Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:03 PM GMT

PDB ID	:	1VQP
Title	:	The structure of the transition state analogue "RAP" bound to the large ribosomal subunit of haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.25 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:

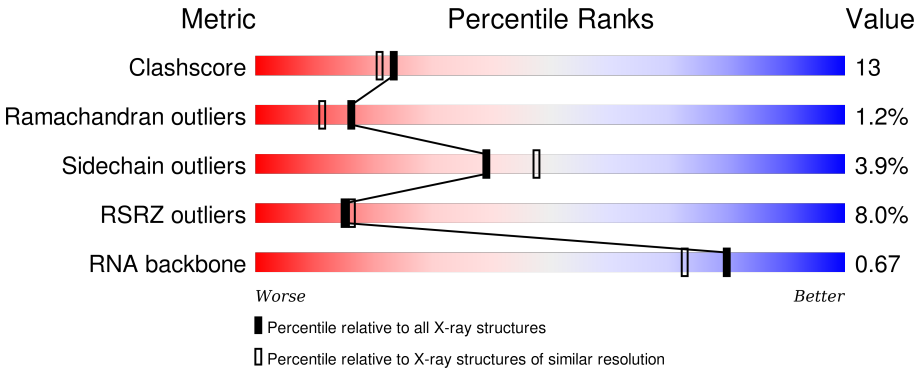
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)
RNA backbone	2183	1002 (2.80-1.74)

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	5% 65% 25% 5% 6%
2	9	122	6% 57% 34% 7% •
3	4	8	38% 63%
4	A	240	6% 63% 32% 5% •
5	B	338	4% 62% 33% •

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Mol	Chain	Length	Quality of chain
6	C	246	2% 67% 29%
7	D	177	25% 36% 36% 7% 21%
8	E	178	8% 67% 28%
9	F	120	13% 58% 39%
10	G	348	5% 5% 92%
11	H	171	14% 60% 32% 6%
12	J	145	3% 63% 29% 6%
13	K	132	3% 63% 34%
14	L	165	10% 59% 27% 12%
15	M	195	3% 66% 31%
16	N	187	20% 55% 39% 5%
17	O	116	3% 69% 30%
18	P	149	4% 70% 24%
19	Q	96	2% 74% 24%
20	R	155	% 72% 23%
21	S	85	7% 75% 20% 5%
22	T	120	11% 56% 39%
23	U	66	3% 55% 26% 20%
24	V	71	28% 51% 37% 8%
25	W	154	5% 58% 41%
26	X	92	10% 49% 37% 11%
27	Y	241	3% 40% 15% 41%
28	Z	83	18% 49% 37% 12%
29	1	57	72% 26%
30	2	50	24% 48% 42% 8%

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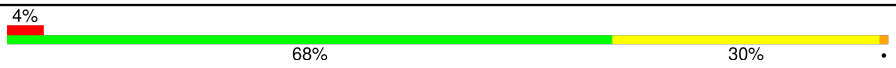
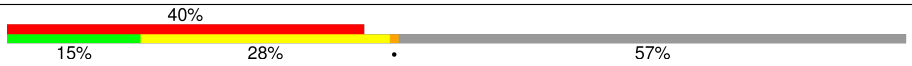
Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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	8001	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8012	-	-	-	X
33	MG	0	8013	-	-	-	X
33	MG	0	8017	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8021	-	-	-	X
33	MG	0	8027	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8039	-	-	-	X
33	MG	0	8054	-	-	-	X
33	MG	0	8058	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8101	-	-	-	X
34	K	0	9001	-	-	-	X
35	NA	0	9105	-	-	-	X
35	NA	0	9114	-	-	-	X
35	NA	0	9120	-	-	-	X
35	NA	0	9124	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9127	-	-	-	X
35	NA	0	9131	-	-	-	X
35	NA	0	9156	-	-	-	X
35	NA	0	9161	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9164	-	-	-	X
35	NA	0	9168	-	-	-	X
35	NA	0	9169	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9173	-	-	-	X
35	NA	0	9174	-	-	-	X
35	NA	0	9177	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	9182	-	-	-	X
35	NA	0	9185	-	-	-	X
35	NA	R	9186	-	-	-	X
36	CL	0	9315	-	-	-	X
37	SR	0	9482	-	-	-	X
37	SR	0	9534	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*(DC)P*(DC)P*(PPU)*(LOF)P*(PO2)P*AP*C*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	132	67	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	C	N	O	0	0	0
			865	529	161	175			

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

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

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

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

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

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

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

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

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

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

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

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

- 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	88	Total	Mg	0	0
			88	88		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	D	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	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
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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	98	Total Sr 98 98	0	0
37	1	2	Total Sr 2 2	0	0
37	H	1	Total Sr 1 1	0	0
37	B	2	Total Sr 2 2	0	0
37	3	1	Total Sr 1 1	0	0
37	A	3	Total Sr 3 3	0	0
37	R	1	Total Sr 1 1	0	0
37	9	3	Total Sr 3 3	0	0
37	L	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	F	1	Total Sr 1 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	3	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5757	Total O 5757 5757	0	0
39	9	139	Total O 139 139	0	0
39	4	6	Total O 6 6	0	0
39	A	124	Total O 124 124	0	0
39	B	140	Total O 140 140	0	0
39	C	172	Total O 172 172	0	0
39	D	50	Total O 50 50	0	0
39	E	40	Total O 40 40	0	0
39	F	25	Total O 25 25	0	0
39	G	16	Total O 16 16	0	0
39	H	69	Total O 69 69	0	0
39	J	52	Total O 52 52	0	0
39	K	59	Total O 59 59	0	0
39	L	83	Total O 83 83	0	0
39	M	131	Total O 131 131	0	0
39	N	58	Total O 58 58	0	0
39	O	39	Total O 39 39	0	0
39	P	57	Total O 57 57	0	0
39	Q	51	Total O 51 51	0	0
39	R	87	Total O 87 87	0	0
39	S	32	Total O 32 32	0	0

