Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 11:45 PM EDT

PDB ID	:	2OTJ
Title	:	13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors	:	Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on	:	2007-02-08
Resolution	:	2.90 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:

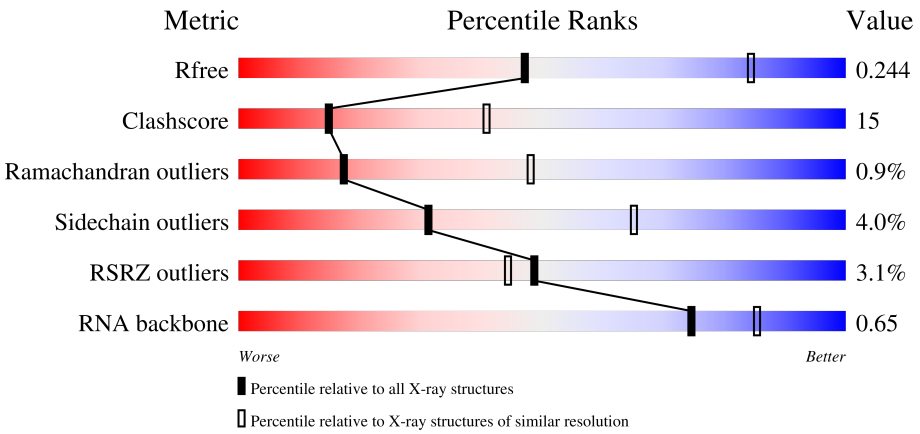
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	49% 39% 6% 6%
2	9	122	2% 38% 48% 13% •
3	A	240	3% 68% 27% • •
4	B	338	62% 34% •

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Mol	Chain	Length	Quality of chain
5	C	246	67% 29% •
6	D	177	22% 44% 34% • 21%
7	E	178	% 71% 25% •
8	F	120	5% 65% 32% • •
9	G	348	% 5% • 92%
10	H	171	9% 69% 22% • 6%
11	J	145	% 66% 28% • •
12	K	132	% 73% 25% •
13	L	165	7% 68% 19% • 12%
14	M	194	74% 24% •
15	N	187	5% 70% 27% • •
16	O	116	79% 20% •
17	P	149	% 72% 22% • •
18	Q	96	77% 21% • •
19	R	155	70% 25% • •
20	S	85	% 74% 21% 5%
21	T	120	2% 73% 24% • •
22	U	66	48% 30% • 20%
23	V	71	20% 59% 30% • 8%
24	W	154	62% 36% •
25	X	92	8% 60% 26% • 11%
26	Y	241	% 42% 15% • 41%
27	Z	73	12% 58% 40% •
28	1	57	67% 32% •
29	2	50	6% 54% 38% 8%

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Mol	Chain	Length	Quality of chain
30	3	92	78% 21%
31	I	161	31% 29% 14% 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
32	13T	0	9000	-	-	X	-
35	NA	0	8506	-	-	-	X
35	NA	0	8516	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8542	-	-	X	-
35	NA	0	8550	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8584	-	-	-	X
36	CL	J	8801	-	-	X	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99043 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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779
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 protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	-	insertion	UNP P60617
H	166	SER	-	insertion	UNP P60617
H	167	PRO	-	insertion	UNP P60617
H	168	ALA	-	insertion	UNP P60617
H	169	GLY	-	insertion	UNP P60617
H	170	ASN	-	insertion	UNP P60617
H	171	ALA	-	insertion	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	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 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	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	UNP P60618
M	194	ALA	-	insertion	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

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

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	Z	73	579	346	116	112	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	insertion	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	1	56	431	258	86	83	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	2	46	396	239	89	67	1	0	0	0

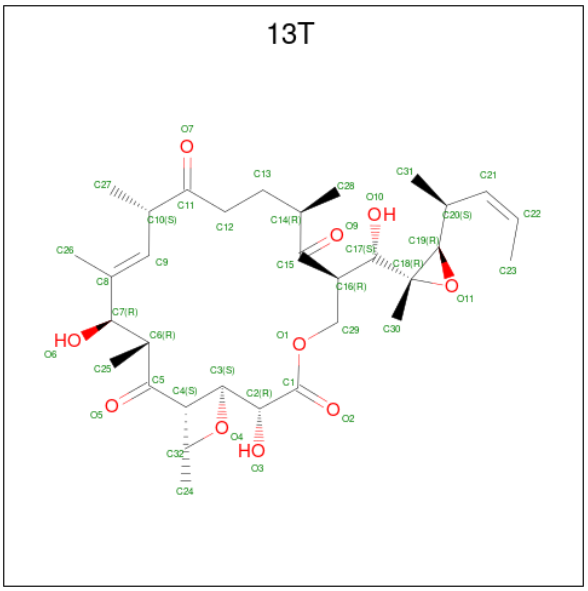
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	3	92	755	458	153	137	7	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is 13-DEOXYTEDANOLIDE (three-letter code: 13T) (formula: $C_{32}H_{50}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
32	0	1	42	32	10	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	1	1	1	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	2	2	2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
34	0	2	2	2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
35	0	74	74	74	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	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	2	Total Cl 2 2	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	5905	Total O 5905 5905	0	0
38	9	140	Total O 140 140	0	0
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	170	Total O 170 170	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	19	Total O 19 19	0	0
38	H	70	Total O 70 70	0	0
38	J	58	Total O 58 58	0	0
38	K	59	Total O 59 59	0	0
38	L	83	Total O 83 83	0	0
38	M	123	Total O 123 123	0	0
38	N	63	Total O 63 63	0	0

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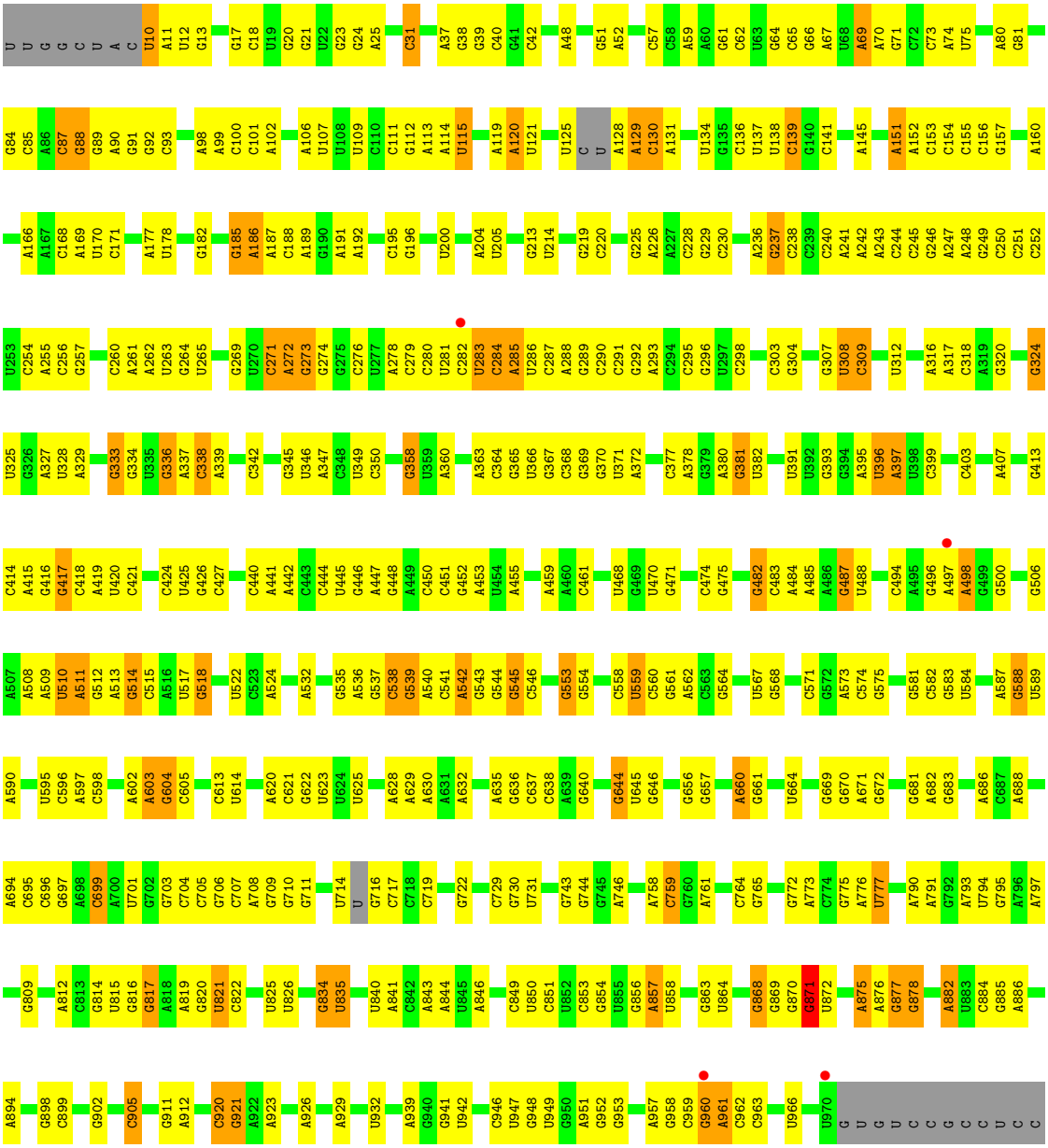
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	44	Total O 44 44	0	0
38	P	56	Total O 56 56	0	0
38	Q	51	Total O 51 51	0	0
38	R	80	Total O 80 80	0	0
38	S	36	Total O 36 36	0	0
38	T	33	Total O 33 33	0	0
38	U	26	Total O 26 26	0	0
38	V	11	Total O 11 11	0	0
38	W	67	Total O 67 67	0	0
38	X	21	Total O 21 21	0	0
38	Y	96	Total O 96 96	0	0
38	Z	31	Total O 31 31	0	0
38	1	56	Total O 56 56	0	0
38	2	45	Total O 45 45	0	0
38	3	66	Total O 66 66	0	0
38	I	8	Total O 8 8	0	0

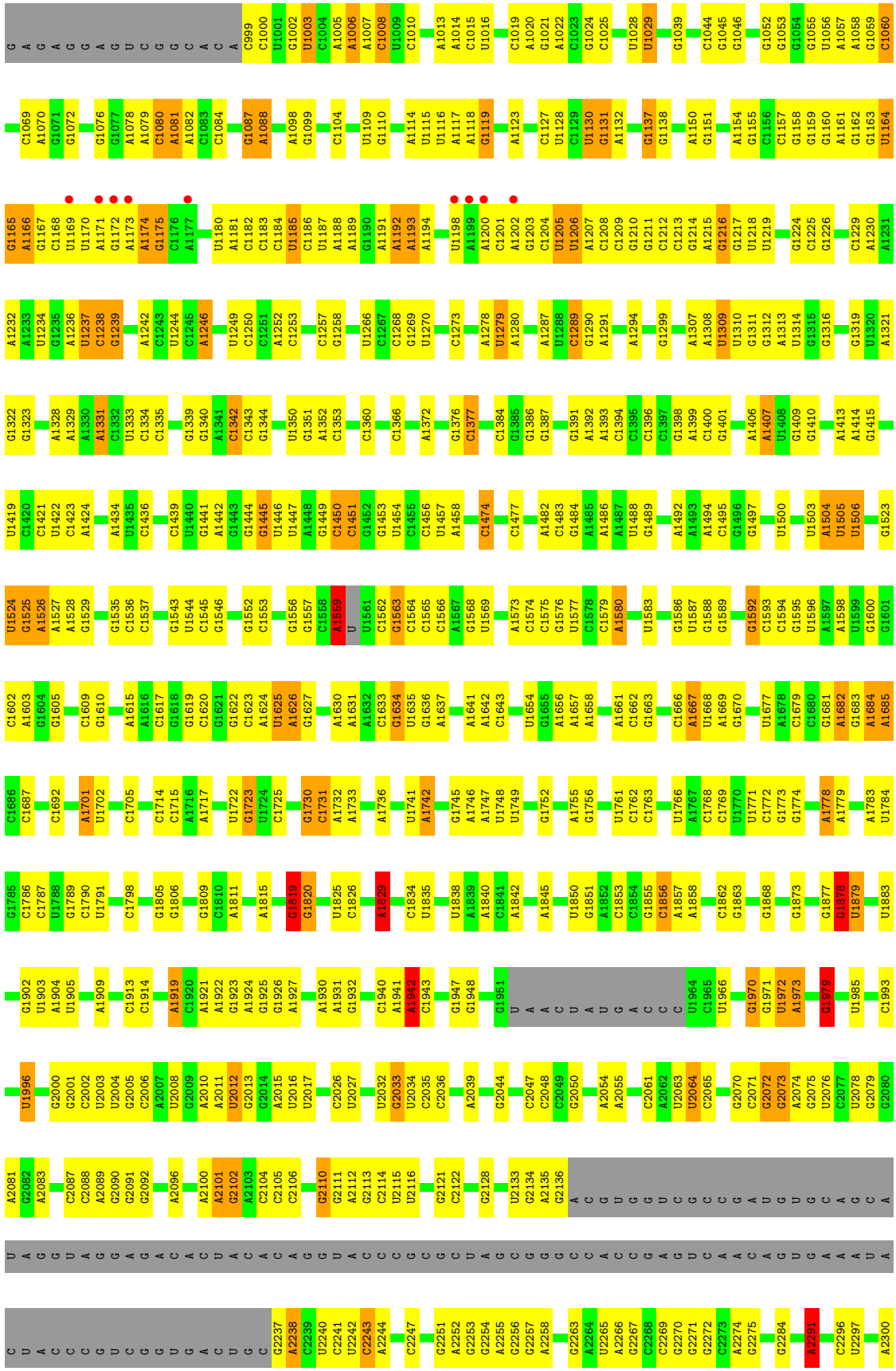
3 Residue-property plots (i)

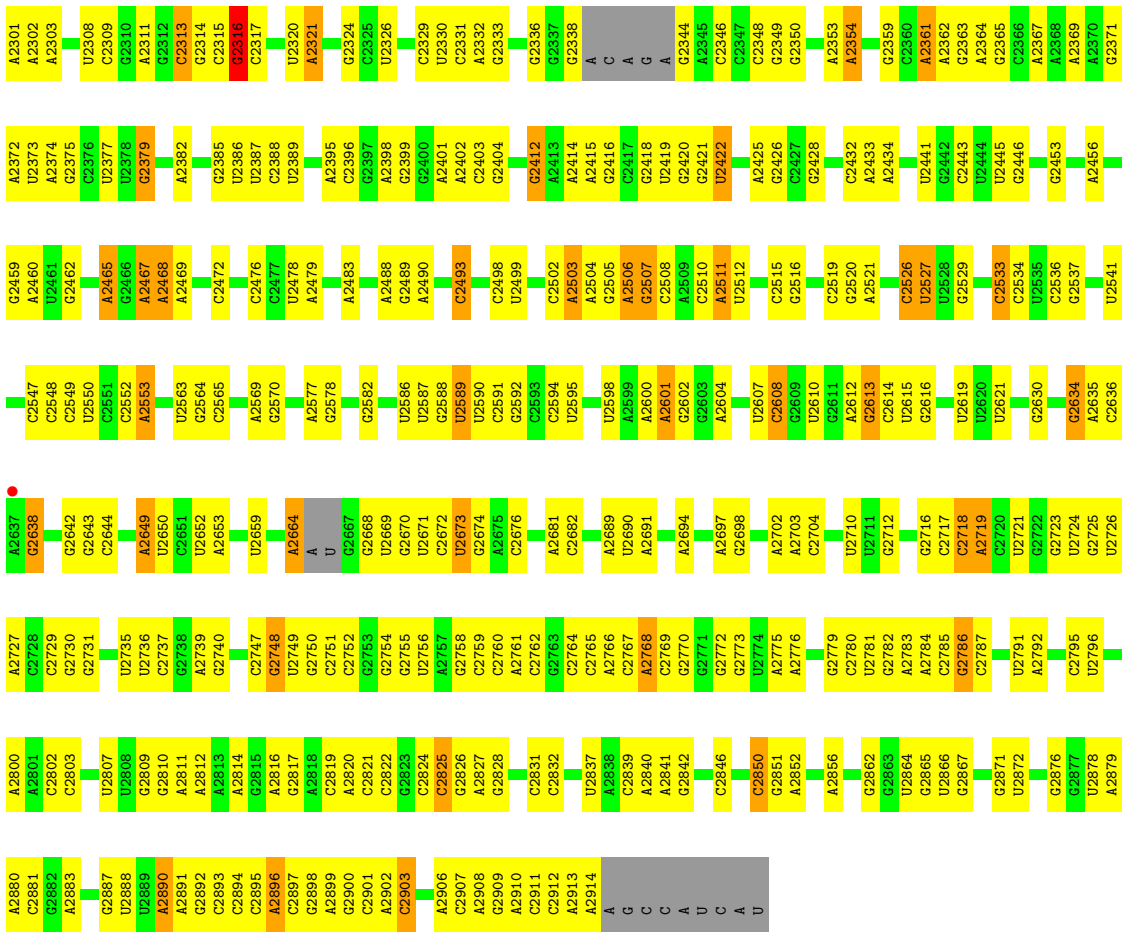
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

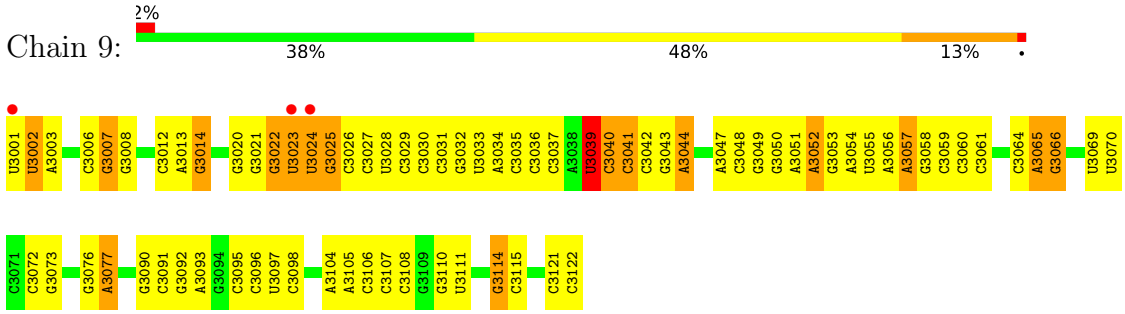



U A G C U C G U C G G U G A C A C U A C A C G G A G G G C A C A
C U A C C C G U G G G A C A C C C C C G G C
G A G A G G A C G G G C C A A C C A
C1069 A1070 G1071 G1072 G1076 G1077 A1078 A1079 C1080 A1081 A1082 C1083 C1084 G1087 A1088 A1098 G1099 C1104 U1109 C1110 A1114 U1115 U1116 A1117 A1118 G1119 A1123 C1127 U1128 C1129 U1130 G1131 A1132 G1137 G1138 A1150 G1151 A1154 G1155 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164
G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 G1224 C1225 G1226 C1229 G1230 A1231
A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 C1257 G1258 U1266 C1267 C1268 G1269 U1270 C1273 A1278 U1279 A1280 A1287 U1288 C1289 G1290 A1291 A1294 G1299 A1307 A1308 U1309 U1310 G1311 G1312 A1313 U1314 G1315 G1316 G1319 U1320 A1321
G1322 G1323 A1328 A1329 A1330 A1331 C1332 U1333 C1334 C1335 G1339 G1340 A1341 C1342 C1343 G1344 U1350 G1351 A1352 C1353 C1360 C1366 A1372 G1376 C1377 C1384 G1385 G1386 G1387 G1391 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399 C1400 G1401 A1406 A1407 U1408 G1409 G1410 A1413 A1414 G1415
U1419 C1420 C1421 U1422 C1423 A1424 A1434 U1435 C1436 C1439 U1440 G1441 A1442 G1443 G1444 G1445 U1446 U1447 A1448 G1449 C1450 C1451 G1452 G1453 U1454 C1455 C1456 U1457 A1458 C1474 C1477 A1482 C1483 G1484 A1485 A1486 A1487 U1488 G1489 A1492 A1493 A1494 G1495 G1496 G1497 U1500 U1503 A1504 U1505 U1506 G1523
U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1537 G1543 U1544 C1545 G1546 G1552 C1553 G1556 G1557 C1558 A1559 U U1561 C1562 G1563 C1564 C1565 C1566 A1567 G1568 U1569 A1573 C1574 C1575 G1576 U1577 C1578 C1579 A1580 U1583 G1586 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 U1599 G1600 G1601
C1602 A1603 G1604 G1605 C1609 G1610 A1615 A1616 C1617 G1618 G1619 C1620 G1621 G1622 C1623 A1624 U1625 A1626 G1627 A1630 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 U1654 G1655 A1656 A1657 A1658 A1661 C1662 G1663 C1666 A1667 U1668 A1669 G1670 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685
C1686 C1687 C1692 A1701 U1702 C1705 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 A1736 U1741 A1742 G1745 A1746 A1747 U1748 U1749 G1752 A1755 G1756 U1761 C1762 C1763 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 G1774 A1778 A1779 A1783 U1784
G1785 C1786 C1787 U1788 G1789 C1790 U1791 C1798 G1805 G1806 G1809 C1810 A1811 A1815 G1819 G1820 U1825 C1826 A1829 C1834 U1835 U1838 A1839 A1840 C1841 A1842 A1845 U1850 G1851 A1852 C1853 C1854 G1855 C1856 A1857 A1858 C1862 G1863 G1868 G1873 G1877 G1878 U1879 U1883
G1902 U1903 A1904 U1905 A1909 C1913 C1914 A1919 C1920 A1921 A1922 G1923 A1924 G1925 G1926 A1927 A1930 A1931 G1932 C1940 A1941 A1942 C1943 G1947 G1948 G1951 U A A C U A U U G A C C U U1964 C1965 U1966 G1970 G1971 U1972 A1973 G1979 U1985 C1993
U1996 G2000 G2001 C2002 U2003 U2004 G2005 C2006 A2007 U2008 G2009 A2010 A2011 U2012 G2013 G2014 A2015 U2016 U2017 C2026 U2027 U2032 G2033 U2034 C2035 C2036 A2039 G2044 C2047 C2048 C2049 G2050 A2054 A2055 C2061 A2062 U2063 U2064 C2065 G2070 C2071 G2072 G2073 A2074 G2075 U2076 C2077 U2078 G2079 G2080
A2081 G2082 A2083 C2087 C2088 A2089 G2090 G2091 G2092 A2096 A2100 A2101 G2102 A2103 C2104 C2105 C2106 G2110 G2111 A2112 G2113 C2114 U2115 U2116 G2121 C2122 G2128 U2133 G2134 A2135 G2136 A C G U G G C U C G C C G A U G U G A C C A G C C A G A G G U G C A A G C A
C U A C C C G U G G G U G A C A C U A C A C G G A G G G C A C A G2237 A2238 A C2239 U2240 C2241 U2242 C2243 A2244 C2247 G2251 A2252 G2253 G2254 A2255 G2256 G2257 A2258 G2263 A2264 U2265 A2266 G2267 C2268 C2269 G2270 G2271 G2272 C2273 A2274 G2275 G2284 A2291 C2296 U2297 A2300



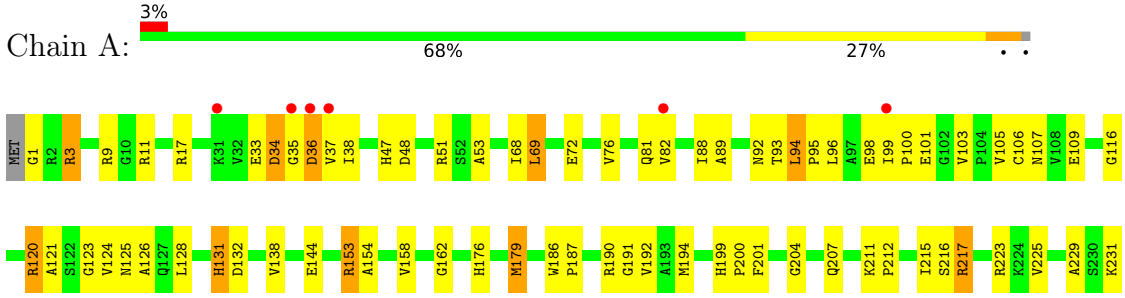
• Molecule 2: 5S ribosomal RNA

Chain 9:



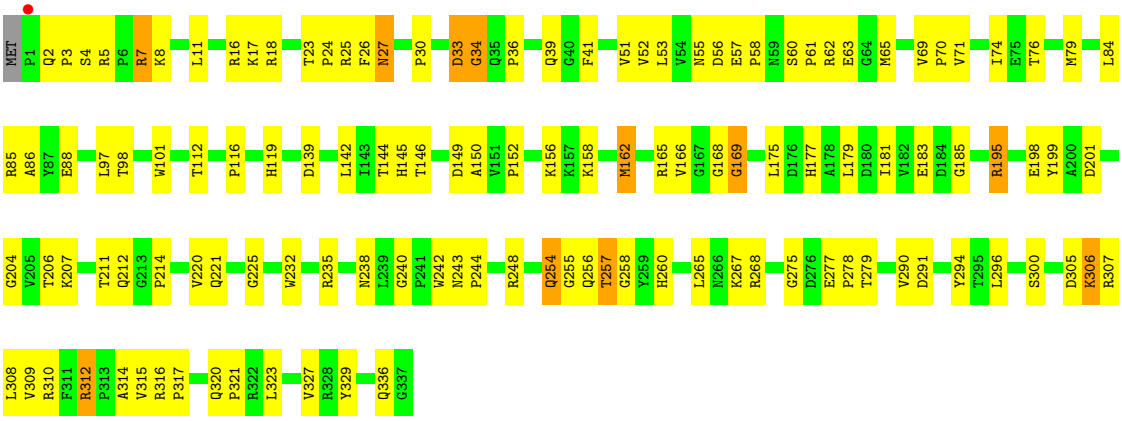
• Molecule 3: 50S ribosomal protein L2P

Chain A:



• Molecule 4: 50S ribosomal protein L3P

Chain B:

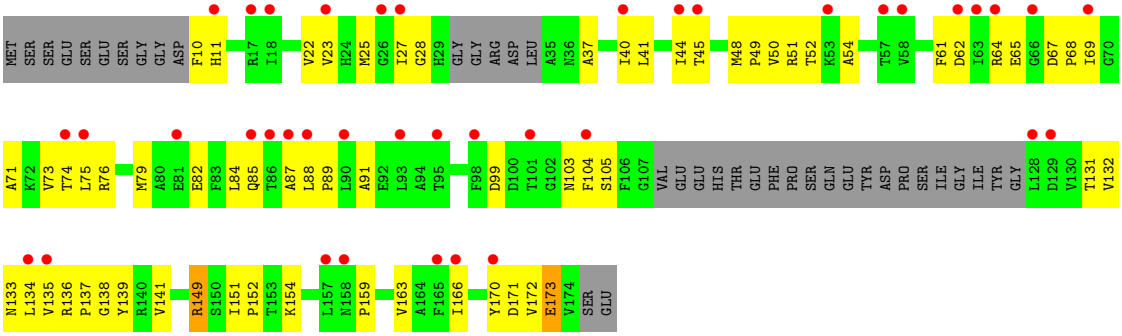


• Molecule 5: 50S ribosomal protein L4P

Chain C:

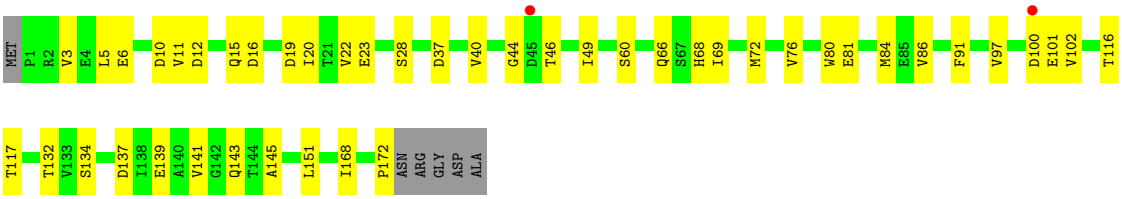
• Molecule 6: 50S ribosomal protein L5P

Chain D:



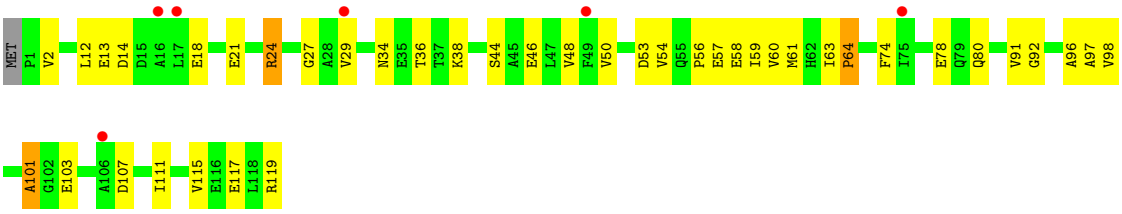
• Molecule 7: 50S ribosomal protein L6P

Chain E:



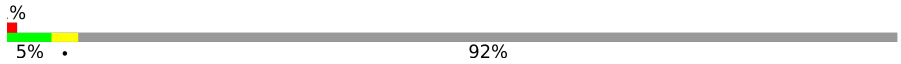
- Molecule 8: 50S ribosomal protein L7Ae

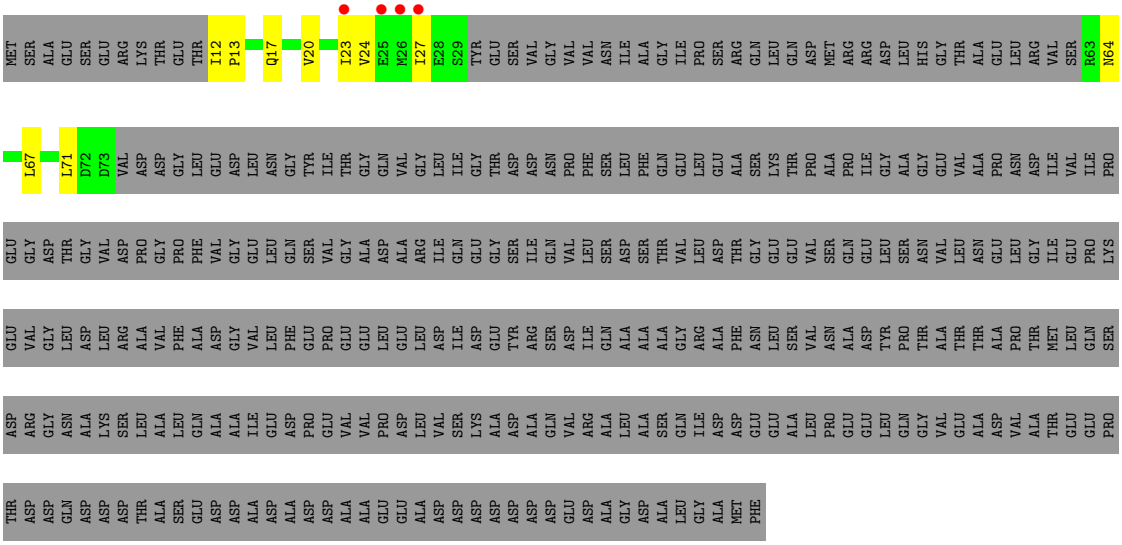
Chain F:



- Molecule 9: 50S ribosomal protein L10E

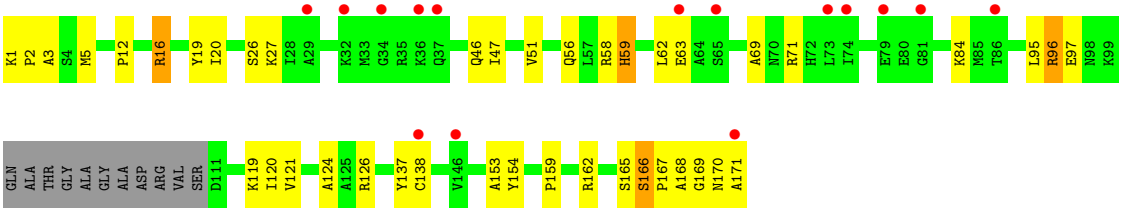
Chain G:





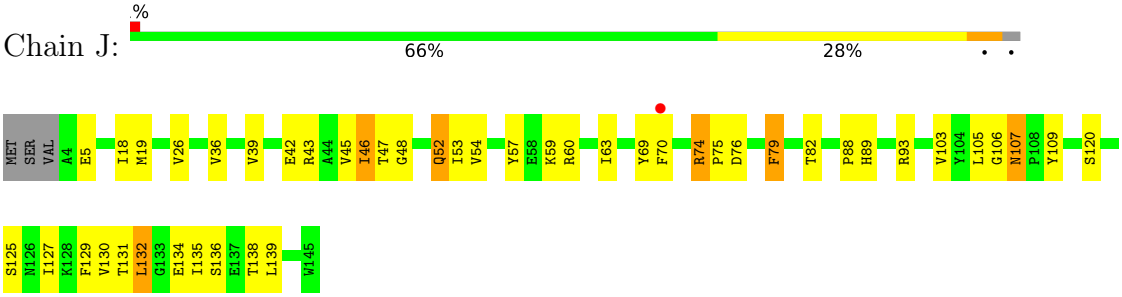
- Molecule 10: 50S ribosomal protein L10e

Chain H:



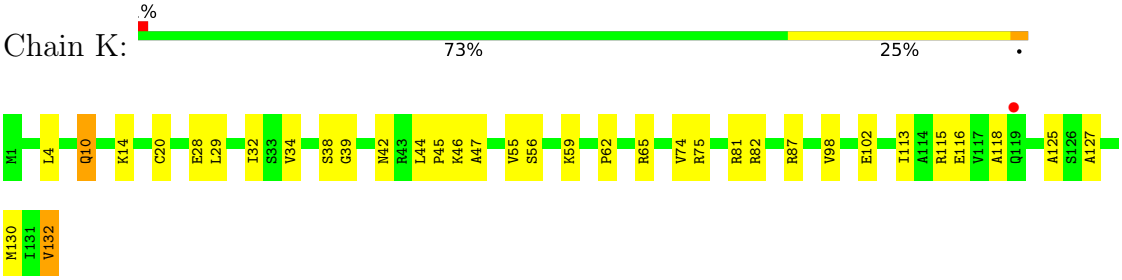
• Molecule 11: 50S ribosomal protein L13P

Chain J:



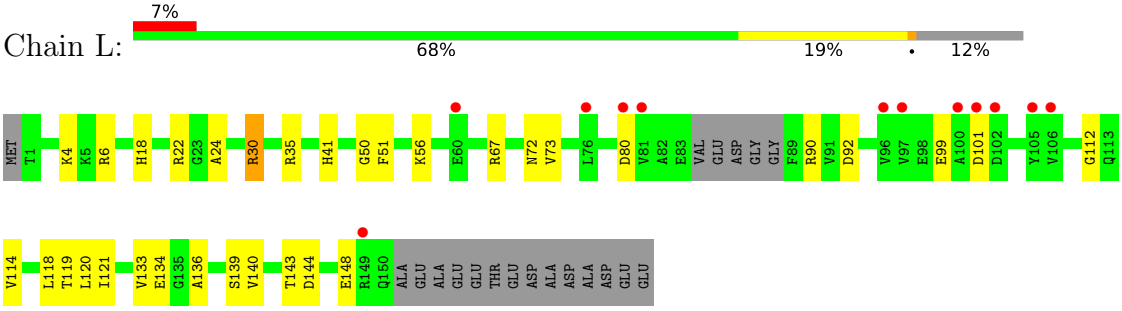
• Molecule 12: 50S ribosomal protein L14P

Chain K:



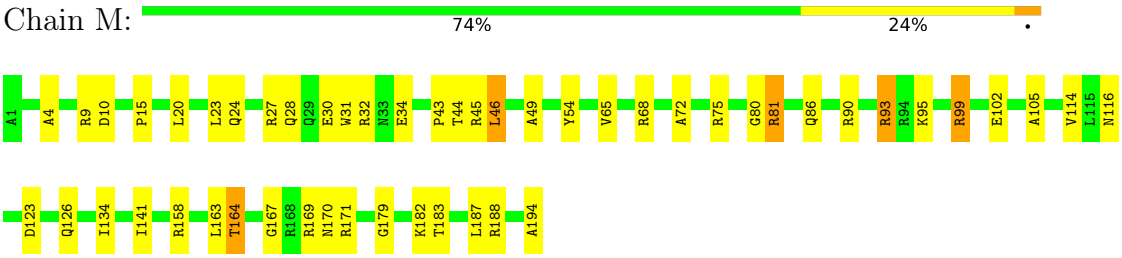
• Molecule 13: 50S ribosomal protein L15P

Chain L:



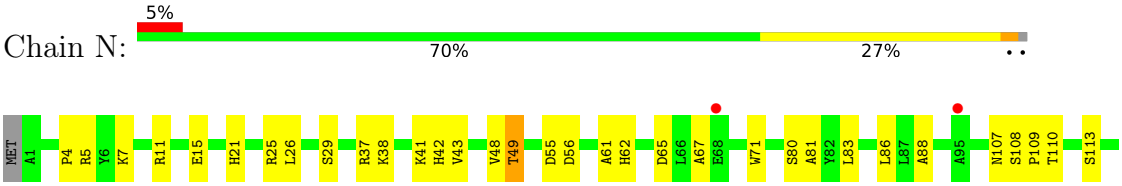
• Molecule 14: 50S ribosomal protein L15e

Chain M:



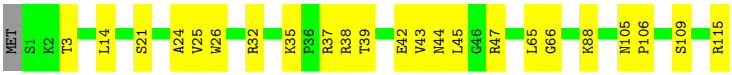
• Molecule 15: 50S ribosomal protein L18P

Chain N:



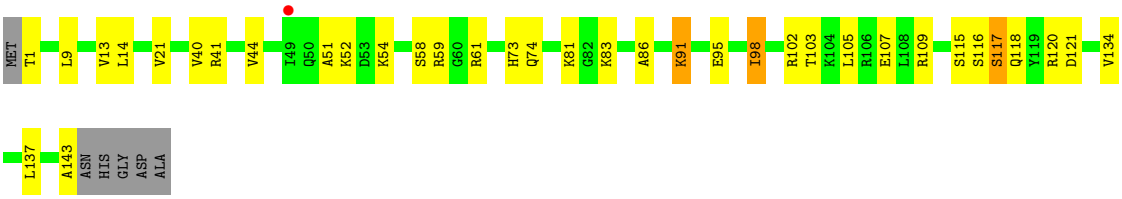
• Molecule 16: 50S ribosomal protein L18e

Chain O:



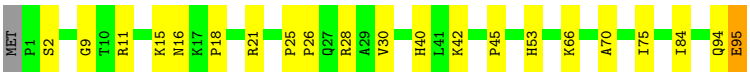
• Molecule 17: 50S ribosomal protein L19e

Chain P:



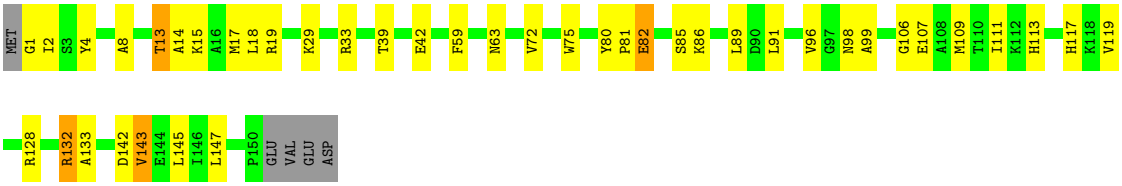
• Molecule 18: 50S ribosomal protein L21e

Chain Q:



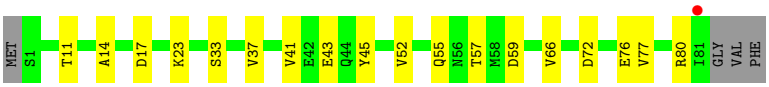
• Molecule 19: 50S ribosomal protein L22P

Chain R:



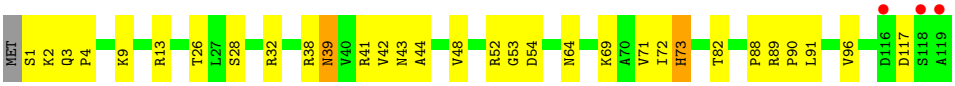
• Molecule 20: 50S ribosomal protein L23P

Chain S:



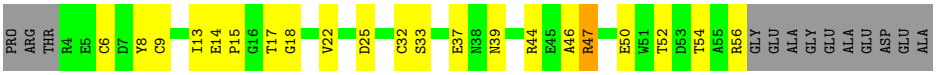
• Molecule 21: 50S ribosomal protein L24P

Chain T:



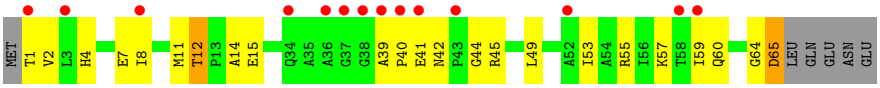
• Molecule 22: 50S ribosomal protein L24e

Chain U:



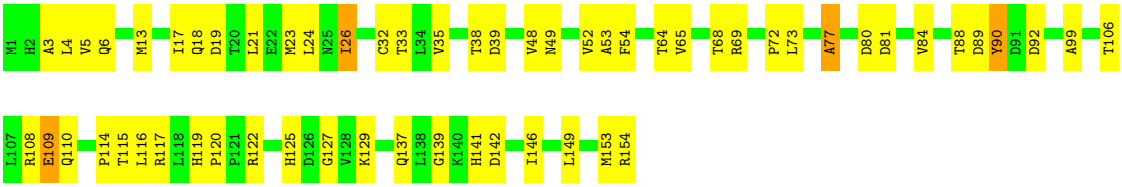
• Molecule 23: 50S ribosomal protein L29P

Chain V:



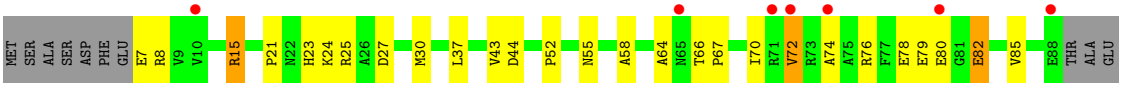
• Molecule 24: 50S ribosomal protein L30P

Chain W:



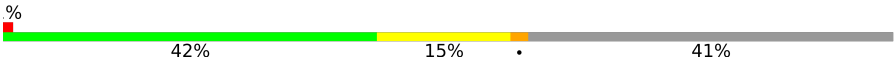
• Molecule 25: 50S ribosomal protein L31e

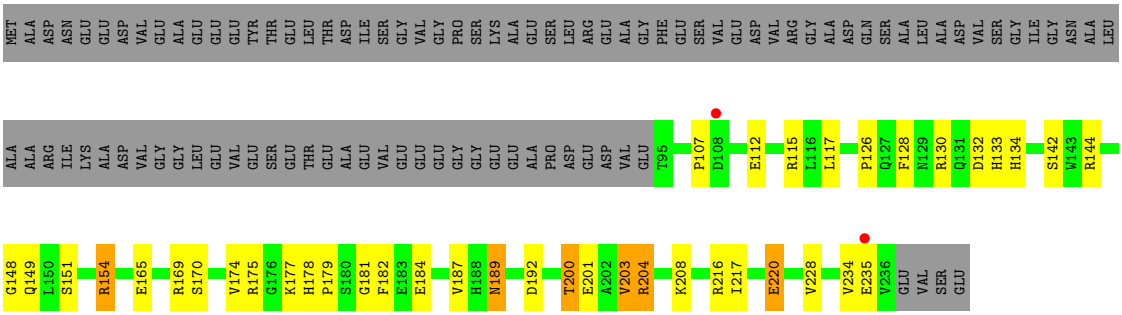
Chain X:



• Molecule 26: 50S ribosomal protein L32e

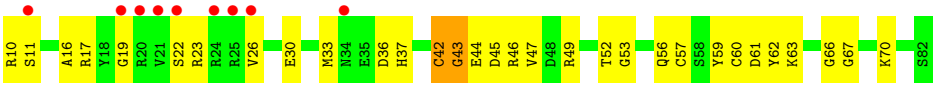
Chain Y:





• Molecule 27: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 28: 50S ribosomal protein L37e

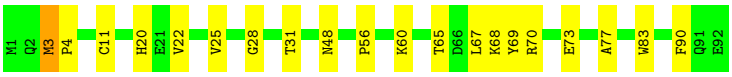
Chain 1:

- Molecule 29: 50S ribosomal protein L39e

Chain 2:

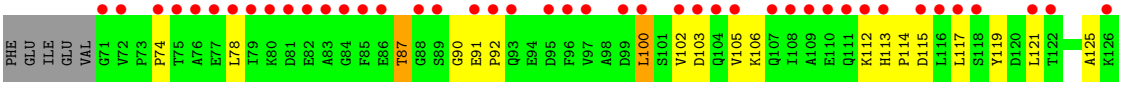
- Molecule 30: 50S ribosomal protein L44E

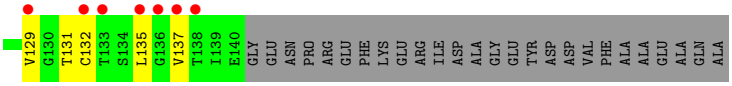
Chain 3:



- Molecule 31: 50S ribosomal protein L11P

Chain I:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.90 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.90) 91.7 (85.48-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.238 0.212 , 0.244	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	99043	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 1.50% 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: 1MA, CD, OMU, PSU, UR3, MG, 13T, NA, K, OMG, CL

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	0.39	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.69	1/4528 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.34	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.58	0/1498
7	E	0.34	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.33	0/241	0.49	0/324
10	H	0.38	0/1287	0.65	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.35	0/1130	0.64	0/1509
14	M	0.37	0/1584	0.63	0/2119
15	N	0.31	0/1474	0.65	1/1999 (0.1%)
16	O	0.36	0/874	0.61	1/1181 (0.1%)
17	P	0.35	0/1147	0.55	0/1528
18	Q	0.37	0/749	0.68	0/1005
19	R	0.36	0/1172	0.64	0/1578
20	S	0.35	0/648	0.59	0/875
21	T	0.34	0/958	0.63	0/1289
22	U	0.36	0/417	0.56	0/562
23	V	0.35	0/502	0.56	0/675
24	W	0.34	0/1219	0.63	0/1655
25	X	0.35	0/664	0.59	0/895
26	Y	0.36	0/1146	0.63	0/1536
27	Z	0.39	0/590	0.64	0/787
28	1	0.40	0/438	0.63	0/578
29	2	0.37	0/401	0.56	0/529
30	3	0.37	0/771	0.57	0/1024
31	I	0.35	0/526	0.57	0/716
All	All	0.38	0/98693	0.67	17/147577 (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	1	42
2	9	0	2
24	W	0	1
All	All	1	45

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.37	130.11	109.50
2	9	3039	U	N1-C1'-C2'	6.50	122.45	114.00
1	0	2316	G	C5'-C4'-C3'	-6.49	105.61	116.00
1	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
1	0	1942	A	C5'-C4'-C3'	6.20	125.92	116.00
15	N	163	PHE	N-CA-C	-5.68	95.66	111.00
16	O	66	GLY	N-CA-C	5.59	127.06	113.10
1	0	871	G	C5'-C4'-O4'	-5.54	102.45	109.10
1	0	1504	A	N9-C1'-C2'	5.52	121.17	114.00
1	0	1819	G	C5'-C4'-C3'	5.40	124.64	116.00
1	0	1829	A	N9-C1'-C2'	-5.39	106.07	112.00
1	0	2313	C	C5'-C4'-O4'	5.31	115.47	109.10
1	0	2291	A	N9-C1'-C2'	5.15	120.70	114.00
1	0	1559	A	C2'-C3'-O3'	5.15	121.94	113.70
1	0	2313	C	O4'-C4'-C3'	-5.07	98.93	104.00
1	0	1878	G	N9-C1'-C2'	-5.04	106.46	112.00
1	0	777	U	O4'-C1'-N1	5.03	112.23	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1131	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1309	U	Sidechain
1	0	131	A	Sidechain
1	0	1376	G	Sidechain
1	0	1445	G	Sidechain
1	0	1458	A	Sidechain
1	0	1635	U	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	1993	C	Sidechain
1	0	220	C	Sidechain
1	0	2308	U	Sidechain
1	0	2316	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	2552	C	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	391	U	Sidechain
1	0	396	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	722	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
2	9	3039	U	Sidechain
2	9	3090	G	Sidechain
24	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	1337	0
2	9	2600	0	1326	95	0
3	A	1753	0	1766	78	0
4	B	2625	0	2533	112	0
5	C	1859	0	1816	74	0
6	D	1094	0	1085	56	0
7	E	1357	0	1266	38	0
8	F	890	0	843	32	0
9	G	240	0	231	9	0
10	H	1266	0	1268	39	0
11	J	1120	0	1098	49	0
12	K	992	0	1031	40	0
13	L	1118	0	1076	28	0
14	M	1560	0	1568	45	0
15	N	1445	0	1401	45	0
16	O	865	0	873	21	0
17	P	1136	0	1123	33	0
18	Q	735	0	728	22	0
19	R	1149	0	1122	41	0
20	S	641	0	605	14	0
21	T	950	0	923	25	0
22	U	410	0	364	21	0
23	V	499	0	511	19	0
24	W	1196	0	1137	57	0
25	X	654	0	653	25	0
26	Y	1130	0	1133	46	0
27	Z	579	0	539	25	0
28	1	431	0	426	21	0
29	2	396	0	413	18	0
30	3	755	0	728	18	0
31	I	519	0	500	23	0
32	0	42	0	50	24	0
33	0	108	0	0	0	0
33	3	2	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	74	0	0	2	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	2	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	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	2	0	0	0	0
37	1	1	0	0	0	0
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	5905	0	0	199	0
38	1	56	0	0	1	0
38	2	45	0	0	4	0
38	3	66	0	0	2	0
38	9	140	0	0	10	0
38	A	112	0	0	8	0
38	B	142	0	0	21	0
38	C	170	0	0	16	0
38	D	45	0	0	8	0
38	E	42	0	0	5	0
38	F	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	G	19	0	0	0	0
38	H	70	0	0	6	0
38	I	8	0	0	1	0
38	J	58	0	0	3	0
38	K	59	0	0	1	0
38	L	83	0	0	10	0
38	M	123	0	0	4	0
38	N	63	0	0	6	0
38	O	44	0	0	3	0
38	P	56	0	0	2	0
38	Q	51	0	0	5	0
38	R	80	0	0	2	0
38	S	36	0	0	2	0
38	T	33	0	0	1	0
38	U	26	0	0	2	0
38	V	11	0	0	1	0
38	W	67	0	0	6	0
38	X	21	0	0	2	0
38	Y	96	0	0	6	0
38	Z	31	0	0	2	0
All	All	99043	0	59948	2276	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 15.

