Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:02 PM GMT

PDB ID	:	1VQ5
Title	:	The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.60 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:

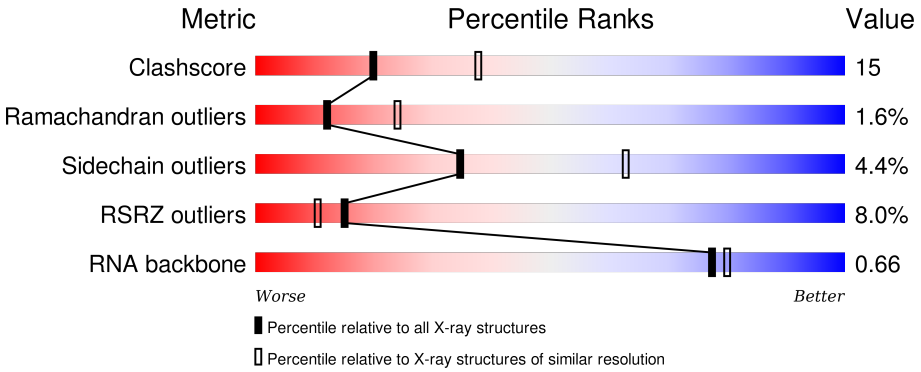
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

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% 61% 28% 5% 6%
2	9	122	3% 58% 32% 10%
3	4	8	38% 63%
4	A	240	7% 60% 34%
5	B	338	10% 50% 45% 5%

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Mol	Chain	Length	Quality of chain
6	C	246	2% 59% 35% 6%
7	D	177	37% 32% 40% 6% 21%
8	E	178	34% 50% 44%
9	F	120	17% 53% 43%
10	G	348	5% 5% 92%
11	H	171	11% 58% 32% 6%
12	J	145	3% 62% 32%
13	K	132	8% 66% 32%
14	L	165	12% 55% 30% 12%
15	M	194	% 70% 28%
16	N	187	15% 50% 44% 6%
17	O	116	2% 71% 27%
18	P	149	3% 64% 30%
19	Q	96	2% 72% 26%
20	R	155	% 63% 32%
21	S	85	6% 66% 28% 5%
22	T	120	7% 58% 38%
23	U	66	9% 47% 33% 20%
24	V	71	27% 45% 44% 8%
25	W	154	% 53% 42% 5%
26	X	92	12% 48% 35% 7% 11%
27	Y	241	4% 40% 16% 41%
28	Z	83	5% 52% 33% 12%
29	1	57	67% 32%
30	2	50	32% 48% 44% 8%

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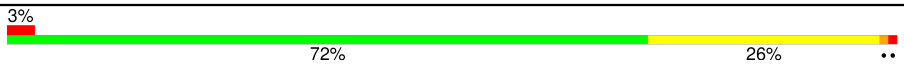
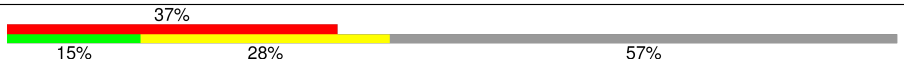
Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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	8060	-	-	-	X
33	MG	Y	8109	-	-	-	X
35	NA	0	9102	-	-	-	X
35	NA	0	9103	-	-	-	X
35	NA	0	9105	-	-	-	X
35	NA	0	9110	-	-	-	X
35	NA	0	9120	-	-	-	X
35	NA	0	9121	-	-	-	X
35	NA	0	9123	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9131	-	-	-	X
35	NA	0	9135	-	-	-	X
35	NA	0	9150	-	-	-	X
35	NA	0	9156	-	-	-	X
35	NA	0	9159	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9164	-	-	-	X
35	NA	0	9165	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9173	-	-	-	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	L	9180	-	-	-	X
35	NA	R	9186	-	-	-	X
36	CL	0	9315	-	-	-	X
36	CL	0	9316	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99060 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'-D(*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	126	61	23	37	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	106	Total	Mg	0	0
			106	106		
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	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	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 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	71	Total Na 71 71	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	R	3	Total Na 3 3	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	10	Total Cl 10 10	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	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	5820	Total O 5820 5820	0	0
38	9	133	Total O 133 133	0	0
38	4	8	Total O 8 8	0	0
38	A	117	Total O 117 117	0	0
38	B	150	Total O 150 150	0	0
38	C	165	Total O 165 165	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	49	Total O 49 49	0	0
38	E	47	Total O 47 47	0	0
38	F	21	Total O 21 21	0	0
38	G	16	Total O 16 16	0	0
38	H	66	Total O 66 66	0	0
38	J	52	Total O 52 52	0	0
38	K	54	Total O 54 54	0	0
38	L	83	Total O 83 83	0	0
38	M	118	Total O 118 118	0	0
38	N	66	Total O 66 66	0	0
38	O	39	Total O 39 39	0	0
38	P	65	Total O 65 65	0	0
38	Q	52	Total O 52 52	0	0
38	R	85	Total O 85 85	0	0
38	S	31	Total O 31 31	0	0
38	T	39	Total O 39 39	0	0
38	U	25	Total O 25 25	0	0
38	V	13	Total O 13 13	0	0
38	W	68	Total O 68 68	0	0
38	X	27	Total O 27 27	0	0
38	Y	92	Total O 92 92	0	0

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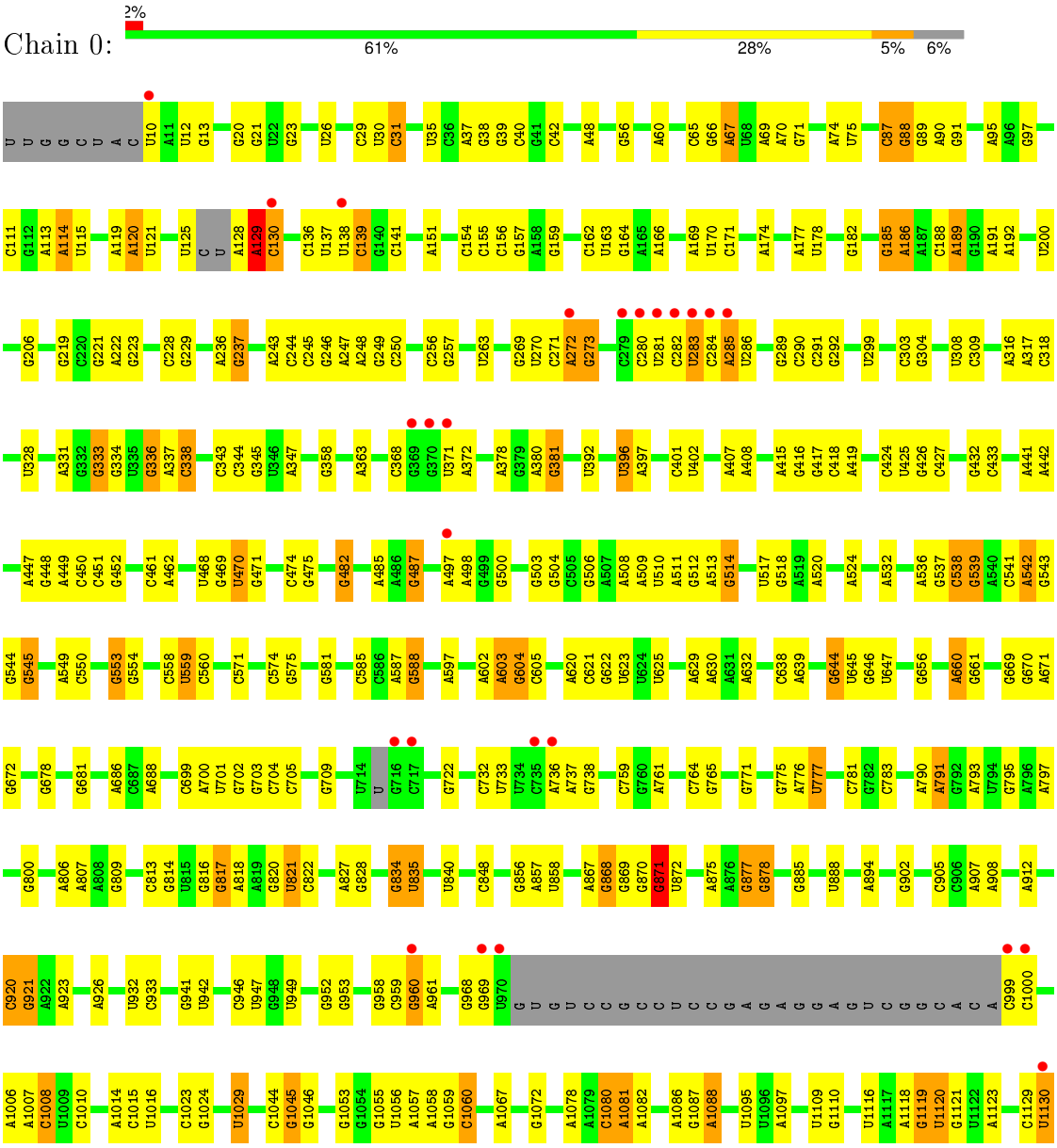
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Z	30	Total O 30 30	0	0
38	1	59	Total O 59 59	0	0
38	2	42	Total O 42 42	0	0
38	3	74	Total O 74 74	0	0
38	I	10	Total O 10 10	0	0

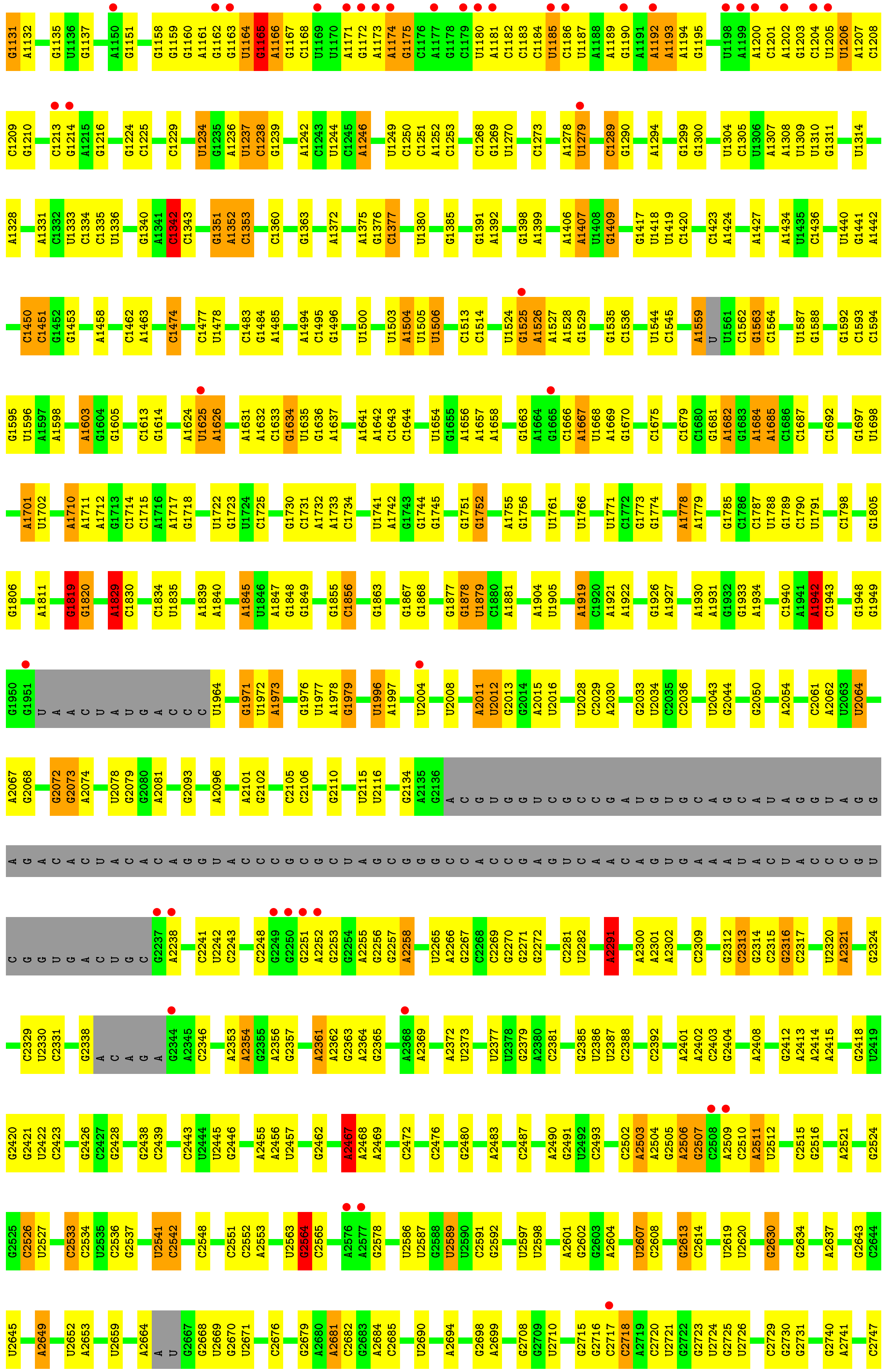
3 Residue-property plots (i)

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:




G1131 A1132 G1135 U1136 G1137 A1150 G1151 G1158 G1159 G1160 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 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208
C1209 G1210 C1213 G1214 A1215 G1216 G1224 C1225 C1229 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 C1268 G1269 U1270 C1273 A1278 U1279 C1289 G1290 A1294 G1299 G1300 U1304 C1305 U1306 A1307 A1308 U1309 U1310 G1311 U1314
A1328 A1331 C1332 U1333 C1334 C1335 U1336 G1340 A1341 C1342 C1343 G1351 A1352 C1353 C1360 G1363 A1372 A1375 G1376 C1377 U1380 G1385 G1391 A1392 G1398 A1399 A1406 A1407 U1408 G1409 G1417 U1418 U1419 C1420 C1423 A1424 A1427 A1434 U1435 C1436 U1440 G1441 A1442
C1450 C1451 G1452 G1453 A1458 C1462 A1463 C1474 C1477 U1478 C1483 G1484 A1485 A1494 C1495 G1496 U1500 U1503 A1504 U1505 U1506 C1513 C1514 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 U1544 C1545 A1559 U U1561 C1562 G1563 C1564 U1587 G1588 G1592 C1593 C1594
G1595 U1596 A1597 A1598 A1603 G1604 G1605 C1613 G1614 A1624 U1625 A1626 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 C1644 U1654 G1655 A1656 A1657 A1658 G1663 A1664 G1665 C1666 A1667 U1668 A1669 G1670 C1675 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 G1697 U1698
A1701 U1702 A1710 A1711 A1712 G1713 C1714 C1715 A1716 A1717 G1718 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 U1741 A1742 G1743 G1744 G1745 G1751 G1752 A1755 G1756 U1761 U1766 U1771 C1772 G1773 G1774 A1778 A1779 G1785 C1786 C1787 U1788 G1789 C1790 U1791 C1798 G1805
G1806 A1811 G1819 G1820 A1829 C1830 C1834 U1835 A1839 A1840 A1845 U1846 A1847 G1848 G1849 G1855 C1856 G1863 G1867 G1868 G1877 G1878 U1879 C1880 A1881 A1904 U1905 A1919 C1920 A1921 A1922 G1926 A1927 A1930 A1931 G1932 G1933 A1934 C1940 A1941 A1942 C1943 G1948 G1949
G1950 G1951 U A A C U A U G A C C C U1964 G1971 U1972 A1973 G1976 U1977 A1978 G1979 U1996 A1997 U2004 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2028 C2029 A2030 G2033 U2034 G2035 C2036 U2043 G2044 G2050 A2054 C2061 A2062 U2063 U2064
A2067 G2068 G2072 G2073 A2074 U2078 G2079 G2080 A2081 G2093 A2096 A2101 G2102 C2105 C2106 G2110 U2115 U2116 G2134 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 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 C2241 U2242 C2243 C2248 G2249 G2250 G2251 A2252 C2253 G2254 A2255 C2256 G2257 A2258 U2265 A2266 C2267 C2268 C2269 G2270 G2271 C2272 C2281 U2282 A2291 A2300 A2301 A2302 C2309 G2312 C2313 C2314 C2315 G2316 C2317 U2320 A2321 G2324
C2329 U2330 C2331 G2338 A C A G A G2344 A2345 C2346 A2353 A2354 G2355 A2356 G2357 A2361 A2362 G2363 A2364 C2365 A2368 A2369 A2372 U2373 U2377 U2378 G2379 A2380 C2381 G2385 U2386 U2387 C2388 C2392 A2401 A2402 C2403 G2404 A2408 G2412 A2413 A2414 A2415 G2418 U2419
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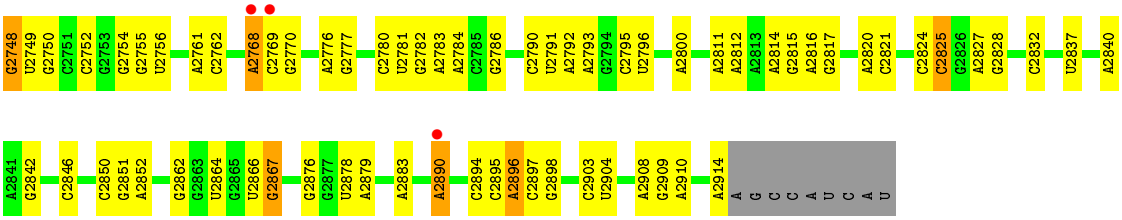
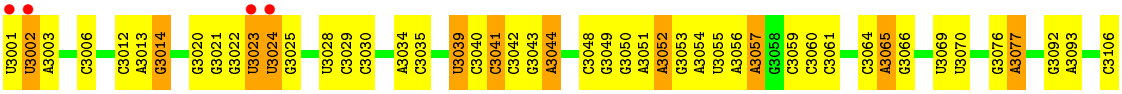
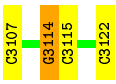
G2525 C2526 U2527 C2533 G2534 U2535 C2536 G2537 U2541 C2542 C2548 C2551 C2552 A2553 U2563 G2564 C2565 A2576 A2577 G2578 U2586 U2587 G2588 U2589 U2590 C2591 G2592 U2597 U2598 A2601 G2602 G2603 A2604 U2607 C2608 G2613 C2614 U2619 U2620 G2630 G2634 A2637 G2643 C2644
U2645 A2649 U2652 A2653 U2659 A2664 A U G2667 G2668 U2669 G2670 U2671 C2676 G2679 A2680 A2681 C2682 G2683 A2684 C2685 U2690 A2694 G2698 A2699 G2708 G2709 U2710 G2715 G2716 C2717 C2718 A2719 C2720 U2721 G2722 G2723 U2724 C2725 U2726 C2729 G2730 G2731 G2740 A2741 C2747



• Molecule 2: 5S ribosomal RNA

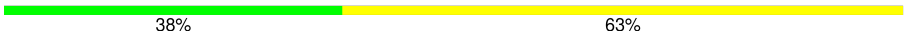
Chain 9:

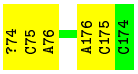




• Molecule 3: 5'-D(*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3')

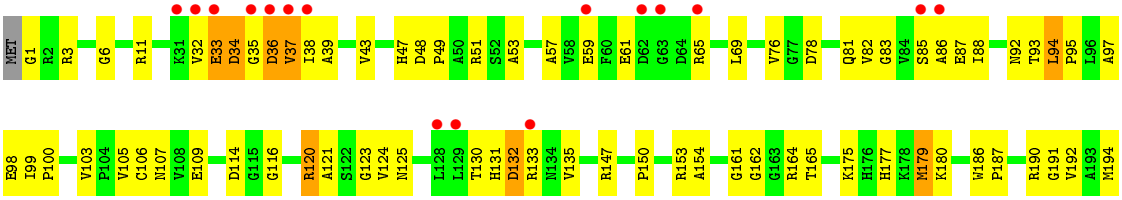
Chain 4:

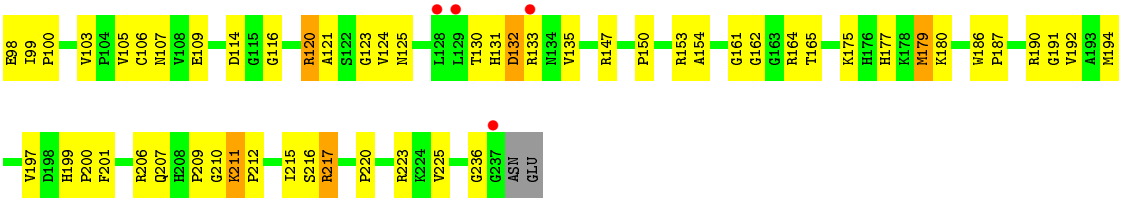




• Molecule 4: 50S ribosomal protein L2P

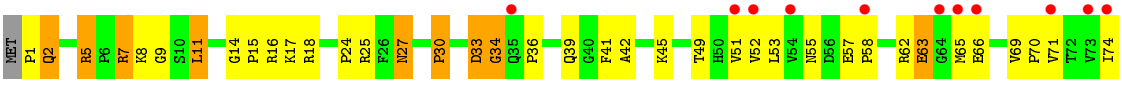
Chain A:

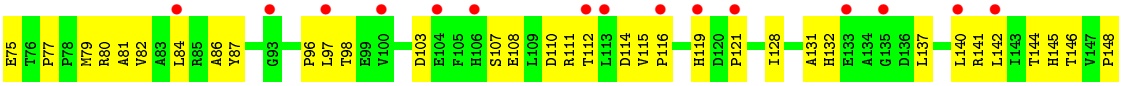


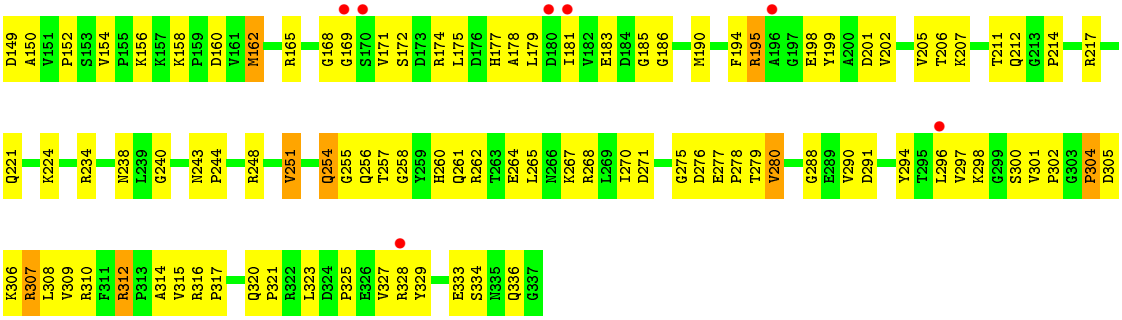


• Molecule 5: 50S ribosomal protein L3P

Chain B:

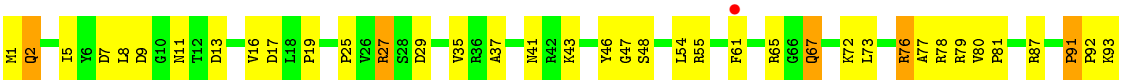


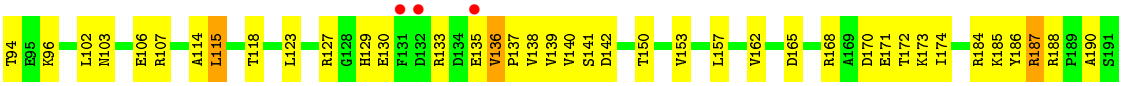




• Molecule 6: 50S ribosomal protein L4E

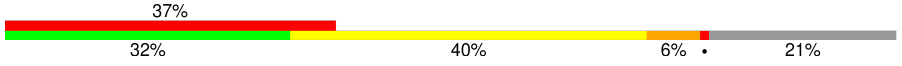
Chain C:

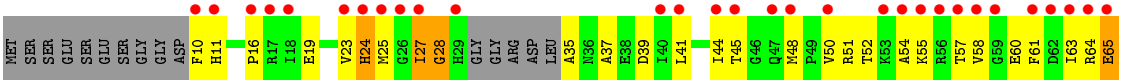


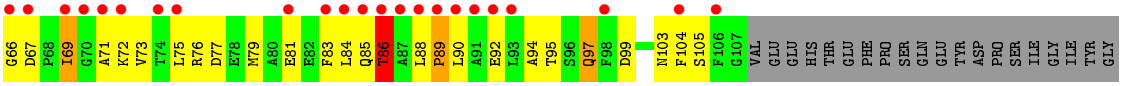


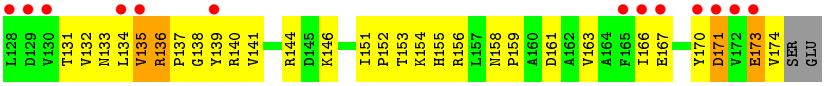
• Molecule 7: 50S ribosomal protein L5P

Chain D:



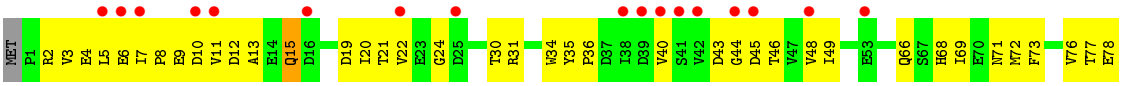


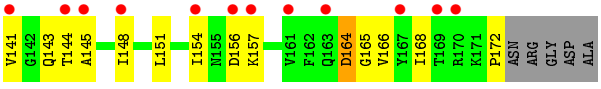




• Molecule 8: 50S ribosomal protein L6P

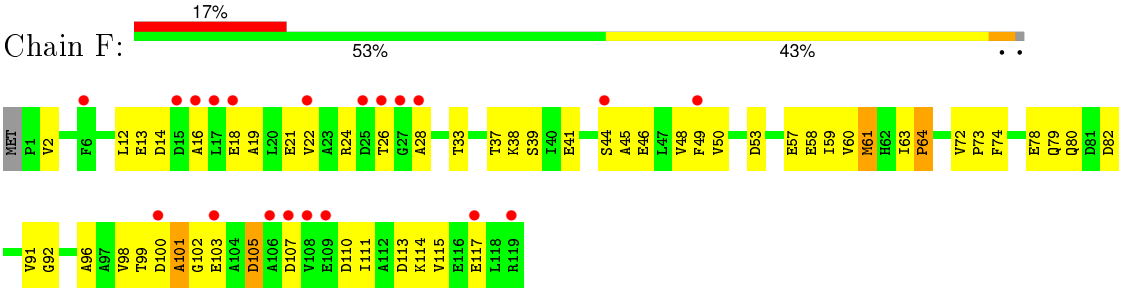
Chain E:





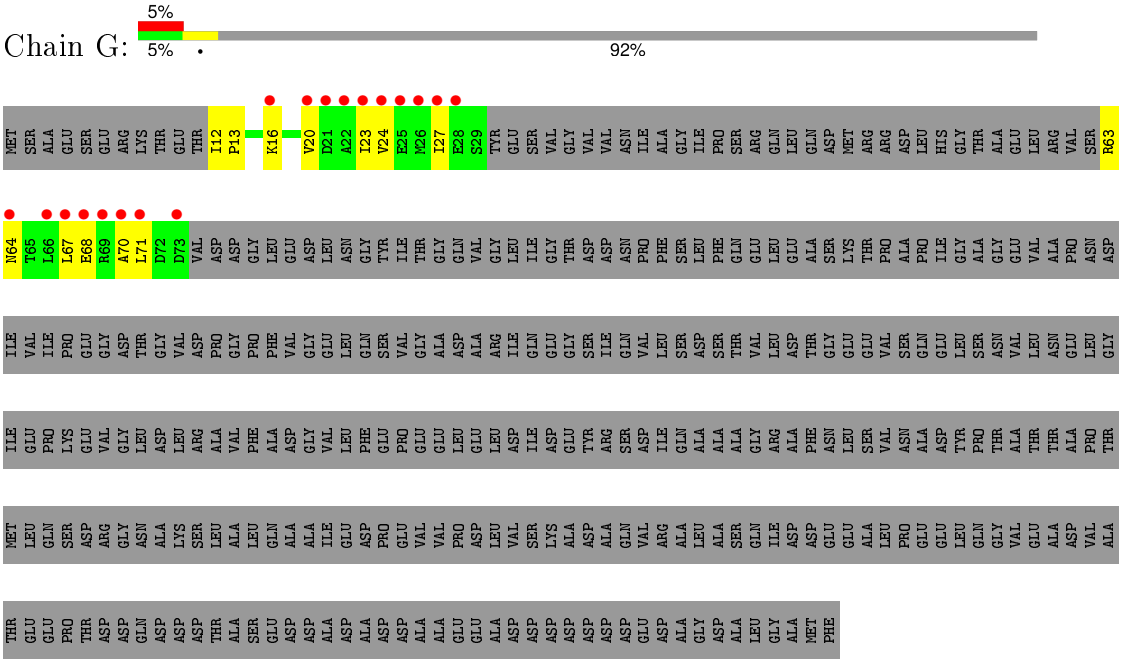
• Molecule 9: 50S ribosomal protein L7AE

Chain F:



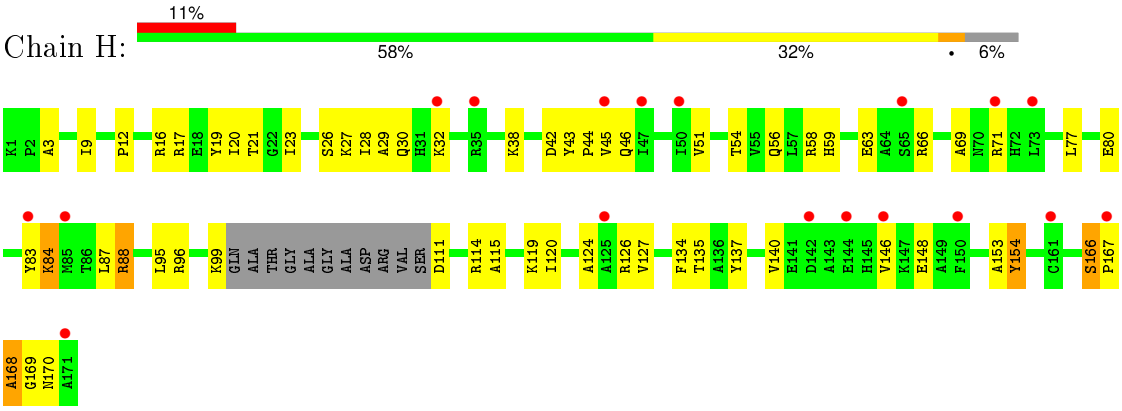
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



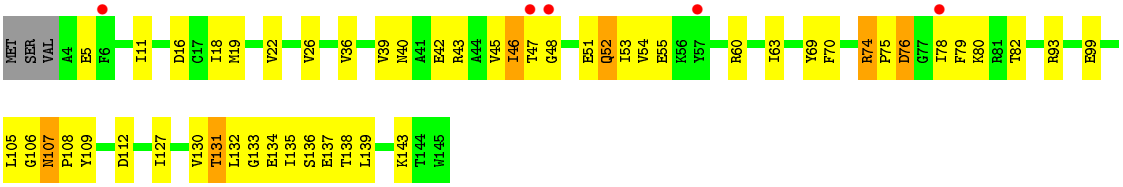
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



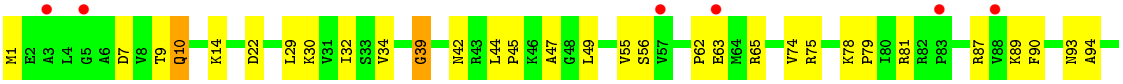
• Molecule 12: 50S ribosomal protein L13P

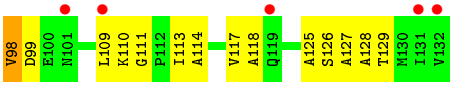
Chain J:



• Molecule 13: 50S ribosomal protein L14P

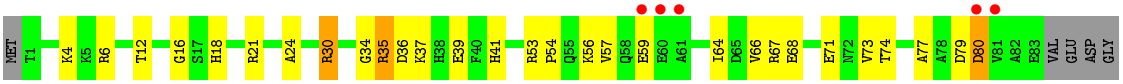
Chain K:





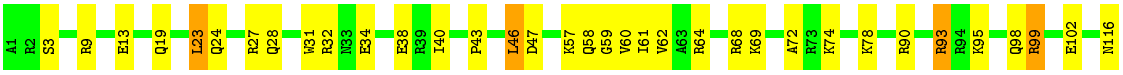
• Molecule 14: 50S ribosomal protein L15P

Chain L:



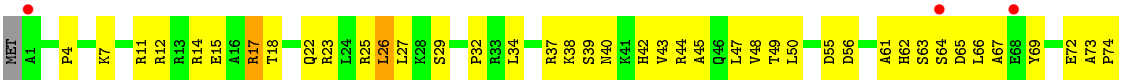
• Molecule 15: 50S Ribosomal Protein L15E

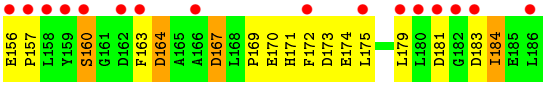
Chain M:



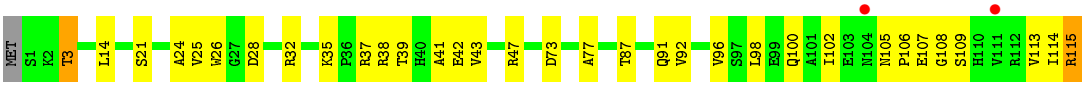
• Molecule 16: 50S ribosomal protein L18P

Chain N:

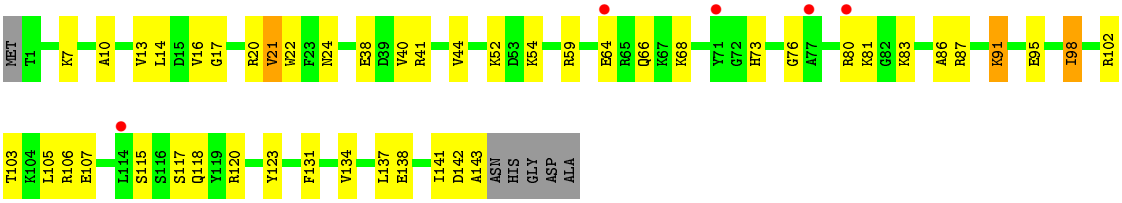




• Molecule 17: 50S ribosomal protein L18e

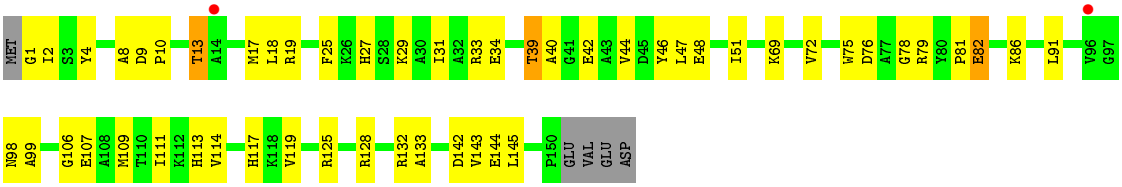


• Molecule 18: 50S ribosomal protein L19E

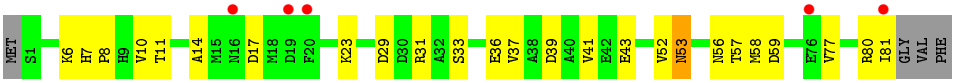


• Molecule 19: 50S ribosomal protein L21e

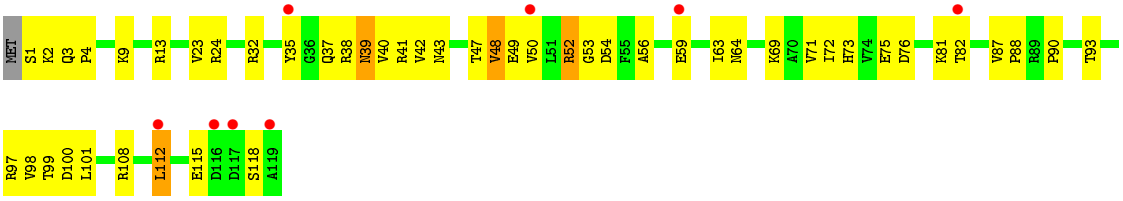
• Molecule 20: 50S ribosomal protein L22P



• Molecule 21: 50S ribosomal protein L23P

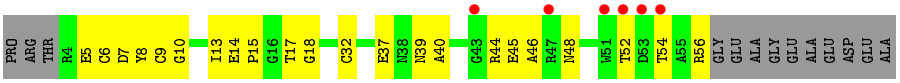


• Molecule 22: 50S ribosomal protein L24P



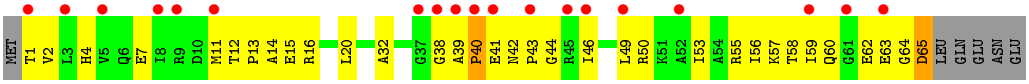
• Molecule 23: 50S ribosomal protein L24E

Chain U:



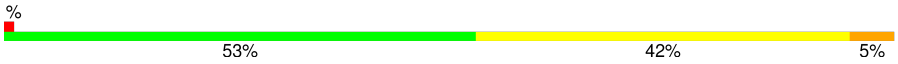
• Molecule 24: 50S ribosomal protein L29P

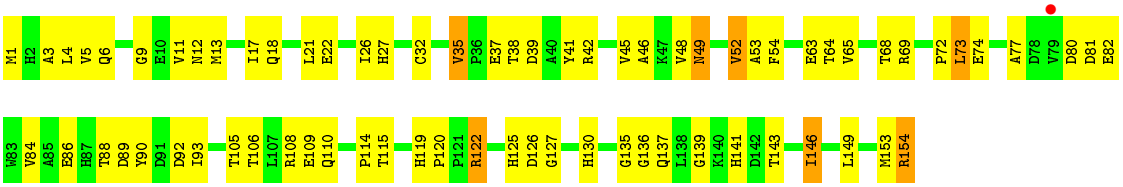
Chain V:



• Molecule 25: 50S ribosomal protein L30P

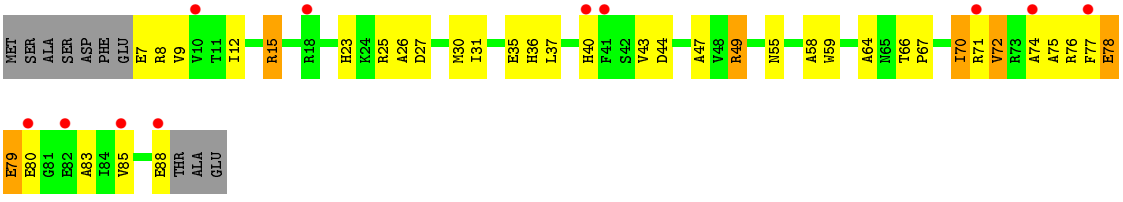
Chain W:





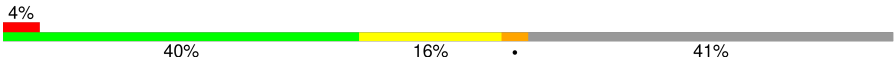
• Molecule 26: 50S ribosomal protein L31e

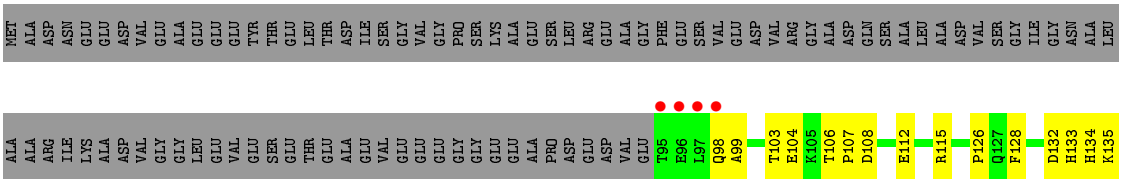
Chain X:

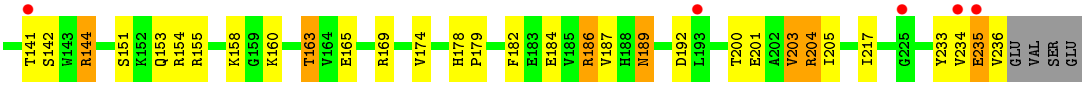


• Molecule 27: 50S ribosomal protein L32E

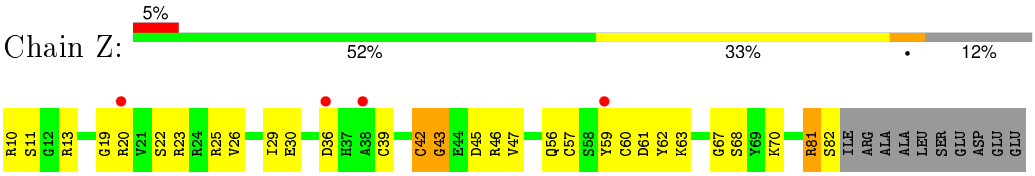
Chain Y:



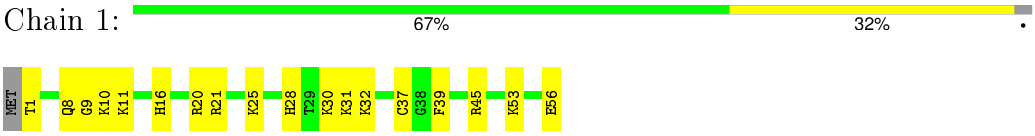




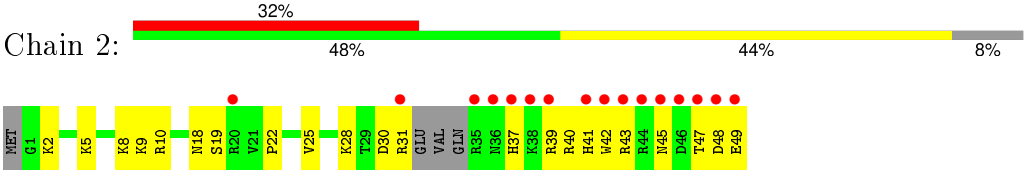
- Molecule 28: 50S ribosomal protein L37Ae



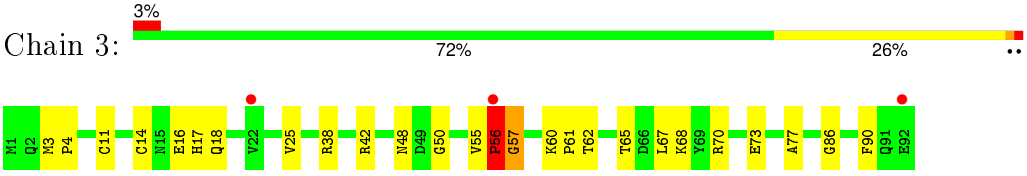
- Molecule 29: 50S ribosomal protein L37e



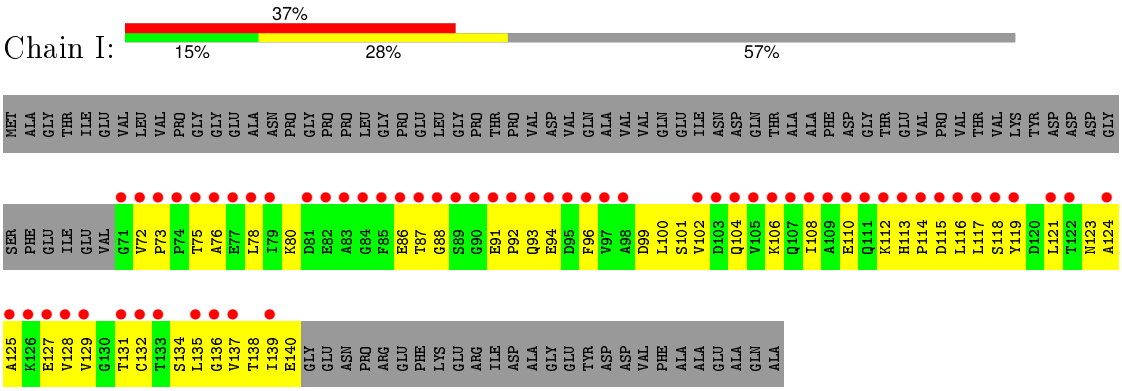
- Molecule 30: 50S ribosomal protein L39e



- 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	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 90.1 (49.67-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.237 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 602690 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, PO2, CD, 5AA, DCZ, 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	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.53	0/83	0.82	0/119
4	A	0.33	0/1786	0.64	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.29	0/241	0.45	0/324
11	H	0.34	0/1287	0.63	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.35	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.62	0/1999
17	O	0.34	0/874	0.59	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.37	0/749	0.68	0/1005
20	R	0.35	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	0/875
22	T	0.32	0/958	0.65	1/1289 (0.1%)
23	U	0.34	0/417	0.56	0/562
24	V	0.28	0/502	0.51	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.37	0/589	0.65	0/787
29	1	0.41	0/438	0.64	0/578
30	2	0.32	0/401	0.55	0/529
31	3	0.38	0/771	0.59	0/1024
32	I	0.29	0/526	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.37	0/98775	0.67	22/147696 (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	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.50	130.40	109.50
1	0	1942	A	C5'-C4'-C3'	7.87	128.58	116.00
2	9	3039	U	N1-C1'-C2'	6.80	122.84	114.00
1	0	871	G	C5'-C4'-O4'	-6.76	100.98	109.10
1	0	1819	G	C5'-C4'-C3'	6.21	125.94	116.00
1	0	2467	A	C1'-O4'-C4'	-5.92	105.17	109.90
1	0	2316	G	C5'-C4'-C3'	-5.90	106.56	116.00
1	0	1504	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	1120	U	C5'-C4'-C3'	-5.77	106.77	116.00
1	0	1504	A	N9-C1'-C2'	5.76	121.49	114.00
1	0	2291	A	N9-C1'-C2'	5.72	121.43	114.00
1	0	1829	A	N9-C1'-C2'	-5.59	105.85	112.00
1	0	2313	C	C5'-C4'-O4'	5.55	115.76	109.10
1	0	1942	A	C5'-C4'-O4'	5.42	115.60	109.10
1	0	206	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	0	129	A	C2'-C3'-O3'	5.34	122.25	113.70
1	0	1165	G	C1'-O4'-C4'	-5.17	105.76	109.90
22	T	52	ARG	N-CA-C	5.15	124.91	111.00
1	0	1942	A	C4'-C3'-C2'	-5.14	97.46	102.60
1	0	2607	U	N1-C1'-C2'	5.13	120.67	114.00
1	0	2313	C	C5'-C4'-C3'	5.07	124.11	116.00
1	0	1971	G	N9-C1'-C2'	5.01	120.51	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain
1	0	1718	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1839	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	189	A	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2551	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	781	C	Sidechain
1	0	791	A	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
25	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	777	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	158	1
6	C	1859	0	1816	111	0
7	D	1094	0	1085	93	0
8	E	1357	0	1266	78	0
9	F	890	0	843	51	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	51	1
14	L	1118	0	1076	53	0
15	M	1560	0	1568	62	0
16	N	1445	0	1401	109	0
17	O	865	0	873	29	0
18	P	1136	0	1123	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Q	735	0	729	23	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	50	0
23	U	410	0	364	21	0
24	V	499	0	511	34	0
25	W	1196	0	1137	95	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	53	0
28	Z	578	0	539	24	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	58	0
33	0	106	0	0	0	0
33	2	1	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	2	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	71	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	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
36	Y	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	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	3	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	9	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0
38	F	21	0	0	3	0
38	G	16	0	0	0	0
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	4	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0
38	X	27	0	0	2	0
38	Y	92	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Z	30	0	0	2	0
All	All	99060	0	59975	2235	3