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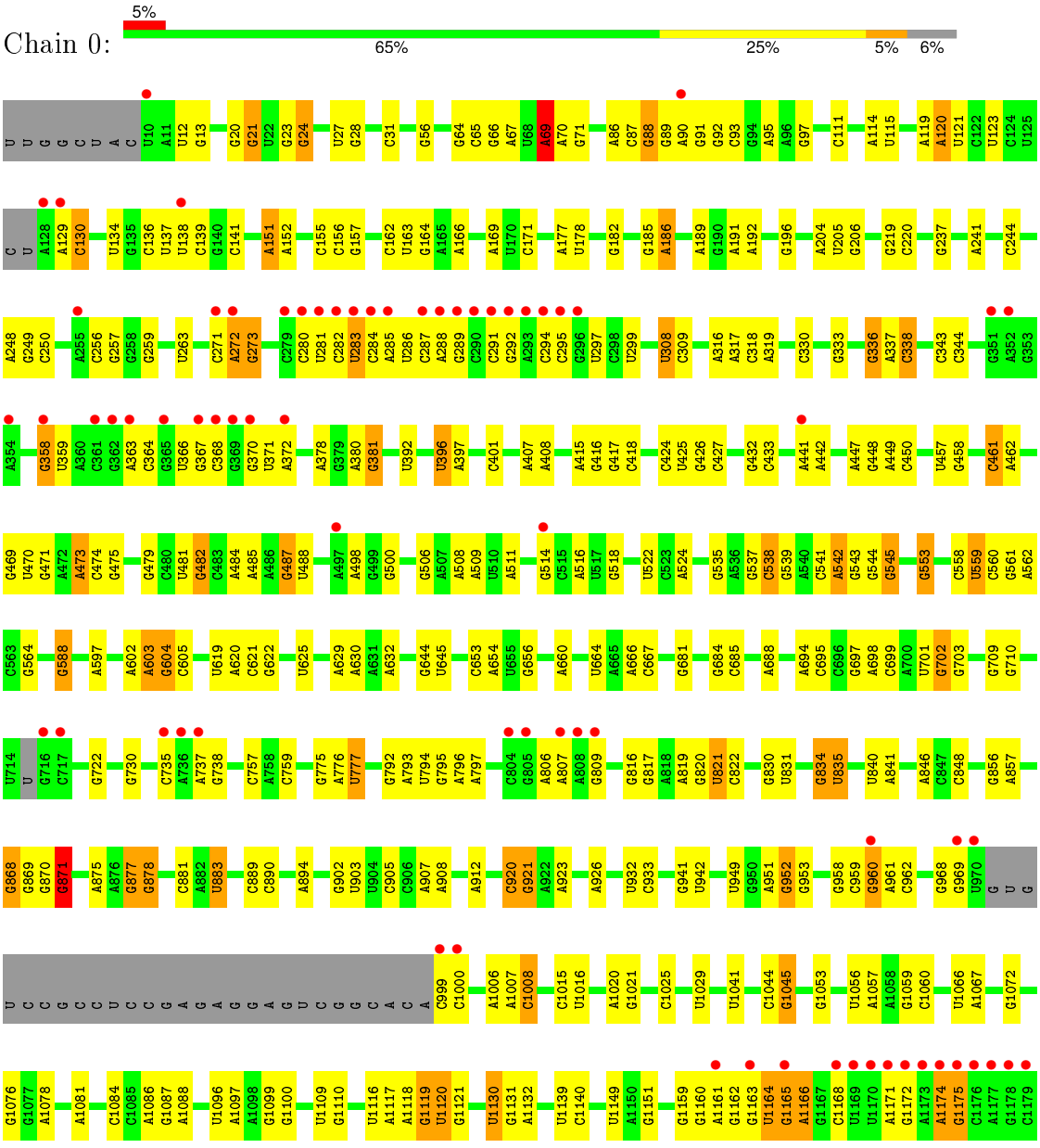
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	T	36	Total O 36 36	0	0
39	U	30	Total O 30 30	0	0
39	V	11	Total O 11 11	0	0
39	W	72	Total O 72 72	0	0
39	X	24	Total O 24 24	0	0
39	Y	88	Total O 88 88	0	0
39	Z	31	Total O 31 31	0	0
39	1	49	Total O 49 49	0	0
39	2	38	Total O 38 38	0	0
39	3	66	Total O 66 66	0	0
39	I	9	Total O 9 9	0	0

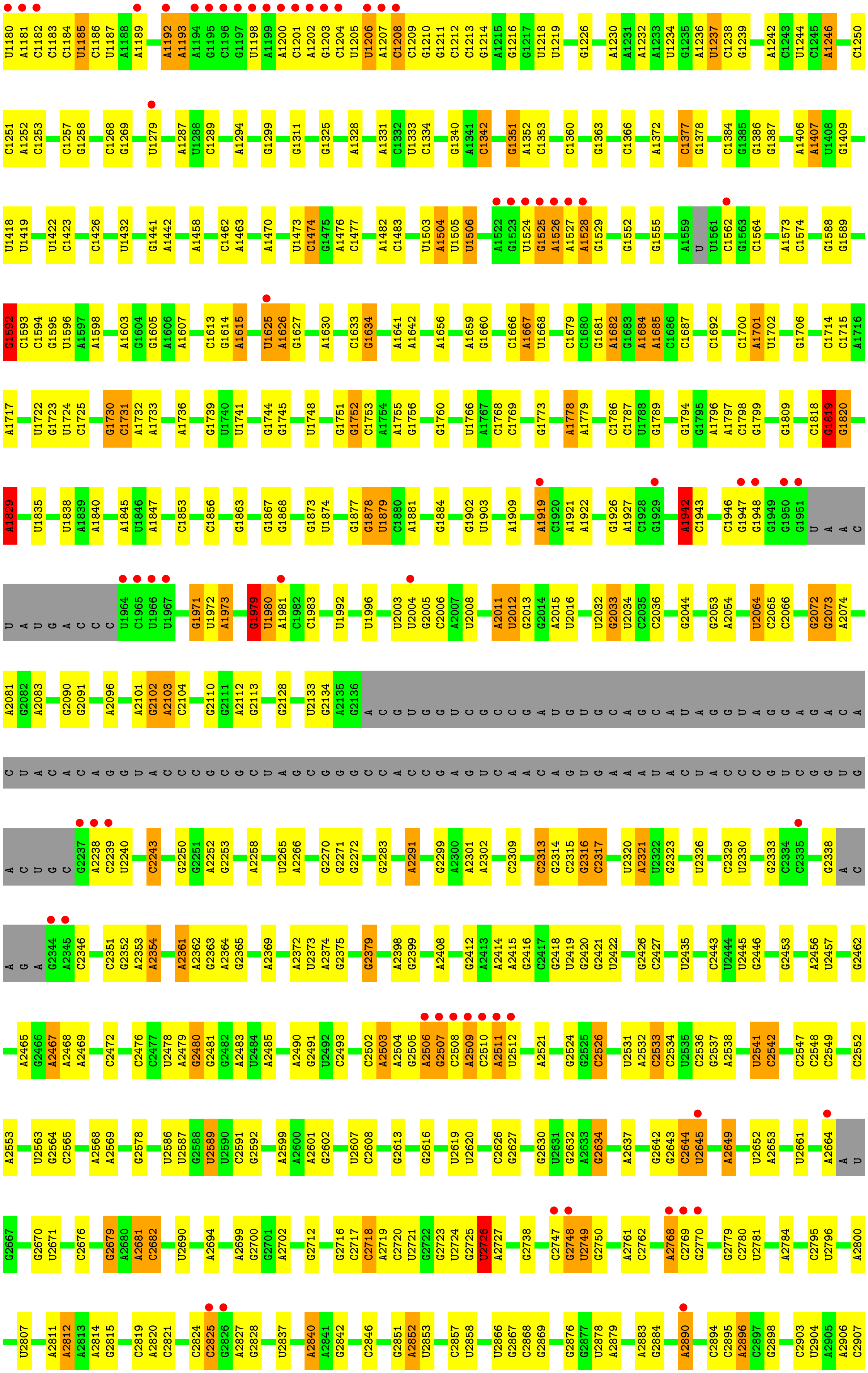
3 Residue-property plots (i)

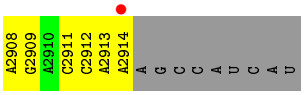
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 23S ribosomal rna

Chain 0:

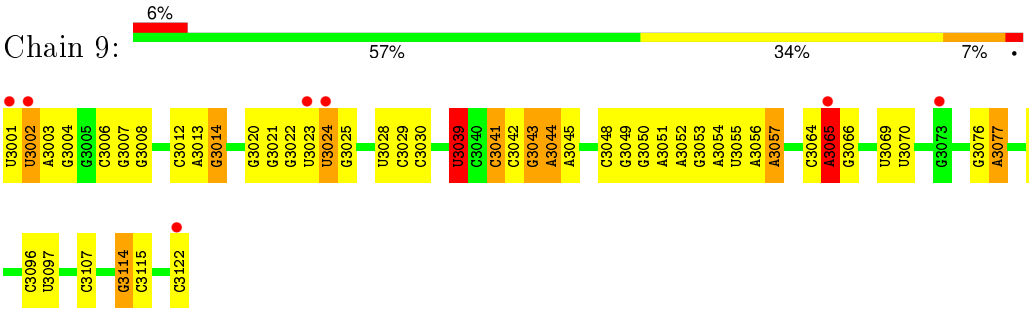



U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 G1226 A1230 A1231 A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 C1250
C1251 A1252 C1253 C1257 G1258 C1268 G1269 U1279 A1287 U1288 C1289 A1294 G1299 G1311 G1325 A1328 A1331 C1332 U1333 C1334 G1340 A1341 C1342 G1351 A1352 C1353 C1360 G1363 C1366 A1372 C1377 G1378 C1384 G1385 G1386 G1387 A1406 A1407 U1408 G1409
U1418 U1419 U1422 C1423 C1426 U1432 G1441 A1442 A1458 C1462 A1463 A1470 U1473 C1474 G1475 A1476 C1477 A1482 C1483 U1503 A1504 U1505 U1506 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1552 G1555 A1559 U U1561 C1562 G1563 C1564 A1573 C1574 G1588 G1589
G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 A1606 A1607 C1613 G1614 A1615 U1625 A1626 G1627 A1630 C1633 G1634 A1641 A1642 A1656 A1659 G1660 C1666 A1667 U1668 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 C1700 A1701 U1702 G1706 C1714 C1715 A1716
A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 A1736 G1739 U1740 U1741 G1744 G1745 U1748 G1751 G1752 C1753 A1754 A1755 G1756 G1760 U1766 A1767 C1768 C1769 G1773 A1778 A1779 C1786 C1787 U1788 G1789 G1794 G1795 A1796 A1797 C1798 G1799 G1809 C1818 G1819 G1820
A1829 U1835 U1838 A1839 A1840 A1845 U1846 A1847 C1853 C1856 G1863 G1867 G1868 G1873 U1874 G1877 G1878 U1879 C1880 A1881 G1884 G1902 U1903 A1909 A1919 C1920 A1921 A1922 G1926 A1927 C1928 G1929 A1942 C1943 C1946 G1947 G1948 G1949 G1950 G1951 U A A C
U A U G A C C C U1964 C1965 U1966 U1967 G1971 U1972 A1973 G1979 U1980 A1981 C1982 C1983 U1992 U1996 U2003 U2004 G2005 C2006 A2007 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2032 G2033 U2034 C2035 C2036 G2044 G2053 A2054 U2064 C2065 C2066 G2072 G2073 A2074
A2081 G2082 A2083 G2090 G2091 A2096 A2101 G2102 A2103 C2104 G2110 G2111 A2112 G2113 G2128 U2133 G2134 A2135 G2136 A C G U G G U C G C C G A U G G U G C A G C A U A G G U A G G A G A C A
C U A C A C A G G U A C C C G C G C U A G C G G G C C A C C G A G U C A A C A G U G A A A U A C U A C C C G U C G G U G
A C U G C G2237 A2238 C2239 U2240 C2243 G2250 G2251 A2252 G2253 A2258 U2265 A2266 G2270 G2271 G2272 G2283 A2291 G2299 A2300 A2301 A2302 C2309 C2313 G2314 C2315 G2316 C2317 U2320 A2321 U2322 G2323 U2326 C2329 U2330 G2333 C2334 C2335 G2338 A C
A G A G2344 A2345 C2346 C2351 G2352 A2353 A2354 A2361 A2362 G2363 A2364 G2365 A2369 A2372 U2373 A2374 G2375 G2379 A2398 G2399 A2408 G2412 A2413 A2414 A2415 G2416 C2417 G2418 U2419 G2420 G2421 U2422 G2426 C2427 U2435 C2443 U2444 U2445 G2446 G2453 A2456 U2457 G2462
A2465 G2466 A2467 A2468 A2469 C2472 C2476 C2477 U2478 A2479 G2480 G2481 G2482 A2483 U2484 A2485 A2490 G2491 U2492 C2493 C2502 A2503 A2504 G2505 A2506 G2507 C2508 A2509 C2510 A2511 U2512 A2521 G2524 G2525 C2526 U2531 A2532 C2533 C2534 U2535 C2536 G2537 A2538 U2541 C2542 C2547 C2548 C2549 C2552
A2553 U2563 G2564 C2565 A2568 A2569 G2578 U2586 U2587 G2588 U2589 U2590 C2591 G2592 A2599 A2600 A2601 G2602 U2607 C2608 G2613 G2616 U2619 U2620 C2626 G2627 G2630 U2631 G2632 A2633 G2634 A2637 G2642 G2643 C2644 U2645 A2649 U2652 A2653 U2661 A2664 A U
G2667 G2670 U2671 C2676 G2679 A2680 A2681 C2682 U2690 A2694 A2699 G2700 G2701 A2702 G2712 G2716 C2717 C2718 A2719 C2720 U2721 G2722 G2723 U2724 G2725 U2726 A2727 G2738 C2747 G2748 U2749 G2750 A2761 C2762 A2768 C2769 G2770 G2779 C2780 U2781 A2784 C2795 U2796 A2800
U2807 A2811 A2812 A2813 A2814 G2815 C2819 A2820 C2821 C2824 C2825 G2826 A2827 G2828 U2837 A2840 A2841 G2842 C2846 G2851 A2852 U2853 C2857 U2858 U2866 G2867 C2868 G2869 G2876 G2877 U2878 A2879 A2883 G2884 A2890 C2894 C2895 A2896 C2897 G2898 C2903 U2904 A2905 A2906 C2907



- Molecule 2: 5S ribosomal RNA

Chain 9:

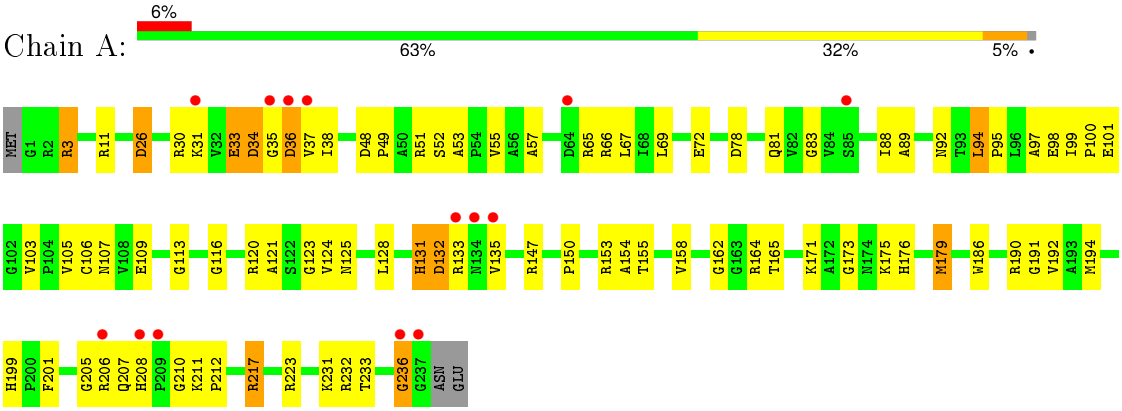


- Molecule 3: 5'-R(*(DC)P*(DC)P*(PPU)*(LOF)P*(PO2)P*AP*C*C)-3'

Chain 4:

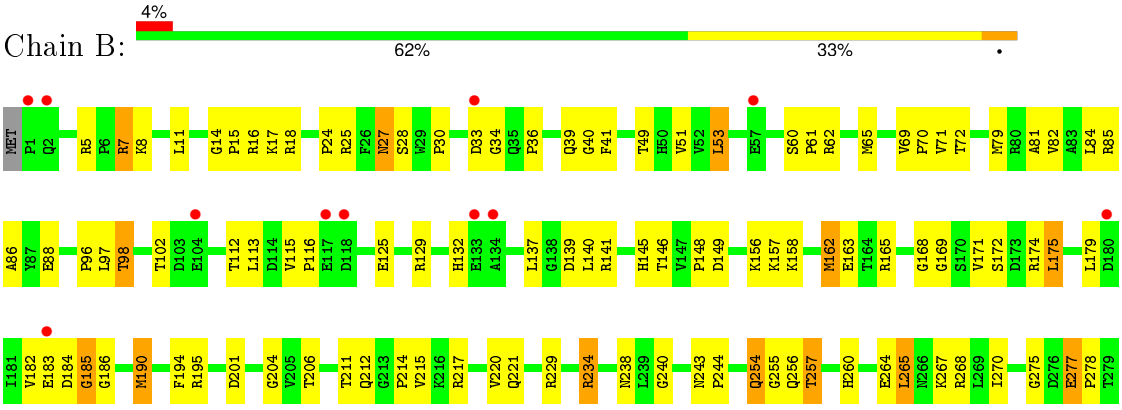
- Molecule 4: 50S ribosomal protein L2P

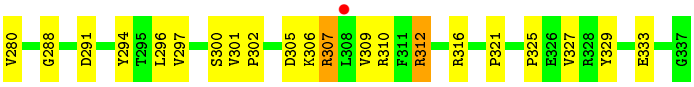
Chain A:



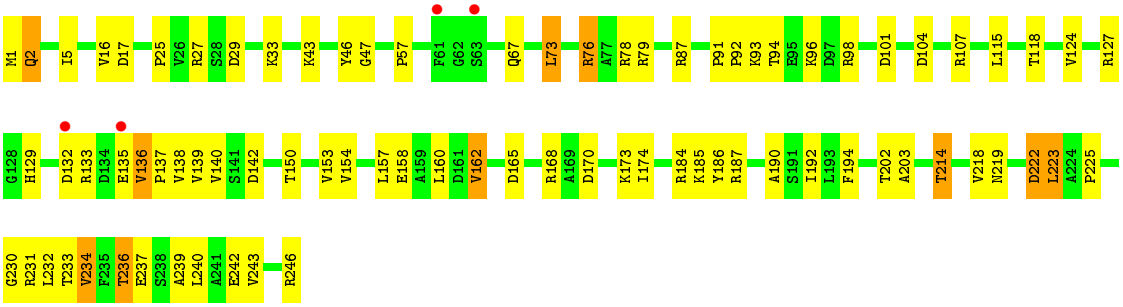
- Molecule 5: 50S ribosomal protein L3P

Chain B:

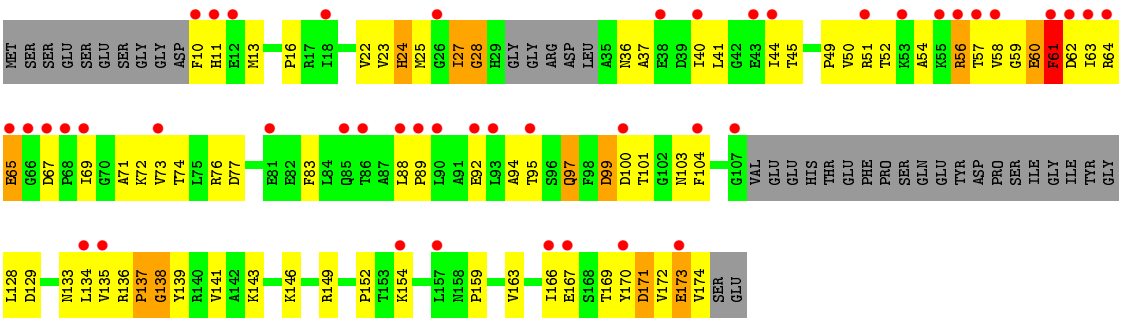




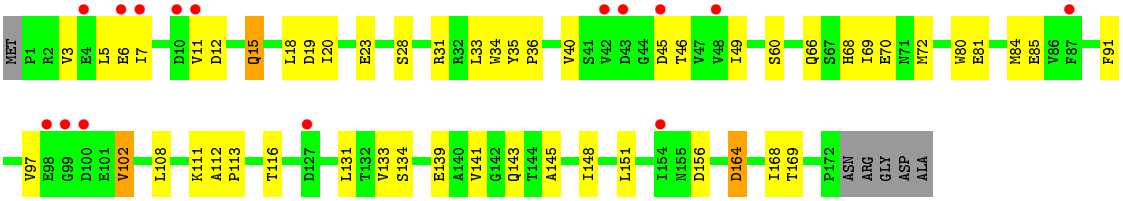
• Molecule 6: 50S ribosomal protein L4E



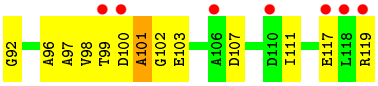
• Molecule 7: 50S ribosomal protein L5P



• Molecule 8: 50S ribosomal protein L6P

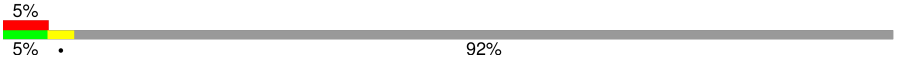


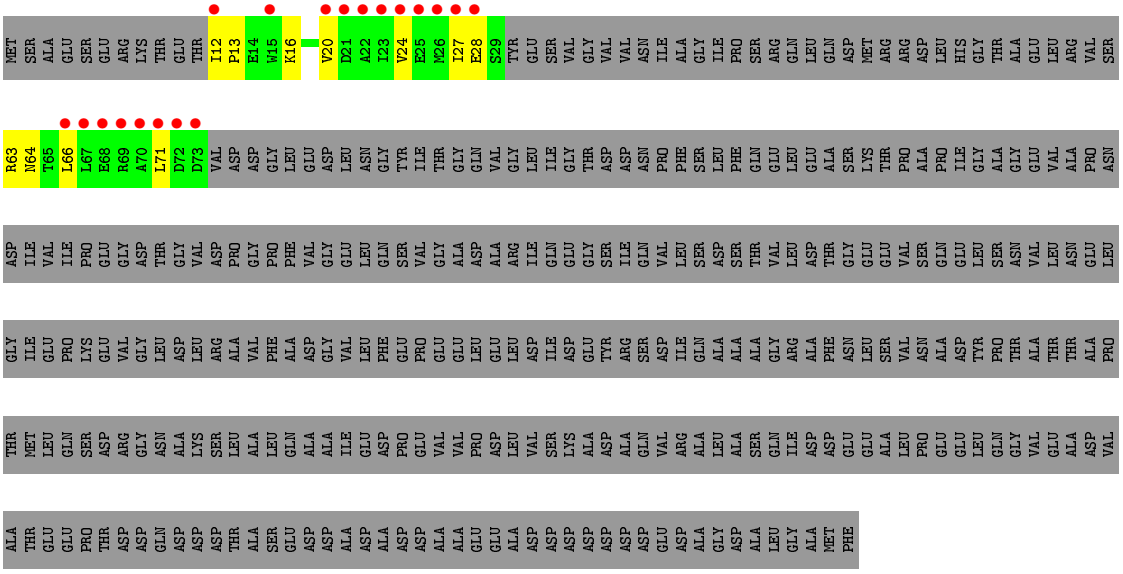
• Molecule 9: 50S ribosomal protein L7AE



• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

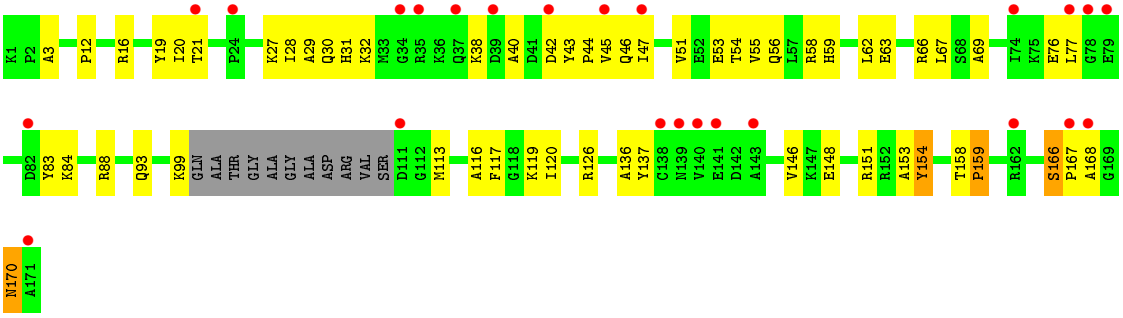
Chain G:





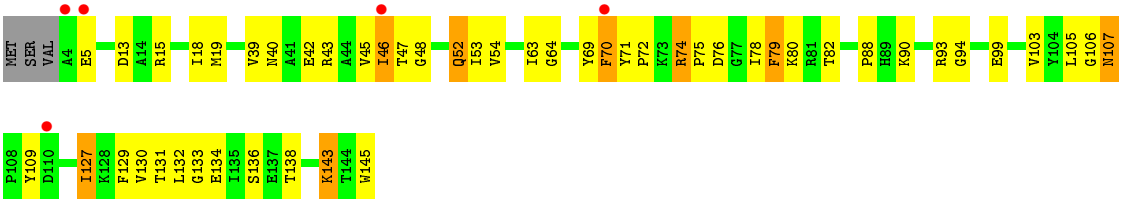
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



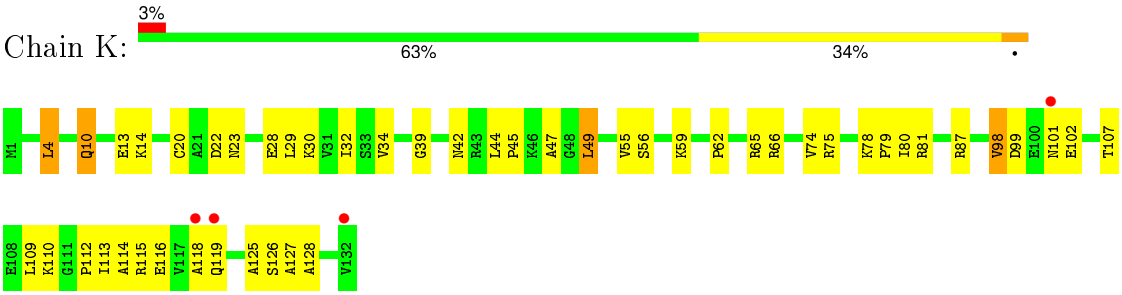
• Molecule 12: 50S ribosomal protein L13P

Chain J:



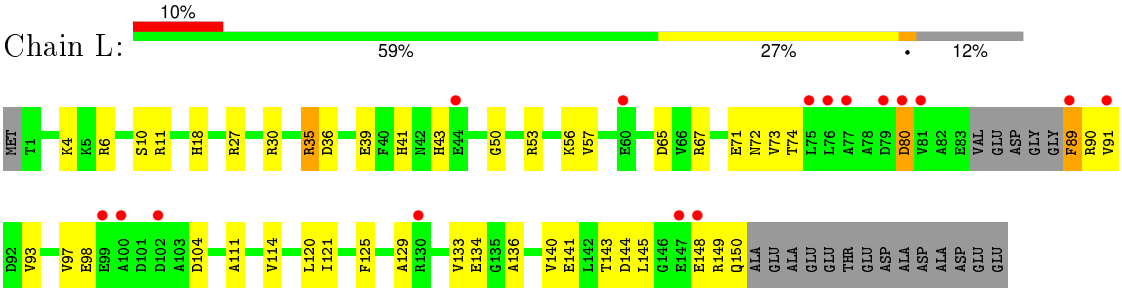
• Molecule 13: 50S ribosomal protein L14P

Chain K:



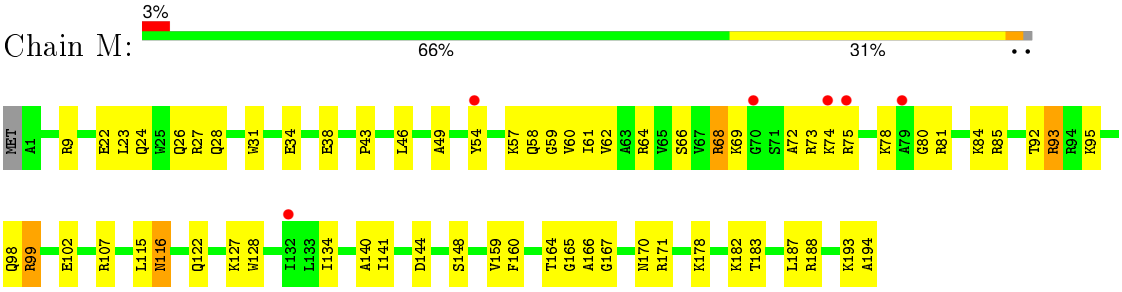
• Molecule 14: 50S ribosomal protein L15P

Chain L:



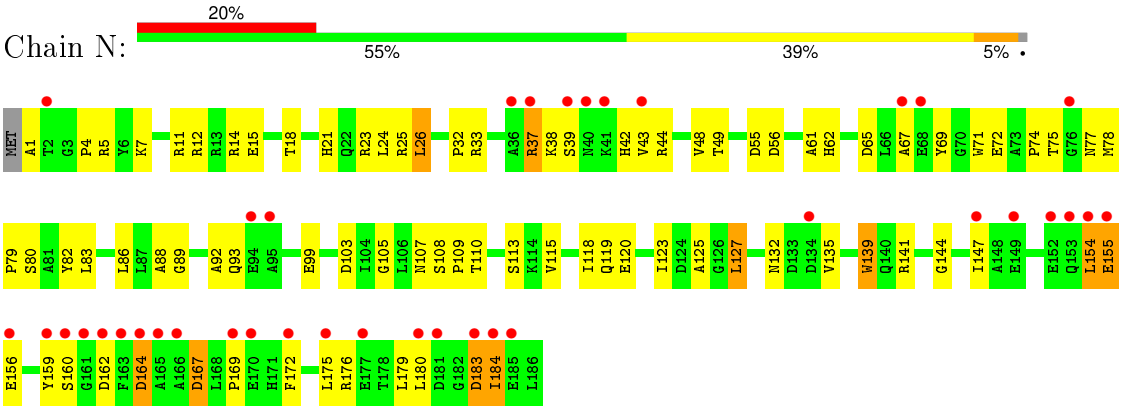
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



