Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:03 PM GMT

PDB ID	:	1VQ7
Title	:	The structure of the transition state analogue "DCA" bound to the large ribosomal subunit of haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

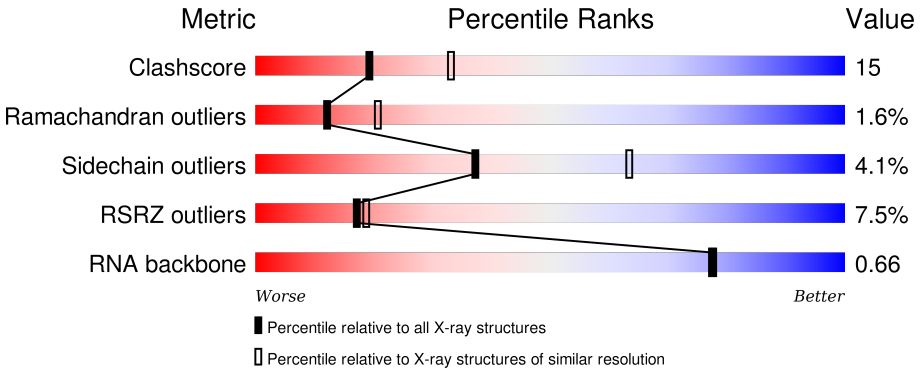
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 60% 28% 5% • 6%
2	9	122	4% 58% 32% 8% •
3	4	8	50% 50%
4	A	240	8% 64% 30% • •
5	B	338	4% 50% 44% 5%

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Mol	Chain	Length	Quality of chain
6	C	246	2% 62% 33% 5%
7	D	177	44% 34% 40% 6% 21%
8	E	178	20% 53% 43%
9	F	120	24% 63% 33%
10	G	348	5% 5% 92%
11	H	171	5% 58% 33% 6%
12	J	145	% 61% 30% 6%
13	K	132	4% 61% 36%
14	L	165	18% 51% 34% 12%
15	M	194	% 71% 27%
16	N	187	22% 49% 45% 6%
17	O	116	3% 71% 26%
18	P	149	3% 58% 36%
19	Q	96	2% 72% 25%
20	R	155	67% 28%
21	S	85	4% 64% 31% 5%
22	T	120	3% 54% 40% 5%
23	U	66	3% 41% 39% 20%
24	V	71	32% 42% 45% 8%
25	W	154	49% 47%
26	X	92	15% 50% 35% 11%
27	Y	241	5% 39% 18% 41%
28	Z	83	7% 53% 33% 12%
29	1	57	72% 26%
30	2	50	30% 54% 36% 8%

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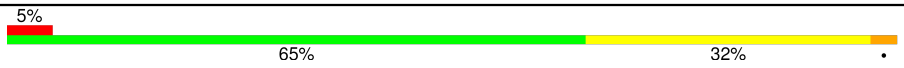
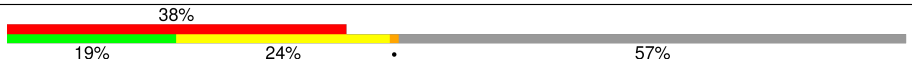
Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8013	-	-	-	X
33	MG	0	8060	-	-	-	X
35	NA	0	9121	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9127	-	-	-	X
35	NA	0	9135	-	-	-	X
35	NA	0	9140	-	-	-	X
35	NA	0	9150	-	-	-	X
35	NA	0	9156	-	-	-	X
35	NA	0	9159	-	-	-	X
35	NA	0	9161	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9164	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9174	-	-	-	X
35	NA	0	9176	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9178	-	-	-	X
35	NA	0	9179	-	-	-	X
35	NA	0	9182	-	-	-	X
35	NA	0	9186	-	-	-	X
35	NA	L	9180	-	-	-	X
36	CL	0	9315	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99063 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	130	63	23	39	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	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	11	Total Cl 11 11	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	R	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0
36	M	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	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
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5809	Total O 5809 5809	0	0
38	9	137	Total O 137 137	0	0
38	4	8	Total O 8 8	0	0
38	A	119	Total O 119 119	0	0
38	B	153	Total O 153 153	0	0
38	C	168	Total O 168 168	0	0
38	D	47	Total O 47 47	0	0
38	E	43	Total O 43 43	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	23	Total O 23 23	0	0
38	G	18	Total O 18 18	0	0
38	H	65	Total O 65 65	0	0
38	J	51	Total O 51 51	0	0
38	K	58	Total O 58 58	0	0
38	L	82	Total O 82 82	0	0
38	M	116	Total O 116 116	0	0
38	N	63	Total O 63 63	0	0
38	O	42	Total O 42 42	0	0
38	P	64	Total O 64 64	0	0
38	Q	51	Total O 51 51	0	0
38	R	84	Total O 84 84	0	0
38	S	30	Total O 30 30	0	0
38	T	42	Total O 42 42	0	0
38	U	29	Total O 29 29	0	0
38	V	14	Total O 14 14	0	0
38	W	68	Total O 68 68	0	0
38	X	27	Total O 27 27	0	0
38	Y	96	Total O 96 96	0	0
38	Z	32	Total O 32 32	0	0
38	1	53	Total O 53 53	0	0

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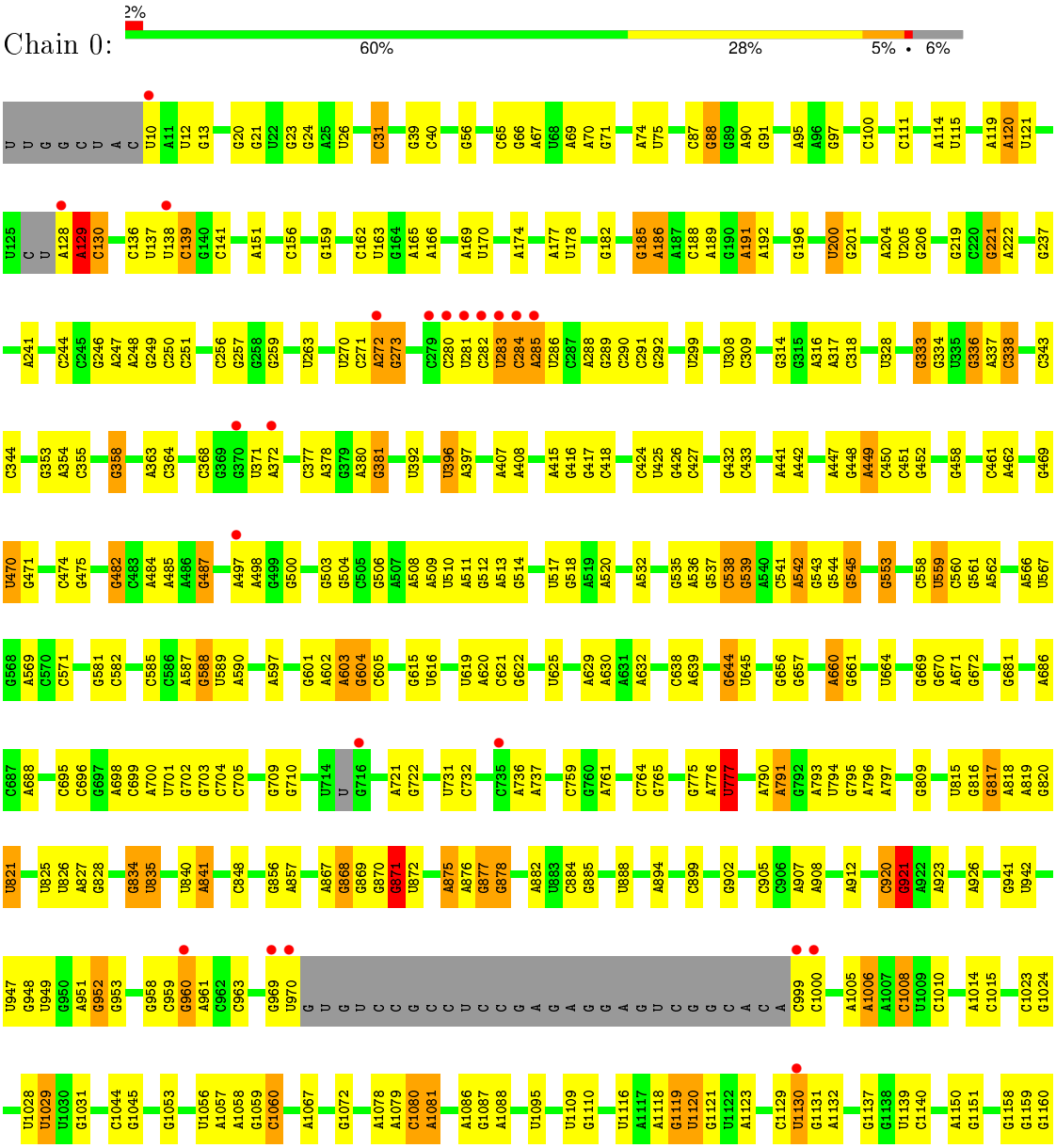
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	2	40	Total O 40 40	0	0
38	3	74	Total O 74 74	0	0
38	I	9	Total O 9 9	0	0

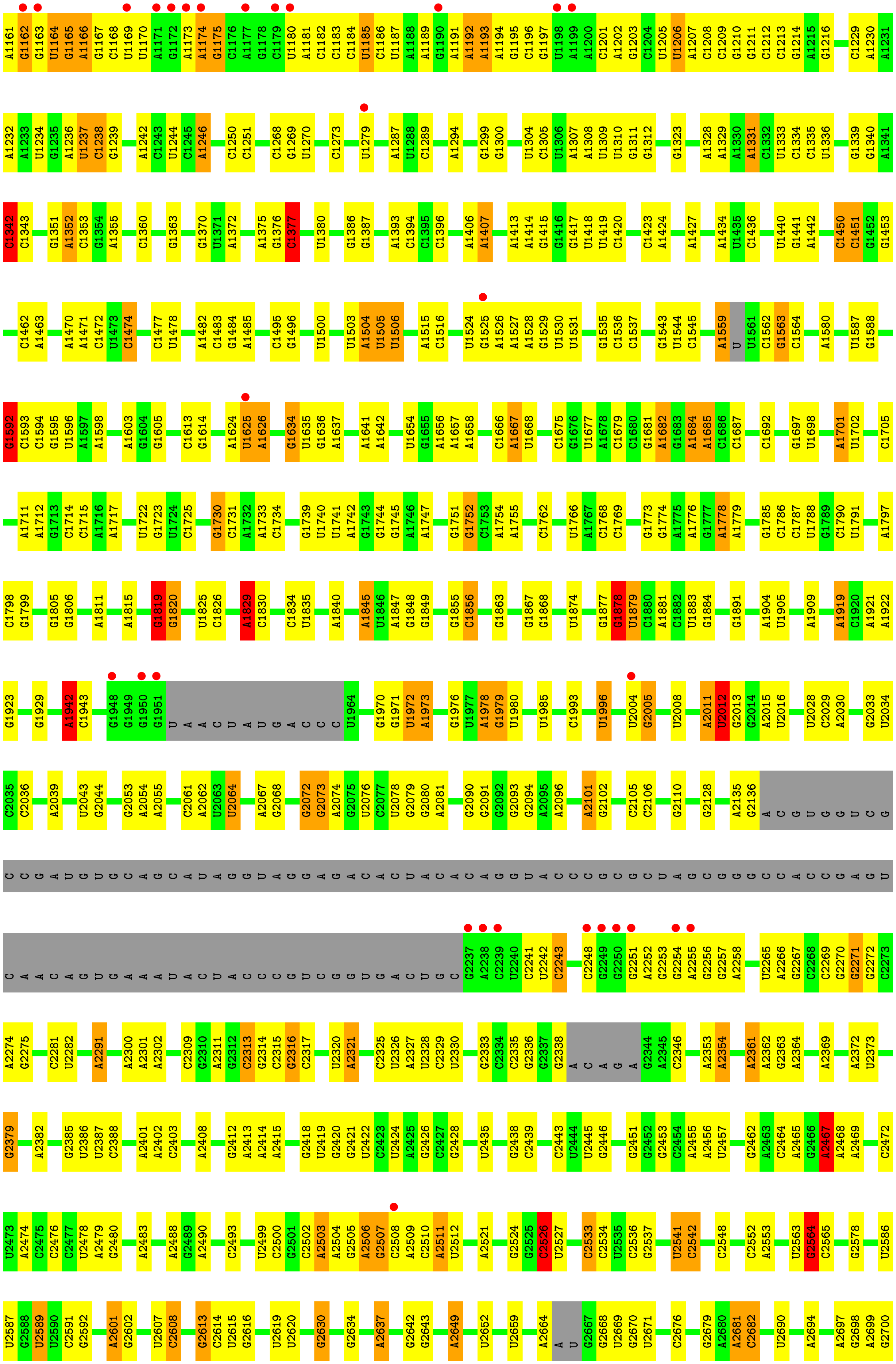
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal rna

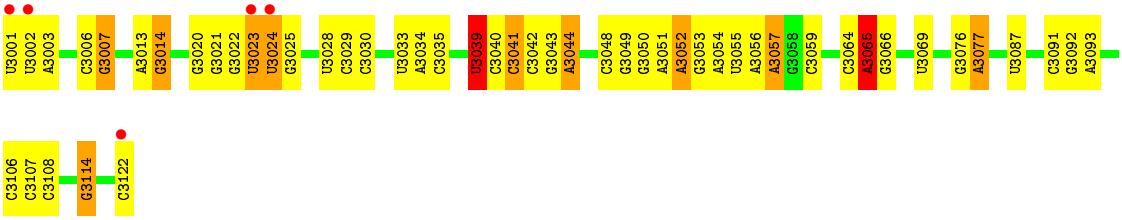
Chain 0:




A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 C1179 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 C1229 A1230 A1231
A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 C1250 C1251 C1268 G1269 U1270 C1273 U1279 A1287 U1288 C1289 A1294 G1299 G1300 U1304 C1305 U1306 A1307 A1308 U1309 U1310 C1311 G1312 G1323 A1328 A1329 A1330 A1331 C1332 U1333 C1334 C1335 U1336 G1339 G1340 A1341
C1342 C1343 G1351 A1352 C1353 G1354 A1355 C1360 G1363 G1370 U1371 A1372 A1375 G1376 C1377 U1380 G1386 G1387 A1393 C1394 C1395 C1396 A1406 A1407 A1413 A1414 G1415 G1416 G1417 U1418 U1419 C1420 C1423 A1424 A1427 A1434 U1435 C1436 U1440 G1441 A1442 C1450 C1451 G1452 G1453
C1462 A1463 A1470 A1471 C1472 U1473 C1474 C1477 U1478 A1482 C1483 G1484 A1485 C1495 G1496 U1500 U1503 A1504 U1505 U1506 A1515 C1516 U1524 G1525 A1526 A1527 A1528 G1529 U1530 U1531 G1535 C1536 C1537 G1543 U1544 C1545 A1559 U U1561 C1562 G1563 C1564 A1580 U1587 G1588
G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 C1613 G1614 A1624 U1625 A1626 G1634 U1635 G1636 A1637 A1641 A1642 U1654 G1655 A1656 A1657 A1658 C1666 A1667 U1668 C1675 G1676 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 G1697 U1698 A1701 U1702 C1705
A1711 A1712 G1713 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 G1739 U1740 U1741 A1742 G1743 G1744 G1745 A1746 A1747 G1751 G1752 C1753 A1754 A1755 C1762 U1766 A1767 C1768 C1769 G1773 U1774 A1775 A1776 G1777 A1778 A1779 G1785 C1786 C1787 U1788 G1789 C1790 U1791 A1797
C1798 G1799 G1805 G1806 A1811 A1815 G1819 G1820 U1825 C1826 A1829 C1830 C1834 U1835 A1840 A1845 U1846 A1847 G1848 G1849 G1855 C1856 G1863 G1867 G1868 U1874 G1877 G1878 U1879 C1880 A1881 C1882 U1883 G1884 G1891 A1904 U1905 A1909 A1919 C1920 A1921 A1922
G1923 G1929 A1942 C1943 G1948 G1949 G1950 G1951 U A A C U A U G A C C C U1964 G1970 G1971 U1972 A1973 G1976 U1977 A1978 G1979 U1980 U1985 C1993 U1996 U2004 G2005 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2028 C2029 A2030 G2033 U2034
C2035 C2036 A2039 U2043 G2044 G2053 A2054 A2055 C2061 A2062 U2063 U2064 A2067 G2068 G2072 G2073 A2074 G2075 U2076 C2077 U2078 G2079 G2080 A2081 G2090 G2091 G2092 G2093 G2094 A2095 A2096 A2101 G2102 C2105 C2106 G2110 G2128 A2135 G2136 A C G U G G U C G
C C G A U G U G C A G C A U A G G U A G G A G A C A C U A C A C A G G U A C C C G C G C U A G C G G G C C A C C G A G U
C A A C A G U G A A A U A C U A C C C G U C G G U G A C U G C G2237 A2238 C2239 U2240 C2241 U2242 C2243 C2248 G2249 G2250 G2251 A2252 G2253 G2254 A2255 G2256 G2257 A2258 U2265 A2266 G2267 C2268 C2269 G2270 G2271 G2272 C2273
A2274 G2275 C2281 U2282 A2291 A2300 A2301 A2302 C2309 G2310 A2311 G2312 C2313 G2314 C2315 G2316 C2317 U2320 A2321 C2325 U2326 A2327 U2328 C2329 U2330 G2333 C2334 C2335 G2336 G2337 G2338 A C A G A G2344 A2345 C2346 A2353 A2354 A2361 A2362 C2363 A2364 A2369 A2372 U2373
G2379 A2382 G2385 U2386 U2387 C2388 A2401 A2402 C2403 A2408 G2412 A2413 A2414 A2415 G2418 U2419 G2420 G2421 U2422 C2423 U2424 A2425 G2426 C2427 G2428 U2435 G2438 C2439 C2443 U2444 U2445 G2446 G2451 G2452 G2453 C2454 A2455 A2456 U2457 G2462 A2463 C2464 A2465 G2466 A2467 A2468 A2469 C2472
U2473 A2474 C2475 C2476 C2477 U2478 A2479 G2480 A2483 A2488 G2489 A2490 C2493 U2499 C2500 G2501 C2502 A2503 A2504 G2505 A2506 G2507 C2508 A2509 C2510 A2511 U2512 A2521 G2524 G2525 C2526 U2527 C2533 C2534 U2535 C2536 G2537 U2541 C2542 C2548 C2552 A2553 U2563 G2564 C2565 G2578 U2586
U2587 G2588 U2589 U2590 C2591 G2592 A2601 G2602 U2607 C2608 G2613 C2614 U2615 G2616 U2619 U2620 G2630 G2634 A2637 G2642 G2643 A2649 U2652 U2659 A2664 A U G2667 G2668 U2669 G2670 U2671 C2676 G2679 A2680 A2681 C2682 U2690 A2694 A2697 G2698 A2699 G2700

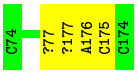
- Molecule 2: 5S ribosomal RNA

Chain 9:



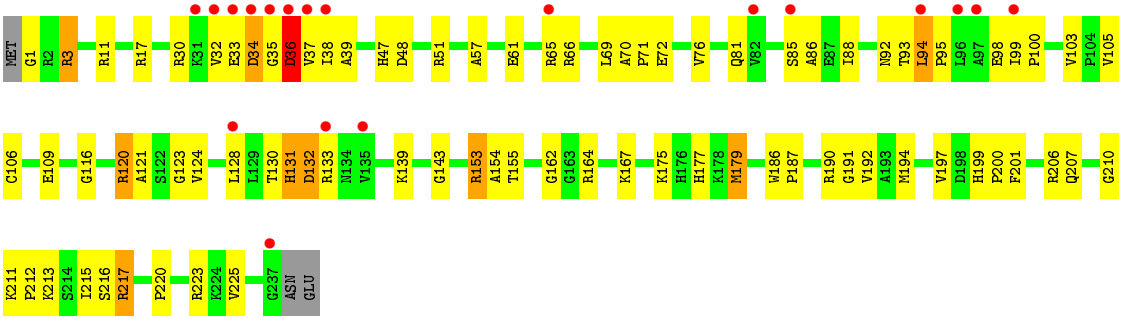
- Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3')

Chain 4:



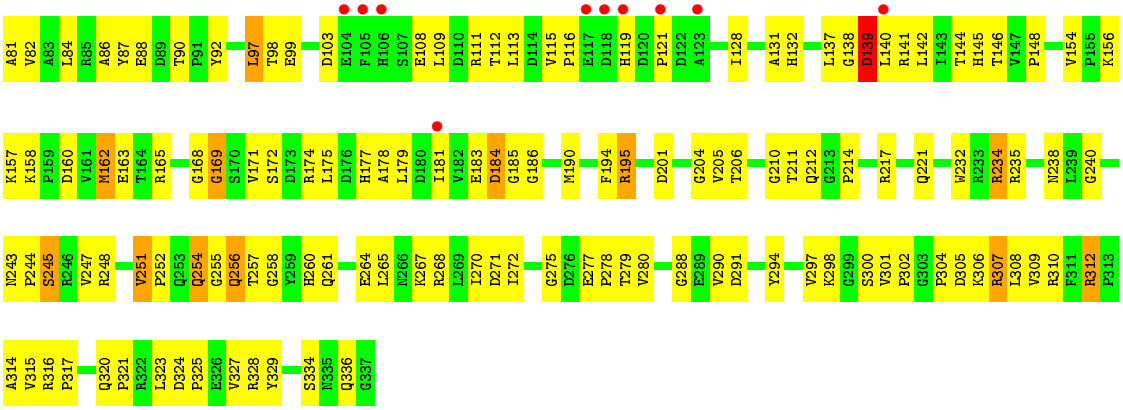
- Molecule 4: 50S ribosomal protein L2P

Chain A:



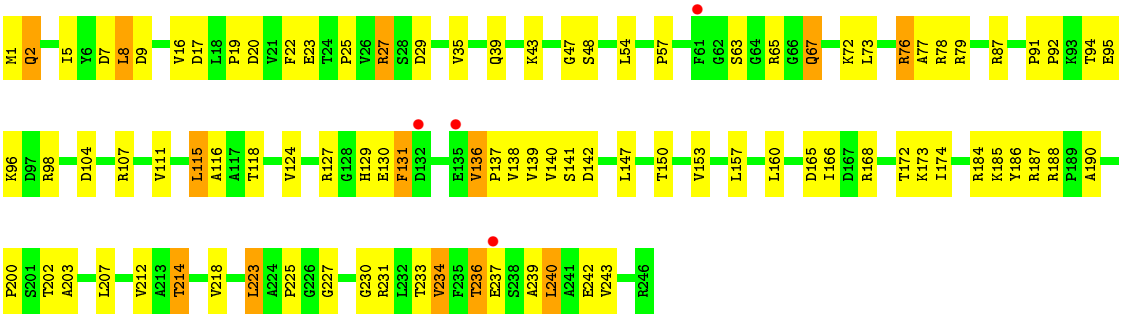
- Molecule 5: 50S ribosomal protein L3P

Chain B:



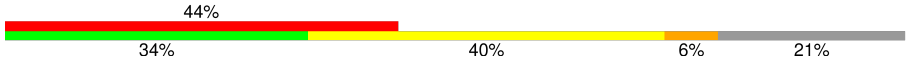
• Molecule 6: 50S ribosomal protein L4E

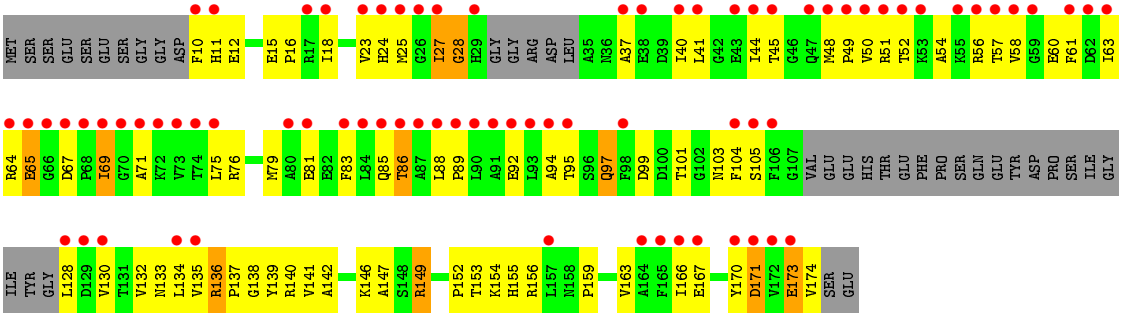
Chain C:



• Molecule 7: 50S ribosomal protein L5P

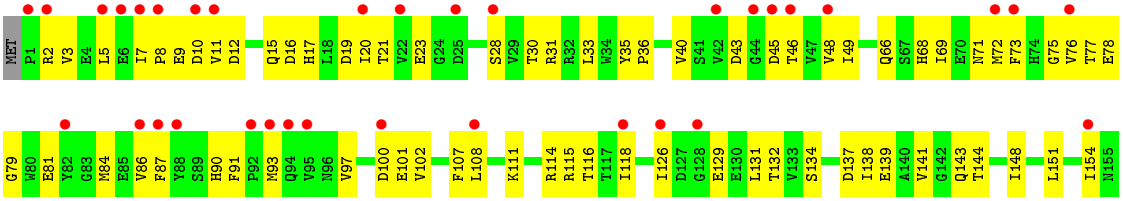
Chain D:

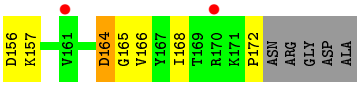




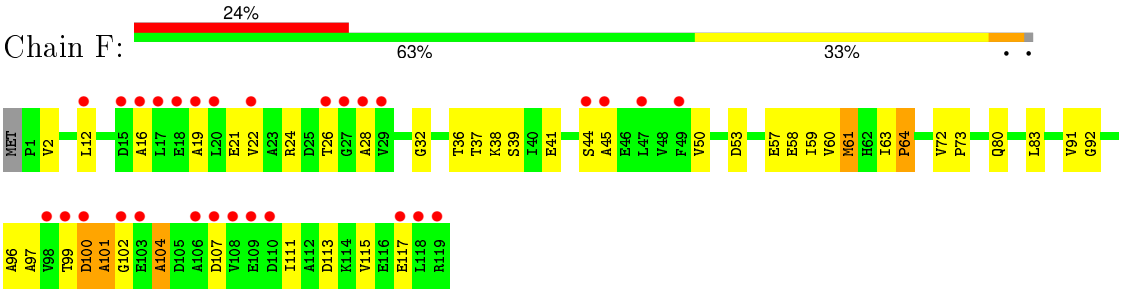
• Molecule 8: 50S ribosomal protein L6P

Chain E:

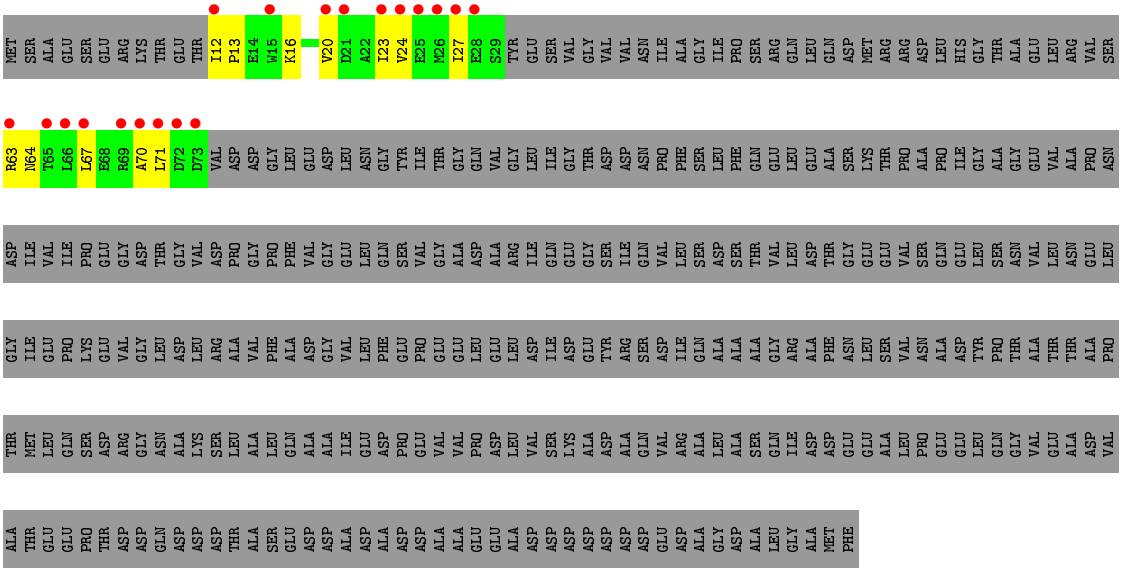




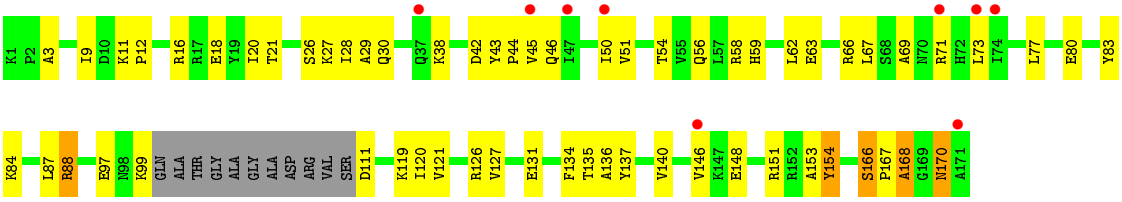
• Molecule 9: 50S ribosomal protein L7AE