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 (2235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:0:156:C:H5"	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.35	1.07
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.31	1.07
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.37	1.06
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.36	1.06
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.33	1.05
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.75	1.02
2:9:3076:G:H3'	2:9:3077:A:H5"	1.39	1.02
6:C:236:THR:HG22	6:C:239:ALA:H	1.24	1.01
1:0:1242:A:H5'	12:J:82:THR:HG23	1.41	1.01
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.43	0.99
1:0:2717:C:H2'	1:0:2718:C:H5"	1.42	0.99
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.77	0.98
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.29	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	0.98	0.97
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.32	0.95
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.49	0.94
1:0:2717:C:C2'	1:0:2718:C:H5"	1.98	0.93
1:0:870:G:H2'	1:0:871:G:H5"	1.48	0.93
1:0:871:G:C8	1:0:871:G:H5'	2.02	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
13:K:10:GLN:H	13:K:10:GLN:NE2	1.66	0.92
1:0:541:C:H2'	1:0:542:A:H5"	1.52	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.34	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.91
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.34	0.91
13:K:10:GLN:H	13:K:10:GLN:HE21	0.94	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.17	0.89
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:H5'	1.36	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	0.93	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.87	0.88
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.56	0.88
2:9:3056:A:H2'	2:9:3057:A:H5"	1.54	0.88
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.53	0.88
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.74	0.88
1:0:1835:U:H5	1:0:1840:A:N7	1.72	0.88
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.54	0.87
1:0:1751:G:H2'	1:0:1752:G:H5"	1.54	0.87
1:0:2364:A:H5"	19:Q:15:LYS:HD3	1.56	0.87
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.37	0.87
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
1:0:1160:G:C5'	1:0:1161:A:H5'	2.04	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.86
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.57	0.86
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.57	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
5:B:307:ARG:HB2	5:B:307:ARG:HH11	1.39	0.85
25:W:13:MET:HE2	25:W:18:GLN:HA	1.57	0.85
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.57	0.85
4:A:35:GLY:O	4:A:36:ASP:HB3	1.76	0.85
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.57	0.85
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.06	0.85
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.59	0.85
1:0:542:A:H5'	1:0:542:A:H8	1.41	0.85
1:0:545:G:H8	1:0:545:G:H5'	1.42	0.84
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.41	0.84
18:P:115:SER:N	18:P:118:GLN:HE21	1.75	0.84
16:N:144:GLY:O	16:N:147:ILE:HG22	1.77	0.84
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.56	0.84
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.84
15:M:166:ALA:HA	15:M:169:ARG:NH1	1.93	0.84
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.58	0.84
7:D:57:THR:HG23	7:D:63:ILE:HA	1.60	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.43	0.83
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.83
26:X:30:MET:HE1	26:X:55:ASN:HA	1.58	0.83
5:B:62:ARG:HA	5:B:65:MET:HE2	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:164:THR:HG22	15:M:167:GLY:N	1.91	0.83
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.59	0.83
2:9:3006:C:H5"	16:N:37:ARG:NH1	1.94	0.83
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.79	0.82
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
24:V:12:THR:HG23	24:V:14:ALA:H	1.42	0.82
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.27	0.82
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.25	0.82
1:0:2904:U:H4'	26:X:8:ARG:NH1	1.95	0.82
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.82
1:0:1159:G:H21	1:0:1189:A:H8	1.27	0.82
23:U:9:CYS:HA	23:U:52:THR:HG23	1.62	0.82
11:H:166:SER:HB2	11:H:167:PRO:CD	2.10	0.82
30:2:41:HIS:N	30:2:45:ASN:HD22	1.77	0.82
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.60	0.82
1:0:381:G:H5"	38:0:4610:HOH:O	1.79	0.81
1:0:282:C:H1'	1:0:368:C:N4	1.94	0.81
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.62	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.81
12:J:107:ASN:ND2	12:J:109:TYR:H	1.79	0.81
1:0:21:G:C5'	20:R:2:ILE:HA	2.12	0.80
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.80
7:D:154:LYS:HD2	7:D:154:LYS:H	1.46	0.80
20:R:39:THR:HG22	20:R:42:GLU:H	1.46	0.80
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.62	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.80
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.63	0.79
1:0:506:G:H22	1:0:509:A:H5"	1.47	0.79
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.63	0.79
1:0:541:C:C2'	1:0:542:A:H5"	2.10	0.79
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.61	0.79
1:0:1160:G:H5'	1:0:1161:A:C5'	2.10	0.79
5:B:27:ASN:H	5:B:27:ASN:HD22	1.30	0.79
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.47	0.79
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.79
25:W:38:THR:HG22	25:W:39:ASP:H	1.47	0.79
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.82	0.79
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.64	0.79
18:P:115:SER:OG	18:P:118:GLN:HG3	1.83	0.78
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.65	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:93:GLN:HE21	16:N:93:GLN:HA	1.47	0.78
6:C:236:THR:H	6:C:239:ALA:HB3	1.49	0.78
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.84	0.77
12:J:45:VAL:HG23	12:J:130:VAL:O	1.83	0.77
1:0:2291:A:C8	1:0:2309:C:H5'	2.19	0.77
25:W:80:ASP:O	25:W:84:VAL:HG23	1.84	0.77
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.83	0.77
7:D:136:ARG:HD2	7:D:155:HIS:O	1.83	0.77
9:F:91:VAL:HG12	9:F:92:GLY:H	1.49	0.77
1:0:559:U:H5'	1:0:559:U:H6	1.49	0.77
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.86	0.77
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.15	0.77
4:A:131:HIS:O	4:A:132:ASP:HB2	1.86	0.76
1:0:2748:G:H2'	38:0:7745:HOH:O	1.84	0.76
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.85	0.76
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.76
5:B:238:ASN:HD22	5:B:240:GLY:H	1.33	0.76
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.64	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.76
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.67	0.76
1:0:870:G:C2'	1:0:871:G:H5"	2.16	0.76
7:D:135:VAL:HG22	7:D:136:ARG:H	1.51	0.76
1:0:56:G:H5"	24:V:50:ARG:HH12	1.49	0.76
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.67	0.75
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.75
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.67	0.75
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.51	0.75
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.50	0.75
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.66	0.75
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.69	0.75
6:C:139:VAL:HG13	38:C:9244:HOH:O	1.85	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.87	0.75
25:W:88:THR:HG22	25:W:89:ASP:H	1.49	0.75
1:0:1641:A:H2'	1:0:1642:A:H5'	1.69	0.75
1:0:1372:A:H3'	38:0:7407:HOH:O	1.87	0.74
11:H:166:SER:CB	11:H:167:PRO:HD3	2.13	0.74
1:0:2862:G:H4'	5:B:336:GLN:O	1.87	0.74
24:V:39:ALA:N	24:V:40:PRO:HD2	2.02	0.74
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.69	0.74
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.18	0.74
38:0:6419:HOH:O	4:A:223:ARG:HG3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.74
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.68	0.74
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.21	0.74
26:X:25:ARG:HD3	26:X:64:ALA:O	1.88	0.74
1:0:2908:A:H2'	1:0:2909:G:O4'	1.88	0.74
29:1:10:LYS:HG3	38:1:9236:HOH:O	1.87	0.74
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.50	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.74
1:0:1116:U:HO2'	1:0:1118:A:H2	1.34	0.74
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.73
1:0:2756:U:H3	1:0:2896:A:H2	1.34	0.73
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.15	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.68	0.73
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.73
16:N:17:ARG:NH1	16:N:17:ARG:HB3	2.03	0.73
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.73
2:9:3014:G:H8	2:9:3014:G:H5'	1.54	0.73
25:W:13:MET:HE1	25:W:17:ILE:HG22	1.71	0.73
16:N:151:ASP:O	16:N:154:LEU:HB2	1.88	0.73
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.70	0.73
2:9:3029:C:H2'	2:9:3030:C:H5'	1.70	0.73
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.70	0.73
12:J:131:THR:HG22	12:J:134:GLU:H	1.53	0.73
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.53	0.73
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.70	0.72
1:0:2716:G:H5"	5:B:206:THR:HG21	1.71	0.72
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.87	0.72
1:0:793:A:H5"	18:P:83:LYS:HG2	1.71	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.72
11:H:27:LYS:H	11:H:59:HIS:HD2	1.37	0.72
4:A:199:HIS:HD2	4:A:201:PHE:H	1.34	0.72
1:0:182:G:H5'	38:0:5431:HOH:O	1.90	0.72
14:L:133:VAL:HA	38:L:9371:HOH:O	1.88	0.72
1:0:1116:U:O2'	1:0:1118:A:H2	1.72	0.72
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.72
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.54	0.72
1:0:506:G:H22	1:0:509:A:C5'	2.03	0.72
26:X:43:VAL:HG12	26:X:44:ASP:H	1.55	0.72
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.71	0.72
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.71
22:T:49:GLU:OE2	22:T:97:ARG:HD2	1.90	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.72	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.72	0.71
1:0:1701:A:H4'	1:0:1702:U:H5"	1.72	0.71
1:0:1184:C:H1'	38:0:7672:HOH:O	1.89	0.71
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.72	0.71
30:2:41:HIS:H	30:2:45:ASN:ND2	1.82	0.71
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.06	0.71
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.06	0.71
1:0:1116:U:H3	1:0:1246:A:H62	1.35	0.71
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.25	0.71
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.01	0.71
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.20	0.71
5:B:168:GLY:H	5:B:174:ARG:HD3	1.56	0.71
1:0:380:A:H2'	38:0:7446:HOH:O	1.90	0.71
1:0:272:A:H5'	1:0:273:G:OP2	1.90	0.71
1:0:188:C:H5"	15:M:163:LEU:HD21	1.73	0.70
32:I:99:ASP:OD1	32:I:138:THR:HB	1.90	0.70
16:N:113:SER:HB2	38:N:9360:HOH:O	1.89	0.70
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.70
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.21	0.70
26:X:43:VAL:HG12	26:X:44:ASP:N	2.05	0.70
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.72	0.70
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.74	0.70
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.55	0.70
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.72	0.70
1:0:2533:C:C6	1:0:2533:C:H5'	2.25	0.70
1:0:2054:A:N3	20:R:128:ARG:NH2	2.39	0.70
7:D:99:ASP:HA	38:D:5675:HOH:O	1.92	0.70
16:N:169:PRO:O	16:N:172:PHE:HB3	1.91	0.70
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.91	0.70
4:A:33:GLU:O	4:A:34:ASP:HB2	1.90	0.70
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.72	0.70
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.56	0.70
6:C:162:VAL:HG12	6:C:192:ILE:HD11	1.72	0.70
5:B:62:ARG:HA	5:B:65:MET:CE	2.21	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.74	0.70
1:0:1118:A:H3'	1:0:1118:A:H8	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.07	0.70
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.07	0.70
1:0:2256:G:H2'	1:0:2257:G:H5'	1.74	0.70
1:0:450:C:OP1	6:C:184:ARG:NH2	2.25	0.70
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.38	0.69
2:9:3006:C:H5"	16:N:37:ARG:HH12	1.57	0.69
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.55	0.69
7:D:99:ASP:HB3	7:D:103:ASN:H	1.55	0.69
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.90	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.75	0.69
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.75	0.69
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.73	0.69
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.56	0.69
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.22	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.69
1:0:1667:A:C8	1:0:1667:A:H5'	2.25	0.69
1:0:1559:A:H1'	38:0:6128:HOH:O	1.93	0.69
5:B:258:GLY:H	5:B:260:HIS:CE1	2.11	0.69
1:0:474:C:O3'	6:C:73:LEU:HD21	1.93	0.69
4:A:121:ALA:O	4:A:124:VAL:HG22	1.92	0.69
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.41	0.69
1:0:1209:C:H2'	1:0:1210:G:H8	1.56	0.69
23:U:52:THR:HG22	23:U:54:THR:H	1.58	0.68
1:0:1603:A:H5'	1:0:1605:G:O4'	1.93	0.68
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.90	0.68
1:0:2679:G:H2'	1:0:2681:A:OP2	1.93	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.92	0.68
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.05	0.68
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.93	0.68
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.75	0.68
1:0:1979:G:H2'	38:0:3601:HOH:O	1.92	0.68
8:E:97:VAL:HG12	38:E:4191:HOH:O	1.93	0.68
16:N:164:ASP:CG	16:N:167:ASP:HA	2.14	0.68
1:0:2851:G:O2'	1:0:2852:A:H5'	1.92	0.68
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.68
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.73	0.68
38:0:3542:HOH:O	32:I:92:PRO:HD2	1.93	0.68
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.75	0.68
1:0:603:A:H5"	1:0:604:G:OP1	1.94	0.68
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.93	0.68
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.23	0.67
1:0:2426:G:H1'	38:0:6350:HOH:O	1.92	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.76	0.67
1:0:2769:C:C2'	1:0:2770:G:H5'	2.23	0.67
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.76	0.67
1:0:56:G:H5"	24:V:50:ARG:NH1	2.07	0.67
25:W:119:HIS:HD2	25:W:120:PRO:O	1.77	0.67
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.75	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.76	0.67
1:0:2840:A:OP1	5:B:211:THR:HG23	1.94	0.67
5:B:140:LEU:HA	38:B:9380:HOH:O	1.95	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
5:B:7:ARG:NH1	5:B:11:LEU:HD21	2.09	0.67
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.75	0.67
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.75	0.67
1:0:1751:G:C2'	1:0:1752:G:H5"	2.24	0.67
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.95	0.67
1:0:2827:A:H2'	1:0:2828:G:O4'	1.95	0.67
1:0:1474:C:C6	1:0:1474:C:H5'	2.23	0.66
2:9:3056:A:C2'	2:9:3057:A:H5"	2.24	0.66
7:D:25:MET:HE1	7:D:41:LEU:HG	1.77	0.66
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.77	0.66
4:A:179:MET:HG2	4:A:186:TRP:CB	2.25	0.66
1:0:1441:G:H1'	38:0:7965:HOH:O	1.96	0.66
6:C:140:VAL:HB	38:C:9247:HOH:O	1.95	0.66
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.95	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.25	0.66
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.09	0.66
1:0:1205:U:H2'	1:0:1206:U:H5"	1.78	0.66
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.77	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.61	0.66
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.95	0.66
1:0:1189:A:H1'	1:0:1209:C:O4'	1.95	0.66
3:4:176:A:O4'	3:4:175:C:H2'	1.95	0.66
14:L:79:ASP:HB3	38:L:9356:HOH:O	1.95	0.66
1:0:560:C:H42	1:0:597:A:H61	1.41	0.66
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.66
23:U:14:GLU:O	23:U:17:THR:HB	1.96	0.66
1:0:88:G:H5'	1:0:88:G:H8	1.61	0.66
15:M:164:THR:CG2	15:M:167:GLY:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2578:G:H5'	1:0:2578:G:H8	1.60	0.65
1:0:21:G:H5"	20:R:1:GLY:O	1.96	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.25	0.65
25:W:38:THR:HG22	25:W:39:ASP:N	2.12	0.65
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.78	0.65
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.79	0.65
8:E:7:ILE:HG22	8:E:45:ASP:O	1.95	0.65
32:I:101:SER:H	32:I:104:GLN:NE2	1.94	0.65
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.78	0.65
29:1:25:LYS:HG3	30:2:49:GLU:H	1.60	0.65
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.79	0.65
1:0:447:A:OP2	22:T:1:SER:HB2	1.96	0.65
24:V:12:THR:HG22	24:V:15:GLU:CG	2.17	0.65
9:F:58:GLU:HA	9:F:61:MET:HG3	1.78	0.65
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.61	0.65
26:X:78:GLU:HG2	26:X:79:GLU:H	1.60	0.65
1:0:2878:U:H2'	1:0:2879:A:O4'	1.95	0.65
1:0:545:G:C8	1:0:545:G:H5'	2.30	0.65
4:A:210:GLY:HA3	38:A:9379:HOH:O	1.97	0.65
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.62	0.65
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.36	0.65
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.65
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.79	0.65
6:C:16:VAL:HG12	6:C:17:ASP:H	1.61	0.65
25:W:65:VAL:HA	25:W:68:THR:HG22	1.79	0.65
16:N:100:ALA:O	16:N:129:ILE:HG23	1.98	0.65
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.79	0.65
11:H:51:VAL:HG21	11:H:127:VAL:HG11	1.79	0.64
1:0:21:G:H4'	20:R:2:ILE:HG22	1.80	0.64
1:0:1667:A:H2'	1:0:1668:U:C6	2.32	0.64
4:A:192:VAL:HG13	38:A:9350:HOH:O	1.96	0.64
1:0:1666:C:O2'	1:0:1667:A:H5"	1.96	0.64
1:0:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.11	0.64
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.63	0.64
11:H:21:THR:O	11:H:120:ILE:HD12	1.98	0.64
1:0:544:G:H2'	1:0:545:G:H5"	1.78	0.64
25:W:106:THR:OG1	25:W:109:GLU:HG3	1.98	0.64
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.79	0.64
8:E:69:ILE:HA	8:E:72:MET:CE	2.27	0.64
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:4899:HOH:O	17:O:39:THR:HB	1.97	0.64
18:P:64:GLU:HG2	38:P:169:HOH:O	1.98	0.64
6:C:16:VAL:HG12	6:C:17:ASP:N	2.12	0.64
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.31	0.64
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.63	0.64
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.80	0.64
5:B:297:VAL:HB	38:B:9407:HOH:O	1.97	0.64
7:D:86:THR:C	7:D:89:PRO:HD2	2.17	0.64
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.64
1:0:2073:G:H5"	38:0:4124:HOH:O	1.98	0.64
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.79	0.64
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.63
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.80	0.63
1:0:1189:A:H1'	1:0:1209:C:C1'	2.27	0.63
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.44	0.63
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.13	0.63
4:A:179:MET:HA	4:A:179:MET:CE	2.28	0.63
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.81	0.63
10:G:16:LYS:O	10:G:20:VAL:HG23	1.98	0.63
2:9:3051:A:H5'	16:N:160:SER:HB3	1.81	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.96	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.11	0.63
2:9:3039:U:H1'	2:9:3044:A:N6	2.13	0.63
5:B:81:ALA:O	5:B:186:GLY:HA3	1.99	0.63
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.97	0.63
1:0:338:C:H4'	6:C:174:ILE:CD1	2.29	0.63
1:0:1116:U:O2'	1:0:1118:A:C2	2.51	0.63
1:0:282:C:O2'	1:0:283:U:H5'	1.98	0.63
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.45	0.63
10:G:64:ASN:N	10:G:64:ASN:HD22	1.94	0.63
11:H:27:LYS:H	11:H:59:HIS:CD2	2.16	0.63
12:J:52:GLN:HG3	12:J:53:ILE:N	2.13	0.63
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.29	0.63
2:9:3041:C:H4'	7:D:48:MET:HB2	1.80	0.63
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.14	0.63
1:0:1058:A:H2'	1:0:1060:C:H5"	1.79	0.63
1:0:542:A:H5'	1:0:542:A:C8	2.29	0.62
25:W:21:LEU:CD2	25:W:26:ILE:HD11	2.28	0.62
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.46	0.62
16:N:110:THR:HB	16:N:113:SER:OG	1.98	0.62
23:U:5:GLU:HG3	23:U:10:GLY:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.45	0.62
5:B:162:MET:HE3	5:B:308:LEU:HD21	1.81	0.62
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.80	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.28	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.30	0.62
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.64	0.62
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.62
2:9:3054:A:O2'	2:9:3055:U:H5'	1.99	0.62
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.82	0.62
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	1.98	0.62
1:0:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.00	0.62
1:0:1625:U:H4'	38:0:4948:HOH:O	1.97	0.62
27:Y:112:GLU:CD	27:Y:115:ARG:HH12	2.01	0.62
1:0:2534:C:H1'	38:0:3800:HOH:O	1.99	0.62
12:J:130:VAL:HG12	12:J:131:THR:N	2.15	0.62
1:0:1206:U:H5'	1:0:1206:U:H6	1.65	0.62
1:0:2251:G:H2'	1:0:2252:A:C8	2.34	0.62
5:B:145:HIS:HD2	5:B:146:THR:O	1.81	0.62
1:0:1634:G:H3'	38:0:4189:HOH:O	2.00	0.62
23:U:52:THR:HG22	23:U:54:THR:N	2.15	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
1:0:299:U:H5'	38:0:7546:HOH:O	1.99	0.62
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.65	0.62
1:0:31:C:H2'	38:0:7888:HOH:O	1.99	0.62
2:9:3001:U:H5"	2:9:3003:A:OP1	2.00	0.62
4:A:199:HIS:CD2	4:A:201:PHE:H	2.16	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.64	0.62
15:M:28:GLN:O	15:M:32:ARG:HG3	2.00	0.62
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.62
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.65	0.61
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.61
1:0:2256:G:H2'	1:0:2257:G:C5'	2.30	0.61
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.80	0.61
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.63	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.61
16:N:152:GLU:C	16:N:154:LEU:H	2.04	0.61
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.30	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
7:D:25:MET:HE3	7:D:37:ALA:CB	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1166:A:H1'	1:0:1192:A:C2	2.36	0.61
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.82	0.61
1:0:119:A:H2'	1:0:120:A:H5"	1.81	0.61
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.61
21:S:33:SER:O	21:S:37:VAL:HG23	1.99	0.61
7:D:138:GLY:N	38:D:7597:HOH:O	2.33	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.61
27:Y:144:ARG:CZ	38:Y:9407:HOH:O	2.48	0.61
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.61
1:0:2491:G:H1'	38:0:7098:HOH:O	1.99	0.61
16:N:80:SER:HB2	38:N:9335:HOH:O	2.01	0.61
1:0:656:G:OP2	17:O:37:ARG:HD2	2.01	0.61
38:0:4951:HOH:O	5:B:300:SER:HB3	1.99	0.61
5:B:144:THR:HB	38:B:9426:HOH:O	2.00	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	0.61
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.31	0.61
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.61
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.81	0.61
8:E:81:GLU:HG2	8:E:134:SER:CB	2.30	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
1:0:969:G:H1	1:0:999:C:H42	1.49	0.61
1:0:1080:C:H4'	1:0:1081:A:OP1	2.00	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.66	0.61
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.63	0.60
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.27	0.60
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.84	0.60
1:0:797:A:H4'	28:Z:10:ARG:N	2.16	0.60
1:0:1182:C:H1'	1:0:1192:A:H8	1.64	0.60
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.82	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.01	0.60
1:0:247:A:H2'	38:0:4218:HOH:O	2.01	0.60
1:0:1535:G:H2'	1:0:1536:C:C6	2.36	0.60
1:0:902:G:N7	14:L:18:HIS:HD2	2.00	0.60
1:0:285:A:H2'	1:0:286:U:O4'	2.00	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
1:0:2346:C:O5'	1:0:2346:C:H6	1.84	0.60
8:E:93:MET:HE1	8:E:165:GLY:N	2.16	0.60
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.81	0.60
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.98	0.60
38:0:5117:HOH:O	12:J:47:THR:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:132:ASN:O	16:N:135:VAL:HG12	2.01	0.60
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.60
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.32	0.60
1:0:2896:A:H5"	38:0:6357:HOH:O	2.01	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.31	0.60
1:0:157:G:H4'	15:M:95:LYS:HE3	1.84	0.60
1:0:1118:A:H62	1:0:1244:U:H3	1.48	0.60
1:0:1741:U:H5'	1:0:1742:A:OP1	2.01	0.60
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.84	0.60
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.67	0.60
17:O:105:ASN:HD21	17:O:109:SER:H	1.49	0.60
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.36	0.60
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.02	0.60
8:E:13:ALA:HB2	8:E:22:VAL:HG22	1.84	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.02	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.60
5:B:168:GLY:N	5:B:174:ARG:HD3	2.16	0.60
6:C:162:VAL:HG13	6:C:232:LEU:HD21	1.83	0.60
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.84	0.60
1:0:447:A:P	22:T:1:SER:HB2	2.42	0.60
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.37	0.60
1:0:2720:C:O2	13:K:87:ARG:NH2	2.35	0.59
7:D:23:VAL:O	7:D:23:VAL:HG23	2.02	0.59
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.14	0.59
5:B:103:ASP:HB2	38:B:9394:HOH:O	2.02	0.59
1:0:2524:G:H21	1:0:2526:C:N4	2.00	0.59
1:0:1500:U:P	18:P:41:ARG:HH22	2.24	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
1:0:2505:G:O2'	1:0:2506:A:H5'	2.02	0.59
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.84	0.59
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.32	0.59
2:9:3013:A:O2'	2:9:3014:G:H5"	2.03	0.59
38:0:7663:HOH:O	5:B:211:THR:HG21	2.01	0.59
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.59
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.82	0.59
1:0:2769:C:H2'	1:0:2770:G:H5'	1.82	0.59
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.82	0.59
20:R:119:VAL:HG12	20:R:119:VAL:O	2.00	0.59
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.59
2:9:3114:G:O6	16:N:11:ARG:HD3	2.02	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:820:G:H5"	38:0:3356:HOH:O	2.01	0.59
22:T:69:LYS:O	22:T:71:VAL:HG23	2.03	0.59
6:C:236:THR:HA	38:C:9247:HOH:O	2.03	0.59
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.30	0.59
1:0:558:C:C2'	1:0:559:U:H5"	2.33	0.59
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.50	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.85	0.59
7:D:135:VAL:HG22	7:D:136:ARG:N	2.17	0.59
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.01	0.59
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.02	0.59
1:0:407:A:H2'	1:0:408:A:C8	2.38	0.59
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.84	0.59
12:J:107:ASN:HD22	12:J:108:PRO:N	2.01	0.59
1:0:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.59
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.38	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.18	0.58
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.38	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
14:L:143:THR:HG22	14:L:145:LEU:H	1.67	0.58
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.83	0.58
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.85	0.58
7:D:86:THR:O	7:D:90:LEU:HG	2.04	0.58
5:B:137:LEU:HD11	5:B:140:LEU:HD21	1.85	0.58
18:P:134:VAL:O	18:P:138:GLU:HG3	2.03	0.58
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.02	0.58
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.58
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.58
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.02	0.58
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.85	0.58
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.85	0.58
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.85	0.58
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.58
20:R:9:ASP:O	20:R:13:THR:HB	2.02	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:45:VAL:HA	11:H:167:PRO:O	2.03	0.58
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.85	0.58
11:H:56:GLN:HE21	11:H:126:ARG:NE	2.00	0.58
23:U:17:THR:HG22	23:U:18:GLY:N	2.18	0.58
8:E:69:ILE:HA	8:E:72:MET:HE3	1.84	0.58
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.85	0.58
1:0:449:A:N7	6:C:43:LYS:HG2	2.19	0.58
1:0:1175:G:H1'	1:0:1193:A:H2'	1.85	0.58
5:B:307:ARG:CB	5:B:307:ARG:HH11	2.12	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.64	0.58
4:A:36:ASP:C	4:A:38:ILE:H	2.07	0.58
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.52	0.58
1:0:1060:C:H6	1:0:1060:C:H5'	1.69	0.58
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.58
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.86	0.58
1:0:1593:C:OP1	18:P:117:SER:HB3	2.04	0.58
1:0:130:C:H2'	38:0:3467:HOH:O	2.02	0.58
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.34	0.58
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.58
13:K:98:VAL:HG13	13:K:99:ASP:N	2.18	0.58
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.84	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.03	0.58
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.86	0.58
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.85	0.58
27:Y:98:GLN:HG3	27:Y:236:VAL:HB	1.84	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
15:M:60:VAL:C	15:M:61:ILE:HD12	2.23	0.58
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.68	0.57
12:J:19:MET:CE	12:J:132:LEU:HD11	2.34	0.57
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.86	0.57
24:V:58:THR:O	24:V:62:GLU:HG3	2.03	0.57
2:9:3029:C:C2'	2:9:3030:C:H5'	2.34	0.57
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.69	0.57
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.86	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
17:O:96:VAL:HA	38:O:4258:HOH:O	2.03	0.57
1:0:1342:C:C2'	1:0:1343:C:H5'	2.34	0.57
2:9:3076:G:C3'	2:9:3077:A:H5"	2.25	0.57
1:0:1377:C:H5'	1:0:1377:C:C6	2.39	0.57
1:0:95:A:H5"	1:0:97:G:O4'	2.03	0.57
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.84	0.57
1:0:1118:A:H8	1:0:1119:G:H5"	1.70	0.57
1:0:2541:U:H5'	38:0:9721:HOH:O	2.04	0.57
1:0:1189:A:H3'	38:0:7881:HOH:O	2.03	0.57
1:0:316:A:N3	1:0:336:G:O2'	2.37	0.57
5:B:58:PRO:HA	5:B:63:GLU:OE1	2.05	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.02	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.19	0.57
6:C:1:MET:HG2	6:C:2:GLN:N	2.12	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.34	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.87	0.57
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.70	0.57
21:S:33:SER:OG	21:S:36:GLU:HG3	2.05	0.57
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.40	0.57
17:O:87:THR:O	17:O:91:GLN:HG3	2.03	0.57
1:0:558:C:O2'	1:0:559:U:H5"	2.05	0.57
8:E:6:GLU:HA	8:E:46:THR:HG22	1.85	0.57
11:H:169:GLY:C	11:H:170:ASN:HD22	2.08	0.57
2:9:3028:U:H5"	16:N:40:ASN:ND2	2.20	0.57
21:S:57:THR:CG2	21:S:58:MET:N	2.67	0.57
1:0:2769:C:H2'	1:0:2770:G:C5'	2.35	0.57
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.78	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.57
5:B:321:PRO:HA	38:B:9461:HOH:O	2.05	0.57
32:I:113:HIS:N	32:I:114:PRO:HD2	2.20	0.57
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.40	0.57
1:0:1185:U:H2'	1:0:1186:C:C6	2.40	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.68	0.57
20:R:132:ARG:HG2	20:R:133:ALA:N	2.20	0.57
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.19	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
14:L:136:ALA:HB3	38:L:9371:HOH:O	2.05	0.56
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.56
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.05	0.56
1:0:90:A:H2'	1:0:91:G:O4'	2.04	0.56
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.05	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.56
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.33	0.56
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.05	0.56
29:1:45:ARG:HB3	38:1:9223:HOH:O	2.05	0.56
1:0:2420:G:O2'	1:0:2421:G:H5'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1352:A:H5"	1:0:1353:C:OP2	2.05	0.56
6:C:170:ASP:O	6:C:171:GLU:HG3	2.05	0.56
7:D:25:MET:CE	7:D:41:LEU:HG	2.35	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.40	0.56
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.18	0.56
20:R:39:THR:HG23	20:R:107:GLU:O	2.05	0.56
18:P:103:THR:O	18:P:107:GLU:HG3	2.05	0.56
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.56
1:0:2502:C:H2'	1:0:2503:A:H5'	1.85	0.56
10:G:12:ILE:N	10:G:13:PRO:HD3	2.20	0.56
1:0:328:U:O4'	6:C:202:THR:HG22	2.04	0.56
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.86	0.56
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.86	0.56
12:J:130:VAL:HG12	12:J:131:THR:H	1.71	0.56
10:G:20:VAL:O	10:G:24:VAL:HG23	2.05	0.56
1:0:138:U:H5"	1:0:139:C:OP2	2.05	0.56
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.20	0.56
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.88	0.56
1:0:200:U:H2'	38:0:3748:HOH:O	2.05	0.56
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.56
1:0:2468:A:H61	31:3:48:ASN:HD21	1.52	0.56
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.36	0.56
2:9:3020:G:O2'	2:9:3021:G:H5'	2.06	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
1:0:1679:C:H5'	38:0:9638:HOH:O	2.06	0.56
20:R:44:VAL:O	20:R:48:GLU:HG3	2.06	0.56
6:C:153:VAL:O	6:C:157:LEU:HG	2.06	0.56
30:2:41:HIS:O	30:2:45:ASN:HB2	2.06	0.56
1:0:1667:A:H2'	1:0:1668:U:H6	1.69	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
7:D:153:THR:O	7:D:156:ARG:HB2	2.06	0.56
16:N:37:ARG:NE	38:N:9333:HOH:O	2.35	0.56
1:0:65:C:O2'	1:0:66:G:H5'	2.05	0.56
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.56
1:0:1163:G:H5'	32:I:115:ASP:O	2.06	0.56
1:0:1086:A:N6	25:W:11:VAL:HG11	2.21	0.56
1:0:462:A:C2	30:2:37:HIS:HB3	2.41	0.56
25:W:122:ARG:HH21	25:W:154:ARG:HD2	1.70	0.56
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.88	0.56
21:S:43:GLU:HB3	38:S:7106:HOH:O	2.05	0.56
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.88	0.56
1:0:1834:C:H2'	1:0:1840:A:N6	2.20	0.56
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.88	0.56
38:0:7252:HOH:O	4:A:211:LYS:HG2	2.05	0.55
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.88	0.55
4:A:192:VAL:HB	38:A:9388:HOH:O	2.06	0.55
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.55
4:A:88:ILE:HG22	4:A:88:ILE:O	2.06	0.55
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.36	0.55
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.05	0.55
1:0:317:A:H5"	22:T:52:ARG:HD2	1.88	0.55
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.06	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.55
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.86	0.55
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.55
38:0:5492:HOH:O	13:K:39:GLY:HA2	2.06	0.55
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.05	0.55
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.36	0.55
1:0:1441:G:O2'	1:0:1442:A:H5'	2.06	0.55
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.06	0.55
1:0:1213:C:O2'	1:0:1214:G:H5'	2.07	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.07	0.55
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.21	0.55
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.37	0.55
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.05	0.55
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
1:0:2812:A:H2	1:0:2814:A:N6	1.97	0.55
14:L:133:VAL:HB	38:L:9355:HOH:O	2.07	0.55
5:B:57:GLU:O	5:B:63:GLU:HB2	2.06	0.55
38:0:4281:HOH:O	22:T:82:THR:HA	2.05	0.55
5:B:214:PRO:HD2	38:B:9320:HOH:O	2.06	0.55