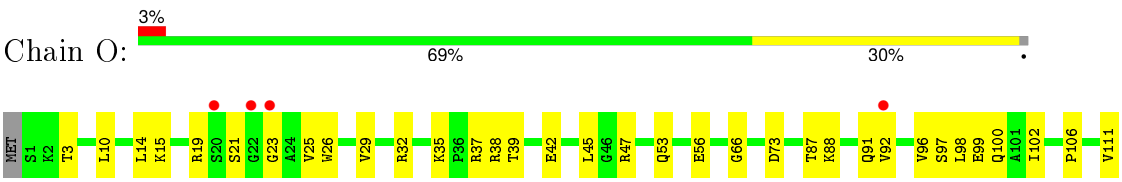
• Molecule 16: 50S ribosomal protein L18P

Chain N:



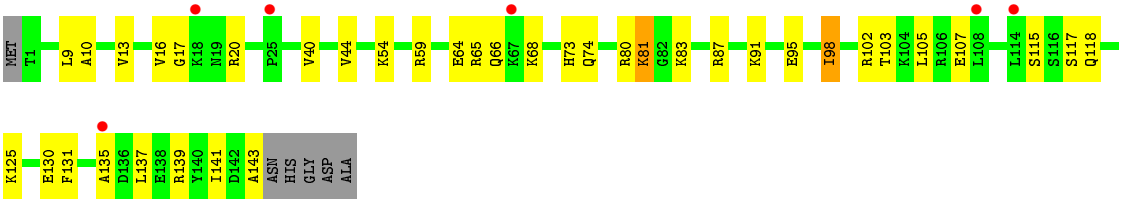
• Molecule 17: 50S ribosomal protein L18e

Chain O:



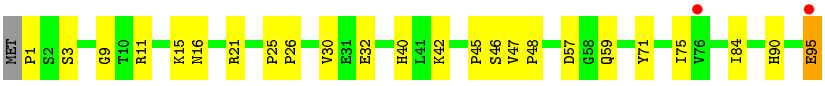
• Molecule 18: 50S ribosomal protein L19E

Chain P:



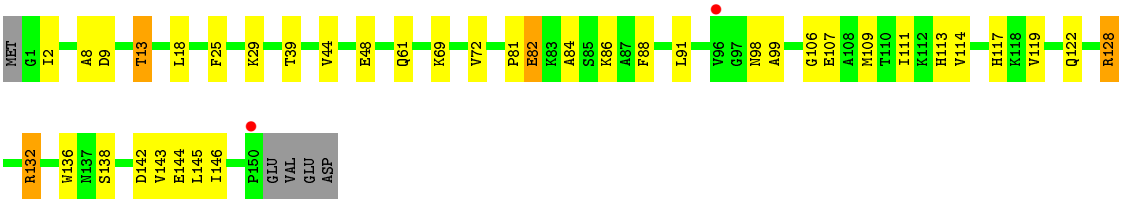
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



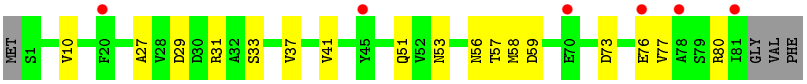
• Molecule 20: 50S ribosomal protein L22P

Chain R:



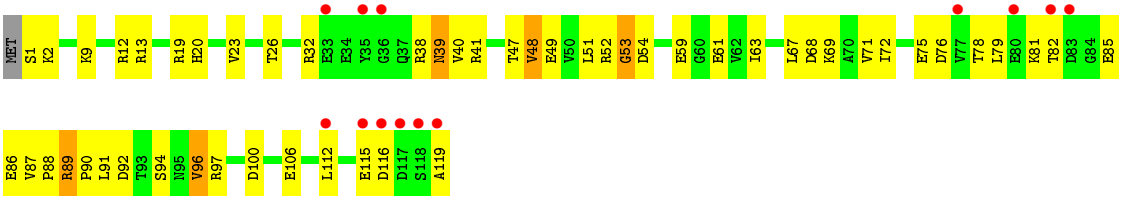
• Molecule 21: 50S ribosomal protein L23P

Chain S:



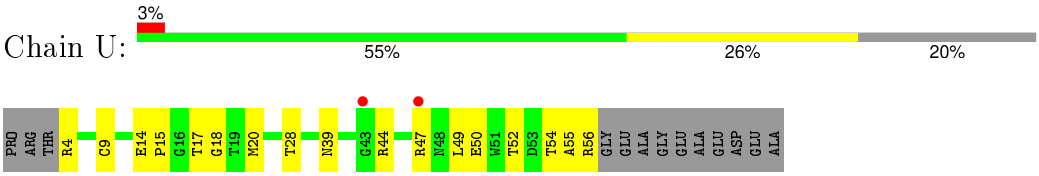
• Molecule 22: 50S ribosomal protein L24P

Chain T:



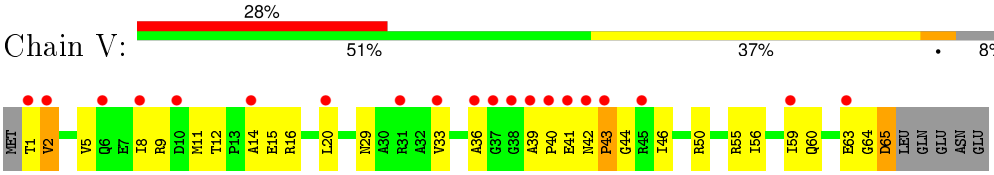
• Molecule 23: 50S ribosomal protein L24E

Chain U:



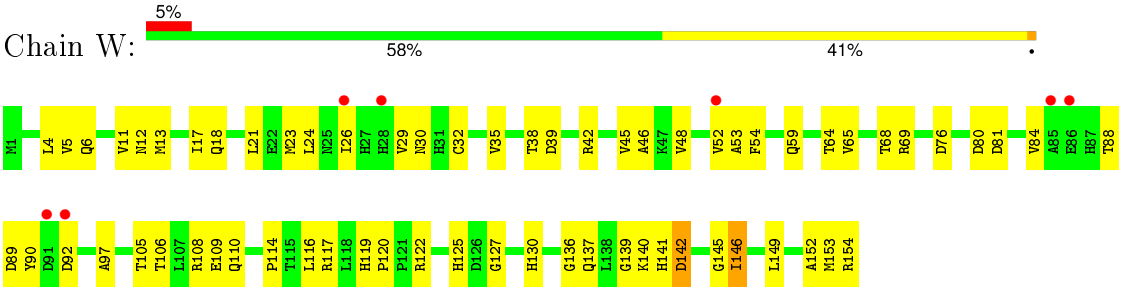
- Molecule 24: 50S ribosomal protein L29P

Chain V:



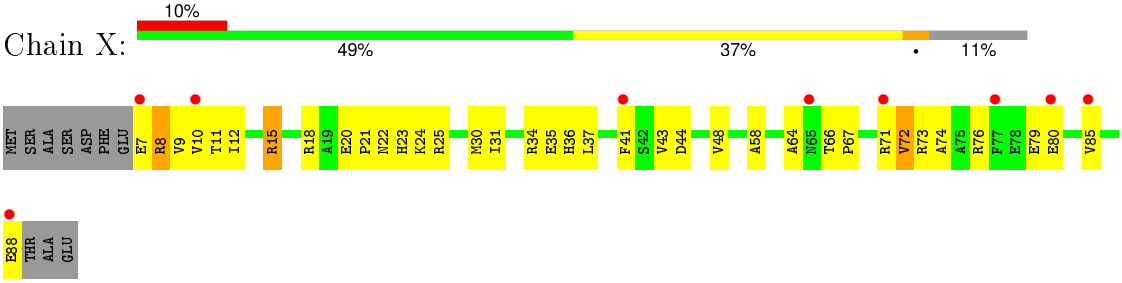
- Molecule 25: 50S ribosomal protein L30P