All (2276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:C8	1:0:871:G:H5'	1.77	1.19
1:0:1160:G:C5'	1:0:1161:A:H5'	1.73	1.18
1:0:1160:G:H5'	1:0:1161:A:C5'	1.79	1.12
1:0:871:G:H5'	1:0:871:G:H8	1.01	1.09
1:0:1002:G:H2'	1:0:1003:U:H5"	1.37	1.07
1:0:1474:C:H6	1:0:1474:C:H5'	1.16	1.06
2:9:3006:C:H5"	15:N:37:ARG:NH1	1.70	1.06
2:9:3056:A:H2'	2:9:3057:A:H5"	1.34	1.05
1:0:1242:A:H5'	11:J:82:THR:HG23	1.34	1.04
1:0:541:C:H2'	1:0:542:A:H5"	1.41	1.03
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.41	1.02
1:0:542:A:H5'	1:0:542:A:H8	1.25	1.01
1:0:1559:A:H1'	38:0:5876:HOH:O	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:C2'	1:0:2718:C:H5"	1.91	1.01
1:0:381:G:H5"	38:0:4329:HOH:O	1.61	1.00
1:0:1474:C:H5'	1:0:1474:C:C6	1.99	0.98
1:0:1701:A:H4'	1:0:1702:U:H5"	1.44	0.98
1:0:1666:C:O2'	1:0:1667:A:H5"	1.64	0.98
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.45	0.98
1:0:156:C:H5"	14:M:171:ARG:HD3	1.41	0.97
1:0:1118:A:H62	1:0:1244:U:H3	1.09	0.97
1:0:2717:C:H2'	1:0:2718:C:H5"	1.46	0.96
1:0:2460:A:H5'	32:0:9000:13T:C23	1.96	0.96
2:9:3092:G:H2'	2:9:3093:A:C8	2.01	0.96
2:9:3076:G:H3'	2:9:3077:A:H5"	1.43	0.95
5:C:236:THR:HG22	5:C:239:ALA:H	1.28	0.95
1:0:871:G:H8	1:0:871:G:C5'	1.80	0.95
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.49	0.94
1:0:1205:U:H2'	1:0:1206:U:H5"	1.50	0.94
1:0:2460:A:H5'	32:0:9000:13T:H233	1.46	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.34	0.93
29:2:41:HIS:H	29:2:45:ASN:HD22	1.16	0.93
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.49	0.93
1:0:289:G:H22	1:0:363:A:H2	0.97	0.93
1:0:1172:G:H5"	38:0:7252:HOH:O	1.69	0.93
1:0:877:G:H5'	1:0:878:G:OP1	1.69	0.93
1:0:282:C:H1'	1:0:368:C:N4	1.84	0.93
1:0:545:G:H5'	1:0:545:G:H8	1.34	0.92
1:0:1372:A:H3'	38:0:7182:HOH:O	1.69	0.92
1:0:2710:U:H1'	38:0:7605:HOH:O	1.68	0.92
12:K:10:GLN:HE21	12:K:10:GLN:H	0.93	0.92
1:0:2506:A:HO2'	1:0:2507:G:H8	0.93	0.92
1:0:506:G:H22	1:0:509:A:C5'	1.82	0.91
1:0:1118:A:C8	1:0:1118:A:H3'	2.05	0.91
1:0:1118:A:H3'	1:0:1118:A:H8	1.33	0.91
1:0:2812:A:H2	1:0:2814:A:H62	1.06	0.91
1:0:541:C:C2'	1:0:542:A:H5"	1.99	0.91
1:0:870:G:H2'	1:0:871:G:H5"	1.50	0.90
1:0:1184:C:H1'	38:0:7452:HOH:O	1.70	0.90
1:0:1603:A:H5'	1:0:1605:G:O4'	1.72	0.90
1:0:93:C:H5"	23:V:1:THR:HB	1.51	0.90
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.54	0.89
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.53	0.89
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2529:G:H3'	38:0:7177:HOH:O	1.70	0.89
1:0:289:G:N2	1:0:363:A:H2	1.70	0.89
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.55	0.88
1:0:317:A:H4'	38:0:3775:HOH:O	1.73	0.88
17:P:115:SER:H	17:P:118:GLN:HE21	1.20	0.88
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.56	0.88
1:0:1209:C:H2'	1:0:1210:G:H8	1.39	0.87
1:0:2508:C:H2'	38:0:6748:HOH:O	1.72	0.87
1:0:1165:G:H4'	1:0:1174:A:O2'	1.74	0.87
1:0:506:G:H22	1:0:509:A:H5"	1.37	0.87
2:9:3049:G:H5"	38:N:8842:HOH:O	1.73	0.87
1:0:1641:A:H2'	1:0:1642:A:H5'	1.55	0.86
1:0:1116:U:H3	1:0:1246:A:H62	1.21	0.86
1:0:2783:A:H3'	38:0:5234:HOH:O	1.75	0.84
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.84
1:0:1701:A:H5'	38:0:6285:HOH:O	1.77	0.84
12:K:10:GLN:HE21	12:K:10:GLN:N	1.76	0.84
1:0:2769:C:C2'	1:0:2770:G:H5'	2.08	0.84
12:K:10:GLN:H	12:K:10:GLN:NE2	1.76	0.84
1:0:182:G:H5'	38:0:5159:HOH:O	1.78	0.83
1:0:2291:A:C8	1:0:2309:C:H5'	2.13	0.83
1:0:21:G:H5'	19:R:2:ILE:HA	1.61	0.83
1:0:272:A:H3'	38:0:7515:HOH:O	1.79	0.83
1:0:272:A:H5'	1:0:273:G:OP2	1.79	0.83
15:N:113:SER:HB2	38:N:8855:HOH:O	1.78	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.76	0.83
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.25	0.83
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.61	0.83
1:0:282:C:O2'	1:0:283:U:H5'	1.79	0.83
2:9:3056:A:C2'	2:9:3057:A:H5"	2.09	0.83
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.59	0.82
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.42	0.82
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.61	0.82
1:0:559:U:H6	1:0:559:U:H5'	1.44	0.82
1:0:69:A:H5'	1:0:69:A:C8	2.14	0.82
1:0:797:A:H4'	27:Z:10:ARG:N	1.94	0.82
24:W:88:THR:HB	38:W:6679:HOH:O	1.79	0.82
1:0:1183:C:H2'	38:0:6249:HOH:O	1.79	0.81
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.62	0.81
1:0:1187:U:HO2'	1:0:1189:A:H2	1.26	0.81
38:0:5223:HOH:O	12:K:39:GLY:HA2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.23	0.81
1:0:236:A:H4'	1:0:237:G:H5'	1.63	0.81
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.62	0.81
1:0:2717:C:O2'	1:0:2718:C:H5"	1.80	0.81
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.62	0.80
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.29	0.80
1:0:515:C:H5"	38:0:5657:HOH:O	1.81	0.80
3:A:199:HIS:HD2	3:A:201:PHE:H	1.27	0.80
1:0:558:C:O2'	1:0:559:U:H5"	1.81	0.80
1:0:1160:G:H5'	1:0:1161:A:H5'	0.88	0.80
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.64	0.80
1:0:541:C:H2'	1:0:542:A:C5'	2.12	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.79
1:0:1835:U:H5	1:0:1840:A:N7	1.79	0.79
1:0:1206:U:H5'	1:0:1206:U:H6	1.47	0.79
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.63	0.79
1:0:292:G:H2'	1:0:358:G:N2	1.97	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.61	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.63	0.79
1:0:2716:G:H5"	4:B:206:THR:HG21	1.63	0.79
12:K:98:VAL:HG13	12:K:102:GLU:HA	1.64	0.79
1:0:1615:A:H5'	38:0:4195:HOH:O	1.83	0.79
1:0:2054:A:N3	19:R:128:ARG:NH2	2.30	0.79
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.18	0.79
1:0:1116:U:HO2'	1:0:1118:A:H2	0.83	0.79
1:0:1119:G:N2	1:0:1246:A:C2	2.51	0.79
1:0:1667:A:H5'	1:0:1667:A:C8	2.18	0.79
20:S:57:THR:HG22	20:S:59:ASP:H	1.48	0.79
27:Z:46:ARG:HD3	27:Z:59:TYR:HB2	1.64	0.79
1:0:1002:G:C2'	1:0:1003:U:H5"	2.13	0.78
1:0:1741:U:H5'	1:0:1742:A:OP1	1.83	0.78
1:0:1441:G:H1'	38:0:7748:HOH:O	1.82	0.78
32:0:9000:13T:H262	32:0:9000:13T:H2	1.65	0.78
1:0:514:G:H4'	38:0:5657:HOH:O	1.83	0.78
1:0:1919:A:H4'	38:0:4858:HOH:O	1.83	0.78
1:0:1878:G:H1'	38:0:6128:HOH:O	1.83	0.78
1:0:1666:C:C2'	1:0:1667:A:H5"	2.14	0.78
1:0:2908:A:H2'	1:0:2909:G:O4'	1.83	0.78
1:0:681:G:N3	1:0:681:G:H5'	1.99	0.77
1:0:871:G:C8	1:0:871:G:C5'	2.59	0.77
1:0:1474:C:H6	1:0:1474:C:C5'	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:G:C5'	19:R:2:ILE:HA	2.13	0.77
1:0:130:C:H2'	38:0:3162:HOH:O	1.84	0.77
1:0:2426:G:H1'	38:0:6098:HOH:O	1.85	0.77
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.66	0.77
1:0:1679:C:H5'	38:0:9320:HOH:O	1.85	0.77
1:0:542:A:H5'	1:0:542:A:C8	2.15	0.77
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.66	0.77
5:C:127:ARG:NH2	5:C:225:PRO:HG2	2.00	0.77
32:0:9000:13T:H21	32:0:9000:13T:C30	2.14	0.76
1:0:1205:U:H2'	1:0:1206:U:C5'	2.15	0.76
32:0:9000:13T:H262	32:0:9000:13T:C2	2.14	0.76
1:0:2769:C:H2'	1:0:2770:G:H5'	1.68	0.76
6:D:154:LYS:H	6:D:154:LYS:HD2	1.50	0.76
1:0:12:U:H2'	1:0:13:G:H5'	1.67	0.76
1:0:1603:A:H5"	1:0:1605:G:H5'	1.67	0.75
1:0:1058:A:H2'	1:0:1060:C:H5"	1.67	0.75
1:0:1701:A:H4'	1:0:1702:U:C5'	2.15	0.75
1:0:2851:G:O2'	1:0:2852:A:H5'	1.87	0.75
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.66	0.75
1:0:2502:C:C2'	1:0:2503:A:H5'	2.16	0.74
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.68	0.74
1:0:558:C:C2'	1:0:559:U:H5"	2.17	0.74
1:0:2010:A:H2'	38:0:5968:HOH:O	1.86	0.74
1:0:2570:G:H5"	38:0:4917:HOH:O	1.86	0.74
1:0:2766:A:H5'	38:B:8824:HOH:O	1.87	0.74
1:0:1205:U:C2'	1:0:1206:U:H5"	2.18	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.31	0.74
1:0:2005:G:H3'	1:0:2005:G:OP2	1.87	0.74
1:0:2768:A:O2'	1:0:2769:C:H5'	1.86	0.74
1:0:396:U:H1'	38:0:7612:HOH:O	1.88	0.74
1:0:899:C:H5'	38:0:3205:HOH:O	1.86	0.74
24:W:84:VAL:HG12	38:W:6679:HOH:O	1.88	0.74
1:0:949:U:H4'	18:Q:95:GLU:HA	1.68	0.74
1:0:69:A:H5'	1:0:69:A:H8	1.52	0.74
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.70	0.74
1:0:711:G:H1'	38:0:7092:HOH:O	1.87	0.73
1:0:797:A:C4'	27:Z:10:ARG:N	2.51	0.73
1:0:1926:G:H2'	1:0:1927:A:H8	1.53	0.73
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.73
2:9:3014:G:H5'	2:9:3014:G:H8	1.51	0.73
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2578:G:H5'	1:0:2578:G:H8	1.53	0.73
1:0:961:A:H4'	38:0:6766:HOH:O	1.89	0.73
1:0:2468:A:H61	30:3:48:ASN:HD21	1.35	0.73
3:A:35:GLY:O	3:A:36:ASP:HB3	1.87	0.73
1:0:2748:G:H1'	38:0:7883:HOH:O	1.87	0.73
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.71	0.73
3:A:51:ARG:HB2	38:A:8897:HOH:O	1.89	0.73
11:J:127:ILE:HG22	36:J:8801:CL:CL	2.25	0.73
22:U:14:GLU:O	22:U:17:THR:HB	1.88	0.73
1:0:288:A:H61	1:0:364:C:H42	1.36	0.73
1:0:544:G:H2'	1:0:545:G:H5"	1.70	0.72
5:C:233:THR:HG22	5:C:234:VAL:H	1.54	0.72
1:0:545:G:H5'	1:0:545:G:C8	2.22	0.72
1:0:587:A:H5"	38:0:7279:HOH:O	1.89	0.72
1:0:2781:U:C2'	1:0:2782:G:H5'	2.19	0.72
1:0:1926:G:H2'	1:0:1927:A:C8	2.24	0.72
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.07	0.72
1:0:2781:U:H2'	1:0:2782:G:H5'	1.70	0.72
1:0:1634:G:H3'	38:0:3901:HOH:O	1.89	0.72
1:0:870:G:C2'	1:0:871:G:H5"	2.17	0.72
1:0:1080:C:H4'	1:0:1081:A:OP1	1.89	0.72
1:0:1350:U:H4'	38:0:5124:HOH:O	1.88	0.72
1:0:1593:C:H5'	17:P:116:SER:O	1.89	0.71
1:0:2505:G:O2'	1:0:2506:A:H5'	1.89	0.71
1:0:2507:G:H2'	1:0:2510:C:H42	1.55	0.71
1:0:2243:C:H5"	38:0:3753:HOH:O	1.88	0.71
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.71	0.71
38:0:3759:HOH:O	21:T:9:LYS:HD3	1.88	0.71
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.55	0.71
1:0:1189:A:H1'	1:0:1209:C:C1'	2.19	0.71
1:0:1189:A:H1'	1:0:1209:C:O4'	1.91	0.71
1:0:2420:G:O2'	1:0:2421:G:H5'	1.90	0.71
1:0:2827:A:H2'	1:0:2828:G:O4'	1.90	0.71
1:0:2862:G:H4'	4:B:336:GLN:O	1.91	0.71
1:0:2878:U:H2'	1:0:2879:A:O4'	1.90	0.71
16:O:32:ARG:HE	16:O:35:LYS:HD2	1.56	0.71
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.73	0.71
2:9:3039:U:H3'	2:9:3040:C:H5"	1.73	0.71
1:0:156:C:H5"	14:M:171:ARG:CD	2.19	0.71
1:0:308:U:H5'	1:0:309:C:OP1	1.90	0.71
1:0:271:C:H41	1:0:378:A:H2	1.36	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:C5'	2.21	0.70
5:C:236:THR:HG22	5:C:239:ALA:N	2.04	0.70
13:L:133:VAL:HA	38:L:8872:HOH:O	1.90	0.70
1:0:1342:C:C2'	1:0:1343:C:H5'	2.20	0.70
1:0:2364:A:H5"	18:Q:15:LYS:HD3	1.73	0.70
19:R:81:PRO:O	19:R:85:SER:HB2	1.91	0.70
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.72	0.70
1:0:214:U:H5'	38:0:6147:HOH:O	1.91	0.70
1:0:2526:C:O2'	1:0:2527:U:H5'	1.91	0.70
1:0:544:G:C2'	1:0:545:G:H5"	2.22	0.70
8:F:58:GLU:HA	8:F:61:MET:HE2	1.74	0.70
3:A:191:GLY:HA2	3:A:194:MET:CE	2.22	0.69
1:0:962:C:H1'	15:N:5:ARG:NH1	2.07	0.69
17:P:115:SER:H	17:P:118:GLN:NE2	1.90	0.69
1:0:2748:G:H2'	38:0:7526:HOH:O	1.91	0.69
17:P:143:ALA:HA	38:P:5521:HOH:O	1.93	0.69
24:W:72:PRO:HG2	24:W:77:ALA:HB3	1.74	0.69
1:0:338:C:H4'	5:C:174:ILE:CD1	2.21	0.69
1:0:2748:G:H5'	38:0:7526:HOH:O	1.92	0.69
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.74	0.69
1:0:960:G:H4'	38:0:7420:HOH:O	1.92	0.69
1:0:1299:G:O6	13:L:6:ARG:HD3	1.92	0.69
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.74	0.69
24:W:80:ASP:O	24:W:84:VAL:HG23	1.92	0.69
1:0:559:U:H5'	1:0:559:U:C6	2.27	0.69
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.75	0.69
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.73	0.69
6:D:103:ASN:ND2	6:D:134:LEU:H	1.90	0.69
1:0:2004:U:H4'	38:0:5313:HOH:O	1.93	0.69
24:W:88:THR:HG22	24:W:89:ASP:H	1.58	0.69
1:0:558:C:H2'	1:0:559:U:C5'	2.23	0.69
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.08	0.69
4:B:238:ASN:HD22	4:B:240:GLY:H	1.41	0.69
1:0:560:C:H42	1:0:597:A:H61	1.39	0.68
1:0:1189:A:H3'	38:0:7666:HOH:O	1.93	0.68
1:0:1242:A:H5'	11:J:82:THR:CG2	2.18	0.68
1:0:657:G:OP1	5:C:27:ARG:NH2	2.26	0.68
32:0:9000:13T:H21	32:0:9000:13T:H301	1.74	0.68
1:0:821:U:H2'	1:0:822:C:H6	1.57	0.68
1:0:1641:A:C2'	1:0:1642:A:H5'	2.23	0.68
36:0:8813:CL:CL	38:0:4691:HOH:O	2.48	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3054:A:O2'	2:9:3055:U:H5'	1.94	0.68
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.94	0.68
10:H:166:SER:HB2	10:H:167:PRO:CD	2.21	0.68
1:0:1183:C:H42	1:0:1184:C:H41	1.42	0.68
1:0:2635:A:O2'	1:0:2636:C:H5'	1.94	0.68
3:A:199:HIS:CD2	3:A:201:PHE:H	2.10	0.68
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.75	0.68
1:0:1244:U:OP1	11:J:18:ILE:HD13	1.93	0.68
1:0:2459:G:H2'	32:0:9000:13T:C23	2.24	0.68
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.22	0.68
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.76	0.68
1:0:603:A:H5"	1:0:604:G:OP1	1.93	0.68
1:0:2812:A:C2	1:0:2814:A:N6	2.55	0.68
24:W:125:HIS:HD2	24:W:127:GLY:H	1.40	0.68
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.68
14:M:134:ILE:HG23	14:M:141:ILE:HD13	1.76	0.68
1:0:138:U:H5"	1:0:139:C:OP2	1.95	0.67
1:0:500:G:H21	19:R:98:ASN:HD21	1.41	0.67
1:0:2374:A:H2'	1:0:2375:G:C8	2.29	0.67
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.67
29:2:35:ARG:HB2	38:2:2691:HOH:O	1.95	0.67
1:0:1189:A:O2'	1:0:1208:C:H2'	1.95	0.67
1:0:1213:C:O2'	1:0:1214:G:H5'	1.94	0.67
1:0:506:G:H22	1:0:509:A:H5'	1.57	0.67
1:0:1118:A:N6	1:0:1244:U:H3	1.87	0.67
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.29	0.67
23:V:57:LYS:HA	23:V:60:GLN:HE21	1.60	0.67
1:0:706:G:HO2'	1:0:707:C:H6	1.43	0.67
1:0:2533:C:H5'	1:0:2533:C:C6	2.28	0.67
11:J:107:ASN:HD22	11:J:109:TYR:H	1.42	0.67
1:0:2717:C:OP1	4:B:207:LYS:HG3	1.95	0.67
11:J:76:ASP:HA	38:J:8868:HOH:O	1.94	0.67
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.77	0.67
1:0:1973:A:H5'	1:0:1973:A:H8	1.59	0.67
1:0:280:C:H2'	1:0:281:U:O4'	1.95	0.66
1:0:2563:U:H2'	1:0:2565:C:O5'	1.96	0.66
4:B:267:LYS:HD3	38:B:8824:HOH:O	1.95	0.66
1:0:2100:A:H5'	38:C:8662:HOH:O	1.93	0.66
1:0:2256:G:H2'	1:0:2257:G:C5'	2.25	0.66
1:0:485:A:N3	1:0:487:G:H5"	2.10	0.66
11:J:74:ARG:HB3	11:J:74:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:10:ARG:HA	38:Z:8715:HOH:O	1.96	0.66
1:0:284:C:H4'	1:0:285:A:O5'	1.96	0.66
1:0:2256:G:H2'	1:0:2257:G:H5'	1.78	0.66
1:0:2489:G:H1'	38:0:7268:HOH:O	1.95	0.66
5:C:1:MET:HG2	5:C:2:GLN:H	1.61	0.66
30:3:73:GLU:HB3	38:3:8854:HOH:O	1.94	0.66
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.24	0.66
1:0:1209:C:H2'	1:0:1210:G:C8	2.26	0.66
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.96	0.66
1:0:1524:U:OP1	1:0:1524:U:H4'	1.94	0.66
1:0:2506:A:O2'	1:0:2507:G:H8	1.72	0.66
1:0:2521:A:OP2	10:H:3:ALA:HB3	1.96	0.66
1:0:694:A:H2'	1:0:695:C:H5'	1.77	0.66
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.78	0.66
19:R:99:ALA:HB1	19:R:109:MET:CE	2.26	0.66
1:0:21:G:H5"	19:R:1:GLY:O	1.97	0.65
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.61	0.65
1:0:2638:G:H1'	38:0:7742:HOH:O	1.96	0.65
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.25	0.65
2:9:3029:C:C2'	2:9:3030:C:H5'	2.26	0.65
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.79	0.65
1:0:2460:A:C5'	32:0:9000:13T:H233	2.23	0.65
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.26	0.65
1:0:136:C:H2'	1:0:137:U:O4'	1.97	0.65
1:0:2890:A:H1'	22:U:56:ARG:NH2	2.11	0.65
4:B:179:LEU:O	4:B:183:GLU:HG2	1.95	0.65
5:C:140:VAL:HB	38:C:8651:HOH:O	1.94	0.65
1:0:1666:C:H2'	1:0:1667:A:C5'	2.26	0.65
1:0:447:A:O2'	1:0:448:G:H5'	1.97	0.65
1:0:558:C:H2'	1:0:559:U:H5'	1.79	0.65
1:0:2414:A:H2'	1:0:2415:A:C8	2.31	0.65
1:0:407:A:H8	38:0:4466:HOH:O	1.79	0.65
1:0:584:U:H3'	38:0:6101:HOH:O	1.96	0.65
1:0:1187:U:O2'	1:0:1189:A:H2	1.78	0.65
1:0:2795:C:O2'	1:0:2796:U:H5'	1.96	0.65
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.79	0.65
2:9:3003:A:N6	2:9:3022:G:H1'	2.12	0.65
1:0:1701:A:H5"	1:0:1702:U:H3'	1.77	0.65
1:0:2320:U:H4'	1:0:2321:A:O4'	1.97	0.64
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.62	0.64
10:H:169:GLY:HA3	38:H:8591:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:403:C:H3'	38:0:6307:HOH:O	1.97	0.64
1:0:1342:C:H2'	1:0:1343:C:H5'	1.79	0.64
1:0:2241:C:O2'	1:0:2242:U:H5'	1.96	0.64
1:0:2787:C:H5	38:0:4641:HOH:O	1.80	0.64
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.28	0.64
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.62	0.64
1:0:281:U:O2'	1:0:282:C:H5'	1.96	0.64
1:0:441:A:H1'	1:0:442:A:N7	2.13	0.64
1:0:2896:A:H5"	38:0:6105:HOH:O	1.97	0.64
6:D:99:ASP:HB3	6:D:103:ASN:H	1.62	0.64
1:0:958:G:H2'	1:0:959:C:C6	2.32	0.64
38:0:4678:HOH:O	4:B:300:SER:HB3	1.97	0.64
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.79	0.64
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.32	0.64
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.79	0.64
2:9:3091:C:H2'	2:9:3092:G:O4'	1.97	0.64
3:A:121:ALA:O	3:A:124:VAL:HG22	1.97	0.64
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.27	0.64
1:0:1185:U:H2'	1:0:1186:C:C6	2.33	0.64
1:0:2459:G:H2'	32:0:9000:13T:H233	1.80	0.64
1:0:2769:C:O2'	1:0:2770:G:H5'	1.96	0.64
1:0:1044:C:H5	38:0:6599:HOH:O	1.81	0.64
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.63	0.64
2:9:3039:U:H1'	2:9:3044:A:H61	1.63	0.64
23:V:42:ASN:HB3	38:V:7247:HOH:O	1.95	0.64
14:M:23:LEU:HD13	14:M:27:ARG:NH2	2.12	0.63
1:0:1200:A:H3'	38:0:5765:HOH:O	1.98	0.63
1:0:1790:C:H2'	1:0:1791:U:H6	1.63	0.63
1:0:2769:C:H2'	1:0:2770:G:C5'	2.27	0.63
2:9:3007:G:H5'	38:9:5071:HOH:O	1.98	0.63
10:H:46:GLN:HE21	10:H:137:TYR:HE2	1.45	0.63
5:C:236:THR:HG21	38:C:8571:HOH:O	1.98	0.63
13:L:114:VAL:HG11	38:L:8872:HOH:O	1.99	0.63
1:0:157:G:H4'	14:M:95:LYS:HE2	1.79	0.63
1:0:1165:G:H1'	1:0:1174:A:H1'	1.79	0.63
1:0:1189:A:H1'	1:0:1209:C:H1'	1.79	0.63
4:B:36:PRO:HG3	4:B:169:GLY:H	1.62	0.63
10:H:166:SER:CB	10:H:167:PRO:HD3	2.27	0.63
16:O:47:ARG:HH11	16:O:47:ARG:HG3	1.63	0.63
18:Q:26:PRO:O	18:Q:30:VAL:HG23	1.98	0.63
1:0:1185:U:H5'	38:0:7452:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1211:G:H2'	1:0:1212:C:H6	1.63	0.63
1:0:1596:U:H2'	1:0:1598:A:OP2	1.99	0.63
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.81	0.63
1:0:447:A:P	21:T:1:SER:HB2	2.39	0.63
13:L:148:GLU:HB2	38:L:8889:HOH:O	1.99	0.63
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.38	0.63
1:0:20:G:H21	19:R:117:HIS:HD2	1.47	0.63
4:B:71:VAL:HG21	4:B:296:LEU:HB3	1.81	0.63
1:0:289:G:O2'	1:0:290:C:H5'	1.99	0.63
1:0:567:U:H5"	38:0:6400:HOH:O	1.98	0.62
1:0:1164:U:H3	1:0:1192:A:H2	1.46	0.62
1:0:1666:C:C2'	1:0:1667:A:C5'	2.77	0.62
1:0:1878:G:O2'	1:0:1879:U:C6	2.49	0.62
1:0:1313:A:H5'	26:Y:208:LYS:O	1.99	0.62
2:9:3092:G:H2'	2:9:3093:A:H8	1.58	0.62
1:0:951:A:C2'	1:0:952:G:H5'	2.29	0.62
1:0:1307:A:H2'	1:0:1308:A:C8	2.34	0.62
1:0:1666:C:H2'	1:0:1667:A:H5'	1.81	0.62
5:C:67:GLN:HG2	38:C:8624:HOH:O	2.00	0.62
18:Q:25:PRO:HB2	38:Q:4350:HOH:O	1.99	0.62
1:0:396:U:O2'	1:0:418:C:H4'	1.99	0.62
1:0:1537:C:H1'	38:0:6583:HOH:O	1.98	0.62
2:9:3036:C:C5	2:9:3037:C:C5	2.88	0.62
1:0:292:G:H2'	1:0:358:G:H22	1.65	0.62
1:0:1377:C:H5'	1:0:1377:C:H6	1.64	0.62
1:0:1667:A:H2'	1:0:1668:U:C6	2.34	0.62
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.80	0.62
15:N:80:SER:HB2	38:N:8832:HOH:O	1.99	0.62
1:0:960:G:N3	1:0:960:G:H2'	2.13	0.62
1:0:1625:U:H4'	38:0:4674:HOH:O	2.00	0.62
25:X:43:VAL:HG12	25:X:44:ASP:N	2.15	0.62
1:0:1441:G:O2'	1:0:1442:A:H5'	2.00	0.62
1:0:1636:G:O2'	1:0:1637:A:H5'	1.99	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.29	0.62
14:M:99:ARG:HH21	14:M:170:ASN:HD22	1.48	0.62
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.82	0.62
1:0:558:C:C2'	1:0:559:U:C5'	2.78	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.82	0.61
23:V:39:ALA:N	23:V:40:PRO:HD2	2.14	0.61
1:0:656:G:H5'	16:O:3:THR:HB	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:8580:NA:NA	38:L:8826:HOH:O	1.71	0.61
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.82	0.61
1:0:597:A:H2'	1:0:598:C:H6	1.65	0.61
35:0:8542:NA:NA	38:0:5663:HOH:O	1.71	0.61
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.80	0.61
23:V:55:ARG:O	23:V:59:ILE:HG12	1.99	0.61
1:0:308:U:C4	1:0:342:C:H1'	2.35	0.61
1:0:470:U:O2'	28:1:16:HIS:HD2	1.82	0.61
1:0:1406:A:H4'	1:0:1407:A:H5"	1.81	0.61
1:0:1528:A:H2'	1:0:1529:G:O4'	2.00	0.61
1:0:1603:A:C5'	1:0:1605:G:H5'	2.30	0.61
1:0:2445:U:H2'	1:0:2446:G:C8	2.36	0.61
1:0:2511:A:H2'	1:0:2512:U:O4'	2.00	0.61
23:V:1:THR:HG23	23:V:2:VAL:H	1.65	0.61
1:0:538:C:OP2	26:Y:134:HIS:HE1	1.84	0.61
1:0:1234:U:N3	4:B:244:PRO:HB3	2.15	0.61
1:0:2338:G:H1'	6:D:105:SER:OG	1.99	0.61
38:0:7359:HOH:O	12:K:45:PRO:HB2	2.01	0.61
12:K:81:ARG:HD3	12:K:87:ARG:NH2	2.15	0.61
18:Q:21:ARG:HA	38:Q:6597:HOH:O	2.00	0.61
1:0:128:A:O2'	1:0:129:A:H5'	2.01	0.61
2:9:3041:C:O4'	6:D:50:VAL:HG22	2.00	0.61
24:W:13:MET:HE1	24:W:18:GLN:HA	1.82	0.61
1:0:1477:C:H5'	1:0:1868:G:C5'	2.30	0.61
2:9:3064:C:H2'	2:9:3065:A:H5'	1.83	0.61
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.82	0.61
1:0:281:U:H2'	1:0:282:C:O4'	2.01	0.61
1:0:2507:G:H2'	1:0:2510:C:N4	2.16	0.61
2:9:3064:C:C2'	2:9:3065:A:H5'	2.31	0.61
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.82	0.61
24:W:137:GLN:NE2	24:W:141:HIS:HE1	1.98	0.61
1:0:1762:C:H2'	1:0:1763:C:H6	1.65	0.61
1:0:2433:A:H2'	1:0:2434:A:C8	2.36	0.61
10:H:27:LYS:H	10:H:59:HIS:CD2	2.19	0.61
1:0:656:G:OP2	16:O:37:ARG:HD2	2.00	0.60
1:0:2134:G:N2	1:0:2242:U:C2	2.69	0.60
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.81	0.60
1:0:517:U:H1'	38:0:7561:HOH:O	2.00	0.60
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.60
2:9:3006:C:H5"	15:N:37:ARG:HH12	1.62	0.60
1:0:338:C:H4'	5:C:174:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:11:THR:H	20:S:14:ALA:HB3	1.65	0.60
1:0:90:A:H2'	1:0:91:G:O4'	2.01	0.60
1:0:669:G:O2'	1:0:670:G:H5'	2.01	0.60
1:0:2659:U:H5"	38:0:4135:HOH:O	2.00	0.60
32:0:9000:13T:H262	32:0:9000:13T:O3	2.01	0.60
29:2:20:ARG:HG2	29:2:21:VAL:H	1.66	0.60
30:3:65:THR:HG23	30:3:67:LEU:HG	1.84	0.60
1:0:255:A:H2'	1:0:256:C:C6	2.36	0.60
1:0:1118:A:C8	1:0:1118:A:C3'	2.70	0.60
27:Z:11:SER:HB3	27:Z:23:ARG:HB2	1.83	0.60
1:0:510:U:H6	38:0:7427:HOH:O	1.85	0.60
1:0:602:A:O2'	1:0:605:C:H4'	2.01	0.60
1:0:1819:G:H2'	1:0:1820:G:H4'	1.83	0.60
1:0:512:G:O3'	1:0:513:A:H8	1.85	0.60
1:0:2359:G:H3'	38:0:5701:HOH:O	2.01	0.60
14:M:187:LEU:CD2	14:M:194:ALA:HB3	2.32	0.60
3:A:48:ASP:HB3	38:A:8897:HOH:O	2.02	0.60
1:0:255:A:H2'	1:0:256:C:H6	1.66	0.59
1:0:2301:A:H5"	1:0:2302:A:H5'	1.84	0.59
4:B:214:PRO:HD2	38:B:8820:HOH:O	2.02	0.59
6:D:65:GLU:HA	38:D:4069:HOH:O	2.02	0.59
6:D:103:ASN:ND2	6:D:133:ASN:HA	2.17	0.59
27:Z:22:SER:O	27:Z:26:VAL:HG23	2.01	0.59
1:0:450:C:OP1	5:C:184:ARG:NH2	2.34	0.59
1:0:1202:A:H2'	1:0:1203:G:H5'	1.85	0.59
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.66	0.59
1:0:1525:G:H5'	1:0:1526:A:OP2	2.02	0.59
6:D:50:VAL:O	6:D:71:ALA:HA	2.02	0.59
1:0:1741:U:O2'	1:0:2723:G:H4'	2.02	0.59
32:0:9000:13T:H3	30:3:56:PRO:HB2	1.83	0.59
2:9:3039:U:H3'	2:9:3040:C:C5'	2.32	0.59
4:B:86:ALA:HA	38:B:8876:HOH:O	2.01	0.59
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.83	0.59
14:M:114:VAL:HG23	36:M:8818:CL:CL	2.39	0.59
19:R:111:ILE:HG23	19:R:145:LEU:HD11	1.83	0.59
27:Z:42:CYS:SG	27:Z:43:GLY:N	2.75	0.59
1:0:1504:A:H5'	38:0:4423:HOH:O	2.02	0.59
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.33	0.59
1:0:966:U:H5'	38:0:3861:HOH:O	2.01	0.59
1:0:1060:C:H6	1:0:1060:C:H5'	1.65	0.59
1:0:2807:U:P	4:B:27:ASN:HD21	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:45:VAL:HG21	11:J:129:PHE:CD1	2.38	0.59
1:0:249:G:O2'	1:0:250:C:H5'	2.03	0.59
1:0:1163:G:H2'	1:0:1164:U:C5	2.37	0.59
23:V:12:THR:HG23	23:V:14:ALA:H	1.68	0.59
1:0:1167:G:O2'	1:0:1168:C:H5'	2.02	0.59
1:0:1183:C:N3	1:0:1184:C:C5	2.71	0.59
1:0:1736:A:H1'	38:0:7569:HOH:O	2.03	0.59
7:E:100:ASP:HB2	38:E:2789:HOH:O	2.02	0.59
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.85	0.59
23:V:49:LEU:O	23:V:53:ILE:HG13	2.01	0.59
1:0:39:G:N2	1:0:444:C:C2	2.71	0.59
1:0:84:G:O2'	1:0:85:C:H5'	2.02	0.59
1:0:2781:U:H2'	1:0:2782:G:C5'	2.31	0.59
38:0:9354:HOH:O	28:1:1:THR:HA	2.03	0.59
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.67	0.59
14:M:30:GLU:O	14:M:34:GLU:HG3	2.02	0.59
1:0:121:U:OP2	29:2:10:ARG:NH2	2.35	0.59
1:0:947:U:H2'	1:0:948:G:C8	2.38	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
27:Z:44:GLU:HG2	27:Z:46:ARG:HD2	1.85	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.34	0.59
35:0:8542:NA:NA	38:0:3317:HOH:O	1.75	0.59
1:0:364:C:H2'	1:0:365:G:O4'	2.03	0.58
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.84	0.58
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.85	0.58
1:0:1014:A:H2'	1:0:1015:C:H5'	1.85	0.58
1:0:1015:C:H2'	1:0:1016:U:H6	1.67	0.58
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.66	0.58
11:J:107:ASN:ND2	11:J:109:TYR:H	2.01	0.58
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.85	0.58
31:I:132:CYS:HB3	31:I:137:VAL:HB	1.83	0.58
1:0:1202:A:C2'	1:0:1203:G:H5'	2.33	0.58
1:0:2252:A:C5	1:0:2253:G:H1'	2.36	0.58
5:C:139:VAL:HG13	38:C:8648:HOH:O	2.02	0.58
25:X:43:VAL:HG12	25:X:44:ASP:H	1.69	0.58
19:R:14:ALA:HB3	19:R:147:LEU:HB2	1.86	0.58
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.58
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.84	0.58
5:C:180:SER:HB2	38:C:8645:HOH:O	2.02	0.58
2:9:3035:C:H5"	38:9:4078:HOH:O	2.03	0.58
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:42:GLU:HB2	38:O:2176:HOH:O	2.04	0.58
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.32	0.58
1:0:42:C:H3'	38:0:4179:HOH:O	2.03	0.58
1:0:87:C:H2'	29:2:28:LYS:O	2.04	0.58
1:0:1168:C:H4'	38:I:5128:HOH:O	2.04	0.58
1:0:2816:A:H5"	1:0:2817:G:H5'	1.86	0.58
13:L:136:ALA:HB3	38:L:8872:HOH:O	2.03	0.58
4:B:25:ARG:HA	4:B:310:ARG:HH21	1.68	0.58
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.31	0.58
13:L:143:THR:HG22	13:L:144:ASP:N	2.18	0.58
1:0:282:C:H1'	1:0:368:C:H42	1.69	0.58
1:0:661:G:C5	1:0:686:A:C2	2.92	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.58
1:0:2703:A:H2'	1:0:2704:C:H6	1.67	0.58
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.86	0.58
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.84	0.58
11:J:103:VAL:HG12	38:J:8868:HOH:O	2.03	0.58
15:N:144:GLY:O	15:N:147:ILE:HG22	2.02	0.58
1:0:875:A:C2	3:A:194:MET:SD	2.97	0.57
1:0:2613:G:O2'	1:0:2614:C:H5'	2.04	0.57
2:9:3057:A:H8	6:D:141:VAL:HG21	1.69	0.57
8:F:53:ASP:OD1	8:F:80:GLN:HB2	2.05	0.57
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.44	0.57
1:0:1183:C:H2'	1:0:1183:C:O2	2.03	0.57
7:E:68:HIS:O	7:E:72:MET:HG3	2.04	0.57
10:H:63:GLU:HA	38:H:8582:HOH:O	2.03	0.57
1:0:2498:C:O2'	1:0:2499:U:H5'	2.04	0.57
38:0:7344:HOH:O	26:Y:149:GLN:HG3	2.02	0.57
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.70	0.57
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.68	0.57
11:J:131:THR:HB	11:J:134:GLU:HG3	1.85	0.57
1:0:877:G:C5'	1:0:878:G:OP1	2.49	0.57
1:0:2478:U:O2'	1:0:2479:A:H5'	2.04	0.57
4:B:258:GLY:H	4:B:260:HIS:CE1	2.21	0.57
1:0:1202:A:H2'	1:0:1203:G:C5'	2.34	0.57
1:0:1226:G:H5'	38:0:4537:HOH:O	2.05	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.57
1:0:1972:U:H2'	1:0:1973:A:C5'	2.35	0.57
1:0:2256:G:O2'	1:0:2257:G:H5'	2.04	0.57
2:9:3072:C:O2'	2:9:3073:G:H5'	2.05	0.57
14:M:24:GLN:NE2	14:M:27:ARG:HH11	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:31:C:H2'	38:0:7673:HOH:O	2.03	0.57
1:0:92:G:H4'	23:V:44:GLY:HA3	1.87	0.57
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.05	0.57
30:3:70:ARG:HG2	30:3:77:ALA:HB2	1.85	0.57
1:0:671:A:O2'	1:0:672:G:H2'	2.05	0.57
23:V:64:GLY:O	23:V:65:ASP:HB2	2.03	0.57
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.85	0.57
1:0:1028:U:H1'	38:0:3649:HOH:O	2.04	0.57
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.70	0.57
2:9:3095:C:O2'	2:9:3096:C:H5'	2.05	0.57
4:B:254:GLN:HG2	4:B:255:GLY:N	2.19	0.57
1:0:88:G:H8	1:0:88:G:H5'	1.70	0.57
1:0:1015:C:H2'	1:0:1016:U:C6	2.40	0.57
1:0:1118:A:H8	1:0:1119:G:H5"	1.69	0.57
1:0:1291:A:H2	38:0:5297:HOH:O	1.86	0.57
1:0:1393:A:H2'	1:0:1394:C:C6	2.40	0.57
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.39	0.57
2:9:3091:C:H1'	38:9:7454:HOH:O	2.04	0.57
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.03	0.57
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.40	0.57
1:0:2781:U:O2'	1:0:2782:G:H5'	2.05	0.57
4:B:152:PRO:HA	38:B:8866:HOH:O	2.04	0.57
10:H:138:CYS:HB2	38:H:8544:HOH:O	2.03	0.57
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
1:0:1193:A:C2	1:0:1194:A:N6	2.73	0.56
1:0:2291:A:N9	1:0:2309:C:H5'	2.20	0.56
2:9:3052:A:H2'	2:9:3053:G:O4'	2.05	0.56
1:0:564:G:H1'	38:0:6311:HOH:O	2.03	0.56
2:9:3057:A:C8	6:D:141:VAL:HG21	2.40	0.56
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.87	0.56
4:B:225:GLY:HA3	38:B:8863:HOH:O	2.05	0.56
10:H:26:SER:HA	10:H:59:HIS:HD2	1.70	0.56
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.56
1:0:2385:G:H2'	1:0:2386:U:C6	2.40	0.56
1:0:2445:U:H2'	1:0:2446:G:H8	1.69	0.56
1:0:2604:A:H5'	38:0:5801:HOH:O	2.05	0.56
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.56
2:9:3044:A:O4'	6:D:76:ARG:NE	2.38	0.56
3:A:99:ILE:O	3:A:131:HIS:HE1	1.87	0.56
21:T:64:ASN:HB3	21:T:73:HIS:HB2	1.88	0.56
24:W:139:GLY:O	24:W:141:HIS:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:187:VAL:HG23	26:Y:192:ASP:HB3	1.86	0.56
1:0:941:G:O2'	1:0:942:U:H5'	2.04	0.56
15:N:147:ILE:HB	38:N:8842:HOH:O	2.04	0.56
1:0:1154:A:H2'	1:0:1155:G:C8	2.40	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.06	0.56
4:B:254:GLN:HG3	38:B:8828:HOH:O	2.06	0.56
8:F:91:VAL:HG12	8:F:92:GLY:N	2.20	0.56
20:S:43:GLU:HB3	38:S:8546:HOH:O	2.04	0.56
1:0:776:A:OP1	28:1:28:HIS:HE1	1.87	0.56
1:0:870:G:OP2	3:A:3:ARG:HD3	2.06	0.56
1:0:1717:A:H5"	17:P:54:LYS:HB2	1.88	0.56
38:0:5467:HOH:O	9:G:12:ILE:HA	2.05	0.56
1:0:111:C:O2'	28:1:20:ARG:HG2	2.06	0.56
1:0:380:A:OP2	14:M:9:ARG:HD2	2.06	0.56
1:0:821:U:H5"	38:0:3050:HOH:O	2.05	0.56
1:0:1181:A:C2	1:0:1192:A:C8	2.94	0.56
1:0:1329:A:H2	38:0:4691:HOH:O	1.89	0.56
1:0:2064:U:H5'	1:0:2652:U:O3'	2.06	0.56
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.88	0.56
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.31	0.56
16:O:32:ARG:O	16:O:32:ARG:HD3	2.05	0.56
24:W:88:THR:HG23	24:W:110:GLN:NE2	2.21	0.56
25:X:43:VAL:HG11	25:X:82:GLU:HA	1.86	0.56
1:0:573:A:O2'	1:0:574:C:H5'	2.06	0.56
1:0:1167:G:H4'	31:I:135:LEU:HD22	1.88	0.56
1:0:1527:A:H1'	1:0:1528:A:C8	2.41	0.56
1:0:2403:C:H2'	1:0:2404:G:O5'	2.06	0.56
22:U:47:ARG:HG2	38:U:4381:HOH:O	2.05	0.56
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.71	0.56
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.54	0.56
1:0:1167:G:H2'	1:0:1168:C:O4'	2.06	0.56
1:0:2255:A:N1	1:0:2256:G:C4	2.74	0.56
5:C:114:ALA:HB1	5:C:223:LEU:HB3	1.88	0.56
21:T:71:VAL:HG11	21:T:90:PRO:CB	2.33	0.56
1:0:21:G:H4'	19:R:2:ILE:HG22	1.88	0.56
1:0:1172:G:H1'	38:0:4978:HOH:O	2.05	0.56
38:0:9539:HOH:O	17:P:81:LYS:HG2	2.05	0.56
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.58	0.56
10:H:20:ILE:HG23	10:H:120:ILE:HD11	1.87	0.56
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.88	0.56
1:0:1168:C:H5"	31:I:87:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1377:C:H2'	1:0:1723:G:O6	2.06	0.55
2:9:3106:C:O2'	2:9:3107:C:H5'	2.07	0.55
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.36	0.55
5:C:65:ARG:HG3	5:C:67:GLN:HB2	1.88	0.55
1:0:333:G:O2'	1:0:334:G:H5'	2.06	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.55
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.89	0.55
4:B:62:ARG:HA	4:B:65:MET:HE3	1.87	0.55
6:D:159:PRO:O	6:D:163:VAL:HG23	2.06	0.55
1:0:1309:U:O2'	1:0:1310:U:H5'	2.06	0.55
38:0:6860:HOH:O	3:A:211:LYS:HD3	2.07	0.55
4:B:79:MET:HE1	38:B:8921:HOH:O	2.06	0.55
6:D:149:ARG:HH12	15:N:15:GLU:HA	1.72	0.55
20:S:57:THR:HG22	20:S:59:ASP:N	2.18	0.55
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.05	0.55
25:X:74:ALA:HB2	25:X:85:VAL:HG13	1.88	0.55
1:0:2839:C:H2'	1:0:2840:A:H5"	1.88	0.55
2:9:3001:U:H5"	2:9:3003:A:OP1	2.07	0.55
24:W:6:GLN:HB2	24:W:26:ILE:CD1	2.36	0.55
1:0:1873:G:H3'	38:0:5213:HOH:O	2.06	0.55
24:W:88:THR:HG22	24:W:89:ASP:N	2.20	0.55
26:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.88	0.55
1:0:926:A:O2'	13:L:41:HIS:CD2	2.60	0.55
1:0:1169:U:H2'	1:0:1170:U:O4'	2.07	0.55
1:0:1180:U:H2'	1:0:1181:A:O4'	2.07	0.55
5:C:246:ARG:NE	38:C:8623:HOH:O	2.38	0.55
7:E:137:ASP:O	7:E:141:VAL:HG23	2.06	0.55
8:F:27:GLY:HA3	8:F:101:ALA:O	2.07	0.55
22:U:52:THR:CG2	22:U:54:THR:HB	2.37	0.55
1:0:553:G:P	26:Y:204:ARG:HH22	2.30	0.55
1:0:960:G:N3	1:0:960:G:C2'	2.69	0.55
1:0:1687:C:O2	28:1:9:GLY:HA2	2.06	0.55
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.88	0.55
1:0:88:G:H2'	1:0:89:G:C8	2.41	0.55
1:0:559:U:H6	1:0:559:U:C5'	2.18	0.55
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.07	0.55
1:0:958:G:H2'	1:0:959:C:H6	1.72	0.55
1:0:1132:A:N6	1:0:1229:C:H2'	2.22	0.55
4:B:62:ARG:HA	4:B:65:MET:CE	2.37	0.55
5:C:77:ALA:O	5:C:78:ARG:HD2	2.06	0.55
29:2:20:ARG:HG2	29:2:21:VAL:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:941:G:C5	1:0:942:U:C4	2.95	0.55
1:0:947:U:H2'	1:0:948:G:H8	1.70	0.55
1:0:1118:A:C8	1:0:1119:G:H5"	2.41	0.55
1:0:856:G:C8	38:0:5435:HOH:O	2.54	0.55
1:0:902:G:N7	13:L:18:HIS:HD2	2.06	0.55
5:C:236:THR:H	5:C:239:ALA:HB3	1.72	0.55
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.54
1:0:1790:C:H2'	1:0:1791:U:C6	2.40	0.54
1:0:2456:A:H5'	38:0:5705:HOH:O	2.06	0.54
38:0:4844:HOH:O	11:J:47:THR:HB	2.07	0.54
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.69	0.54
8:F:58:GLU:CD	14:M:27:ARG:HH22	2.10	0.54
1:0:120:A:H2'	1:0:120:A:N3	2.22	0.54
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.54
4:B:41:PHE:HA	4:B:79:MET:HE2	1.90	0.54
24:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.54
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.87	0.54
1:0:255:A:C5	1:0:256:C:C4	2.96	0.54
1:0:468:U:H3'	38:0:7553:HOH:O	2.07	0.54
1:0:1137:G:H1'	38:0:3885:HOH:O	2.07	0.54
1:0:1588:G:C6	1:0:1589:G:N1	2.75	0.54
3:A:33:GLU:O	3:A:34:ASP:HB2	2.07	0.54
14:M:24:GLN:HE22	14:M:27:ARG:HH11	1.55	0.54
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.88	0.54
31:I:113:HIS:N	31:I:114:PRO:HD2	2.22	0.54
1:0:2266:A:OP2	14:M:90:ARG:NH2	2.41	0.54
1:0:2425:A:H2'	38:0:9228:HOH:O	2.06	0.54
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.22	0.54
1:0:2826:G:C6	1:0:2913:A:N6	2.75	0.54
2:9:3076:G:C3'	2:9:3077:A:H5"	2.30	0.54
38:9:3472:HOH:O	15:N:41:LYS:HD3	2.08	0.54
19:R:39:THR:HB	19:R:42:GLU:HG3	1.90	0.54
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.37	0.54
1:0:226:A:H1'	1:0:393:G:C5	2.43	0.54
1:0:705:C:O2	1:0:705:C:H2'	2.08	0.54
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.54
5:C:22:PHE:HA	5:C:116:ALA:HA	1.88	0.54
5:C:233:THR:HG22	5:C:234:VAL:N	2.21	0.54
8:F:29:VAL:HG12	8:F:98:VAL:HA	1.90	0.54
21:T:53:GLY:HA3	38:T:6384:HOH:O	2.08	0.54
1:0:506:G:N2	1:0:509:A:H5"	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1171:A:H2'	1:0:1172:G:H5'	1.90	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
1:0:1603:A:H5'	1:0:1605:G:C4'	2.38	0.54
1:0:1783:A:O2'	1:0:1784:U:H5'	2.08	0.54
1:0:2001:G:O2'	1:0:2002:C:H5'	2.07	0.54
1:0:2346:C:H6	1:0:2346:C:O5'	1.90	0.54