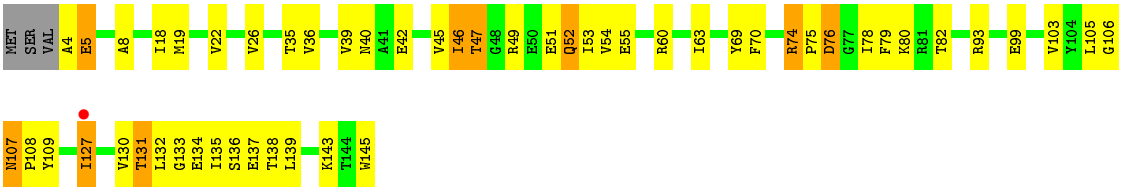
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

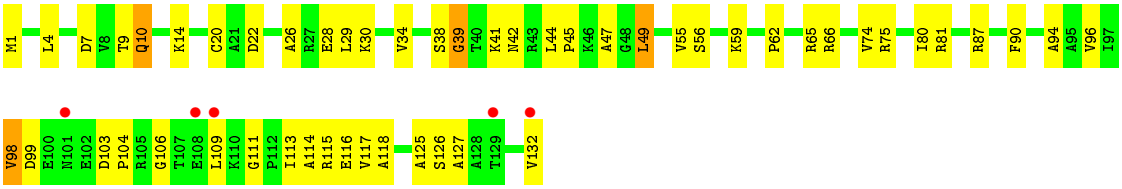


• Molecule 12: 50S ribosomal protein L13P



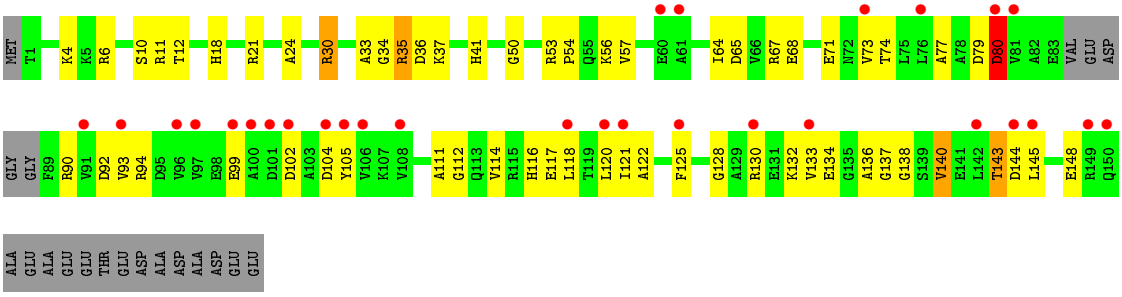
• Molecule 13: 50S ribosomal protein L14P

Chain K:



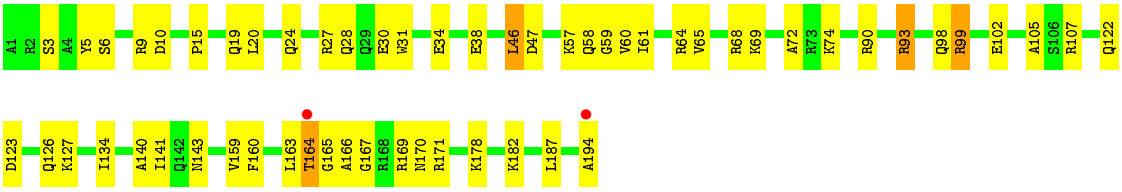
• Molecule 14: 50S ribosomal protein L15P

Chain L:



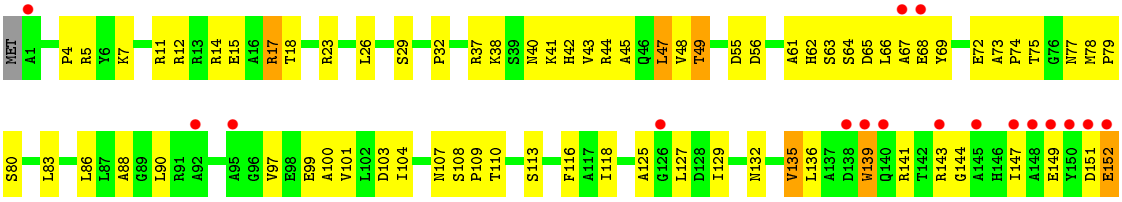
• Molecule 15: 50S Ribosomal Protein L15E

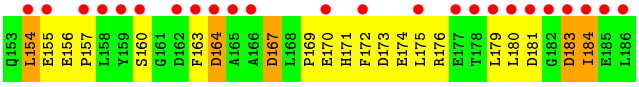
Chain M:



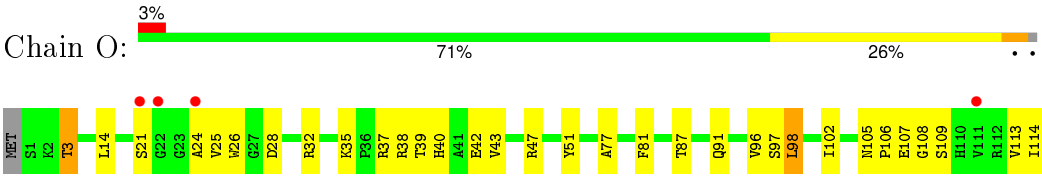
• Molecule 16: 50S ribosomal protein L18P

Chain N:

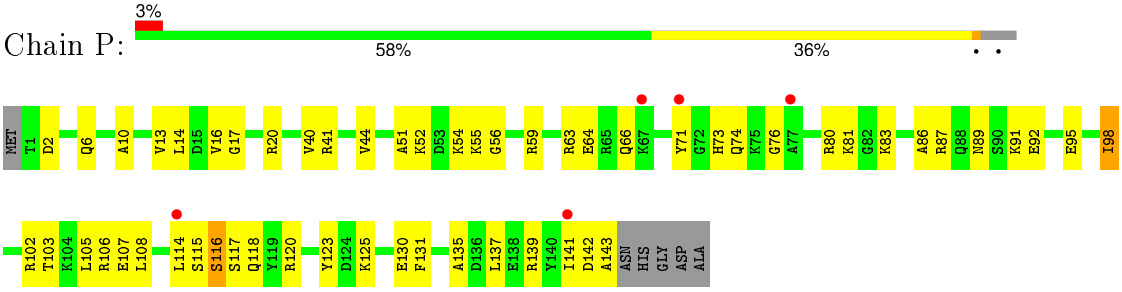




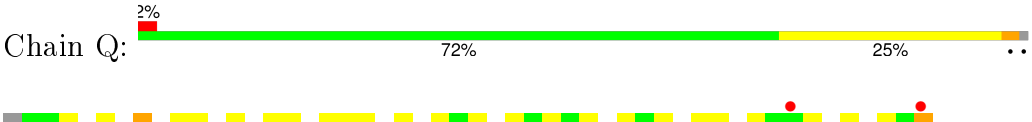
• Molecule 17: 50S ribosomal protein L18e



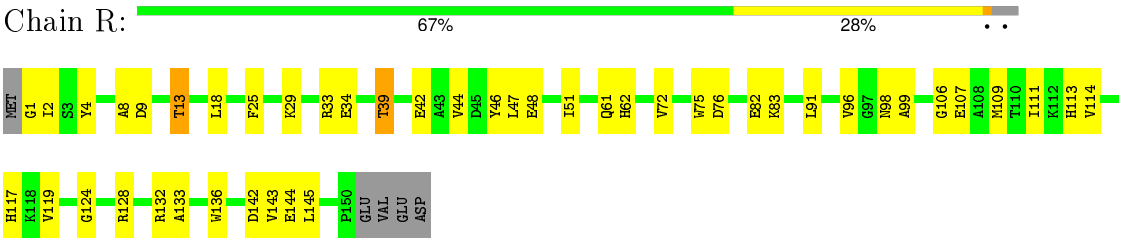
• Molecule 18: 50S ribosomal protein L19E



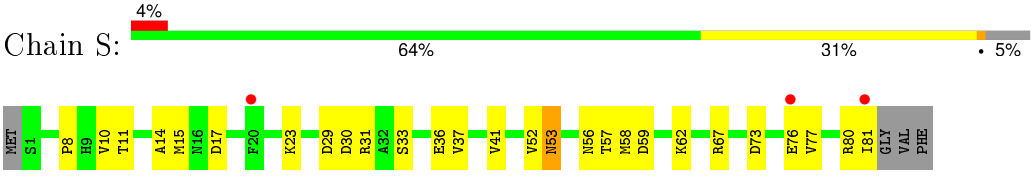
• Molecule 19: 50S ribosomal protein L21e



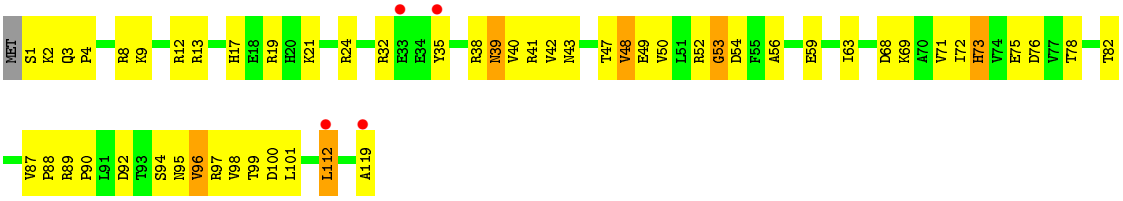
• Molecule 20: 50S ribosomal protein L22P



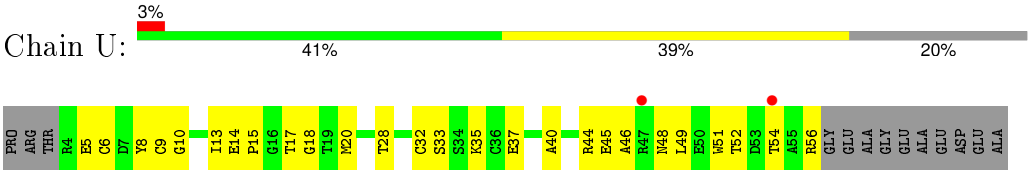
• Molecule 21: 50S ribosomal protein L23P



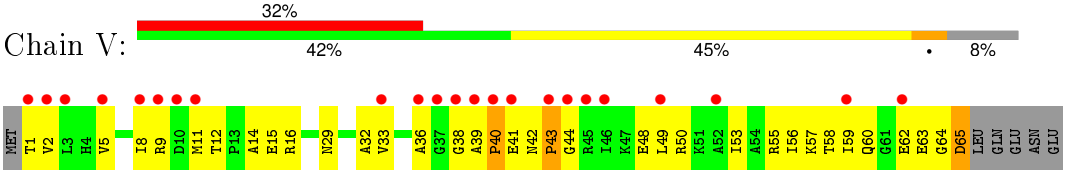
• Molecule 22: 50S ribosomal protein L24P



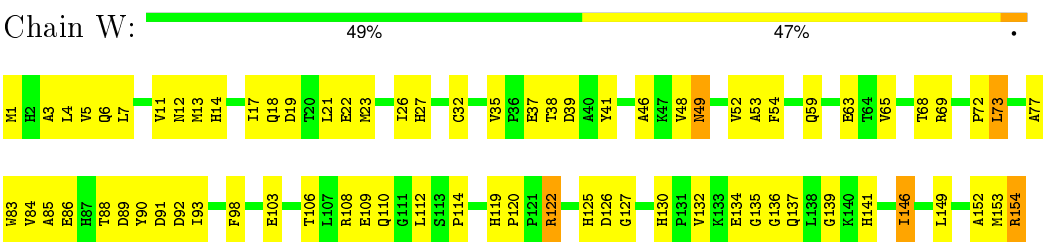
- Molecule 23: 50S ribosomal protein L24E



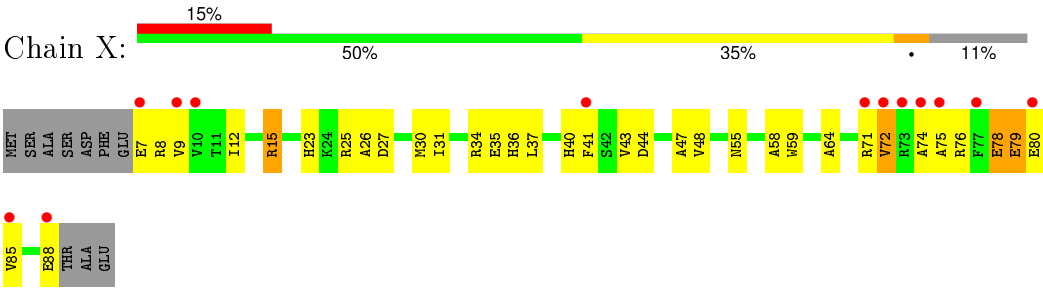
- Molecule 24: 50S ribosomal protein L29P



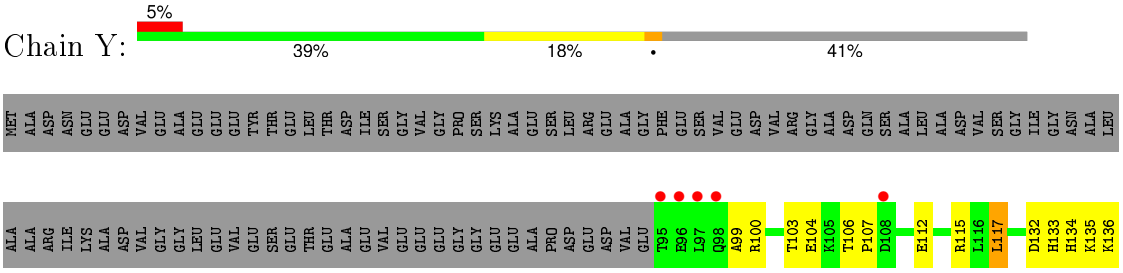
- Molecule 25: 50S ribosomal protein L30P

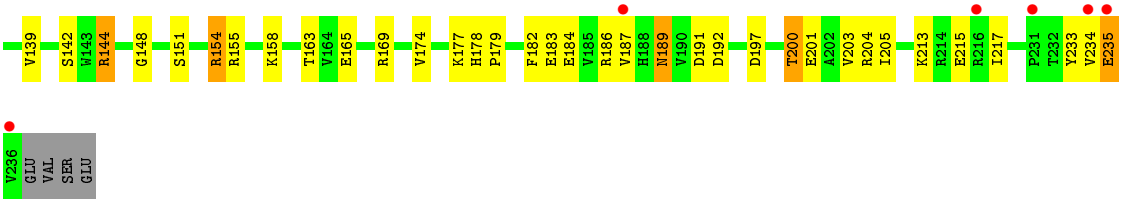


- Molecule 26: 50S ribosomal protein L31e

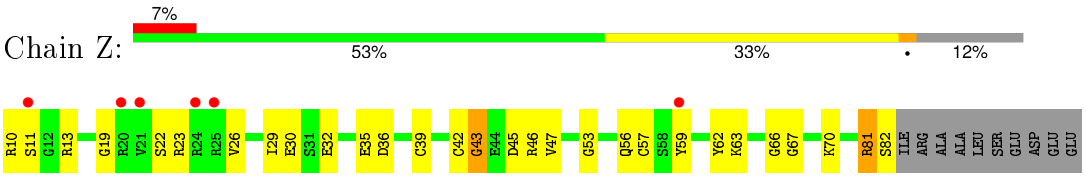


- Molecule 27: 50S ribosomal protein L32E

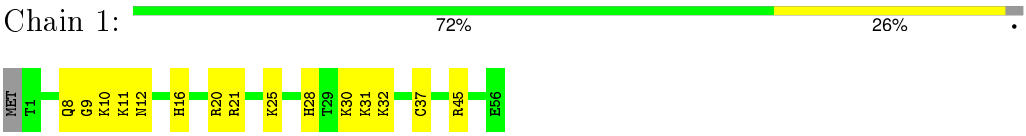




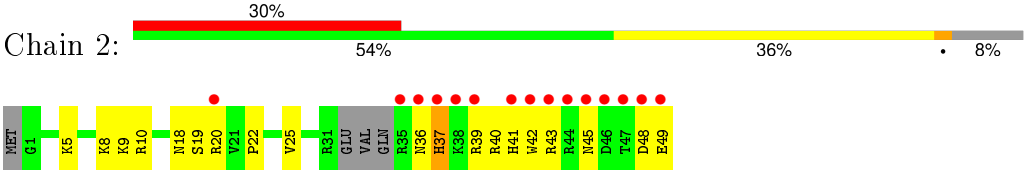
- Molecule 28: 50S ribosomal protein L37Ae



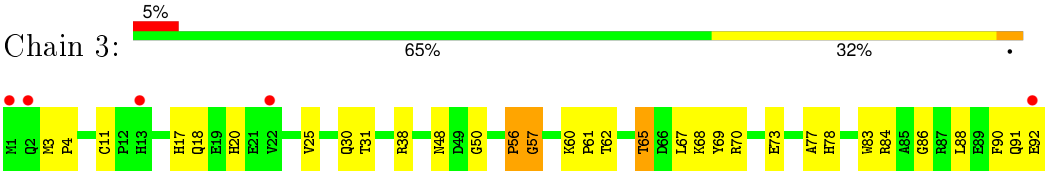
- Molecule 29: 50S ribosomal protein L37e



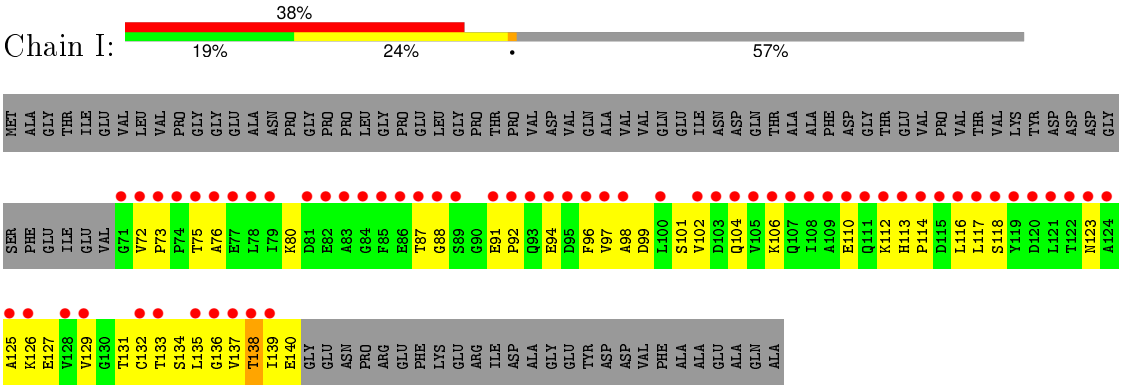
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.15Å 300.13Å 573.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 89.0 (49.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.244 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 600554 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99063	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.37	0/65959	0.69	23/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.43	0/102	0.65	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.38	0/1884	0.66	0/2551
7	D	0.30	0/1111	0.54	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.31	0/901	0.55	0/1224
10	G	0.27	0/241	0.45	0/324
11	H	0.33	0/1287	0.65	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.65	0/1509
15	M	0.35	0/1584	0.62	0/2119
16	N	0.29	0/1474	0.63	0/1999
17	O	0.34	0/874	0.60	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.35	0/749	0.67	0/1005
20	R	0.36	0/1172	0.63	0/1578
21	S	0.33	0/648	0.60	0/875
22	T	0.31	0/958	0.63	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.63	0/1655
26	X	0.33	0/664	0.58	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.36	0/589	0.65	0/787
29	1	0.41	0/438	0.66	0/578
30	2	0.32	0/401	0.52	0/529
31	3	0.39	0/771	0.61	0/1024
32	I	0.31	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.36	0/98794	0.67	24/147726 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	54
2	9	0	3
All	All	1	57