Chain W:



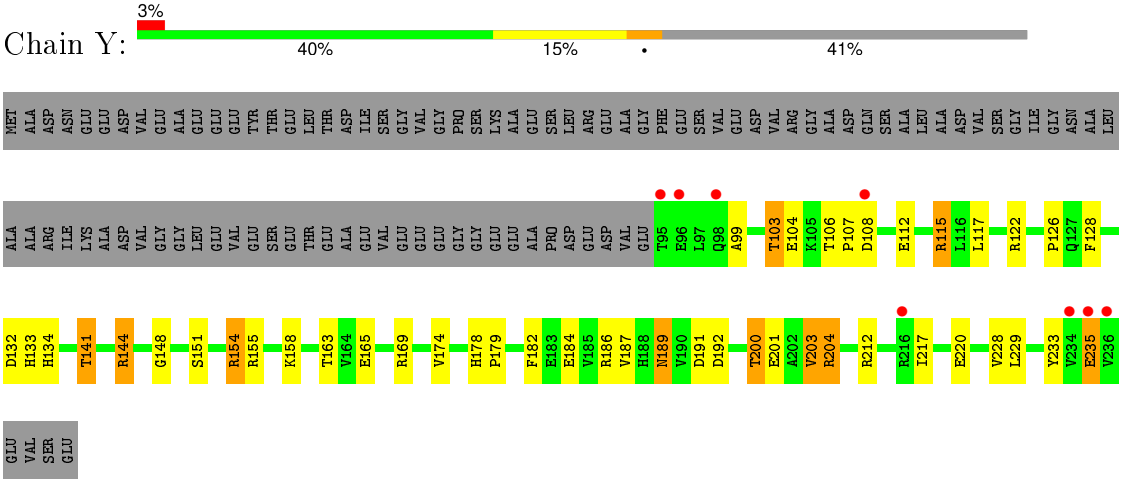
- Molecule 26: 50S ribosomal protein L31e

Chain X:



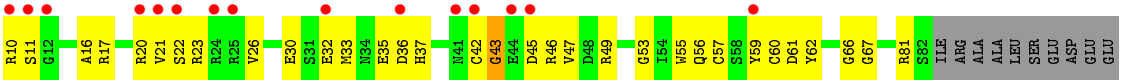
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



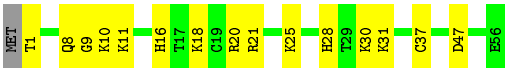
- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



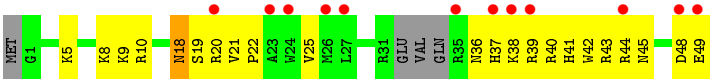
• Molecule 29: 50S ribosomal protein L37e

Chain 1:



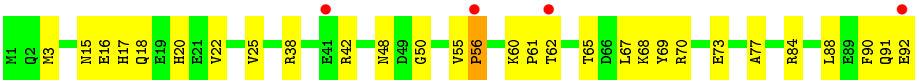
• Molecule 30: 50S ribosomal protein L39e

Chain 2:



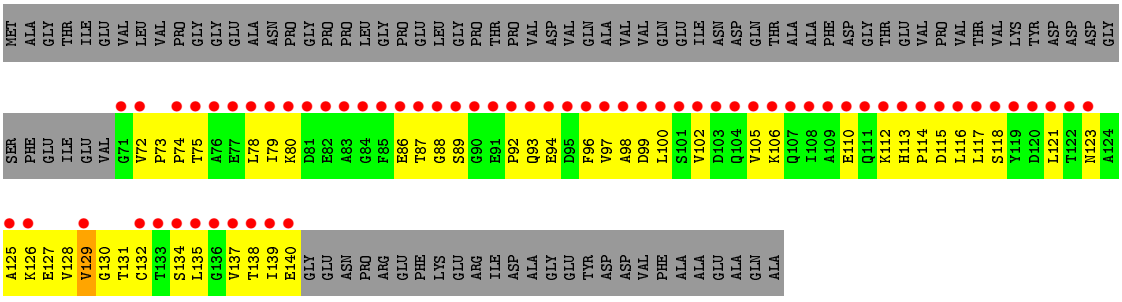
• Molecule 31: 50S ribosomal protein L44E

Chain 3:



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.61Å 298.19Å 574.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 37.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 90.5 (37.18-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.247 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.6	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 840903 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99070	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, PO2, CD, HFA, DCZ, OMU, UR3, 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	0.36	0/65959	0.70	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.51	0/83	0.79	0/119
4	A	0.32	0/1786	0.67	0/2408
5	B	0.32	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	1/2551 (0.0%)
7	D	0.28	0/1111	0.53	0/1498
8	E	0.30	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.32	0/1287	0.65	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.65	0/1509
15	M	0.33	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.61	0/1999
17	O	0.31	0/874	0.58	1/1181 (0.1%)
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.34	0/749	0.69	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.29	0/958	0.62	0/1289
23	U	0.32	0/417	0.57	0/562
24	V	0.26	0/502	0.51	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.32	0/664	0.57	0/895
27	Y	0.35	0/1146	0.64	0/1536
28	Z	0.31	0/589	0.60	0/787
29	1	0.43	0/438	0.65	0/578
30	2	0.34	0/401	0.57	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.35	0/98775	0.68	29/147696 (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	0	45
2	9	0	2
All	All	0	47

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	871	G	C5'-C4'-O4'	-8.48	98.93	109.10
1	0	1942	A	C5'-C4'-C3'	7.65	128.23	116.00
1	0	1819	G	C5'-C4'-C3'	7.08	127.34	116.00
1	0	777	U	O4'-C1'-N1	7.08	113.87	108.20
2	9	3039	U	N1-C1'-C2'	6.91	122.98	114.00
1	0	1979	G	C2'-C3'-O3'	6.69	124.40	113.70
1	0	1592	G	N9-C1'-C2'	6.36	122.26	114.00
1	0	1819	G	C1'-O4'-C4'	-6.15	104.98	109.90
1	0	2467	A	C1'-O4'-C4'	-6.00	105.10	109.90
1	0	1504	A	C1'-O4'-C4'	-5.94	105.15	109.90
6	C	73	LEU	CA-CB-CG	-5.82	101.92	115.30
1	0	1829	A	N9-C1'-C2'	-5.77	105.66	112.00
1	0	1819	G	C4'-C3'-C2'	-5.76	96.84	102.60
1	0	2291	A	N9-C1'-C2'	5.71	121.42	114.00
1	0	206	G	C5'-C4'-C3'	-5.43	107.31	116.00
1	0	2726	U	N1-C1'-C2'	5.38	121.00	114.00
1	0	1120	U	C5'-C4'-C3'	-5.32	107.48	116.00
1	0	883	U	N1-C1'-C2'	5.30	120.89	114.00
1	0	1615	A	C5'-C4'-C3'	5.28	124.44	116.00
1	0	535	G	N9-C1'-C2'	5.27	120.86	114.00
1	0	841	A	C1'-O4'-C4'	-5.26	105.69	109.90
1	0	2313	C	C5'-C4'-O4'	5.24	115.38	109.10
1	0	134	U	C5'-C4'-C3'	-5.17	107.72	116.00
17	O	66	GLY	N-CA-C	5.16	126.00	113.10
21	S	27	ALA	N-CA-C	-5.11	97.22	111.00
1	0	2301	A	N9-C1'-C2'	5.09	120.62	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	69	A	C5'-C4'-O4'	-5.08	103.00	109.10
20	R	128	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	0	473	A	C5'-C4'-C3'	5.01	124.02	116.00