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.87	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.87	0.55
1:0:2533:C:H6	1:0:2533:C:C5'	2.18	0.55
8:E:81:GLU:O	8:E:172:PRO:HD3	2.07	0.55
8:E:11:VAL:HG12	8:E:12:ASP:N	2.22	0.55
1:0:503:G:H2'	1:0:504:G:H8	1.72	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.55
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2526:C:O2'	1:0:2527:U:H5'	2.07	0.55
1:0:820:G:H3'	38:0:3356:HOH:O	2.05	0.55
1:0:1342:C:O2'	1:0:1343:C:H5'	2.05	0.55
6:C:25:PRO:HG2	38:C:9123:HOH:O	2.06	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.71	0.55
25:W:88:THR:HG22	25:W:89:ASP:N	2.21	0.55
6:C:218:VAL:HG12	38:C:9220:HOH:O	2.04	0.55
1:0:2241:C:H2'	1:0:2242:U:H6	1.70	0.55
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.72	0.55
38:0:6533:HOH:O	27:Y:158:LYS:HD3	2.06	0.55
1:0:2824:C:H5"	1:0:2825:C:H5'	1.88	0.55
1:0:2909:G:H2'	1:0:2910:A:C8	2.42	0.55
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.42	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
1:0:316:A:H5'	22:T:54:ASP:OD2	2.06	0.55
25:W:1:MET:N	25:W:37:GLU:HG3	2.22	0.55
1:0:816:G:H5'	1:0:1598:A:H4'	1.89	0.55
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.41	0.55
25:W:52:VAL:HG22	25:W:53:ALA:H	1.72	0.54
1:0:2781:U:H2'	1:0:2782:G:H5'	1.88	0.54
11:H:170:ASN:HD22	11:H:170:ASN:N	2.04	0.54
17:O:106:PRO:HG2	17:O:107:GLU:OE1	2.07	0.54
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.22	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
1:0:159:G:OP1	15:M:74:LYS:HE3	2.07	0.54
25:W:82:GLU:O	25:W:86:GLU:HG3	2.07	0.54
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.69	0.54
5:B:36:PRO:HA	5:B:168:GLY:CA	2.33	0.54
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.37	0.54
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.90	0.54
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.90	0.54
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.54
25:W:13:MET:HE2	25:W:18:GLN:CA	2.34	0.54
1:0:1120:U:H5'	1:0:1121:G:OP2	2.07	0.54
1:0:544:G:C2'	1:0:545:G:H5"	2.37	0.54
1:0:969:G:H1	1:0:999:C:N4	2.05	0.54
8:E:95:VAL:O	8:E:126:ILE:HD12	2.08	0.54
15:M:57:LYS:HE2	15:M:140:ALA:O	2.07	0.54
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.89	0.54
16:N:44:ARG:HG3	16:N:45:ALA:N	2.22	0.54
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1202:A:H2'	1:0:1203:G:H5'	1.88	0.54
24:V:39:ALA:O	24:V:41:GLU:N	2.36	0.54
1:0:2248:C:H3'	38:0:5709:HOH:O	2.07	0.54
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.07	0.54
9:F:21:GLU:O	9:F:24:ARG:HG2	2.08	0.54
1:0:10:U:O4	1:0:532:A:OP2	2.25	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.22	0.54
5:B:71:VAL:HG11	5:B:296:LEU:HB3	1.89	0.54
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.54
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.90	0.54
8:E:77:THR:OG1	8:E:78:GLU:N	2.40	0.54
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.54
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.90	0.54
9:F:38:LYS:NZ	15:M:3:SER:HA	2.22	0.54
8:E:132:THR:HG23	8:E:132:THR:O	2.08	0.54
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.54
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.17	0.54
31:3:62:THR:HB	38:3:9351:HOH:O	2.08	0.54
1:0:1596:U:H2'	1:0:1598:A:OP2	2.08	0.54
18:P:141:ILE:C	18:P:143:ALA:H	2.12	0.54
1:0:2755:G:H1'	38:0:4963:HOH:O	2.08	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.89	0.54
25:W:13:MET:CE	25:W:17:ILE:HG22	2.38	0.54
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.02	0.54
1:0:396:U:O2'	1:0:418:C:H4'	2.08	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.08	0.54
21:S:77:VAL:O	21:S:80:ARG:HG2	2.07	0.54
1:0:2064:U:H5'	1:0:2652:U:O3'	2.08	0.54
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.25	0.53
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.09	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.36	0.53
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.08	0.53
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.53
1:0:2385:G:H2'	1:0:2386:U:C6	2.43	0.53
1:0:1943:C:H4'	4:A:211:LYS:O	2.08	0.53
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.90	0.53
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.90	0.53
2:9:3064:C:H2'	2:9:3065:A:H5'	1.90	0.53
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.09	0.53
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.08	0.53
1:0:625:U:H5"	1:0:1044:C:N4	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.53
38:0:4905:HOH:O	4:A:6:GLY:HA3	2.08	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.53
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.39	0.53
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.90	0.53
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.08	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.53
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.09	0.53
1:0:960:G:N3	1:0:960:G:H2'	2.23	0.53
1:0:380:A:OP2	15:M:9:ARG:HD2	2.09	0.53
1:0:1166:A:H61	1:0:1180:U:H3	1.56	0.53
1:0:2768:A:H2'	1:0:2769:C:O4'	2.07	0.53
1:0:2241:C:O2'	1:0:2242:U:H5'	2.09	0.53
31:3:73:GLU:HB3	38:3:9363:HOH:O	2.07	0.53
17:O:73:ASP:HA	17:O:92:VAL:O	2.07	0.53
5:B:280:VAL:HG13	5:B:334:SER:HA	1.89	0.53
12:J:47:THR:HG22	12:J:48:GLY:H	1.74	0.53
4:A:32:VAL:HG12	4:A:34:ASP:H	1.72	0.53
4:A:36:ASP:O	4:A:38:ILE:N	2.40	0.53
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.53
18:P:143:ALA:HA	38:P:190:HOH:O	2.08	0.53
1:0:396:U:OP2	31:3:38:ARG:HD2	2.07	0.53
1:0:818:A:O2'	28:Z:13:ARG:HD3	2.08	0.53
13:K:125:ALA:C	13:K:127:ALA:H	2.12	0.53
5:B:175:LEU:C	5:B:175:LEU:HD23	2.28	0.53
38:0:5796:HOH:O	15:M:58:GLN:HG3	2.08	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.41	0.53
1:0:121:U:OP2	30:2:10:ARG:NH2	2.28	0.53
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.23	0.53
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.23	0.53
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.53
1:0:2265:U:H2'	1:0:2266:A:C8	2.44	0.53
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.39	0.53
10:G:67:LEU:O	10:G:71:LEU:HG	2.08	0.53
25:W:149:LEU:HG	25:W:153:MET:HE2	1.90	0.53
1:0:588:G:O6	25:W:154:ARG:NH1	2.42	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.53
5:B:175:LEU:O	5:B:175:LEU:HD23	2.07	0.53
9:F:96:ALA:HA	38:F:3111:HOH:O	2.08	0.53
5:B:248:ARG:O	5:B:251:VAL:HG13	2.08	0.53
7:D:25:MET:CE	7:D:37:ALA:HB1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:9:CYS:CA	23:U:52:THR:HG23	2.36	0.53
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.53
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.53
1:0:790:A:H2'	1:0:791:A:O4'	2.09	0.53
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.90	0.53
32:I:131:THR:HG22	32:I:131:THR:O	2.09	0.53
1:0:1299:G:N7	14:L:6:ARG:NH1	2.56	0.53
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.09	0.53
8:E:13:ALA:CB	8:E:22:VAL:HG22	2.39	0.53
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.53
1:0:1477:C:H5'	1:0:1868:G:C5'	2.39	0.53
3:4:74:DCZ:C2'	3:4:75:DC:H5'	2.38	0.53
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.91	0.53
1:0:644:G:N3	1:0:644:G:H5'	2.23	0.53
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.53
1:0:797:A:C4'	28:Z:10:ARG:N	2.71	0.52
1:0:244:C:OP2	9:F:38:LYS:HE3	2.09	0.52
1:0:1406:A:H4'	1:0:1407:A:H5"	1.90	0.52
25:W:108:ARG:HE	25:W:114:PRO:CG	2.23	0.52
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.52
1:0:185:G:O3'	1:0:186:A:H4'	2.09	0.52
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.24	0.52
1:0:1741:U:O2'	1:0:2723:G:H4'	2.09	0.52
1:0:1477:C:H5'	1:0:1868:G:H5'	1.90	0.52
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.09	0.52
1:0:2423:C:H5"	38:0:7262:HOH:O	2.08	0.52
32:I:139:ILE:C	32:I:140:GLU:HG3	2.28	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.52
7:D:170:TYR:O	7:D:171:ASP:HB3	2.10	0.52
27:Y:133:HIS:HD2	38:Y:9379:HOH:O	1.93	0.52
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.73	0.52
14:L:114:VAL:HG11	38:L:9371:HOH:O	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.39	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.40	0.52
9:F:19:ALA:O	9:F:22:VAL:HG22	2.09	0.52
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.44	0.52
1:0:1632:A:H2'	1:0:1633:C:H5'	1.91	0.52
1:0:468:U:H3'	38:0:7773:HOH:O	2.10	0.52
1:0:2072:G:C6	1:0:2533:C:H1'	2.45	0.52
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.52
1:0:2769:C:O2'	1:0:2770:G:H5'	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3051:A:H5'	16:N:160:SER:CB	2.39	0.52
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.89	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.44	0.52
1:0:1130:U:H2'	1:0:1131:G:O4'	2.09	0.52
7:D:85:GLN:O	7:D:86:THR:HG23	2.09	0.52
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.44	0.52
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.92	0.52
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.92	0.52
21:S:56:ASN:O	30:2:8:LYS:NZ	2.35	0.52
8:E:137:ASP:O	8:E:141:VAL:HG23	2.09	0.52
6:C:140:VAL:HG12	6:C:141:SER:N	2.24	0.52
25:W:4:LEU:O	25:W:32:CYS:HA	2.10	0.52
32:I:75:THR:N	32:I:112:LYS:HZ1	2.08	0.52
12:J:45:VAL:HG22	12:J:46:ILE:N	2.24	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.57	0.52
24:V:39:ALA:C	24:V:41:GLU:H	2.13	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.72	0.52
27:Y:155:ARG:NH1	38:Y:9358:HOH:O	2.42	0.52
31:3:14:CYS:HB3	31:3:16:GLU:HG2	1.90	0.52
14:L:21:ARG:N	38:L:9329:HOH:O	2.43	0.52
5:B:177:HIS:O	5:B:181:ILE:HG13	2.09	0.52
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.91	0.52
16:N:72:GLU:HG2	16:N:72:GLU:O	2.10	0.52
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.58	0.52
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.75	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
1:0:958:G:H2'	1:0:959:C:C6	2.45	0.52
7:D:163:VAL:HA	38:D:6326:HOH:O	2.10	0.52
7:D:67:ASP:O	7:D:69:ILE:HG13	2.10	0.52
1:0:1701:A:H5'	38:0:6532:HOH:O	2.10	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
1:0:1669:A:H2'	1:0:1670:G:C8	2.45	0.52
30:2:39:ARG:HG2	38:2:3143:HOH:O	2.09	0.52
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.44	0.52
7:D:88:LEU:C	7:D:90:LEU:H	2.13	0.52
1:0:447:A:O2'	1:0:448:G:H5'	2.10	0.52
1:0:447:A:OP1	22:T:2:LYS:HG2	2.10	0.52
5:B:148:PRO:HB2	5:B:156:LYS:O	2.10	0.52
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.25	0.52
4:A:86:ALA:HB3	4:A:94:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.92	0.52
9:F:113:ASP:O	9:F:117:GLU:HG3	2.10	0.52
12:J:74:ARG:O	12:J:78:ILE:HG12	2.11	0.51
1:0:2054:A:H2	20:R:128:ARG:HH22	1.51	0.51
1:0:2769:C:H2'	1:0:2770:G:O4'	2.10	0.51
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.51
5:B:217:ARG:CG	5:B:257:THR:HG22	2.37	0.51
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.93	0.51
1:0:524:A:H5"	20:R:29:LYS:HD3	1.93	0.51
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.51
5:B:52:VAL:C	5:B:53:LEU:HD12	2.30	0.51
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.40	0.51
3:4:74:DCZ:H2'1	3:4:75:DC:O4'	2.10	0.51
1:0:848:C:H5'	38:0:7491:HOH:O	2.09	0.51
21:S:81:ILE:HG12	38:S:4527:HOH:O	2.10	0.51
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.91	0.51
1:0:2252:A:C6	1:0:2253:G:H1'	2.45	0.51
1:0:2717:C:O2'	1:0:2718:C:H5"	2.11	0.51
26:X:30:MET:CE	26:X:55:ASN:HA	2.37	0.51
26:X:78:GLU:CG	26:X:79:GLU:H	2.23	0.51
2:9:3049:G:O2'	2:9:3050:G:H5'	2.10	0.51
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.76	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.92	0.51
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.26	0.51
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.25	0.51
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.41	0.51
8:E:95:VAL:HG22	8:E:104:ILE:HG12	1.92	0.51
1:0:669:G:O2'	1:0:670:G:H5'	2.10	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.93	0.51
1:0:1375:A:H2'	1:0:1376:G:H5'	1.93	0.51
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.46	0.51
32:I:134:SER:O	32:I:135:LEU:HD23	2.11	0.51
1:0:1641:A:C2'	1:0:1642:A:H5'	2.39	0.51
16:N:149:GLU:O	16:N:152:GLU:HB2	2.10	0.51
5:B:108:GLU:HA	5:B:110:ASP:OD1	2.11	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
1:0:512:G:O3'	1:0:513:A:H8	1.94	0.51
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.51
1:0:1119:G:H22	1:0:1246:A:H2	1.50	0.51
32:I:131:THR:O	32:I:135:LEU:HG	2.10	0.51
2:9:3057:A:C8	7:D:141:VAL:HG21	2.46	0.51
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.51
1:0:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
1:0:1787:C:H2'	1:0:1788:U:H6	1.75	0.51
12:J:51:GLU:O	12:J:55:GLU:HG3	2.10	0.51
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.37	0.51
11:H:167:PRO:O	11:H:168:ALA:HB2	2.11	0.51
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.40	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.94	0.51
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.10	0.51
1:0:517:U:H1'	38:0:7782:HOH:O	2.10	0.51
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.93	0.51
23:U:6:CYS:C	23:U:8:TYR:H	2.14	0.51
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.11	0.51
24:V:4:HIS:HB3	38:V:6622:HOH:O	2.10	0.51
4:A:179:MET:HE3	4:A:179:MET:HA	1.93	0.51
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.26	0.51
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.10	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51
1:0:834:G:H4'	1:0:835:U:OP2	2.11	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.45	0.51
1:0:1123:A:C6	1:0:1238:C:H5'	2.46	0.51
25:W:46:ALA:O	25:W:49:ASN:HB2	2.10	0.51
20:R:33:ARG:NH1	38:R:9345:HOH:O	2.44	0.51
5:B:150:ALA:O	5:B:152:PRO:HD3	2.10	0.51
4:A:212:PRO:HB2	38:A:9353:HOH:O	2.10	0.51
7:D:84:LEU:C	7:D:86:THR:H	2.13	0.51
1:0:1086:A:C6	25:W:11:VAL:HG11	2.45	0.51
8:E:131:LEU:HD12	8:E:166:VAL:HG11	1.92	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.11	0.51
6:C:79:ARG:O	6:C:87:ARG:HG2	2.10	0.51
38:0:7104:HOH:O	15:M:178:LYS:HB2	2.09	0.51
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.91	0.51
1:0:289:G:H22	1:0:363:A:H2	1.57	0.51
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.23	0.50
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.10	0.50
1:0:1123:A:C2	1:0:1129:C:H4'	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.44	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.12	0.50
4:A:37:VAL:HG22	38:A:9391:HOH:O	2.11	0.50
21:S:6:LYS:O	21:S:7:HIS:HB3	2.11	0.50
1:0:1289:C:H3'	38:0:6650:HOH:O	2.10	0.50
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.50
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.38	0.50
1:0:1044:C:H3'	1:0:1045:G:H5"	1.93	0.50
1:0:1940:C:H4'	38:0:7555:HOH:O	2.11	0.50
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.46	0.50
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.92	0.50
6:C:236:THR:HG21	38:C:9171:HOH:O	2.11	0.50
9:F:91:VAL:CG1	9:F:92:GLY:H	2.21	0.50
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.50
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.50
11:H:28:ILE:HG23	38:H:9179:HOH:O	2.11	0.50
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.46	0.50
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.11	0.50
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.50
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.93	0.50
15:M:164:THR:HG23	15:M:165:GLY:N	2.25	0.50
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.93	0.50
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.27	0.50
18:P:134:VAL:O	18:P:137:LEU:HB3	2.11	0.50
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.50
9:F:37:THR:O	9:F:41:GLU:HG3	2.10	0.50
1:0:1423:C:O2'	1:0:1424:A:H5'	2.11	0.50
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.50
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.12	0.50
25:W:21:LEU:CD1	25:W:26:ILE:HD11	2.40	0.50
38:9:7568:HOH:O	16:N:107:ASN:HB3	2.11	0.50
14:L:143:THR:CG2	14:L:144:ASP:N	2.74	0.50
8:E:84:MET:HE3	8:E:148:ILE:HG21	1.94	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.47	0.50
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.79	0.50
30:2:40:ARG:CD	30:2:47:THR:HG22	2.42	0.50
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.77	0.50
29:1:28:HIS:O	29:1:32:LYS:N	2.44	0.50
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.94	0.50
8:E:101:GLU:HB2	8:E:116:THR:O	2.11	0.50
15:M:46:LEU:HG	38:M:9416:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:441:A:H1'	1:0:442:A:N7	2.27	0.50
38:0:3205:HOH:O	12:J:46:ILE:HA	2.12	0.50
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.62	0.50
21:S:57:THR:HG22	21:S:58:MET:N	2.26	0.50
24:V:38:GLY:C	24:V:40:PRO:HD2	2.32	0.50
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.93	0.50
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.47	0.50
1:0:920:C:H5'	1:0:921:G:C4	2.46	0.50
1:0:2668:G:H2'	1:0:2669:U:C6	2.47	0.50
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.28	0.50
1:0:1201:C:H5"	38:0:6487:HOH:O	2.12	0.50
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.45	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.12	0.50
10:G:64:ASN:N	10:G:64:ASN:ND2	2.59	0.50
1:0:1375:A:C2'	1:0:1376:G:H5'	2.41	0.50
11:H:83:TYR:C	11:H:83:TYR:CD1	2.85	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.25	0.50
7:D:146:LYS:HZ3	16:N:107:ASN:ND2	2.07	0.50
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.94	0.50
1:0:2064:U:H4'	1:0:2653:A:OP1	2.11	0.50
20:R:27:HIS:O	20:R:31:ILE:HG13	2.12	0.50
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.50
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.33	0.49
9:F:46:GLU:OE2	9:F:100:ASP:HA	2.12	0.49
1:0:2036:C:O4'	13:K:44:LEU:HG	2.12	0.49
4:A:36:ASP:HB2	4:A:85:SER:H	1.77	0.49
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.93	0.49
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.27	0.49
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.94	0.49
30:2:5:LYS:O	30:2:9:LYS:HG3	2.12	0.49
8:E:119:HIS:O	8:E:140:ALA:HB1	2.12	0.49
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.12	0.49
5:B:294:TYR:HE2	38:B:9454:HOH:O	1.95	0.49
25:W:5:VAL:HG11	25:W:153:MET:CE	2.41	0.49
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.94	0.49
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.12	0.49
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.49
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.12	0.49
6:C:61:PHE:HB3	38:C:9242:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2710:U:H1'	38:0:7824:HOH:O	2.12	0.49
19:Q:16:ASN:HB2	38:Q:6597:HOH:O	2.11	0.49
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.94	0.49
2:9:3023:U:O2'	2:9:3024:U:H4'	2.12	0.49
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.49
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.77	0.49
38:0:3592:HOH:O	13:K:9:THR:HA	2.11	0.49
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.49
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.94	0.49
4:A:179:MET:HG2	4:A:186:TRP:CG	2.47	0.49
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.94	0.49
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.43	0.49
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.27	0.49
4:A:94:LEU:N	4:A:94:LEU:HD23	2.27	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.12	0.49
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.45	0.49
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.19	0.49
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.49
1:0:1820:G:C6	1:0:2030:A:C2	3.00	0.49
11:H:63:GLU:HA	38:H:9179:HOH:O	2.12	0.49
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.12	0.49
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.49
9:F:101:ALA:HA	38:F:5413:HOH:O	2.13	0.49
1:0:263:U:O4'	9:F:59:ILE:HD13	2.12	0.49
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.94	0.49
1:0:2392:C:H4'	38:Q:2875:HOH:O	2.13	0.49
1:0:1462:C:H2'	1:0:1463:A:C8	2.48	0.49
14:L:35:ARG:HD3	14:L:35:ARG:C	2.33	0.49
1:0:1733:A:H4'	5:B:212:GLN:HA	1.94	0.49
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
1:0:705:C:H2'	1:0:705:C:O2	2.13	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.94	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.12	0.49
25:W:26:ILE:HG22	38:W:5420:HOH:O	2.12	0.49
22:T:48:VAL:HG22	22:T:97:ARG:O	2.13	0.49
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:661:G:C5	1:0:686:A:C2	3.01	0.49
5:B:82:VAL:HG12	5:B:82:VAL:O	2.13	0.49
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.13	0.49
25:W:139:GLY:O	25:W:141:HIS:CD2	2.66	0.49
1:0:1202:A:H2'	1:0:1203:G:C5'	2.43	0.49
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.95	0.49
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.49
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.78	0.49
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.49
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.12	0.49
1:0:2894:C:O2'	1:0:2895:C:H5'	2.12	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
38:0:9532:HOH:O	4:A:11:ARG:HD3	2.12	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.24	0.49
1:0:2252:A:C5	1:0:2253:G:H1'	2.47	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
1:0:585:C:H5"	38:0:5151:HOH:O	2.13	0.49
38:0:5676:HOH:O	4:A:164:ARG:CZ	2.60	0.49
22:T:71:VAL:HG12	22:T:72:ILE:N	2.27	0.48
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.76	0.48
9:F:107:ASP:O	9:F:111:ILE:HG13	2.12	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.13	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
1:0:1878:G:H1'	38:0:6378:HOH:O	2.11	0.48
15:M:78:LYS:HD3	38:M:9434:HOH:O	2.13	0.48
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.48	0.48
4:A:32:VAL:HG12	4:A:34:ASP:N	2.27	0.48
15:M:166:ALA:HA	15:M:169:ARG:HH12	1.73	0.48
32:I:75:THR:OG1	32:I:112:LYS:NZ	2.45	0.48
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.48
17:O:77:ALA:HA	17:O:96:VAL:O	2.13	0.48
1:0:926:A:H5'	14:L:39:GLU:OE2	2.13	0.48
1:0:221:G:H2'	1:0:222:A:C8	2.48	0.48
8:E:9:GLU:HG3	8:E:10:ASP:N	2.28	0.48
4:A:215:ILE:HG13	4:A:216:SER:N	2.28	0.48
14:L:104:ASP:O	14:L:105:TYR:HB3	2.12	0.48
1:0:1427:A:H61	1:0:1440:U:C1'	2.25	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.43	0.48
1:0:282:C:H1'	1:0:368:C:H42	1.74	0.48
20:R:39:THR:HB	20:R:42:GLU:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:41:ARG:NH1	22:T:42:VAL:O	2.46	0.48
8:E:15:GLN:HG2	8:E:19:ASP:O	2.13	0.48
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.12	0.48
1:0:941:G:C5	1:0:942:U:C4	3.01	0.48
1:0:74:A:H2'	1:0:75:U:C6	2.48	0.48
1:0:1135:G:H5'	38:0:6188:HOH:O	2.12	0.48
21:S:23:LYS:HE2	38:S:3430:HOH:O	2.12	0.48
1:0:800:G:H4'	38:0:7283:HOH:O	2.13	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
1:0:2762:C:H3'	38:0:3673:HOH:O	2.13	0.48
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.27	0.48
1:0:1165:G:H1'	1:0:1174:A:H1'	1.96	0.48
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.48	0.48
32:I:96:PHE:HA	32:I:136:GLY:CA	2.44	0.48
1:0:1352:A:N1	6:C:48:SER:HB3	2.27	0.48
9:F:14:ASP:O	9:F:18:GLU:HG3	2.13	0.48
24:V:56:ILE:O	24:V:60:GLN:HG3	2.14	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
19:Q:14:LEU:HD21	19:Q:43:ILE:HD12	1.95	0.48
1:0:2730:G:O2'	1:0:2731:G:H5'	2.13	0.48
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.79	0.48
26:X:30:MET:CE	26:X:58:ALA:HB3	2.44	0.48
5:B:254:GLN:NE2	38:B:9390:HOH:O	2.46	0.48
22:T:75:GLU:O	22:T:76:ASP:HB2	2.12	0.48
8:E:15:GLN:NE2	8:E:40:VAL:O	2.46	0.48
1:0:1717:A:H5"	18:P:54:LYS:HB2	1.96	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.13	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.13	0.48
1:0:536:A:H3'	38:0:5327:HOH:O	2.12	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.13	0.48
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.94	0.48
1:0:1666:C:H2'	1:0:1667:A:C5'	2.44	0.48
12:J:133:GLY:O	12:J:137:GLU:HG3	2.14	0.48
8:E:69:ILE:HA	8:E:72:MET:HE2	1.95	0.48
5:B:84:LEU:HD23	5:B:142:LEU:CD2	2.42	0.48
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.42	0.48
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.48
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.40	0.48
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.45	0.48
1:0:827:A:H2'	1:0:828:G:O4'	2.14	0.48
7:D:27:ILE:HD11	7:D:37:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:87:THR:HG22	32:I:88:GLY:N	2.28	0.48
1:0:1201:C:H2'	1:0:1202:A:H5'	1.95	0.48
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.32	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.48
4:A:105:VAL:HG12	4:A:106:CYS:N	2.28	0.48
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.79	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.34	0.48
1:0:1829:A:H2'	1:0:1830:C:H5'	1.96	0.48
11:H:154:TYR:CD1	11:H:154:TYR:C	2.87	0.48
6:C:138:VAL:O	6:C:234:VAL:HA	2.13	0.48
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.48
1:0:1785:G:OP1	18:P:76:GLY:HA3	2.13	0.48
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.48
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.48
1:0:2718:C:H6	1:0:2718:C:H5'	1.78	0.48
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.29	0.48
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.45	0.48
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.95	0.48
14:L:80:ASP:HB2	14:L:90:ARG:O	2.14	0.48
1:0:2685:C:H1'	38:0:3745:HOH:O	2.13	0.48
1:0:1380:U:O4	1:0:2043:U:H4'	2.13	0.48
26:X:49:ARG:HG3	26:X:49:ARG:O	2.09	0.48
1:0:1790:C:H2'	1:0:1791:U:H6	1.79	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:1087:G:H4'	1:0:1088:A:OP1	2.14	0.48
1:0:1544:U:H2'	1:0:1545:C:H6	1.79	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.27	0.48
1:0:1130:U:H5'	38:0:7873:HOH:O	2.13	0.48
24:V:49:LEU:O	24:V:53:ILE:HG13	2.14	0.48
1:0:1300:G:H1'	38:0:4964:HOH:O	2.14	0.48
38:0:6937:HOH:O	27:Y:165:GLU:HB3	2.13	0.48
1:0:2613:G:O2'	1:0:2614:C:H5'	2.14	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.82	0.48
1:0:1202:A:C2'	1:0:1203:G:H5'	2.43	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2256:G:O2'	1:0:2257:G:H5'	2.14	0.47
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.13	0.47
1:0:170:U:H2'	1:0:171:C:H5'	1.95	0.47
6:C:236:THR:CG2	6:C:239:ALA:H	2.12	0.47
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:91:VAL:CG1	9:F:92:GLY:N	2.74	0.47
2:9:3039:U:H3'	2:9:3040:C:H5"	1.96	0.47
1:0:378:A:OP1	15:M:9:ARG:NH2	2.45	0.47
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.44	0.47
1:0:1681:G:H5"	1:0:1682:A:H5'	1.95	0.47
12:J:135:ILE:O	12:J:139:LEU:HG	2.13	0.47
5:B:195:ARG:CZ	5:B:323:LEU:HD13	2.44	0.47
1:0:2361:A:H2'	1:0:2362:A:C8	2.49	0.47
5:B:310:ARG:HD2	38:B:9452:HOH:O	2.14	0.47
12:J:46:ILE:O	12:J:46:ILE:HG12	2.13	0.47
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.47
1:0:1180:U:H2'	1:0:1181:A:C8	2.49	0.47
19:Q:18:PRO:O	19:Q:21:ARG:HB2	2.15	0.47
1:0:2782:G:O6	1:0:2790:C:H5"	2.14	0.47
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.44	0.47
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.49	0.47
5:B:128:ILE:O	5:B:131:ALA:HB3	2.14	0.47
1:0:415:A:O2'	1:0:416:G:H5'	2.15	0.47
6:C:37:ALA:O	6:C:41:ASN:ND2	2.48	0.47
1:0:1097:A:H5"	25:W:125:HIS:NE2	2.30	0.47
6:C:2:GLN:HB3	38:C:9181:HOH:O	2.14	0.47
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.47
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.97	0.47
1:0:821:U:H2'	1:0:822:C:H6	1.79	0.47
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.47
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.96	0.47
38:0:9672:HOH:O	29:1:1:THR:HA	2.13	0.47
1:0:2403:C:H3'	38:0:5482:HOH:O	2.15	0.47
1:0:1919:A:H4'	38:0:5131:HOH:O	2.13	0.47
16:N:27:LEU:HD22	16:N:50:LEU:HD13	1.96	0.47
16:N:37:ARG:NH2	38:N:9333:HOH:O	2.47	0.47
20:R:39:THR:HB	20:R:42:GLU:CD	2.35	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
18:P:10:ALA:O	18:P:13:VAL:HG12	2.14	0.47
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.97	0.47
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.15	0.47
6:C:234:VAL:HG22	6:C:234:VAL:O	2.14	0.47
1:0:2897:C:H2'	1:0:2898:G:H8	1.79	0.47
9:F:101:ALA:HB3	9:F:105:ASP:OD1	2.15	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1666:C:C2'	1:0:1667:A:H5"	2.45	0.47
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.29	0.47
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.47
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.46	0.47
5:B:162:MET:CE	5:B:308:LEU:HD21	2.44	0.47
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.45	0.47
15:M:61:ILE:N	15:M:61:ILE:HD12	2.29	0.47
3:4:74:DCZ:H2'1	3:4:75:DC:H5'	1.96	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.15	0.47
1:0:37:A:H2'	1:0:38:G:C8	2.49	0.47
1:0:587:A:H5"	38:0:7501:HOH:O	2.15	0.47
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.15	0.47
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.44	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.14	0.47
5:B:238:ASN:HD22	5:B:240:GLY:N	2.07	0.47
1:0:475:G:OP1	6:C:73:LEU:HD22	2.15	0.47
24:V:42:ASN:O	24:V:44:GLY:N	2.48	0.47
1:0:660:A:H4'	1:0:661:G:O5'	2.15	0.47
1:0:1495:C:H2'	1:0:1496:G:C8	2.50	0.47
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.15	0.47
5:B:16:ARG:NH1	38:B:9418:HOH:O	2.47	0.47
2:9:3055:U:H4'	2:9:3056:A:C8	2.50	0.47
12:J:75:PRO:HD3	12:J:136:SER:OG	2.15	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
6:C:55:ARG:NH2	29:1:56:GLU:OE2	2.39	0.47
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.15	0.47
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.14	0.47
38:0:5785:HOH:O	5:B:298:LYS:HD3	2.14	0.47
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.47
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.96	0.47
1:0:2428:G:N7	31:3:60:LYS:NZ	2.63	0.47
1:0:1183:C:N4	1:0:1184:C:H41	2.13	0.47
18:P:103:THR:HB	38:P:180:HOH:O	2.15	0.47
9:F:38:LYS:HZ3	15:M:3:SER:HA	1.80	0.47
1:0:2361:A:H5"	38:0:9323:HOH:O	2.15	0.47
1:0:1118:A:C8	1:0:1119:G:H5"	2.49	0.46
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.09	0.46
32:I:138:THR:HG22	32:I:139:ILE:H	1.79	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
5:B:258:GLY:H	5:B:260:HIS:HE1	1.56	0.46
8:E:73:PHE:O	8:E:76:VAL:HG22	2.14	0.46
25:W:11:VAL:O	25:W:12:ASN:HB2	2.14	0.46
1:0:553:G:P	27:Y:204:ARG:HH22	2.38	0.46
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.80	0.46
7:D:35:ALA:N	38:D:5576:HOH:O	2.47	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.79	0.46
9:F:26:THR:HG21	9:F:103:GLU:HG3	1.97	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.15	0.46
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.50	0.46
6:C:130:GLU:HA	6:C:130:GLU:OE1	2.15	0.46
4:A:35:GLY:O	4:A:36:ASP:CB	2.56	0.46
12:J:39:VAL:HG13	12:J:106:GLY:O	2.15	0.46
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.80	0.46
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.46	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.50	0.46
18:P:13:VAL:HG13	18:P:14:LEU:N	2.31	0.46
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.98	0.46
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.15	0.46
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.46
1:0:485:A:N3	1:0:487:G:H5"	2.30	0.46
25:W:130:HIS:O	25:W:136:GLY:HA3	2.14	0.46
1:0:1172:G:H1'	38:0:5254:HOH:O	2.15	0.46
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.48	0.46
32:I:106:LYS:O	32:I:110:GLU:HG3	2.15	0.46
1:0:2748:G:H1'	38:0:8206:HOH:O	2.14	0.46
2:9:3050:G:H2'	2:9:3051:A:C8	2.50	0.46
38:0:3949:HOH:O	17:O:3:THR:HG21	2.15	0.46
8:E:87:PHE:O	8:E:93:MET:HE3	2.15	0.46
1:0:2694:A:H5"	8:E:90:HIS:CE1	2.51	0.46
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.80	0.46
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.97	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.79	0.46
38:0:9868:HOH:O	25:W:119:HIS:HE1	1.97	0.46
10:G:64:ASN:O	10:G:68:GLU:HG3	2.16	0.46
1:0:776:A:OP1	29:1:28:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2301:A:H5"	1:0:2302:A:H5'	1.98	0.46
1:0:1385:G:O3'	26:X:49:ARG:NH1	2.48	0.46
28:Z:81:ARG:O	28:Z:82:SER:C	2.53	0.46
1:0:2866:U:H4'	1:0:2867:G:H5'	1.97	0.46
1:0:424:C:H2'	1:0:425:U:C6	2.50	0.46
6:C:242:GLU:HG3	38:C:9178:HOH:O	2.15	0.46
1:0:29:C:O2'	1:0:30:U:H5'	2.16	0.46
1:0:1119:G:H8	12:J:52:GLN:NE2	2.13	0.46
25:W:149:LEU:HG	25:W:153:MET:CE	2.46	0.46
23:U:9:CYS:HA	23:U:52:THR:CG2	2.39	0.46
16:N:110:THR:HB	16:N:113:SER:HG	1.79	0.46
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.45	0.46
1:0:775:G:OP1	29:1:16:HIS:HE1	1.99	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.96	0.46
1:0:2708:G:N2	13:K:1:MET:O	2.47	0.46
1:0:236:A:H4'	1:0:237:G:H5'	1.97	0.46
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.98	0.46
1:0:2487:C:H5	38:0:5168:HOH:O	1.98	0.46
24:V:1:THR:O	24:V:4:HIS:CE1	2.69	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
14:L:145:LEU:O	14:L:148:GLU:HG3	2.15	0.46
1:0:2064:U:H5'	1:0:2652:U:H4'	1.98	0.46
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.81	0.46
18:P:40:VAL:O	18:P:44:VAL:HG23	2.15	0.46
1:0:482:G:H4'	1:0:508:A:N1	2.31	0.46
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.98	0.46
1:0:1278:A:H4'	1:0:1279:U:C4	2.50	0.46
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.16	0.46
1:0:558:C:H2'	1:0:559:U:H5"	1.97	0.46
1:0:2269:C:C2'	1:0:2270:G:H5'	2.46	0.46
1:0:1205:U:C2'	1:0:1206:U:H5"	2.45	0.46
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.46
1:0:2415:A:N3	16:N:26:LEU:HD13	2.31	0.46
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.45	0.46
1:0:1427:A:N6	1:0:1440:U:H1'	2.31	0.46
11:H:154:TYR:HD1	11:H:154:TYR:C	2.18	0.46
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.14	0.46
1:0:2324:G:H4'	1:0:2418:G:O2'	2.15	0.46
1:0:87:C:H2'	30:2:28:LYS:O	2.16	0.46
1:0:21:G:H5"	20:R:2:ILE:HA	1.96	0.46
16:N:154:LEU:C	16:N:156:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1086:A:OP1	25:W:9:GLY:N	2.43	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.51	0.46
1:0:2445:U:H2'	1:0:2446:G:C8	2.51	0.46
15:M:64:ARG:HD2	38:M:9383:HOH:O	2.15	0.46
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	1.97	0.46
1:0:2670:G:O2'	1:0:2671:U:H5'	2.16	0.46
12:J:52:GLN:HG3	12:J:53:ILE:H	1.80	0.46
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.44	0.46
1:0:88:G:H2'	1:0:89:G:C8	2.51	0.46
29:1:25:LYS:HD2	30:2:49:GLU:N	2.30	0.46
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.46
9:F:48:VAL:HG23	9:F:74:PHE:HB2	1.97	0.46
1:0:1878:G:O2'	1:0:1879:U:C6	2.67	0.46
36:0:9303:CL:CL	30:2:2:LYS:HE3	2.52	0.46
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.98	0.46
1:0:2832:C:H5	38:0:7432:HOH:O	1.98	0.46
4:A:165:THR:O	4:A:165:THR:HG22	2.15	0.46
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.44	0.46
25:W:21:LEU:HD21	25:W:48:VAL:HG13	1.98	0.46
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.51	0.46
1:0:2365:G:H4'	19:Q:45:PRO:O	2.16	0.46
12:J:107:ASN:HD22	12:J:107:ASN:C	2.16	0.46
1:0:793:A:C5'	18:P:83:LYS:HG2	2.41	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.46
9:F:33:THR:HG21	9:F:59:ILE:O	2.16	0.46
1:0:1613:C:H2'	1:0:1614:G:O4'	2.15	0.46
7:D:140:ARG:O	7:D:144:ARG:HG2	2.16	0.46
38:0:4054:HOH:O	22:T:9:LYS:HD3	2.16	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.45	0.45
20:R:17:MET:CE	20:R:19:ARG:CZ	2.94	0.45
32:I:96:PHE:HA	32:I:136:GLY:HA3	1.97	0.45
1:0:2472:C:O2'	1:0:2634:G:H4'	2.16	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.98	0.45
4:A:36:ASP:C	4:A:38:ILE:N	2.69	0.45
32:I:102:VAL:O	32:I:106:LYS:HG3	2.17	0.45
7:D:166:ILE:HB	38:D:6326:HOH:O	2.15	0.45
7:D:81:GLU:C	7:D:83:PHE:H	2.20	0.45
26:X:43:VAL:CG1	26:X:44:ASP:H	2.24	0.45
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.45
16:N:34:LEU:HD22	16:N:129:ILE:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.98	0.45
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.45
1:0:289:G:N2	1:0:363:A:H2	2.15	0.45
1:0:1168:C:H4'	38:I:5128:HOH:O	2.15	0.45
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.47	0.45
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.80	0.45