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.68	130.79	109.50
1	0	1942	A	C5'-C4'-C3'	8.39	129.43	116.00
1	0	1979	G	C2'-C3'-O3'	7.72	126.49	109.50
1	0	871	G	C5'-C4'-O4'	-7.18	100.48	109.10
2	9	3039	U	N1-C1'-C2'	7.03	123.14	114.00
1	0	1504	A	N9-C1'-C2'	6.38	122.30	114.00
1	0	1819	G	C5'-C4'-C3'	6.19	125.91	116.00
1	0	1120	U	C5'-C4'-C3'	-6.15	106.17	116.00
1	0	2316	G	C5'-C4'-C3'	-6.09	106.25	116.00
1	0	2313	C	C5'-C4'-O4'	6.06	116.38	109.10
1	0	1504	A	C1'-O4'-C4'	-5.96	105.13	109.90
1	0	2012	U	N1-C1'-C2'	5.87	121.62	114.00
1	0	2467	A	C1'-O4'-C4'	-5.70	105.34	109.90
1	0	129	A	C2'-C3'-O3'	5.63	122.71	113.70
1	0	921	G	N9-C1'-C2'	5.51	121.17	114.00
1	0	206	G	C5'-C4'-C3'	-5.51	107.19	116.00
1	0	1592	G	N9-C1'-C2'	5.51	121.16	114.00
1	0	1942	A	C4'-C3'-C2'	-5.43	97.17	102.60
1	0	1878	G	O4'-C1'-N9	5.32	112.46	108.20
1	0	1942	A	C5'-C4'-O4'	5.24	115.38	109.10
1	0	535	G	N9-C1'-C2'	5.14	120.68	114.00
1	0	777	U	O4'-C1'-N1	5.06	112.25	108.20
1	0	841	A	C1'-O4'-C4'	-5.05	105.86	109.90
1	0	1942	A	C1'-O4'-C4'	-5.02	105.88	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1323	G	Sidechain
1	0	1342	C	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1978	A	Sidechain
1	0	1993	C	Sidechain
1	0	2076	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	246	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	449	A	Sidechain
1	0	458	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	791	A	Sidechain
1	0	795	G	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	882	A	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
2	9	3087	U	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	29813	813	0
2	9	2600	0	1326	57	0
3	4	130	0	77	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	167	0
6	C	1859	0	1816	100	0
7	D	1094	0	1085	85	0
8	E	1357	0	1266	84	0
9	F	890	0	843	43	0
10	G	240	0	231	14	0
11	H	1266	0	1268	64	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	57	0
14	L	1118	0	1076	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	1560	0	1568	58	0
16	N	1445	0	1401	104	0
17	O	865	0	873	32	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	21	0
20	R	1149	0	1122	60	0
21	S	641	0	605	21	0
22	T	950	0	923	56	0
23	U	410	0	364	29	0
24	V	499	0	511	35	0
25	W	1196	0	1137	95	0
26	X	654	0	653	34	0
27	Y	1130	0	1133	56	0
28	Z	578	0	539	25	0
29	1	431	0	426	21	0
30	2	396	0	413	28	0
31	3	755	0	728	27	0
32	I	519	0	500	47	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	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	5809	0	0	103	0
38	1	53	0	0	2	0
38	2	40	0	0	3	0
38	3	74	0	0	4	0
38	4	8	0	0	1	0
38	9	137	0	0	5	0
38	A	119	0	0	13	0
38	B	153	0	0	15	0
38	C	168	0	0	12	0
38	D	47	0	0	10	0
38	E	43	0	0	7	0
38	F	23	0	0	3	0
38	G	18	0	0	2	0
38	H	65	0	0	4	0
38	I	9	0	0	2	0
38	J	51	0	0	4	0
38	K	58	0	0	6	0
38	L	82	0	0	12	0
38	M	116	0	0	5	0
38	N	63	0	0	10	0
38	O	42	0	0	3	0
38	P	64	0	0	3	0
38	Q	51	0	0	3	0
38	R	84	0	0	3	0
38	S	30	0	0	1	0
38	T	42	0	0	2	0
38	U	29	0	0	2	0
38	V	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	68	0	0	2	0
38	X	27	0	0	2	0
38	Y	96	0	0	5	0
38	Z	32	0	0	2	0
All	All	99063	0	59977	2271	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 (2271) 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)
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.28	1.16
5:B:62:ARG:HA	5:B:65:MET:HE3	1.29	1.14
1:0:156:C:H5"	15:M:171:ARG:HD3	1.29	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.20	1.11
1:0:1242:A:H5'	12:J:82:THR:HG23	1.34	1.09
6:C:236:THR:HG22	6:C:239:ALA:H	1.16	1.08
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.30	1.08
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.34	1.07
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.72	1.04
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.21	1.04
2:9:3076:G:H3'	2:9:3077:A:H5"	1.38	1.01
1:0:1751:G:H2'	1:0:1752:G:H5"	1.40	1.01
20:R:39:THR:HG22	20:R:42:GLU:H	1.26	1.00
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.40	1.00
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.40	1.00
2:9:3006:C:H5"	16:N:37:ARG:NH1	1.76	1.00
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.42	0.99
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.77	0.99
1:0:2717:C:H2'	1:0:2718:C:H5"	1.46	0.98
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.45	0.97
13:K:10:GLN:H	13:K:10:GLN:NE2	1.61	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	1.10	0.97
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.47	0.96
7:D:154:LYS:HD2	7:D:154:LYS:H	1.29	0.96
1:0:871:G:C8	1:0:871:G:H5'	2.02	0.94
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.50	0.94
13:K:10:GLN:N	13:K:10:GLN:HE21	1.65	0.94
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.49	0.93
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:HO2'	1:0:1189:A:H2	1.04	0.93
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.51	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.32	0.92
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.35	0.92
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.11	0.92
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.52	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.92
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.52	0.91
12:J:131:THR:HG22	12:J:134:GLU:H	1.34	0.91
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.11	0.91
15:M:164:THR:HG22	15:M:167:GLY:H	1.33	0.91
6:C:1:MET:HG2	6:C:2:GLN:H	1.33	0.91
1:0:541:C:H2'	1:0:542:A:H5"	1.53	0.91
1:0:2717:C:C2'	1:0:2718:C:H5"	2.01	0.90
1:0:1835:U:H5	1:0:1840:A:N7	1.69	0.90
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.90
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.53	0.90
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.54	0.89
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.89
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.52	0.89
1:0:542:A:H5'	1:0:542:A:H8	1.37	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	1.01	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.88	0.89
1:0:1701:A:H4'	1:0:1702:U:H5"	1.55	0.89
1:0:1372:A:H3'	38:0:7406:HOH:O	1.72	0.89
1:0:21:G:H5'	20:R:2:ILE:HA	1.55	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.88
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.74	0.87
16:N:144:GLY:O	16:N:147:ILE:HG22	1.74	0.87
5:B:248:ARG:O	5:B:251:VAL:HG12	1.73	0.87
1:0:1160:G:C5'	1:0:1161:A:H5'	2.05	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.75	0.86
26:X:30:MET:HE1	26:X:55:ASN:HA	1.57	0.86
1:0:870:G:H2'	1:0:871:G:H5"	1.55	0.86
2:9:3056:A:H2'	2:9:3057:A:H5"	1.57	0.85
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.24	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.24	0.85
2:9:3006:C:H5"	16:N:37:ARG:HH12	1.34	0.85
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.58	0.85
1:0:1159:G:H21	1:0:1189:A:H8	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.59	0.84
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.58	0.84
1:0:21:G:C5'	20:R:2:ILE:HA	2.07	0.84
5:B:321:PRO:HA	38:B:9463:HOH:O	1.78	0.83
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.60	0.83
5:B:98:THR:HG22	5:B:99:GLU:H	1.44	0.83
1:0:2291:A:C8	1:0:2309:C:H5'	2.13	0.83
1:0:2586:U:H3	1:0:2592:G:H22	1.26	0.83
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.79	0.83
2:9:3051:A:H5'	16:N:160:SER:HB3	1.61	0.83
1:0:1160:G:H5'	1:0:1161:A:C5'	2.08	0.82
32:I:138:THR:HG22	32:I:139:ILE:H	1.43	0.82
23:U:9:CYS:HA	23:U:52:THR:HG23	1.61	0.82
13:K:10:GLN:H	13:K:10:GLN:HE21	0.84	0.82
23:U:52:THR:HG22	23:U:54:THR:H	1.43	0.82
1:0:871:G:H8	1:0:871:G:H5'	1.44	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.82	0.82
1:0:2364:A:H5"	19:Q:15:LYS:HD3	1.59	0.82
6:C:139:VAL:HG13	38:C:9246:HOH:O	1.80	0.81
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.43	0.81
21:S:57:THR:HG22	21:S:59:ASP:H	1.44	0.81
1:0:2105:C:H5'	38:4:7924:HOH:O	1.79	0.81
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.44	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.61	0.81
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.63	0.81
1:0:2908:A:H2'	1:0:2909:G:O4'	1.80	0.81
11:H:166:SER:HB2	11:H:167:PRO:CD	2.09	0.81
5:B:51:VAL:HG23	5:B:329:TYR:O	1.81	0.81
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.61	0.81
5:B:179:LEU:O	5:B:183:GLU:HG2	1.81	0.80
25:W:88:THR:HB	38:W:6679:HOH:O	1.82	0.80
7:D:25:MET:HE2	7:D:41:LEU:HG	1.63	0.80
25:W:88:THR:HG22	25:W:89:ASP:H	1.44	0.80
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.12	0.80
1:0:282:C:H1'	1:0:368:C:N4	1.97	0.79
1:0:1593:C:H5'	18:P:116:SER:O	1.82	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.62	0.79
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.64	0.79
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.65	0.79
1:0:559:U:H5'	1:0:559:U:H6	1.47	0.79
1:0:1559:A:H1'	38:0:6127:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:289:G:H22	1:0:363:A:H2	1.30	0.79
6:C:236:THR:H	6:C:239:ALA:HB3	1.47	0.78
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.82	0.78
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.81	0.78
1:0:1751:G:C2'	1:0:1752:G:H5"	2.13	0.78
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.65	0.78
22:T:41:ARG:HH11	22:T:41:ARG:HG2	1.47	0.78
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.49	0.78
1:0:2840:A:OP1	5:B:211:THR:HG23	1.84	0.78
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.14	0.78
4:A:131:HIS:O	4:A:132:ASP:HB2	1.83	0.78
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.82	0.78
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.48	0.78
2:9:3039:U:H1'	2:9:3044:A:H61	1.48	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.77
25:W:65:VAL:HA	25:W:68:THR:HG22	1.66	0.77
1:0:1603:A:H5'	1:0:1605:G:O4'	1.84	0.77
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.66	0.77
1:0:541:C:C2'	1:0:542:A:H5"	2.12	0.77
25:W:106:THR:OG1	25:W:109:GLU:HG3	1.85	0.77
1:0:2533:C:H5'	1:0:2533:C:H6	1.49	0.77
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.66	0.77
11:H:27:LYS:H	11:H:59:HIS:HD2	1.30	0.77
27:Y:117:LEU:HD12	27:Y:174:VAL:CG1	2.14	0.77
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.14	0.77
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.66	0.77
1:0:159:G:OP1	15:M:74:LYS:HE3	1.84	0.77
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.50	0.77
1:0:1209:C:H2'	1:0:1210:G:H8	1.49	0.77
12:J:107:ASN:ND2	12:J:109:TYR:H	1.83	0.77
1:0:2608:C:H2'	38:0:8228:HOH:O	1.85	0.77
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.67	0.76
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.66	0.76
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.50	0.76
24:V:1:THR:HG23	24:V:2:VAL:H	1.49	0.76
25:W:52:VAL:HG22	25:W:53:ALA:H	1.49	0.76
7:D:57:THR:HG23	7:D:63:ILE:HA	1.68	0.76
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.66	0.76
38:0:4965:HOH:O	5:B:300:SER:HB3	1.86	0.76
11:H:166:SER:CB	11:H:167:PRO:HD3	2.14	0.76
1:0:111:C:O2'	29:1:20:ARG:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:O2'	1:0:1118:A:H2	1.68	0.76
5:B:98:THR:HG22	5:B:99:GLU:N	2.00	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	1.27	0.76
26:X:78:GLU:HG2	26:X:79:GLU:H	1.49	0.76
16:N:113:SER:HB2	38:N:9357:HOH:O	1.85	0.75
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.85	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.75
1:0:871:G:H8	1:0:871:G:C5'	1.98	0.75
1:0:2679:G:H2'	1:0:2681:A:OP2	1.86	0.75
1:0:244:C:OP2	9:F:38:LYS:HE3	1.85	0.75
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.68	0.75
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.86	0.75
2:9:3014:G:H8	2:9:3014:G:H5'	1.51	0.75
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.68	0.75
1:0:281:U:H2'	1:0:282:C:O4'	1.87	0.75
1:0:447:A:OP2	22:T:1:SER:HB2	1.85	0.75
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.68	0.75
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.69	0.74
1:0:2094:G:H4'	5:B:245:SER:HB3	1.67	0.74
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.74
18:P:115:SER:OG	18:P:118:GLN:HG3	1.87	0.74
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.67	0.74
32:I:101:SER:H	32:I:104:GLN:NE2	1.85	0.74
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.69	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.69	0.74
24:V:39:ALA:N	24:V:40:PRO:HD2	2.03	0.74
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.69	0.74
24:V:12:THR:HG22	24:V:15:GLU:CG	2.15	0.74
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.53	0.74
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.70	0.74
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.17	0.74
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.68	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.36	0.74
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.70	0.74
1:0:793:A:H5"	18:P:83:LYS:HG2	1.70	0.74
1:0:545:G:H8	1:0:545:G:H5'	1.52	0.73
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.18	0.73
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.73
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.73
5:B:62:ARG:CA	5:B:65:MET:HE3	2.15	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.73
1:0:2426:G:H1'	38:0:6343:HOH:O	1.87	0.73
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.73
4:A:191:GLY:HA2	4:A:194:MET:CE	2.19	0.73
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.89	0.73
1:0:2256:G:H2'	1:0:2257:G:H5'	1.71	0.72
7:D:99:ASP:HB3	7:D:103:ASN:H	1.54	0.72
1:0:381:G:H5"	38:0:4621:HOH:O	1.89	0.72
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.70	0.72
1:0:182:G:H5'	38:0:5437:HOH:O	1.88	0.72
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.90	0.72
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.89	0.72
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.89	0.72
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.71	0.72
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.70	0.72
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.93	0.72
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.72	0.72
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.20	0.71
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.05	0.71
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.72	0.71
14:L:133:VAL:HA	38:L:9370:HOH:O	1.89	0.71
1:0:2827:A:H2'	1:0:2828:G:O4'	1.89	0.71
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.71
8:E:69:ILE:HA	8:E:72:MET:CE	2.20	0.71
9:F:91:VAL:HG12	9:F:92:GLY:H	1.55	0.71
1:0:820:G:H5"	38:0:3359:HOH:O	1.90	0.71
5:B:307:ARG:HB2	5:B:307:ARG:HH11	1.56	0.70
1:0:2054:A:N3	20:R:128:ARG:NH2	2.38	0.70
1:0:21:G:H5"	20:R:1:GLY:O	1.91	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.90	0.70
1:0:450:C:OP1	6:C:184:ARG:NH2	2.24	0.70
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.73	0.70
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.73	0.70
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.09	0.70
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.89	0.70
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.03	0.70
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.74	0.70
1:0:796:A:HO2'	28:Z:10:ARG:N	1.89	0.70
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.73	0.70
5:B:145:HIS:HD2	5:B:146:THR:O	1.72	0.70
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2468:A:H61	31:3:48:ASN:HD21	1.37	0.70
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.22	0.70
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.74	0.70
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.07	0.70
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.74	0.70
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.72	0.69
5:B:139:ASP:HB2	5:B:165:ARG:HE	1.56	0.69
1:0:1667:A:C8	1:0:1667:A:H5'	2.24	0.69
25:W:38:THR:HG22	25:W:39:ASP:H	1.58	0.69
20:R:44:VAL:O	20:R:48:GLU:HG3	1.92	0.69
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.72	0.69
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.58	0.69
38:0:7097:HOH:O	15:M:178:LYS:HB2	1.91	0.69
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.40	0.69
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.27	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.91	0.69
4:A:223:ARG:HG3	38:A:9398:HOH:O	1.91	0.69
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.73	0.69
20:R:9:ASP:O	20:R:13:THR:HB	1.92	0.69
1:0:338:C:H4'	6:C:174:ILE:CD1	2.23	0.69
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.58	0.69
21:S:57:THR:HG22	21:S:59:ASP:N	2.07	0.69
27:Y:117:LEU:HD12	27:Y:174:VAL:HG13	1.75	0.69
9:F:38:LYS:NZ	15:M:3:SER:HA	2.08	0.69
1:0:1184:C:H1'	38:0:7669:HOH:O	1.92	0.69
1:0:1206:U:H6	1:0:1206:U:H5'	1.58	0.68
1:0:1166:A:H1'	1:0:1192:A:C2	2.29	0.68
1:0:1116:U:H3	1:0:1246:A:H62	1.39	0.68
1:0:870:G:C2'	1:0:871:G:H5"	2.23	0.68
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.74	0.68
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.08	0.68
9:F:91:VAL:HG12	9:F:92:GLY:N	2.08	0.68
30:2:41:HIS:N	30:2:45:ASN:HD22	1.88	0.68
4:A:199:HIS:HD2	4:A:201:PHE:H	1.38	0.68
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.76	0.68
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.24	0.68
1:0:1666:C:O2'	1:0:1667:A:H5"	1.93	0.68
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.19	0.68
1:0:2502:C:H2'	1:0:2503:A:H5'	1.75	0.68
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.59	0.68
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1236:A:C8	12:J:63:ILE:HD11	2.30	0.67
1:0:1474:C:C6	1:0:1474:C:H5'	2.22	0.67
1:0:2533:C:C6	1:0:2533:C:H5'	2.28	0.67
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.74	0.67
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.77	0.67
18:P:103:THR:HA	18:P:106:ARG:NH1	2.09	0.67
4:A:121:ALA:O	4:A:124:VAL:HG22	1.93	0.67
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.67
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.77	0.67
17:O:32:ARG:HD3	17:O:32:ARG:O	1.94	0.67
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.24	0.67
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.95	0.67
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.09	0.67
4:A:179:MET:HA	4:A:179:MET:CE	2.25	0.67
1:0:317:A:H5"	22:T:52:ARG:HD2	1.76	0.67
20:R:39:THR:HG22	20:R:42:GLU:N	2.05	0.67
1:0:558:C:C2'	1:0:559:U:H5"	2.25	0.67
1:0:2768:A:H2'	1:0:2769:C:O4'	1.94	0.67
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.59	0.67
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.77	0.66
6:C:236:THR:CG2	6:C:239:ALA:H	2.00	0.66
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.28	0.66
1:0:542:A:H5'	1:0:542:A:C8	2.26	0.66
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.60	0.66
1:0:1634:G:H3'	38:0:4200:HOH:O	1.94	0.66
16:N:169:PRO:O	16:N:172:PHE:HB3	1.96	0.66
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.66
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.56	0.66
1:0:560:C:H42	1:0:597:A:H61	1.42	0.66
1:0:1118:A:H3'	1:0:1118:A:H8	1.61	0.66
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.77	0.66
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.78	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.61	0.66
1:0:681:G:N3	1:0:681:G:H5'	2.11	0.66
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.11	0.66
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.77	0.66
1:0:506:G:H22	1:0:509:A:H5"	1.61	0.66
19:Q:26:PRO:O	19:Q:30:VAL:HG23	1.95	0.66
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.96	0.66
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.44	0.65
2:9:3028:U:H5"	16:N:40:ASN:ND2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:52:GLN:HG3	12:J:53:ILE:N	2.10	0.65
1:0:1189:A:H1'	1:0:1209:C:O4'	1.96	0.65
23:U:14:GLU:O	23:U:17:THR:HB	1.96	0.65
6:C:7:ASP:OD2	6:C:9:ASP:HB2	1.96	0.65
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.26	0.65
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.79	0.65
1:0:2502:C:C2'	1:0:2503:A:H5'	2.27	0.65
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.78	0.65
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.61	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.27	0.65
1:0:2769:C:C2'	1:0:2770:G:H5'	2.27	0.65
25:W:149:LEU:HG	25:W:153:MET:HE2	1.79	0.65
5:B:297:VAL:HB	38:B:9412:HOH:O	1.95	0.65
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.61	0.65
8:E:97:VAL:HG12	38:E:4191:HOH:O	1.96	0.65
7:D:23:VAL:HG12	7:D:130:VAL:HG22	1.79	0.65
2:9:3056:A:C2'	2:9:3057:A:H5"	2.26	0.65
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.65
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.78	0.65
1:0:272:A:H5'	1:0:273:G:OP2	1.96	0.65
1:0:95:A:H5"	1:0:97:G:O4'	1.96	0.65
2:9:3092:G:H2'	2:9:3093:A:C8	2.31	0.65
22:T:47:THR:HB	22:T:100:ASP:HB3	1.79	0.65
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.00	0.65
2:9:3013:A:O2'	2:9:3014:G:H5"	1.96	0.65
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.77	0.65
1:0:1118:A:H3'	1:0:1118:A:C8	2.32	0.64
24:V:38:GLY:C	24:V:40:PRO:HD2	2.17	0.64
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.79	0.64
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.96	0.64
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.78	0.64
15:M:9:ARG:HB2	15:M:47:ASP:OD2	1.96	0.64
1:0:2578:G:H5'	1:0:2578:G:H8	1.62	0.64
17:O:21:SER:OG	17:O:106:PRO:HB2	1.97	0.64
1:0:657:G:OP1	6:C:27:ARG:NH2	2.29	0.64
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.79	0.64
12:J:39:VAL:HG13	12:J:106:GLY:O	1.97	0.64
1:0:603:A:H5"	1:0:604:G:OP1	1.96	0.64
6:C:242:GLU:HG3	38:C:9177:HOH:O	1.96	0.64
1:0:2878:U:H2'	1:0:2879:A:O4'	1.96	0.64
1:0:1116:U:O2'	1:0:1118:A:C2	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3039:U:H1'	2:9:3044:A:N6	2.12	0.64
6:C:218:VAL:HG12	38:C:9222:HOH:O	1.96	0.64
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.37	0.64
18:P:64:GLU:HG2	38:P:168:HOH:O	1.97	0.64
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.79	0.64
1:0:447:A:P	22:T:1:SER:HB2	2.38	0.64
10:G:12:ILE:N	10:G:13:PRO:HD3	2.13	0.64
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.10	0.64
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.78	0.64
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.12	0.64
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.78	0.64
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.64
32:I:76:ALA:O	32:I:80:LYS:HG3	1.98	0.64
24:V:12:THR:HG23	24:V:14:ALA:H	1.62	0.64
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.63	0.64
5:B:36:PRO:HA	5:B:168:GLY:CA	2.25	0.63
3:4:176:A:O4'	3:4:175:C:H2'	1.99	0.63
1:0:1299:G:O6	14:L:6:ARG:HD3	1.97	0.63
1:0:31:C:H4'	38:0:7630:HOH:O	1.98	0.63
23:U:52:THR:HG22	23:U:54:THR:N	2.11	0.63
8:E:69:ILE:HA	8:E:72:MET:HE2	1.81	0.63
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.78	0.63
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.19	0.63
7:D:25:MET:CE	7:D:37:ALA:HB1	2.29	0.63
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.78	0.63
8:E:144:THR:O	8:E:148:ILE:HG13	1.98	0.63
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.79	0.63
9:F:96:ALA:HA	38:F:3111:HOH:O	1.98	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.98	0.63
4:A:36:ASP:O	4:A:38:ILE:N	2.32	0.63
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.28	0.63
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.28	0.63
1:0:2524:G:H21	1:0:2526:C:N4	1.97	0.63
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.81	0.63
1:0:1701:A:H4'	1:0:1702:U:C5'	2.27	0.63
38:0:4293:HOH:O	22:T:82:THR:HA	1.99	0.63
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	1.99	0.63
30:2:20:ARG:HB3	38:2:5444:HOH:O	1.97	0.63
20:R:39:THR:HG23	20:R:107:GLU:O	1.99	0.63
5:B:138:GLY:O	5:B:139:ASP:O	2.17	0.63
1:0:1175:G:H1'	1:0:1193:A:H2'	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3029:C:C2'	2:9:3030:C:H5'	2.29	0.63
1:0:119:A:H2'	1:0:120:A:H5"	1.81	0.63
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.79	0.63
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.47	0.63
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.29	0.63
12:J:107:ASN:HD22	12:J:108:PRO:N	1.97	0.62
26:X:25:ARG:HD3	26:X:64:ALA:O	1.99	0.62
1:0:1641:A:H2'	1:0:1642:A:H5'	1.80	0.62
8:E:15:GLN:HG2	8:E:19:ASP:O	1.99	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.30	0.62
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.00	0.62
10:G:64:ASN:N	10:G:64:ASN:HD22	1.95	0.62
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.80	0.62
2:9:3014:G:C8	2:9:3014:G:H5'	2.33	0.62
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.81	0.62
11:H:170:ASN:HD22	11:H:170:ASN:N	1.96	0.62
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.29	0.62
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.81	0.62
7:D:136:ARG:HD2	7:D:155:HIS:O	1.99	0.62
9:F:19:ALA:O	9:F:22:VAL:HG22	1.98	0.62
16:N:32:PRO:HD2	16:N:99:GLU:O	1.99	0.62
1:0:88:G:H5'	1:0:88:G:H8	1.65	0.62
1:0:544:G:H2'	1:0:545:G:H5"	1.82	0.62
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.12	0.62
1:0:1053:G:OP1	11:H:12:PRO:HG3	1.99	0.62
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.99	0.62
7:D:50:VAL:O	7:D:71:ALA:HA	2.00	0.62
1:0:2534:C:H1'	38:0:3802:HOH:O	1.99	0.62
10:G:16:LYS:O	10:G:20:VAL:HG23	1.99	0.62
1:0:2824:C:H5"	1:0:2825:C:H5'	1.81	0.62
38:0:7630:HOH:O	22:T:9:LYS:HB2	1.99	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:2896:A:H5"	38:0:6350:HOH:O	2.00	0.62
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.99	0.62
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.15	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.62
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.30	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
1:0:138:U:H5"	1:0:139:C:OP2	2.00	0.62
1:0:558:C:O2'	1:0:559:U:H5"	2.00	0.61
1:0:447:A:O2'	1:0:448:G:H5'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:H2'	1:0:2257:G:C5'	2.29	0.61
1:0:2717:C:H2'	1:0:2718:C:C5'	2.27	0.61
24:V:1:THR:HG23	24:V:2:VAL:N	2.15	0.61
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.81	0.61
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.98	0.61
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.81	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.65	0.61
32:I:138:THR:HG22	32:I:139:ILE:N	2.15	0.61
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.30	0.61
27:Y:144:ARG:CZ	38:Y:8201:HOH:O	2.48	0.61
1:0:1120:U:H5"	1:0:1120:U:C6	2.35	0.61
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.15	0.61
7:D:25:MET:CE	7:D:41:LEU:HG	2.30	0.61
6:C:1:MET:HG2	6:C:2:GLN:N	2.10	0.61
32:I:99:ASP:OD1	32:I:138:THR:HB	2.00	0.61
7:D:163:VAL:HA	38:D:6326:HOH:O	2.01	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
7:D:23:VAL:O	7:D:23:VAL:HG23	2.01	0.61
1:0:506:G:H22	1:0:509:A:H5'	1.66	0.61
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.61
4:A:33:GLU:O	4:A:34:ASP:HB2	1.98	0.61
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.97	0.61
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.99	0.61
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.66	0.61
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.31	0.61
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.01	0.61
1:0:2248:C:H3'	38:0:5712:HOH:O	2.01	0.61
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.83	0.61
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.82	0.61
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.00	0.61
1:0:1943:C:H4'	4:A:211:LYS:O	2.01	0.61
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.15	0.61
4:A:179:MET:HG2	4:A:186:TRP:CB	2.31	0.61
11:H:63:GLU:HA	38:H:9178:HOH:O	2.00	0.61
1:0:316:A:H5'	22:T:54:ASP:OD2	2.01	0.61
8:E:9:GLU:HG3	8:E:10:ASP:N	2.16	0.61
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.82	0.61
8:E:93:MET:HE1	8:E:165:GLY:N	2.15	0.61
11:H:9:ILE:O	11:H:9:ILE:HG22	2.01	0.61
1:0:1741:U:O2'	1:0:2723:G:H4'	2.01	0.61
8:E:7:ILE:HG22	8:E:45:ASP:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.61
4:A:192:VAL:HG13	38:A:9356:HOH:O	2.00	0.61
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.31	0.61
19:Q:53:HIS:CE1	19:Q:55:ARG:HG3	2.35	0.61
12:J:133:GLY:O	12:J:137:GLU:HG3	2.01	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.32	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.82	0.60
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.83	0.60
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.60
16:N:110:THR:HB	16:N:113:SER:OG	2.02	0.60
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.60
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.34	0.60
16:N:37:ARG:NE	38:N:9331:HOH:O	2.34	0.60
1:0:2716:G:H5"	5:B:206:THR:HG21	1.84	0.60
38:0:3594:HOH:O	13:K:9:THR:HA	2.01	0.60
1:0:1717:A:H5"	18:P:54:LYS:HB2	1.83	0.60
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.16	0.60
1:0:2346:C:O5'	1:0:2346:C:H6	1.85	0.60
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.33	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
1:0:121:U:OP2	30:2:10:ARG:NH2	2.28	0.60
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.01	0.60
7:D:153:THR:O	7:D:156:ARG:HB2	2.01	0.60
29:1:10:LYS:HG3	38:1:2979:HOH:O	2.01	0.60
1:0:1667:A:H2'	1:0:1668:U:C6	2.37	0.60
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.84	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.02	0.60
1:0:475:G:H5'	6:C:73:LEU:HD23	1.84	0.60
14:L:143:THR:HG22	14:L:144:ASP:N	2.17	0.60
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.84	0.60
1:0:541:C:H2'	1:0:542:A:C5'	2.28	0.60
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.31	0.60
8:E:23:GLU:HG2	8:E:28:SER:CB	2.31	0.60
1:0:1878:G:H1'	38:0:6371:HOH:O	2.02	0.60
23:U:52:THR:CG2	23:U:54:THR:HB	2.32	0.60
25:W:88:THR:HG22	25:W:89:ASP:N	2.16	0.60
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.84	0.60
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.02	0.60
1:0:474:C:O3'	6:C:73:LEU:HD21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:151:ASP:O	16:N:154:LEU:HB2	2.01	0.60
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.84	0.60
13:K:115:ARG:HB3	13:K:132:VAL:OXT	2.02	0.59
20:R:132:ARG:HG2	20:R:133:ALA:N	2.17	0.59
21:S:56:ASN:O	30:2:8:LYS:NZ	2.34	0.59
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.37	0.59
1:0:1119:G:OP2	12:J:49:ARG:HD3	2.02	0.59
7:D:154:LYS:H	7:D:154:LYS:CD	2.06	0.59
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.84	0.59
1:0:2241:C:O2'	1:0:2242:U:H5'	2.01	0.59
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.82	0.59
1:0:1080:C:H4'	1:0:1081:A:OP1	2.01	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.31	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
1:0:20:G:H21	20:R:117:HIS:HD2	1.49	0.59
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.85	0.59
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.84	0.59
6:C:115:LEU:O	6:C:118:THR:HB	2.03	0.59
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.03	0.59
18:P:103:THR:O	18:P:107:GLU:HG3	2.02	0.59
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.01	0.59
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.85	0.59
5:B:140:LEU:HD23	38:B:9384:HOH:O	2.02	0.59
38:0:7658:HOH:O	5:B:211:THR:HG21	2.01	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.68	0.59
1:0:247:A:H2'	38:0:4229:HOH:O	2.03	0.59
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.83	0.59
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.59
13:K:55:VAL:HG12	13:K:56:SER:N	2.18	0.59
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.35	0.59
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.32	0.59
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.33	0.59
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.84	0.59
12:J:130:VAL:HG12	12:J:131:THR:N	2.17	0.59
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.67	0.59
16:N:154:LEU:HD12	16:N:156:GLU:O	2.02	0.59
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.84	0.59
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.02	0.59
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1462:C:H2'	1:0:1463:A:C8	2.38	0.59
1:0:1834:C:H2'	1:0:1840:A:N6	2.17	0.59
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.59
1:0:1666:C:C2'	1:0:1667:A:H5"	2.33	0.59
6:C:16:VAL:HG12	6:C:17:ASP:H	1.66	0.59
4:A:199:HIS:CD2	4:A:201:PHE:H	2.19	0.59
1:0:775:G:OP1	29:1:16:HIS:HE1	1.85	0.59
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.02	0.59
5:B:238:ASN:HD22	5:B:240:GLY:N	1.94	0.59
1:0:289:G:N2	1:0:363:A:H2	1.99	0.59
12:J:99:GLU:HA	38:J:9370:HOH:O	2.02	0.59
5:B:177:HIS:O	5:B:181:ILE:HG13	2.02	0.59
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.58
38:0:5498:HOH:O	13:K:39:GLY:HA2	2.02	0.58
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.84	0.58
25:W:149:LEU:HG	25:W:153:MET:CE	2.33	0.58
9:F:58:GLU:HA	9:F:61:MET:HE2	1.85	0.58
1:0:1189:A:H1'	1:0:1209:C:C1'	2.34	0.58
8:E:69:ILE:HA	8:E:72:MET:HE3	1.84	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58
1:0:1118:A:H8	1:0:1119:G:H5"	1.68	0.58
1:0:2541:U:H5'	38:0:9722:HOH:O	2.04	0.58
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.58
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.58
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.18	0.58
1:0:1527:A:H1'	1:0:1528:A:C8	2.39	0.58
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.19	0.58
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.03	0.58
1:0:2601:A:N1	13:K:38:SER:HB2	2.19	0.58
1:0:2710:U:H1'	38:0:7817:HOH:O	2.03	0.58
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.04	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.85	0.58
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.84	0.58
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.03	0.58
29:1:25:LYS:HG3	30:2:49:GLU:H	1.69	0.58
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.06	0.58
1:0:553:G:P	27:Y:204:ARG:HH22	2.26	0.58
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.39	0.58
5:B:98:THR:CG2	5:B:99:GLU:H	2.14	0.58
17:O:105:ASN:HD21	17:O:109:SER:H	1.48	0.58
5:B:81:ALA:O	5:B:186:GLY:HA3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1766:U:O2	1:0:1778:A:H5'	2.03	0.58
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.85	0.58
25:W:108:ARG:HE	25:W:114:PRO:CG	2.15	0.58
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.17	0.58
1:0:1741:U:H5'	1:0:1742:A:OP1	2.04	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.68	0.58
16:N:47:LEU:HD12	16:N:97:VAL:HG11	1.86	0.58
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.03	0.58
1:0:1086:A:C6	25:W:11:VAL:HG11	2.38	0.58
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.86	0.57
1:0:1120:U:H6	1:0:1120:U:H5"	1.69	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.86	0.57
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.68	0.57
1:0:2488:A:H2	38:0:7489:HOH:O	1.87	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.30	0.57
7:D:64:ARG:HB3	7:D:67:ASP:OD2	2.04	0.57
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.04	0.57
1:0:2361:A:H8	1:0:2361:A:H5'	1.69	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.57
1:0:1189:A:H3'	38:0:7875:HOH:O	2.03	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.04	0.57
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.34	0.57
4:A:36:ASP:C	4:A:38:ILE:H	2.06	0.57
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.69	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.85	0.57
8:E:81:GLU:HG2	8:E:134:SER:CB	2.31	0.57
16:N:80:SER:HB2	38:N:9333:HOH:O	2.05	0.57
12:J:8:ALA:HA	12:J:35:THR:HG22	1.84	0.57
11:H:97:GLU:HB3	11:H:121:VAL:HG11	1.87	0.57
3:4:77:2OP:HA	3:4:177:PAE:O2	2.04	0.57
2:9:3020:G:O2'	2:9:3021:G:H5'	2.05	0.57
6:C:95:GLU:N	6:C:95:GLU:OE1	2.34	0.57
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.03	0.57
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.29	0.57
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.34	0.57
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.57
1:0:656:G:OP2	17:O:37:ARG:HD2	2.05	0.57
1:0:1625:U:H4'	38:0:4961:HOH:O	2.03	0.57
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.68	0.57
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.85	0.57
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:155:GLU:O	16:N:156:GLU:HG3	2.04	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.34	0.57
1:0:1441:G:O2'	1:0:1442:A:H5'	2.04	0.57
5:B:62:ARG:HA	5:B:65:MET:CE	2.19	0.57
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.87	0.57
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.87	0.57
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.04	0.57
6:C:168:ARG:NH2	6:C:190:ALA:O	2.38	0.57
1:0:1596:U:H2'	1:0:1598:A:OP2	2.05	0.57
6:C:16:VAL:HG12	6:C:17:ASP:N	2.20	0.57
1:0:1500:U:P	18:P:41:ARG:HH22	2.28	0.57
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.86	0.57
32:I:92:PRO:O	32:I:94:GLU:HG3	2.05	0.57
6:C:25:PRO:HG2	38:C:9122:HOH:O	2.04	0.57
2:9:3076:G:C3'	2:9:3077:A:H5"	2.25	0.57
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.86	0.57
25:W:13:MET:CE	25:W:17:ILE:HG22	2.34	0.57
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.39	0.57
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.70	0.57
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.20	0.57
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.35	0.57
13:K:74:VAL:HG21	13:K:96:VAL:HG23	1.85	0.57
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.38	0.57
1:0:503:G:H2'	1:0:504:G:H8	1.69	0.57
23:U:9:CYS:CA	23:U:52:THR:HG23	2.32	0.56
1:0:848:C:H5'	38:0:7487:HOH:O	2.04	0.56
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.86	0.56
1:0:2649:A:C8	1:0:2649:A:H5'	2.40	0.56
26:X:31:ILE:O	26:X:35:GLU:HG3	2.04	0.56
1:0:902:G:N7	14:L:18:HIS:HD2	2.03	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
26:X:30:MET:CE	26:X:55:ASN:HA	2.32	0.56
8:E:15:GLN:NE2	8:E:40:VAL:O	2.37	0.56
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.53	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.06	0.56
31:3:3:MET:O	31:3:90:PHE:HA	2.05	0.56
31:3:73:GLU:HB3	38:3:9360:HOH:O	2.05	0.56
11:H:27:LYS:N	11:H:59:HIS:HD2	2.01	0.56
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.56
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.05	0.56