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.88	0.54
2:9:3003:A:OP2	2:9:3025:G:N2	2.40	0.54
5:C:236:THR:CG2	5:C:239:ALA:H	2.11	0.54
8:F:21:GLU:O	8:F:24:ARG:HG2	2.07	0.54
1:0:1667:A:H2'	1:0:1668:U:H6	1.72	0.54
38:0:4623:HOH:O	16:O:39:THR:HB	2.07	0.54
2:9:3076:G:H3'	2:9:3077:A:C5'	2.28	0.54
5:C:1:MET:HG2	5:C:2:GLN:N	2.21	0.54
10:H:46:GLN:HG3	10:H:137:TYR:CE2	2.43	0.54
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.90	0.54
1:0:1421:C:H2'	1:0:1422:U:H6	1.73	0.54
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.23	0.54
1:0:1568:G:O2'	1:0:1569:U:H5'	2.07	0.54
38:0:4376:HOH:O	3:A:212:PRO:HB2	2.08	0.54
2:9:3055:U:H4'	2:9:3056:A:C8	2.43	0.54
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.38	0.54
1:0:1319:G:H1'	38:0:4701:HOH:O	2.07	0.54
1:0:1450:C:C4'	1:0:1451:C:OP2	2.53	0.54
1:0:1931:A:H2'	1:0:1932:G:H5'	1.90	0.54
8:F:117:GLU:C	8:F:119:ARG:H	2.10	0.54
1:0:328:U:O4'	5:C:202:THR:HG22	2.07	0.54
1:0:645:U:OP2	13:L:4:LYS:HE2	2.08	0.54
1:0:794:U:H3	1:0:819:A:H61	1.54	0.54
1:0:1173:A:H2	38:0:6282:HOH:O	1.91	0.54
1:0:1762:C:H2'	1:0:1763:C:C6	2.43	0.54
1:0:2064:U:H4'	1:0:2653:A:OP1	2.08	0.54
3:A:51:ARG:NH1	3:A:120:ARG:O	2.41	0.54
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.54
5:C:236:THR:HA	38:C:8651:HOH:O	2.08	0.54
17:P:91:LYS:O	17:P:95:GLU:HG3	2.08	0.54
1:0:125:U:H2'	38:0:3769:HOH:O	2.07	0.53
1:0:349:U:O2'	1:0:350:C:H5'	2.09	0.53
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.53
1:0:820:G:H5'	1:0:821:U:H5'	1.90	0.53
1:0:841:A:H5"	38:0:6906:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.08	0.53
1:0:1396:C:H1'	17:P:1:THR:O	2.08	0.53
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.38	0.53
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.43	0.53
4:B:279:THR:OG1	4:B:290:VAL:HB	2.08	0.53
1:0:2361:A:H5'	1:0:2361:A:H8	1.73	0.53
1:0:2488:A:H61	1:0:2534:C:H42	1.54	0.53
4:B:74:ILE:HG22	4:B:76:THR:HG23	1.91	0.53
1:0:1444:G:O2'	1:0:1445:G:H5'	2.08	0.53
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.36	0.53
23:V:4:HIS:O	23:V:8:ILE:HG13	2.08	0.53
1:0:40:C:H4'	38:0:6998:HOH:O	2.08	0.53
1:0:399:C:H5'	14:M:179:GLY:O	2.09	0.53
1:0:660:A:H4'	1:0:661:G:O5'	2.08	0.53
1:0:2472:C:O2'	1:0:2634:G:H4'	2.08	0.53
1:0:2784:A:H1'	7:E:60:SER:OG	2.08	0.53
8:F:56:PRO:HG2	14:M:43:PRO:O	2.08	0.53
20:S:57:THR:HG22	20:S:59:ASP:HB2	1.90	0.53
22:U:9:CYS:HA	22:U:52:THR:HG23	1.90	0.53
1:0:2064:U:H5'	1:0:2652:U:H4'	1.91	0.53
1:0:2526:C:C6	1:0:2526:C:H5'	2.43	0.53
4:B:162:MET:CE	4:B:308:LEU:HD21	2.39	0.53
24:W:64:THR:O	24:W:68:THR:HG22	2.08	0.53
1:0:271:C:H4'	1:0:272:A:OP1	2.08	0.53
1:0:622:G:O2'	1:0:623:U:H5'	2.08	0.53
1:0:2382:A:H5'	38:3:8831:HOH:O	2.09	0.53
1:0:2735:U:H2'	1:0:2736:U:C6	2.44	0.53
4:B:23:THR:HG23	4:B:308:LEU:HD23	1.91	0.53
5:C:40:ALA:O	5:C:43:LYS:HB2	2.08	0.53
8:F:96:ALA:HA	38:F:3111:HOH:O	2.09	0.53
11:J:46:ILE:HA	38:J:8828:HOH:O	2.09	0.53
18:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.90	0.53
24:W:68:THR:HG23	24:W:69:ARG:HG2	1.91	0.53
1:0:420:U:H2'	1:0:421:C:C6	2.44	0.53
1:0:821:U:H2'	1:0:822:C:C6	2.41	0.53
1:0:1314:U:H2'	38:0:5885:HOH:O	2.09	0.53
1:0:2071:C:H5'	38:0:9529:HOH:O	2.09	0.53
17:P:14:LEU:HD13	17:P:51:ALA:HB2	1.91	0.53
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.90	0.53
20:S:52:VAL:HG22	20:S:66:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:129:LYS:HG2	38:W:1990:HOH:O	2.07	0.53
31:I:103:ASP:HA	31:I:106:LYS:HD2	1.91	0.53
1:0:12:U:C2'	1:0:13:G:H5'	2.38	0.53
1:0:282:C:O2'	1:0:283:U:C5'	2.53	0.53
1:0:1342:C:O2'	1:0:1343:C:H5'	2.09	0.53
1:0:1456:C:H2'	1:0:1457:U:C6	2.44	0.53
1:0:1855:G:H4'	1:0:1856:C:O5'	2.09	0.53
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.44	0.53
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.09	0.53
6:D:163:VAL:HA	38:D:6326:HOH:O	2.07	0.53
6:D:166:ILE:HB	38:D:6326:HOH:O	2.09	0.53
1:0:1181:A:N1	1:0:1192:A:O2'	2.38	0.53
1:0:1213:C:C2'	1:0:1214:G:H5'	2.39	0.53
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.42	0.53
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.43	0.53
9:G:64:ASN:HD22	9:G:64:ASN:N	2.06	0.53
21:T:32:ARG:NH1	21:T:38:ARG:HH12	2.07	0.53
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.89	0.53
1:0:1159:G:H21	1:0:1189:A:H8	1.55	0.53
1:0:1236:A:H2'	1:0:1237:U:O4'	2.09	0.53
1:0:1309:U:C2'	1:0:1310:U:H5'	2.40	0.53
1:0:2269:C:C2'	1:0:2270:G:H5'	2.39	0.53
6:D:135:VAL:HG22	6:D:136:ARG:H	1.74	0.53
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.89	0.53
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.06	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.38	0.52
1:0:625:U:H5"	1:0:1044:C:N4	2.24	0.52
1:0:1733:A:H4'	4:B:212:GLN:HA	1.90	0.52
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.52
1:0:2837:U:H2'	38:0:6833:HOH:O	2.08	0.52
2:9:3031:C:H2'	2:9:3032:G:O4'	2.10	0.52
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.91	0.52
10:H:56:GLN:HE21	10:H:126:ARG:NE	2.00	0.52
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.39	0.52
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.90	0.52
1:0:371:U:H2'	1:0:372:A:H8	1.75	0.52
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.38	0.52
2:9:3060:C:O2'	2:9:3061:C:H5'	2.09	0.52
4:B:16:ARG:NH1	38:B:8913:HOH:O	2.42	0.52
14:M:169:ARG:HD2	38:M:8886:HOH:O	2.09	0.52
1:0:603:A:H4'	1:0:604:G:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1588:G:C6	1:0:1589:G:C6	2.98	0.52
10:H:69:ALA:HB2	10:H:153:ALA:HB2	1.90	0.52
15:N:38:LYS:HE2	15:N:107:ASN:ND2	2.24	0.52
20:S:76:GLU:HB3	38:S:8547:HOH:O	2.09	0.52
1:0:544:G:H2'	1:0:545:G:C5'	2.40	0.52
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.91	0.52
1:0:2601:A:N1	12:K:38:SER:HB2	2.25	0.52
1:0:2894:C:O2'	1:0:2895:C:H5'	2.09	0.52
1:0:304:G:H1'	1:0:347:A:N6	2.24	0.52
1:0:1384:C:H5'	25:X:30:MET:HG2	1.92	0.52
1:0:1755:A:H2'	1:0:1756:G:O4'	2.09	0.52
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.52
1:0:1972:U:C2'	1:0:1973:A:H5"	2.39	0.52
1:0:2237:G:H1'	38:0:4862:HOH:O	2.10	0.52
19:R:33:ARG:NH1	38:R:8838:HOH:O	2.41	0.52
30:3:3:MET:O	30:3:90:PHE:HA	2.10	0.52
1:0:289:G:N2	1:0:363:A:C2	2.57	0.52
1:0:1421:C:H2'	1:0:1422:U:C6	2.45	0.52
1:0:2769:C:H2'	1:0:2770:G:O4'	2.10	0.52
2:9:3029:C:H2'	2:9:3030:C:C5'	2.36	0.52
6:D:82:GLU:HA	6:D:85:GLN:HE21	1.74	0.52
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.57	0.52
21:T:26:THR:HA	21:T:39:ASN:HB3	1.91	0.52
1:0:204:A:H2'	1:0:205:U:H5'	1.91	0.52
1:0:346:U:H4'	38:0:6837:HOH:O	2.08	0.52
1:0:707:C:C2	1:0:708:A:C8	2.97	0.52
1:0:1169:U:C5	1:0:1170:U:C4	2.97	0.52
1:0:1641:A:H2'	1:0:1642:A:C5'	2.33	0.52
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.90	0.52
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.91	0.52
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.25	0.52
13:L:148:GLU:HA	38:L:8871:HOH:O	2.10	0.52
22:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.52
24:W:88:THR:HG22	24:W:90:TYR:HD1	1.74	0.52
1:0:567:U:C5'	38:0:6400:HOH:O	2.57	0.52
1:0:951:A:O2'	1:0:952:G:H5'	2.10	0.52
9:G:23:ILE:O	9:G:27:ILE:HG13	2.10	0.52
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.40	0.52
1:0:59:A:H5'	38:0:4342:HOH:O	2.09	0.52
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.52
1:0:1661:A:C8	38:0:5210:HOH:O	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1878:G:O2'	1:0:1879:U:P	2.68	0.52
1:0:2460:A:H5'	32:0:9000:13T:H231	1.90	0.52
1:0:2766:A:O2'	1:0:2767:C:H5'	2.10	0.52
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.16	0.52
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.52
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.92	0.52
5:C:95:GLU:HG3	38:C:8673:HOH:O	2.09	0.52
1:0:475:G:OP1	5:C:73:LEU:HD22	2.09	0.51
1:0:1119:G:H22	1:0:1246:A:H2	1.48	0.51
38:0:7541:HOH:O	30:3:60:LYS:HG3	2.10	0.51
2:9:3020:G:O2'	2:9:3021:G:H5'	2.10	0.51
14:M:164:THR:HG22	14:M:167:GLY:H	1.74	0.51
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.92	0.51
1:0:291:C:H2'	1:0:292:G:O4'	2.10	0.51
1:0:2010:A:C2'	38:0:5968:HOH:O	2.50	0.51
1:0:2361:A:H5"	38:0:9001:HOH:O	2.08	0.51
1:0:2388:C:O2'	1:0:2389:U:H5'	2.10	0.51
1:0:2467:A:O2'	1:0:2468:A:H2'	2.10	0.51
38:0:4733:HOH:O	19:R:29:LYS:HD3	2.10	0.51
5:C:242:GLU:HB2	38:C:8579:HOH:O	2.09	0.51
1:0:64:G:H2'	1:0:65:C:O4'	2.10	0.51
1:0:119:A:H2'	1:0:120:A:H5"	1.93	0.51
1:0:254:C:O2	1:0:254:C:H2'	2.09	0.51
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.51
1:0:1500:U:P	17:P:41:ARG:HH22	2.33	0.51
1:0:1545:C:H2'	1:0:1546:G:O4'	2.10	0.51
1:0:2266:A:H2'	1:0:2267:G:C8	2.45	0.51
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.74	0.51
8:F:91:VAL:HG12	8:F:92:GLY:H	1.76	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.93	0.51
1:0:1398:G:O2'	1:0:1399:A:H5'	2.11	0.51
1:0:1594:C:OP2	17:P:120:ARG:HD2	2.11	0.51
1:0:2036:C:O4'	12:K:44:LEU:HG	2.10	0.51
2:9:3034:A:H2'	2:9:3035:C:O4'	2.11	0.51
2:9:3092:G:C6	2:9:3093:A:C6	2.98	0.51
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.09	0.51
18:Q:75:ILE:HD13	18:Q:84:ILE:HD11	1.93	0.51
26:Y:189:ASN:C	26:Y:189:ASN:HD22	2.14	0.51
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.93	0.51
1:0:714:U:H3'	38:0:6939:HOH:O	2.09	0.51
1:0:894:A:C2	5:C:87:ARG:NH2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.51
1:0:2887:G:H2'	1:0:2888:U:C6	2.45	0.51
4:B:85:ARG:NH1	38:B:8930:HOH:O	2.42	0.51
13:L:72:ASN:HB2	38:L:8881:HOH:O	2.09	0.51
15:N:132:ASN:O	15:N:135:VAL:HG12	2.09	0.51
1:0:2379:G:N3	1:0:2418:G:H2'	2.25	0.51
1:0:2871:G:H2'	1:0:2872:U:C6	2.46	0.51
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.10	0.51
11:J:54:VAL:HG11	11:J:138:THR:HG21	1.93	0.51
17:P:115:SER:N	17:P:118:GLN:HE21	2.00	0.51
17:P:134:VAL:O	17:P:137:LEU:HB3	2.11	0.51
1:0:558:C:H2'	1:0:559:U:H5"	1.88	0.51
1:0:1314:U:H5"	1:0:1316:G:O4'	2.11	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.92	0.51
1:0:1819:G:H5'	38:0:4720:HOH:O	2.09	0.51
1:0:2578:G:H5'	1:0:2578:G:C8	2.41	0.51
2:9:3013:A:O2'	2:9:3014:G:H5"	2.11	0.51
2:9:3039:U:H1'	2:9:3044:A:N6	2.26	0.51
6:D:62:ASP:HA	38:D:4233:HOH:O	2.11	0.51
7:E:69:ILE:HA	7:E:72:MET:CE	2.40	0.51
15:N:169:PRO:O	15:N:172:PHE:HB3	2.11	0.51
1:0:324:G:C6	1:0:325:U:C5	2.99	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
1:0:589:U:H2'	1:0:590:A:H8	1.74	0.51
1:0:1163:G:H5'	31:I:115:ASP:O	2.10	0.51
1:0:1543:G:N1	1:0:1641:A:OP2	2.38	0.51
1:0:1787:C:H4'	1:0:2883:A:O4'	2.11	0.51
1:0:1856:C:H5'	1:0:1858:A:O4'	2.10	0.51
4:B:145:HIS:HD2	4:B:146:THR:O	1.94	0.51
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.92	0.51
1:0:228:C:H2'	1:0:229:G:H5'	1.92	0.51
1:0:1116:U:O2'	1:0:1118:A:C2	2.50	0.51
1:0:1878:G:C1'	38:0:6128:HOH:O	2.49	0.51
1:0:2893:C:O2'	1:0:2894:C:H5'	2.11	0.51
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.93	0.51
7:E:101:GLU:HB3	7:E:117:THR:HA	1.92	0.51
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.93	0.51
1:0:168:C:O5'	1:0:168:C:H6	1.93	0.51
1:0:329:A:OP2	5:C:206:ASN:HB2	2.11	0.51
1:0:1119:G:H8	11:J:52:GLN:HE22	1.59	0.51
1:0:1600:G:OP2	1:0:1600:G:H8	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2765:C:H2'	1:0:2766:A:H8	1.76	0.51
5:C:132:ASP:HB3	38:C:8560:HOH:O	2.10	0.51
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.08	0.51
1:0:1119:G:H8	11:J:52:GLN:NE2	2.08	0.50
1:0:1586:G:O2'	1:0:1587:U:H5'	2.11	0.50
1:0:2106:C:H5'	1:0:2284:G:H21	1.77	0.50
1:0:2135:A:O2'	1:0:2136:G:H5'	2.10	0.50
1:0:2269:C:O2'	1:0:2270:G:H5'	2.11	0.50
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.93	0.50
1:0:17:G:H2'	1:0:18:C:C6	2.47	0.50
1:0:588:G:O6	24:W:154:ARG:NH1	2.43	0.50
1:0:710:G:C2'	1:0:711:G:H5'	2.41	0.50
1:0:1556:G:O2'	1:0:1557:G:H5'	2.11	0.50
1:0:1862:C:H1'	38:0:7211:HOH:O	2.10	0.50
1:0:2515:C:H2'	1:0:2516:G:O4'	2.11	0.50
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.93	0.50
6:D:103:ASN:HD22	6:D:134:LEU:H	1.57	0.50
24:W:4:LEU:HB2	24:W:33:THR:HG22	1.92	0.50
26:Y:117:LEU:HD12	26:Y:174:VAL:CG1	2.41	0.50
28:1:28:HIS:CE1	28:1:31:LYS:HE2	2.46	0.50
1:0:814:G:H4'	38:0:3133:HOH:O	2.12	0.50
1:0:1287:A:O4'	24:W:117:ARG:HD3	2.12	0.50
1:0:1413:A:H2'	1:0:1414:A:O4'	2.11	0.50
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.27	0.50
19:R:119:VAL:HG21	19:R:142:ASP:CG	2.31	0.50
1:0:1188:A:H5'	38:0:7415:HOH:O	2.11	0.50
1:0:1406:A:H4'	1:0:1407:A:C5'	2.42	0.50
32:0:9000:13T:C23	32:0:9000:13T:C31	2.90	0.50
2:9:3023:U:O2'	2:9:3024:U:H4'	2.11	0.50
11:J:107:ASN:HD22	11:J:107:ASN:C	2.14	0.50
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.26	0.50
31:I:78:LEU:HD12	31:I:112:LYS:NZ	2.26	0.50
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.44	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:1985:U:C2	1:0:1996:U:O4'	2.64	0.50
1:0:2717:C:C2'	1:0:2718:C:C5'	2.78	0.50
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.45	0.50
2:9:3104:A:O2'	2:9:3105:A:H5'	2.12	0.50
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.94	0.50
5:C:102:LEU:HD12	38:C:8515:HOH:O	2.11	0.50
19:R:119:VAL:HG12	19:R:119:VAL:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:84:G:C2'	1:0:85:C:H5'	2.42	0.50
1:0:240:C:O2	1:0:240:C:H2'	2.12	0.50
1:0:793:A:H5"	17:P:83:LYS:HG2	1.94	0.50
1:0:2664:A:H8	1:0:2664:A:OP1	1.95	0.50
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.94	0.50
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.46	0.50
6:D:172:VAL:HG12	6:D:173:GLU:N	2.27	0.50
12:K:74:VAL:HG13	12:K:113:ILE:HG12	1.92	0.50
13:L:24:ALA:HB2	13:L:30:ARG:HD2	1.93	0.50
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.93	0.50
28:1:10:LYS:HG3	38:1:8731:HOH:O	2.11	0.50
1:0:370:G:O2'	1:0:371:U:H5'	2.12	0.50
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.76	0.50
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.94	0.50
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.93	0.50
19:R:59:PHE:O	19:R:63:ASN:HB3	2.12	0.50
21:T:41:ARG:NH1	21:T:42:VAL:O	2.45	0.50
21:T:69:LYS:O	21:T:71:VAL:HG23	2.12	0.50
24:W:125:HIS:CD2	24:W:127:GLY:H	2.25	0.50
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.94	0.50
1:0:363:A:O2'	1:0:364:C:H5'	2.12	0.50
1:0:1130:U:H5'	38:0:7657:HOH:O	2.11	0.50
1:0:1207:A:C8	1:0:1208:C:C5	3.00	0.50
1:0:1878:G:O2'	1:0:1879:U:H6	1.93	0.50
1:0:2253:G:C2	1:0:2254:G:C8	3.00	0.50
1:0:2336:G:H1'	38:0:6297:HOH:O	2.12	0.50
1:0:2506:A:N6	1:0:2511:A:O2'	2.44	0.50
1:0:2668:G:H2'	1:0:2669:U:C6	2.46	0.50
1:0:2779:G:H21	7:E:143:GLN:NE2	2.10	0.50
3:A:89:ALA:HB3	38:A:8913:HOH:O	2.11	0.50
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.93	0.50
5:C:214:THR:HG23	38:C:8636:HOH:O	2.10	0.50
9:G:12:ILE:N	9:G:13:PRO:HD3	2.27	0.50
1:0:424:C:H2'	1:0:425:U:H6	1.77	0.50
1:0:1154:A:H2'	1:0:1155:G:H8	1.75	0.50
1:0:1163:G:N2	38:0:6056:HOH:O	2.45	0.50
10:H:47:ILE:HG12	10:H:165:SER:HA	1.93	0.50
25:X:25:ARG:HD3	25:X:64:ALA:O	2.12	0.50
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.11	0.50
1:0:93:C:H5"	23:V:1:THR:CB	2.33	0.49
1:0:635:A:H2'	1:0:636:G:H5"	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2296:C:H2'	1:0:2297:U:C6	2.47	0.49
1:0:2764:C:O2'	1:0:2765:C:H5'	2.12	0.49
1:0:2831:C:H2'	1:0:2832:C:H5'	1.93	0.49
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.42	0.49
13:L:80:ASP:HB2	13:L:90:ARG:O	2.12	0.49
15:N:43:VAL:HG11	15:N:81:ALA:HA	1.94	0.49
21:T:71:VAL:HG12	21:T:72:ILE:N	2.27	0.49
1:0:710:G:O2'	1:0:711:G:H5'	2.12	0.49
1:0:1423:C:O2'	1:0:1424:A:H5'	2.12	0.49
1:0:2896:A:N3	1:0:2896:A:H2'	2.28	0.49
2:9:3055:U:H4'	2:9:3056:A:H8	1.77	0.49
4:B:26:PHE:HE1	4:B:310:ARG:HB3	1.77	0.49
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.49
10:H:162:ARG:HD3	38:H:8585:HOH:O	2.12	0.49
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.49
1:0:775:G:OP1	28:1:16:HIS:HE1	1.95	0.49
1:0:1497:G:H4'	1:0:1627:G:O2'	2.12	0.49
1:0:1909:A:N1	1:0:2128:G:H1'	2.26	0.49
3:A:179:MET:HG2	3:A:186:TRP:CG	2.46	0.49
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.45	0.49
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.76	0.49
13:L:134:GLU:HG3	38:L:8855:HOH:O	2.12	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.12	0.49
1:0:1008:C:H5"	10:H:16:ARG:HH12	1.76	0.49
1:0:1642:A:C8	1:0:1643:C:C5	3.00	0.49
1:0:2363:G:O2'	18:Q:11:ARG:HG3	2.13	0.49
1:0:2493:C:O2	1:0:2493:C:H2'	2.11	0.49
1:0:2866:U:C5	22:U:50:GLU:HB2	2.47	0.49
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.77	0.49
1:0:494:C:H2'	1:0:496:G:OP2	2.13	0.49
1:0:946:C:H2'	1:0:947:U:C6	2.47	0.49
1:0:1972:U:H2'	1:0:1973:A:H5"	1.93	0.49
1:0:2004:U:O2	1:0:2004:U:H2'	2.11	0.49
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.49
10:H:27:LYS:H	10:H:59:HIS:HD2	1.59	0.49
11:J:19:MET:HE2	11:J:79:PHE:HA	1.94	0.49
26:Y:107:PRO:HD3	26:Y:182:PHE:CE1	2.47	0.49
27:Z:53:GLY:HA2	27:Z:67:GLY:O	2.12	0.49
1:0:251:C:O2'	1:0:252:C:H5'	2.12	0.49
1:0:318:C:H5'	1:0:339:A:C2	2.48	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.78	0.49
1:0:1474:C:C6	1:0:1474:C:C5'	2.81	0.49
1:0:2122:C:H3'	38:0:5295:HOH:O	2.13	0.49
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.38	0.49
4:B:267:LYS:HA	38:B:8824:HOH:O	2.11	0.49
11:J:75:PRO:HD3	11:J:136:SER:OG	2.13	0.49
1:0:710:G:OP1	16:O:24:ALA:HB3	2.13	0.49
1:0:1278:A:H4'	1:0:1279:U:C4	2.48	0.49
1:0:1488:U:H4'	1:0:1489:G:OP1	2.12	0.49
1:0:1681:G:H5"	1:0:1682:A:H5'	1.94	0.49
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.27	0.49
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.11	0.49
1:0:645:U:O2	1:0:761:A:H2	1.96	0.49
1:0:1331:A:OP2	26:Y:142:SER:OG	2.27	0.49
1:0:2694:A:C6	1:0:2702:A:C8	3.01	0.49
38:0:5640:HOH:O	17:P:58:SER:HB3	2.11	0.49
10:H:51:VAL:HG13	10:H:159:PRO:HG3	1.95	0.49
1:0:152:A:O2'	1:0:153:C:H5'	2.13	0.49
1:0:514:G:OP1	1:0:514:G:H2'	2.12	0.49
1:0:558:C:H5'	38:0:5262:HOH:O	2.13	0.49
1:0:1422:U:H2'	1:0:1423:C:C6	2.48	0.49
1:0:1484:G:H2'	38:0:9098:HOH:O	2.13	0.49
1:0:2102:G:C2	1:0:2104:C:C4	3.01	0.49
1:0:2316:G:H4'	38:0:6098:HOH:O	2.12	0.49
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.49
4:B:36:PRO:HA	4:B:168:GLY:CA	2.39	0.49
4:B:294:TYR:HE2	38:B:8945:HOH:O	1.95	0.49
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.28	0.49
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.48	0.49
28:1:25:LYS:O	28:1:25:LYS:HG2	2.13	0.49
1:0:23:G:C6	1:0:24:G:N1	2.81	0.49
1:0:949:U:O2'	18:Q:40:HIS:HE1	1.96	0.49
1:0:1098:A:H2'	1:0:1099:G:O4'	2.12	0.49
1:0:1311:G:C2	1:0:1312:G:C8	3.01	0.49
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.49
1:0:1421:C:O2'	1:0:1422:U:H5'	2.13	0.49
1:0:1834:C:H2'	1:0:1840:A:N6	2.27	0.49
1:0:2300:A:H4'	1:0:2301:A:O5'	2.13	0.49
1:0:2387:U:H2'	1:0:2388:C:C6	2.48	0.49
1:0:2453:G:H3'	38:0:5931:HOH:O	2.13	0.49
38:0:6679:HOH:O	21:T:38:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:6699:HOH:O	26:Y:165:GLU:HB3	2.13	0.49
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.43	0.49
1:0:447:A:OP2	21:T:1:SER:HB2	2.12	0.48
1:0:522:U:O2'	1:0:1366:C:H5'	2.13	0.48
1:0:559:U:C6	1:0:559:U:C3'	2.96	0.48
1:0:1165:G:C4'	1:0:1174:A:O2'	2.55	0.48
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.39	0.48
17:P:115:SER:OG	17:P:118:GLN:HG3	2.12	0.48
24:W:115:THR:HG23	38:W:5420:HOH:O	2.13	0.48
1:0:816:G:C6	1:0:817:G:N1	2.80	0.48
1:0:999:C:H2'	1:0:1000:C:O4'	2.14	0.48
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.48
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.95	0.48
13:L:67:ARG:HB2	13:L:112:GLY:HA3	1.94	0.48
30:3:65:THR:HB	30:3:83:TRP:H	1.78	0.48
1:0:292:G:H1'	1:0:360:A:N6	2.28	0.48
1:0:474:C:O2'	5:C:73:LEU:HD21	2.13	0.48
1:0:1477:C:H5'	1:0:1868:G:H5'	1.95	0.48
1:0:1947:G:H2'	1:0:1948:G:H8	1.78	0.48
1:0:2349:G:O2'	1:0:2350:G:H5'	2.12	0.48
1:0:2703:A:H2'	1:0:2704:C:C6	2.48	0.48
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.28	0.48
5:C:107:ARG:NE	38:C:8657:HOH:O	2.35	0.48
10:H:170:ASN:HD22	10:H:170:ASN:N	2.10	0.48
12:K:130:MET:SD	22:U:25:ASP:O	2.71	0.48
14:M:99:ARG:CD	14:M:167:GLY:HA2	2.42	0.48
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.34	0.48
25:X:23:HIS:CD2	25:X:24:LYS:HG3	2.49	0.48
1:0:10:U:O4	1:0:532:A:OP2	2.32	0.48
1:0:154:C:H2'	1:0:155:C:H6	1.78	0.48
1:0:441:A:H8	1:0:441:A:O5'	1.96	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.48
1:0:1211:G:O2'	1:0:1212:C:H5'	2.14	0.48
1:0:1589:G:N2	1:0:1605:G:H1'	2.28	0.48
1:0:2374:A:H2'	1:0:2375:G:H8	1.78	0.48
38:0:9792:HOH:O	13:L:30:ARG:NH2	2.44	0.48
3:A:53:ALA:HB3	38:A:8897:HOH:O	2.12	0.48
14:M:49:ALA:C	14:M:54:TYR:HB3	2.34	0.48
14:M:164:THR:CG2	14:M:167:GLY:H	2.27	0.48
31:I:113:HIS:CE1	31:I:121:LEU:HD22	2.48	0.48
1:0:188:C:H5"	14:M:163:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:597:A:C4	1:0:598:C:C5	3.01	0.48
1:0:1193:A:H2	1:0:1194:A:N6	2.12	0.48
1:0:2055:A:H4'	19:R:132:ARG:NH2	2.28	0.48
2:9:3054:A:C2	2:9:3055:U:N3	2.81	0.48
4:B:17:LYS:O	4:B:260:HIS:HD2	1.95	0.48
10:H:97:GLU:HB3	10:H:121:VAL:HG11	1.96	0.48
16:O:47:ARG:HG3	16:O:47:ARG:NH1	2.29	0.48
19:R:39:THR:HB	19:R:42:GLU:CG	2.43	0.48
1:0:366:U:H2'	1:0:367:G:O4'	2.12	0.48
1:0:470:U:O2'	28:1:16:HIS:CD2	2.64	0.48
1:0:597:A:H2'	1:0:598:C:C6	2.46	0.48
1:0:1081:A:C6	1:0:1082:A:N1	2.82	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.95	0.48
1:0:1942:A:O2'	1:0:1943:C:H5'	2.14	0.48
1:0:2403:C:H3'	38:0:5214:HOH:O	2.13	0.48
1:0:2616:G:H1'	38:0:9423:HOH:O	2.14	0.48
2:9:3058:G:C8	2:9:3059:C:C5	3.02	0.48
7:E:11:VAL:HG12	7:E:12:ASP:N	2.29	0.48
10:H:20:ILE:HG23	10:H:120:ILE:CD1	2.44	0.48
1:0:613:C:H2'	1:0:614:U:H6	1.79	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.14	0.48
1:0:963:C:O2	1:0:1005:A:N1	2.46	0.48
1:0:1118:A:N6	1:0:1244:U:N3	2.57	0.48
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.32	0.48
1:0:1552:G:C6	1:0:1553:C:C4	3.01	0.48
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.48
1:0:2324:G:N2	1:0:2377:U:H1'	2.29	0.48
1:0:2553:A:H2'	1:0:2553:A:N3	2.28	0.48
4:B:221:GLN:HE22	12:K:42:ASN:ND2	2.03	0.48
11:J:42:GLU:O	11:J:131:THR:HG23	2.14	0.48
11:J:74:ARG:NH1	11:J:76:ASP:HB2	2.29	0.48
24:W:3:ALA:O	24:W:54:PHE:HA	2.14	0.48
27:Z:33:MET:SD	27:Z:49:ARG:HD2	2.53	0.48
29:2:41:HIS:HD2	29:2:44:ARG:H	1.62	0.48
1:0:886:A:OP2	1:0:2113:G:H5'	2.14	0.48
1:0:1217:G:C2	1:0:1218:U:C2	3.02	0.48
1:0:1842:A:C4	1:0:1979:G:C6	3.01	0.48
1:0:1921:A:O2'	1:0:1922:A:H5'	2.14	0.48
1:0:1942:A:H3'	38:0:7336:HOH:O	2.12	0.48
1:0:2032:U:H2'	1:0:2033:G:C5'	2.44	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.95	0.48
3:A:200:PRO:HD3	38:A:8819:HOH:O	2.14	0.48
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.42	0.48
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.14	0.48
11:J:45:VAL:HG23	11:J:130:VAL:O	2.14	0.48
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.93	0.48
1:0:1044:C:H5"	38:0:9021:HOH:O	2.12	0.48
1:0:1573:A:N7	1:0:1574:C:C2	2.82	0.48
1:0:1669:A:H2'	1:0:1670:G:C8	2.49	0.48
1:0:1747:A:C8	12:K:44:LEU:HD13	2.49	0.48
1:0:1789:G:O6	17:P:73:HIS:HE1	1.97	0.48
1:0:2070:G:H5"	38:0:3786:HOH:O	2.14	0.48
1:0:2488:A:H2	38:0:7268:HOH:O	1.96	0.48
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.95	0.48
5:C:51:TYR:HA	5:C:54:LEU:HD12	1.96	0.48
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.43	0.48
23:V:39:ALA:C	23:V:41:GLU:H	2.16	0.48
1:0:629:A:H2'	1:0:630:A:O4'	2.14	0.48
1:0:1587:U:H2'	1:0:1588:G:O4'	2.13	0.48
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.48
2:9:3051:A:H5'	15:N:160:SER:HB3	1.96	0.48
6:D:51:ARG:HH11	6:D:68:PRO:HB3	1.79	0.48
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.96	0.48
15:N:67:ALA:HA	15:N:71:TRP:CB	2.42	0.48
16:O:39:THR:O	16:O:115:ARG:NH2	2.47	0.48
1:0:57:C:H5"	38:0:6753:HOH:O	2.14	0.47
1:0:324:G:O2'	1:0:325:U:H5'	2.14	0.47
1:0:664:U:O4	1:0:681:G:H5"	2.14	0.47
1:0:2044:G:OP1	25:X:23:HIS:HE1	1.97	0.47
1:0:2114:C:OP1	3:A:1:GLY:HA2	2.13	0.47
1:0:2689:A:H2'	1:0:2690:U:H5'	1.96	0.47
1:0:2831:C:C2'	1:0:2832:C:H5'	2.44	0.47
4:B:84:LEU:HD23	4:B:142:LEU:HD23	1.95	0.47
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.44	0.47
25:X:66:THR:HG23	25:X:67:PRO:HD2	1.96	0.47
1:0:709:G:O2'	16:O:25:VAL:HG12	2.14	0.47
1:0:941:G:C6	1:0:942:U:C4	3.02	0.47
1:0:1188:A:C6	1:0:1189:A:C6	3.02	0.47
1:0:1477:C:C5'	1:0:1868:G:H5"	2.43	0.47
1:0:2649:A:H5'	1:0:2649:A:H8	1.78	0.47
1:0:2765:C:H2'	1:0:2766:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.79	0.47
7:E:10:ASP:HA	38:E:6017:HOH:O	2.14	0.47
28:1:25:LYS:HD2	29:2:48:ASP:HA	1.96	0.47
1:0:255:A:C8	1:0:256:C:C5	3.02	0.47
1:0:264:G:H1'	1:0:265:U:H5	1.79	0.47
1:0:1339:G:C6	1:0:1340:G:N1	2.82	0.47
1:0:1398:G:H2'	1:0:1399:A:C8	2.49	0.47
1:0:2112:A:H2'	1:0:2113:G:C8	2.49	0.47
1:0:2297:U:H1'	38:0:5179:HOH:O	2.13	0.47
1:0:2330:U:H4'	1:0:2331:C:OP1	2.15	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.31	0.47
1:0:2802:C:H2'	1:0:2803:C:C6	2.50	0.47
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.27	0.47
4:B:150:ALA:O	4:B:152:PRO:HD3	2.14	0.47
1:0:106:A:O2'	1:0:107:U:H5'	2.14	0.47
1:0:155:C:OP2	14:M:188:ARG:HD3	2.13	0.47
1:0:271:C:C2	1:0:273:G:O4'	2.67	0.47
1:0:293:A:C4	1:0:360:A:C2	3.03	0.47
38:0:9215:HOH:O	3:A:11:ARG:HD3	2.15	0.47
2:9:3002:U:OP2	2:9:3002:U:H4'	2.15	0.47
2:9:3049:G:H2'	2:9:3050:G:O4'	2.14	0.47
2:9:3114:G:O6	15:N:11:ARG:HD3	2.13	0.47
4:B:112:THR:OG1	4:B:158:LYS:HG3	2.14	0.47
11:J:135:ILE:O	11:J:139:LEU:HG	2.15	0.47
21:T:73:HIS:CD2	21:T:88:PRO:HG3	2.49	0.47
1:0:80:A:H3'	21:T:43:ASN:OD1	2.15	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:1592:G:O2'	1:0:1593:C:O5'	2.33	0.47
13:L:143:THR:HG21	38:L:8836:HOH:O	2.14	0.47
30:3:3:MET:HG3	30:3:4:PRO:HD2	1.96	0.47
1:0:69:A:H8	1:0:69:A:C5'	2.25	0.47
1:0:247:A:H2'	38:0:3931:HOH:O	2.13	0.47
1:0:876:A:H2'	1:0:876:A:N3	2.29	0.47
1:0:1562:C:O2	1:0:1562:C:H2'	2.12	0.47
1:0:1574:C:H2'	1:0:1575:C:C6	2.50	0.47
1:0:2026:C:O2'	1:0:2027:U:H5'	2.15	0.47
1:0:2115:U:H2'	1:0:2116:U:C6	2.49	0.47
1:0:2403:C:C2'	1:0:2404:G:O5'	2.62	0.47
15:N:108:SER:HA	15:N:109:PRO:HD3	1.74	0.47
24:W:52:VAL:HG22	24:W:53:ALA:H	1.79	0.47
26:Y:189:ASN:HD22	26:Y:192:ASP:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:475:G:H5'	5:C:73:LEU:CD2	2.44	0.47
1:0:524:A:C5'	19:R:29:LYS:HE2	2.45	0.47
1:0:644:G:H5'	1:0:644:G:N3	2.30	0.47
1:0:729:C:C2	1:0:743:G:C2	3.03	0.47
1:0:758:A:H2'	1:0:759:C:O4'	2.15	0.47
1:0:1007:A:H2'	10:H:19:TYR:CZ	2.50	0.47
1:0:1069:C:C2'	1:0:1070:A:H5'	2.44	0.47
1:0:1079:A:H4'	1:0:2078:U:H5'	1.97	0.47
1:0:1202:A:O2'	1:0:1203:G:H5'	2.14	0.47
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.47
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.47	0.47
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.15	0.47
1:0:2274:A:O2'	1:0:2275:G:H5'	2.14	0.47
1:0:2371:G:H5'	38:0:5013:HOH:O	2.14	0.47
1:0:2419:U:H5"	1:0:2420:G:H5'	1.97	0.47
1:0:2421:G:H3'	1:0:2422:U:C5'	2.45	0.47
1:0:2421:G:H3'	1:0:2422:U:H5"	1.97	0.47
1:0:2615:U:C5	1:0:2616:G:C6	3.03	0.47
1:0:2754:G:O2'	1:0:2755:G:H5'	2.15	0.47
2:9:3048:C:H4'	15:N:141:ARG:NH2	2.30	0.47
4:B:275:GLY:O	4:B:291:ASP:HA	2.15	0.47
10:H:2:PRO:HD2	10:H:5:MET:SD	2.55	0.47
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.97	0.47
14:M:65:VAL:HG21	14:M:105:ALA:HB2	1.97	0.47
16:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.47
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.45	0.47
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.97	0.47
24:W:90:TYR:CE2	24:W:99:ALA:HB2	2.50	0.47
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.96	0.47
1:0:920:C:H5'	1:0:921:G:C4	2.50	0.47
1:0:951:A:H2'	1:0:952:G:H5'	1.96	0.47
1:0:1731:C:H1'	38:0:6446:HOH:O	2.14	0.47
1:0:1746:A:O4'	1:0:1747:A:C2	2.67	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.45	0.47
1:0:2111:G:H1'	38:0:9044:HOH:O	2.14	0.47
3:A:17:ARG:HD2	38:A:8836:HOH:O	2.13	0.47
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.79	0.47
22:U:33:SER:O	22:U:37:GLU:HG3	2.14	0.47
26:Y:117:LEU:HD12	26:Y:174:VAL:HG11	1.97	0.47
28:1:28:HIS:HD2	28:1:30:LYS:H	1.61	0.47
1:0:329:A:C5	1:0:347:A:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:524:A:H5'	19:R:29:LYS:HE2	1.97	0.47
1:0:905:C:H3'	38:0:5188:HOH:O	2.15	0.47
1:0:1013:A:H1'	38:0:9156:HOH:O	2.15	0.47
1:0:1114:A:O2'	1:0:1115:U:H5'	2.15	0.47
1:0:1268:C:O2'	1:0:1269:G:H5'	2.14	0.47
1:0:1593:C:OP1	17:P:117:SER:HB3	2.15	0.47
1:0:1921:A:C6	1:0:1922:A:C2	3.03	0.47
1:0:2244:A:H1'	38:M:8866:HOH:O	2.14	0.47
1:0:2274:A:H1'	14:M:86:GLN:NE2	2.30	0.47
1:0:2468:A:H4'	38:0:3550:HOH:O	2.14	0.47
1:0:2502:C:H2'	1:0:2503:A:C5'	2.43	0.47
1:0:2768:A:C2'	1:0:2769:C:O4'	2.61	0.47
38:0:6273:HOH:O	17:P:59:ARG:HD3	2.15	0.47
38:0:6996:HOH:O	18:Q:9:GLY:HA2	2.15	0.47
2:9:3047:A:C2	2:9:3048:C:C2	3.03	0.47
3:A:109:GLU:HG2	3:A:116:GLY:H	1.79	0.47
24:W:149:LEU:HG	24:W:153:MET:CE	2.45	0.47
1:0:312:U:C2	1:0:320:G:N2	2.83	0.47
1:0:377:C:H5	38:0:3309:HOH:O	1.98	0.47
1:0:1015:C:O5'	1:0:1015:C:H6	1.98	0.47
1:0:1857:A:N6	1:0:2247:C:H1'	2.30	0.47
1:0:1878:G:H5'	38:0:4380:HOH:O	2.15	0.47
3:A:215:ILE:HG13	3:A:216:SER:N	2.30	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
6:D:135:VAL:HG22	6:D:136:ARG:N	2.29	0.47
7:E:37:ASP:OD1	11:J:125:SER:HB3	2.15	0.47
8:F:34:ASN:HA	14:M:4:ALA:HB2	1.97	0.47
1:0:513:A:N3	38:0:3663:HOH:O	2.36	0.46
1:0:559:U:C6	1:0:559:U:H3'	2.51	0.46
1:0:812:A:H1'	38:0:3966:HOH:O	2.14	0.46
1:0:851:C:H5	38:0:6802:HOH:O	1.96	0.46
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.46
1:0:1773:G:N2	1:0:1774:G:C8	2.83	0.46
1:0:2047:C:H2'	1:0:2048:C:H6	1.80	0.46
1:0:2063:U:O4	1:0:2083:A:H2	1.98	0.46
1:0:2255:A:C6	1:0:2256:G:C5	3.03	0.46
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.46
2:9:3097:U:H2'	2:9:3098:C:H6	1.79	0.46
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.97	0.46
18:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.15	0.46
21:T:71:VAL:HG13	21:T:91:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:38:THR:HG22	24:W:39:ASP:N	2.30	0.46
26:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.48	0.46
1:0:31:C:H4'	38:0:7414:HOH:O	2.16	0.46
1:0:111:C:O2'	1:0:112:G:H5'	2.16	0.46
1:0:1183:C:C2	1:0:1184:C:C5	3.03	0.46
1:0:1447:U:H3'	1:0:1506:U:O2	2.15	0.46
1:0:1838:U:O2'	1:0:2644:C:H5'	2.15	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.16	0.46
1:0:2255:A:C2	1:0:2256:G:C4	3.03	0.46
32:0:9000:13T:C23	32:0:9000:13T:H311	2.46	0.46
2:9:3028:U:H2'	2:9:3029:C:C6	2.50	0.46
1:0:694:A:C2'	1:0:695:C:H5'	2.43	0.46
1:0:1198:U:C6	1:0:1200:A:OP2	2.68	0.46
1:0:1207:A:N6	38:0:5644:HOH:O	2.48	0.46
1:0:1211:G:H2'	1:0:1212:C:C6	2.47	0.46
1:0:1523:G:C6	1:0:1524:U:O4	2.67	0.46
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.46
1:0:1878:G:O2'	1:0:1879:U:C5	2.65	0.46
1:0:1913:C:H2'	1:0:1914:C:H6	1.80	0.46
1:0:2269:C:H2'	1:0:2270:G:C5'	2.46	0.46
1:0:2764:C:H1'	38:0:7458:HOH:O	2.16	0.46
3:A:126:ALA:HB1	3:A:138:VAL:CG1	2.45	0.46
8:F:111:ILE:O	8:F:115:VAL:HG23	2.15	0.46
1:0:559:U:H2'	1:0:560:C:O4'	2.14	0.46
1:0:704:C:H2'	1:0:705:C:H6	1.81	0.46
1:0:843:A:C2	1:0:846:A:C8	3.04	0.46
1:0:1913:C:H2'	1:0:1914:C:C6	2.50	0.46
1:0:1931:A:C2'	1:0:1932:G:H5'	2.45	0.46
1:0:2459:G:C2'	32:0:9000:13T:C23	2.94	0.46
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.48	0.46
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.31	0.46
16:O:105:ASN:HD21	16:O:109:SER:H	1.62	0.46
31:I:100:LEU:HD22	31:I:105:VAL:CG2	2.46	0.46
1:0:317:A:OP1	21:T:52:ARG:O	2.33	0.46
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.46
1:0:1204:C:H2'	1:0:1205:U:O4'	2.16	0.46
1:0:2459:G:H2'	32:0:9000:13T:H232	1.98	0.46
1:0:2821:C:H2'	1:0:2822:C:H6	1.80	0.46
15:N:65:ASP:HB3	38:N:8821:HOH:O	2.14	0.46
1:0:39:G:C2	1:0:444:C:C2	3.04	0.46
1:0:1173:A:H3'	38:0:4360:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1619:G:C5	1:0:1620:C:C4	3.03	0.46
1:0:2114:C:O2'	1:0:2115:U:H5'	2.16	0.46
1:0:2332:A:H3'	1:0:2333:G:H8	1.80	0.46
3:A:3:ARG:H	3:A:3:ARG:HG2	1.55	0.46
3:A:179:MET:HG2	3:A:186:TRP:CB	2.45	0.46
14:M:183:THR:HG22	14:M:194:ALA:HB1	1.96	0.46
22:U:13:ILE:HG12	22:U:32:CYS:HB3	1.97	0.46
1:0:281:U:C2'	1:0:282:C:H5'	2.46	0.46
1:0:857:A:H4'	3:A:176:HIS:CD2	2.51	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.98	0.46
1:0:1850:U:H2'	1:0:1851:G:C8	2.50	0.46
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.98	0.46
6:D:10:PHE:CG	6:D:11:HIS:N	2.84	0.46
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.96	0.46
19:R:39:THR:HG23	19:R:107:GLU:O	2.16	0.46
1:0:475:G:H5'	5:C:73:LEU:HD23	1.96	0.46
1:0:1684:A:O2'	1:0:1685:A:H5"	2.15	0.46
1:0:2121:G:O2'	1:0:2122:C:H5'	2.16	0.46
1:0:2729:C:O2'	1:0:2730:G:H5'	2.15	0.46
3:A:36:ASP:O	3:A:38:ILE:N	2.49	0.46
13:L:56:LYS:NZ	38:L:8873:HOH:O	2.49	0.46
22:U:52:THR:HG22	22:U:54:THR:N	2.31	0.46
26:Y:216:ARG:HD2	38:Y:8868:HOH:O	2.14	0.46
31:I:78:LEU:HD12	31:I:112:LYS:HZ2	1.79	0.46
1:0:1218:U:H2'	1:0:1219:U:C6	2.51	0.46
1:0:2263:G:H1'	38:0:6618:HOH:O	2.16	0.46
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.46
26:Y:184:GLU:OE2	26:Y:204:ARG:HD2	2.15	0.46
1:0:17:G:H2'	1:0:18:C:H6	1.81	0.46
1:0:101:C:H2'	1:0:102:A:C8	2.51	0.46
1:0:113:A:H2'	1:0:115:U:O4	2.16	0.46
1:0:1166:A:H1'	1:0:1192:A:C2	2.50	0.46
1:0:1182:C:O2'	1:0:1183:C:H5	1.99	0.46
1:0:2050:G:H5"	19:R:80:TYR:O	2.16	0.46
1:0:2549:C:H4'	38:0:7504:HOH:O	2.16	0.46
1:0:2672:C:H1'	38:B:8930:HOH:O	2.15	0.46
1:0:2911:C:H2'	1:0:2912:C:C6	2.51	0.46
38:0:7403:HOH:O	31:I:90:GLY:HA2	2.16	0.46
6:D:51:ARG:NH1	6:D:68:PRO:HB3	2.31	0.46
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.98	0.46
7:E:69:ILE:HA	7:E:72:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:107:ASP:O	8:F:111:ILE:HG13	2.15	0.46
10:H:170:ASN:N	10:H:170:ASN:ND2	2.64	0.46
11:J:26:VAL:HG13	11:J:36:VAL:HG11	1.98	0.46
14:M:134:ILE:CG2	14:M:141:ILE:HD13	2.43	0.46
20:S:57:THR:CG2	20:S:59:ASP:HB2	2.45	0.46
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.45	0.46
1:0:189:A:OP1	14:M:171:ARG:NH2	2.49	0.45
1:0:583:G:H2'	1:0:584:U:C6	2.51	0.45
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.97	0.45
1:0:1583:U:H1'	38:0:9979:HOH:O	2.15	0.45
1:0:2000:G:O2'	1:0:2001:G:H5'	2.16	0.45
1:0:2253:G:O2'	1:0:2254:G:H5'	2.16	0.45
1:0:2730:G:O2'	1:0:2731:G:H5'	2.15	0.45
2:9:3107:C:H2'	2:9:3108:C:C6	2.51	0.45
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.98	0.45
10:H:1:LYS:HA	10:H:2:PRO:HD3	1.73	0.45
11:J:45:VAL:HG22	11:J:46:ILE:N	2.30	0.45
20:S:77:VAL:O	20:S:80:ARG:HG2	2.17	0.45
1:0:939:A:H5'	38:0:5419:HOH:O	2.16	0.45
1:0:1127:C:C5	1:0:1128:U:C4	3.04	0.45
1:0:1321:A:H2'	1:0:1322:G:C8	2.51	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.51	0.45
1:0:1741:U:C4	1:0:2033:G:C8	3.04	0.45
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.45
1:0:2092:G:H5"	1:0:2613:G:OP1	2.15	0.45
1:0:2570:G:H8	38:0:4917:HOH:O	2.00	0.45
1:0:2820:A:H2'	1:0:2821:C:O4'	2.17	0.45
10:H:95:LEU:HD11	10:H:124:ALA:HB2	1.99	0.45
16:O:32:ARG:HB2	38:O:4656:HOH:O	2.17	0.45
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.17	0.45
23:V:7:GLU:O	23:V:11:MET:HG3	2.15	0.45
26:Y:220:GLU:HG3	38:Y:8849:HOH:O	2.16	0.45