1:0:1120:U:H5"	1:0:1120:U:C6	2.51	0.45
1:0:894:A:C2	6:C:87:ARG:NH2	2.84	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
5:B:97:LEU:HD21	38:B:9444:HOH:O	2.17	0.45
1:0:2372:A:H2'	1:0:2373:U:C6	2.52	0.45
21:S:52:VAL:C	21:S:53:ASN:HD22	2.20	0.45
1:0:500:G:H21	20:R:98:ASN:HD21	1.62	0.45
1:0:156:C:H5"	15:M:171:ARG:CD	2.24	0.45
32:I:112:LYS:O	32:I:116:LEU:HG	2.16	0.45
22:T:49:GLU:HG3	22:T:97:ARG:HB3	1.97	0.45
13:K:75:ARG:O	13:K:93:ASN:HA	2.16	0.45
1:0:2415:A:C2	16:N:25:ARG:HB3	2.52	0.45
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.45
20:R:132:ARG:CZ	38:R:9383:HOH:O	2.65	0.45
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.99	0.45
1:0:1309:U:O2'	1:0:1310:U:H5'	2.15	0.45
14:L:34:GLY:C	14:L:36:ASP:H	2.20	0.45
26:X:7:GLU:HA	26:X:74:ALA:O	2.16	0.45
12:J:47:THR:O	12:J:53:ILE:HD11	2.17	0.45
4:A:36:ASP:CG	4:A:85:SER:HB2	2.36	0.45
7:D:159:PRO:O	7:D:163:VAL:HG23	2.16	0.45
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.45
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.45
1:0:2467:A:H1'	38:0:5014:HOH:O	2.17	0.45
1:0:2563:U:H2'	1:0:2565:C:O5'	2.16	0.45
1:0:270:U:H1'	38:0:4020:HOH:O	2.16	0.45
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.45
6:C:165:ASP:O	6:C:168:ARG:HB3	2.17	0.45
1:0:2385:G:H2'	1:0:2386:U:H6	1.80	0.45
9:F:46:GLU:O	9:F:73:PRO:HD2	2.17	0.45
1:0:678:G:OP2	6:C:107:ARG:NH2	2.50	0.45
1:0:290:C:O2'	1:0:291:C:H5'	2.15	0.45
26:X:75:ALA:O	26:X:83:ALA:HA	2.16	0.45
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.17	0.45
15:M:167:GLY:O	15:M:171:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:HG12	4:A:192:VAL:O	2.17	0.45
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.99	0.45
38:0:3990:HOH:O	8:E:143:GLN:HG2	2.16	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.17	0.45
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.86	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.17	0.45
1:0:1314:U:H2'	38:0:6137:HOH:O	2.15	0.45
6:C:214:THR:HG23	38:C:9234:HOH:O	2.15	0.45
1:0:2816:A:H5"	1:0:2817:G:H5'	1.99	0.45
1:0:2004:U:H4'	38:0:5579:HOH:O	2.16	0.45
1:0:1711:A:O2'	1:0:1712:A:H5'	2.17	0.45
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.52	0.45
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.46	0.45
16:N:93:GLN:NE2	16:N:93:GLN:HA	2.23	0.45
1:0:559:U:H2'	1:0:560:C:O4'	2.17	0.45
16:N:140:GLN:HA	16:N:143:ARG:HD3	1.99	0.45
5:B:86:ALA:HA	38:B:9380:HOH:O	2.16	0.45
5:B:51:VAL:HG13	5:B:51:VAL:O	2.16	0.45
8:E:43:ASP:O	8:E:45:ASP:N	2.47	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.45
38:0:7005:HOH:O	16:N:4:PRO:HD2	2.16	0.45
1:0:703:G:O2'	1:0:704:C:H5'	2.17	0.45
14:L:66:VAL:HG23	14:L:67:ARG:N	2.32	0.45
1:0:2281:C:C2'	1:0:2282:U:H5'	2.46	0.45
26:X:66:THR:HG22	26:X:67:PRO:O	2.17	0.45
1:0:907:A:H2'	1:0:908:A:H8	1.81	0.45
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.47	0.45
12:J:47:THR:HG22	12:J:48:GLY:N	2.31	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.29	0.45
5:B:276:ASP:HB3	5:B:291:ASP:OD1	2.17	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
24:V:46:ILE:HA	24:V:49:LEU:HD12	1.99	0.45
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.45
1:0:243:A:H61	1:0:269:G:H1'	1.81	0.45
1:0:23:G:H1'	1:0:520:A:N6	2.32	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45
38:0:5725:HOH:O	10:G:12:ILE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:133:ARG:HG2	6:C:135:GLU:O	2.17	0.45
1:0:920:C:H5"	1:0:921:G:O5'	2.17	0.45
1:0:2698:G:H2'	1:0:2699:A:O4'	2.16	0.45
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.82	0.45
8:E:34:TRP:HA	38:E:4572:HOH:O	2.17	0.45
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.32	0.45
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.15	0.45
1:0:451:C:O2'	1:0:452:G:H5'	2.17	0.45
2:9:3106:C:O2'	2:9:3107:C:H5'	2.16	0.45
32:I:132:CYS:C	32:I:134:SER:H	2.19	0.44
8:E:15:GLN:CG	8:E:20:ILE:HG12	2.47	0.44
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.16	0.44
16:N:39:SER:HB3	16:N:42:HIS:H	1.82	0.44
1:0:1289:C:O2'	1:0:1290:G:H5'	2.16	0.44
16:N:63:SER:HB2	16:N:75:THR:HB	1.99	0.44
14:L:12:THR:HG21	14:L:16:GLY:O	2.17	0.44
1:0:1304:U:H2'	1:0:1305:C:C6	2.52	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.16	0.44
31:3:65:THR:CG2	31:3:67:LEU:HG	2.47	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.17	0.44
12:J:99:GLU:HA	38:J:9371:HOH:O	2.17	0.44
1:0:1942:A:O2'	1:0:1943:C:H5'	2.17	0.44
25:W:38:THR:O	25:W:42:ARG:HB2	2.17	0.44
5:B:198:GLU:HA	38:B:9461:HOH:O	2.15	0.44
8:E:43:ASP:HA	38:E:5864:HOH:O	2.16	0.44
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.57	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.44
1:0:816:G:C6	1:0:817:G:N1	2.85	0.44
38:0:9937:HOH:O	9:F:38:LYS:HE2	2.17	0.44
1:0:1200:A:H4'	38:0:7550:HOH:O	2.17	0.44
38:0:9851:HOH:O	18:P:81:LYS:HG2	2.18	0.44
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.00	0.44
1:0:1657:A:H2'	1:0:1658:A:C8	2.52	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.44
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.99	0.44
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.44
1:0:2715:G:O2'	5:B:262:ARG:HD2	2.17	0.44
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.44
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.86	0.44
1:0:35:U:H5'	6:C:47:GLY:O	2.17	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:133:ARG:NE	6:C:135:GLU:O	2.50	0.44
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.44
1:0:2061:C:C2'	1:0:2062:A:H5'	2.48	0.44
1:0:2438:G:H2'	1:0:2439:C:O4'	2.17	0.44
4:A:53:ALA:HB3	38:A:9400:HOH:O	2.17	0.44
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.15	0.44
1:0:2036:C:C4'	13:K:44:LEU:HG	2.47	0.44
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.44
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.99	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.52	0.44
16:N:18:THR:HG21	38:N:9348:HOH:O	2.17	0.44
32:I:92:PRO:O	32:I:94:GLU:HG3	2.16	0.44
27:Y:112:GLU:OE1	27:Y:115:ARG:NH1	2.50	0.44
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.98	0.44
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.98	0.44
38:0:7568:HOH:O	4:A:177:HIS:HE1	2.01	0.44
1:0:1249:U:H2'	1:0:1250:C:C6	2.52	0.44
7:D:158:ASN:HB2	7:D:161:ASP:OD2	2.16	0.44
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.16	0.44
13:K:90:PHE:CD1	13:K:90:PHE:N	2.86	0.44
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.99	0.44
25:W:88:THR:CG2	25:W:110:GLN:HE21	2.22	0.44
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.52	0.44
16:N:154:LEU:HD12	16:N:156:GLU:O	2.17	0.44
6:C:246:ARG:NE	38:C:9220:HOH:O	2.51	0.44
9:F:50:VAL:HG11	9:F:60:VAL:HG11	1.99	0.44
32:I:101:SER:OG	32:I:104:GLN:HG3	2.18	0.44
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.44
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.44
1:0:1544:U:H2'	1:0:1545:C:C6	2.53	0.44
1:0:2403:C:H2'	1:0:2404:G:O5'	2.17	0.44
1:0:2061:C:H2'	1:0:2062:A:H5'	2.00	0.44
1:0:113:A:OP2	1:0:114:A:H2'	2.18	0.44
8:E:21:THR:HG23	8:E:30:THR:OG1	2.17	0.44
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.18	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.44
26:X:70:ILE:HG23	26:X:70:ILE:O	2.17	0.44
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.16	0.44
6:C:16:VAL:CG1	6:C:17:ASP:N	2.80	0.44
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.47	0.44
22:T:48:VAL:HG22	22:T:97:ARG:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:H5'	17:O:3:THR:CG2	2.48	0.44
1:0:968:G:H1'	11:H:32:LYS:HD2	2.00	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
16:N:11:ARG:NH2	38:N:9316:HOH:O	2.51	0.44
20:R:40:ALA:O	20:R:44:VAL:HG23	2.18	0.44
1:0:1632:A:C2'	1:0:1633:C:H5'	2.47	0.44
11:H:38:LYS:HE2	11:H:42:ASP:CB	2.47	0.44
1:0:1067:A:H5'	38:0:4638:HOH:O	2.18	0.44
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.22	0.44
25:W:122:ARG:NH1	25:W:122:ARG:HG2	2.25	0.44
5:B:212:GLN:HG2	5:B:257:THR:OG1	2.17	0.44
7:D:44:ILE:HG12	7:D:83:PHE:CE1	2.49	0.44
4:A:130:THR:HG22	4:A:131:HIS:N	2.32	0.44
7:D:76:ARG:O	7:D:77:ASP:HB2	2.16	0.44
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.00	0.44
7:D:173:GLU:O	7:D:174:VAL:C	2.56	0.44
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.21	0.44
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.44
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.99	0.44
1:0:926:A:O2'	14:L:41:HIS:CD2	2.70	0.44
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.16	0.44
6:C:65:ARG:HG3	6:C:67:GLN:HB2	2.00	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
1:0:2015:A:H2'	1:0:2016:U:O4'	2.17	0.44
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.44
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.17	0.44
23:U:52:THR:CG2	23:U:54:THR:HB	2.48	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
6:C:233:THR:HG22	6:C:234:VAL:H	1.83	0.44
1:0:1829:A:H5"	38:0:3389:HOH:O	2.16	0.44
5:B:14:GLY:HA3	38:B:9410:HOH:O	2.17	0.44
1:0:425:U:H4'	38:0:7160:HOH:O	2.17	0.44
16:N:63:SER:O	16:N:66:LEU:HB2	2.17	0.44
16:N:64:SER:C	16:N:66:LEU:H	2.21	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.18	0.44
25:W:73:LEU:O	25:W:74:GLU:HG2	2.18	0.44
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.00	0.44
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.75	0.44
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.75	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.44
5:B:7:ARG:HD3	5:B:9:GLY:O	2.18	0.44
1:0:248:A:H5'	1:0:249:G:OP2	2.18	0.44
1:0:1204:C:H1'	38:0:5023:HOH:O	2.18	0.44
1:0:2511:A:H2'	1:0:2512:U:O4'	2.18	0.44
1:0:2329:C:O2'	1:0:2330:U:H5'	2.17	0.44
18:P:91:LYS:O	18:P:95:GLU:HG3	2.18	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.33	0.44
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.83	0.44
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.15	0.44
25:W:143:THR:N	38:W:3520:HOH:O	2.51	0.44
5:B:304:PRO:HD2	5:B:307:ARG:NH1	2.32	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
6:C:5:ILE:CD1	6:C:16:VAL:HG23	2.40	0.43
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.00	0.43
25:W:64:THR:O	25:W:68:THR:HG22	2.18	0.43
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.99	0.43
25:W:105:THR:HG23	25:W:106:THR:N	2.31	0.43
6:C:136:VAL:HA	6:C:137:PRO:C	2.39	0.43
1:0:999:C:H2'	1:0:1000:C:O4'	2.18	0.43
17:O:96:VAL:HG12	17:O:100:GLN:HB2	1.99	0.43
1:0:958:G:H2'	1:0:959:C:H6	1.82	0.43
1:0:2684:A:H2'	1:0:2685:C:C6	2.53	0.43
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.53	0.43
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.43
1:0:1224:G:H2'	1:0:1225:C:C6	2.52	0.43
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.18	0.43
1:0:1926:G:H2'	1:0:1927:A:C8	2.53	0.43
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.43
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.48	0.43
16:N:154:LEU:O	16:N:155:GLU:CB	2.65	0.43
2:9:3049:G:C2'	2:9:3050:G:H5'	2.48	0.43
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.43
5:B:175:LEU:O	5:B:178:ALA:HB3	2.18	0.43
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.31	0.43
4:A:43:VAL:HG21	4:A:59:GLU:OE2	2.18	0.43
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.99	0.43
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.43
1:0:806:A:H2'	1:0:807:A:O4'	2.18	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
1:0:1168:C:H5"	32:I:87:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.43
5:B:51:VAL:HG13	5:B:53:LEU:CD1	2.48	0.43
6:C:168:ARG:NH2	6:C:190:ALA:O	2.51	0.43
7:D:58:VAL:HG12	7:D:60:GLU:HG2	2.00	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43
1:0:1504:A:H5'	38:0:4704:HOH:O	2.17	0.43
1:0:2684:A:H1'	38:0:3235:HOH:O	2.18	0.43
1:0:1682:A:H2'	38:0:3108:HOH:O	2.18	0.43
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.43
20:R:114:VAL:HA	20:R:144:GLU:O	2.18	0.43
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:946:C:H2'	1:0:947:U:C6	2.53	0.43
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.43
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.43
14:L:130:ARG:O	14:L:134:GLU:HG3	2.18	0.43
24:V:12:THR:HG23	24:V:14:ALA:N	2.21	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.43
20:R:99:ALA:CB	20:R:109:MET:HE1	2.39	0.43
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.43
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.43
5:B:51:VAL:HG13	5:B:53:LEU:HD11	2.00	0.43
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.43
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.33	0.43
1:0:1528:A:H2'	1:0:1529:G:O4'	2.18	0.43
1:0:1973:A:H8	1:0:1973:A:H5'	1.83	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:2338:G:H1'	7:D:105:SER:OG	2.18	0.43
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.54	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.18	0.43
1:0:574:C:H2'	1:0:575:G:O4'	2.19	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.18	0.43
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.43
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.43
1:0:926:A:O2'	14:L:41:HIS:HD2	2.01	0.43
14:L:59:GLU:HG2	14:L:104:ASP:CG	2.39	0.43
20:R:47:LEU:O	20:R:51:ILE:HG13	2.18	0.43
1:0:2365:G:P	19:Q:15:LYS:HG3	2.59	0.43
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.59	0.43
38:0:7762:HOH:O	31:3:60:LYS:HG3	2.17	0.43
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:79:MET:O	5:B:80:ARG:HG3	2.19	0.43
8:E:145:ALA:HB1	8:E:168:ILE:HD11	2.01	0.43
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.19	0.43
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.53	0.43
4:A:51:ARG:NH1	4:A:120:ARG:O	2.51	0.43
5:B:27:ASN:N	5:B:27:ASN:HD22	2.01	0.43
15:M:182:LYS:HD2	15:M:193:LYS:HB2	1.99	0.43
1:0:475:G:H5'	6:C:73:LEU:HD23	2.00	0.43
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.37	0.43
1:0:120:A:H2'	1:0:120:A:N3	2.34	0.43
1:0:1878:G:O2'	1:0:1879:U:OP2	2.35	0.43
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.84	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.43
1:0:622:G:O2'	1:0:623:U:H5'	2.19	0.43
8:E:156:ASP:N	8:E:156:ASP:OD1	2.51	0.43
7:D:152:PRO:O	7:D:156:ARG:HG2	2.18	0.43
1:0:1189:A:O2'	1:0:1208:C:H2'	2.18	0.43
1:0:392:U:O2'	15:M:182:LYS:HE2	2.18	0.43
5:B:52:VAL:O	5:B:53:LEU:HD12	2.19	0.43
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.54	0.43
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.83	0.43
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.48	0.43
1:0:644:G:H1'	38:0:6645:HOH:O	2.19	0.43
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.86	0.43
1:0:1419:U:H5'	1:0:1420:C:OP2	2.18	0.43
6:C:150:THR:HA	6:C:203:ALA:O	2.18	0.43
1:0:2379:G:H5'	1:0:2381:C:O4'	2.18	0.43
1:0:1636:G:O2'	1:0:1637:A:H5'	2.18	0.43
1:0:1930:A:H2'	1:0:1931:A:C8	2.53	0.43
10:G:23:ILE:O	10:G:27:ILE:HG13	2.19	0.43
4:A:114:ASP:C	4:A:114:ASP:OD1	2.56	0.43
6:C:236:THR:O	6:C:239:ALA:N	2.51	0.43
38:0:7650:HOH:O	4:A:211:LYS:NZ	2.51	0.43
15:M:182:LYS:O	15:M:194:ALA:HB2	2.18	0.43
13:K:113:ILE:HG22	13:K:114:ALA:O	2.19	0.43
15:M:59:GLY:C	15:M:141:ILE:HD11	2.39	0.43
2:9:3003:A:H2	2:9:3021:G:N3	2.17	0.43
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.47	0.43
7:D:170:TYR:CD1	7:D:170:TYR:N	2.86	0.43
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.43
1:0:154:C:P	15:M:188:ARG:HH12	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2715:G:N2	5:B:264:GLU:OE1	2.52	0.43
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.43
26:X:76:ARG:O	26:X:77:PHE:HB3	2.18	0.43
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.01	0.43
5:B:17:LYS:O	5:B:260:HIS:HD2	2.02	0.43
15:M:31:TRP:HA	15:M:34:GLU:HG3	2.01	0.43
1:0:2780:C:H2'	1:0:2781:U:C6	2.54	0.43
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.34	0.43
1:0:222:A:H2'	1:0:223:G:O4'	2.18	0.43
5:B:14:GLY:HA2	5:B:15:PRO:C	2.40	0.43
11:H:80:GLU:HA	38:H:9183:HOH:O	2.18	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
38:0:9991:HOH:O	27:Y:163:THR:HG23	2.19	0.43
1:0:912:A:C4	1:0:1294:A:C2	3.07	0.43
1:0:709:G:O2'	17:O:25:VAL:CG1	2.67	0.43
1:0:2134:G:C6	1:0:2258:A:C8	3.07	0.43
18:P:22:TRP:CH2	18:P:24:ASN:HA	2.54	0.43
32:I:132:CYS:CB	32:I:137:VAL:HB	2.35	0.42
32:I:92:PRO:HG3	38:I:6825:HOH:O	2.18	0.42
5:B:79:MET:C	5:B:80:ARG:HG3	2.39	0.42
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.42
8:E:145:ALA:O	8:E:148:ILE:HB	2.19	0.42
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.49	0.42
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.01	0.42
1:0:1675:C:H5"	30:2:5:LYS:HD2	2.01	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.01	0.42
32:I:124:ALA:O	32:I:128:VAL:HG23	2.19	0.42
6:C:91:PRO:O	6:C:93:LYS:HG3	2.19	0.42
1:0:1008:C:H5"	11:H:16:ARG:HH12	1.84	0.42
1:0:737:A:H2'	1:0:738:G:O4'	2.19	0.42
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.19	0.42
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.42
7:D:23:VAL:CG2	7:D:23:VAL:O	2.66	0.42
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.47	0.42
1:0:2251:G:H2'	1:0:2252:A:H8	1.81	0.42
1:0:795:G:N3	1:0:817:G:C2	2.87	0.42
1:0:1309:U:H2'	1:0:1310:U:O4'	2.19	0.42
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.20	0.42
1:0:2820:A:H2'	1:0:2821:C:O4'	2.18	0.42
1:0:2067:A:H2'	1:0:2068:G:O4'	2.19	0.42
38:E:2512:HOH:O	12:J:127:ILE:HD11	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2815:G:N7	12:J:80:LYS:NZ	2.65	0.42
15:M:43:PRO:HG3	15:M:62:VAL:HG21	2.01	0.42
1:0:638:C:H2'	1:0:639:A:C8	2.54	0.42
5:B:207:LYS:HG2	5:B:304:PRO:HB3	2.01	0.42
12:J:130:VAL:CG1	12:J:131:THR:N	2.82	0.42
16:N:34:LEU:HA	16:N:47:LEU:CD2	2.49	0.42
11:H:20:ILE:HG23	11:H:120:ILE:HD11	2.00	0.42
1:0:2467:A:O2'	1:0:2468:A:H2'	2.19	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
14:L:59:GLU:HG2	14:L:104:ASP:OD2	2.19	0.42
8:E:35:TYR:CD2	8:E:36:PRO:HD2	2.54	0.42
19:Q:64:GLU:HA	19:Q:64:GLU:OE1	2.19	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.58	0.42
1:0:2255:A:C6	1:0:2256:G:C5	3.08	0.42
15:M:24:GLN:O	15:M:28:GLN:HG3	2.19	0.42
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.42
13:K:22:ASP:O	13:K:110:LYS:HE3	2.20	0.42
1:0:2564:G:OP2	1:0:2565:C:H5"	2.19	0.42
2:9:3034:A:H2'	2:9:3035:C:O4'	2.19	0.42
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.55	0.42
1:0:2314:G:C2'	1:0:2315:C:H5'	2.49	0.42
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.49	0.42
23:U:37:GLU:O	23:U:40:ALA:HB3	2.20	0.42
6:C:16:VAL:CG1	6:C:17:ASP:H	2.30	0.42
25:W:38:THR:CG2	25:W:39:ASP:N	2.82	0.42
7:D:81:GLU:C	7:D:83:PHE:N	2.73	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.45	0.42
7:D:95:THR:HG1	7:D:174:VAL:HG22	1.81	0.42
1:0:2346:C:O2'	7:D:52:THR:HG21	2.19	0.42
5:B:277:GLU:N	5:B:278:PRO:CD	2.83	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.42
20:R:125:ARG:HG2	38:R:9344:HOH:O	2.19	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.49	0.42
6:C:13:ASP:OD1	6:C:13:ASP:O	2.37	0.42
22:T:71:VAL:CG1	22:T:72:ILE:N	2.82	0.42
7:D:66:GLY:O	7:D:67:ASP:HB3	2.18	0.42
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.50	0.42
20:R:17:MET:HE3	20:R:19:ARG:NE	2.34	0.42
27:Y:144:ARG:NH2	38:Y:9407:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2524:G:H21	1:0:2526:C:H41	1.68	0.42
5:B:55:ASN:HB3	5:B:63:GLU:HA	2.01	0.42
8:E:108:LEU:HD11	8:E:164:ASP:HB2	2.02	0.42
19:Q:93:ARG:NH1	19:Q:93:ARG:HG3	2.35	0.42
1:0:37:A:H2'	1:0:38:G:H8	1.84	0.42
28:Z:39:CYS:HA	28:Z:47:VAL:CG2	2.50	0.42
1:0:67:A:H5"	1:0:69:A:C8	2.55	0.42
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.03	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.53	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.00	0.42
1:0:2761:A:H2'	38:0:5903:HOH:O	2.18	0.42
1:0:514:G:OP1	1:0:514:G:H2'	2.20	0.42
1:0:1160:G:O2'	1:0:1190:G:H1'	2.19	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.49	0.42
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.33	0.42
26:X:30:MET:HE2	26:X:58:ALA:HB3	2.02	0.42
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.42
7:D:88:LEU:O	7:D:90:LEU:N	2.53	0.42
26:X:15:ARG:HB3	26:X:15:ARG:NH1	2.34	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.19	0.42
1:0:820:G:O2'	1:0:856:G:H4'	2.19	0.42
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.37	0.42
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.42
1:0:1380:U:H5'	38:0:9533:HOH:O	2.20	0.42
1:0:1483:C:O2'	1:0:1484:G:H5'	2.19	0.42
1:0:347:A:O2'	6:C:205:ARG:NH2	2.53	0.42
1:0:1771:U:O2	28:Z:19:GLY:HA2	2.19	0.42
1:0:1409:G:H5'	38:0:4024:HOH:O	2.19	0.42
1:0:783:C:OP1	4:A:180:LYS:HE3	2.19	0.42
1:0:371:U:H2'	1:0:372:A:H8	1.84	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.85	0.42
6:C:237:GLU:HB2	38:C:9226:HOH:O	2.18	0.42
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.45	0.42
4:A:130:THR:HG22	4:A:131:HIS:O	2.19	0.42
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.02	0.42
32:I:99:ASP:O	32:I:100:LEU:HD23	2.20	0.42
1:0:1058:A:H2'	1:0:1060:C:C5'	2.48	0.42
1:0:1634:G:H2'	1:0:1635:U:C6	2.54	0.42
11:H:66:ARG:HD3	38:H:9179:HOH:O	2.19	0.42
4:A:109:GLU:HG2	4:A:116:GLY:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.08	0.42
1:0:236:A:H8	1:0:236:A:OP1	2.03	0.42
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.01	0.42
1:0:1525:G:H5'	1:0:1526:A:OP2	2.20	0.42
5:B:270:ILE:O	5:B:271:ASP:HB2	2.19	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.84	0.42
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.42
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.42
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.81	0.42
14:L:120:LEU:HD12	14:L:133:VAL:HG21	2.01	0.42
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.49	0.42
1:0:475:G:OP1	6:C:73:LEU:CD2	2.68	0.42
6:C:27:ARG:CG	6:C:27:ARG:HH11	2.32	0.42
1:0:2266:A:H2'	1:0:2267:G:C8	2.55	0.42
1:0:164:G:O3'	14:L:30:ARG:HB2	2.20	0.42
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.20	0.42
1:0:125:U:H2'	38:0:4064:HOH:O	2.18	0.42
1:0:1697:G:O2'	1:0:1698:U:H5'	2.20	0.42
1:0:1331:A:OP2	27:Y:142:SER:OG	2.34	0.42
1:0:1335:C:H2'	1:0:1336:U:C6	2.55	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.54	0.42
1:0:645:U:O2	1:0:761:A:H2	2.03	0.42
1:0:42:C:H1'	38:0:4957:HOH:O	2.19	0.42
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.85	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.73	0.42
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.42
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.85	0.42
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.85	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.31	0.42
26:X:78:GLU:CG	26:X:79:GLU:N	2.82	0.42
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.20	0.42
5:B:280:VAL:HG22	5:B:333:GLU:O	2.19	0.42
9:F:99:THR:HA	38:F:3461:HOH:O	2.19	0.42
1:0:700:A:C2	14:L:71:GLU:HG2	2.55	0.42
27:Y:153:GLN:HG3	27:Y:160:LYS:O	2.20	0.42
1:0:813:C:H2'	1:0:814:G:O4'	2.20	0.42
11:H:166:SER:HB3	38:H:9143:HOH:O	2.20	0.41
1:0:2269:C:H2'	1:0:2270:G:C5'	2.50	0.41
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.41
16:N:73:ALA:HB2	16:N:163:PHE:CE2	2.55	0.41
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:704:C:H2'	1:0:705:C:H6	1.85	0.41
8:E:4:GLU:HG2	8:E:48:VAL:HG22	2.02	0.41
1:0:2330:U:H4'	1:0:2331:C:OP1	2.20	0.41
30:2:19:SER:HB3	38:2:4479:HOH:O	2.20	0.41
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.41
20:R:82:GLU:O	20:R:86:LYS:HG3	2.20	0.41
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.68	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.83	0.41
7:D:23:VAL:HG22	7:D:73:VAL:HB	2.02	0.41
16:N:157:PRO:HA	38:N:9323:HOH:O	2.21	0.41
16:N:67:ALA:C	16:N:69:TYR:N	2.74	0.41
18:P:16:VAL:HG12	18:P:17:GLY:N	2.35	0.41
6:C:27:ARG:CG	6:C:27:ARG:NH1	2.83	0.41
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.40	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.01	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.87	0.41
14:L:67:ARG:O	14:L:71:GLU:HG3	2.20	0.41
1:0:2821:C:O2'	5:B:114:ASP:O	2.36	0.41
1:0:1948:G:O2'	1:0:1949:G:H5'	2.21	0.41
1:0:2604:A:H5'	38:0:6052:HOH:O	2.19	0.41
1:0:401:C:H2'	1:0:402:U:C6	2.55	0.41
4:A:161:GLY:O	28:Z:68:SER:OG	2.34	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
1:0:419:A:H1'	1:0:1921:A:C2	2.55	0.41
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.41
11:H:17:ARG:HD3	11:H:23:ILE:CD1	2.50	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.83	0.41
1:0:1046:G:N3	1:0:1082:A:H2	2.18	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.55	0.41
1:0:39:G:H2'	1:0:40:C:O4'	2.20	0.41
20:R:9:ASP:HA	20:R:10:PRO:HD2	1.92	0.41
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.35	0.41
1:0:1701:A:H5"	1:0:1702:U:H3'	2.01	0.41
5:B:258:GLY:N	5:B:260:HIS:CE1	2.85	0.41
1:0:1377:C:C5'	1:0:1377:C:H6	2.32	0.41
6:C:27:ARG:HG2	6:C:27:ARG:NH1	2.34	0.41
1:0:138:U:OP2	1:0:139:C:H5	2.03	0.41
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.53	0.41
18:P:141:ILE:C	18:P:143:ALA:N	2.73	0.41
22:T:43:ASN:ND2	22:T:108:ARG:CZ	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1398:G:O2'	1:0:1399:A:H5'	2.20	0.41
4:A:82:VAL:HG13	4:A:93:THR:HB	2.01	0.41
1:0:128:A:O2'	1:0:129:A:H5'	2.20	0.41
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.92	0.41
15:M:181:GLU:N	15:M:181:GLU:OE1	2.48	0.41
13:K:9:THR:O	13:K:10:GLN:C	2.58	0.41
7:D:151:ILE:HA	7:D:152:PRO:HD3	1.95	0.41
25:W:115:THR:HG23	38:W:5420:HOH:O	2.21	0.41
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.41
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.29	0.41
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.41
17:O:21:SER:OG	17:O:106:PRO:HB2	2.20	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.41
25:W:125:HIS:CD2	25:W:127:GLY:H	2.38	0.41
5:B:119:HIS:O	5:B:121:PRO:HD3	2.20	0.41
30:2:30:ASP:O	30:2:31:ARG:HB2	2.20	0.41
1:0:1023:C:O2'	1:0:1024:G:H5'	2.20	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.20	0.41
4:A:217:ARG:HG3	38:A:9325:HOH:O	2.20	0.41
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.41
1:0:870:G:C3'	1:0:871:G:H5"	2.50	0.41
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.82	0.41
1:0:2269:C:H2'	1:0:2270:G:H5'	2.01	0.41
13:K:113:ILE:HG22	13:K:114:ALA:N	2.34	0.41
13:K:75:ARG:HE	13:K:94:ALA:HB3	1.85	0.41
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.50	0.41
8:E:11:VAL:HG13	8:E:76:VAL:HG21	2.03	0.41
16:N:183:ASP:O	16:N:184:ILE:O	2.38	0.41
1:0:538:C:H5"	1:0:539:G:C8	2.55	0.41
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.01	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:1734:C:OP1	5:B:234:ARG:NH1	2.50	0.41
6:C:236:THR:HG22	6:C:239:ALA:CB	2.50	0.41
25:W:48:VAL:CG1	25:W:48:VAL:O	2.68	0.41
5:B:255:GLY:O	5:B:257:THR:HG23	2.21	0.41
12:J:42:GLU:HG2	12:J:43:ARG:HG3	2.03	0.41
1:0:2768:A:O2'	1:0:2769:C:H5'	2.21	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.20	0.41
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.41
1:0:1528:A:H62	1:0:1663:G:H21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1080:C:H6	1:0:1080:C:O5'	2.04	0.41
1:0:820:G:H5'	1:0:821:U:H5'	2.03	0.41
1:0:137:U:H2'	1:0:139:C:C5	2.56	0.41
9:F:26:THR:HB	9:F:102:GLY:HA3	2.03	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
1:0:2078:U:O2'	1:0:2079:G:H5'	2.21	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.56	0.41
16:N:101:VAL:HG12	38:N:9328:HOH:O	2.19	0.41
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.85	0.41
6:C:114:ALA:HB1	6:C:223:LEU:HB3	2.03	0.41
1:0:1185:U:H2'	1:0:1186:C:H6	1.84	0.41
1:0:2754:G:O2'	1:0:2755:G:H5'	2.21	0.41
5:B:16:ARG:HD3	38:B:9410:HOH:O	2.19	0.41
1:0:736:A:H2'	1:0:737:A:O4'	2.21	0.41
1:0:1391:G:H2'	1:0:1392:A:H5'	2.02	0.41
1:0:1744:G:H2'	1:0:1745:G:H5'	2.02	0.41
19:Q:53:HIS:ND1	19:Q:55:ARG:HB2	2.36	0.41
1:0:1269:G:H2'	1:0:1270:U:C6	2.56	0.41
1:0:2377:U:O5'	1:0:2377:U:H6	2.03	0.41
11:H:9:ILE:O	11:H:9:ILE:HG22	2.20	0.41
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.20	0.41
5:B:51:VAL:O	5:B:53:LEU:HD13	2.21	0.41
18:P:16:VAL:CG1	18:P:17:GLY:N	2.84	0.41
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.54	0.41
1:0:2413:A:H2'	1:0:2414:A:O4'	2.20	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
31:3:48:ASN:ND2	31:3:50:GLY:H	2.17	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.86	0.41
1:0:958:G:O2'	1:0:959:C:H5'	2.20	0.41
16:N:29:SER:OG	16:N:101:VAL:HG21	2.20	0.41
11:H:95:LEU:HD11	11:H:124:ALA:HB2	2.03	0.41
1:0:2353:A:H4'	1:0:2354:A:O5'	2.20	0.41
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.19	0.41
1:0:189:A:OP1	15:M:171:ARG:NH2	2.53	0.41
27:Y:187:VAL:CG1	27:Y:205:ILE:HA	2.51	0.41
1:0:2718:C:P	5:B:45:LYS:HZ1	2.44	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.41
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.50	0.41
4:A:33:GLU:O	4:A:34:ASP:CB	2.61	0.41
25:W:3:ALA:O	25:W:54:PHE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:281:U:O2'	1:0:282:C:H5'	2.20	0.41
32:I:113:HIS:N	32:I:114:PRO:CD	2.83	0.41
12:J:131:THR:HG22	12:J:133:GLY:N	2.35	0.41
6:C:223:LEU:HA	6:C:223:LEU:HD12	1.94	0.41
22:T:40:VAL:HG22	22:T:41:ARG:N	2.36	0.41
17:O:32:ARG:HH11	17:O:115:ARG:HH21	1.69	0.41
1:0:1180:U:H4'	32:I:91:GLU:OE2	2.21	0.41
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.03	0.41
2:9:3114:G:H2'	2:9:3115:C:C6	2.56	0.41
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.56	0.41
6:C:133:ARG:HD2	38:C:9206:HOH:O	2.20	0.41
5:B:175:LEU:C	5:B:175:LEU:CD2	2.89	0.41
7:D:105:SER:HB2	7:D:131:THR:HG23	2.01	0.41
1:0:926:A:C4'	14:L:39:GLU:HG2	2.51	0.41
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.86	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.54	0.41
2:9:3107:C:H5	38:9:3167:HOH:O	2.03	0.41
11:H:38:LYS:O	11:H:84:LYS:HE2	2.21	0.41
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.56	0.41
11:H:146:VAL:HG22	38:H:9176:HOH:O	2.21	0.41
2:9:3060:C:O2'	2:9:3061:C:H5'	2.20	0.41
22:T:23:VAL:C	22:T:93:THR:HG21	2.41	0.41
1:0:2387:U:H2'	1:0:2388:C:C6	2.56	0.41
17:O:24:ALA:O	17:O:28:ASP:HB2	2.20	0.41
22:T:47:THR:HB	22:T:100:ASP:HB3	2.01	0.41
1:0:1194:A:O2'	1:0:1195:G:H5'	2.21	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
17:O:41:ALA:HA	38:O:5104:HOH:O	2.21	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.53	0.41
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.36	0.41
5:B:224:LYS:HA	5:B:224:LYS:HD3	1.94	0.41
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.94	0.41
1:0:2365:G:OP1	19:Q:15:LYS:HG3	2.21	0.41
25:W:153:MET:O	25:W:154:ARG:C	2.59	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
28:Z:13:ARG:NH1	38:Z:9218:HOH:O	2.53	0.41
1:0:2265:U:H2'	1:0:2266:A:H8	1.86	0.41
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.02	0.41
7:D:10:PHE:CG	7:D:11:HIS:N	2.89	0.41
1:0:1419:U:H2'	1:0:1685:A:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
32:I:78:LEU:HD13	32:I:108:ILE:HG23	2.03	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.21	0.40
13:K:44:LEU:HA	13:K:45:PRO:HD2	1.96	0.40
25:W:72:PRO:CG	25:W:77:ALA:HB3	2.39	0.40
7:D:57:THR:HG23	7:D:63:ILE:CA	2.42	0.40
1:0:1158:G:O2'	1:0:1159:G:H5'	2.21	0.40
1:0:380:A:C2	15:M:13:GLU:HB3	2.56	0.40
15:M:9:ARG:HB2	15:M:47:ASP:OD2	2.20	0.40
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.40
16:N:181:ASP:O	16:N:184:ILE:HG22	2.21	0.40
7:D:55:LYS:HA	38:D:6752:HOH:O	2.21	0.40
4:A:165:THR:O	4:A:165:THR:CG2	2.69	0.40
38:0:9988:HOH:O	6:C:214:THR:HB	2.20	0.40
1:0:1761:U:H5'	18:P:81:LYS:O	2.22	0.40
22:T:47:THR:HG22	22:T:99:THR:OG1	2.21	0.40
2:9:3059:C:H5'	38:9:5233:HOH:O	2.21	0.40
1:0:228:C:H2'	1:0:229:G:H5'	2.03	0.40
1:0:1789:G:O6	18:P:73:HIS:HE1	2.04	0.40
1:0:1714:C:O2'	1:0:1715:C:H5'	2.21	0.40
13:K:89:LYS:HA	38:K:7064:HOH:O	2.21	0.40
1:0:1933:G:O2'	1:0:1934:A:H5'	2.20	0.40
1:0:732:C:O2'	1:0:733:U:H5'	2.21	0.40
1:0:571:C:H6	1:0:571:C:O5'	2.03	0.40
1:0:1943:C:H5"	4:A:209:PRO:HG3	2.03	0.40
1:0:1562:C:N4	38:0:6128:HOH:O	2.55	0.40
5:B:80:ARG:HA	5:B:186:GLY:O	2.21	0.40
1:0:1741:U:H3'	38:0:3074:HOH:O	2.21	0.40
1:0:1311:G:O6	6:C:173:LYS:HE3	2.22	0.40
1:0:2619:UR3:H5'	3:4:76:5AA:H103	2.03	0.40
1:0:1855:G:H4'	1:0:1856:C:O5'	2.21	0.40
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.56	0.40
1:0:1513:C:O2'	1:0:1514:C:H5'	2.21	0.40
1:0:1996:U:O2'	1:0:1997:A:H5'	2.21	0.40
5:B:171:VAL:HG23	5:B:172:SER:N	2.35	0.40
1:0:2740:G:H2'	1:0:2741:A:O4'	2.21	0.40
1:0:1643:C:O2'	1:0:1644:C:H5'	2.22	0.40
6:C:187:ARG:NH2	38:C:9162:HOH:O	2.51	0.40
38:0:7751:HOH:O	5:B:2:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:119:TYR:CD1	32:I:119:TYR:N	2.89	0.40
14:L:89:PHE:CD1	14:L:89:PHE:N	2.89	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
1:0:1167:G:H4'	32:I:135:LEU:CD2	2.51	0.40
25:W:48:VAL:HG12	25:W:48:VAL:O	2.21	0.40
11:H:54:THR:HA	11:H:127:VAL:O	2.22	0.40
2:9:3029:C:H2'	2:9:3030:C:C5'	2.45	0.40
11:H:26:SER:HA	11:H:59:HIS:HD2	1.85	0.40
6:C:118:THR:O	6:C:136:VAL:HG13	2.21	0.40
8:E:144:THR:O	8:E:148:ILE:HG13	2.21	0.40
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.68	0.40
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.56	0.40
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.57	0.40
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.52	0.40
1:0:790:A:H1'	1:0:1710:A:O2'	2.22	0.40
1:0:1631:A:H2'	1:0:1632:A:C8	2.56	0.40
9:F:99:THR:O	9:F:99:THR:HG23	2.21	0.40
25:W:125:HIS:HE1	38:W:3071:HOH:O	2.05	0.40
13:K:22:ASP:OD1	13:K:22:ASP:C	2.60	0.40
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.40
1:0:2379:G:N7	1:0:2408:A:N1	2.70	0.40
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.03	0.40
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.40
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.95	0.40
1:0:1434:A:H2'	1:0:1436:C:C5	2.56	0.40
1:0:2050:G:OP1	20:R:79:ARG:HB3	2.21	0.40
1:0:2115:U:H2'	1:0:2116:U:C6	2.56	0.40
1:0:646:G:H2'	1:0:647:U:C6	2.56	0.40
1:0:1167:G:H3'	38:0:7702:HOH:O	2.20	0.40
25:W:137:GLN:HG3	25:W:137:GLN:O	2.21	0.40
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.04	0.40
5:B:183:GLU:OE1	5:B:183:GLU:HA	2.21	0.40
7:D:99:ASP:HB2	7:D:103:ASN:HB2	2.04	0.40
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.56	0.40
16:N:183:ASP:O	16:N:184:ILE:C	2.59	0.40
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.84	0.40
24:V:59:ILE:O	24:V:63:GLU:HG2	2.21	0.40
20:R:132:ARG:NH1	38:R:9383:HOH:O	2.54	0.40
14:L:68:GLU:HG3	38:L:9342:HOH:O	2.22	0.40
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.74	0.40
1:0:2314:G:O2'	1:0:2315:C:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1744:G:C2'	1:0:1745:G:H5'	2.51	0.40
1:0:2776:A:H2'	1:0:2777:G:O4'	2.20	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.21	0.40
20:R:69:LYS:HE2	20:R:78:GLY:O	2.21	0.40
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.40
22:T:37:GLN:OE1	22:T:118:SER:HA	2.21	0.40
1:0:1624:A:H4'	1:0:1626:A:H5"	2.03	0.40
5:B:33:ASP:HB3	5:B:34:GLY:H	1.57	0.40
1:0:549:A:O2'	1:0:550:C:H5'	2.21	0.40
7:D:19:GLU:HG3	38:D:6165:HOH:O	2.21	0.40
30:2:40:ARG:HG2	30:2:40:ARG:NH1	2.37	0.40
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.18	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.64	0.40
12:J:11:ILE:HD11	12:J:109:TYR:CD2	2.57	0.40
1:0:56:G:C5'	24:V:50:ARG:HH12	2.27	0.40
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.14	0.40
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.51	0.40
27:Y:144:ARG:NH1	38:Y:9373:HOH:O	2.54	0.40
29:1:28:HIS:CD2	29:1:31:LYS:H	2.39	0.40
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.52	0.40
6:C:173:LYS:O	6:C:186:TYR:HA	2.22	0.40
15:M:40:ILE:HG21	15:M:64:ARG:NH2	2.36	0.40
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.88	0.40
38:0:9429:HOH:O	6:C:103:ASN:HB3	2.20	0.40
1:0:2515:C:H2'	1:0:2516:G:O4'	2.21	0.40
6:C:80:VAL:HA	6:C:81:PRO:HD3	1.95	0.40
1:0:2093:G:H5"	38:B:9327:HOH:O	2.21	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.04	0.40
1:0:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
11:H:114:ARG:O	11:H:115:ALA:C	2.60	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3_655]	2.13	0.07