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.70	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.35	0.56
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.20	0.56
12:J:76:ASP:HA	38:J:9365:HOH:O	2.05	0.56
2:9:3051:A:H5'	16:N:160:SER:CB	2.32	0.56
1:0:2420:G:O2'	1:0:2421:G:H5'	2.06	0.56
18:P:115:SER:H	18:P:118:GLN:NE2	1.86	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.56
1:0:449:A:N7	6:C:43:LYS:HG2	2.21	0.56
16:N:72:GLU:HG2	16:N:72:GLU:O	2.06	0.56
25:W:52:VAL:HG22	25:W:53:ALA:N	2.20	0.56
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.36	0.56
1:0:2301:A:H5"	1:0:2302:A:H5'	1.87	0.56
25:W:59:GLN:HE22	25:W:98:PHE:HB2	1.69	0.56
7:D:86:THR:C	7:D:89:PRO:HD2	2.26	0.56
1:0:2769:C:H2'	1:0:2770:G:H5'	1.88	0.56
1:0:1677:U:OP2	30:2:8:LYS:NZ	2.37	0.56
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.36	0.56
22:T:41:ARG:NH1	22:T:42:VAL:O	2.38	0.56
11:H:170:ASN:N	11:H:170:ASN:ND2	2.53	0.56
5:B:16:ARG:NH1	38:B:9422:HOH:O	2.38	0.56
1:0:2748:G:H2'	38:0:7739:HOH:O	2.05	0.56
8:E:137:ASP:O	8:E:141:VAL:HG23	2.06	0.56
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.20	0.56
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.69	0.56
9:F:38:LYS:HZ1	15:M:3:SER:HA	1.68	0.56
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.70	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.05	0.55
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.05	0.55
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.35	0.55
1:0:475:G:C5'	6:C:73:LEU:HD23	2.37	0.55
1:0:1211:G:O2'	1:0:1212:C:H5'	2.05	0.55
1:0:709:G:O2'	17:O:25:VAL:HG12	2.07	0.55
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.36	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.30	0.55
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.36	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.04	0.55
26:X:78:GLU:HG2	26:X:79:GLU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.52	0.55
24:V:39:ALA:O	24:V:41:GLU:N	2.33	0.55
38:0:6997:HOH:O	16:N:4:PRO:HD2	2.06	0.55
1:0:2036:C:O4'	13:K:44:LEU:HG	2.06	0.55
21:S:77:VAL:O	21:S:80:ARG:HG2	2.06	0.55
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.35	0.55
15:M:60:VAL:C	15:M:61:ILE:HD12	2.26	0.55
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.05	0.55
5:B:98:THR:CG2	5:B:99:GLU:N	2.70	0.55
9:F:22:VAL:HG21	9:F:104:ALA:HB2	1.89	0.55
2:9:3054:A:O2'	2:9:3055:U:H5'	2.07	0.55
38:0:5127:HOH:O	12:J:47:THR:HB	2.06	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.06	0.55
7:D:138:GLY:N	38:D:7597:HOH:O	2.39	0.55
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.42	0.55
8:E:132:THR:O	8:E:132:THR:HG23	2.05	0.55
1:0:282:C:H1'	1:0:368:C:H42	1.68	0.55
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.36	0.55
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.87	0.55
9:F:37:THR:O	9:F:41:GLU:HG3	2.07	0.55
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.06	0.55
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.88	0.55
6:C:138:VAL:O	6:C:234:VAL:HA	2.07	0.55
1:0:1058:A:H2'	1:0:1060:C:H5"	1.89	0.55
1:0:704:C:H2'	1:0:705:C:H6	1.71	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.87	0.55
6:C:236:THR:HA	38:C:9249:HOH:O	2.06	0.55
38:0:5728:HOH:O	10:G:12:ILE:HA	2.05	0.55
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.72	0.55
1:0:1123:A:C6	1:0:1238:C:H5'	2.41	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.63	0.55
25:W:65:VAL:CA	25:W:68:THR:HG22	2.35	0.55
25:W:46:ALA:O	25:W:49:ASN:HB2	2.06	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.72	0.55
16:N:86:LEU:O	16:N:90:LEU:HG	2.07	0.55
1:0:1185:U:H2'	1:0:1186:C:C6	2.41	0.55
27:Y:155:ARG:NH1	38:Y:8144:HOH:O	2.40	0.55
5:B:103:ASP:HB2	38:B:9399:HOH:O	2.06	0.55
1:0:644:G:N3	1:0:644:G:H5'	2.21	0.55
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.88	0.55
7:D:135:VAL:HG22	7:D:136:ARG:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1441:G:H1'	38:0:7960:HOH:O	2.06	0.55
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.42	0.55
1:0:263:U:O4'	9:F:59:ILE:HD13	2.07	0.55
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.42	0.54
1:0:1333:U:H2'	1:0:1334:C:C6	2.42	0.54
20:R:39:THR:HB	20:R:42:GLU:CD	2.27	0.54
2:9:3028:U:H5"	16:N:40:ASN:HD21	1.72	0.54
20:R:29:LYS:NZ	38:R:9338:HOH:O	2.40	0.54
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.89	0.54
20:R:39:THR:HB	20:R:42:GLU:CG	2.37	0.54
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.42	0.54
1:0:56:G:H5"	24:V:50:ARG:NH1	2.22	0.54
1:0:1406:A:H4'	1:0:1407:A:H5"	1.89	0.54
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.90	0.54
25:W:125:HIS:CD2	25:W:127:GLY:H	2.25	0.54
1:0:299:U:H5'	38:0:7544:HOH:O	2.08	0.54
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.20	0.54
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.22	0.54
8:E:9:GLU:HG3	8:E:10:ASP:H	1.73	0.54
14:L:148:GLU:HA	38:L:9369:HOH:O	2.07	0.54
12:J:135:ILE:O	12:J:139:LEU:HG	2.07	0.54
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.23	0.54
1:0:870:G:OP2	4:A:3:ARG:HD3	2.08	0.54
5:B:86:ALA:HA	38:B:9384:HOH:O	2.07	0.54
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.72	0.54
5:B:14:GLY:HA3	38:B:9415:HOH:O	2.08	0.54
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.10	0.54
1:0:380:A:H2'	38:0:7443:HOH:O	2.07	0.54
15:M:24:GLN:O	15:M:28:GLN:HG3	2.07	0.54
1:0:1352:A:N1	6:C:48:SER:HB3	2.23	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.38	0.54
1:0:2055:A:H4'	20:R:132:ARG:NH2	2.23	0.54
1:0:2815:G:N7	12:J:80:LYS:NZ	2.55	0.54
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.54
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.54
1:0:797:A:H4'	28:Z:10:ARG:N	2.23	0.54
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.54
1:0:1451:C:H5'	1:0:1505:U:H3	1.73	0.54
5:B:144:THR:HG22	5:B:145:HIS:N	2.23	0.54
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.07	0.54
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2054:A:C2	20:R:128:ARG:NH2	2.72	0.54
25:W:11:VAL:O	25:W:12:ASN:HB2	2.08	0.54
1:0:669:G:O2'	1:0:670:G:H5'	2.08	0.54
1:0:1477:C:H5'	1:0:1868:G:C5'	2.38	0.54
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.89	0.54
1:0:462:A:C2	30:2:37:HIS:HB3	2.43	0.54
5:B:82:VAL:HG12	5:B:82:VAL:O	2.08	0.54
12:J:45:VAL:HG22	12:J:46:ILE:N	2.23	0.53
1:0:1667:A:H2'	1:0:1668:U:H6	1.72	0.53
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.53
7:D:159:PRO:O	7:D:163:VAL:HG23	2.08	0.53
1:0:2769:C:O2'	1:0:2770:G:H5'	2.09	0.53
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.53
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.08	0.53
1:0:625:U:H5"	1:0:1044:C:N4	2.23	0.53
2:9:3107:C:H2'	2:9:3108:C:C6	2.43	0.53
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.72	0.53
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.41	0.53
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.43	0.53
1:0:1679:C:H5'	38:0:9641:HOH:O	2.07	0.53
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.90	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.09	0.53
7:D:170:TYR:O	7:D:171:ASP:HB3	2.08	0.53
5:B:84:LEU:HD23	5:B:178:ALA:HB1	1.90	0.53
6:C:140:VAL:HB	38:C:9249:HOH:O	2.08	0.53
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.90	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.89	0.53
1:0:2467:A:O2'	1:0:2468:A:H2'	2.09	0.53
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.89	0.53
1:0:396:U:OP2	31:3:38:ARG:HD2	2.08	0.53
5:B:27:ASN:H	5:B:27:ASN:HD22	1.57	0.53
38:0:7567:HOH:O	4:A:177:HIS:HE1	1.91	0.53
7:D:154:LYS:HD2	7:D:154:LYS:N	2.12	0.53
8:E:81:GLU:O	8:E:172:PRO:HD3	2.08	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.53
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.90	0.53
1:0:2769:C:H2'	1:0:2770:G:O4'	2.08	0.53
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.91	0.53
1:0:2565:C:H4'	38:0:5126:HOH:O	2.08	0.53
1:0:558:C:H2'	1:0:559:U:H5"	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:9935:HOH:O	9:F:38:LYS:HE2	2.08	0.53
1:0:475:G:OP1	6:C:73:LEU:HD22	2.08	0.53
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.90	0.53
25:W:1:MET:HB2	25:W:103:GLU:HG2	1.89	0.53
32:I:96:PHE:HA	32:I:136:GLY:CA	2.39	0.53
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.07	0.53
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
1:0:2748:G:H1'	38:0:8202:HOH:O	2.09	0.53
1:0:1250:C:O2'	1:0:1251:C:H5'	2.08	0.53
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.91	0.53
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.37	0.53
38:0:7754:HOH:O	31:3:60:LYS:HG3	2.08	0.53
14:L:92:ASP:HA	14:L:121:ILE:HB	1.91	0.53
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.53
1:0:517:U:H1'	38:0:7774:HOH:O	2.09	0.53
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.91	0.53
1:0:2241:C:H2'	1:0:2242:U:C6	2.44	0.53
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.42	0.53
1:0:1636:G:O2'	1:0:1637:A:H5'	2.08	0.53
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.24	0.53
24:V:56:ILE:O	24:V:60:GLN:HG3	2.09	0.53
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.91	0.53
1:0:947:U:H2'	1:0:948:G:H8	1.73	0.53
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.09	0.53
15:M:6:SER:O	15:M:10:ASP:HB2	2.09	0.53
27:Y:136:LYS:HB3	27:Y:139:VAL:HG23	1.91	0.53
6:C:150:THR:HA	6:C:203:ALA:O	2.09	0.53
1:0:441:A:H1'	1:0:442:A:N7	2.24	0.53
12:J:130:VAL:HG12	12:J:131:THR:H	1.72	0.52
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.39	0.52
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.73	0.52
5:B:162:MET:CE	5:B:310:ARG:HD3	2.37	0.52
18:P:103:THR:HB	38:P:180:HOH:O	2.09	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.43	0.52
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.52
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.91	0.52
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.38	0.52
25:W:82:GLU:O	25:W:86:GLU:HG3	2.09	0.52
23:U:33:SER:O	23:U:37:GLU:HG3	2.09	0.52
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.74	0.52
6:C:118:THR:O	6:C:136:VAL:HG13	2.08	0.52
23:U:17:THR:HG22	23:U:18:GLY:N	2.24	0.52
23:U:52:THR:HG22	23:U:54:THR:HB	1.90	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.10	0.52
17:O:39:THR:O	17:O:115:ARG:NH2	2.39	0.52
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.24	0.52
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.52
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.90	0.52
5:B:128:ILE:O	5:B:131:ALA:HB3	2.09	0.52
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.52
5:B:258:GLY:H	5:B:260:HIS:CE1	2.27	0.52
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.09	0.52
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.52
14:L:143:THR:CG2	14:L:144:ASP:N	2.72	0.52
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.73	0.52
11:H:21:THR:O	11:H:120:ILE:HD12	2.09	0.52
6:C:79:ARG:O	6:C:87:ARG:HG2	2.09	0.52
38:0:9851:HOH:O	18:P:81:LYS:HG2	2.09	0.52
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.09	0.52
24:V:12:THR:HG23	24:V:14:ALA:N	2.25	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.91	0.52
4:A:105:VAL:HG12	4:A:106:CYS:N	2.24	0.52
1:0:137:U:H2'	1:0:139:C:C5	2.44	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52
32:I:113:HIS:N	32:I:114:PRO:HD2	2.24	0.52
1:0:1484:G:H2'	38:0:9420:HOH:O	2.08	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.91	0.52
5:B:214:PRO:HD2	38:B:9321:HOH:O	2.08	0.52
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.43	0.52
16:N:132:ASN:O	16:N:135:VAL:HG12	2.10	0.52
1:0:2694:A:H5"	8:E:90:HIS:CE1	2.44	0.52
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.91	0.52
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.91	0.52
1:0:703:G:O2'	1:0:704:C:H5'	2.10	0.52
1:0:1923:G:H4'	31:3:31:THR:O	2.09	0.52
1:0:328:U:O4'	6:C:202:THR:HG22	2.10	0.52
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.52
1:0:2839:C:H4'	5:B:18:ARG:NH2	2.24	0.52
1:0:777:U:O2'	29:1:11:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1787:C:H2'	1:0:1788:U:H6	1.74	0.52
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.40	0.52
1:0:1537:C:H1'	38:0:6819:HOH:O	2.10	0.52
38:0:7247:HOH:O	4:A:211:LYS:HG2	2.08	0.52
1:0:2094:G:C4'	5:B:245:SER:HB3	2.36	0.52
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.39	0.52
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.39	0.52
1:0:1462:C:H2'	1:0:1463:A:H8	1.74	0.52
17:O:87:THR:O	17:O:91:GLN:HG3	2.09	0.52
1:0:1535:G:H2'	1:0:1536:C:C6	2.45	0.52
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.92	0.52
1:0:1482:A:O2'	1:0:1483:C:H5'	2.10	0.52
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.10	0.52
30:2:5:LYS:O	30:2:9:LYS:HG3	2.10	0.52
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.52
11:H:46:GLN:HG3	11:H:137:TYR:CE2	2.44	0.52
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.24	0.52
2:9:3114:G:O6	16:N:11:ARG:HD3	2.10	0.52
38:0:9868:HOH:O	25:W:119:HIS:HE1	1.93	0.52
32:I:92:PRO:C	32:I:94:GLU:H	2.13	0.52
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.83	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.73	0.52
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.75	0.52
1:0:1189:A:O2'	1:0:1208:C:H2'	2.09	0.52
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.90	0.52
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.52
11:H:27:LYS:H	11:H:59:HIS:CD2	2.21	0.52
14:L:136:ALA:HB3	38:L:9370:HOH:O	2.09	0.52
1:0:1741:U:H3'	38:0:3073:HOH:O	2.10	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.76	0.52
1:0:2252:A:C5	1:0:2253:G:H1'	2.45	0.52
1:0:2730:G:O2'	1:0:2731:G:H5'	2.10	0.52
1:0:2372:A:H2'	1:0:2373:U:C6	2.45	0.52
2:9:3057:A:C8	7:D:141:VAL:HG21	2.45	0.51
2:9:3050:G:H2'	2:9:3051:A:C8	2.45	0.51
1:0:290:C:O2'	1:0:291:C:H5'	2.10	0.51
14:L:10:SER:O	14:L:12:THR:N	2.41	0.51
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.92	0.51
20:R:82:GLU:HG3	20:R:83:LYS:N	2.25	0.51
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.51
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:122:ARG:NH1	25:W:152:ALA:O	2.43	0.51
1:0:1173:A:H4'	1:0:1174:A:C8	2.45	0.51
29:1:28:HIS:HD2	29:1:30:LYS:H	1.57	0.51
38:0:5678:HOH:O	4:A:164:ARG:CZ	2.58	0.51
1:0:1130:U:H2'	1:0:1131:G:O4'	2.10	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
1:0:1427:A:H61	1:0:1440:U:H1'	1.76	0.51
1:0:185:G:O3'	1:0:186:A:H4'	2.10	0.51
1:0:188:C:H5"	15:M:163:LEU:HD21	1.92	0.51
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.10	0.51
4:A:35:GLY:O	4:A:36:ASP:CB	2.58	0.51
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.10	0.51
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.44	0.51
5:B:171:VAL:HG23	5:B:172:SER:N	2.24	0.51
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.11	0.51
12:J:45:VAL:HG23	12:J:130:VAL:O	2.10	0.51
25:W:65:VAL:HA	25:W:68:THR:CG2	2.37	0.51
13:K:74:VAL:HG13	13:K:113:ILE:HG12	1.91	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51
5:B:119:HIS:O	5:B:121:PRO:HD3	2.09	0.51
1:0:2090:G:H2'	1:0:2091:G:C8	2.45	0.51
14:L:104:ASP:O	14:L:105:TYR:HB3	2.09	0.51
1:0:2064:U:H5'	1:0:2652:U:H4'	1.93	0.51
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.43	0.51
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.25	0.51
38:0:7630:HOH:O	22:T:9:LYS:HD2	2.09	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.40	0.51
32:I:131:THR:O	32:I:131:THR:HG22	2.11	0.51
6:C:1:MET:HG2	6:C:2:GLN:NE2	2.25	0.51
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.93	0.51
16:N:64:SER:C	16:N:66:LEU:H	2.14	0.51
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.41	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.10	0.51
1:0:2526:C:O2'	1:0:2527:U:H5'	2.09	0.51
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.10	0.51
32:I:75:THR:HA	32:I:112:LYS:NZ	2.25	0.51
22:T:4:PRO:O	22:T:8:ARG:HG3	2.10	0.51
6:C:236:THR:HG22	6:C:239:ALA:CB	2.41	0.51
7:D:67:ASP:O	7:D:69:ILE:HG13	2.11	0.51
11:H:9:ILE:HD12	11:H:54:THR:CG2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2720:C:O2	13:K:87:ARG:NH2	2.44	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.51
1:0:1166:A:H61	1:0:1180:U:H3	1.57	0.51
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.41	0.51
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.09	0.51
2:9:3064:C:H2'	2:9:3065:A:H5'	1.93	0.51
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.10	0.51
20:R:99:ALA:CB	20:R:109:MET:HE1	2.32	0.51
5:B:254:GLN:NE2	38:B:9395:HOH:O	2.43	0.51
31:3:62:THR:HB	38:3:9350:HOH:O	2.11	0.51
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.91	0.51
27:Y:100:ARG:NH1	27:Y:215:GLU:HA	2.26	0.51
1:0:1942:A:O2'	1:0:1943:C:H5'	2.11	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.94	0.51
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.54	0.51
1:0:2748:G:H5'	38:0:7739:HOH:O	2.11	0.51
9:F:99:THR:HG23	9:F:99:THR:O	2.11	0.51
1:0:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
15:M:164:THR:HG22	15:M:167:GLY:N	2.13	0.51
18:P:115:SER:C	18:P:117:SER:H	2.14	0.51
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.16	0.51
1:0:2072:G:C6	1:0:2533:C:H1'	2.46	0.51
1:0:2073:G:H5"	38:0:4132:HOH:O	2.11	0.51
1:0:396:U:O2'	1:0:418:C:H4'	2.10	0.51
1:0:1733:A:H4'	5:B:212:GLN:HA	1.92	0.50
11:H:28:ILE:HG23	38:H:9178:HOH:O	2.10	0.50
11:H:66:ARG:HD3	38:H:9178:HOH:O	2.11	0.50
1:0:1878:G:O2'	1:0:1879:U:OP2	2.29	0.50
1:0:2325:C:H1'	38:0:4453:HOH:O	2.11	0.50
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.50
14:L:79:ASP:HB3	38:L:9357:HOH:O	2.11	0.50
1:0:156:C:H5"	15:M:171:ARG:CD	2.21	0.50
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.11	0.50
12:J:19:MET:CE	12:J:132:LEU:HD11	2.41	0.50
17:O:25:VAL:HG23	17:O:26:TRP:N	2.26	0.50
25:W:1:MET:N	25:W:37:GLU:HG3	2.26	0.50
1:0:200:U:H2'	38:0:3752:HOH:O	2.10	0.50
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.93	0.50
24:V:58:THR:O	24:V:62:GLU:HG3	2.11	0.50
1:0:2862:G:H4'	5:B:336:GLN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.41	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.88	0.50
1:0:544:G:C2'	1:0:545:G:H5"	2.40	0.50
20:R:114:VAL:HA	20:R:144:GLU:O	2.11	0.50
1:0:1427:A:H61	1:0:1440:U:C1'	2.25	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.46	0.50
24:V:49:LEU:O	24:V:53:ILE:HG13	2.10	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.12	0.50
22:T:71:VAL:HG12	22:T:72:ILE:N	2.26	0.50
1:0:2851:G:C2'	1:0:2852:A:H5'	2.40	0.50
1:0:2717:C:O2'	1:0:2718:C:H5"	2.11	0.50
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.94	0.50
1:0:1185:U:OP1	32:I:126:LYS:HD3	2.11	0.50
16:N:154:LEU:C	16:N:156:GLU:H	2.15	0.50
1:0:1515:A:H2'	1:0:1516:C:C6	2.46	0.50
1:0:536:A:H3'	38:0:5332:HOH:O	2.10	0.50
23:U:44:ARG:HB3	38:U:3805:HOH:O	2.11	0.50
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.50
4:A:88:ILE:HG22	4:A:88:ILE:O	2.12	0.50
38:0:5260:HOH:O	11:H:58:ARG:HG3	2.11	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.50
9:F:101:ALA:HA	38:F:5413:HOH:O	2.11	0.50
1:0:588:G:O6	25:W:154:ARG:NH1	2.44	0.50
25:W:4:LEU:O	25:W:32:CYS:HA	2.11	0.50
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.40	0.50
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.25	0.50
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.65	0.50
1:0:1528:A:H2'	1:0:1529:G:O4'	2.11	0.50
16:N:183:ASP:O	16:N:184:ILE:O	2.28	0.50
1:0:130:C:H2'	38:0:3469:HOH:O	2.11	0.50
1:0:424:C:H2'	1:0:425:U:C6	2.46	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.12	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.12	0.50
25:W:65:VAL:O	25:W:68:THR:HG22	2.12	0.50
1:0:2270:G:C4'	4:A:223:ARG:HH12	2.22	0.50
1:0:1180:U:H4'	32:I:91:GLU:OE2	2.11	0.50
4:A:36:ASP:CG	4:A:85:SER:HB2	2.30	0.50
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.94	0.50
5:B:280:VAL:HG13	5:B:334:SER:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:9535:HOH:O	4:A:11:ARG:HD3	2.12	0.50
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.76	0.50
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.39	0.50
5:B:148:PRO:HB2	5:B:156:LYS:O	2.12	0.50
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.44	0.50
1:0:2524:G:H21	1:0:2526:C:H41	1.59	0.50
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.50
25:W:125:HIS:HD2	25:W:127:GLY:H	1.59	0.50
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.26	0.50
5:B:109:LEU:HG	5:B:113:LEU:HD12	1.94	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.50
4:A:17:ARG:HD2	38:A:9339:HOH:O	2.12	0.50
4:A:215:ILE:HG13	4:A:216:SER:N	2.27	0.50
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.92	0.50
1:0:2387:U:H2'	1:0:2388:C:C6	2.47	0.50
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.28	0.49
5:B:139:ASP:HB2	5:B:165:ARG:NE	2.24	0.49
6:C:65:ARG:HG3	6:C:67:GLN:HB2	1.93	0.49
26:X:34:ARG:NH1	26:X:48:VAL:O	2.44	0.49
21:S:37:VAL:O	21:S:41:VAL:HG23	2.12	0.49
1:0:1008:C:H5"	11:H:16:ARG:HH12	1.77	0.49
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.49
1:0:1701:A:H5"	1:0:1702:U:H3'	1.95	0.49
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.49
12:J:107:ASN:HD22	12:J:107:ASN:C	2.15	0.49
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.94	0.49
8:E:11:VAL:HG13	8:E:76:VAL:HG21	1.94	0.49
1:0:2472:C:O2'	1:0:2634:G:H4'	2.12	0.49
9:F:113:ASP:O	9:F:117:GLU:HG3	2.12	0.49
32:I:139:ILE:HG22	32:I:140:GLU:N	2.27	0.49
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.76	0.49
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.41	0.49
1:0:1150:A:C2	10:G:20:VAL:HG21	2.47	0.49
1:0:284:C:H4'	1:0:285:A:O5'	2.12	0.49
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.49
1:0:2385:G:H2'	1:0:2386:U:C6	2.48	0.49
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.77	0.49
2:9:3006:C:C5'	16:N:37:ARG:HH12	2.16	0.49
12:J:131:THR:HG22	12:J:134:GLU:N	2.16	0.49
25:W:59:GLN:HE22	25:W:98:PHE:CA	2.25	0.49
1:0:2265:U:H2'	1:0:2266:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:111:VAL:HB	38:C:9121:HOH:O	2.11	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
1:0:380:A:OP2	15:M:9:ARG:HD2	2.12	0.49
26:X:43:VAL:CG1	26:X:44:ASP:N	2.74	0.49
20:R:33:ARG:NH1	38:R:9341:HOH:O	2.45	0.49
1:0:512:G:O3'	1:0:513:A:H8	1.95	0.49
1:0:2004:U:H2'	1:0:2004:U:O2	2.12	0.49
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.95	0.49
4:A:130:THR:HG22	4:A:131:HIS:O	2.11	0.49
1:0:2681:A:H4'	1:0:2682:C:H5'	1.95	0.49
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
1:0:1681:G:H5"	1:0:1682:A:H5'	1.93	0.49
27:Y:133:HIS:HD2	38:Y:8170:HOH:O	1.94	0.49
38:0:3270:HOH:O	31:3:84:ARG:HB2	2.11	0.49
1:0:21:G:H4'	20:R:2:ILE:HG22	1.95	0.49
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.76	0.49
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.79	0.49
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.39	0.49
1:0:2054:A:H2	20:R:128:ARG:HH22	1.57	0.49
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.48	0.49
14:L:145:LEU:O	14:L:148:GLU:HG3	2.13	0.49
1:0:2883:A:H2'	1:0:2884:G:O4'	2.13	0.49
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.26	0.49
1:0:834:G:H4'	1:0:835:U:OP2	2.13	0.49
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.49
1:0:1666:C:H2'	1:0:1667:A:H5'	1.94	0.49
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.94	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
13:K:41:LYS:O	13:K:42:ASN:HB2	2.13	0.49
38:0:4910:HOH:O	17:O:39:THR:HB	2.13	0.49
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.48	0.49
1:0:2821:C:H4'	5:B:116:PRO:HB3	1.95	0.49
1:0:1697:G:O2'	1:0:1698:U:H5'	2.12	0.49
1:0:177:A:H2'	1:0:178:U:O4'	2.12	0.49
38:0:5799:HOH:O	15:M:58:GLN:HG3	2.13	0.49
7:D:128:LEU:HD23	7:D:128:LEU:C	2.33	0.49
2:9:3029:C:H2'	2:9:3030:C:C5'	2.39	0.49
4:A:95:PRO:HA	4:A:153:ARG:HA	1.95	0.49
16:N:163:PHE:O	16:N:164:ASP:OD1	2.31	0.49
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.16	0.49
1:0:2780:C:H2'	1:0:2781:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.43	0.49
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.95	0.49
1:0:2338:G:H1'	7:D:105:SER:OG	2.12	0.49
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.48	0.49
11:H:166:SER:CB	11:H:167:PRO:CD	2.82	0.49
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.49
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.28	0.49
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.49
1:0:2335:C:H2'	1:0:2336:G:C8	2.48	0.49
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.49
6:C:20:ASP:O	6:C:23:GLU:HB2	2.13	0.49
15:M:64:ARG:HD2	38:M:9382:HOH:O	2.13	0.49
2:9:3049:G:H2'	2:9:3050:G:O4'	2.13	0.48
12:J:75:PRO:HD3	12:J:136:SER:OG	2.13	0.48
10:G:64:ASN:N	10:G:64:ASN:ND2	2.60	0.48
27:Y:144:ARG:NH1	38:Y:8164:HOH:O	2.45	0.48
38:0:3957:HOH:O	17:O:3:THR:HG21	2.12	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
1:0:1415:G:H5'	29:1:12:ASN:O	2.12	0.48
5:B:255:GLY:O	5:B:257:THR:HG23	2.13	0.48
20:R:113:HIS:O	20:R:145:LEU:HD12	2.13	0.48
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.94	0.48
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.27	0.48
4:A:93:THR:HG23	4:A:154:ALA:O	2.12	0.48
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.95	0.48
16:N:154:LEU:O	16:N:155:GLU:HB3	2.13	0.48
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.13	0.48
14:L:80:ASP:HB2	14:L:90:ARG:O	2.13	0.48
1:0:1734:C:OP1	5:B:234:ARG:HD3	2.13	0.48
1:0:485:A:N3	1:0:487:G:H5"	2.28	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
8:E:21:THR:HG23	8:E:30:THR:OG1	2.12	0.48
31:3:65:THR:HB	31:3:83:TRP:H	1.78	0.48
1:0:1624:A:H5'	1:0:1626:A:O4'	2.13	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.34	0.48
1:0:820:G:H5'	1:0:821:U:H5'	1.95	0.48
18:P:41:ARG:O	18:P:44:VAL:HB	2.13	0.48
11:H:167:PRO:O	11:H:168:ALA:HB2	2.13	0.48
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.48
4:A:132:ASP:OD1	4:A:133:ARG:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.96	0.48
17:O:35:LYS:O	17:O:40:HIS:NE2	2.47	0.48
7:D:135:VAL:HG22	7:D:136:ARG:N	2.28	0.48
21:S:11:THR:O	21:S:15:MET:HG2	2.13	0.48
1:0:474:C:O3'	6:C:73:LEU:CD2	2.61	0.48
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.95	0.48
1:0:90:A:H2'	1:0:91:G:O4'	2.13	0.48
1:0:1503:U:H2'	1:0:1504:A:O4'	2.13	0.48
5:B:277:GLU:N	5:B:278:PRO:HD2	2.28	0.48
26:X:75:ALA:O	26:X:83:ALA:HA	2.14	0.48
30:2:41:HIS:O	30:2:45:ASN:HB2	2.13	0.48
5:B:251:VAL:HG23	5:B:252:PRO:HD2	1.95	0.48
6:C:19:PRO:HD2	6:C:240:LEU:HD21	1.95	0.48
14:L:114:VAL:HG11	38:L:9370:HOH:O	2.12	0.48
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.48
16:N:100:ALA:O	16:N:129:ILE:HG23	2.13	0.48
38:0:6529:HOH:O	27:Y:158:LYS:HD3	2.13	0.48
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.13	0.48
1:0:638:C:H2'	1:0:639:A:C8	2.48	0.48
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.43	0.48
14:L:134:GLU:HA	14:L:138:GLY:O	2.13	0.48
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.61	0.48
25:W:7:LEU:CD1	25:W:53:ALA:HB2	2.44	0.48
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.14	0.48
8:E:101:GLU:HB2	8:E:116:THR:O	2.13	0.48
1:0:2361:A:H2'	1:0:2362:A:C8	2.47	0.48
1:0:251:C:H5"	15:M:143:ASN:HD22	1.77	0.48
1:0:661:G:C5	1:0:686:A:C2	3.02	0.48
1:0:74:A:H2'	1:0:75:U:C6	2.48	0.48
2:9:3001:U:H5"	2:9:3003:A:OP1	2.14	0.48
25:W:137:GLN:HG3	25:W:137:GLN:O	2.14	0.48
20:R:8:ALA:CB	20:R:13:THR:HG21	2.39	0.48
1:0:2073:G:OP2	1:0:2490:A:H5'	2.14	0.48
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.48
1:0:545:G:C8	1:0:545:G:H5'	2.40	0.48
32:I:102:VAL:O	32:I:106:LYS:HG3	2.14	0.48
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.95	0.48
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.95	0.48
18:P:16:VAL:CG1	18:P:17:GLY:N	2.76	0.48
14:L:143:THR:HG22	14:L:145:LEU:H	1.79	0.48
31:3:67:LEU:HD21	31:3:88:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:21:ARG:N	38:L:9329:HOH:O	2.46	0.48
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.96	0.48
25:W:7:LEU:HD12	25:W:53:ALA:HB2	1.96	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.49	0.48
16:N:15:GLU:HB3	16:N:17:ARG:CG	2.42	0.48
8:E:84:MET:HE3	8:E:131:LEU:HD13	1.94	0.48
4:A:105:VAL:HG13	4:A:155:THR:O	2.14	0.48
4:A:36:ASP:HB2	4:A:85:SER:H	1.78	0.48
1:0:1657:A:H2'	1:0:1658:A:C8	2.49	0.48
1:0:2900:G:H2'	1:0:2901:C:O4'	2.14	0.48
4:A:210:GLY:HA3	38:A:9383:HOH:O	2.13	0.48
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.95	0.48
1:0:1919:A:H4'	38:0:5141:HOH:O	2.13	0.48
1:0:1119:G:H22	1:0:1246:A:H2	1.52	0.48
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.48
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.14	0.48
1:0:1201:C:H2'	1:0:1202:A:H5'	1.95	0.48
1:0:2866:U:H4'	1:0:2867:G:H5'	1.94	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.48
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.44	0.48
1:0:2909:G:H2'	1:0:2910:A:H8	1.79	0.48
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.28	0.48
1:0:1163:G:H2'	1:0:1164:U:C5	2.49	0.48
9:F:58:GLU:HA	9:F:61:MET:HG3	1.95	0.48
5:B:305:ASP:O	5:B:306:LYS:CB	2.61	0.48
5:B:140:LEU:HD13	5:B:175:LEU:HA	1.95	0.48
1:0:2421:G:H4'	38:0:5073:HOH:O	2.14	0.48
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.48	0.48
10:G:67:LEU:O	10:G:71:LEU:HG	2.13	0.48
4:A:39:ALA:O	4:A:61:GLU:HG3	2.14	0.48
1:0:189:A:OP1	15:M:171:ARG:NH2	2.47	0.47
21:S:57:THR:CG2	21:S:58:MET:N	2.77	0.47
26:X:78:GLU:CG	26:X:79:GLU:H	2.24	0.47
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
1:0:1086:A:N6	25:W:11:VAL:HG11	2.29	0.47
1:0:2807:U:P	5:B:27:ASN:HD21	2.36	0.47
2:9:3064:C:C2'	2:9:3065:A:H5'	2.43	0.47
16:N:42:HIS:HB3	16:N:62:HIS:CE1	2.49	0.47
1:0:794:U:H3	1:0:819:A:H61	1.63	0.47
4:A:51:ARG:NH1	4:A:120:ARG:O	2.47	0.47
5:B:275:GLY:O	5:B:291:ASP:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1811:A:C2	1:0:2752:C:H1'	2.49	0.47
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.95	0.47
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.14	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.14	0.47
11:H:63:GLU:O	11:H:67:LEU:HB2	2.14	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
12:J:8:ALA:HA	12:J:35:THR:CG2	2.44	0.47
1:0:2445:U:H2'	1:0:2446:G:C8	2.49	0.47
1:0:2078:U:O2'	1:0:2079:G:H5'	2.14	0.47
1:0:1805:G:H2'	1:0:1806:G:H8	1.78	0.47
10:G:63:ARG:N	38:G:2569:HOH:O	2.46	0.47
23:U:9:CYS:HA	23:U:52:THR:CG2	2.38	0.47
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.96	0.47
1:0:2838:A:H2'	1:0:2839:C:C6	2.50	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.96	0.47
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.27	0.47
1:0:2241:C:H2'	1:0:2242:U:H6	1.79	0.47
5:B:140:LEU:HA	38:B:9384:HOH:O	2.14	0.47
1:0:2424:U:H1'	19:Q:7:LEU:HD12	1.96	0.47
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.13	0.47
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.21	0.47
15:M:99:ARG:HD2	15:M:167:GLY:CA	2.35	0.47
6:C:237:GLU:HA	38:C:9228:HOH:O	2.13	0.47
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.96	0.47
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.30	0.47
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.47
15:M:59:GLY:C	15:M:141:ILE:HD11	2.35	0.47
31:3:65:THR:HG21	31:3:83:TRP:CZ3	2.49	0.47
6:C:214:THR:HG23	38:C:9236:HOH:O	2.14	0.47
1:0:392:U:O2'	15:M:182:LYS:HE2	2.15	0.47
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.95	0.47
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.14	0.47
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.74	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.59	0.47
1:0:1191:A:H2'	1:0:1193:A:H5'	1.96	0.47
38:0:3544:HOH:O	32:I:92:PRO:HD2	2.13	0.47
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.47	0.47
1:0:128:A:O2'	1:0:129:A:H5'	2.14	0.47
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.47
15:M:107:ARG:NH1	38:M:9374:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.28	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.50	0.47
1:0:1023:C:O2'	1:0:1024:G:H5'	2.15	0.47
2:9:3052:A:H2'	2:9:3053:G:O4'	2.15	0.47
21:S:53:ASN:N	21:S:53:ASN:HD22	2.12	0.47
1:0:39:G:H2'	1:0:40:C:O4'	2.15	0.47
1:0:960:G:N3	1:0:960:G:C2'	2.78	0.47
12:J:52:GLN:HG3	12:J:53:ILE:H	1.78	0.47
20:R:96:VAL:O	20:R:99:ALA:HB3	2.15	0.47
5:B:238:ASN:ND2	5:B:240:GLY:H	1.98	0.47
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.79	0.47
6:C:22:PHE:HA	6:C:116:ALA:HA	1.96	0.47
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.48	0.47
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.30	0.47
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.97	0.47
1:0:2768:A:O2'	1:0:2769:C:H5'	2.14	0.47
38:0:3999:HOH:O	8:E:143:GLN:HG2	2.14	0.47
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.47
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.45	0.47
6:C:233:THR:HG22	6:C:234:VAL:N	2.30	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.45	0.47
1:0:2252:A:C6	1:0:2253:G:H1'	2.48	0.47
2:9:3041:C:H4'	7:D:48:MET:HB2	1.95	0.47
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.96	0.47
1:0:1132:A:N6	1:0:1229:C:H2'	2.30	0.47
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.97	0.47
20:R:47:LEU:O	20:R:51:ILE:HG13	2.14	0.47
1:0:2314:G:C2'	1:0:2315:C:H5'	2.45	0.47
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.13	0.47
1:0:1167:G:H2'	1:0:1168:C:O4'	2.15	0.47
6:C:165:ASP:O	6:C:168:ARG:HB3	2.15	0.47
4:A:128:LEU:HD21	4:A:131:HIS:CE1	2.50	0.47
1:0:2541:U:H4'	1:0:2542:C:OP1	2.15	0.47
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.97	0.47
5:B:307:ARG:CB	5:B:307:ARG:HH11	2.25	0.47
5:B:139:ASP:CB	5:B:165:ARG:HE	2.26	0.47
1:0:1820:G:C6	1:0:2030:A:C2	3.02	0.47
1:0:561:G:H2'	1:0:562:A:H8	1.79	0.47
1:0:10:U:O4	1:0:532:A:OP2	2.33	0.47
2:9:3023:U:O2'	2:9:3024:U:H4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:132:CYS:C	32:I:134:SER:H	2.16	0.47
1:0:1165:G:O2'	1:0:1174:A:H1'	2.15	0.47
4:A:179:MET:HA	4:A:179:MET:HE2	1.96	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
10:G:12:ILE:N	10:G:13:PRO:CD	2.78	0.47
1:0:1060:C:H6	1:0:1060:C:H5'	1.80	0.47
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.47	0.47
1:0:1687:C:O2	29:1:9:GLY:HA2	2.15	0.47
1:0:407:A:H2'	1:0:408:A:C8	2.50	0.47
32:I:133:THR:N	38:I:5371:HOH:O	2.48	0.47
1:0:790:A:H2'	1:0:791:A:O4'	2.15	0.47
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.47
7:D:166:ILE:HB	38:D:6326:HOH:O	2.13	0.47
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.47
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.49	0.47
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.45	0.47
1:0:1787:C:H4'	1:0:2883:A:O4'	2.15	0.47
4:A:51:ARG:HB2	38:A:9402:HOH:O	2.15	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.50	0.47
5:B:271:ASP:OD1	5:B:272:ILE:N	2.48	0.47
5:B:48:MET:HG2	5:B:72:THR:HA	1.97	0.47
24:V:8:ILE:HA	24:V:11:MET:CE	2.44	0.46
1:0:1118:A:C3'	1:0:1118:A:C8	2.94	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.80	0.46
23:U:52:THR:HG21	23:U:54:THR:HB	1.96	0.46
1:0:317:A:OP1	22:T:52:ARG:O	2.33	0.46
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.15	0.46
1:0:1855:G:H4'	1:0:1856:C:O5'	2.15	0.46
1:0:2613:G:O2'	1:0:2614:C:H5'	2.15	0.46
9:F:26:THR:HG21	9:F:102:GLY:C	2.35	0.46
1:0:2135:A:O2'	1:0:2136:G:H5'	2.15	0.46
1:0:1375:A:H2'	1:0:1376:G:H5'	1.97	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.15	0.46
16:N:67:ALA:C	16:N:69:TYR:H	2.17	0.46
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.96	0.46
1:0:249:G:O2'	1:0:250:C:H5'	2.15	0.46
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.56	0.46
22:T:48:VAL:HG22	22:T:96:VAL:HG13	1.97	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.95	0.46
16:N:152:GLU:C	16:N:154:LEU:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:H5'	17:O:3:THR:CG2	2.45	0.46
1:0:1747:A:C8	13:K:44:LEU:HD13	2.50	0.46
25:W:35:VAL:CG2	25:W:41:TYR:CD2	2.98	0.46
1:0:2335:C:H2'	1:0:2336:G:H8	1.81	0.46
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.16	0.46
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.50	0.46
14:L:24:ALA:HB2	14:L:30:ARG:HD2	1.97	0.46
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.46
31:3:91:GLN:O	31:3:92:GLU:HB2	2.14	0.46
32:I:98:ALA:O	32:I:137:VAL:HA	2.16	0.46
16:N:164:ASP:OD1	16:N:167:ASP:CA	2.60	0.46
1:0:2255:A:H2'	1:0:2256:G:O4'	2.16	0.46
1:0:538:C:H5"	1:0:539:G:C8	2.51	0.46
4:A:94:LEU:N	4:A:94:LEU:HD23	2.30	0.46
1:0:589:U:H2'	1:0:590:A:H8	1.79	0.46
1:0:1413:A:H2'	1:0:1414:A:O4'	2.15	0.46
1:0:1790:C:H2'	1:0:1791:U:H6	1.80	0.46
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.16	0.46
1:0:899:C:H5'	38:0:3511:HOH:O	2.14	0.46
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.46
1:0:2478:U:O2'	1:0:2479:A:H5'	2.14	0.46
1:0:571:C:H6	1:0:571:C:O5'	1.98	0.46
15:M:164:THR:HB	38:M:9319:HOH:O	2.15	0.46
2:9:3039:U:H3'	2:9:3040:C:H5"	1.98	0.46
8:E:68:HIS:O	8:E:72:MET:HG3	2.15	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.16	0.46
1:0:960:G:H3'	1:0:960:G:N3	2.31	0.46
18:P:14:LEU:HD13	18:P:51:ALA:HB2	1.96	0.46
1:0:1380:U:O4	1:0:2043:U:H4'	2.16	0.46
5:B:157:LYS:HG2	38:B:9467:HOH:O	2.16	0.46
23:U:20:MET:CG	23:U:28:THR:HG23	2.46	0.46
7:D:37:ALA:O	7:D:40:ILE:HG12	2.16	0.46
25:W:13:MET:HE1	25:W:18:GLN:HA	1.98	0.46
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.45	0.46
1:0:2897:C:H2'	1:0:2898:G:H8	1.80	0.46
1:0:949:U:H4'	19:Q:95:GLU:HA	1.97	0.46
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.48	0.46
1:0:1342:C:C2'	1:0:1343:C:H5'	2.46	0.46
25:W:83:TRP:CZ3	25:W:112:LEU:HD21	2.51	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:108:SER:HA	16:N:109:PRO:HD3	1.72	0.46
7:D:81:GLU:C	7:D:83:PHE:H	2.19	0.46
1:0:797:A:O4'	28:Z:10:ARG:N	2.49	0.46
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.37	0.46
1:0:2507:G:H2'	1:0:2510:C:H42	1.81	0.46
13:K:49:LEU:HD21	13:K:74:VAL:O	2.16	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.16	0.46
22:T:75:GLU:O	22:T:76:ASP:HB2	2.15	0.46
1:0:1375:A:C2'	1:0:1376:G:H5'	2.45	0.46
22:T:78:THR:HB	22:T:87:VAL:O	2.16	0.46
1:0:241:A:C2	1:0:378:A:H4'	2.51	0.46
6:C:147:LEU:HA	38:C:9210:HOH:O	2.15	0.46
8:E:77:THR:OG1	8:E:78:GLU:N	2.43	0.46
1:0:1530:U:H2'	1:0:1531:U:O4'	2.16	0.46
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.83	0.46
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.46
24:V:57:LYS:HA	24:V:60:GLN:NE2	2.28	0.46
1:0:1181:A:N1	1:0:1192:A:O2'	2.46	0.46
4:A:105:VAL:CG1	4:A:106:CYS:N	2.79	0.46
1:0:314:G:N2	1:0:316:A:H3'	2.31	0.46