27:Z:56:GLN:HA	27:Z:62:TYR:O	2.16	0.45
1:0:365:G:C6	1:0:366:U:C4	3.04	0.45
1:0:419:A:H1'	1:0:1921:A:C2	2.51	0.45
1:0:512:G:O3'	1:0:513:A:C8	2.69	0.45
1:0:541:C:C2'	1:0:542:A:C5'	2.82	0.45
1:0:706:G:O2'	1:0:707:C:H6	1.99	0.45
1:0:814:G:N2	1:0:815:U:H1'	2.31	0.45
1:0:920:C:H5"	1:0:921:G:O5'	2.17	0.45
1:0:1855:G:H8	3:A:144:GLU:OE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2314:G:C2'	1:0:2315:C:H5'	2.46	0.45
1:0:2582:G:H5"	4:B:3:PRO:HB3	1.98	0.45
1:0:2831:C:H2'	1:0:2832:C:C5'	2.46	0.45
2:9:3107:C:C5	38:9:3167:HOH:O	2.68	0.45
15:N:139:TRP:HA	15:N:139:TRP:CE3	2.52	0.45
17:P:83:LYS:O	17:P:86:ALA:HB3	2.16	0.45
23:V:39:ALA:N	23:V:40:PRO:CD	2.80	0.45
23:V:45:ARG:HH11	23:V:45:ARG:HG3	1.82	0.45
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.98	0.45
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.16	0.45
29:2:20:ARG:HB3	38:2:5444:HOH:O	2.17	0.45
1:0:51:G:O2'	1:0:52:A:H5'	2.16	0.45
1:0:200:U:H2'	38:0:3446:HOH:O	2.15	0.45
1:0:229:G:O2'	1:0:230:C:H5'	2.16	0.45
1:0:1477:C:H5'	1:0:1868:G:H5"	1.97	0.45
1:0:1588:G:C5	1:0:1589:G:C6	3.05	0.45
1:0:2105:C:H2'	1:0:2106:C:C6	2.52	0.45
1:0:2237:G:O2'	1:0:2238:A:C8	2.69	0.45
1:0:2428:G:N7	30:3:60:LYS:NZ	2.61	0.45
1:0:2649:A:H5'	1:0:2649:A:C8	2.52	0.45
3:A:82:VAL:HG13	3:A:93:THR:HB	1.98	0.45
26:Y:130:ARG:HB2	26:Y:142:SER:O	2.16	0.45
1:0:407:A:H5'	38:0:6034:HOH:O	2.15	0.45
1:0:2016:U:H2'	1:0:2017:U:C6	2.51	0.45
1:0:2864:U:C5	1:0:2865:G:C6	3.04	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.81	0.45
38:0:9988:HOH:O	13:L:22:ARG:HG2	2.15	0.45
2:9:3008:G:O6	15:N:11:ARG:NH1	2.39	0.45
2:9:3026:C:O2'	2:9:3027:C:H5'	2.17	0.45
3:A:109:GLU:HG2	3:A:116:GLY:N	2.31	0.45
4:B:162:MET:CE	4:B:310:ARG:HD3	2.47	0.45
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.45
1:0:453:A:H4'	1:0:455:A:N7	2.32	0.45
1:0:1730:G:H4'	1:0:1731:C:H6	1.82	0.45
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.51	0.45
25:X:76:ARG:HH11	25:X:76:ARG:CG	2.28	0.45
25:X:76:ARG:HG3	25:X:76:ARG:NH1	2.28	0.45
26:Y:117:LEU:HA	26:Y:174:VAL:HG11	1.98	0.45
1:0:111:C:C2'	1:0:112:G:H5'	2.47	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.16	0.45
1:0:560:C:H2'	1:0:561:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1164:U:OP1	31:I:74:PRO:HA	2.17	0.45
1:0:1544:U:O2'	1:0:1545:C:H5'	2.17	0.45
1:0:1771:U:O2'	1:0:1773:G:N7	2.48	0.45
1:0:2110:G:C2	1:0:2478:U:C2	3.04	0.45
1:0:2326:U:H4'	1:0:2412:G:C4'	2.46	0.45
1:0:2772:G:O2'	1:0:2773:G:H5'	2.16	0.45
1:0:2891:A:C2	1:0:2892:G:C4	3.05	0.45
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.45
1:0:244:C:OP2	8:F:38:LYS:HE3	2.17	0.45
1:0:289:G:N1	1:0:363:A:C2	2.81	0.45
1:0:696:C:O2'	1:0:731:U:OP1	2.33	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.16	0.45
1:0:1029:U:O2'	1:0:1273:C:OP1	2.32	0.45
1:0:1123:A:N1	1:0:1238:C:H5'	2.32	0.45
1:0:1150:A:C2	9:G:20:VAL:HG21	2.52	0.45
1:0:1252:A:H2'	1:0:1253:C:O4'	2.17	0.45
1:0:1682:A:O2'	1:0:1683:G:H5"	2.17	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.47	0.45
1:0:1940:C:H4'	38:0:7336:HOH:O	2.17	0.45
1:0:1973:A:H5'	1:0:1973:A:C8	2.45	0.45
1:0:2073:G:OP2	1:0:2490:A:H5'	2.16	0.45
7:E:15:GLN:HG2	7:E:19:ASP:O	2.17	0.45
13:L:143:THR:HG22	13:L:144:ASP:H	1.81	0.45
15:N:110:THR:HB	15:N:113:SER:OG	2.17	0.45
24:W:5:VAL:HG11	24:W:153:MET:CE	2.47	0.45
30:3:69:TYR:O	30:3:77:ALA:HA	2.16	0.45
1:0:292:G:H1'	1:0:360:A:H61	1.81	0.45
1:0:542:A:C5'	1:0:542:A:C8	2.95	0.45
1:0:1076:G:C2	1:0:1084:C:C2	3.05	0.45
1:0:2075:G:C6	1:0:2076:U:C4	3.05	0.45
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.45
1:0:2614:C:O2'	1:0:2615:U:H5'	2.17	0.45
1:0:2906:A:H5'	1:0:2907:C:O4'	2.17	0.45
4:B:277:GLU:N	4:B:278:PRO:HD2	2.31	0.45
5:C:2:GLN:HB3	38:C:8582:HOH:O	2.15	0.45
1:0:488:U:O2'	21:T:82:THR:HG21	2.17	0.45
1:0:670:G:H2'	1:0:671:A:C8	2.52	0.45
1:0:926:A:O2'	13:L:41:HIS:HD2	2.00	0.45
1:0:1238:C:H5"	1:0:1239:G:OP2	2.17	0.45
1:0:2133:U:H4'	1:0:2134:G:H5'	1.98	0.45
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:236:THR:HG22	5:C:239:ALA:CB	2.47	0.45
17:P:9:LEU:O	17:P:13:VAL:HG23	2.17	0.45
24:W:139:GLY:O	24:W:141:HIS:CD2	2.70	0.45
1:0:248:A:H5'	1:0:249:G:OP2	2.18	0.44
1:0:426:G:H2'	1:0:427:C:O4'	2.17	0.44
1:0:538:C:N4	1:0:2061:C:H1'	2.32	0.44
1:0:660:A:N6	1:0:746:A:O4'	2.50	0.44
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.44
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.44
1:0:1279:U:O2	1:0:1279:U:H2'	2.17	0.44
1:0:2346:C:O2'	6:D:52:THR:HG21	2.17	0.44
1:0:2354:A:C2	1:0:2367:A:C8	3.04	0.44
1:0:2594:C:O2'	1:0:2595:U:H5'	2.17	0.44
6:D:40:ILE:HG23	38:D:5583:HOH:O	2.17	0.44
11:J:53:ILE:O	11:J:57:TYR:HD1	2.00	0.44
15:N:179:LEU:HD23	15:N:184:ILE:CD1	2.47	0.44
18:Q:75:ILE:CD1	18:Q:84:ILE:HD11	2.47	0.44
22:U:52:THR:HG22	22:U:54:THR:HB	1.98	0.44
25:X:78:GLU:HG2	25:X:79:GLU:H	1.82	0.44
26:Y:235:GLU:CD	26:Y:235:GLU:H	2.21	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.18	0.44
1:0:536:A:H3'	38:0:5051:HOH:O	2.16	0.44
1:0:957:A:H8	1:0:957:A:O5'	2.00	0.44
1:0:1494:A:O2'	1:0:1505:U:O2	2.34	0.44
1:0:2719:A:C2	4:B:70:PRO:HG3	2.52	0.44
2:9:3058:G:H1'	38:9:3839:HOH:O	2.16	0.44
2:9:3097:U:H2'	2:9:3098:C:C6	2.51	0.44
3:A:107:ASN:OD1	3:A:116:GLY:HA3	2.17	0.44
4:B:60:SER:HA	4:B:61:PRO:HD3	1.85	0.44
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.52	0.44
11:J:45:VAL:CG2	11:J:129:PHE:HD1	2.30	0.44
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.98	0.44
26:Y:151:SER:HB3	26:Y:154:ARG:HB3	2.00	0.44
1:0:111:C:H2'	1:0:112:G:C5'	2.46	0.44
1:0:263:U:C2	8:F:59:ILE:CD1	3.01	0.44
1:0:697:G:H4'	1:0:730:G:O3'	2.17	0.44
1:0:834:G:H3'	1:0:835:U:H4'	1.99	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.44
1:0:1244:U:H4'	1:0:1246:A:O4'	2.17	0.44
1:0:1269:G:H2'	1:0:1270:U:C6	2.53	0.44
1:0:1334:C:O2'	1:0:1335:C:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1972:U:C2'	1:0:1973:A:C5'	2.96	0.44
1:0:2133:U:H4'	1:0:2134:G:C5'	2.47	0.44
1:0:2716:G:O2'	1:0:2717:C:H5'	2.18	0.44
1:0:2900:G:C2'	1:0:2901:C:H5'	2.47	0.44
3:A:95:PRO:HA	3:A:153:ARG:HA	1.98	0.44
14:M:15:PRO:HA	14:M:20:LEU:HD23	2.00	0.44
15:N:154:LEU:C	15:N:156:GLU:H	2.20	0.44
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.52	0.44
1:0:2256:G:H2'	1:0:2257:G:O5'	2.17	0.44
1:0:2610:U:H4'	38:0:9479:HOH:O	2.18	0.44
4:B:18:ARG:HE	4:B:256:GLN:NE2	2.15	0.44
4:B:307:ARG:HA	38:B:8850:HOH:O	2.17	0.44
5:C:34:ALA:HB3	5:C:220:THR:HG21	2.00	0.44
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.85	0.44
1:0:710:G:N2	1:0:719:C:C2	2.86	0.44
1:0:1309:U:C4	1:0:1310:U:C5	3.06	0.44
1:0:1667:A:H8	1:0:1667:A:C5'	2.18	0.44
1:0:1714:C:O2'	1:0:1715:C:H5'	2.18	0.44
1:0:1748:U:C5	1:0:1749:U:C4	3.06	0.44
1:0:2846:C:H4'	4:B:156:LYS:HB3	1.98	0.44
4:B:144:THR:HB	38:B:8921:HOH:O	2.18	0.44
1:0:170:U:H2'	1:0:171:C:H5'	1.98	0.44
1:0:538:C:H5"	1:0:539:G:C8	2.53	0.44
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.44
1:0:929:A:O5'	1:0:929:A:H8	2.01	0.44
1:0:1117:A:C2	1:0:1244:U:C2	3.06	0.44
1:0:1500:U:OP2	17:P:41:ARG:NH2	2.51	0.44
1:0:1523:G:H2'	1:0:1524:U:C6	2.53	0.44
1:0:1602:C:OP2	27:Z:46:ARG:NH2	2.51	0.44
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.18	0.44
1:0:2504:A:H4'	10:H:71:ARG:HH11	1.83	0.44
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.44
32:0:9000:13T:O2	32:0:9000:13T:H323	2.18	0.44
4:B:199:TYR:CE2	4:B:268:ARG:HB2	2.53	0.44
7:E:132:THR:HB	38:E:2227:HOH:O	2.17	0.44
12:K:14:LYS:CB	12:K:45:PRO:HG2	2.46	0.44
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.97	0.44
23:V:45:ARG:HG3	23:V:45:ARG:NH1	2.32	0.44
1:0:1419:U:H2'	1:0:1685:A:C2	2.53	0.44
1:0:2416:G:O2'	15:N:25:ARG:HG2	2.17	0.44
1:0:2432:C:H1'	32:0:9000:13T:O9	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:321:PRO:HA	38:B:8952:HOH:O	2.16	0.44
5:C:129:HIS:CE1	5:C:232:LEU:H	2.36	0.44
24:W:13:MET:CE	24:W:17:ILE:HG22	2.48	0.44
24:W:90:TYR:CD1	24:W:90:TYR:N	2.85	0.44
1:0:413:G:H2'	1:0:414:C:C6	2.52	0.44
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.44
1:0:500:G:H21	19:R:98:ASN:ND2	2.13	0.44
1:0:622:G:P	26:Y:148:GLY:HA3	2.58	0.44
1:0:637:C:H2'	1:0:638:C:C6	2.52	0.44
1:0:920:C:H4'	1:0:921:G:N2	2.32	0.44
1:0:1069:C:O2'	1:0:1070:A:H5'	2.18	0.44
1:0:1280:A:OP1	1:0:1280:A:H3'	2.18	0.44
1:0:1730:G:H4'	1:0:1731:C:C6	2.53	0.44
1:0:1773:G:C8	27:Z:16:ALA:HA	2.53	0.44
1:0:2361:A:H2'	1:0:2362:A:C8	2.52	0.44
1:0:2577:A:H5'	38:0:7734:HOH:O	2.17	0.44
1:0:2802:C:H2'	1:0:2803:C:H6	1.81	0.44
1:0:2899:A:O2'	1:0:2900:G:H5'	2.18	0.44
38:0:7396:HOH:O	21:T:2:LYS:HE2	2.17	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
15:N:171:HIS:CE1	38:N:8862:HOH:O	2.71	0.44
1:0:238:C:H4'	1:0:287:C:OP1	2.18	0.44
1:0:276:C:H6	1:0:276:C:O5'	2.01	0.44
1:0:303:C:O2'	1:0:304:G:H5'	2.18	0.44
1:0:307:G:C2	1:0:309:C:C4	3.05	0.44
1:0:821:U:H4'	27:Z:17:ARG:NH1	2.33	0.44
1:0:1236:A:C8	11:J:63:ILE:HD11	2.53	0.44
1:0:2385:G:H2'	1:0:2386:U:H6	1.79	0.44
1:0:2691:A:OP1	1:0:2691:A:H8	2.01	0.44
2:9:3039:U:H3	2:9:3042:C:H5"	1.83	0.44
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.99	0.44
4:B:185:GLY:HA2	38:B:8929:HOH:O	2.17	0.44
1:0:699:C:C2	1:0:743:G:N2	2.86	0.43
1:0:1159:G:H1	1:0:1208:C:H42	1.64	0.43
1:0:1191:A:H2'	1:0:1193:A:H5'	2.00	0.43
1:0:1205:U:C2'	1:0:1206:U:C5'	2.87	0.43
1:0:1761:U:H5'	17:P:81:LYS:O	2.18	0.43
27:Z:36:ASP:HB3	27:Z:45:ASP:HB3	1.99	0.43
1:0:37:A:H2'	1:0:38:G:C8	2.52	0.43
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:338:C:H4'	5:C:174:ILE:HD12	1.98	0.43
1:0:1183:C:H42	1:0:1184:C:N4	2.12	0.43
1:0:1215:A:O3'	1:0:1216:G:C4'	2.66	0.43
1:0:1829:A:H5"	38:0:3081:HOH:O	2.17	0.43
1:0:1923:G:H4'	30:3:31:THR:O	2.18	0.43
1:0:2101:A:H2'	5:C:63:SER:OG	2.18	0.43
1:0:2821:C:H4'	4:B:116:PRO:HG3	2.00	0.43
1:0:2850:C:H6	1:0:2850:C:H5'	1.83	0.43
5:C:51:TYR:CE2	28:1:53:LYS:HB3	2.53	0.43
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.51	0.43
1:0:195:C:H2'	1:0:196:G:H5'	2.00	0.43
1:0:1377:C:H6	1:0:1377:C:C5'	2.28	0.43
1:0:1624:A:H5'	1:0:1626:A:O4'	2.17	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.19	0.43
1:0:2089:A:O2'	1:0:2090:G:H5'	2.18	0.43
32:0:9000:13T:H2	32:0:9000:13T:C26	2.42	0.43
38:0:7442:HOH:O	4:B:211:THR:HG21	2.19	0.43
1:0:99:A:C8	1:0:100:C:C5	3.06	0.43
1:0:304:G:H1'	1:0:347:A:H61	1.83	0.43
1:0:772:G:H2'	1:0:773:A:O4'	2.17	0.43
1:0:1118:A:N6	1:0:1244:U:C2	2.86	0.43
1:0:1343:C:H2'	1:0:1344:G:O5'	2.19	0.43
1:0:1409:G:C2	1:0:1410:G:C8	3.06	0.43
1:0:1903:U:O2'	1:0:1904:A:N7	2.49	0.43
1:0:2002:C:H2'	1:0:2003:U:H5'	2.00	0.43
1:0:2252:A:C6	1:0:2253:G:H1'	2.54	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.01	0.43
5:C:115:LEU:HD12	5:C:115:LEU:HA	1.87	0.43
6:D:170:TYR:O	6:D:171:ASP:HB3	2.18	0.43
7:E:22:VAL:O	7:E:76:VAL:HG11	2.18	0.43
8:F:101:ALA:HA	38:F:5413:HOH:O	2.18	0.43
12:K:34:VAL:HG21	12:K:46:LYS:O	2.19	0.43
12:K:132:VAL:HG21	22:U:22:VAL:HG11	2.00	0.43
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.34	0.43
20:S:33:SER:O	20:S:37:VAL:HG23	2.18	0.43
1:0:137:U:H2'	1:0:139:C:C5	2.53	0.43
1:0:187:A:H3'	1:0:188:C:H6	1.83	0.43
1:0:242:A:N6	1:0:269:G:H1'	2.34	0.43
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.43
1:0:2786:G:H2'	38:0:7180:HOH:O	2.17	0.43
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:185:LYS:HD3	5:C:186:TYR:CE1	2.53	0.43
5:C:193:LEU:HD13	5:C:222:ASP:HB2	2.00	0.43
6:D:49:PRO:HA	6:D:73:VAL:HG22	2.01	0.43
7:E:80:TRP:O	7:E:134:SER:HA	2.17	0.43
15:N:7:LYS:HE3	18:Q:21:ARG:O	2.19	0.43
19:R:132:ARG:HG2	19:R:133:ALA:N	2.32	0.43
27:Z:30:GLU:HG2	27:Z:33:MET:HE2	1.99	0.43
1:0:69:A:C8	1:0:69:A:C5'	2.95	0.43
1:0:645:U:H2'	1:0:646:G:C8	2.54	0.43
1:0:1130:U:H4'	38:0:6133:HOH:O	2.18	0.43
1:0:1183:C:O2	1:0:1183:C:C2'	2.67	0.43
1:0:1186:C:H5"	31:I:119:TYR:CE1	2.53	0.43
1:0:1439:C:O5'	1:0:1439:C:H6	2.01	0.43
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.43
1:0:2779:G:N2	1:0:2796:U:C2	2.87	0.43
1:0:2812:A:H2	1:0:2814:A:N6	1.91	0.43
1:0:2840:A:OP1	4:B:211:THR:HG23	2.19	0.43
4:B:4:SER:O	4:B:5:ARG:HB2	2.19	0.43
4:B:88:GLU:HG3	4:B:88:GLU:O	2.18	0.43
8:F:56:PRO:CG	14:M:44:THR:HA	2.48	0.43
9:G:20:VAL:O	9:G:24:VAL:HG23	2.19	0.43
24:W:26:ILE:HB	38:W:5420:HOH:O	2.18	0.43
1:0:365:G:C5	1:0:366:U:C5	3.07	0.43
1:0:947:U:O2'	1:0:948:G:H5'	2.18	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.43
1:0:1215:A:O3'	1:0:1216:G:H4'	2.19	0.43
1:0:1257:C:O2'	1:0:1258:G:H5'	2.18	0.43
1:0:1386:G:O2'	1:0:1387:G:H5'	2.19	0.43
1:0:1772:C:H5'	1:0:1773:G:C5	2.53	0.43
1:0:1778:A:H2'	1:0:1779:A:H5'	2.00	0.43
1:0:1883:U:H5'	1:0:2012:U:OP2	2.19	0.43
1:0:1904:A:H2'	1:0:1905:U:O4'	2.19	0.43
1:0:2460:A:C4	32:0:9000:13T:H20	2.53	0.43
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.34	0.43
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.49	0.43
11:J:47:THR:HG22	11:J:48:GLY:N	2.34	0.43
14:M:46:LEU:HG	38:M:8913:HOH:O	2.18	0.43
24:W:106:THR:OG1	24:W:109:GLU:HB2	2.19	0.43
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.43
1:0:445:U:O2'	1:0:446:G:H5'	2.18	0.43
1:0:1415:G:H5'	28:1:12:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1434:A:H2'	1:0:1436:C:C5	2.53	0.43
1:0:1565:C:O2'	1:0:1566:C:H5'	2.19	0.43
1:0:1850:U:O4'	1:0:1941:A:C2	2.71	0.43
1:0:2036:C:C4'	12:K:44:LEU:HG	2.48	0.43
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.43
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.43
1:0:2856:A:OP1	25:X:15:ARG:NH2	2.51	0.43
38:0:6721:HOH:O	18:Q:2:SER:HA	2.19	0.43
38:0:9208:HOH:O	4:B:248:ARG:NH2	2.51	0.43
2:9:3069:U:OP1	15:N:4:PRO:HG3	2.18	0.43
4:B:33:ASP:HB3	4:B:34:GLY:H	1.60	0.43
11:J:127:ILE:CG2	36:J:8801:CL:CL	3.00	0.43
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.54	0.43
31:I:125:ALA:O	31:I:129:VAL:HG23	2.19	0.43
1:0:134:U:C2	1:0:145:A:C2	3.07	0.43
1:0:228:C:C2'	1:0:229:G:H5'	2.49	0.43
1:0:1191:A:H2	1:0:1206:U:H3	1.67	0.43
1:0:1825:U:O2'	1:0:1826:C:H5'	2.19	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.43
1:0:2254:G:C2	1:0:2255:A:C8	3.06	0.43
1:0:2372:A:H2'	1:0:2373:U:H6	1.82	0.43
32:0:9000:13T:H3	30:3:56:PRO:CB	2.48	0.43
6:D:138:GLY:N	38:D:7597:HOH:O	2.51	0.43
7:E:20:ILE:HD11	7:E:40:VAL:HG11	2.01	0.43
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.49	0.43
12:K:125:ALA:C	12:K:127:ALA:H	2.22	0.43
24:W:5:VAL:HG11	24:W:153:MET:HE3	1.99	0.43
1:0:73:C:O2'	1:0:74:A:H5'	2.18	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.34	0.43
1:0:815:U:O2'	1:0:1598:A:H4'	2.18	0.43
1:0:1080:C:O5'	1:0:1080:C:H6	2.02	0.43
1:0:1114:A:H2'	1:0:1115:U:C6	2.54	0.43
1:0:1163:G:H1	1:0:1184:C:N4	2.17	0.43
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.52	0.43
1:0:1667:A:C2	1:0:1668:U:C2	3.07	0.43
1:0:1805:G:H2'	1:0:1806:G:H8	1.83	0.43
1:0:2255:A:H2'	1:0:2256:G:O4'	2.18	0.43
1:0:2255:A:O2'	1:0:2256:G:H5'	2.18	0.43
1:0:2348:C:H1'	6:D:131:THR:HG21	2.01	0.43
1:0:2598:U:O2	1:0:2600:A:H8	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:177:HIS:O	4:B:181:ILE:HG13	2.19	0.43
11:J:45:VAL:HG21	11:J:129:PHE:HD1	1.82	0.43
14:M:80:GLY:O	14:M:81:ARG:HD3	2.18	0.43
22:U:17:THR:HG22	22:U:18:GLY:N	2.34	0.43
24:W:4:LEU:O	24:W:32:CYS:HA	2.18	0.43
26:Y:107:PRO:HD3	26:Y:182:PHE:CD1	2.54	0.43
29:2:40:ARG:HG3	29:2:45:ASN:CB	2.48	0.43
1:0:559:U:C5	1:0:560:C:C5	3.07	0.42
1:0:571:C:O5'	1:0:571:C:H6	2.01	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.00	0.42
1:0:1242:A:OP2	11:J:60:ARG:NH2	2.47	0.42
1:0:1930:A:H2'	1:0:1931:A:C8	2.54	0.42
1:0:2291:A:H8	38:0:6467:HOH:O	2.01	0.42
1:0:2504:A:H4'	10:H:71:ARG:NH1	2.34	0.42
1:0:2519:C:O2'	1:0:2520:G:H5'	2.19	0.42
1:0:2712:G:H5'	38:0:5223:HOH:O	2.18	0.42
32:0:9000:13T:H233	32:0:9000:13T:H311	2.01	0.42
38:0:6400:HOH:O	24:W:122:ARG:NH2	2.45	0.42
5:C:194:PHE:HA	5:C:234:VAL:HG13	2.01	0.42
6:D:103:ASN:HD22	6:D:133:ASN:HA	1.84	0.42
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.34	0.42
28:1:53:LYS:HA	28:1:53:LYS:HD3	1.85	0.42
1:0:169:A:H1'	30:3:48:ASN:ND2	2.34	0.42
1:0:177:A:H2'	1:0:178:U:O4'	2.19	0.42
1:0:682:A:H2'	1:0:683:G:O4'	2.19	0.42
1:0:952:G:OP1	18:Q:42:LYS:HE2	2.20	0.42
1:0:1138:G:H4'	38:0:5719:HOH:O	2.19	0.42
1:0:1552:G:H2'	1:0:1553:C:C6	2.54	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
2:9:3041:C:C2	6:D:50:VAL:HG21	2.54	0.42
6:D:44:ILE:HG23	6:D:45:THR:HG23	2.00	0.42
10:H:47:ILE:HG21	38:H:8579:HOH:O	2.20	0.42
16:O:21:SER:OG	16:O:106:PRO:HB2	2.18	0.42
16:O:105:ASN:HD21	16:O:109:SER:N	2.18	0.42
19:R:4:TYR:CE1	19:R:15:LYS:HD3	2.53	0.42
21:T:28:SER:O	21:T:32:ARG:HG3	2.18	0.42
26:Y:178:HIS:CG	26:Y:179:PRO:HD2	2.54	0.42
1:0:151:A:H2'	1:0:152:A:O4'	2.18	0.42
1:0:284:C:C4'	1:0:285:A:O5'	2.64	0.42
1:0:644:G:O2'	36:0:8814:CL:CL	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1544:U:H2'	1:0:1545:C:C6	2.54	0.42
1:0:1970:G:H2'	1:0:1970:G:N3	2.35	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
1:0:2608:C:H3'	38:0:7790:HOH:O	2.18	0.42
1:0:2785:C:H4'	1:0:2786:G:OP2	2.19	0.42
38:0:4740:HOH:O	15:N:21:HIS:HD2	2.01	0.42
4:B:165:ARG:HG2	4:B:166:VAL:N	2.35	0.42
4:B:204:GLY:HA3	38:B:8948:HOH:O	2.18	0.42
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.19	0.42
20:S:37:VAL:O	20:S:41:VAL:HG23	2.19	0.42
25:X:30:MET:HE1	25:X:55:ASN:HA	2.00	0.42
1:0:1486:A:C5	29:2:2:LYS:HG3	2.55	0.42
1:0:2296:C:H2'	1:0:2297:U:H6	1.82	0.42
1:0:2415:A:H2'	1:0:2416:G:H5'	2.00	0.42
2:9:3001:U:H4'	2:9:3003:A:OP1	2.19	0.42
14:M:167:GLY:O	14:M:171:ARG:HG3	2.19	0.42
16:O:44:ASN:HA	16:O:65:LEU:O	2.19	0.42
22:U:6:CYS:HB2	22:U:32:CYS:HB3	2.00	0.42
1:0:263:U:C4	8:F:54:VAL:HG13	2.54	0.42
1:0:395:A:H4'	38:0:9964:HOH:O	2.20	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.19	0.42
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.42
1:0:2035:C:O5'	1:0:2035:C:H6	2.02	0.42
1:0:2395:A:C6	1:0:2396:C:C4	3.07	0.42
1:0:2502:C:O2'	1:0:2503:A:H5'	2.18	0.42
1:0:2909:G:O2'	1:0:2910:A:H5'	2.20	0.42
2:9:3031:C:H1'	38:9:1137:HOH:O	2.18	0.42
12:K:28:GLU:HB3	12:K:59:LYS:HB2	2.01	0.42
13:L:73:VAL:HG11	13:L:118:LEU:HD21	2.01	0.42
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.55	0.42
17:P:103:THR:O	17:P:107:GLU:HG3	2.20	0.42
28:1:26:SER:HB3	28:1:35:SER:OG	2.20	0.42
1:0:475:G:C5'	5:C:73:LEU:HD23	2.50	0.42
1:0:482:G:O4'	1:0:511:A:C2	2.72	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
1:0:1046:G:N3	1:0:1082:A:H2	2.17	0.42
1:0:1175:G:H1'	1:0:1193:A:H2'	2.01	0.42
1:0:2105:C:O2'	1:0:2284:G:N2	2.52	0.42
1:0:2265:U:H2'	1:0:2266:A:C8	2.55	0.42
1:0:2607:U:H4'	38:0:9438:HOH:O	2.18	0.42
2:9:3034:A:H8	2:9:3034:A:O5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:9:ARG:NH1	38:A:8822:HOH:O	2.53	0.42
11:J:39:VAL:HG13	11:J:106:GLY:O	2.20	0.42
14:M:28:GLN:O	14:M:32:ARG:HG3	2.18	0.42
15:N:170:GLU:O	15:N:174:GLU:HG3	2.20	0.42
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.42
25:X:80:GLU:HB3	38:X:5564:HOH:O	2.17	0.42
26:Y:151:SER:HB3	26:Y:154:ARG:CB	2.49	0.42
1:0:316:A:H5'	21:T:54:ASP:OD2	2.20	0.42
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.42
1:0:535:G:C6	1:0:2064:U:C5	3.08	0.42
1:0:876:A:N3	1:0:876:A:C2'	2.83	0.42
1:0:1323:G:N2	1:0:1335:C:C2	2.88	0.42
32:0:9000:13T:H323	32:0:9000:13T:C1	2.49	0.42
38:0:3186:HOH:O	14:M:9:ARG:HG3	2.19	0.42
2:9:3059:C:H5'	38:9:5233:HOH:O	2.18	0.42
2:9:3110:G:C5	2:9:3111:U:C5	3.07	0.42
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.42
11:J:59:LYS:O	11:J:63:ILE:HG13	2.19	0.42
30:3:22:VAL:HG11	30:3:67:LEU:HD13	2.01	0.42
1:0:447:A:OP1	21:T:2:LYS:HG2	2.20	0.42
1:0:595:U:H2'	1:0:596:C:H6	1.85	0.42
1:0:1161:A:O5'	1:0:1161:A:H8	2.02	0.42
1:0:1579:C:H4'	1:0:1580:A:OP1	2.19	0.42
1:0:2078:U:O2'	1:0:2079:G:H5'	2.20	0.42
1:0:2256:G:C2'	1:0:2257:G:C5'	2.93	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.42
38:0:3652:HOH:O	16:O:3:THR:HG21	2.19	0.42
38:0:4574:HOH:O	5:C:50:GLU:HG2	2.20	0.42
2:9:3013:A:H3'	2:9:3014:G:H5'	2.02	0.42
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.42
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.02	0.42
5:C:218:VAL:HG12	38:C:8623:HOH:O	2.19	0.42
12:K:4:LEU:HD23	12:K:4:LEU:HA	1.83	0.42
13:L:120:LEU:HD12	13:L:133:VAL:HG21	2.02	0.42
1:0:282:C:O2'	1:0:283:U:C4'	2.68	0.42
1:0:318:C:H5'	1:0:339:A:N3	2.35	0.42
1:0:589:U:H2'	1:0:590:A:C8	2.54	0.42
1:0:825:U:H5"	1:0:826:U:OP1	2.20	0.42
1:0:856:G:H2'	38:0:5435:HOH:O	2.18	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.20	0.42
1:0:1923:G:H2'	1:0:1924:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2758:G:H2'	1:0:2759:C:C6	2.55	0.42
2:9:3059:C:H2'	2:9:3060:C:C6	2.55	0.42
6:D:25:MET:HE1	6:D:37:ALA:O	2.20	0.42
6:D:64:ARG:HD3	6:D:67:ASP:HB3	2.02	0.42
22:U:6:CYS:C	22:U:8:TYR:H	2.21	0.42
26:Y:170:SER:OG	26:Y:175:ARG:HG3	2.19	0.42
1:0:561:G:C2	1:0:562:A:C5	3.08	0.42
1:0:1055:G:OP2	10:H:96:ARG:NH1	2.53	0.42
1:0:1482:A:O2'	1:0:1483:C:H5'	2.20	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.42
1:0:2240:U:O2'	1:0:2241:C:H5'	2.19	0.42
1:0:2521:A:P	10:H:3:ALA:HB3	2.60	0.42
1:0:2612:A:H4'	38:0:3685:HOH:O	2.19	0.42
1:0:2824:C:O3'	1:0:2825:C:H6	2.01	0.42
2:9:3114:G:H2'	2:9:3115:C:C6	2.55	0.42
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.01	0.42
4:B:79:MET:HB2	4:B:79:MET:HE3	1.99	0.42
4:B:305:ASP:O	4:B:306:LYS:CB	2.68	0.42
6:D:23:VAL:HG21	6:D:45:THR:HG21	2.02	0.42
19:R:132:ARG:NH2	38:R:8879:HOH:O	2.52	0.42
1:0:517:U:C2'	1:0:518:G:H5'	2.50	0.41
1:0:941:G:C2'	1:0:942:U:H5'	2.50	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
1:0:1019:C:O2	18:Q:94:GLN:NE2	2.53	0.41
1:0:1762:C:H4'	38:0:4662:HOH:O	2.19	0.41
1:0:2032:U:O2'	1:0:2033:G:H5"	2.20	0.41
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.55	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:2589:U:H2'	1:0:2590:U:C6	2.55	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
2:9:3059:C:H6	2:9:3059:C:O5'	2.03	0.41
2:9:3105:A:C2'	2:9:3106:C:H5'	2.49	0.41
3:A:76:VAL:HG23	27:Z:63:LYS:HB3	2.00	0.41
3:A:131:HIS:O	3:A:132:ASP:HB2	2.20	0.41
4:B:260:HIS:HE1	38:B:8883:HOH:O	2.03	0.41
6:D:25:MET:SD	6:D:40:ILE:HD11	2.60	0.41
6:D:48:MET:HA	6:D:49:PRO:HD3	1.87	0.41
19:R:18:LEU:HD12	19:R:143:VAL:HG11	2.02	0.41
1:0:381:G:OP2	14:M:45:ARG:NH2	2.50	0.41
1:0:497:A:H2'	1:0:498:A:C5'	2.50	0.41
1:0:553:G:H2'	1:0:554:G:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:699:C:C6	1:0:744:G:C4	3.08	0.41
1:0:1904:A:C8	1:0:1905:U:C5	3.08	0.41
1:0:2112:A:H2'	1:0:2113:G:H8	1.85	0.41
1:0:2254:G:O2'	1:0:2255:A:H5'	2.20	0.41
1:0:2402:A:H1'	38:0:3163:HOH:O	2.20	0.41
1:0:2689:A:C2'	1:0:2690:U:H5'	2.50	0.41
1:0:2754:G:C2'	1:0:2755:G:H5'	2.50	0.41
6:D:49:PRO:HG3	38:D:5828:HOH:O	2.21	0.41
8:F:14:ASP:O	8:F:18:GLU:HG3	2.20	0.41
8:F:48:VAL:HG23	8:F:74:PHE:HB3	2.01	0.41
14:M:164:THR:HG22	14:M:167:GLY:N	2.35	0.41
22:U:17:THR:CG2	22:U:18:GLY:N	2.83	0.41
28:1:25:LYS:HD2	29:2:49:GLU:H	1.84	0.41
31:I:100:LEU:HD22	31:I:105:VAL:HG23	2.02	0.41
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.41
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.41
1:0:459:A:H5"	38:0:9047:HOH:O	2.20	0.41
1:0:694:A:H4'	1:0:2441:U:OP1	2.21	0.41
1:0:902:G:N7	13:L:18:HIS:CD2	2.85	0.41
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.41
1:0:1225:C:H2'	1:0:1226:G:O4'	2.21	0.41
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.41
1:0:1576:G:H2'	1:0:1577:U:H6	1.85	0.41
1:0:2434:A:O3'	30:3:28:GLY:HA3	2.20	0.41
2:9:3033:U:H2'	38:9:3797:HOH:O	2.19	0.41
2:9:3042:C:O2	6:D:76:ARG:NH1	2.52	0.41
2:9:3105:A:H2'	2:9:3106:C:H5'	2.03	0.41
7:E:84:MET:HG2	7:E:168:ILE:HA	2.02	0.41
10:H:171:ALA:HA	38:H:8570:HOH:O	2.20	0.41
11:J:19:MET:CE	11:J:132:LEU:HD11	2.51	0.41
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.35	0.41
24:W:4:LEU:CD1	24:W:24:LEU:HD13	2.50	0.41
26:Y:112:GLU:CD	26:Y:115:ARG:NH1	2.74	0.41
27:Z:30:GLU:HB2	38:Z:8715:HOH:O	2.20	0.41
28:1:25:LYS:HE2	38:2:7213:HOH:O	2.20	0.41
31:I:91:GLU:HA	31:I:92:PRO:HD2	1.84	0.41
1:0:81:G:N3	1:0:98:A:C2	2.89	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.54	0.41
1:0:1422:U:H4'	38:0:7732:HOH:O	2.19	0.41
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.41
1:0:1943:C:C4'	3:A:212:PRO:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.86	0.41
1:0:2634:G:OP2	3:A:204:GLY:N	2.53	0.41
1:0:2825:C:H4'	1:0:2826:G:O5'	2.20	0.41
11:J:19:MET:HE1	11:J:132:LEU:HD11	2.02	0.41
11:J:74:ARG:HH11	11:J:74:ARG:CB	2.30	0.41
15:N:42:HIS:CG	15:N:62:HIS:HE1	2.38	0.41
25:X:7:GLU:HA	25:X:74:ALA:O	2.20	0.41
1:0:61:G:C6	1:0:62:C:C4	3.09	0.41
1:0:308:U:C4	1:0:342:C:C1'	3.03	0.41
1:0:849:C:O2'	1:0:850:U:H5'	2.21	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.56	0.41
1:0:1024:G:C6	1:0:1025:C:C4	3.08	0.41
1:0:1052:G:N3	1:0:1052:G:H2'	2.35	0.41
1:0:1400:C:O2'	1:0:1401:G:H5'	2.21	0.41
1:0:1923:G:H2'	1:0:1924:A:C8	2.56	0.41
2:9:3001:U:H5'	2:9:3121:C:O2	2.20	0.41
2:9:3001:U:O3'	2:9:3003:A:C5'	2.69	0.41
2:9:3092:G:C6	2:9:3093:A:N6	2.88	0.41
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.86	0.41
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.48	0.41
14:M:182:LYS:HB2	14:M:194:ALA:HB2	2.01	0.41
24:W:149:LEU:HG	24:W:153:MET:HE2	2.03	0.41
25:X:74:ALA:CB	25:X:85:VAL:HG22	2.51	0.41
27:Z:67:GLY:N	27:Z:70:LYS:O	2.54	0.41
1:0:255:A:C5	1:0:256:C:C5	3.09	0.41
1:0:863:G:C6	1:0:864:U:C4	3.08	0.41
1:0:1206:U:H6	1:0:1206:U:C5'	2.23	0.41
1:0:2775:A:C6	1:0:2776:A:C6	3.08	0.41
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.51	0.41
18:Q:16:ASN:OD1	18:Q:45:PRO:HB2	2.20	0.41
24:W:19:ASP:O	24:W:23:MET:HG3	2.20	0.41
31:I:129:VAL:HG12	31:I:129:VAL:O	2.21	0.41
1:0:25:A:O2'	1:0:640:G:H5'	2.21	0.41
1:0:298:C:H6	1:0:298:C:O5'	2.04	0.41
1:0:1181:A:C2'	1:0:1182:C:H5'	2.51	0.41
1:0:1224:G:H2'	1:0:1225:C:C6	2.55	0.41
1:0:2549:C:O2'	1:0:2550:U:H5'	2.20	0.41
4:B:7:ARG:HH11	4:B:7:ARG:HG2	1.85	0.41
7:E:5:LEU:HD21	7:E:66:GLN:HG3	2.01	0.41
14:M:123:ASP:OD1	14:M:126:GLN:HG2	2.19	0.41
24:W:119:HIS:HD2	24:W:120:PRO:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:247:A:H1'	38:0:3892:HOH:O	2.21	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.20	0.41
1:0:539:G:H2'	1:0:540:A:C8	2.56	0.41
1:0:912:A:C4	1:0:1294:A:C2	3.09	0.41
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.41
1:0:1609:C:H2'	1:0:1610:G:H8	1.84	0.41
1:0:1622:G:H2'	1:0:1623:C:H5'	2.02	0.41
1:0:2036:C:C1'	12:K:44:LEU:HG	2.51	0.41
1:0:2303:A:H2	38:Q:5641:HOH:O	2.03	0.41
1:0:2365:G:H4'	18:Q:45:PRO:O	2.20	0.41
1:0:2716:G:H5"	4:B:206:THR:CG2	2.44	0.41
2:9:3003:A:H61	2:9:3022:G:H1'	1.83	0.41
12:K:132:VAL:HG21	22:U:22:VAL:CG1	2.50	0.41
13:L:92:ASP:HA	13:L:121:ILE:HB	2.02	0.41
14:M:158:ARG:HB2	14:M:163:LEU:HB2	2.03	0.41
19:R:72:VAL:CG1	19:R:75:TRP:HB3	2.50	0.41
20:S:45:TYR:O	20:S:80:ARG:NH2	2.53	0.41
26:Y:144:ARG:NH2	38:Y:8912:HOH:O	2.54	0.41
1:0:66:G:C2	1:0:109:U:C4	3.08	0.41
1:0:169:A:H4'	38:M:8837:HOH:O	2.20	0.41
1:0:287:C:H6	1:0:287:C:O5'	2.04	0.41
1:0:327:A:H4'	1:0:329:A:C8	2.55	0.41
1:0:368:C:H2'	1:0:369:G:H5'	2.02	0.41
1:0:483:C:C4	1:0:484:A:C6	3.09	0.41
1:0:567:U:O2'	1:0:568:G:H5'	2.20	0.41
1:0:581:G:O2'	1:0:582:C:H5'	2.21	0.41
1:0:911:G:H5'	1:0:932:U:OP1	2.21	0.41
1:0:1115:U:O2'	1:0:1116:U:H5'	2.20	0.41
1:0:1116:U:C2	1:0:1246:A:N6	2.89	0.41
1:0:1157:C:O2'	1:0:1158:G:H5'	2.20	0.41
1:0:1166:A:P	1:0:1174:A:H4'	2.61	0.41
1:0:1619:G:C6	1:0:1620:C:N3	2.89	0.41
1:0:1630:A:O2'	1:0:1631:A:H5'	2.21	0.41
1:0:1666:C:H2'	1:0:1667:A:H8	1.86	0.41
1:0:1786:C:OP1	17:P:74:GLN:HG2	2.21	0.41
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.41
1:0:2398:A:H2'	1:0:2399:G:O4'	2.21	0.41
1:0:2415:A:O2'	15:N:29:SER:HB3	2.21	0.41
1:0:2569:A:H2'	1:0:2570:G:O5'	2.20	0.41
1:0:2607:U:C4	4:B:242:TRP:CZ2	3.08	0.41
1:0:2727:A:N1	1:0:2756:U:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2768:A:H5"	38:0:4432:HOH:O	2.21	0.41
2:9:3001:U:C4'	2:9:3003:A:OP1	2.69	0.41
2:9:3040:C:OP1	2:9:3041:C:H5	2.04	0.41
2:9:3065:A:O2'	2:9:3066:G:P	2.79	0.41
2:9:3104:A:C2'	2:9:3105:A:H5'	2.50	0.41
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.51	0.41
3:A:186:TRP:CG	3:A:187:PRO:HA	2.56	0.41
4:B:23:THR:HG23	4:B:308:LEU:CD2	2.51	0.41
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.56	0.41
4:B:52:VAL:O	4:B:53:LEU:HD12	2.21	0.41
4:B:265:LEU:HD21	4:B:316:ARG:HD3	2.01	0.41
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.56	0.41
5:C:228:ALA:HA	5:C:229:PRO:HD3	1.90	0.41
6:D:151:ILE:HA	6:D:152:PRO:HD3	1.92	0.41
11:J:42:GLU:HG2	11:J:43:ARG:HG3	2.03	0.41
19:R:113:HIS:O	19:R:145:LEU:HD12	2.20	0.41
21:T:3:GLN:HA	21:T:4:PRO:HD3	1.76	0.41
21:T:32:ARG:NH1	21:T:38:ARG:NH1	2.69	0.41
24:W:81:ASP:OD1	24:W:92:ASP:HB2	2.20	0.41
31:I:131:THR:O	31:I:135:LEU:HG	2.21	0.41
1:0:380:A:O4'	1:0:382:U:H1'	2.21	0.41
1:0:397:A:H1'	1:0:417:G:H1'	2.02	0.41
1:0:716:G:C6	1:0:717:C:N4	2.89	0.41
1:0:1182:C:O5'	1:0:1182:C:H6	2.02	0.41
1:0:1299:G:N2	38:0:4691:HOH:O	2.53	0.41
1:0:1594:C:OP1	17:P:109:ARG:NH1	2.54	0.41
1:0:1662:C:H2'	1:0:1663:G:O4'	2.21	0.41
1:0:2004:U:H5"	1:0:2005:G:C8	2.56	0.41
1:0:2363:G:H2'	1:0:2364:A:O4'	2.21	0.41
1:0:2791:U:H1'	1:0:2792:A:H5"	2.03	0.41
1:0:2791:U:H4'	1:0:2792:A:OP1	2.21	0.41
1:0:2897:C:O2'	1:0:2898:G:H5'	2.21	0.41
32:0:9000:13T:H261	32:0:9000:13T:H10	1.80	0.41
3:A:68:ILE:HD11	38:A:8863:HOH:O	2.20	0.41
13:L:119:THR:HA	13:L:139:SER:O	2.21	0.41
17:P:115:SER:O	17:P:117:SER:N	2.46	0.41
26:Y:144:ARG:NE	38:Y:8912:HOH:O	2.54	0.41
1:0:228:C:H2'	1:0:229:G:C5'	2.51	0.40
1:0:445:U:C1'	38:0:7326:HOH:O	2.68	0.40
1:0:545:G:H2'	1:0:546:C:O4'	2.21	0.40
1:0:1449:G:N3	1:0:1449:G:H2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1745:G:H5'	38:0:4341:HOH:O	2.20	0.40
1:0:1925:G:O2'	1:0:1926:G:H5'	2.21	0.40
1:0:2072:G:H3'	1:0:2073:G:C5'	2.52	0.40
1:0:2549:C:H2'	1:0:2550:U:O4'	2.22	0.40
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.40
1:0:2887:G:H2'	1:0:2888:U:O4'	2.21	0.40
3:A:33:GLU:CD	3:A:33:GLU:H	2.24	0.40
4:B:198:GLU:HA	38:B:8952:HOH:O	2.20	0.40
4:B:305:ASP:O	4:B:306:LYS:HB2	2.21	0.40
4:B:336:GLN:NE2	38:B:8822:HOH:O	2.53	0.40
7:E:22:VAL:O	7:E:28:SER:HA	2.22	0.40
7:E:69:ILE:HA	7:E:72:MET:HE2	2.03	0.40
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.21	0.40
9:G:67:LEU:O	9:G:71:LEU:HG	2.21	0.40
19:R:89:LEU:HD23	19:R:89:LEU:HA	1.84	0.40
26:Y:189:ASN:ND2	26:Y:192:ASP:N	2.69	0.40
1:0:535:G:O6	1:0:2064:U:C6	2.75	0.40
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.40
1:0:567:U:O5'	1:0:567:U:H6	2.04	0.40
1:0:699:C:H6	1:0:744:G:O4'	2.03	0.40
1:0:1310:U:P	5:C:168:ARG:HH11	2.44	0.40
1:0:1457:U:H5	38:0:7859:HOH:O	2.04	0.40
1:0:1494:A:H1'	1:0:1495:C:C6	2.56	0.40
1:0:1574:C:O5'	1:0:1574:C:H6	2.04	0.40
1:0:1642:A:N7	1:0:1643:C:C4	2.89	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:2064:U:H2'	1:0:2065:C:H6	1.86	0.40
1:0:2344:G:H2'	1:0:2344:G:N3	2.36	0.40
1:0:2361:A:H2'	1:0:2362:A:O4'	2.21	0.40
1:0:2453:G:O3'	13:L:50:GLY:HA2	2.21	0.40
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.54	0.40
26:Y:134:HIS:H	26:Y:134:HIS:CD2	2.38	0.40
1:0:74:A:H2'	1:0:75:U:C6	2.55	0.40
1:0:574:C:H2'	1:0:575:G:O4'	2.21	0.40
1:0:844:A:C6	1:0:882:A:C6	3.09	0.40
1:0:1268:C:O2'	26:Y:169:ARG:HB2	2.21	0.40
1:0:1902:G:H2'	1:0:1903:U:O4'	2.21	0.40
1:0:2642:G:H2'	1:0:2643:G:O4'	2.22	0.40
1:0:2902:A:H4'	1:0:2903:C:OP1	2.21	0.40
3:A:105:VAL:HG12	3:A:106:CYS:N	2.36	0.40
6:D:25:MET:HE3	6:D:37:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:72:ALA:HB2	14:M:93:ARG:HG2	2.03	0.40
17:P:121:ASP:HB2	38:P:5891:HOH:O	2.21	0.40
24:W:13:MET:CE	24:W:18:GLN:HA	2.49	0.40
24:W:65:VAL:HG12	24:W:116:LEU:HD13	2.04	0.40
26:Y:177:LYS:HD3	26:Y:181:GLY:O	2.22	0.40
1:0:243:A:H2	1:0:274:G:N3	2.19	0.40
1:0:260:C:C4	1:0:261:A:C5	3.10	0.40
1:0:474:C:O3'	5:C:73:LEU:HD21	2.22	0.40
1:0:485:A:HO2'	1:0:487:G:H8	1.68	0.40
1:0:517:U:H2'	1:0:518:G:H5'	2.03	0.40
1:0:559:U:C6	1:0:559:U:C4'	3.04	0.40
1:0:705:C:O2	1:0:705:C:C2'	2.70	0.40
1:0:1006:A:N1	1:0:2311:A:H1'	2.37	0.40
1:0:1087:G:H4'	1:0:1088:A:OP1	2.22	0.40
1:0:1180:U:O2'	31:I:92:PRO:HD2	2.21	0.40
1:0:1189:A:C3'	38:0:7666:HOH:O	2.62	0.40
1:0:1308:A:O4'	5:C:226:GLY:HA3	2.21	0.40
1:0:1309:U:H2'	1:0:1310:U:O4'	2.21	0.40
1:0:1705:C:P	17:P:59:ARG:HH12	2.45	0.40
1:0:1741:U:H3'	38:0:9763:HOH:O	2.20	0.40
1:0:2673:U:C4	1:0:2674:G:C6	3.10	0.40
1:0:2754:G:HO2'	1:0:2755:G:H5'	1.85	0.40
2:9:3110:G:C2'	2:9:3111:U:H5'	2.51	0.40
38:9:466:HOH:O	18:Q:25:PRO:HB3	2.21	0.40
5:C:175:LYS:HD2	5:C:187:ARG:HB3	2.04	0.40
6:D:25:MET:CE	6:D:37:ALA:HB1	2.51	0.40
6:D:64:ARG:HB3	6:D:67:ASP:OD2	2.22	0.40
12:K:62:PRO:HG3	12:K:65:ARG:NH2	2.37	0.40
16:O:14:LEU:HB3	16:O:26:TRP:O	2.21	0.40
16:O:45:LEU:CD1	16:O:88:LYS:HD2	2.51	0.40
25:X:30:MET:CE	25:X:58:ALA:HB3	2.52	0.40
1:0:160:A:C4	1:0:177:A:C2	3.09	0.40
1:0:245:C:H2'	1:0:246:G:H5'	2.04	0.40
1:0:820:G:H5'	1:0:821:U:C5'	2.51	0.40
1:0:1329:A:H5"	38:0:3790:HOH:O	2.20	0.40
1:0:1334:C:H2'	1:0:1335:C:H6	1.86	0.40
1:0:1453:G:H2'	1:0:1454:U:O4'	2.22	0.40
1:0:1544:U:H2'	1:0:1545:C:H6	1.87	0.40
1:0:1617:C:C4	1:0:1643:C:H4'	2.57	0.40
1:0:2739:A:C6	1:0:2740:G:C5	3.09	0.40
7:E:6:GLU:HA	7:E:46:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:58:GLU:HA	8:F:61:MET:CE	2.47	0.40
14:M:28:GLN:HA	14:M:31:TRP:HB2	2.03	0.40
17:P:40:VAL:O	17:P:44:VAL:HG23	2.22	0.40
19:R:17:MET:HE3	19:R:19:ARG:HH21	1.86	0.40
23:V:39:ALA:O	23:V:41:GLU:N	2.51	0.40
25:X:8:ARG:NH1	38:X:2479:HOH:O	2.49	0.40
27:Z:49:ARG:NH2	27:Z:52:THR:HA	2.37	0.40
29:2:49:GLU:HB2	38:2:131:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	212 (90%)	21 (9%)	2 (1%)	17	48
4	B	335/338 (99%)	310 (92%)	21 (6%)	4 (1%)	13	40
5	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	19	51
6	D	134/177 (76%)	113 (84%)	18 (13%)	3 (2%)	6	24
7	E	170/178 (96%)	163 (96%)	6 (4%)	1 (1%)	25	58
8	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	5	20
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	8	28
11	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	11	36
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	121 (86%)	20 (14%)	0	100	100
14	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
15	N	184/187 (98%)	167 (91%)	13 (7%)	4 (2%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
17	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	22	54
18	Q	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	14	42
19	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
20	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	17	48
22	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
24	W	152/154 (99%)	150 (99%)	0	2 (1%)	12	37
25	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	12	37
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	60 (84%)	9 (13%)	2 (3%)	5	19
28	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
31	I	68/161 (42%)	62 (91%)	6 (9%)	0	100	100
All	All	3705/4419 (84%)	3436 (93%)	237 (6%)	32 (1%)	17	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	101	ALA
10	H	166	SER
11	J	5	GLU
15	N	154	LEU
15	N	183	ASP
15	N	184	ILE
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
6	D	27	ILE
6	D	137	PRO
6	D	173	GLU
8	F	44	SER
24	W	49	ASN
3	A	37	VAL