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%)	206 (88%)	24 (10%)	5 (2%)	9 16
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	11 21
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	39 65
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	1 1
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	30 56
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	5 7
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	10 19
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	14 28
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	8 14
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	14 28
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100 100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	5 7
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	21 42
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100 100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100 100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	14 28
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100 100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100 100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	9 18
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	5 8
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	26 51
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	7 12
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100 100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	2 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	8 15
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100 100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	12 24

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	GLU
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	37	VAL
5	B	34	GLY
5	B	169	GLY
6	C	8	LEU
7	D	65	GLU
7	D	137	PRO
7	D	173	GLU
9	F	44	SER
11	H	166	SER
24	V	43	PRO
5	B	107	SER
7	D	86	THR
11	H	140	VAL
13	K	126	SER
14	L	80	ASP
14	L	143	THR
16	N	113	SER
16	N	164	ASP
23	U	7	ASP
26	X	78	GLU
28	Z	42	CYS
5	B	185	GLY
7	D	171	ASP
8	E	44	GLY

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Mol	Chain	Res	Type
9	F	61	MET
9	F	64	PRO
12	J	143	LYS
16	N	167	ASP
26	X	70	ILE
31	3	56	PRO
5	B	2	GLN
7	D	89	PRO
16	N	160	SER
25	W	49	ASN
28	Z	20	ARG
31	3	57	GLY
7	D	16	PRO
7	D	97	GLN
28	Z	43	GLY
4	A	211	LYS
4	A	236	GLY
7	D	28	GLY
24	V	40	PRO
7	D	27	ILE
17	O	108	GLY
20	R	106	GLY
7	D	69	ILE
7	D	135	VAL
13	K	39	GLY
20	R	81	PRO
5	B	30	PRO
13	K	111	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	179/182 (98%)	169 (94%)	10 (6%)	26 50
5	B	282/283 (100%)	265 (94%)	17 (6%)	24 47
6	C	193/193 (100%)	176 (91%)	17 (9%)	12 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	D	117/148 (79%)	112 (96%)	5 (4%)	35 64
8	E	152/156 (97%)	148 (97%)	4 (3%)	54 80
9	F	93/94 (99%)	92 (99%)	1 (1%)	80 93
10	G	27/283 (10%)	27 (100%)	0	100 100
11	H	132/138 (96%)	126 (96%)	6 (4%)	34 62
12	J	118/121 (98%)	109 (92%)	9 (8%)	16 32
13	K	106/106 (100%)	101 (95%)	5 (5%)	32 59
14	L	113/127 (89%)	107 (95%)	6 (5%)	28 53
15	M	158/158 (100%)	151 (96%)	7 (4%)	35 63
16	N	149/150 (99%)	144 (97%)	5 (3%)	44 72
17	O	93/94 (99%)	90 (97%)	3 (3%)	46 74
18	P	113/117 (97%)	109 (96%)	4 (4%)	43 71
19	Q	79/80 (99%)	76 (96%)	3 (4%)	40 68
20	R	117/122 (96%)	114 (97%)	3 (3%)	54 80
21	S	71/74 (96%)	69 (97%)	2 (3%)	51 78
22	T	105/106 (99%)	101 (96%)	4 (4%)	40 68
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	50 (98%)	1 (2%)	63 85
25	W	130/130 (100%)	124 (95%)	6 (5%)	33 61
26	X	66/74 (89%)	61 (92%)	5 (8%)	16 32
27	Y	120/196 (61%)	111 (92%)	9 (8%)	17 33
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%)	76 (96%)	3 (4%)	40 68
32	I	58/130 (45%)	57 (98%)	1 (2%)	68 88
All	All	3093/3611 (86%)	2956 (96%)	137 (4%)	35 63