1:0:2413:A:H2'	1:0:2414:A:O4'	2.15	0.46
1:0:1874:U:OP1	4:A:51:ARG:HD2	2.16	0.46
1:0:1309:U:O2'	1:0:1310:U:H5'	2.16	0.46
1:0:2819:C:H2'	1:0:2820:A:C8	2.50	0.46
22:T:40:VAL:HG23	22:T:119:ALA:OXT	2.16	0.46
24:V:29:ASN:O	24:V:33:VAL:HG23	2.16	0.46
1:0:31:C:H2'	38:0:7883:HOH:O	2.15	0.46
1:0:1168:C:H4'	38:I:5128:HOH:O	2.16	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.98	0.46
14:L:130:ARG:HA	38:L:9356:HOH:O	2.16	0.46
1:0:2846:C:OP1	5:B:158:LYS:HD2	2.15	0.46
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.31	0.46
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.36	0.46
1:0:660:A:H4'	1:0:661:G:O5'	2.16	0.46
1:0:1849:G:H1'	1:0:2011:A:N1	2.31	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46
26:X:30:MET:CE	26:X:58:ALA:HB3	2.46	0.46
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.46
1:0:1164:U:H3	1:0:1192:A:H2	1.64	0.46
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.97	0.46
5:B:66:GLU:O	5:B:67:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1768:C:H2'	1:0:1769:C:O4'	2.15	0.46
1:0:926:A:O2'	14:L:41:HIS:CD2	2.69	0.46
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.36	0.46
13:K:90:PHE:CD1	13:K:90:PHE:N	2.84	0.46
38:0:3205:HOH:O	12:J:46:ILE:HA	2.15	0.45
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.45
1:0:1419:U:H5'	1:0:1420:C:OP2	2.16	0.45
7:D:173:GLU:HG3	7:D:174:VAL:H	1.81	0.45
1:0:1120:U:H5'	1:0:1121:G:OP2	2.15	0.45
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.34	0.45
31:3:65:THR:HG23	31:3:67:LEU:HG	1.98	0.45
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.45
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.45
1:0:1825:U:O2'	1:0:1826:C:H5'	2.16	0.45
25:W:90:TYR:N	25:W:90:TYR:CD1	2.84	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
32:I:132:CYS:C	32:I:134:SER:N	2.69	0.45
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.98	0.45
1:0:1634:G:H2'	1:0:1635:U:C6	2.51	0.45
1:0:2346:C:O2'	7:D:52:THR:HG21	2.16	0.45
1:0:2795:C:O2'	1:0:2796:U:H5'	2.15	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.16	0.45
22:T:12:ARG:O	22:T:19:ARG:NH2	2.49	0.45
14:L:117:GLU:HB3	14:L:137:GLY:O	2.17	0.45
13:K:98:VAL:HG13	13:K:99:ASP:N	2.30	0.45
5:B:24:PRO:O	5:B:25:ARG:HD3	2.15	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
1:0:2563:U:H2'	1:0:2565:C:O5'	2.17	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
5:B:270:ILE:O	5:B:271:ASP:HB2	2.17	0.45
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.14	0.45
1:0:1139:U:H2'	1:0:1140:C:C6	2.51	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
1:0:2379:G:N3	1:0:2418:G:H2'	2.32	0.45
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.98	0.45
32:I:97:VAL:O	32:I:97:VAL:HG12	2.16	0.45
32:I:131:THR:O	32:I:135:LEU:HG	2.16	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
1:0:292:G:H2'	1:0:358:G:N2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:13:MET:HE2	25:W:18:GLN:N	2.31	0.45
32:I:101:SER:OG	32:I:104:GLN:HG3	2.16	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
9:F:32:GLY:N	38:F:3111:HOH:O	2.49	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.47	0.45
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.81	0.45
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.52	0.45
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.45	0.45
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.45
1:0:671:A:O2'	1:0:672:G:H2'	2.17	0.45
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.51	0.45
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.03	0.45
1:0:816:G:C6	1:0:817:G:N1	2.84	0.45
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.97	0.45
1:0:2428:G:N7	31:3:60:LYS:NZ	2.61	0.45
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.45
32:I:75:THR:CA	32:I:112:LYS:NZ	2.79	0.45
17:O:96:VAL:HA	38:O:4258:HOH:O	2.17	0.45
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.99	0.45
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.45
1:0:1118:A:H62	1:0:1244:U:H3	1.63	0.45
4:A:211:LYS:NZ	38:A:9415:HOH:O	2.43	0.45
1:0:21:G:H5"	20:R:2:ILE:HA	1.95	0.45
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.98	0.45
8:E:31:ARG:HH12	8:E:68:HIS:CE1	2.35	0.45
1:0:1299:G:N7	14:L:6:ARG:NH1	2.64	0.45
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.17	0.45
5:B:17:LYS:O	5:B:260:HIS:HD2	1.99	0.45
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.98	0.45
4:A:48:ASP:HB3	38:A:9402:HOH:O	2.15	0.45
1:0:2508:C:H2'	38:0:6980:HOH:O	2.15	0.45
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.45
1:0:1269:G:H2'	1:0:1270:U:C6	2.52	0.45
5:B:33:ASP:O	5:B:34:GLY:O	2.34	0.45
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45
1:0:1595:G:O2'	1:0:1596:U:H5'	2.16	0.45
9:F:91:VAL:CG1	9:F:92:GLY:N	2.79	0.45
31:3:48:ASN:ND2	31:3:50:GLY:H	2.14	0.45
1:0:1891:G:H1'	1:0:1972:U:C2	2.51	0.45
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:57:VAL:O	14:L:57:VAL:HG12	2.17	0.45
21:S:52:VAL:C	21:S:53:ASN:HD22	2.19	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.17	0.45
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.45
21:S:30:ASP:HA	21:S:62:LYS:HE3	1.99	0.45
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.46	0.45
1:0:2101:A:H2'	6:C:63:SER:OG	2.17	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.84	0.45
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.82	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.68	0.45
1:0:820:G:O2'	1:0:856:G:H4'	2.17	0.45
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.51	0.45
22:T:48:VAL:HG21	22:T:96:VAL:CG1	2.47	0.45
1:0:2637:A:N6	3:4:176:A:H2'	2.32	0.45
1:0:952:G:N3	1:0:2302:A:H2'	2.32	0.45
8:E:71:ASN:ND2	8:E:138:ILE:HD13	2.31	0.45
1:0:1477:C:O2'	1:0:1478:U:H5'	2.17	0.45
1:0:2266:A:H2'	1:0:2267:G:C8	2.52	0.45
1:0:960:G:H2'	1:0:960:G:N3	2.31	0.45
13:K:103:ASP:O	13:K:104:PRO:C	2.56	0.45
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.51	0.45
25:W:132:VAL:C	25:W:134:GLU:H	2.20	0.45
38:9:3472:HOH:O	16:N:41:LYS:HD3	2.16	0.45
11:H:45:VAL:HA	11:H:167:PRO:O	2.16	0.45
22:T:71:VAL:CG1	22:T:72:ILE:N	2.79	0.45
6:C:240:LEU:HD23	6:C:240:LEU:O	2.17	0.45
1:0:2541:U:C2	1:0:2620:U:O4	2.69	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.81	0.45
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.98	0.45
26:X:41:PHE:O	26:X:43:VAL:HG23	2.17	0.45
4:A:139:LYS:HE2	4:A:143:GLY:HA2	1.99	0.45
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.45
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.45
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.17	0.45
4:A:213:LYS:NZ	38:A:9362:HOH:O	2.46	0.45
1:0:2401:A:H2'	1:0:2402:A:C8	2.52	0.45
38:0:4963:HOH:O	21:S:67:ARG:HD3	2.16	0.45
1:0:1829:A:H2'	1:0:1830:C:H5'	1.99	0.45
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.45
13:K:20:CYS:HB3	13:K:26:ALA:O	2.17	0.45
1:0:165:A:H5"	14:L:33:ALA:HB2	1.99	0.45
13:K:66:ARG:HD3	38:K:2777:HOH:O	2.17	0.45
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.45
6:C:166:ILE:CD1	6:C:207:LEU:HD13	2.46	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.45
38:0:5788:HOH:O	5:B:298:LYS:HD3	2.15	0.45
7:D:63:ILE:HG13	7:D:64:ARG:N	2.32	0.44
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.82	0.44
1:0:291:C:H2'	1:0:292:G:O4'	2.17	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.17	0.44
1:0:2419:U:H5"	1:0:2420:G:H5'	1.99	0.44
1:0:1058:A:H2'	1:0:1060:C:C5'	2.47	0.44
1:0:2451:G:O2'	31:3:38:ARG:NH2	2.50	0.44
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.47	0.44
1:0:1300:G:H1'	38:0:4978:HOH:O	2.17	0.44
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.99	0.44
1:0:2435:U:H1'	38:0:5700:HOH:O	2.17	0.44
1:0:700:A:C2	14:L:71:GLU:HG2	2.52	0.44
20:R:124:GLY:HA3	20:R:136:TRP:O	2.17	0.44
1:0:1189:A:H1'	1:0:1209:C:H1'	1.97	0.44
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.85	0.44
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.99	0.44
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.47	0.44
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.47	0.44
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.99	0.44
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.18	0.44
32:I:112:LYS:C	32:I:114:PRO:HD2	2.37	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.65	0.44
21:S:33:SER:OG	21:S:36:GLU:HG3	2.16	0.44
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.83	0.44
24:V:5:VAL:HG11	24:V:9:ARG:NH1	2.32	0.44
18:P:108:LEU:HB2	18:P:114:LEU:HD12	2.00	0.44
1:0:1329:A:N1	36:0:9313:CL:CL	2.87	0.44
1:0:500:G:H21	20:R:98:ASN:HD21	1.63	0.44
7:D:140:ARG:O	7:D:140:ARG:HG2	2.17	0.44
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.46	0.44
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.44
1:0:447:A:OP1	22:T:2:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.44
13:K:106:GLY:HA3	38:K:5264:HOH:O	2.16	0.44
1:0:2821:C:H4'	5:B:116:PRO:CB	2.48	0.44
1:0:1495:C:H2'	1:0:1496:G:C8	2.52	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
1:0:2403:C:H3'	38:0:5489:HOH:O	2.18	0.44
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.99	0.44
1:0:736:A:H2'	1:0:737:A:O4'	2.17	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.35	0.44
7:D:18:ILE:HG12	7:D:134:LEU:CD2	2.47	0.44
1:0:1183:C:N4	1:0:1184:C:H41	2.15	0.44
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.44
1:0:2036:C:C1'	13:K:44:LEU:HG	2.47	0.44
1:0:396:U:H1'	38:0:7824:HOH:O	2.15	0.44
29:1:28:HIS:O	29:1:32:LYS:N	2.48	0.44
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.44
18:P:55:LYS:CG	18:P:56:GLY:N	2.80	0.44
1:0:2894:C:O2'	1:0:2895:C:H5'	2.17	0.44
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.05	0.44
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.17	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.32	0.44
20:R:114:VAL:HB	20:R:145:LEU:HD13	2.00	0.44
9:F:91:VAL:CG1	9:F:92:GLY:H	2.28	0.44
1:0:820:G:H3'	38:0:3359:HOH:O	2.18	0.44
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.99	0.44
14:L:92:ASP:OD1	14:L:94:ARG:HB2	2.17	0.44
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.83	0.44
1:0:1309:U:C2'	1:0:1310:U:H5'	2.48	0.44
5:B:294:TYR:HE2	38:B:9456:HOH:O	2.01	0.44
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.00	0.44
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.82	0.44
1:0:2542:C:H5"	1:0:2608:C:N4	2.33	0.44
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.47	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.83	0.44
5:B:138:GLY:O	5:B:139:ASP:C	2.55	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.85	0.44
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.44
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.18	0.44
10:G:20:VAL:O	10:G:24:VAL:HG23	2.18	0.44
5:B:195:ARG:NH2	5:B:323:LEU:HD13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.48	0.44
1:0:2011:A:H4'	1:0:2012:U:O5'	2.18	0.44
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
1:0:2281:C:C2'	1:0:2282:U:H5'	2.47	0.44
6:C:153:VAL:O	6:C:157:LEU:HG	2.17	0.44
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.44
1:0:1909:A:N1	1:0:2128:G:H1'	2.33	0.44
1:0:289:G:O2'	1:0:290:C:H5'	2.18	0.44
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.17	0.44
16:N:67:ALA:C	16:N:69:TYR:N	2.71	0.44
1:0:1976:G:H1'	1:0:2005:G:N2	2.33	0.44
17:O:96:VAL:HG12	17:O:97:SER:N	2.33	0.44
12:J:42:GLU:HG3	12:J:145:TRP:CD1	2.53	0.44
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.17	0.44
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.44
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.98	0.44
5:B:251:VAL:HG13	38:B:9371:HOH:O	2.18	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.44
1:0:2782:G:O6	1:0:2790:C:H5"	2.17	0.44
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.80	0.44
1:0:553:G:P	27:Y:204:ARG:NH2	2.90	0.44
1:0:2004:U:H2'	1:0:2005:G:OP1	2.18	0.44
1:0:1202:A:H2'	1:0:1203:G:H5'	1.99	0.44
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.53	0.44
1:0:2243:C:H5"	38:0:4058:HOH:O	2.17	0.44
27:Y:177:LYS:HE2	27:Y:183:GLU:OE2	2.17	0.44
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.48	0.44
17:O:24:ALA:O	17:O:28:ASP:HB2	2.18	0.44
1:0:818:A:O2'	28:Z:13:ARG:HD3	2.18	0.44
15:M:165:GLY:O	15:M:169:ARG:HG3	2.18	0.44
1:0:1167:G:O2'	1:0:1168:C:H5'	2.18	0.44
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.44
6:C:7:ASP:C	6:C:9:ASP:H	2.21	0.44
1:0:508:A:H2'	1:0:509:A:H5"	2.00	0.43
1:0:841:A:OP2	20:R:128:ARG:HD2	2.18	0.43
8:E:7:ILE:HD11	8:E:11:VAL:HG12	2.00	0.43
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.51	0.43
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.43
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1744:G:H2'	1:0:1745:G:H5'	1.98	0.43
1:0:585:C:H5"	38:0:5161:HOH:O	2.17	0.43
1:0:100:C:O2	22:T:17:HIS:HB3	2.18	0.43
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.98	0.43
6:C:115:LEU:HD21	6:C:243:VAL:CG1	2.38	0.43
23:U:17:THR:CG2	23:U:18:GLY:N	2.81	0.43
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.33	0.43
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.51	0.43
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.33	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.17	0.43
28:Z:13:ARG:NH1	38:Z:9219:HOH:O	2.51	0.43
1:0:1929:G:H1'	38:0:5438:HOH:O	2.18	0.43
32:I:118:SER:HB2	32:I:123:ASN:HB2	2.00	0.43
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.43
1:0:1883:U:C2'	1:0:1884:G:H5'	2.48	0.43
1:0:1067:A:H5'	38:0:4650:HOH:O	2.16	0.43
12:J:103:VAL:HG12	38:J:9365:HOH:O	2.19	0.43
5:B:36:PRO:HD3	5:B:169:GLY:H	1.83	0.43
2:9:3055:U:H4'	2:9:3056:A:C8	2.53	0.43
2:9:3042:C:O2	7:D:76:ARG:NH1	2.51	0.43
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.43
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.43
1:0:2781:U:C2'	1:0:2782:G:H5'	2.48	0.43
16:N:151:ASP:HB3	38:N:9324:HOH:O	2.17	0.43
2:9:3106:C:O2'	2:9:3107:C:H5'	2.18	0.43
1:0:2775:A:C6	1:0:2799:A:C8	3.06	0.43
11:H:154:TYR:CD1	11:H:154:TYR:C	2.91	0.43
1:0:2274:A:O2'	1:0:2275:G:H5'	2.18	0.43
7:D:142:ALA:HA	7:D:149:ARG:O	2.19	0.43
1:0:2015:A:H2'	1:0:2016:U:O4'	2.18	0.43
6:C:131:PHE:CD2	6:C:131:PHE:N	2.86	0.43
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.79	0.43
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.43
24:V:39:ALA:C	24:V:41:GLU:H	2.17	0.43
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.00	0.43
1:0:2039:A:OP2	5:B:234:ARG:NH2	2.51	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
1:0:1268:C:O2'	1:0:1269:G:H5'	2.18	0.43
1:0:2438:G:H2'	1:0:2439:C:O4'	2.18	0.43
5:B:232:TRP:CD1	5:B:235:ARG:HD2	2.54	0.43
18:P:71:TYR:HD2	18:P:73:HIS:CD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:5:GLU:HG3	23:U:10:GLY:O	2.18	0.43
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.51	0.43
2:9:3054:A:H2	38:9:3535:HOH:O	2.01	0.43
32:I:138:THR:CG2	32:I:139:ILE:H	2.23	0.43
1:0:2890:A:C8	23:U:56:ARG:NE	2.87	0.43
3:4:176:A:OP1	3:4:175:C:H5"	2.17	0.43
1:0:1625:U:H5"	38:0:6274:HOH:O	2.18	0.43
25:W:59:GLN:HE22	25:W:98:PHE:N	2.17	0.43
1:0:1423:C:O2'	1:0:1424:A:H5'	2.18	0.43
38:0:4151:HOH:O	11:H:11:LYS:HE2	2.18	0.43
16:N:147:ILE:HB	38:N:9342:HOH:O	2.19	0.43
5:B:51:VAL:HG22	5:B:53:LEU:CD1	2.49	0.43
5:B:254:GLN:HG3	38:B:9331:HOH:O	2.17	0.43
1:0:1451:C:H5'	1:0:1505:U:N3	2.34	0.43
22:T:48:VAL:HG22	22:T:97:ARG:C	2.39	0.43
23:U:6:CYS:C	23:U:8:TYR:H	2.22	0.43
8:E:11:VAL:HG12	8:E:12:ASP:N	2.34	0.43
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.99	0.43
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.99	0.43
16:N:42:HIS:HB3	16:N:62:HIS:HE1	1.82	0.43
7:D:48:MET:HA	7:D:49:PRO:HD3	1.79	0.43
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.43
1:0:1169:U:H2'	1:0:1170:U:O4'	2.18	0.43
15:M:98:GLN:O	15:M:102:GLU:HG3	2.19	0.43
1:0:1119:G:H8	12:J:52:GLN:NE2	2.17	0.43
7:D:23:VAL:HG11	7:D:83:PHE:CZ	2.54	0.43
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.49	0.43
24:V:1:THR:CG2	24:V:2:VAL:N	2.79	0.43
8:E:49:ILE:HD11	8:E:69:ILE:HD12	2.01	0.43
15:M:30:GLU:O	15:M:34:GLU:HG3	2.18	0.43
7:D:139:TYR:N	38:D:3723:HOH:O	2.51	0.43
14:L:145:LEU:O	14:L:145:LEU:HD23	2.19	0.43
1:0:920:C:H5"	1:0:921:G:O5'	2.19	0.43
6:C:8:LEU:HD13	6:C:147:LEU:HD21	1.99	0.43
1:0:2511:A:H2'	1:0:2512:U:O4'	2.19	0.43
1:0:2061:C:C2'	1:0:2062:A:H5'	2.49	0.43
27:Y:165:GLU:HB3	38:Y:8182:HOH:O	2.17	0.43
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.33	0.43
5:B:26:PHE:CE1	5:B:310:ARG:HB3	2.54	0.43
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.18	0.43
4:A:36:ASP:CB	4:A:85:SER:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.43
2:9:3052:A:H8	2:9:3052:A:O5'	2.02	0.43
22:T:40:VAL:HG23	22:T:119:ALA:C	2.38	0.43
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.81	0.43
6:C:98:ARG:NH1	38:C:9154:HOH:O	2.50	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.43
1:0:645:U:OP2	14:L:4:LYS:CE	2.67	0.43
5:B:7:ARG:HD3	5:B:9:GLY:O	2.19	0.43
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.01	0.43
7:D:81:GLU:C	7:D:83:PHE:N	2.72	0.43
2:9:3056:A:C3'	2:9:3057:A:H5"	2.49	0.43
1:0:1206:U:H2'	1:0:1207:A:O4'	2.18	0.43
18:P:55:LYS:HG2	18:P:56:GLY:N	2.33	0.43
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.01	0.43
1:0:2382:A:H5'	38:3:9334:HOH:O	2.18	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
1:0:1942:A:H3'	38:0:7554:HOH:O	2.19	0.43
18:P:40:VAL:O	18:P:44:VAL:HG23	2.19	0.43
5:B:88:GLU:HB3	5:B:97:LEU:HG	2.00	0.43
15:M:159:VAL:HG13	15:M:160:PHE:N	2.33	0.43
1:0:2816:A:H5"	1:0:2817:G:H5'	2.01	0.43
1:0:721:A:H4'	17:O:51:TYR:CD1	2.53	0.43
18:P:6:GLN:OE1	18:P:6:GLN:N	2.47	0.43
6:C:236:THR:O	6:C:237:GLU:C	2.57	0.42
1:0:1118:A:C8	1:0:1119:G:H5"	2.51	0.42
1:0:1942:A:H4'	38:A:9312:HOH:O	2.19	0.42
7:D:57:THR:HG23	7:D:63:ILE:HG22	2.00	0.42
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.42
1:0:282:C:H2'	1:0:283:U:O4'	2.18	0.42
1:0:1705:C:C5'	18:P:59:ARG:HH12	2.32	0.42
1:0:1654:U:H5"	38:0:7627:HOH:O	2.18	0.42
9:F:22:VAL:CG2	9:F:104:ALA:HB2	2.49	0.42
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.18	0.42
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.42
15:M:46:LEU:HG	38:M:9413:HOH:O	2.18	0.42
30:2:19:SER:HB3	38:2:4479:HOH:O	2.19	0.42
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.84	0.42
1:0:1331:A:OP2	27:Y:142:SER:OG	2.27	0.42
1:0:969:G:H1	1:0:999:C:H42	1.67	0.42
1:0:2740:G:H2'	1:0:2741:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.42
1:0:559:U:H2'	1:0:560:C:O4'	2.19	0.42
1:0:544:G:H2'	1:0:545:G:C5'	2.49	0.42
1:0:1377:C:C5'	1:0:1377:C:H6	2.31	0.42
20:R:25:PHE:CE2	20:R:29:LYS:CE	3.01	0.42
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.23	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.42
1:0:2708:G:N2	13:K:1:MET:O	2.52	0.42
16:N:44:ARG:HG3	16:N:45:ALA:N	2.34	0.42
16:N:104:ILE:HG13	16:N:104:ILE:O	2.18	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.42
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.52	0.42
13:K:45:PRO:HB2	38:K:7169:HOH:O	2.18	0.42
16:N:149:GLU:O	16:N:152:GLU:HB2	2.19	0.42
38:0:6997:HOH:O	16:N:5:ARG:HB2	2.19	0.42
8:E:166:VAL:HB	38:E:6341:HOH:O	2.19	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.42
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.42
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.33	0.42
1:0:2327:A:H2'	1:0:2328:U:O4'	2.19	0.42
7:D:101:THR:HG22	38:D:7400:HOH:O	2.19	0.42
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.42
1:0:1711:A:O2'	1:0:1712:A:H5'	2.19	0.42
20:R:39:THR:CG2	20:R:42:GLU:HG3	2.49	0.42
1:0:1167:G:H4'	32:I:135:LEU:HD22	2.01	0.42
1:0:875:A:C2	4:A:194:MET:SD	3.12	0.42
1:0:1205:U:H2'	1:0:1206:U:C5'	2.49	0.42
22:T:47:THR:HG22	22:T:99:THR:OG1	2.19	0.42
9:F:83:LEU:HD11	9:F:96:ALA:HB3	2.02	0.42
9:F:107:ASP:O	9:F:111:ILE:HG13	2.20	0.42
1:0:1675:C:H5"	30:2:5:LYS:HD2	2.01	0.42
1:0:2719:A:C2	5:B:70:PRO:HG3	2.54	0.42
12:J:4:ALA:O	12:J:5:GLU:O	2.37	0.42
15:M:123:ASP:OD1	15:M:126:GLN:HG2	2.19	0.42
1:0:1544:U:H2'	1:0:1545:C:H6	1.84	0.42
2:9:3007:G:H5'	38:N:9345:HOH:O	2.17	0.42
1:0:2499:U:O2'	1:0:2500:C:H5'	2.18	0.42
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.32	0.42
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.01	0.42
4:A:200:PRO:HD3	38:A:9319:HOH:O	2.19	0.42
8:E:31:ARG:NH1	38:E:5919:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1175:G:H1'	1:0:1193:A:C2'	2.47	0.42
32:I:92:PRO:C	32:I:94:GLU:N	2.72	0.42
25:W:59:GLN:HE22	25:W:98:PHE:CB	2.30	0.42
6:C:107:ARG:NE	38:C:9256:HOH:O	2.27	0.42
1:0:2372:A:H2'	1:0:2373:U:H6	1.84	0.42
1:0:1427:A:N6	1:0:1440:U:H1'	2.34	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
22:T:40:VAL:HA	22:T:119:ALA:O	2.19	0.42
1:0:969:G:H1	1:0:999:C:N4	2.17	0.42
1:0:1773:G:N2	1:0:1774:G:C8	2.87	0.42
5:B:90:THR:C	5:B:92:TYR:H	2.22	0.42
6:C:124:VAL:HA	6:C:230:GLY:O	2.18	0.42
1:0:1785:G:OP1	18:P:76:GLY:HA3	2.20	0.42
1:0:2728:C:H2'	1:0:2729:C:C6	2.54	0.42
1:0:2453:G:H5'	38:0:4985:HOH:O	2.18	0.42
11:H:38:LYS:HE2	11:H:42:ASP:HB2	2.01	0.42
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.02	0.42
16:N:103:ASP:OD1	16:N:103:ASP:C	2.57	0.42
2:9:3049:G:C2'	2:9:3050:G:H5'	2.50	0.42
4:A:153:ARG:HD3	38:A:9328:HOH:O	2.18	0.42
4:A:186:TRP:CG	4:A:187:PRO:HA	2.54	0.42
8:E:84:MET:HE3	8:E:148:ILE:HG21	2.02	0.42
1:0:2415:A:O2'	16:N:29:SER:HB3	2.19	0.42
12:J:80:LYS:NZ	38:J:9370:HOH:O	2.52	0.42
18:P:143:ALA:HA	38:P:190:HOH:O	2.20	0.42
1:0:581:G:O2'	1:0:582:C:H5'	2.19	0.42
2:9:3059:C:H5'	38:9:5233:HOH:O	2.19	0.42
1:0:963:C:O2	1:0:1005:A:N1	2.52	0.42
1:0:333:G:O2'	1:0:334:G:H5'	2.20	0.42
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.02	0.42
1:0:196:G:H2'	38:L:9371:HOH:O	2.18	0.42
1:0:1562:C:N4	38:0:6127:HOH:O	2.53	0.42
16:N:163:PHE:O	16:N:164:ASP:O	2.38	0.42
16:N:171:HIS:CE1	38:N:9364:HOH:O	2.73	0.42
1:0:1185:U:H2'	1:0:1186:C:H6	1.82	0.42
38:0:4910:HOH:O	17:O:35:LYS:HD3	2.20	0.42
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.49	0.42
30:2:36:ASN:O	30:2:39:ARG:HG3	2.19	0.42
1:0:2474:A:N6	3:4:176:A:OP2	2.53	0.42
18:P:92:GLU:HA	18:P:95:GLU:OE1	2.20	0.42
2:9:3107:C:H2'	2:9:3108:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.42
1:0:1587:U:H2'	1:0:1588:G:O4'	2.19	0.42
7:D:56:ARG:N	38:D:6752:HOH:O	2.53	0.42
8:E:43:ASP:HA	38:E:5864:HOH:O	2.19	0.42
1:0:970:U:H2'	38:0:6568:HOH:O	2.19	0.42
6:C:115:LEU:HA	6:C:115:LEU:HD12	1.92	0.42
25:W:84:VAL:HG21	25:W:93:ILE:HG12	2.00	0.42
13:K:75:ARG:HH21	13:K:94:ALA:CB	2.32	0.42
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.54	0.42
1:0:603:A:H4'	1:0:604:G:O5'	2.19	0.42
8:E:107:PHE:CD2	8:E:108:LEU:HD13	2.55	0.42
1:0:462:A:N3	30:2:37:HIS:HB3	2.35	0.42
5:B:279:THR:CG2	5:B:280:VAL:N	2.83	0.42
1:0:2728:C:H2'	1:0:2729:C:H6	1.83	0.42
1:0:581:G:H5'	38:0:7877:HOH:O	2.19	0.42
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.19	0.42
1:0:1471:A:H2'	1:0:1472:C:C6	2.55	0.42
12:J:22:VAL:O	12:J:26:VAL:HG23	2.20	0.42
24:V:12:THR:CG2	24:V:15:GLU:H	2.33	0.42
1:0:1187:U:O2'	1:0:1189:A:H2	1.82	0.42
24:V:1:THR:HG22	24:V:48:GLU:OE1	2.20	0.42
5:B:210:GLY:HA2	5:B:256:GLN:NE2	2.35	0.42
1:0:484:A:N1	1:0:506:G:H4'	2.35	0.42
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.50	0.42
1:0:664:U:O4	1:0:681:G:H5"	2.19	0.42
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.20	0.42
4:A:86:ALA:HB3	4:A:94:LEU:HD13	2.02	0.42
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.38	0.42
6:C:173:LYS:O	6:C:186:TYR:HA	2.20	0.42
1:0:2333:G:P	7:D:56:ARG:HH22	2.42	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.42
1:0:371:U:H2'	1:0:372:A:H8	1.85	0.42
1:0:2786:G:H2'	38:0:7404:HOH:O	2.20	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.55	0.42
1:0:1594:C:O2'	1:0:1595:G:H5'	2.20	0.42
8:E:31:ARG:NH1	8:E:68:HIS:ND1	2.66	0.42
1:0:2254:G:O2'	1:0:2255:A:H5'	2.20	0.42
14:L:133:VAL:HB	38:L:9356:HOH:O	2.18	0.42
1:0:1163:G:N2	38:0:6299:HOH:O	2.53	0.42
1:0:1684:A:O2'	1:0:1685:A:H5"	2.19	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
28:Z:81:ARG:O	28:Z:82:SER:C	2.57	0.42
1:0:1312:G:OP1	27:Y:213:LYS:NZ	2.46	0.42
1:0:731:U:O2'	1:0:732:C:H5'	2.20	0.42
11:H:50:ILE:HG23	11:H:131:GLU:O	2.20	0.42
6:C:140:VAL:HG12	6:C:141:SER:N	2.34	0.41
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.53	0.41
4:A:93:THR:HA	4:A:154:ALA:O	2.19	0.41
27:Y:134:HIS:CD2	27:Y:134:HIS:H	2.38	0.41
1:0:1878:G:H5"	38:0:3103:HOH:O	2.19	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.50	0.41
1:0:569:A:H5"	1:0:587:A:N1	2.35	0.41
6:C:35:VAL:HG21	6:C:227:GLY:HA2	2.02	0.41
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.19	0.41
1:0:2271:G:N3	1:0:2271:G:H2'	2.35	0.41
25:W:21:LEU:HD21	25:W:48:VAL:HG13	2.01	0.41
1:0:1593:C:O2'	1:0:1594:C:H5'	2.20	0.41
13:K:132:VAL:O	13:K:132:VAL:HG12	2.20	0.41
16:N:181:ASP:O	16:N:184:ILE:HG22	2.20	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.88	0.41
5:B:279:THR:HG22	5:B:280:VAL:N	2.35	0.41
15:M:182:LYS:NZ	38:M:9325:HOH:O	2.53	0.41
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.20	0.41
1:0:1393:A:H2'	1:0:1394:C:C6	2.55	0.41
1:0:1028:U:H5'	1:0:1031:G:O4'	2.20	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.87	0.41
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.41
5:B:168:GLY:H	5:B:174:ARG:HD2	1.85	0.41
5:B:53:LEU:HD11	5:B:327:VAL:HG22	2.01	0.41
32:I:129:VAL:O	32:I:129:VAL:HG12	2.21	0.41
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.43	0.41
1:0:2541:U:O2'	1:0:2542:C:H5'	2.19	0.41
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.41
4:A:179:MET:HG2	4:A:186:TRP:CG	2.55	0.41
1:0:2780:C:H2'	1:0:2781:U:H6	1.84	0.41
29:1:25:LYS:HD2	30:2:49:GLU:N	2.34	0.41
1:0:1776:A:C8	1:0:1778:A:O4'	2.73	0.41
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.20	0.41
1:0:705:C:H2'	1:0:705:C:O2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:87:TYR:OH	5:B:163:GLU:OE2	2.27	0.41
1:0:2754:G:O2'	1:0:2755:G:H5'	2.20	0.41
1:0:288:A:H61	1:0:364:C:H42	1.69	0.41
12:J:45:VAL:CG2	12:J:46:ILE:N	2.83	0.41
5:B:247:VAL:HG13	5:B:251:VAL:HG11	2.03	0.41
1:0:2269:C:C2'	1:0:2270:G:H5'	2.50	0.41
29:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.34	0.41
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	2.02	0.41
1:0:2832:C:H5	38:0:7429:HOH:O	2.03	0.41
14:L:128:GLY:O	14:L:132:LYS:HG3	2.20	0.41
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.41
1:0:2072:G:H3'	1:0:2073:G:C5'	2.51	0.41
25:W:13:MET:CE	25:W:18:GLN:HA	2.51	0.41
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.21	0.41
38:9:1056:HOH:O	16:N:7:LYS:HE2	2.21	0.41
1:0:1180:U:H2'	1:0:1181:A:O4'	2.21	0.41
23:U:6:CYS:HA	23:U:13:ILE:HD11	2.03	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
16:N:154:LEU:O	16:N:155:GLU:CB	2.68	0.41
1:0:1044:C:H5"	38:0:9342:HOH:O	2.21	0.41
14:L:140:VAL:O	14:L:140:VAL:HG12	2.19	0.41
1:0:1131:G:C6	1:0:1230:A:C4	3.09	0.41
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.85	0.41
1:0:1921:A:O2'	1:0:1922:A:H5'	2.20	0.41
11:H:80:GLU:HA	38:H:9182:HOH:O	2.20	0.41
14:L:34:GLY:C	14:L:36:ASP:H	2.24	0.41
1:0:2464:C:H5"	1:0:2465:A:OP1	2.20	0.41
26:X:7:GLU:HA	26:X:74:ALA:O	2.19	0.41
1:0:2670:G:O2'	1:0:2671:U:H5'	2.21	0.41
1:0:827:A:H2'	1:0:828:G:O4'	2.20	0.41
31:3:30:GLN:HB3	31:3:30:GLN:HE21	1.61	0.41
16:N:37:ARG:NH2	38:N:9331:HOH:O	2.53	0.41
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.85	0.41
1:0:2812:A:C2	1:0:2814:A:N6	2.75	0.41
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.13	0.41
1:0:1477:C:H5'	1:0:1868:G:H5"	2.03	0.41
1:0:2564:G:OP2	1:0:2565:C:H5"	2.21	0.41
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.41
1:0:1006:A:N1	1:0:2311:A:H1'	2.35	0.41
1:0:1355:A:H2'	38:0:4429:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2842:G:H2'	1:0:2843:A:H5'	2.03	0.41
8:E:16:ASP:O	8:E:17:HIS:HB2	2.19	0.41
6:C:130:GLU:HA	6:C:130:GLU:OE1	2.21	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.44	0.41
7:D:27:ILE:HG22	7:D:28:GLY:N	2.34	0.41
11:H:9:ILE:HG23	11:H:126:ARG:NE	2.36	0.41
5:B:217:ARG:CG	5:B:257:THR:HG22	2.48	0.41
1:0:120:A:H2'	1:0:120:A:N3	2.36	0.41
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.41
1:0:1419:U:H2'	1:0:1685:A:C2	2.56	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.41
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.03	0.41
1:0:250:C:H2'	1:0:251:C:C6	2.55	0.41
1:0:2379:G:N7	1:0:2408:A:N1	2.68	0.41
1:0:204:A:C2'	1:0:205:U:H5'	2.51	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
11:H:51:VAL:HG21	11:H:127:VAL:HG11	2.03	0.41
1:0:1762:C:H4'	38:0:4949:HOH:O	2.19	0.41
1:0:2455:A:H2'	1:0:2456:A:O4'	2.20	0.41
38:0:7175:HOH:O	19:Q:16:ASN:HB2	2.21	0.41
1:0:2735:U:H2'	1:0:2736:U:C6	2.55	0.41
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.41
1:0:2668:G:H2'	1:0:2669:U:C6	2.56	0.41
1:0:825:U:H5"	1:0:826:U:OP1	2.21	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.20	0.41
32:I:132:CYS:O	32:I:135:LEU:N	2.52	0.41
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.41
1:0:2255:A:C6	1:0:2256:G:C5	3.09	0.41
18:P:59:ARG:O	18:P:63:ARG:HG3	2.21	0.41
25:W:5:VAL:HG11	25:W:153:MET:CE	2.51	0.41
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.03	0.41
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.55	0.41
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.90	0.41
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.20	0.41
1:0:1307:A:H2'	1:0:1308:A:C8	2.56	0.41
5:B:184:ASP:HB2	5:B:185:GLY:H	1.71	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.91	0.41
1:0:451:C:O2'	1:0:452:G:H5'	2.21	0.41
1:0:377:C:H5	38:0:3616:HOH:O	2.03	0.41
17:O:81:PHE:N	17:O:81:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:P	12:J:49:ARG:HH11	2.44	0.41
13:K:10:GLN:N	13:K:10:GLN:NE2	2.43	0.41
12:J:131:THR:CG2	12:J:134:GLU:HG3	2.51	0.41
18:P:115:SER:C	18:P:117:SER:N	2.74	0.41
6:C:19:PRO:HG2	6:C:22:PHE:CD1	2.56	0.41
12:J:39:VAL:CG1	12:J:40:ASN:N	2.84	0.41
1:0:482:G:H4'	1:0:508:A:N1	2.36	0.41
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.55	0.41
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.85	0.41
10:G:12:ILE:HG13	38:G:6833:HOH:O	2.21	0.41
4:A:36:ASP:C	4:A:38:ILE:N	2.71	0.41
1:0:1778:A:H2'	1:0:1779:A:H5'	2.02	0.41
8:E:75:GLY:HA2	8:E:79:GLY:HA2	2.03	0.41
6:C:39:GLN:O	6:C:43:LYS:HD3	2.20	0.41
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.55	0.41
9:F:111:ILE:O	9:F:115:VAL:HG23	2.21	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.03	0.41
1:0:894:A:C2	6:C:87:ARG:NH2	2.88	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.86	0.41
1:0:200:U:O2'	1:0:201:G:H5'	2.21	0.41
23:U:49:LEU:HG	38:U:3805:HOH:O	2.20	0.41
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.85	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.41
1:0:2079:G:H2'	1:0:2080:G:O4'	2.21	0.41
22:T:19:ARG:NH1	22:T:68:ASP:O	2.54	0.41
1:0:645:U:O2	1:0:761:A:H2	2.04	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41
1:0:1386:G:O2'	1:0:1387:G:H5'	2.21	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
15:M:65:VAL:HG21	15:M:105:ALA:HB2	2.03	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.21	0.41
1:0:1396:C:H4'	18:P:2:ASP:OD1	2.21	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.41
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.20	0.41
1:0:432:G:O2'	1:0:433:C:H5'	2.20	0.41
1:0:876:A:H2'	1:0:876:A:N3	2.35	0.41
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.53	0.41
22:T:41:ARG:O	22:T:43:ASN:ND2	2.53	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.56	0.41
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.51	0.41
6:C:77:ALA:O	6:C:78:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1123:A:C2	1:0:1129:C:H4'	2.56	0.41
2:9:3041:C:H5"	7:D:48:MET:SD	2.61	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
15:M:72:ALA:HB2	15:M:93:ARG:HG2	2.03	0.41
1:0:710:G:OP1	17:O:24:ALA:HB3	2.21	0.41
1:0:1744:G:C2'	1:0:1745:G:H5'	2.51	0.41
11:H:99:LYS:CG	11:H:119:LYS:HD3	2.51	0.41
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.21	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.41
5:B:57:GLU:OE1	5:B:60:SER:HB2	2.21	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.77	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.56	0.41
15:M:164:THR:HG22	15:M:166:ALA:N	2.36	0.40
1:0:542:A:O2'	1:0:543:G:H5'	2.21	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.63	0.40
16:N:164:ASP:CG	16:N:167:ASP:HA	2.39	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
1:0:1543:G:N1	1:0:1641:A:OP2	2.41	0.40
1:0:907:A:H4'	1:0:1328:A:C2	2.56	0.40
8:E:73:PHE:O	8:E:76:VAL:HG22	2.21	0.40
1:0:475:G:H5'	6:C:73:LEU:CD2	2.50	0.40
1:0:1682:A:H5"	38:0:9769:HOH:O	2.20	0.40
1:0:1790:C:H2'	1:0:1791:U:C6	2.55	0.40
38:0:4650:HOH:O	25:W:14:HIS:HA	2.20	0.40
11:H:154:TYR:HD1	11:H:154:TYR:C	2.24	0.40
2:9:3033:U:H2'	38:9:3797:HOH:O	2.21	0.40
1:0:2615:U:C5	1:0:2616:G:C6	3.09	0.40
1:0:1370:G:O5'	20:R:62:HIS:HB3	2.21	0.40
1:0:353:G:O2'	1:0:354:A:H5'	2.22	0.40
20:R:99:ALA:CB	20:R:109:MET:CE	2.95	0.40
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.40
1:0:2506:A:O2'	1:0:2507:G:P	2.79	0.40
7:D:86:THR:HG23	38:D:7477:HOH:O	2.21	0.40
1:0:474:C:O2'	6:C:73:LEU:HD21	2.21	0.40
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.04	0.40
1:0:702:G:O2'	1:0:703:G:H5'	2.22	0.40
1:0:2690:U:H4'	8:E:111:LYS:CE	2.51	0.40
16:N:63:SER:HB2	16:N:75:THR:HB	2.03	0.40
1:0:10:U:H1'	1:0:532:A:H62	1.86	0.40
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.56	0.40
1:0:2765:C:H2'	1:0:2766:A:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:354:A:H2'	1:0:355:C:C6	2.56	0.40
1:0:1739:G:O2'	1:0:1740:U:H5'	2.21	0.40
16:N:157:PRO:HA	38:N:9322:HOH:O	2.21	0.40
1:0:1434:A:H2'	1:0:1436:C:C5	2.56	0.40
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.41	0.40
23:U:35:LYS:HE2	23:U:51:TRP:CH2	2.56	0.40
16:N:101:VAL:HG12	38:N:9327:HOH:O	2.22	0.40
27:Y:197:ASP:OD1	27:Y:197:ASP:C	2.60	0.40
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.73	0.40
1:0:1730:G:H2'	1:0:1730:G:N3	2.36	0.40
12:J:130:VAL:CG1	12:J:131:THR:N	2.85	0.40
5:B:53:LEU:HD12	5:B:327:VAL:HA	2.04	0.40
4:A:223:ARG:CZ	38:A:9317:HOH:O	2.69	0.40
4:A:194:MET:CE	4:A:199:HIS:HB2	2.51	0.40
7:D:104:PHE:CE2	7:D:166:ILE:CD1	3.04	0.40
8:E:87:PHE:O	8:E:93:MET:HE3	2.21	0.40
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.93	0.40
16:N:67:ALA:O	16:N:69:TYR:N	2.54	0.40
23:U:37:GLU:O	23:U:40:ALA:HB3	2.22	0.40
1:0:1139:U:H2'	1:0:1140:C:H6	1.85	0.40
1:0:2061:C:H2'	1:0:2062:A:H5'	2.04	0.40
1:0:999:C:H2'	1:0:1000:C:O4'	2.21	0.40
1:0:2453:G:H4'	14:L:50:GLY:C	2.41	0.40
12:J:51:GLU:O	12:J:55:GLU:HG3	2.20	0.40
1:0:566:A:H2'	1:0:567:U:O4'	2.21	0.40
18:P:135:ALA:O	18:P:139:ARG:HG3	2.22	0.40
1:0:1613:C:H2'	1:0:1614:G:O4'	2.21	0.40
1:0:1985:U:C2	1:0:1996:U:O4'	2.75	0.40
25:W:85:ALA:HB2	25:W:91:ASP:O	2.21	0.40
1:0:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
20:R:76:ASP:N	20:R:76:ASP:OD1	2.53	0.40
1:0:1158:G:O2'	1:0:1159:G:H5'	2.21	0.40
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.40
1:0:338:C:H4'	6:C:174:ILE:HD12	2.03	0.40
11:H:63:GLU:OE1	11:H:66:ARG:NH1	2.54	0.40
5:B:175:LEU:O	5:B:175:LEU:HD23	2.21	0.40
11:H:20:ILE:CG2	11:H:120:ILE:HD11	2.52	0.40
14:L:125:PHE:CE2	14:L:140:VAL:HG22	2.56	0.40
1:0:601:G:O2'	1:0:602:A:H5'	2.21	0.40
1:0:1079:A:H4'	1:0:2078:U:H5'	2.04	0.40
28:Z:67:GLY:N	28:Z:70:LYS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1311:G:C2	1:0:1312:G:C8	3.09	0.40
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.94	0.40
1:0:2456:A:H2'	1:0:2457:U:C6	2.56	0.40
2:9:3034:A:H2'	2:9:3035:C:O4'	2.21	0.40
1:0:2067:A:H2'	1:0:2068:G:O4'	2.21	0.40
21:S:81:ILE:HG12	38:S:9134:HOH:O	2.21	0.40
1:0:615:G:H2'	1:0:616:U:C6	2.56	0.40
1:0:1194:A:C2'	1:0:1195:G:H5'	2.51	0.40
1:0:1196:C:H2'	1:0:1197:G:H5'	2.04	0.40
20:R:106:GLY:HA2	20:R:109:MET:HE3	2.02	0.40
12:J:39:VAL:HG12	12:J:40:ASN:CG	2.42	0.40
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.22	0.40
5:B:316:ARG:N	5:B:317:PRO:HD3	2.37	0.40
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.35	0.40
8:E:102:VAL:HG11	8:E:148:ILE:HG12	2.03	0.40
7:D:173:GLU:CG	7:D:174:VAL:H	2.35	0.40
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.40
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.34	0.40
20:R:61:GLN:CD	38:R:9338:HOH:O	2.60	0.40
4:A:65:ARG:C	4:A:66:ARG:HG3	2.42	0.40
11:H:88:ARG:H	11:H:88:ARG:HG2	1.68	0.40
5:B:76:THR:N	5:B:77:PRO:HD3	2.37	0.40
1:0:622:G:P	27:Y:148:GLY:HA3	2.62	0.40
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	2.04	0.40
1:0:1335:C:H2'	1:0:1336:U:C6	2.57	0.40
1:0:2093:G:H5"	38:B:9326:HOH:O	2.21	0.40
25:W:130:HIS:O	25:W:136:GLY:HA3	2.22	0.40
1:0:912:A:C4	1:0:1294:A:C2	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	11 19
5	B	335/338 (99%)	298 (89%)	31 (9%)	6 (2%)	11 18
6	C	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	39 61
7	D	134/177 (76%)	101 (75%)	23 (17%)	10 (8%)	1 1
8	E	170/178 (96%)	158 (93%)	12 (7%)	0	100 100
9	F	117/120 (98%)	108 (92%)	3 (3%)	6 (5%)	2 2
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
11	H	156/171 (91%)	145 (93%)	8 (5%)	3 (2%)	10 16
12	J	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	14 24
13	K	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	8 12
14	L	141/165 (86%)	121 (86%)	16 (11%)	4 (3%)	6 9
15	M	192/194 (99%)	183 (95%)	9 (5%)	0	100 100
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	4 5
17	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	21 37
18	P	141/149 (95%)	138 (98%)	2 (1%)	1 (1%)	26 46
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100 100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100 100
21	S	79/85 (93%)	76 (96%)	3 (4%)	0	100 100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21 37
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100 100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	5 6
25	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	26 46
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	15 26
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
28	Z	71/83 (86%)	60 (84%)	9 (13%)	2 (3%)	6 9
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100 100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	7 11
31	3	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	8 13
32	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	13 22
All	All	3705/4430 (84%)	3373 (91%)	273 (7%)	59 (2%)	12 21