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Mol	Chain	Res	Type
15	N	139	TRP
27	Z	42	CYS
5	C	79	ARG
10	H	16	ARG
10	H	168	ALA
17	P	117	SER
25	X	70	ILE
4	B	2	GLN
5	C	8	LEU
8	F	64	PRO
21	T	44	ALA
24	W	77	ALA
4	B	306	LYS
7	E	44	GLY
11	J	89	HIS
18	Q	18	PRO
27	Z	43	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	170 (95%)	9 (5%)	24	57
4	B	282/283 (100%)	268 (95%)	14 (5%)	24	57
5	C	193/193 (100%)	178 (92%)	15 (8%)	12	34
6	D	117/148 (79%)	115 (98%)	2 (2%)	60	86
7	E	152/156 (97%)	149 (98%)	3 (2%)	55	82
8	F	93/94 (99%)	89 (96%)	4 (4%)	29	62
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	126 (96%)	6 (4%)	27	61
11	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
12	K	106/106 (100%)	104 (98%)	2 (2%)	57	84
13	L	113/127 (89%)	107 (95%)	6 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	158/158 (100%)	149 (94%)	9 (6%)	20	51
15	N	149/150 (99%)	146 (98%)	3 (2%)	55	82
16	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
17	P	113/117 (97%)	109 (96%)	4 (4%)	36	70
18	Q	79/80 (99%)	78 (99%)	1 (1%)	69	90
19	R	117/122 (96%)	113 (97%)	4 (3%)	37	71
20	S	71/74 (96%)	70 (99%)	1 (1%)	67	89
21	T	105/106 (99%)	99 (94%)	6 (6%)	20	51
22	U	44/52 (85%)	43 (98%)	1 (2%)	50	80
23	V	51/57 (90%)	49 (96%)	2 (4%)	32	66
24	W	130/130 (100%)	124 (95%)	6 (5%)	27	60
25	X	66/74 (89%)	61 (92%)	5 (8%)	13	36
26	Y	120/196 (61%)	114 (95%)	6 (5%)	24	57
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/47 (98%)	45 (98%)	1 (2%)	52	81
29	2	42/46 (91%)	40 (95%)	2 (5%)	25	58
30	3	79/79 (100%)	78 (99%)	1 (1%)	69	90
31	I	58/129 (45%)	56 (97%)	2 (3%)	37	71
All	All	3093/3602 (86%)	2969 (96%)	124 (4%)	31	65