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU

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Mol	Chain	Res	Type
4	A	36	ASP
4	A	69	LEU
4	A	78	ASP
4	A	94	LEU
4	A	120	ARG
4	A	125	ASN
4	A	179	MET
4	A	217	ARG
5	B	5	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	33	ASP
5	B	49	THR
5	B	63	GLU
5	B	98	THR
5	B	149	ASP
5	B	162	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	280	VAL
5	B	304	PRO
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	106	GLU
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	246	ARG

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Mol	Chain	Res	Type
7	D	24	HIS
7	D	61	PHE
7	D	86	THR
7	D	133	ASN
7	D	136	ARG
8	E	15	GLN
8	E	102	VAL
8	E	126	ILE
8	E	164	ASP
9	F	105	ASP
11	H	30	GLN
11	H	84	LYS
11	H	88	ARG
11	H	96	ARG
11	H	111	ASP
11	H	154	TYR
12	J	16	ASP
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
13	K	129	THR
14	L	4	LYS
14	L	30	ARG
14	L	35	ARG
14	L	99	GLU
14	L	102	ASP
14	L	104	ASP
15	M	23	LEU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN

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Mol	Chain	Res	Type
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	93	GLN
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	115	ARG
18	P	21	VAL
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
20	R	39	THR
20	R	82	GLU
21	S	10	VAL
21	S	53	ASN
22	T	39	ASN
22	T	48	VAL
22	T	112	LEU
22	T	115	GLU
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
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	49	ARG
26	X	72	VAL
26	X	79	GLU
27	Y	141	THR
27	Y	144	ARG
27	Y	163	THR
27	Y	174	VAL
27	Y	186	ARG

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Mol	Chain	Res	Type
27	Y	189	ASN
27	Y	203	VAL
27	Y	204	ARG
27	Y	235	GLU
30	2	18	ASN
31	3	11	CYS
31	3	42	ARG
31	3	56	PRO
32	I	86	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	92	ASN
4	A	176	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
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	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	52	GLN

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Mol	Chain	Res	Type
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	26	GLN
15	M	58	GLN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	93	GLN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
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
20	R	113	HIS
20	R	117	HIS
21	S	25	GLN
21	S	53	ASN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	2	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS

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Mol	Chain	Res	Type
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	2	GLN
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%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	250 (8%)	33 (1%)

All (250) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	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

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Mol	Chain	Res	Type
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
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	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A

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Mol	Chain	Res	Type
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1131	G
1	0	1137	G

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Mol	Chain	Res	Type
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	1234	U
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
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	1592	G
1	0	1603	A
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

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Mol	Chain	Res	Type
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
1	0	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
1	0	1996	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G

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Mol	Chain	Res	Type
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	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
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	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A

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Mol	Chain	Res	Type
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2864	U
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	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
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	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	869	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1246	A

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Mol	Chain	Res	Type
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	1856	C
1	0	1942	A
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	2637	A
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	1,35	12,22,23	1.04	1 (8%)	19,31,34	3.16	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.06	2 (11%)	21,38,41	2.52	3 (14%)
1	UR3	0	2619	1	12,22,23	0.88	0	16,32,35	0.73	0
1	PSU	0	2621	1	13,21,22	1.64	2 (15%)	18,30,33	6.08	3 (16%)
1	1MA	0	628	1	14,25,26	1.09	1 (7%)	15,37,40	1.16	1 (6%)
3	5AA	4	76	1,3	16,26,27	0.63	0	15,38,41	1.19	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	1,35	-	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.83	1.48	1.52
1	0	2588	OMG	C8-N7	-2.06	1.30	1.34
1	0	2587	OMU	C4-N3	2.57	1.37	1.33
1	0	2621	PSU	C4-N3	2.81	1.38	1.33
1	0	628	1MA	C6-N6	2.99	1.34	1.29
1	0	2588	OMG	C6-N1	3.20	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	-21.25	114.77	128.33
1	0	2588	OMG	C5-C6-N1	-8.70	111.70	123.59
1	0	628	1MA	C2-N3-C4	-3.56	110.89	116.40
1	0	2587	OMU	C5-C4-N3	-3.32	114.59	123.12
1	0	2588	OMG	N3-C2-N1	-2.33	123.90	127.44
1	0	2621	PSU	C6-N1-C2	2.53	119.54	115.47
3	4	76	5AA	C2-N1-C6	3.48	118.83	111.43
1	0	2588	OMG	C6-N1-C2	6.60	125.09	115.94
1	0	2587	OMU	C4-N3-C2	13.17	127.18	114.14
1	0	2621	PSU	C4-N3-C2	13.97	127.32	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
3	4	76	5AA	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%)	0.14	71 (2%) 59 53	24, 51, 98, 161	0
2	9	122/122 (100%)	0.30	4 (3%) 50 43	46, 68, 96, 153	0
3	4	4/8 (50%)	0.01	0 100 100	42, 42, 46, 46	0
4	A	237/240 (98%)	0.55	17 (7%) 18 13	31, 55, 94, 120	0
5	B	337/338 (99%)	1.02	33 (9%) 10 6	33, 65, 94, 103	0
6	C	246/246 (100%)	0.03	5 (2%) 68 63	26, 51, 75, 86	0
7	D	140/177 (79%)	2.36	66 (47%) 0 0	64, 110, 134, 141	0
8	E	172/178 (96%)	1.72	60 (34%) 0 0	50, 81, 105, 115	0
9	F	119/120 (99%)	0.86	20 (16%) 2 1	57, 81, 107, 122	0
10	G	29/348 (8%)	3.00	18 (62%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	0.95	18 (11%) 7 4	42, 63, 94, 101	0
12	J	142/145 (97%)	0.73	5 (3%) 48 40	42, 59, 82, 97	0
13	K	132/132 (100%)	0.87	11 (8%) 14 9	37, 62, 86, 90	0
14	L	145/165 (87%)	0.79	20 (13%) 4 2	28, 74, 118, 131	0
15	M	194/194 (100%)	0.16	2 (1%) 84 81	33, 48, 64, 72	0
16	N	186/187 (99%)	0.87	28 (15%) 3 1	43, 69, 118, 124	0
17	O	115/116 (99%)	0.22	2 (1%) 73 68	43, 61, 79, 89	0
18	P	143/149 (95%)	0.56	5 (3%) 48 40	46, 62, 75, 81	0
19	Q	95/96 (98%)	0.39	2 (2%) 67 61	40, 50, 66, 77	0
20	R	150/155 (96%)	0.23	2 (1%) 79 75	36, 51, 72, 82	0
21	S	81/85 (95%)	0.38	5 (6%) 24 18	48, 65, 85, 94	0
22	T	119/120 (99%)	0.47	8 (6%) 21 15	44, 61, 90, 111	0
23	U	53/66 (80%)	1.02	6 (11%) 7 4	48, 63, 80, 88	0
24	V	65/71 (91%)	1.45	19 (29%) 1 0	59, 83, 117, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	0.43	1 (0%) 90 88	41, 57, 78, 88	0
26	X	82/92 (89%)	0.83	11 (13%) 4 2	49, 66, 89, 106	0
27	Y	142/241 (58%)	0.54	9 (6%) 23 17	32, 51, 74, 95	0
28	Z	73/83 (87%)	0.29	4 (5%) 29 21	45, 64, 78, 96	0
29	1	56/57 (98%)	-0.06	0 100 100	31, 38, 46, 61	0
30	2	46/50 (92%)	1.70	16 (34%) 0 0	40, 70, 123, 128	0
31	3	92/92 (100%)	0.41	3 (3%) 50 43	37, 60, 74, 89	0
32	I	70/162 (43%)	4.04	60 (85%) 0 0	108, 129, 152, 155	0
All	All	6650/7482 (88%)	0.52	531 (7%) 15 10	24, 58, 109, 161	0