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	34	GLY
5	B	139	ASP
5	B	184	ASP
7	D	173	GLU
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
12	J	5	GLU
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	81	ARG
32	I	138	THR
4	A	34	ASP
4	A	132	ASP
6	C	8	LEU
7	D	27	ILE
14	L	80	ASP
16	N	164	ASP
31	3	57	GLY
5	B	169	GLY
7	D	137	PRO
7	D	171	ASP
9	F	61	MET
13	K	39	GLY
13	K	126	SER
14	L	143	THR
16	N	167	ASP
17	O	108	GLY
22	T	53	GLY
24	V	43	PRO
25	W	49	ASN
30	2	37	HIS
31	3	56	PRO
5	B	2	GLN
7	D	16	PRO
7	D	28	GLY
7	D	65	GLU
7	D	97	GLN
7	D	147	ALA
12	J	143	LYS

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Mol	Chain	Res	Type
13	K	111	GLY
16	N	65	ASP
26	X	78	GLU
28	Z	43	GLY
5	B	67	GLU
9	F	44	SER
9	F	64	PRO
11	H	140	VAL
14	L	11	ARG
14	L	35	ARG
16	N	68	GLU
18	P	116	SER
9	F	100	ASP
9	F	104	ALA
7	D	69	ILE
24	V	40	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	179/182 (98%)	170 (95%)	9 (5%)	30 53
5	B	282/283 (100%)	266 (94%)	16 (6%)	25 46
6	C	193/193 (100%)	178 (92%)	15 (8%)	16 29
7	D	117/148 (79%)	111 (95%)	6 (5%)	29 52
8	E	152/156 (97%)	151 (99%)	1 (1%)	88 97
9	F	93/94 (99%)	93 (100%)	0	100 100
10	G	27/283 (10%)	27 (100%)	0	100 100
11	H	132/138 (96%)	124 (94%)	8 (6%)	23 42
12	J	118/121 (98%)	109 (92%)	9 (8%)	16 30
13	K	106/106 (100%)	102 (96%)	4 (4%)	40 67
14	L	113/127 (89%)	107 (95%)	6 (5%)	28 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	M	158/158 (100%)	153 (97%)	5 (3%)	46 74
16	N	149/150 (99%)	142 (95%)	7 (5%)	32 56
17	O	93/94 (99%)	89 (96%)	4 (4%)	35 61
18	P	113/117 (97%)	110 (97%)	3 (3%)	52 79
19	Q	79/80 (99%)	76 (96%)	3 (4%)	40 67
20	R	117/122 (96%)	115 (98%)	2 (2%)	68 89
21	S	71/74 (96%)	70 (99%)	1 (1%)	74 91
22	T	105/106 (99%)	99 (94%)	6 (6%)	25 46
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	49 (96%)	2 (4%)	39 66
25	W	130/130 (100%)	126 (97%)	4 (3%)	47 75
26	X	66/74 (89%)	62 (94%)	4 (6%)	23 42
27	Y	120/196 (61%)	112 (93%)	8 (7%)	20 37
28	Z	60/68 (88%)	60 (100%)	0	100 100
29	1	46/47 (98%)	46 (100%)	0	100 100
30	2	42/46 (91%)	41 (98%)	1 (2%)	57 82
31	3	79/79 (100%)	77 (98%)	2 (2%)	55 82
32	I	58/130 (45%)	58 (100%)	0	100 100
All	All	3093/3611 (86%)	2967 (96%)	126 (4%)	37 63