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	36	ASP
3	A	69	LEU
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP

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Mol	Chain	Res	Type
4	B	56	ASP
4	B	97	LEU
4	B	98	THR
4	B	149	ASP
4	B	162	MET
4	B	175	LEU
4	B	195	ARG
4	B	254	GLN
4	B	257	THR
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG
5	C	91	PRO
5	C	94	THR
5	C	115	LEU
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	236	THR
5	C	240	LEU
6	D	61	PHE
6	D	149	ARG
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
8	F	24	ARG
8	F	46	GLU
8	F	103	GLU
10	H	59	HIS
10	H	62	LEU
10	H	84	LYS
10	H	96	ARG
10	H	119	LYS
10	H	154	TYR
11	J	46	ILE
11	J	52	GLN

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Mol	Chain	Res	Type
11	J	74	ARG
11	J	79	PHE
11	J	93	ARG
11	J	107	ASN
11	J	120	SER
11	J	132	LEU
12	K	10	GLN
12	K	132	VAL
13	L	30	ARG
13	L	35	ARG
13	L	51	PHE
13	L	99	GLU
13	L	101	ASP
13	L	140	VAL
14	M	10	ASP
14	M	46	LEU
14	M	68	ARG
14	M	75	ARG
14	M	81	ARG
14	M	93	ARG
14	M	99	ARG
14	M	116	ASN
14	M	164	THR
15	N	26	LEU
15	N	49	THR
15	N	138	ASP
16	O	43	VAL
17	P	21	VAL
17	P	52	LYS
17	P	91	LYS
17	P	98	ILE
18	Q	95	GLU
19	R	13	THR
19	R	82	GLU
19	R	132	ARG
19	R	143	VAL
20	S	72	ASP
21	T	39	ASN
21	T	48	VAL
21	T	73	HIS
21	T	89	ARG
21	T	96	VAL

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Mol	Chain	Res	Type
21	T	117	ASP
22	U	47	ARG
23	V	12	THR
23	V	65	ASP
24	W	26	ILE
24	W	35	VAL
24	W	73	LEU
24	W	109	GLU
24	W	142	ASP
24	W	146	ILE
25	X	15	ARG
25	X	27	ASP
25	X	52	PRO
25	X	72	VAL
25	X	82	GLU
26	Y	154	ARG
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL
26	Y	204	ARG
26	Y	220	GLU
28	1	47	ASP
29	2	18	ASN
29	2	31	ARG
30	3	3	MET
31	I	87	THR
31	I	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	176	HIS
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	129	HIS

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Mol	Chain	Res	Type
6	D	85	GLN
6	D	103	ASN
6	D	133	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	46	GLN
10	H	56	GLN
10	H	59	HIS
10	H	170	ASN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	42	ASN
13	L	18	HIS
13	L	41	HIS
13	L	42	ASN
13	L	116	HIS
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
14	M	170	ASN
15	N	21	HIS
15	N	107	ASN
17	P	50	GLN
17	P	73	HIS
17	P	118	GLN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	123	GLN
20	S	9	HIS
20	S	53	ASN
21	T	39	ASN
22	U	39	ASN
22	U	48	ASN
23	V	60	GLN
24	W	28	HIS
24	W	110	GLN
24	W	119	HIS

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Mol	Chain	Res	Type
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	134	HIS
26	Y	149	GLN
26	Y	188	HIS
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	18	ASN
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	30	GLN
30	3	48	ASN
31	I	93	GLN
31	I	107	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	241 (8%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	259 (9%)	34 (1%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
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

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Mol	Chain	Res	Type
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
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	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
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	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	588	G
1	0	604	G
1	0	620	A
1	0	632	A

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Mol	Chain	Res	Type
1	0	644	G
1	0	660	A
1	0	688	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	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
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	1003	U
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	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G

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Mol	Chain	Res	Type
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	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	1192	A
1	0	1193	A
1	0	1205	U
1	0	1206	U
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	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G

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Mol	Chain	Res	Type
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	1730	G
1	0	1731	C
1	0	1732	A
1	0	1742	A
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	1979	G
1	0	1996	U
1	0	2006	C
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

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Mol	Chain	Res	Type
1	0	2110	G
1	0	2238	A
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	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2468	A
1	0	2469	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
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	2634	G
1	0	2638	G
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C

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Mol	Chain	Res	Type
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	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2867	G
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	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G
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 (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U

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Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1165	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1506	U
1	0	1563	G
1	0	1667	A
1	0	1685	A
1	0	1942	A
1	0	2313	C
1	0	2361	A
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
2	9	3065	A

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

5 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	1MA	0	628	1	16,25,26	1.33	3 (18%)	18,37,40	1.05	2 (11%)
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	19,38,41	0.71	1 (5%)
1	OMU	0	2587	1	19,22,23	0.32	0	26,31,34	0.42	0
1	PSU	0	2621	1	18,21,22	1.50	2 (11%)	22,30,33	1.31	3 (13%)
1	UR3	0	2619	1	19,22,23	0.48	0	26,32,35	0.68	1 (3%)

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	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.98	1.43	1.36
1	0	628	1MA	C2-N3	3.37	1.33	1.29
1	0	2588	OMG	C5-C6	-3.09	1.41	1.47
1	0	2621	PSU	C6-C5	2.66	1.38	1.35
1	0	628	1MA	C6-N6	2.42	1.33	1.27
1	0	2588	OMG	C8-N7	-2.37	1.31	1.35
1	0	628	1MA	C8-N7	-2.14	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.52	120.66	118.20
1	0	2621	PSU	C6-N1-C2	-2.86	119.75	122.68
1	0	2621	PSU	O2-C2-N1	2.79	125.86	122.79
1	0	628	1MA	N1-C2-N3	2.69	129.16	126.02
1	0	628	1MA	C5-C6-N1	2.53	117.67	113.90
1	0	2619	UR3	C4-N3-C2	2.43	126.86	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2588	OMG	O6-C6-C5	2.12	128.50	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
32	13T	0	9000	-	41,43,43	2.02	10 (24%)	51,63,63	1.75	9 (17%)

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
32	13T	0	9000	-	-	15/73/81/81	0/1/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	13T	C18-C19	7.20	1.56	1.47
32	0	9000	13T	C10-C9	3.89	1.57	1.51
32	0	9000	13T	O2-C1	3.33	1.29	1.21
32	0	9000	13T	O5-C5	3.27	1.26	1.21
32	0	9000	13T	C9-C8	3.21	1.40	1.33
32	0	9000	13T	O7-C11	2.98	1.26	1.21
32	0	9000	13T	C29-C16	2.69	1.55	1.52
32	0	9000	13T	C27-C10	2.37	1.57	1.54
32	0	9000	13T	C26-C8	2.25	1.54	1.50
32	0	9000	13T	O1-C1	2.11	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	9000	13T	C18-O11-C19	7.60	65.36	60.79
32	0	9000	13T	O4-C3-C4	4.13	115.61	105.83
32	0	9000	13T	O11-C18-C19	-4.10	56.62	59.38
32	0	9000	13T	C27-C10-C9	2.56	113.14	110.75
32	0	9000	13T	O11-C19-C18	-2.55	58.01	59.83
32	0	9000	13T	C7-C6-C5	-2.21	106.74	109.48
32	0	9000	13T	C19-C20-C21	-2.21	108.45	113.94
32	0	9000	13T	C29-O1-C1	2.15	121.09	116.84
32	0	9000	13T	O1-C1-O2	2.11	128.12	124.13

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	9000	13T	C2-C3-O4-C32
32	0	9000	13T	C1-C2-C3-O4
32	0	9000	13T	O6-C7-C8-C9
32	0	9000	13T	O6-C7-C8-C26
32	0	9000	13T	C6-C7-C8-C9
32	0	9000	13T	C6-C7-C8-C26
32	0	9000	13T	C18-C19-C20-C21
32	0	9000	13T	O11-C19-C20-C21
32	0	9000	13T	O11-C19-C20-C31
32	0	9000	13T	C14-C15-C16-C29
32	0	9000	13T	O9-C15-C16-C17
32	0	9000	13T	C14-C15-C16-C17
32	0	9000	13T	O9-C15-C16-C29
32	0	9000	13T	C12-C13-C14-C15
32	0	9000	13T	C31-C20-C21-C22

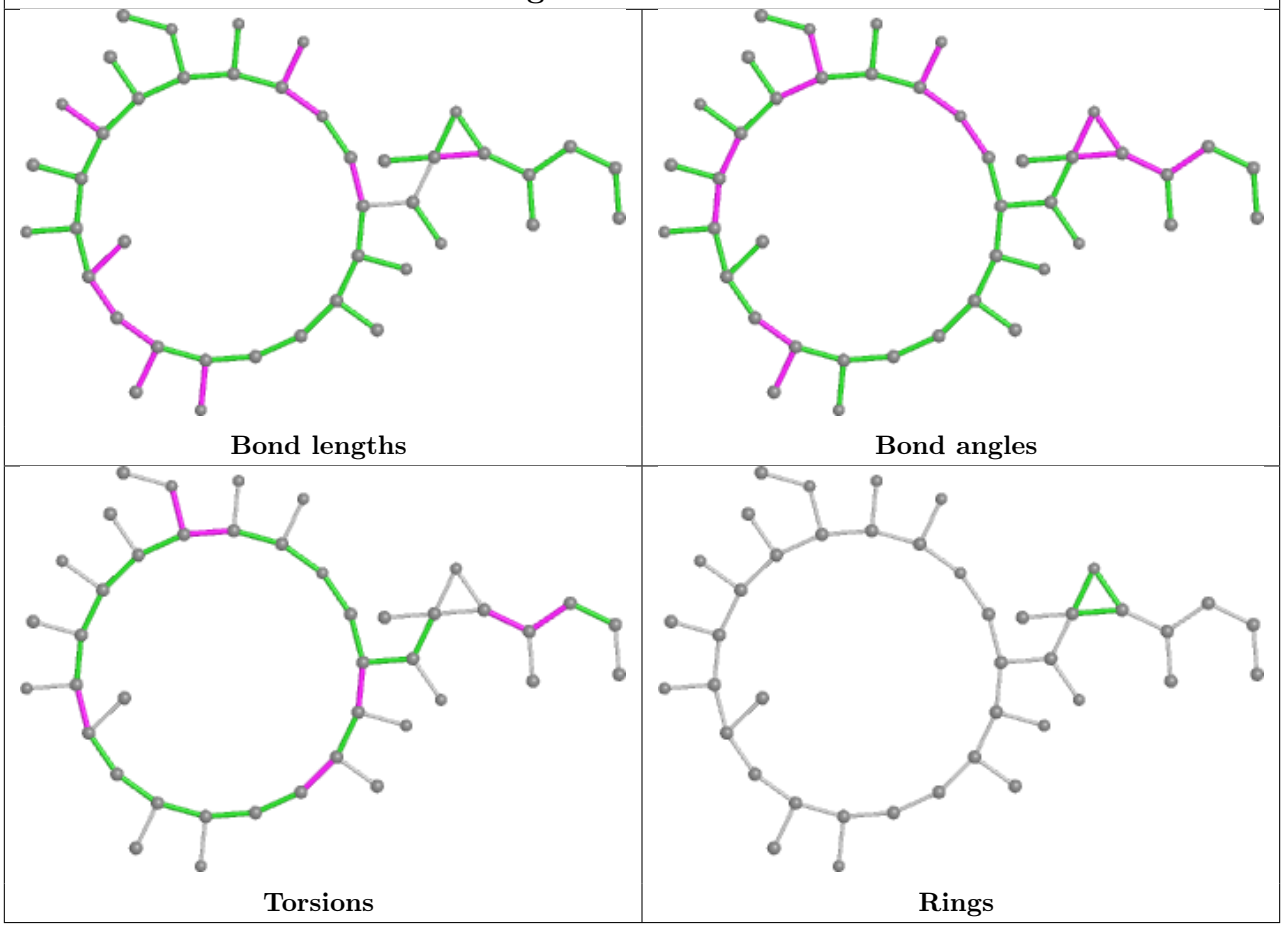
There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	13T	24	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 13T 0 9000



