33	MG	0	8032	1/1	0.98	0.05	35,35,35,35	0
35	NA	0	9153	1/1	0.98	0.10	25,25,25,25	0
33	MG	0	8034	1/1	0.98	0.10	32,32,32,32	0
33	MG	0	8067	1/1	0.98	0.08	46,46,46,46	0
33	MG	0	8035	1/1	0.98	0.07	51,51,51,51	0
33	MG	0	8117	1/1	0.98	0.10	40,40,40,40	0
33	MG	9	8052	1/1	0.98	0.05	47,47,47,47	0
35	NA	J	9146	1/1	0.98	0.10	35,35,35,35	0
35	NA	0	9118	1/1	0.98	0.21	47,47,47,47	0
35	NA	M	9147	1/1	0.98	0.21	33,33,33,33	0
35	NA	0	9119	1/1	0.98	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8070	1/1	0.98	0.04	45,45,45,45	0
33	MG	A	8065	1/1	0.98	0.21	52,52,52,52	0
33	MG	0	8037	1/1	0.98	0.07	44,44,44,44	0
33	MG	B	8055	1/1	0.98	0.14	52,52,52,52	0
33	MG	0	8072	1/1	0.98	0.24	55,55,55,55	0
33	MG	0	8074	1/1	0.98	0.09	40,40,40,40	0
36	CL	0	9313	1/1	0.98	0.13	61,61,61,61	0
33	MG	0	8016	1/1	0.98	0.21	44,44,44,44	0
33	MG	0	8017	1/1	0.98	0.10	33,33,33,33	0
35	NA	0	9130	1/1	0.98	0.08	44,44,44,44	0
34	K	0	9002	1/1	0.98	0.08	54,54,54,54	0
33	MG	0	8053	1/1	0.98	0.17	58,58,58,58	0
33	MG	0	8022	1/1	0.98	0.07	35,35,35,35	0
35	NA	0	9134	1/1	0.98	0.10	37,37,37,37	0
36	CL	J	9301	1/1	0.98	0.19	73,73,73,73	0
33	MG	0	8023	1/1	0.98	0.18	48,48,48,48	0
35	NA	0	9136	1/1	0.98	0.07	56,56,56,56	0
33	MG	0	8004	1/1	0.98	0.05	27,27,27,27	0
36	CL	L	9310	1/1	0.98	0.15	61,61,61,61	0
36	CL	M	9318	1/1	0.98	0.15	50,50,50,50	0
33	MG	0	8058	1/1	0.98	0.12	57,57,57,57	0
33	MG	0	8107	1/1	0.98	0.09	38,38,38,38	0
35	NA	0	9143	1/1	0.98	0.07	36,36,36,36	0
33	MG	0	8013	1/1	0.98	0.19	41,41,41,41	0
33	MG	0	8061	1/1	0.98	0.08	45,45,45,45	0
33	MG	0	8011	1/1	0.98	0.15	23,23,23,23	0
33	MG	0	8002	1/1	0.99	0.06	39,39,39,39	0
33	MG	0	8025	1/1	0.99	0.11	35,35,35,35	0
33	MG	Y	8109	1/1	0.99	0.09	39,39,39,39	0
33	MG	0	8026	1/1	0.99	0.13	31,31,31,31	0
33	MG	0	8003	1/1	0.99	0.14	40,40,40,40	0
33	MG	0	8100	1/1	0.99	0.18	82,82,82,82	0
33	MG	0	8001	1/1	0.99	0.10	38,38,38,38	0
33	MG	0	8029	1/1	0.99	0.17	36,36,36,36	0
33	MG	0	8077	1/1	0.99	0.13	35,35,35,35	0
36	CL	0	9311	1/1	0.99	0.10	52,52,52,52	0
33	MG	0	8079	1/1	0.99	0.12	38,38,38,38	0
33	MG	0	8006	1/1	0.99	0.05	33,33,33,33	0
35	NA	0	9139	1/1	0.99	0.13	22,22,22,22	0
33	MG	0	8033	1/1	0.99	0.13	32,32,32,32	0
33	MG	0	8015	1/1	0.99	0.12	31,31,31,31	0
33	MG	0	8110	1/1	0.99	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8007	1/1	0.99	0.07	24,24,24,24	0
33	MG	0	8036	1/1	0.99	0.13	35,35,35,35	0
36	CL	B	9319	1/1	0.99	0.14	60,60,60,60	0
33	MG	0	8008	1/1	0.99	0.08	37,37,37,37	0
33	MG	0	8038	1/1	0.99	0.16	26,26,26,26	0
33	MG	0	8060	1/1	0.99	0.31	49,49,49,49	0
33	MG	0	8018	1/1	0.99	0.15	47,47,47,47	0
33	MG	0	8019	1/1	0.99	0.09	38,38,38,38	0
33	MG	0	8118	1/1	0.99	0.09	40,40,40,40	0
33	MG	0	8020	1/1	0.99	0.11	24,24,24,24	0
35	NA	0	9120	1/1	0.99	0.10	43,43,43,43	0
33	MG	0	8091	1/1	0.99	0.07	57,57,57,57	0
33	MG	0	8021	1/1	0.99	0.17	30,30,30,30	0
33	MG	0	8009	1/1	0.99	0.10	35,35,35,35	0
37	CD	U	9201	1/1	0.99	0.09	69,69,69,69	0
37	CD	Z	9203	1/1	0.99	0.09	68,68,68,68	0
33	MG	0	8010	1/1	0.99	0.11	29,29,29,29	0
33	MG	0	8005	1/1	1.00	0.14	37,37,37,37	0
33	MG	0	8030	1/1	1.00	0.15	26,26,26,26	0
37	CD	1	9202	1/1	1.00	0.05	68,68,68,68	0
33	MG	0	8031	1/1	1.00	0.08	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.