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	36	ASP
4	A	69	LEU
4	A	94	LEU
4	A	120	ARG
4	A	131	HIS
4	A	153	ARG
4	A	179	MET
4	A	217	ARG
5	B	5	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN

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Mol	Chain	Res	Type
5	B	53	LEU
5	B	97	LEU
5	B	139	ASP
5	B	162	MET
5	B	195	ARG
5	B	234	ARG
5	B	245	SER
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	115	LEU
6	C	131	PHE
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	61	PHE
7	D	86	THR
7	D	133	ASN
7	D	136	ARG
7	D	149	ARG
8	E	164	ASP
11	H	18	GLU
11	H	30	GLN
11	H	62	LEU
11	H	84	LYS
11	H	88	ARG
11	H	111	ASP
11	H	154	TYR
11	H	170	ASN

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Mol	Chain	Res	Type
12	J	46	ILE
12	J	47	THR
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP
14	L	99	GLU
14	L	102	ASP
14	L	140	VAL
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	47	LEU
16	N	49	THR
16	N	135	VAL
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	98	LEU
17	O	115	ARG
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR

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Mol	Chain	Res	Type
20	R	39	THR
21	S	53	ASN
22	T	39	ASN
22	T	48	VAL
22	T	73	HIS
22	T	89	ARG
22	T	96	VAL
22	T	112	LEU
24	V	43	PRO
24	V	65	ASP
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	72	VAL
26	X	79	GLU
27	Y	117	LEU
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	191	ASP
27	Y	200	THR
27	Y	235	GLU
30	2	18	ASN
31	3	56	PRO
31	3	65	THR

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

Mol	Chain	Res	Type
4	A	92	ASN
4	A	125	ASN
4	A	127	GLN
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN

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Mol	Chain	Res	Type
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	71	ASN
8	E	90	HIS
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	132	GLN
11	H	170	ASN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	58	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN

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Mol	Chain	Res	Type
20	R	113	HIS
20	R	117	HIS
20	R	123	GLN
21	S	9	HIS
21	S	25	GLN
21	S	53	ASN
22	T	39	ASN
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	2	HIS
25	W	6	GLN
25	W	27	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	98	GLN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	4	1/8 (12%)	0	0
All	All	2867/3052 (93%)	251 (8%)	33 (1%)

All (251) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G

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Mol	Chain	Res	Type
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
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
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	905	C
1	0	920	C

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Mol	Chain	Res	Type
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1162	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	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C

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Mol	Chain	Res	Type
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G

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Mol	Chain	Res	Type
1	0	1980	U
1	0	1996	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A

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Mol	Chain	Res	Type
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	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	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A

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

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	87	C
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
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	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1692	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMU	0	2587	1	12,22,23	1.04	1 (8%)	19,31,34	3.14	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.06	2 (11%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.86	0	16,32,35	0.75	0
1	PSU	0	2621	1	13,21,22	1.66	2 (15%)	18,30,33	6.07	3 (16%)
1	1MA	0	628	1	14,25,26	1.02	1 (7%)	15,37,40	1.16	1 (6%)
3	5AA	4	76	1,3	16,26,27	1.05	1 (6%)	15,38,41	1.20	1 (6%)

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	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.07	1.47	1.52
3	4	76	5AA	C3'-N3'	-3.33	1.42	1.47
1	0	2588	OMG	C8-N7	-2.04	1.30	1.34
1	0	2621	PSU	C4-N3	2.50	1.37	1.33
1	0	2587	OMU	C4-N3	2.59	1.37	1.33
1	0	628	1MA	C6-N6	2.84	1.34	1.29
1	0	2588	OMG	C6-N1	3.25	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	N1-C2-N3	-21.26	114.77	128.33
1	0	2588	OMG	C5-C6-N1	-8.77	111.59	123.59
1	0	628	1MA	C2-N3-C4	-3.60	110.83	116.40
1	0	2587	OMU	C5-C4-N3	-3.30	114.67	123.12
1	0	2588	OMG	N3-C2-N1	-2.30	123.95	127.44
1	0	2621	PSU	C6-N1-C2	2.57	119.60	115.47
3	4	76	5AA	C2-N1-C6	3.47	118.82	111.43
1	0	2588	OMG	C6-N1-C2	6.64	125.15	115.94
1	0	2587	OMU	C4-N3-C2	13.12	127.14	114.14
1	0	2621	PSU	C4-N3-C2	13.82	127.20	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 234 ligands modelled in this entry, 234 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.30	54 (1%) 68 72	24, 49, 93, 155	0
2	9	122/122 (100%)	-0.11	5 (4%) 41 46	45, 66, 91, 152	0
3	4	5/8 (62%)	-0.51	0 100 100	41, 45, 47, 49	0
4	A	237/240 (98%)	0.45	19 (8%) 15 16	30, 51, 89, 114	0
5	B	337/338 (99%)	0.37	12 (3%) 46 51	31, 61, 90, 100	0
6	C	246/246 (100%)	-0.00	4 (1%) 74 78	28, 48, 71, 82	0
7	D	140/177 (79%)	2.68	77 (55%) 0 0	59, 106, 130, 136	0
8	E	172/178 (96%)	1.19	36 (20%) 1 1	52, 76, 101, 111	0
9	F	119/120 (99%)	1.08	29 (24%) 1 1	52, 74, 100, 116	0
10	G	29/348 (8%)	2.78	19 (65%) 0 0	74, 92, 104, 108	0
11	H	160/171 (93%)	0.45	9 (5%) 28 31	42, 60, 91, 100	0
12	J	142/145 (97%)	0.19	1 (0%) 89 90	40, 56, 77, 99	0
13	K	132/132 (100%)	0.26	5 (3%) 44 49	35, 58, 80, 85	0
14	L	145/165 (87%)	0.93	29 (20%) 1 1	28, 69, 114, 127	0
15	M	194/194 (100%)	0.10	2 (1%) 84 86	32, 43, 59, 66	0
16	N	186/187 (99%)	0.92	41 (22%) 1 1	40, 64, 113, 119	0
17	O	115/116 (99%)	0.21	4 (3%) 48 53	39, 58, 75, 90	0
18	P	143/149 (95%)	0.36	5 (3%) 48 53	43, 58, 70, 78	0
19	Q	95/96 (98%)	0.20	2 (2%) 67 71	38, 47, 60, 72	0
20	R	150/155 (96%)	-0.02	0 100 100	33, 48, 65, 76	0
21	S	81/85 (95%)	0.25	3 (3%) 45 50	45, 59, 78, 88	0
22	T	119/120 (99%)	0.49	4 (3%) 49 54	40, 58, 85, 96	0
23	U	53/66 (80%)	0.35	2 (3%) 44 49	46, 62, 76, 86	0
24	V	65/71 (91%)	1.73	23 (35%) 0 0	56, 76, 112, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	0.12	0 100 100	39, 55, 74, 86	0
26	X	82/92 (89%)	0.72	14 (17%) 2 2	46, 63, 85, 101	0
27	Y	142/241 (58%)	0.33	11 (7%) 16 18	30, 49, 70, 92	0
28	Z	73/83 (87%)	0.24	6 (8%) 14 15	46, 60, 76, 94	0
29	1	56/57 (98%)	-0.31	0 100 100	27, 34, 39, 52	0
30	2	46/50 (92%)	1.71	15 (32%) 1 0	36, 65, 120, 122	0
31	3	92/92 (100%)	0.38	5 (5%) 29 33	35, 55, 71, 87	0
32	I	70/162 (43%)	4.72	61 (87%) 0 0	108, 126, 148, 149	0
All	All	6651/7482 (88%)	0.23	497 (7%) 17 19	24, 55, 103, 155	0

All (497) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	96	PHE	15.7
32	I	133	THR	14.1
24	V	1	THR	13.6
32	I	102	VAL	12.9
32	I	93	GLN	12.0
7	D	63	ILE	10.0
30	2	38	LYS	9.6
16	N	166	ALA	9.6
7	D	88	LEU	9.1
32	I	116	LEU	9.0
2	9	3001	U	8.9
32	I	71	GLY	8.8
7	D	69	ILE	8.7
10	G	23	ILE	8.5
32	I	79	ILE	8.4
10	G	27	ILE	7.8
32	I	109	ALA	7.7
32	I	117	LEU	7.7
7	D	57	THR	7.7
7	D	26	GLY	7.6
24	V	39	ALA	7.6
7	D	44	ILE	7.5
30	2	41	HIS	7.4
4	A	37	VAL	7.3
7	D	64	ARG	7.2
32	I	113	HIS	7.1

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Mol	Chain	Res	Type	RSRZ
24	V	40	PRO	7.1
32	I	137	VAL	7.0
24	V	38	GLY	6.9
7	D	84	LEU	6.8
32	I	118	SER	6.8
32	I	75	THR	6.7
7	D	85	GLN	6.7
30	2	44	ARG	6.6
7	D	58	VAL	6.5
7	D	172	VAL	6.5
32	I	105	VAL	6.5
7	D	170	TYR	6.3
32	I	88	GLY	6.2
7	D	61	PHE	6.2
7	D	66	GLY	6.1
32	I	85	PHE	6.1
32	I	103	ASP	5.9
7	D	75	LEU	5.7
10	G	24	VAL	5.7
30	2	42	TRP	5.7
32	I	111	GLN	5.7
32	I	77	GLU	5.7
30	2	48	ASP	5.6
30	2	45	ASN	5.5
24	V	43	PRO	5.5
7	D	10	PHE	5.5
30	2	49	GLU	5.5
30	2	37	HIS	5.5
1	0	2237	G	5.4
32	I	129	VAL	5.4
26	X	88	GLU	5.4
8	E	42	VAL	5.3
7	D	23	VAL	5.3
7	D	41	LEU	5.3
8	E	44	GLY	5.3
1	0	1173	A	5.3
2	9	3024	U	5.1
7	D	40	ILE	5.1
7	D	87	ALA	5.1
32	I	119	TYR	5.0
32	I	115	ASP	4.9
32	I	81	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
32	I	114	PRO	4.9
2	9	3023	U	4.9
32	I	94	GLU	4.8
32	I	92	PRO	4.8
32	I	126	LYS	4.8
7	D	165	PHE	4.7
32	I	74	PRO	4.7
7	D	56	ARG	4.7
16	N	159	TYR	4.6
32	I	97	VAL	4.6
32	I	72	VAL	4.6
32	I	78	LEU	4.6
1	0	1177	A	4.5
7	D	68	PRO	4.5
1	0	960	G	4.5
16	N	160	SER	4.5
21	S	81	ILE	4.5
4	A	31	LYS	4.5
7	D	98	PHE	4.5
7	D	90	LEU	4.4
1	0	282	C	4.4
1	0	2238	A	4.4
11	H	73	LEU	4.4
1	0	1172	G	4.4
7	D	18	ILE	4.4
9	F	17	LEU	4.4
7	D	89	PRO	4.4
32	I	106	LYS	4.4
10	G	71	LEU	4.3
32	I	89	SER	4.3
32	I	121	LEU	4.3
14	L	97	VAL	4.3
24	V	37	GLY	4.3
9	F	119	ARG	4.3
16	N	67	ALA	4.3
7	D	51	ARG	4.3
8	E	11	VAL	4.2
30	2	39	ARG	4.2
30	2	36	ASN	4.2
7	D	65	GLU	4.2
14	L	106	VAL	4.2
7	D	166	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
7	D	86	THR	4.2
16	N	152	GLU	4.2
10	G	26	MET	4.2
14	L	60	GLU	4.2
24	V	41	GLU	4.1
32	I	136	GLY	4.1
8	E	87	PHE	4.1
32	I	73	PRO	4.1
7	D	59	GLY	4.1
30	2	47	THR	4.1
32	I	76	ALA	4.1
7	D	62	ASP	4.1
7	D	49	PRO	4.0
32	I	91	GLU	4.0
9	F	16	ALA	4.0
32	I	107	GLN	4.0
7	D	128	LEU	4.0
1	0	1951	G	4.0
16	N	158	LEU	4.0
1	0	970	U	4.0
32	I	139	ILE	4.0
7	D	92	GLU	3.9
7	D	93	LEU	3.9
7	D	106	PHE	3.9
14	L	80	ASP	3.9
7	D	27	ILE	3.9
7	D	104	PHE	3.9
32	I	95	ASP	3.9
7	D	134	LEU	3.9
1	0	1199	A	3.9
32	I	135	LEU	3.9
27	Y	236	VAL	3.9
32	I	125	ALA	3.8
7	D	73	VAL	3.8
8	E	76	VAL	3.8
8	E	100	ASP	3.8
9	F	106	ALA	3.8
1	0	1171	A	3.8
7	D	135	VAL	3.8
1	0	1525	G	3.8
14	L	105	TYR	3.8
4	A	35	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
27	Y	235	GLU	3.7
7	D	81	GLU	3.7
8	E	8	PRO	3.7
32	I	104	GLN	3.7
7	D	25	MET	3.7
9	F	45	ALA	3.7
32	I	98	ALA	3.7
32	I	132	CYS	3.7
7	D	70	GLY	3.6
8	E	88	TYR	3.6
8	E	45	ASP	3.6
32	I	128	VAL	3.6
17	O	22	GLY	3.6
30	2	43	ARG	3.6
9	F	117	GLU	3.6
5	B	119	HIS	3.6
9	F	44	SER	3.5
7	D	71	ALA	3.5
26	X	41	PHE	3.5
32	I	138	THR	3.5
1	0	10	U	3.5
32	I	86	GLU	3.5
14	L	142	LEU	3.5
16	N	175	LEU	3.5
7	D	167	GLU	3.5
1	0	735	C	3.5
4	A	36	ASP	3.5
23	U	47	ARG	3.4
14	L	104	ASP	3.4
16	N	164	ASP	3.4
11	H	45	VAL	3.4
14	L	149	ARG	3.4
24	V	8	ILE	3.4
4	A	85	SER	3.4
7	D	130	VAL	3.3
26	X	85	VAL	3.3
26	X	71	ARG	3.3
16	N	149	GLU	3.3
27	Y	98	GLN	3.3
32	I	122	THR	3.3
32	I	110	GLU	3.3
1	0	1279	U	3.2