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%)	-0.50	14 (0%) 91 91	23, 50, 93, 150	0
2	9	122/122 (100%)	-0.69	3 (2%) 57 55	43, 69, 91, 151	0
3	A	237/240 (98%)	-0.21	7 (2%) 50 45	32, 55, 86, 105	0
4	B	337/338 (99%)	-0.28	1 (0%) 94 94	33, 60, 82, 90	0
5	C	246/246 (100%)	-0.44	0 100 100	30, 50, 73, 82	0
6	D	140/177 (79%)	1.26	39 (27%) 0 0	63, 103, 124, 130	0
7	E	172/178 (96%)	-0.13	2 (1%) 79 79	55, 73, 90, 96	0
8	F	119/120 (99%)	0.38	6 (5%) 28 25	57, 74, 96, 106	0
9	G	29/348 (8%)	0.78	4 (13%) 2 2	81, 94, 103, 103	0
10	H	160/171 (93%)	0.44	15 (9%) 8 6	52, 67, 93, 100	0
11	J	142/145 (97%)	-0.36	1 (0%) 87 87	45, 56, 74, 94	0
12	K	132/132 (100%)	-0.44	1 (0%) 86 86	41, 54, 75, 81	0
13	L	145/165 (87%)	0.27	12 (8%) 11 8	32, 71, 107, 118	0
14	M	194/194 (100%)	-0.52	0 100 100	36, 47, 60, 64	0
15	N	186/187 (99%)	0.10	9 (4%) 30 27	50, 67, 110, 119	0
16	O	115/116 (99%)	-0.34	0 100 100	44, 59, 71, 76	0
17	P	143/149 (95%)	-0.30	1 (0%) 87 87	46, 60, 70, 75	0
18	Q	95/96 (98%)	-0.44	0 100 100	43, 52, 64, 72	0
19	R	150/155 (96%)	-0.43	0 100 100	38, 50, 68, 73	0
20	S	81/85 (95%)	-0.05	1 (1%) 79 79	52, 65, 81, 85	0
21	T	119/120 (99%)	-0.08	3 (2%) 57 55	47, 62, 83, 96	0
22	U	53/66 (80%)	-0.20	0 100 100	51, 61, 75, 81	0
23	V	65/71 (91%)	1.28	14 (21%) 0 0	59, 79, 109, 114	0
24	W	154/154 (100%)	-0.39	0 100 100	42, 56, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	82/92 (89%)	0.17	7 (8%) 10 8	52, 64, 87, 97	0
26	Y	142/241 (58%)	-0.57	2 (1%) 75 75	30, 51, 70, 86	0
27	Z	73/73 (100%)	0.30	9 (12%) 4 3	58, 69, 80, 94	0
28	1	56/57 (98%)	-0.44	0 100 100	31, 37, 43, 51	0
29	2	46/50 (92%)	0.16	3 (6%) 18 14	41, 69, 90, 99	0
30	3	92/92 (100%)	-0.35	0 100 100	42, 60, 71, 82	0
31	I	70/161 (43%)	3.20	50 (71%) 0 0	109, 119, 135, 135	0
All	All	6646/7463 (89%)	-0.24	204 (3%) 49 44	23, 57, 100, 151	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	I	75	THR	9.2
31	I	79	ILE	8.7
23	V	1	THR	8.2
31	I	109	ALA	8.2
6	D	63	ILE	7.9
31	I	113	HIS	7.7
31	I	71	GLY	7.7
31	I	118	SER	7.5
13	L	100	ALA	6.7
23	V	40	PRO	6.7
23	V	39	ALA	6.7
31	I	96	PHE	6.7
15	N	166	ALA	6.6
23	V	43	PRO	6.4
13	L	97	VAL	6.4
31	I	93	GLN	5.9
31	I	102	VAL	5.8
25	X	88	GLU	5.8
31	I	137	VAL	5.6
6	D	57	THR	5.6
31	I	76	ALA	5.5
6	D	64	ARG	5.3
31	I	105	VAL	5.3
10	H	73	LEU	5.2
31	I	133	THR	5.0
25	X	80	GLU	4.8
23	V	38	GLY	4.7
31	I	103	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
31	I	107	GLN	4.5
6	D	85	GLN	4.5
31	I	77	GLU	4.5
31	I	85	PHE	4.4
6	D	18	ILE	4.4
27	Z	22	SER	4.3
20	S	81	ILE	4.3
6	D	90	LEU	4.3
4	B	1	PRO	4.3
27	Z	26	VAL	4.2
27	Z	11	SER	4.2
23	V	41	GLU	4.2
3	A	37	VAL	4.0
31	I	111	GLN	4.0
1	0	1172	G	4.0
31	I	83	ALA	4.0
13	L	102	ASP	3.9
31	I	84	GLY	3.8
29	2	39	ARG	3.8
8	F	17	LEU	3.7
31	I	115	ASP	3.7
31	I	116	LEU	3.7
27	Z	21	VAL	3.7
23	V	37	GLY	3.7
6	D	69	ILE	3.6
31	I	104	GLN	3.5
10	H	138	CYS	3.5
6	D	88	LEU	3.4
31	I	108	ILE	3.4
10	H	32	LYS	3.4
6	D	87	ALA	3.4
8	F	49	PHE	3.4
31	I	121	LEU	3.3
31	I	74	PRO	3.3
1	0	1198	U	3.3
9	G	27	ILE	3.2
31	I	132	CYS	3.2
29	2	35	ARG	3.2
6	D	23	VAL	3.2
27	Z	19	GLY	3.2
3	A	237	GLY	3.2
2	9	3001	U	3.1

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Mol	Chain	Res	Type	RSRZ
13	L	76	LEU	3.1
15	N	165	ALA	3.1
23	V	52	ALA	3.1
6	D	157	LEU	3.1
31	I	91	GLU	3.1
10	H	65	SER	3.1
25	X	71	ARG	3.1
2	9	3024	U	3.1
31	I	117	LEU	3.0
10	H	37	GLN	3.0
6	D	17	ARG	3.0
15	N	183	ASP	3.0
31	I	81	ASP	3.0
6	D	66	GLY	3.0
3	A	31	LYS	3.0
6	D	81	GLU	3.0
8	F	106	ALA	2.9
1	0	1199	A	2.9
15	N	185	GLU	2.9
29	2	49	GLU	2.9
31	I	126	LYS	2.8
6	D	95	THR	2.8
31	I	122	THR	2.8
7	E	45	ASP	2.8
23	V	34	GLN	2.8
1	0	1177	A	2.8
26	Y	108	ASP	2.8
1	0	960	G	2.8
21	T	116	ASP	2.8
31	I	97	VAL	2.8
31	I	110	GLU	2.8
9	G	23	ILE	2.7
10	H	79	GLU	2.7
13	L	101	ASP	2.7
6	D	135	VAL	2.7
6	D	53	LYS	2.7
31	I	72	VAL	2.7
9	G	25	GLU	2.7
6	D	45	THR	2.7
25	X	65	ASN	2.7
1	0	1171	A	2.7
6	D	134	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
31	I	99	ASP	2.7
6	D	166	ILE	2.6
31	I	89	SER	2.6
31	I	138	THR	2.6
31	I	82	GLU	2.6
23	V	59	ILE	2.6
6	D	128	LEU	2.6
10	H	86	THR	2.6
1	0	497	A	2.6
10	H	171	ALA	2.6
1	0	970	U	2.6
13	L	80	ASP	2.6
10	H	146	VAL	2.5
13	L	105	TYR	2.5
6	D	40	ILE	2.5
6	D	101	THR	2.5
6	D	62	ASP	2.5
31	I	86	GLU	2.5
6	D	44	ILE	2.5
6	D	11	HIS	2.5
6	D	58	VAL	2.5
8	F	29	VAL	2.5
6	D	75	LEU	2.5
10	H	36	LYS	2.5
13	L	60	GLU	2.5
8	F	16	ALA	2.5
6	D	93	LEU	2.5
15	N	95	ALA	2.4
21	T	119	ALA	2.4
1	0	1169	U	2.4
31	I	78	LEU	2.4
13	L	106	VAL	2.4
25	X	74	ALA	2.4
25	X	10	VAL	2.4
26	Y	235	GLU	2.3
6	D	26	GLY	2.3
6	D	165	PHE	2.3
31	I	136	GLY	2.3
7	E	100	ASP	2.3
31	I	129	VAL	2.3
10	H	29	ALA	2.3
6	D	74	THR	2.3

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Mol	Chain	Res	Type	RSRZ
6	D	104	PHE	2.3
6	D	129	ASP	2.3
3	A	35	GLY	2.2
21	T	118	SER	2.2
31	I	135	LEU	2.2
23	V	8	ILE	2.2
6	D	158	ASN	2.2
10	H	63	GLU	2.2
6	D	170	TYR	2.2
13	L	149	ARG	2.2
1	0	2637	A	2.2
2	9	3023	U	2.2
17	P	49	ILE	2.2
6	D	98	PHE	2.2
31	I	80	LYS	2.2
15	N	68	GLU	2.2
27	Z	20	ARG	2.2
6	D	86	THR	2.2
15	N	178	THR	2.2
10	H	81	GLY	2.2
10	H	74	ILE	2.2
3	A	82	VAL	2.2
23	V	3	LEU	2.1
6	D	27	ILE	2.1
12	K	119	GLN	2.1
27	Z	34	ASN	2.1
23	V	36	ALA	2.1
31	I	92	PRO	2.1
23	V	58	THR	2.1
31	I	100	LEU	2.1
15	N	137	ALA	2.1
1	0	1202	A	2.1
13	L	81	VAL	2.1
13	L	96	VAL	2.1
27	Z	25	ARG	2.0
11	J	70	PHE	2.0
1	0	282	C	2.0
10	H	34	GLY	2.0
31	I	88	GLY	2.0
31	I	112	LYS	2.0
25	X	72	VAL	2.0
27	Z	24	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	36	ASP	2.0
3	A	99	ILE	2.0
8	F	75	ILE	2.0
1	0	1173	A	2.0
15	N	138	ASP	2.0
31	I	95	ASP	2.0
1	0	1200	A	2.0
9	G	26	MET	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	OMU	0	2587	21/22	0.95	0.12	38,39,40,41	0
1	1MA	0	628	23/24	0.96	0.17	33,35,36,37	0
1	UR3	0	2619	21/22	0.96	0.15	36,38,39,40	0
1	OMG	0	2588	24/25	0.97	0.13	37,38,39,40	0
1	PSU	0	2621	20/21	0.97	0.12	30,32,39,40	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
33	MG	0	8113	1/1	0.23	0.16	44,44,44,44	0
35	NA	9	8551	1/1	0.38	0.38	92,92,92,92	0
35	NA	0	8538	1/1	0.47	0.09	55,55,55,55	0
35	NA	0	8559	1/1	0.48	0.37	53,53,53,53	0
33	MG	0	8096	1/1	0.48	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8507	1/1	0.53	0.24	69,69,69,69	0
35	NA	0	8513	1/1	0.54	0.07	72,72,72,72	0
33	MG	0	8104	1/1	0.54	0.37	78,78,78,78	0
35	NA	0	8531	1/1	0.55	0.39	57,57,57,57	0
35	NA	0	8585	1/1	0.60	0.38	65,65,65,65	0
35	NA	0	8571	1/1	0.61	0.30	59,59,59,59	0
35	NA	0	8577	1/1	0.63	0.75	81,81,81,81	0
33	MG	0	8080	1/1	0.64	0.15	39,39,39,39	0
36	CL	0	8815	1/1	0.64	0.14	89,89,89,89	0
35	NA	0	8502	1/1	0.66	0.20	57,57,57,57	0
35	NA	0	8550	1/1	0.66	0.61	65,65,65,65	0
35	NA	0	8528	1/1	0.68	0.50	54,54,54,54	0
33	MG	0	8111	1/1	0.68	0.08	46,46,46,46	0
35	NA	0	8569	1/1	0.69	0.25	64,64,64,64	0
33	MG	0	8117	1/1	0.69	0.09	34,34,34,34	0
33	MG	0	8100	1/1	0.71	0.10	42,42,42,42	0
33	MG	0	8102	1/1	0.71	0.29	50,50,50,50	0
35	NA	0	8582	1/1	0.72	0.21	85,85,85,85	0
33	MG	0	8046	1/1	0.72	0.07	56,56,56,56	0
35	NA	0	8509	1/1	0.72	0.11	48,48,48,48	0
35	NA	0	8510	1/1	0.72	0.15	45,45,45,45	0
35	NA	0	8560	1/1	0.74	0.24	60,60,60,60	0
35	NA	9	8583	1/1	0.74	0.15	73,73,73,73	0
35	NA	0	8535	1/1	0.74	0.35	54,54,54,54	0
35	NA	0	8575	1/1	0.75	0.32	72,72,72,72	0
35	NA	J	8546	1/1	0.76	0.25	39,39,39,39	0
33	MG	0	8045	1/1	0.76	0.12	67,67,67,67	0
33	MG	0	8075	1/1	0.77	0.05	56,56,56,56	0
35	NA	0	8506	1/1	0.77	0.71	49,49,49,49	0
33	MG	9	8095	1/1	0.77	0.15	77,77,77,77	0
35	NA	0	8517	1/1	0.77	0.13	37,37,37,37	0
35	NA	0	8584	1/1	0.77	0.70	90,90,90,90	0
35	NA	0	8564	1/1	0.78	0.37	49,49,49,49	0
35	NA	0	8527	1/1	0.78	0.24	61,61,61,61	0
35	NA	0	8516	1/1	0.78	0.42	49,49,49,49	0
35	NA	H	8522	1/1	0.79	0.35	77,77,77,77	0
33	MG	0	8094	1/1	0.80	0.15	59,59,59,59	0
36	CL	0	8816	1/1	0.80	0.13	69,69,69,69	0
35	NA	0	8581	1/1	0.81	0.08	42,42,42,42	0
35	NA	0	8524	1/1	0.81	0.11	48,48,48,48	0
35	NA	0	8562	1/1	0.81	0.49	70,70,70,70	0
33	MG	0	8052	1/1	0.81	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8565	1/1	0.81	0.57	47,47,47,47	0
33	MG	0	8084	1/1	0.82	0.14	58,58,58,58	0
33	MG	K	8069	1/1	0.82	0.06	51,51,51,51	0
33	MG	0	8063	1/1	0.82	0.09	63,63,63,63	0
33	MG	0	8071	1/1	0.82	0.07	50,50,50,50	0
33	MG	0	8047	1/1	0.83	0.12	57,57,57,57	0
35	NA	0	8521	1/1	0.83	0.41	77,77,77,77	0
35	NA	0	8529	1/1	0.84	0.09	68,68,68,68	0
33	MG	0	8061	1/1	0.84	0.16	44,44,44,44	0
33	MG	0	8024	1/1	0.84	1.00	65,65,65,65	0
35	NA	C	8504	1/1	0.84	0.08	35,35,35,35	0
33	MG	0	8035	1/1	0.84	0.11	46,46,46,46	0
33	MG	0	8112	1/1	0.84	0.07	39,39,39,39	0
35	NA	0	8566	1/1	0.84	0.18	48,48,48,48	0
35	NA	0	8568	1/1	0.84	0.20	87,87,87,87	0
36	CL	L	8810	1/1	0.84	0.10	59,59,59,59	0
33	MG	0	8097	1/1	0.85	0.07	45,45,45,45	0
33	MG	0	8072	1/1	0.85	0.09	57,57,57,57	0
35	NA	0	8579	1/1	0.85	0.23	65,65,65,65	0
33	MG	0	8057	1/1	0.85	0.05	41,41,41,41	0
36	CL	0	8822	1/1	0.85	0.48	90,90,90,90	0
33	MG	0	8015	1/1	0.85	0.17	35,35,35,35	0
35	NA	0	8515	1/1	0.86	0.22	49,49,49,49	0
32	13T	0	9000	42/42	0.86	0.25	58,67,73,74	0
33	MG	0	8058	1/1	0.86	0.11	42,42,42,42	0
35	NA	0	8544	1/1	0.86	0.07	29,29,29,29	0
33	MG	0	8116	1/1	0.86	0.10	56,56,56,56	0
35	NA	S	8512	1/1	0.87	0.42	57,57,57,57	0
36	CL	0	8812	1/1	0.87	0.09	49,49,49,49	0
35	NA	0	8561	1/1	0.87	0.32	50,50,50,50	0
35	NA	0	8556	1/1	0.87	0.44	61,61,61,61	0
34	K	0	8401	1/1	0.87	0.73	84,84,84,84	0
36	CL	J	8821	1/1	0.87	0.21	77,77,77,77	0
33	MG	0	8076	1/1	0.87	0.06	49,49,49,49	0
35	NA	0	8572	1/1	0.88	0.39	73,73,73,73	0
33	MG	0	8013	1/1	0.88	0.19	38,38,38,38	0
35	NA	0	8557	1/1	0.88	0.13	45,45,45,45	0
35	NA	0	8555	1/1	0.88	0.99	85,85,85,85	0
36	CL	N	8807	1/1	0.88	0.14	71,71,71,71	0
36	CL	O	8808	1/1	0.88	0.09	67,67,67,67	0
37	CD	O	8705	1/1	0.88	0.10	186,186,186,186	0
33	MG	Y	8109	1/1	0.89	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8008	1/1	0.89	0.08	29,29,29,29	0
35	NA	0	8558	1/1	0.89	0.56	75,75,75,75	0
33	MG	0	8029	1/1	0.89	0.12	42,42,42,42	0
35	NA	0	8518	1/1	0.89	0.34	58,58,58,58	0
33	MG	0	8011	1/1	0.89	0.18	39,39,39,39	0
33	MG	0	8020	1/1	0.90	0.12	39,39,39,39	0
35	NA	M	8547	1/1	0.90	0.07	41,41,41,41	0
33	MG	0	8115	1/1	0.90	0.07	45,45,45,45	0
33	MG	0	8062	1/1	0.90	0.22	13,13,13,13	0
35	NA	0	8563	1/1	0.90	0.42	68,68,68,68	0
33	MG	0	8022	1/1	0.90	0.08	37,37,37,37	0
35	NA	0	8554	1/1	0.90	0.15	42,42,42,42	0
33	MG	0	8081	1/1	0.90	0.13	43,43,43,43	0
33	MG	0	8018	1/1	0.90	0.15	39,39,39,39	0
33	MG	0	8090	1/1	0.90	0.23	73,73,73,73	0
33	MG	0	8028	1/1	0.90	0.06	33,33,33,33	0
35	NA	0	8532	1/1	0.90	0.23	44,44,44,44	0
33	MG	0	8091	1/1	0.91	0.10	65,65,65,65	0
35	NA	0	8542	1/1	0.91	0.29	15,15,15,15	0
33	MG	0	8114	1/1	0.91	0.35	54,54,54,54	0
36	CL	B	8819	1/1	0.91	0.10	53,53,53,53	0
36	CL	J	8802	1/1	0.91	0.15	76,76,76,76	0
35	NA	0	8505	1/1	0.91	0.23	37,37,37,37	0
35	NA	0	8567	1/1	0.91	0.46	61,61,61,61	0
35	NA	0	8552	1/1	0.91	0.13	68,68,68,68	0
33	MG	0	8040	1/1	0.91	0.34	53,53,53,53	0
33	MG	0	8031	1/1	0.91	0.10	30,30,30,30	0
33	MG	0	8036	1/1	0.92	0.06	41,41,41,41	0
33	MG	0	8093	1/1	0.92	0.10	61,61,61,61	0
33	MG	0	8070	1/1	0.92	0.15	43,43,43,43	0
33	MG	0	8023	1/1	0.92	0.24	61,61,61,61	0
35	NA	0	8574	1/1	0.92	0.60	67,67,67,67	0
33	MG	0	8050	1/1	0.92	0.19	74,74,74,74	0
33	MG	0	8088	1/1	0.92	0.10	33,33,33,33	0
35	NA	0	8533	1/1	0.92	0.12	39,39,39,39	0
33	MG	0	8010	1/1	0.92	0.16	11,11,11,11	0
33	MG	0	8103	1/1	0.92	0.19	78,78,78,78	0
33	MG	0	8083	1/1	0.93	0.07	41,41,41,41	0
35	NA	0	8539	1/1	0.93	0.30	40,40,40,40	0
36	CL	0	8803	1/1	0.93	0.15	56,56,56,56	0
35	NA	0	8540	1/1	0.93	0.26	50,50,50,50	0
33	MG	0	8025	1/1	0.93	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8526	1/1	0.93	0.30	70,70,70,70	0
35	NA	0	8549	1/1	0.93	0.26	53,53,53,53	0
33	MG	0	8049	1/1	0.93	0.17	36,36,36,36	0
33	MG	0	8089	1/1	0.93	0.13	62,62,62,62	0
33	MG	0	8044	1/1	0.93	0.08	55,55,55,55	0
33	MG	0	8001	1/1	0.93	0.12	44,44,44,44	0
33	MG	0	8079	1/1	0.93	0.15	27,27,27,27	0
33	MG	0	8067	1/1	0.93	0.09	37,37,37,37	0
33	MG	0	8037	1/1	0.93	0.07	42,42,42,42	0
33	MG	0	8019	1/1	0.94	0.04	34,34,34,34	0
33	MG	0	8033	1/1	0.94	0.04	38,38,38,38	0
35	NA	A	8545	1/1	0.94	0.16	61,61,61,61	0
33	MG	0	8006	1/1	0.94	0.09	36,36,36,36	0
33	MG	3	8078	1/1	0.94	0.10	16,16,16,16	0
35	NA	0	8541	1/1	0.94	0.09	46,46,46,46	0
35	NA	0	8570	1/1	0.94	0.39	65,65,65,65	0
35	NA	Q	8548	1/1	0.94	0.11	46,46,46,46	0
35	NA	R	8537	1/1	0.94	0.14	45,45,45,45	0
33	MG	0	8021	1/1	0.94	0.09	37,37,37,37	0
35	NA	0	8534	1/1	0.94	0.07	40,40,40,40	0
35	NA	R	8586	1/1	0.95	0.35	23,23,23,23	0
35	NA	0	8530	1/1	0.95	0.09	45,45,45,45	0
33	MG	0	8051	1/1	0.95	0.12	56,56,56,56	0
33	MG	0	8085	1/1	0.95	0.12	48,48,48,48	0
36	CL	0	8813	1/1	0.95	0.06	54,54,54,54	0
33	MG	0	8038	1/1	0.95	0.12	31,31,31,31	0
33	MG	0	8042	1/1	0.95	0.05	33,33,33,33	0
34	K	0	8402	1/1	0.95	0.13	61,61,61,61	0
36	CL	A	8809	1/1	0.95	0.19	82,82,82,82	0
35	NA	0	8536	1/1	0.95	0.07	54,54,54,54	0
36	CL	J	8801	1/1	0.95	0.06	58,58,58,58	0
33	MG	0	8098	1/1	0.95	0.11	42,42,42,42	0
33	MG	0	8099	1/1	0.95	0.33	70,70,70,70	0
33	MG	0	8074	1/1	0.95	0.04	30,30,30,30	0
33	MG	0	8043	1/1	0.95	0.13	47,47,47,47	0
33	MG	0	8092	1/1	0.95	0.12	72,72,72,72	0
36	CL	Y	8817	1/1	0.95	0.15	70,70,70,70	0
33	MG	B	8055	1/1	0.95	0.15	64,64,64,64	0
33	MG	0	8041	1/1	0.96	0.23	68,68,68,68	0
33	MG	A	8065	1/1	0.96	0.14	45,45,45,45	0
33	MG	A	8066	1/1	0.96	0.05	73,73,73,73	0
35	NA	0	8514	1/1	0.96	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	CL	0	8814	1/1	0.96	0.11	57,57,57,57	0
33	MG	0	8034	1/1	0.96	0.10	25,25,25,25	0
33	MG	0	8004	1/1	0.96	0.18	37,37,37,37	0
33	MG	T	8073	1/1	0.96	0.10	57,57,57,57	0
33	MG	0	8108	1/1	0.96	0.03	77,77,77,77	0
35	NA	0	8520	1/1	0.96	0.23	36,36,36,36	0
33	MG	0	8053	1/1	0.96	0.13	43,43,43,43	0
33	MG	0	8086	1/1	0.96	0.07	42,42,42,42	0
33	MG	0	8087	1/1	0.96	0.09	63,63,63,63	0
33	MG	0	8077	1/1	0.96	0.16	36,36,36,36	0
36	CL	M	8818	1/1	0.96	0.09	44,44,44,44	0
33	MG	0	8048	1/1	0.96	0.09	49,49,49,49	0
33	MG	0	8005	1/1	0.96	0.10	32,32,32,32	0
33	MG	0	8101	1/1	0.96	0.08	45,45,45,45	0
36	CL	3	8804	1/1	0.96	0.09	56,56,56,56	0
35	NA	0	8508	1/1	0.96	0.26	58,58,58,58	0
37	CD	Z	8703	1/1	0.96	0.09	71,71,71,71	0
33	MG	0	8007	1/1	0.97	0.17	26,26,26,26	0
33	MG	0	8003	1/1	0.97	0.10	36,36,36,36	0
35	NA	0	8578	1/1	0.97	0.10	57,57,57,57	0
33	MG	0	8009	1/1	0.97	0.15	36,36,36,36	0
33	MG	0	8082	1/1	0.97	0.34	84,84,84,84	0
33	MG	0	8016	1/1	0.97	0.07	18,18,18,18	0
33	MG	0	8054	1/1	0.97	0.16	30,30,30,30	0
33	MG	0	8056	1/1	0.97	0.10	56,56,56,56	0
33	MG	0	8032	1/1	0.97	0.07	35,35,35,35	0
33	MG	0	8017	1/1	0.97	0.16	31,31,31,31	0
33	MG	0	8059	1/1	0.97	0.05	39,39,39,39	0
35	NA	0	8573	1/1	0.97	0.20	56,56,56,56	0
33	MG	0	8002	1/1	0.97	0.03	40,40,40,40	0
33	MG	0	8060	1/1	0.98	0.17	45,45,45,45	0
33	MG	3	8118	1/1	0.98	0.21	50,50,50,50	0
35	NA	0	8543	1/1	0.98	0.20	35,35,35,35	0
35	NA	0	8576	1/1	0.98	0.16	33,33,33,33	0
35	NA	0	8511	1/1	0.98	0.12	56,56,56,56	0
33	MG	0	8107	1/1	0.98	0.12	38,38,38,38	0
33	MG	0	8068	1/1	0.98	0.09	56,56,56,56	0
35	NA	L	8580	1/1	0.98	0.24	1,1,1,1	0
36	CL	Y	8820	1/1	0.98	0.05	44,44,44,44	0
33	MG	0	8026	1/1	0.98	0.09	33,33,33,33	0
35	NA	0	8553	1/1	0.98	0.11	44,44,44,44	0
35	NA	0	8525	1/1	0.98	0.39	59,59,59,59	0

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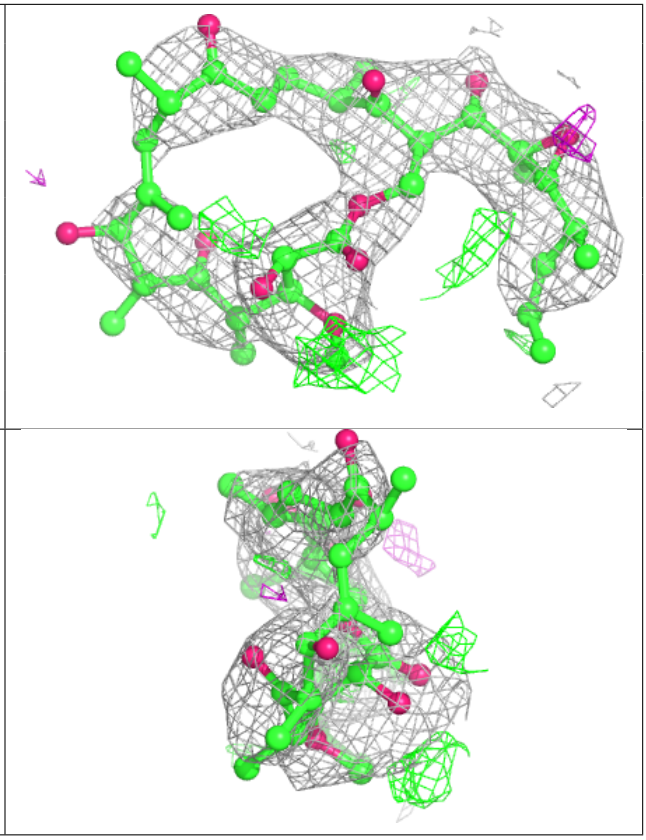
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	CD	3	8704	1/1	0.98	0.08	65,65,65,65	0
33	MG	0	8106	1/1	0.99	0.07	71,71,71,71	0
35	NA	0	8523	1/1	0.99	0.22	38,38,38,38	0
35	NA	0	8501	1/1	0.99	0.06	50,50,50,50	0
36	CL	0	8805	1/1	0.99	0.13	71,71,71,71	0
36	CL	0	8811	1/1	0.99	0.11	58,58,58,58	0
33	MG	0	8064	1/1	0.99	0.09	41,41,41,41	0
35	NA	0	8503	1/1	0.99	0.30	1,1,1,1	0
36	CL	R	8806	1/1	0.99	0.03	49,49,49,49	0
33	MG	0	8039	1/1	0.99	0.07	64,64,64,64	0
33	MG	0	8110	1/1	0.99	0.10	53,53,53,53	0
33	MG	0	8030	1/1	0.99	0.07	35,35,35,35	0
33	MG	0	8012	1/1	0.99	0.14	39,39,39,39	0
37	CD	U	8701	1/1	0.99	0.10	67,67,67,67	0
35	NA	0	8519	1/1	0.99	0.16	17,17,17,17	0
37	CD	1	8702	1/1	0.99	0.08	65,65,65,65	0
33	MG	0	8027	1/1	0.99	0.03	40,40,40,40	0
33	MG	0	8014	1/1	1.00	0.10	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 13T 0 9000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.