All (531) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	93	GLN	12.0
32	I	133	THR	9.6
24	V	1	THR	8.3
7	D	88	LEU	8.2
32	I	137	VAL	8.1
7	D	69	ILE	7.7
10	G	27	ILE	7.7
32	I	114	PRO	7.1
32	I	96	PHE	6.9
32	I	71	GLY	6.9
2	9	3001	U	6.8
7	D	44	ILE	6.7
32	I	111	GLN	6.7
30	2	36	ASN	6.7
30	2	44	ARG	6.6
24	V	43	PRO	6.6
7	D	58	VAL	6.5
7	D	84	LEU	6.5
7	D	63	ILE	6.5
30	2	37	HIS	6.5
7	D	89	PRO	6.5
10	G	23	ILE	6.4
32	I	121	LEU	6.4
7	D	90	LEU	6.3
32	I	81	ASP	6.3
32	I	78	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
30	2	38	LYS	6.2
32	I	113	HIS	6.2
4	A	37	VAL	6.0
7	D	57	THR	6.0
24	V	39	ALA	5.9
32	I	116	LEU	5.9
32	I	135	LEU	5.9
30	2	48	ASP	5.8
7	D	10	PHE	5.7
1	0	282	C	5.7
32	I	110	GLU	5.7
30	2	49	GLU	5.6
32	I	72	VAL	5.6
32	I	88	GLY	5.6
30	2	41	HIS	5.5
32	I	132	CYS	5.5
7	D	26	GLY	5.5
1	0	1173	A	5.4
7	D	134	LEU	5.4
7	D	92	GLU	5.4
1	0	2237	G	5.4
7	D	85	GLN	5.4
32	I	77	GLU	5.4
7	D	56	ARG	5.3
32	I	73	PRO	5.3
8	E	100	ASP	5.3
32	I	117	LEU	5.3
7	D	65	GLU	5.3
7	D	64	ARG	5.2
10	G	24	VAL	5.2
1	0	1177	A	5.2
7	D	170	TYR	5.1
32	I	89	SER	5.1
32	I	102	VAL	5.1
7	D	61	PHE	5.0
32	I	125	ALA	5.0
24	V	40	PRO	4.9
4	A	36	ASP	4.9
10	G	71	LEU	4.9
7	D	75	LEU	4.9
14	L	80	ASP	4.8
8	E	10	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
7	D	172	VAL	4.7
32	I	109	ALA	4.7
7	D	40	ILE	4.7
8	E	45	ASP	4.7
26	X	88	GLU	4.7
2	9	3024	U	4.7
2	9	3023	U	4.6
30	2	42	TRP	4.6
23	U	54	THR	4.5
7	D	70	GLY	4.5
7	D	41	LEU	4.5
8	E	42	VAL	4.4
7	D	130	VAL	4.4
14	L	60	GLU	4.4
32	I	97	VAL	4.4
10	G	67	LEU	4.4
10	G	28	GLU	4.4
1	0	1525	G	4.4
9	F	119	ARG	4.3
32	I	85	PHE	4.3
13	K	132	VAL	4.3
32	I	118	SER	4.2
32	I	103	ASP	4.2
32	I	79	ILE	4.2
32	I	128	VAL	4.2
7	D	87	ALA	4.2
10	G	26	MET	4.2
32	I	139	ILE	4.1
1	0	1951	G	4.1
8	E	93	MET	4.1
32	I	86	GLU	4.1
7	D	18	ILE	4.0
11	H	47	ILE	4.0
16	N	147	ILE	4.0
32	I	107	GLN	4.0
7	D	86	THR	4.0
1	0	735	C	3.9
8	E	95	VAL	3.9
8	E	83	GLY	3.9
8	E	92	PRO	3.9
28	Z	59	TYR	3.9
30	2	47	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	0	2238	A	3.9
9	F	16	ALA	3.9
16	N	166	ALA	3.9
32	I	129	VAL	3.9
1	0	1199	A	3.9
8	E	99	GLY	3.9
7	D	50	VAL	3.9
16	N	172	PHE	3.8
16	N	160	SER	3.8
7	D	98	PHE	3.8
22	T	112	LEU	3.8
5	B	180	ASP	3.8
32	I	124	ALA	3.8
8	E	148	ILE	3.8
32	I	75	THR	3.8
32	I	91	GLU	3.7
8	E	11	VAL	3.7
9	F	18	GLU	3.7
1	0	970	U	3.7
1	0	1279	U	3.7
32	I	92	PRO	3.7
32	I	95	ASP	3.7
8	E	118	ILE	3.7
5	B	104	GLU	3.7
1	0	1172	G	3.7
21	S	81	ILE	3.7
24	V	38	GLY	3.6
32	I	84	GLY	3.6
18	P	77	ALA	3.6
10	G	20	VAL	3.6
9	F	44	SER	3.6
27	Y	235	GLU	3.6
7	D	27	ILE	3.6
26	X	74	ALA	3.6
8	E	102	VAL	3.6
26	X	85	VAL	3.6
5	B	119	HIS	3.6
14	L	105	TYR	3.6
1	0	960	G	3.6
10	G	22	ALA	3.6
5	B	181	ILE	3.5
30	2	20	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
30	2	45	ASN	3.5
30	2	35	ARG	3.5
9	F	117	GLU	3.5
24	V	37	GLY	3.5
7	D	55	LYS	3.5
5	B	106	HIS	3.5
1	0	280	C	3.5
7	D	66	GLY	3.5
9	F	27	GLY	3.5
16	N	181	ASP	3.5
1	0	2004	U	3.5
8	E	48	VAL	3.5
10	G	64	ASN	3.5
7	D	59	GLY	3.5
7	D	93	LEU	3.4
22	T	50	VAL	3.4
1	0	1190	G	3.4
14	L	124	ASP	3.4
16	N	68	GLU	3.4
11	H	83	TYR	3.4
32	I	119	TYR	3.4
23	U	47	ARG	3.4
7	D	173	GLU	3.4
8	E	82	TYR	3.4
16	N	64	SER	3.4
14	L	149	ARG	3.4
10	G	73	ASP	3.4
7	D	104	PHE	3.3
4	A	237	GLY	3.3
1	0	497	A	3.3
10	G	16	LYS	3.3
16	N	152	GLU	3.3
32	I	131	THR	3.3
14	L	104	ASP	3.3
1	0	284	C	3.3
5	B	64	GLY	3.3
1	0	283	U	3.3
1	0	1198	U	3.3
32	I	83	ALA	3.3
32	I	104	GLN	3.3
7	D	67	ASP	3.3
22	T	117	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
7	D	11	HIS	3.3
8	E	105	GLU	3.3
16	N	163	PHE	3.2
13	K	101	ASN	3.2
5	B	116	PRO	3.2
7	D	106	PHE	3.2
32	I	115	ASP	3.2
28	Z	20	ARG	3.2
4	A	32	VAL	3.2
24	V	59	ILE	3.2
1	0	1185	U	3.2
1	0	1130	U	3.2
1	0	285	A	3.2
14	L	108	VAL	3.1
30	2	43	ARG	3.1
7	D	166	ILE	3.1
14	L	91	VAL	3.1
19	Q	95	GLU	3.1
8	E	109	GLY	3.1
1	0	1163	G	3.1
16	N	175	LEU	3.1
24	V	41	GLU	3.1
7	D	25	MET	3.1
8	E	170	ARG	3.1
8	E	22	VAL	3.1
27	Y	96	GLU	3.1
32	I	106	LYS	3.0
8	E	122	THR	3.0
8	E	128	GLY	3.0
7	D	83	PHE	3.0
7	D	135	VAL	3.0
7	D	24	HIS	3.0
1	0	1202	A	3.0
4	A	35	GLY	3.0
1	0	10	U	3.0
9	F	106	ALA	3.0
32	I	87	THR	3.0
8	E	126	ILE	3.0
1	0	1174	A	3.0
31	3	92	GLU	2.9
9	F	25	ASP	2.9
32	I	105	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
21	S	76	GLU	2.9
8	E	161	VAL	2.9
7	D	91	ALA	2.9
16	N	159	TYR	2.9
2	9	3002	U	2.9
22	T	59	GLU	2.9
18	P	114	LEU	2.9
7	D	62	ASP	2.9
13	K	3	ALA	2.9
5	B	135	GLY	2.9
11	H	50	ILE	2.9
16	N	180	LEU	2.9
11	H	144	GLU	2.9
1	0	1000	C	2.9
8	E	88	TYR	2.9
1	0	2249	G	2.8
9	F	107	ASP	2.8
17	O	111	VAL	2.8
23	U	53	ASP	2.8
4	A	133	ARG	2.8
7	D	29	HIS	2.8
8	E	87	PHE	2.8
8	E	121	ASP	2.8
7	D	16	PRO	2.8
9	F	17	LEU	2.8
1	0	2508	C	2.8
32	I	94	GLU	2.8
22	T	116	ASP	2.8
9	F	15	ASP	2.8
1	0	969	G	2.8
7	D	47	GLN	2.8
7	D	17	ARG	2.8
14	L	81	VAL	2.8
11	H	171	ALA	2.8
21	S	16	ASN	2.8
8	E	44	GLY	2.8
16	N	182	GLY	2.8
1	0	138	U	2.7
1	0	272	A	2.7
7	D	23	VAL	2.7
22	T	119	ALA	2.7
27	Y	95	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	A	31	LYS	2.7
5	B	133	GLU	2.7
8	E	108	LEU	2.7
31	3	22	VAL	2.7
1	0	279	C	2.7
1	0	1171	A	2.7
27	Y	97	LEU	2.7
16	N	157	PRO	2.7
1	0	1181	A	2.7
10	G	21	ASP	2.7
24	V	52	ALA	2.7
32	I	74	PRO	2.7
10	G	68	GLU	2.7
24	V	45	ARG	2.7
32	I	136	GLY	2.7
11	H	65	SER	2.7
5	B	97	LEU	2.6
5	B	328	ARG	2.6
1	0	2769	C	2.6
6	C	237	GLU	2.6
26	X	10	VAL	2.6
7	D	45	THR	2.6
7	D	171	ASP	2.6
5	B	140	LEU	2.6
8	E	145	ALA	2.6
14	L	61	ALA	2.6
24	V	49	LEU	2.6
26	X	82	GLU	2.6
8	E	154	ILE	2.6
10	G	69	ARG	2.6
11	H	71	ARG	2.6
9	F	26	THR	2.6
10	G	66	LEU	2.6
11	H	142	ASP	2.6
5	B	35	GLN	2.6
10	G	70	ALA	2.6
16	N	137	ALA	2.6
5	B	54	VAL	2.6
9	F	103	GLU	2.6
9	F	109	GLU	2.6
5	B	196	ALA	2.6
16	N	138	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
16	N	183	ASP	2.5
13	K	119	GLN	2.5
8	E	81	GLU	2.5
1	0	2509	A	2.5
13	K	5	GLY	2.5
32	I	76	ALA	2.5
1	0	1192	A	2.5
9	F	108	VAL	2.5
11	H	161	CYS	2.5
4	A	128	LEU	2.5
7	D	74	THR	2.5
1	0	999	C	2.5
1	0	1200	A	2.5
32	I	90	GLY	2.5
13	K	63	GLU	2.5
5	B	142	LEU	2.5
7	D	128	LEU	2.5
8	E	97	VAL	2.5
20	R	96	VAL	2.5
27	Y	141	THR	2.5
5	B	65	MET	2.5
8	E	86	VAL	2.5
7	D	81	GLU	2.5
32	I	112	LYS	2.4
11	H	45	VAL	2.4
14	L	100	ALA	2.4
8	E	144	THR	2.4
8	E	16	ASP	2.4
19	Q	20	ASP	2.4
32	I	126	LYS	2.4
14	L	133	VAL	2.4
8	E	41	SER	2.4
7	D	129	ASP	2.4
11	H	150	PHE	2.4
8	E	6	GLU	2.4
30	2	31	ARG	2.4
5	B	52	VAL	2.4
16	N	1	ALA	2.4
8	E	157	LYS	2.4
1	0	370	G	2.4
13	K	109	LEU	2.4
4	A	38	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
8	E	38	ILE	2.4
18	P	71	TYR	2.4
8	E	80	TRP	2.4
8	E	111	LYS	2.4
13	K	131	ILE	2.4
1	0	1213	C	2.4
14	L	150	GLN	2.4
1	0	1150	A	2.4
6	C	61	PHE	2.4
5	B	51	VAL	2.4
5	B	74	ILE	2.4
5	B	100	VAL	2.4
8	E	40	VAL	2.4
20	R	14	ALA	2.4
22	T	82	THR	2.4
1	0	281	U	2.4
16	N	127	LEU	2.3
16	N	94	GLU	2.3
18	P	64	GLU	2.3
13	K	88	VAL	2.3
24	V	9	ARG	2.3
1	0	1204	C	2.3
24	V	3	LEU	2.3
8	E	104	ILE	2.3
30	2	46	ASP	2.3
23	U	52	THR	2.3
1	0	736	A	2.3
1	0	2768	A	2.3
11	H	35	ARG	2.3
16	N	143	ARG	2.3
7	D	71	ALA	2.3
8	E	119	HIS	2.3
1	0	2577	A	2.3
4	A	129	LEU	2.3
11	H	167	PRO	2.3
7	D	53	LYS	2.3
14	L	97	VAL	2.3
8	E	53	GLU	2.3
4	A	63	GLY	2.3
11	H	73	LEU	2.3
6	C	131	PHE	2.3
8	E	124	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
27	Y	234	VAL	2.3
1	0	130	C	2.3
24	V	61	GLY	2.3
30	2	39	ARG	2.3
32	I	98	ALA	2.3
1	0	371	U	2.3
1	0	1625	U	2.3
5	B	73	VAL	2.3
25	W	79	VAL	2.3
8	E	117	THR	2.3
26	X	18	ARG	2.3
27	Y	98	GLN	2.3
4	A	62	ASP	2.3
16	N	162	ASP	2.3
24	V	11	MET	2.3
24	V	5	VAL	2.3
1	0	2344	G	2.3
5	B	113	LEU	2.2
6	C	135	GLU	2.2
6	C	132	ASP	2.2
4	A	65	ARG	2.2
23	U	51	TRP	2.2
12	J	57	TYR	2.2
1	0	716	G	2.2
1	0	1665	G	2.2
1	0	2251	G	2.2
31	3	56	PRO	2.2
1	0	1186	C	2.2
5	B	71	VAL	2.2
14	L	102	ASP	2.2
1	0	2250	G	2.2
1	0	717	C	2.2
1	0	2717	C	2.2
13	K	57	VAL	2.2
14	L	106	VAL	2.2
5	B	112	THR	2.2
24	V	8	ILE	2.2
7	D	54	ALA	2.2
1	0	1162	G	2.2
8	E	132	THR	2.2
16	N	158	LEU	2.2
28	Z	36	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
7	D	139	TYR	2.2
4	A	85	SER	2.2
8	E	89	SER	2.2
8	E	163	GLN	2.2
14	L	118	LEU	2.2
7	D	165	PHE	2.2
16	N	150	TYR	2.2
26	X	80	GLU	2.2
5	B	93	GLY	2.2
1	0	2890	A	2.2
11	H	85	MET	2.2
32	I	127	GLU	2.2
1	0	369	G	2.2
1	0	1169	U	2.2
16	N	81	ALA	2.2
14	L	96	VAL	2.2
5	B	296	LEU	2.1
5	B	169	GLY	2.1
17	O	104	ASN	2.1
16	N	156	GLU	2.1
1	0	1179	C	2.1
15	M	164	THR	2.1
16	N	179	LEU	2.1
27	Y	193	LEU	2.1
5	B	170	SER	2.1
23	U	43	GLY	2.1
8	E	167	TYR	2.1
14	L	59	GLU	2.1
26	X	40	HIS	2.1
7	D	72	LYS	2.1
9	F	22	VAL	2.1
15	M	165	GLY	2.1
13	K	83	PRO	2.1
18	P	80	ARG	2.1
8	E	127	ASP	2.1
1	0	1205	U	2.1
7	D	48	MET	2.1
8	E	7	ILE	2.1
11	H	32	LYS	2.1
4	A	86	ALA	2.1
8	E	5	LEU	2.1
11	H	146	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
12	J	47	THR	2.1
32	I	82	GLU	2.1
5	B	121	PRO	2.1
7	D	167	GLU	2.1
10	G	25	GLU	2.1
1	0	2252	A	2.1
12	J	6	PHE	2.1
9	F	100	ASP	2.1
22	T	35	TYR	2.1
9	F	28	ALA	2.1
5	B	84	LEU	2.1
8	E	169	THR	2.1
5	B	58	PRO	2.1
1	0	1180	U	2.1
21	S	19	ASP	2.1
5	B	66	GLU	2.1
24	V	63	GLU	2.1
12	J	78	ILE	2.0
21	S	20	PHE	2.0
24	V	46	ILE	2.0
1	0	2368	A	2.0
12	J	48	GLY	2.0
28	Z	38	ALA	2.0
8	E	141	VAL	2.0
9	F	49	PHE	2.0
14	L	130	ARG	2.0
32	I	108	ILE	2.0
8	E	39	ASP	2.0
27	Y	225	GLY	2.0
8	E	134	SER	2.0
1	0	1214	G	2.0
16	N	186	LEU	2.0
4	A	59	GLU	2.0
26	X	71	ARG	2.0
8	E	156	ASP	2.0
9	F	6	PHE	2.0
26	X	41	PHE	2.0
26	X	77	PHE	2.0
11	H	125	ALA	2.0
4	A	33	GLU	2.0
32	I	122	THR	2.0
8	E	25	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	0	2576	A	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	0.94	0.18	-	31,34,40,41	0
1	1MA	0	628	23/24	0.93	0.21	-	28,34,37,38	0
1	OMU	0	2587	21/22	0.93	0.17	-	31,35,40,41	0
1	OMG	0	2588	24/25	0.90	0.20	-	30,33,38,40	0
1	UR3	0	2619	21/22	0.92	0.22	-	33,38,39,42	0
3	5AA	4	76	24/25	0.93	0.23	-	40,44,46,47	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	9121	1/1	0.73	0.84	39.55	55,55,55,55	0
35	NA	0	9162	1/1	0.75	0.55	39.07	64,64,64,64	0
35	NA	0	9178	1/1	0.90	0.47	30.30	57,57,57,57	0
35	NA	0	9135	1/1	0.87	0.41	17.13	52,52,52,52	0
35	NA	0	9174	1/1	0.88	0.34	14.00	62,62,62,62	0
35	NA	0	9177	1/1	0.60	0.45	13.13	68,68,68,68	0
35	NA	L	9180	1/1	0.96	0.46	12.91	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	9156	1/1	0.86	0.31	12.86	49,49,49,49	0
36	CL	0	9315	1/1	0.79	0.26	10.86	80,80,80,80	0
35	NA	0	9182	1/1	0.64	0.49	9.55	81,81,81,81	0
35	NA	0	9176	1/1	0.69	0.33	9.11	49,49,49,49	0
35	NA	0	9164	1/1	0.85	0.28	8.26	53,53,53,53	0
35	NA	0	9123	1/1	0.89	0.30	6.79	44,44,44,44	0
35	NA	0	9120	1/1	0.95	0.27	6.41	52,52,52,52	0
33	MG	0	8060	1/1	0.92	0.23	6.14	46,46,46,46	0
35	NA	R	9186	1/1	0.57	0.42	6.07	78,78,78,78	0
35	NA	0	9103	1/1	0.95	0.26	5.48	43,43,43,43	0
35	NA	0	9179	1/1	0.89	0.29	5.17	70,70,70,70	0
33	MG	Y	8109	1/1	0.83	0.34	4.45	44,44,44,44	0
35	NA	0	9165	1/1	0.89	0.23	4.30	47,47,47,47	0
35	NA	0	9110	1/1	0.54	0.34	3.66	43,43,43,43	0
35	NA	0	9173	1/1	0.84	0.21	3.53	62,62,62,62	0
35	NA	0	9150	1/1	0.95	0.23	3.50	42,42,42,42	0
35	NA	0	9131	1/1	0.86	0.20	3.18	41,41,41,41	0
35	NA	0	9105	1/1	0.69	0.26	3.16	44,44,44,44	0
35	NA	0	9102	1/1	0.61	0.25	2.99	45,45,45,45	0
35	NA	0	9125	1/1	0.82	0.21	2.90	59,59,59,59	0
35	NA	0	9172	1/1	0.92	0.25	2.41	62,62,62,62	0
36	CL	0	9316	1/1	0.88	0.30	2.28	66,66,66,66	0
35	NA	0	9159	1/1	0.96	0.24	2.20	50,50,50,50	0
36	CL	O	9308	1/1	0.98	0.27	1.93	79,79,79,79	0
33	MG	0	8080	1/1	0.90	0.18	1.93	41,41,41,41	0
35	NA	0	9161	1/1	0.82	0.22	1.78	56,56,56,56	0
36	CL	0	9312	1/1	0.94	0.28	1.49	59,59,59,59	0
35	NA	0	9140	1/1	0.92	0.25	1.40	47,47,47,47	0
35	NA	0	9171	1/1	0.85	0.21	1.23	52,52,52,52	0
35	NA	0	9153	1/1	0.97	0.20	1.08	21,21,21,21	0
33	MG	0	8028	1/1	0.95	0.18	1.04	41,41,41,41	0
35	NA	0	9114	1/1	0.93	0.21	1.00	64,64,64,64	0
35	NA	0	9124	1/1	0.59	0.21	0.78	66,66,66,66	0
33	MG	0	8032	1/1	0.85	0.20	0.44	41,41,41,41	0
35	NA	0	9133	1/1	0.76	0.15	-0.05	34,34,34,34	0
33	MG	0	8053	1/1	0.70	0.16	-0.11	57,57,57,57	0
35	NA	Q	9148	1/1	0.89	0.22	-0.20	38,38,38,38	0
35	NA	0	9143	1/1	0.97	0.17	-0.22	33,33,33,33	0
36	CL	B	9319	1/1	0.92	0.22	-0.38	55,55,55,55	0
35	NA	A	9145	1/1	0.90	0.20	-0.44	48,48,48,48	0
36	CL	L	9310	1/1	0.87	0.16	-0.53	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	9117	1/1	0.85	0.26	-0.66	61,61,61,61	0
36	CL	M	9318	1/1	0.98	0.17	-0.73	47,47,47,47	0
33	MG	0	8017	1/1	0.97	0.14	-0.78	29,29,29,29	0
33	MG	0	8013	1/1	0.91	0.19	-0.90	33,33,33,33	0
36	CL	J	9321	1/1	0.78	0.18	-0.93	55,55,55,55	0
33	MG	0	8021	1/1	0.78	0.17	-0.96	32,32,32,32	0
37	CD	Z	9203	1/1	0.97	0.09	-0.99	67,67,67,67	0
33	MG	0	8018	1/1	0.83	0.16	-1.08	42,42,42,42	0
33	MG	0	8038	1/1	0.80	0.17	-1.09	32,32,32,32	0
33	MG	0	8086	1/1	0.91	0.12	-1.13	50,50,50,50	0
33	MG	A	8065	1/1	0.96	0.17	-1.16	45,45,45,45	0
35	NA	C	9104	1/1	0.85	0.14	-1.21	40,40,40,40	0
35	NA	0	9126	1/1	0.81	0.17	-1.26	41,41,41,41	0
35	NA	0	9166	1/1	0.88	0.13	-1.28	69,69,69,69	0
33	MG	0	8058	1/1	0.69	0.15	-1.37	56,56,56,56	0
33	MG	B	8055	1/1	0.78	0.20	-1.46	62,62,62,62	0
33	MG	0	8096	1/1	0.90	0.15	-1.48	53,53,53,53	0
33	MG	0	8064	1/1	0.87	0.15	-1.48	30,30,30,30	0
33	MG	0	8057	1/1	0.87	0.15	-1.77	42,42,42,42	0
35	NA	R	9137	1/1	0.89	0.14	-1.78	44,44,44,44	0
33	MG	0	8035	1/1	0.92	0.12	-1.86	49,49,49,49	0
33	MG	T	8073	1/1	0.92	0.13	-1.87	59,59,59,59	0
35	NA	M	9147	1/1	0.97	0.14	-1.96	25,25,25,25	0
33	MG	0	8067	1/1	0.96	0.16	-2.07	49,49,49,49	0
35	NA	H	9109	1/1	0.89	0.14	-2.12	34,34,34,34	0
33	MG	0	8019	1/1	0.98	0.14	-2.27	35,35,35,35	0
35	NA	R	9138	1/1	0.89	0.14	-2.28	63,63,63,63	0
33	MG	0	8002	1/1	0.92	0.14	-2.51	39,39,39,39	0
33	MG	0	8074	1/1	0.99	0.08	-2.57	37,37,37,37	0
35	NA	0	9144	1/1	0.81	0.13	-2.59	33,33,33,33	0
33	MG	0	8108	1/1	0.90	0.11	-2.63	58,58,58,58	0
34	K	0	9002	1/1	0.92	0.13	-2.71	48,48,48,48	0
33	MG	0	8070	1/1	0.90	0.10	-2.85	57,57,57,57	0
34	K	0	9001	1/1	0.98	0.14	-2.89	71,71,71,71	0
35	NA	0	9127	1/1	0.91	0.12	-2.96	42,42,42,42	0
37	CD	U	9201	1/1	0.87	0.11	-3.09	74,74,74,74	0
33	MG	0	8033	1/1	0.80	0.11	-3.11	38,38,38,38	0
33	MG	0	8012	1/1	0.93	0.13	-3.12	32,32,32,32	0
37	CD	1	9202	1/1	0.91	0.07	-3.19	62,62,62,62	0
33	MG	4	8118	1/1	0.91	0.13	-3.26	41,41,41,41	0
33	MG	3	8078	1/1	0.86	0.10	-3.32	43,43,43,43	0
33	MG	0	8044	1/1	0.84	0.13	-3.47	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8003	1/1	0.84	0.15	-3.57	31,31,31,31	0
33	MG	B	8056	1/1	0.76	0.10	-3.60	47,47,47,47	0
35	NA	J	9146	1/1	0.92	0.08	-3.66	42,42,42,42	0
35	NA	9	9183	1/1	0.89	0.14	-3.69	60,60,60,60	0
33	MG	0	8110	1/1	0.96	0.15	-3.74	32,32,32,32	0
33	MG	0	8020	1/1	0.95	0.13	-3.79	31,31,31,31	0
35	NA	0	9139	1/1	0.84	0.16	-3.79	31,31,31,31	0
33	MG	0	8112	1/1	0.97	0.06	-3.83	39,39,39,39	0
33	MG	0	8001	1/1	0.92	0.11	-3.99	35,35,35,35	0
35	NA	0	9108	1/1	0.93	0.10	-4.09	49,49,49,49	0
36	CL	3	9304	1/1	0.80	0.12	-4.18	61,61,61,61	0
33	MG	0	8015	1/1	0.90	0.12	-4.39	33,33,33,33	0
33	MG	0	8062	1/1	0.96	0.07	-4.40	51,51,51,51	0
33	MG	0	8107	1/1	0.91	0.10	-4.57	53,53,53,53	0
36	CL	0	9305	1/1	0.98	0.10	-4.85	55,55,55,55	0
33	MG	9	8052	1/1	0.68	0.12	-5.01	54,54,54,54	0
33	MG	0	8054	1/1	0.98	0.10	-5.06	29,29,29,29	0
33	MG	0	8007	1/1	0.85	0.12	-5.06	27,27,27,27	0
33	MG	0	8039	1/1	0.96	0.05	-5.13	52,52,52,52	0
33	MG	0	8008	1/1	0.83	0.08	-5.69	37,37,37,37	0
35	NA	0	9132	1/1	0.98	0.06	-5.74	34,34,34,34	0
33	MG	0	8084	1/1	0.72	0.13	-5.97	38,38,38,38	0
33	MG	0	8010	1/1	0.92	0.11	-6.17	28,28,28,28	0
33	MG	0	8077	1/1	0.90	0.09	-6.19	28,28,28,28	0
33	MG	0	8014	1/1	0.91	0.07	-6.41	43,43,43,43	0
35	NA	0	9168	1/1	0.94	0.08	-6.83	49,49,49,49	0
35	NA	0	9167	1/1	0.96	0.07	-7.21	52,52,52,52	0
33	MG	0	8004	1/1	0.97	0.09	-9.28	34,34,34,34	0
33	MG	0	8006	1/1	0.82	0.09	-9.68	37,37,37,37	0
33	MG	0	8048	1/1	0.95	0.07	-10.03	56,56,56,56	0
33	MG	0	8022	1/1	0.92	0.09	-11.41	35,35,35,35	0
35	NA	0	9130	1/1	0.93	0.11	-	45,45,45,45	0
33	MG	0	8050	1/1	0.79	0.14	-	69,69,69,69	0
33	MG	0	8090	1/1	0.59	0.31	-	65,65,65,65	0
35	NA	0	9181	1/1	0.79	0.34	-	56,56,56,56	0
33	MG	0	8031	1/1	0.94	0.13	-	30,30,30,30	0
35	NA	0	9119	1/1	0.88	0.10	-	44,44,44,44	0
33	MG	0	8043	1/1	0.96	0.11	-	47,47,47,47	0
35	NA	0	9149	1/1	0.89	0.18	-	38,38,38,38	0
33	MG	0	8082	1/1	0.86	0.16	-	76,76,76,76	0
36	CL	N	9307	1/1	0.73	0.33	-	72,72,72,72	0
33	MG	0	8029	1/1	0.97	0.07	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	9170	1/1	0.64	0.29	-	49,49,49,49	0
35	NA	0	9101	1/1	0.82	0.25	-	40,40,40,40	0
35	NA	0	9142	1/1	0.81	0.26	-	47,47,47,47	0
33	MG	0	8072	1/1	0.86	0.26	-	60,60,60,60	0
35	NA	0	9155	1/1	0.64	0.49	-	79,79,79,79	0
35	NA	0	9115	1/1	0.94	0.14	-	37,37,37,37	0
33	MG	0	8087	1/1	0.95	0.27	-	59,59,59,59	0
33	MG	0	8089	1/1	0.94	0.10	-	56,56,56,56	0
35	NA	0	9129	1/1	0.67	0.24	-	57,57,57,57	0
35	NA	0	9157	1/1	0.68	0.11	-	73,73,73,73	0
35	NA	0	9107	1/1	0.95	0.17	-	46,46,46,46	0
35	NA	9	9151	1/1	0.86	0.14	-	64,64,64,64	0
33	MG	0	8059	1/1	0.70	0.15	-	51,51,51,51	0
35	NA	0	9160	1/1	0.95	0.35	-	46,46,46,46	0
33	MG	0	8026	1/1	0.87	0.10	-	24,24,24,24	0
35	NA	0	9113	1/1	0.81	0.35	-	67,67,67,67	0
33	MG	0	8068	1/1	0.53	0.07	-	60,60,60,60	0
33	MG	0	8079	1/1	0.79	0.10	-	29,29,29,29	0
35	NA	H	9122	1/1	0.86	0.17	-	72,72,72,72	0
33	MG	0	8103	1/1	0.65	0.25	-	65,65,65,65	0
36	CL	J	9301	1/1	0.68	0.20	-	78,78,78,78	0
33	MG	0	8024	1/1	0.97	0.17	-	39,39,39,39	0
33	MG	0	8047	1/1	0.81	0.18	-	86,86,86,86	0
35	NA	0	9111	1/1	0.72	0.21	-	61,61,61,61	0
33	MG	0	8101	1/1	0.70	0.39	-	72,72,72,72	0
33	MG	9	8095	1/1	0.81	0.10	-	77,77,77,77	0
36	CL	0	9313	1/1	0.94	0.13	-	60,60,60,60	0
33	MG	0	8040	1/1	0.95	0.14	-	56,56,56,56	0
35	NA	0	9184	1/1	0.32	0.88	-	83,83,83,83	0
35	NA	0	9163	1/1	0.93	0.19	-	65,65,65,65	0
33	MG	2	8076	1/1	0.97	0.14	-	55,55,55,55	0
33	MG	0	8030	1/1	0.91	0.16	-	35,35,35,35	0
33	MG	0	8061	1/1	0.92	0.08	-	37,37,37,37	0
33	MG	0	8114	1/1	0.93	0.07	-	56,56,56,56	0
33	MG	0	8011	1/1	0.93	0.19	-	20,20,20,20	0
36	CL	0	9314	1/1	0.94	0.11	-	49,49,49,49	0
35	NA	0	9154	1/1	0.97	0.14	-	33,33,33,33	0
33	MG	0	8075	1/1	0.93	0.16	-	57,57,57,57	0
36	CL	0	9322	1/1	0.96	0.19	-	77,77,77,77	0
35	NA	0	9118	1/1	0.97	0.22	-	62,62,62,62	0
33	MG	0	8042	1/1	0.96	0.06	-	44,44,44,44	0
33	MG	0	8005	1/1	0.94	0.19	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	S	9112	1/1	0.73	0.29	-	73,73,73,73	0
37	CD	3	9204	1/1	0.98	0.06	-	64,64,64,64	0
33	MG	0	8116	1/1	0.45	0.18	-	62,62,62,62	0
35	NA	0	9128	1/1	0.93	0.09	-	43,43,43,43	0
33	MG	0	8051	1/1	0.94	0.08	-	72,72,72,72	0
33	MG	0	8016	1/1	0.91	0.29	-	50,50,50,50	0
33	MG	0	8083	1/1	0.94	0.09	-	42,42,42,42	0
35	NA	0	9185	1/1	0.89	0.36	-	51,51,51,51	0
33	MG	0	8085	1/1	0.91	0.19	-	72,72,72,72	0
33	MG	0	8036	1/1	0.90	0.13	-	35,35,35,35	0
35	NA	0	9116	1/1	0.94	0.17	-	42,42,42,42	0
36	CL	J	9302	1/1	0.63	0.21	-	79,79,79,79	0
33	MG	0	8049	1/1	0.78	0.43	-	81,81,81,81	0
33	MG	0	8111	1/1	0.81	0.10	-	52,52,52,52	0
36	CL	0	9311	1/1	0.88	0.16	-	53,53,53,53	0
33	MG	0	8099	1/1	0.82	0.17	-	53,53,53,53	0
33	MG	0	8045	1/1	0.85	0.19	-	73,73,73,73	0
33	MG	0	8092	1/1	0.78	0.45	-	90,90,90,90	0
33	MG	0	8034	1/1	0.72	0.13	-	38,38,38,38	0
34	K	0	9003	1/1	0.88	0.20	-	64,64,64,64	0
33	MG	0	8027	1/1	0.90	0.09	-	37,37,37,37	0
33	MG	0	8119	1/1	0.92	0.20	-	62,62,62,62	0
33	MG	0	8117	1/1	0.72	0.15	-	37,37,37,37	0
35	NA	0	9141	1/1	0.89	0.10	-	45,45,45,45	0
33	MG	0	8102	1/1	0.94	0.09	-	58,58,58,58	0
36	CL	0	9317	1/1	0.91	0.09	-	61,61,61,61	0
33	MG	0	8025	1/1	0.65	0.14	-	46,46,46,46	0
37	CD	O	9205	1/1	0.93	0.04	-	143,143,143,143	0
33	MG	0	8097	1/1	0.95	0.09	-	40,40,40,40	0
33	MG	0	8104	1/1	0.83	0.17	-	55,55,55,55	0
33	MG	0	8041	1/1	0.92	0.25	-	79,79,79,79	0
36	CL	0	9303	1/1	0.94	0.12	-	53,53,53,53	0
33	MG	0	8046	1/1	0.92	0.09	-	59,59,59,59	0
33	MG	0	8094	1/1	0.92	0.11	-	73,73,73,73	0
35	NA	B	9158	1/1	0.78	0.84	-	70,70,70,70	0
33	MG	0	8106	1/1	0.90	0.07	-	54,54,54,54	0
33	MG	0	8063	1/1	0.30	0.19	-	71,71,71,71	0
33	MG	0	8113	1/1	0.70	0.20	-	52,52,52,52	0
33	MG	0	8081	1/1	0.90	0.16	-	52,52,52,52	0
33	MG	0	8091	1/1	0.49	0.07	-	79,79,79,79	0
35	NA	0	9169	1/1	0.83	0.33	-	60,60,60,60	0
35	NA	0	9152	1/1	0.94	0.50	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8071	1/1	0.86	0.18	-	66,66,66,66	0
35	NA	0	9134	1/1	0.93	0.15	-	41,41,41,41	0
35	NA	0	9175	1/1	0.94	0.34	-	52,52,52,52	0
36	CL	A	9309	1/1	0.93	0.25	-	61,61,61,61	0
33	MG	0	8115	1/1	0.91	0.09	-	57,57,57,57	0
33	MG	0	8088	1/1	0.80	0.14	-	38,38,38,38	0
36	CL	R	9306	1/1	0.95	0.13	-	57,57,57,57	0
33	MG	0	8093	1/1	0.79	0.19	-	66,66,66,66	0
33	MG	0	8100	1/1	0.89	0.43	-	70,70,70,70	0
35	NA	0	9136	1/1	0.92	0.09	-	55,55,55,55	0
33	MG	K	8069	1/1	0.85	0.09	-	52,52,52,52	0
33	MG	A	8066	1/1	0.94	0.05	-	66,66,66,66	0
33	MG	0	8023	1/1	0.82	0.24	-	52,52,52,52	0
36	CL	Y	9320	1/1	0.92	0.12	-	52,52,52,52	0
35	NA	0	9106	1/1	0.90	0.37	-	38,38,38,38	0
33	MG	0	8098	1/1	0.94	0.10	-	47,47,47,47	0
33	MG	0	8037	1/1	0.89	0.11	-	45,45,45,45	0
33	MG	0	8009	1/1	0.89	0.13	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.