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Mol	Chain	Res	Type	RSRZ
7	D	29	HIS	3.2
14	L	96	VAL	3.2
26	X	10	VAL	3.2
16	N	148	ALA	3.2
32	I	124	ALA	3.2
9	F	22	VAL	3.2
9	F	49	PHE	3.2
1	0	280	C	3.2
7	D	17	ARG	3.2
16	N	157	PRO	3.2
11	H	37	GLN	3.2
7	D	171	ASP	3.2
18	P	114	LEU	3.1
4	A	38	ILE	3.1
14	L	130	ARG	3.1
7	D	45	THR	3.1
10	G	73	ASP	3.1
7	D	157	LEU	3.1
9	F	26	THR	3.1
16	N	143	ARG	3.1
10	G	20	VAL	3.1
9	F	103	GLU	3.1
30	2	20	ARG	3.1
14	L	145	LEU	3.0
30	2	35	ARG	3.0
26	X	72	VAL	3.0
7	D	24	HIS	3.0
26	X	80	GLU	3.0
6	C	61	PHE	3.0
22	T	35	TYR	3.0
4	A	33	GLU	3.0
8	E	48	VAL	3.0
14	L	102	ASP	3.0
9	F	18	GLU	3.0
22	T	119	ALA	3.0
32	I	108	ILE	3.0
14	L	150	GLN	3.0
9	F	12	LEU	3.0
1	0	272	A	3.0
1	0	2004	U	3.0
14	L	133	VAL	3.0
8	E	5	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
8	E	108	LEU	3.0
14	L	76	LEU	3.0
8	E	10	ASP	3.0
14	L	121	ILE	3.0
1	0	2769	C	3.0
1	0	2254	G	2.9
16	N	154	LEU	2.9
26	X	77	PHE	2.9
7	D	53	LYS	2.9
4	A	34	ASP	2.9
5	B	181	ILE	2.9
10	G	67	LEU	2.9
14	L	120	LEU	2.9
1	0	370	G	2.9
10	G	28	GLU	2.9
1	0	497	A	2.9
26	X	73	ARG	2.9
1	0	2508	C	2.9
32	I	87	THR	2.9
1	0	2250	G	2.9
16	N	180	LEU	2.9
22	T	112	LEU	2.9
16	N	140	GLN	2.9
8	E	118	ILE	2.9
24	V	33	VAL	2.9
2	9	3122	C	2.9
16	N	182	GLY	2.9
14	L	81	VAL	2.8
7	D	55	LYS	2.8
11	H	146	VAL	2.8
16	N	139	TRP	2.8
9	F	107	ASP	2.8
4	A	32	VAL	2.8
5	B	106	HIS	2.8
16	N	138	ASP	2.8
9	F	108	VAL	2.8
16	N	95	ALA	2.8
31	3	92	GLU	2.8
1	0	283	U	2.8
27	Y	95	THR	2.8
1	0	999	C	2.8
16	N	183	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
24	V	59	ILE	2.8
7	D	48	MET	2.8
9	F	19	ALA	2.8
7	D	129	ASP	2.8
8	E	7	ILE	2.7
18	P	141	ILE	2.7
4	A	237	GLY	2.7
9	F	98	VAL	2.7
14	L	108	VAL	2.7
27	Y	108	ASP	2.7
24	V	3	LEU	2.7
1	0	1163	G	2.7
7	D	94	ALA	2.7
6	C	135	GLU	2.7
5	B	105	PHE	2.7
1	0	2251	G	2.7
4	A	97	ALA	2.7
7	D	164	ALA	2.7
1	0	284	C	2.7
4	A	133	ARG	2.7
16	N	68	GLU	2.7
1	0	2850	C	2.7
1	0	285	A	2.7
7	D	173	GLU	2.6
23	U	54	THR	2.6
24	V	36	ALA	2.6
7	D	11	HIS	2.6
10	G	66	LEU	2.6
11	H	47	ILE	2.6
28	Z	11	SER	2.6
7	D	47	GLN	2.6
1	0	1169	U	2.6
1	0	1179	C	2.6
2	9	3002	U	2.6
18	P	71	TYR	2.6
8	E	95	VAL	2.6
8	E	161	VAL	2.6
1	0	1198	U	2.6
8	E	128	GLY	2.6
9	F	118	LEU	2.6
32	I	100	LEU	2.6
32	I	112	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	281	U	2.6
16	N	155	GLU	2.6
24	V	9	ARG	2.6
28	Z	59	TYR	2.6
9	F	20	LEU	2.6
10	G	25	GLU	2.6
8	E	170	ARG	2.5
10	G	69	ARG	2.5
28	Z	21	VAL	2.5
1	0	2239	C	2.5
5	B	117	GLU	2.5
11	H	50	ILE	2.5
7	D	67	ASP	2.5
31	3	22	VAL	2.5
8	E	126	ILE	2.5
1	0	1162	G	2.5
14	L	118	LEU	2.5
28	Z	20	ARG	2.5
10	G	65	THR	2.5
16	N	147	ILE	2.5
16	N	150	TYR	2.5
31	3	1	MET	2.5
16	N	145	ALA	2.5
16	N	165	ALA	2.5
7	D	83	PHE	2.5
24	V	45	ARG	2.5
24	V	46	ILE	2.5
7	D	80	ALA	2.5
15	M	194	ALA	2.5
7	D	43	GLU	2.5
14	L	125	PHE	2.5
5	B	1	PRO	2.5
1	0	1948	G	2.5
4	A	94	LEU	2.5
16	N	184	ILE	2.5
1	0	1000	C	2.5
16	N	162	ASP	2.4
1	0	1625	U	2.4
19	Q	95	GLU	2.4
14	L	100	ALA	2.4
10	G	21	ASP	2.4
24	V	2	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
9	F	99	THR	2.4
8	E	93	MET	2.4
17	O	24	ALA	2.4
5	B	123	ALA	2.4
32	I	84	GLY	2.4
4	A	82	VAL	2.4
14	L	73	VAL	2.4
19	Q	76	VAL	2.4
16	N	181	ASP	2.4
7	D	105	SER	2.4
1	0	1190	G	2.4
4	A	96	LEU	2.4
5	B	104	GLU	2.4
14	L	99	GLU	2.4
9	F	47	LEU	2.3
26	X	9	VAL	2.3
1	0	2249	G	2.3
27	Y	96	GLU	2.3
1	0	372	A	2.3
7	D	50	VAL	2.3
7	D	72	LYS	2.3
31	3	13	HIS	2.3
18	P	77	ALA	2.3
5	B	35	GLN	2.3
10	G	15	TRP	2.3
27	Y	97	LEU	2.3
14	L	93	VAL	2.3
6	C	132	ASP	2.3
9	F	15	ASP	2.3
9	F	100	ASP	2.3
10	G	72	ASP	2.3
24	V	11	MET	2.3
24	V	52	ALA	2.3
26	X	74	ALA	2.3
32	I	120	ASP	2.3
1	0	1950	G	2.3
21	S	20	PHE	2.3
9	F	109	GLU	2.3
10	G	12	ILE	2.3
11	H	74	ILE	2.3
10	G	63	ARG	2.3
31	3	2	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
14	L	144	ASP	2.3
24	V	44	GLY	2.3
13	K	132	VAL	2.3
10	G	70	ALA	2.2
32	I	83	ALA	2.2
16	N	186	LEU	2.2
24	V	49	LEU	2.2
15	M	164	THR	2.2
8	E	6	GLU	2.2
14	L	91	VAL	2.2
28	Z	24	ARG	2.2
18	P	67	LYS	2.2
16	N	172	PHE	2.2
7	D	74	THR	2.2
8	E	46	THR	2.2
5	B	121	PRO	2.2
8	E	86	VAL	2.2
17	O	111	VAL	2.2
8	E	72	MET	2.2
14	L	61	ALA	2.2
13	K	101	ASN	2.2
4	A	65	ARG	2.2
8	E	2	ARG	2.2
16	N	178	THR	2.2
6	C	237	GLU	2.2
11	H	171	ALA	2.2
16	N	179	LEU	2.2
9	F	29	VAL	2.2
1	0	1130	U	2.2
9	F	110	ASP	2.2
16	N	92	ALA	2.2
27	Y	216	ARG	2.2
4	A	99	ILE	2.2
1	0	279	C	2.2
7	D	38	GLU	2.2
24	V	62	GLU	2.2
26	X	82	GLU	2.2
5	B	118	ASP	2.2
24	V	10	ASP	2.2
1	0	1180	U	2.2
9	F	27	GLY	2.2
16	N	177	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
7	D	52	THR	2.2
30	2	46	ASP	2.2
1	0	138	U	2.2
16	N	126	GLY	2.1
8	E	94	GLN	2.1
9	F	102	GLY	2.1
1	0	128	A	2.1
1	0	716	G	2.1
8	E	22	VAL	2.1
26	X	75	ALA	2.1
13	K	108	GLU	2.1
16	N	170	GLU	2.1
16	N	163	PHE	2.1
1	0	2248	C	2.1
8	E	28	SER	2.1
9	F	28	ALA	2.1
1	0	969	G	2.1
14	L	101	ASP	2.1
8	E	20	ILE	2.1
8	E	154	ILE	2.1
12	J	127	ILE	2.1
5	B	140	LEU	2.1
13	K	129	THR	2.1
8	E	25	ASP	2.1
27	Y	234	VAL	2.1
17	O	21	SER	2.1
16	N	1	ALA	2.1
24	V	5	VAL	2.1
32	I	123	ASN	2.1
16	N	185	GLU	2.1
8	E	73	PHE	2.1
13	K	109	LEU	2.1
7	D	37	ALA	2.0
27	Y	187	VAL	2.0
4	A	128	LEU	2.0
16	N	151	ASP	2.0
11	H	71	ARG	2.0
21	S	76	GLU	2.0
22	T	33	GLU	2.0
26	X	7	GLU	2.0
28	Z	25	ARG	2.0
32	I	82	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	135	VAL	2.0
1	0	1174	A	2.0
27	Y	231	PRO	2.0
7	D	91	ALA	2.0
1	0	2255	A	2.0
8	E	1	PRO	2.0
8	E	92	PRO	2.0
7	D	95	THR	2.0
8	E	82	TYR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	PSU	0	2621	20/21	0.98	0.13	-	28,31,39,40	0
1	OMU	0	2587	21/22	0.98	0.13	-	31,34,37,38	0
1	UR3	0	2619	21/22	0.99	0.15	-	33,38,40,43	0
1	OMG	0	2588	24/25	0.98	0.13	-	30,34,37,38	0
1	1MA	0	628	23/24	0.99	0.16	-	31,35,37,38	0
3	5AA	4	76	24/25	0.99	0.14	-	39,44,45,46	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	9161	1/1	0.95	0.25	33.16	49,49,49,49	0
35	NA	0	9171	1/1	0.83	0.26	21.62	60,60,60,60	0
35	NA	0	9174	1/1	0.84	0.26	15.19	59,59,59,59	0
35	NA	0	9140	1/1	0.95	0.33	11.23	49,49,49,49	0
35	NA	L	9180	1/1	0.93	0.38	11.03	50,50,50,50	0
35	NA	0	9179	1/1	0.97	0.20	9.97	57,57,57,57	0
35	NA	0	9172	1/1	0.83	0.31	9.77	59,59,59,59	0
35	NA	0	9162	1/1	0.97	0.26	9.58	58,58,58,58	0
35	NA	0	9178	1/1	0.97	0.30	9.07	53,53,53,53	0
35	NA	0	9176	1/1	0.91	0.24	8.97	43,43,43,43	0
35	NA	0	9150	1/1	0.88	0.21	8.63	44,44,44,44	0
33	MG	0	8060	1/1	0.97	0.20	8.48	39,39,39,39	0
35	NA	0	9182	1/1	0.65	0.28	8.42	74,74,74,74	0
35	NA	0	9121	1/1	0.95	0.26	7.65	50,50,50,50	0
36	CL	0	9315	1/1	0.90	0.21	7.53	69,69,69,69	0
35	NA	0	9186	1/1	0.83	0.33	7.52	75,75,75,75	0
35	NA	0	9177	1/1	0.94	0.22	6.07	55,55,55,55	0
35	NA	0	9135	1/1	0.95	0.20	6.07	43,43,43,43	0
35	NA	0	9156	1/1	0.94	0.21	5.17	50,50,50,50	0
35	NA	0	9159	1/1	0.94	0.19	5.12	50,50,50,50	0
33	MG	0	8013	1/1	0.95	0.23	3.67	33,33,33,33	0
35	NA	0	9125	1/1	0.95	0.17	3.59	64,64,64,64	0
35	NA	0	9127	1/1	0.96	0.17	3.34	39,39,39,39	0
35	NA	0	9164	1/1	0.95	0.16	2.31	52,52,52,52	0
35	NA	0	9120	1/1	0.98	0.14	1.75	56,56,56,56	0
33	MG	0	8038	1/1	0.98	0.17	1.49	28,28,28,28	0
33	MG	B	8055	1/1	0.97	0.20	1.48	60,60,60,60	0
35	NA	0	9103	1/1	0.98	0.15	1.42	44,44,44,44	0
35	NA	0	9173	1/1	0.94	0.14	1.29	42,42,42,42	0
33	MG	0	8012	1/1	0.98	0.15	1.09	35,35,35,35	0
33	MG	0	8058	1/1	0.97	0.17	0.89	45,45,45,45	0
33	MG	0	8066	1/1	0.97	0.17	0.88	114,114,114,114	0
35	NA	0	9133	1/1	0.97	0.16	0.84	27,27,27,27	0
35	NA	0	9113	1/1	0.88	0.14	0.75	59,59,59,59	0
35	NA	0	9168	1/1	0.97	0.13	0.52	52,52,52,52	0
35	NA	Q	9148	1/1	0.98	0.20	0.34	36,36,36,36	0
35	NA	0	9165	1/1	0.89	0.17	0.03	39,39,39,39	0
35	NA	0	9102	1/1	0.95	0.14	0.00	42,42,42,42	0
33	MG	0	8028	1/1	0.98	0.15	-0.03	43,43,43,43	0
36	CL	0	9313	1/1	0.96	0.15	-0.05	62,62,62,62	0
35	NA	0	9110	1/1	0.97	0.13	-0.14	37,37,37,37	0
36	CL	J	9321	1/1	0.97	0.15	-0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	A	9145	1/1	0.96	0.18	-0.20	39,39,39,39	0
35	NA	H	9109	1/1	0.98	0.13	-0.32	31,31,31,31	0
33	MG	0	8032	1/1	0.97	0.16	-0.33	39,39,39,39	0
35	NA	0	9166	1/1	0.91	0.12	-0.34	77,77,77,77	0
35	NA	0	9169	1/1	0.95	0.15	-0.39	46,46,46,46	0
33	MG	0	8027	1/1	0.96	0.12	-0.48	44,44,44,44	0
33	MG	0	8018	1/1	0.97	0.13	-0.50	40,40,40,40	0
36	CL	B	9319	1/1	0.96	0.14	-0.64	47,47,47,47	0
35	NA	M	9147	1/1	0.98	0.13	-0.67	18,18,18,18	0
35	NA	0	9131	1/1	0.97	0.13	-0.67	35,35,35,35	0
35	NA	0	9117	1/1	0.86	0.21	-0.72	72,72,72,72	0
33	MG	B	8056	1/1	0.98	0.15	-0.83	49,49,49,49	0
35	NA	J	9146	1/1	0.92	0.14	-0.84	37,37,37,37	0
33	MG	0	8064	1/1	0.99	0.12	-0.87	25,25,25,25	0
33	MG	0	8070	1/1	0.97	0.12	-0.89	53,53,53,53	0
33	MG	0	8020	1/1	0.97	0.14	-1.02	32,32,32,32	0
35	NA	0	9138	1/1	0.94	0.12	-1.04	51,51,51,51	0
35	NA	0	9124	1/1	0.86	0.09	-1.12	59,59,59,59	0
33	MG	0	8086	1/1	0.97	0.07	-1.14	50,50,50,50	0
36	CL	M	9318	1/1	0.99	0.13	-1.24	36,36,36,36	0
37	CD	3	9204	1/1	0.91	0.10	-1.26	62,62,62,62	0
37	CD	Z	9203	1/1	0.99	0.08	-1.33	61,61,61,61	0
35	NA	0	9105	1/1	0.93	0.13	-1.37	35,35,35,35	0
33	MG	A	8065	1/1	0.97	0.14	-1.46	42,42,42,42	0
36	CL	O	9308	1/1	0.93	0.11	-1.47	68,68,68,68	0
35	NA	9	9183	1/1	0.93	0.12	-1.48	55,55,55,55	0
33	MG	0	8021	1/1	0.98	0.14	-1.67	25,25,25,25	0
33	MG	0	8017	1/1	0.98	0.10	-1.68	31,31,31,31	0
37	CD	U	9201	1/1	0.99	0.06	-1.82	73,73,73,73	0
33	MG	0	8062	1/1	0.95	0.11	-1.99	53,53,53,53	0
33	MG	0	8019	1/1	0.97	0.10	-2.03	33,33,33,33	0
36	CL	0	9305	1/1	0.98	0.10	-2.18	52,52,52,52	0
33	MG	0	8003	1/1	0.97	0.13	-2.32	26,26,26,26	0
33	MG	0	8057	1/1	0.91	0.13	-2.35	39,39,39,39	0
33	MG	0	8107	1/1	0.88	0.06	-2.37	45,45,45,45	0
33	MG	0	8015	1/1	0.98	0.10	-2.47	30,30,30,30	0
35	NA	R	9137	1/1	0.87	0.08	-2.53	42,42,42,42	0
33	MG	0	8074	1/1	0.98	0.07	-2.55	34,34,34,34	0
33	MG	0	8084	1/1	0.97	0.11	-2.60	40,40,40,40	0
33	MG	0	8096	1/1	0.98	0.09	-2.61	38,38,38,38	0
33	MG	0	8053	1/1	0.90	0.09	-2.73	51,51,51,51	0
35	NA	0	9132	1/1	0.98	0.09	-2.85	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8067	1/1	0.97	0.12	-2.93	52,52,52,52	0
35	NA	0	9123	1/1	0.98	0.13	-2.94	52,52,52,52	0
33	MG	0	8014	1/1	0.93	0.10	-3.07	42,42,42,42	0
36	CL	0	9316	1/1	0.96	0.09	-3.10	56,56,56,56	0
33	MG	0	8039	1/1	0.97	0.08	-3.12	49,49,49,49	0
36	CL	3	9304	1/1	0.94	0.06	-3.22	47,47,47,47	0
33	MG	0	8035	1/1	0.97	0.08	-3.38	50,50,50,50	0
36	CL	0	9312	1/1	0.99	0.07	-3.40	52,52,52,52	0
33	MG	3	8078	1/1	0.89	0.07	-3.49	46,46,46,46	0
33	MG	0	8108	1/1	0.97	0.09	-3.52	56,56,56,56	0
37	CD	1	9202	1/1	0.99	0.02	-3.56	54,54,54,54	0
33	MG	T	8073	1/1	0.99	0.05	-3.67	49,49,49,49	0
35	NA	0	9144	1/1	0.98	0.06	-3.82	35,35,35,35	0
33	MG	0	8100	1/1	0.96	0.10	-3.91	68,68,68,68	0
33	MG	Y	8109	1/1	0.97	0.08	-3.98	40,40,40,40	0
33	MG	4	8119	1/1	0.97	0.08	-4.04	41,41,41,41	0
33	MG	0	8077	1/1	0.98	0.10	-4.52	29,29,29,29	0
33	MG	0	8001	1/1	0.94	0.07	-4.77	36,36,36,36	0
33	MG	0	8054	1/1	0.97	0.11	-4.81	24,24,24,24	0
35	NA	0	9139	1/1	0.98	0.09	-4.90	22,22,22,22	0
35	NA	T	9143	1/1	0.99	0.06	-5.26	31,31,31,31	0
33	MG	0	8112	1/1	0.96	0.05	-5.28	37,37,37,37	0
33	MG	0	8007	1/1	0.97	0.09	-5.32	23,23,23,23	0
33	MG	0	8033	1/1	0.98	0.08	-5.33	39,39,39,39	0
33	MG	0	8044	1/1	0.97	0.06	-5.55	47,47,47,47	0
33	MG	0	8080	1/1	0.94	0.06	-5.97	37,37,37,37	0
34	K	0	9002	1/1	0.96	0.07	-6.41	43,43,43,43	0
33	MG	0	8008	1/1	0.95	0.08	-6.53	35,35,35,35	0
33	MG	9	8052	1/1	0.96	0.07	-6.76	50,50,50,50	0
33	MG	0	8004	1/1	0.99	0.08	-7.08	33,33,33,33	0
35	NA	0	9153	1/1	0.98	0.05	-7.20	17,17,17,17	0
34	K	0	9001	1/1	0.92	0.09	-8.61	66,66,66,66	0
33	MG	0	8091	1/1	0.97	0.07	-8.89	74,74,74,74	0
33	MG	0	8002	1/1	0.97	0.03	-9.16	28,28,28,28	0
33	MG	0	8110	1/1	0.98	0.06	-10.51	34,34,34,34	0
33	MG	0	8010	1/1	0.98	0.07	-13.49	30,30,30,30	0
33	MG	0	8006	1/1	0.96	0.09	-19.56	32,32,32,32	0
33	MG	0	8009	1/1	0.99	0.10	-	31,31,31,31	0
35	NA	0	9167	1/1	0.93	0.09	-	40,40,40,40	0
36	CL	N	9307	1/1	0.96	0.16	-	61,61,61,61	0
36	CL	J	9302	1/1	0.91	0.13	-	70,70,70,70	0
33	MG	0	8045	1/1	0.80	0.23	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	9184	1/1	0.82	0.10	-	75,75,75,75	0
33	MG	0	8034	1/1	0.98	0.12	-	39,39,39,39	0
35	NA	0	9142	1/1	0.89	0.21	-	52,52,52,52	0
35	NA	0	9134	1/1	0.97	0.14	-	34,34,34,34	0
35	NA	0	9141	1/1	0.85	0.12	-	46,46,46,46	0
35	NA	C	9104	1/1	0.96	0.09	-	32,32,32,32	0
33	MG	0	8083	1/1	0.99	0.08	-	35,35,35,35	0
33	MG	0	8005	1/1	0.99	0.09	-	24,24,24,24	0
35	NA	0	9130	1/1	0.97	0.09	-	36,36,36,36	0
33	MG	0	8031	1/1	0.99	0.08	-	30,30,30,30	0
33	MG	0	8115	1/1	0.94	0.14	-	52,52,52,52	0
35	NA	S	9112	1/1	0.77	0.49	-	76,76,76,76	0
35	NA	0	9163	1/1	0.83	0.34	-	71,71,71,71	0
35	NA	0	9108	1/1	0.94	0.12	-	48,48,48,48	0
35	NA	0	9181	1/1	0.94	0.14	-	51,51,51,51	0
33	MG	0	8046	1/1	0.95	0.04	-	52,52,52,52	0
33	MG	0	8026	1/1	0.98	0.12	-	24,24,24,24	0
36	CL	A	9309	1/1	0.98	0.21	-	58,58,58,58	0
35	NA	0	9128	1/1	0.98	0.07	-	40,40,40,40	0
33	MG	0	8022	1/1	0.97	0.06	-	35,35,35,35	0
33	MG	0	8117	1/1	0.98	0.08	-	32,32,32,32	0
36	CL	J	9301	1/1	0.93	0.12	-	72,72,72,72	0
36	CL	0	9314	1/1	0.93	0.09	-	50,50,50,50	0
33	MG	0	8081	1/1	0.99	0.14	-	43,43,43,43	0
33	MG	0	8030	1/1	0.87	0.11	-	35,35,35,35	0
33	MG	0	8076	1/1	0.90	0.11	-	57,57,57,57	0
33	MG	0	8088	1/1	0.96	0.06	-	39,39,39,39	0
33	MG	0	8025	1/1	0.99	0.13	-	48,48,48,48	0
33	MG	0	8063	1/1	0.95	0.09	-	53,53,53,53	0
33	MG	0	8040	1/1	0.94	0.09	-	45,45,45,45	0
33	MG	0	8072	1/1	0.93	0.20	-	51,51,51,51	0
33	MG	0	8029	1/1	0.99	0.19	-	32,32,32,32	0
33	MG	0	8036	1/1	0.97	0.14	-	39,39,39,39	0
33	MG	0	8023	1/1	0.96	0.20	-	53,53,53,53	0
35	NA	0	9101	1/1	0.97	0.22	-	46,46,46,46	0
33	MG	0	8104	1/1	0.86	0.17	-	53,53,53,53	0
33	MG	0	8024	1/1	0.97	0.15	-	49,49,49,49	0
35	NA	0	9152	1/1	0.97	0.30	-	60,60,60,60	0
35	NA	0	9119	1/1	0.91	0.13	-	42,42,42,42	0
33	MG	0	8075	1/1	0.94	0.05	-	39,39,39,39	0
35	NA	0	9157	1/1	0.95	0.07	-	60,60,60,60	0
35	NA	9	9151	1/1	0.50	0.14	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8085	1/1	0.79	0.24	-	93,93,93,93	0
35	NA	0	9175	1/1	0.94	0.23	-	42,42,42,42	0
35	NA	0	9107	1/1	0.91	0.13	-	43,43,43,43	0
33	MG	0	8093	1/1	0.96	0.13	-	56,56,56,56	0
35	NA	0	9136	1/1	0.96	0.08	-	53,53,53,53	0
33	MG	0	8102	1/1	0.97	0.09	-	51,51,51,51	0
35	NA	0	9115	1/1	0.95	0.14	-	37,37,37,37	0
36	CL	0	9322	1/1	0.90	0.31	-	76,76,76,76	0
33	MG	0	8094	1/1	0.96	0.16	-	62,62,62,62	0
33	MG	0	8043	1/1	0.90	0.09	-	42,42,42,42	0
35	NA	0	9185	1/1	0.86	0.36	-	60,60,60,60	0
33	MG	0	8101	1/1	0.91	0.17	-	69,69,69,69	0
35	NA	0	9155	1/1	0.92	0.26	-	60,60,60,60	0
35	NA	H	9122	1/1	0.81	0.26	-	77,77,77,77	0
33	MG	0	8087	1/1	0.97	0.21	-	57,57,57,57	0
36	CL	0	9320	1/1	0.98	0.11	-	48,48,48,48	0
35	NA	0	9114	1/1	0.94	0.17	-	66,66,66,66	0
36	CL	0	9311	1/1	0.98	0.14	-	51,51,51,51	0
35	NA	0	9160	1/1	0.96	0.24	-	41,41,41,41	0
36	CL	L	9310	1/1	0.94	0.09	-	58,58,58,58	0
33	MG	0	8106	1/1	0.95	0.09	-	51,51,51,51	0
36	CL	0	9303	1/1	0.96	0.15	-	54,54,54,54	0
36	CL	0	9317	1/1	0.99	0.05	-	61,61,61,61	0
35	NA	0	9116	1/1	0.84	0.13	-	36,36,36,36	0
33	MG	0	8048	1/1	0.91	0.13	-	60,60,60,60	0
33	MG	0	8041	1/1	0.96	0.23	-	59,59,59,59	0
35	NA	0	9170	1/1	0.95	0.41	-	61,61,61,61	0
33	MG	9	8095	1/1	0.62	0.11	-	72,72,72,72	0
33	MG	0	8068	1/1	0.98	0.07	-	58,58,58,58	0
33	MG	0	8116	1/1	0.93	0.07	-	50,50,50,50	0
33	MG	0	8071	1/1	0.87	0.08	-	53,53,53,53	0
33	MG	0	8089	1/1	0.98	0.07	-	60,60,60,60	0
33	MG	0	8082	1/1	0.84	0.14	-	66,66,66,66	0
35	NA	0	9126	1/1	0.89	0.14	-	40,40,40,40	0
33	MG	0	8050	1/1	0.90	0.07	-	63,63,63,63	0
35	NA	0	9106	1/1	0.96	0.17	-	34,34,34,34	0
33	MG	0	8099	1/1	0.98	0.14	-	59,59,59,59	0
33	MG	0	8098	1/1	0.97	0.11	-	45,45,45,45	0
35	NA	B	9158	1/1	0.91	1.05	-	69,69,69,69	0
33	MG	0	8061	1/1	0.98	0.09	-	34,34,34,34	0
36	CL	R	9306	1/1	0.98	0.12	-	53,53,53,53	0
33	MG	0	8079	1/1	0.98	0.12	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8016	1/1	0.98	0.19	-	35,35,35,35	0
33	MG	0	8111	1/1	0.96	0.08	-	57,57,57,57	0
33	MG	0	8118	1/1	0.93	0.10	-	63,63,63,63	0
33	MG	0	8092	1/1	0.76	0.48	-	95,95,95,95	0
33	MG	0	8114	1/1	0.81	0.12	-	64,64,64,64	0
33	MG	0	8090	1/1	0.84	0.39	-	80,80,80,80	0
34	K	0	9003	1/1	0.61	0.32	-	82,82,82,82	0
33	MG	0	8037	1/1	0.96	0.10	-	46,46,46,46	0
35	NA	0	9129	1/1	0.90	0.14	-	53,53,53,53	0
33	MG	0	8103	1/1	0.96	0.19	-	66,66,66,66	0
33	MG	0	8113	1/1	0.93	0.10	-	45,45,45,45	0
33	MG	0	8042	1/1	0.93	0.07	-	45,45,45,45	0
35	NA	0	9149	1/1	0.96	0.09	-	36,36,36,36	0
33	MG	0	8011	1/1	0.99	0.11	-	23,23,23,23	0
33	MG	K	8069	1/1	0.98	0.11	-	41,41,41,41	0
37	CD	O	9205	1/1	0.90	0.07	-	137,137,137,137	0
33	MG	0	8049	1/1	0.84	0.39	-	90,90,90,90	0
33	MG	0	8047	1/1	0.85	0.19	-	102,102,102,102	0
33	MG	0	8051	1/1	0.91	0.12	-	56,56,56,56	0
35	NA	0	9118	1/1	0.97	0.12	-	54,54,54,54	0
33	MG	0	8059	1/1	0.92	0.09	-	51,51,51,51	0
35	NA	0	9154	1/1	0.98	0.09	-	26,26,26,26	0
35	NA	0	9111	1/1	0.93	0.24	-	65,65,65,65	0
33	MG	0	8097	1/1	0.98	0.10	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.