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1458	A	Sidechain
1	0	1744	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1979	G	Sidechain
1	0	2036	C	Sidechain
1	0	2316	G	Sidechain
1	0	24	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2616	G	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2679	G	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	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	686	0
2	9	2600	0	1326	56	0
3	4	132	0	79	4	0
4	A	1753	0	1766	110	0
5	B	2625	0	2531	132	0
6	C	1859	0	1816	92	0
7	D	1094	0	1085	87	0
8	E	1357	0	1266	57	0
9	F	890	0	843	45	0
10	G	240	0	231	10	0
11	H	1266	0	1268	61	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	48	0
15	M	1560	0	1568	61	0
16	N	1445	0	1401	85	0
17	O	865	0	873	33	0
18	P	1136	0	1123	34	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	S	641	0	605	15	0
22	T	950	0	923	56	0
23	U	410	0	364	17	0
24	V	499	0	511	34	0
25	W	1196	0	1137	85	0
26	X	654	0	653	39	0
27	Y	1130	0	1133	50	0
28	Z	578	0	539	23	0
29	1	431	0	426	22	0
30	2	396	0	413	32	0
31	3	755	0	728	25	0
32	I	519	0	500	56	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	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	64	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	H	1	0	0	0	0
35	J	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	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5757	0	0	88	0
39	1	49	0	0	1	0
39	2	38	0	0	2	0
39	3	66	0	0	2	0
39	4	6	0	0	0	0
39	9	139	0	0	7	0
39	A	124	0	0	16	0
39	B	140	0	0	18	0
39	C	172	0	0	16	0
39	D	50	0	0	12	0
39	E	40	0	0	3	0
39	F	25	0	0	2	0
39	G	16	0	0	1	0
39	H	69	0	0	6	0
39	I	9	0	0	0	0
39	J	52	0	0	3	0
39	K	59	0	0	3	0
39	L	83	0	0	9	0
39	M	131	0	0	5	0
39	N	58	0	0	4	0
39	O	39	0	0	5	0
39	P	57	0	0	1	0
39	Q	51	0	0	5	0
39	R	87	0	0	3	0
39	S	32	0	0	0	0
39	T	36	0	0	6	0
39	U	30	0	0	3	0
39	V	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	W	72	0	0	3	0
39	X	24	0	0	4	0
39	Y	88	0	0	7	0
39	Z	31	0	0	2	0
All	All	99070	0	59977	2013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2013) 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)
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.27	1.09
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.28	1.07
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.31	1.06
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.06
9:F:91:VAL:HG12	9:F:92:GLY:H	1.24	1.03
1:0:1160:G:H5'	1:0:1161:A:H5'	1.40	1.02
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.25	1.01
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.40	1.01
2:9:3076:G:H3'	2:9:3077:A:H5"	1.42	1.00
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.09	0.99
30:2:18:ASN:HD21	30:2:40:ARG:H	1.09	0.99
1:0:156:C:H5"	15:M:171:ARG:HD3	1.40	0.99
1:0:871:G:C8	1:0:871:G:H5'	1.98	0.99
7:D:25:MET:HE2	7:D:41:LEU:HG	1.44	0.99
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.46	0.98
1:0:21:G:H5'	20:R:2:ILE:HA	1.46	0.97
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.46	0.97
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.47	0.96
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.49	0.94
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.82	0.94
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.50	0.94
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.03	0.93
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.50	0.93
1:0:1372:A:H3'	39:0:7674:HOH:O	1.69	0.93
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.92
5:B:238:ASN:HD22	5:B:240:GLY:H	1.18	0.92
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.52	0.92
1:0:2840:A:OP1	5:B:211:THR:HG23	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:H	13:K:10:GLN:NE2	1.68	0.91
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.17	0.91
1:0:2717:C:H2'	1:0:2718:C:H5"	1.52	0.91
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.70	0.91
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.35	0.90
1:0:542:A:H5'	1:0:542:A:H8	1.35	0.90
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.54	0.90
13:K:10:GLN:N	13:K:10:GLN:HE21	1.69	0.90
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.37	0.90
6:C:1:MET:HG2	6:C:2:GLN:H	1.34	0.90
1:0:2506:A:HO2'	1:0:2507:G:H8	0.94	0.90
18:P:115:SER:H	18:P:118:GLN:HE21	1.11	0.90
16:N:113:SER:HB2	39:N:9352:HOH:O	1.73	0.89
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.52	0.89
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.56	0.88
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.55	0.88
5:B:140:LEU:HA	39:B:9578:HOH:O	1.72	0.88
1:0:871:G:H8	1:0:871:G:H5'	1.39	0.88
16:N:144:GLY:O	16:N:147:ILE:HG22	1.73	0.88
1:0:2896:A:H5"	39:0:6619:HOH:O	1.74	0.87
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.36	0.87
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.56	0.87
1:0:2717:C:C2'	1:0:2718:C:H5"	2.03	0.87
1:0:870:G:H2'	1:0:871:G:H5"	1.54	0.87
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.87
2:9:3056:A:H2'	2:9:3057:A:H5"	1.54	0.86
30:2:41:HIS:H	30:2:45:ASN:HD22	1.18	0.86
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.76	0.86
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.58	0.86
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.55	0.86
5:B:86:ALA:HA	39:B:9578:HOH:O	1.75	0.85
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.58	0.85
25:W:88:THR:HB	39:W:6679:HOH:O	1.75	0.85
1:0:1242:A:H5'	12:J:82:THR:HG23	1.57	0.85
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.58	0.85
1:0:1041:U:H5'	39:L:9491:HOH:O	1.74	0.85
6:C:104:ASP:HA	6:C:107:ARG:NH1	1.91	0.85
9:F:58:GLU:HA	9:F:61:MET:HE2	1.57	0.85
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.59	0.85
1:0:2716:G:H5"	5:B:206:THR:HG21	1.59	0.84
25:W:122:ARG:HG2	25:W:152:ALA:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:199:HIS:HD2	4:A:201:PHE:H	1.23	0.84
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.61	0.83
4:A:192:VAL:HG22	39:A:9621:HOH:O	1.76	0.83
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.13	0.83
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.42	0.83
39:0:5401:HOH:O	12:J:47:THR:HB	1.78	0.83
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.60	0.83
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.58	0.83
1:0:1973:A:H5'	1:0:1973:A:H8	1.44	0.83
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.83
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.43	0.83
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.82
24:V:1:THR:HG23	24:V:2:VAL:H	1.45	0.82
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.94	0.82
4:A:192:VAL:HB	39:A:9584:HOH:O	1.78	0.82
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.60	0.82
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.60	0.82
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.95	0.82
25:W:137:GLN:HE21	25:W:141:HIS:CE1	1.96	0.82
25:W:125:HIS:HD2	25:W:127:GLY:H	1.28	0.81
1:0:541:C:H2'	1:0:542:A:H5"	1.62	0.81
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.62	0.81
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.45	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.81
20:R:99:ALA:HB1	20:R:109:MET:CE	2.11	0.81
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.63	0.80
25:W:13:MET:HE1	25:W:18:GLN:HA	1.60	0.80
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.46	0.80
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.97	0.80
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.11	0.80
32:I:78:LEU:HD12	32:I:112:LYS:NZ	1.95	0.80
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.64	0.80
12:J:74:ARG:NH1	12:J:76:ASP:HB2	1.97	0.80
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.47	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
1:0:1667:A:H8	1:0:1667:A:H5'	1.46	0.79
6:C:236:THR:HG22	6:C:239:ALA:N	1.96	0.79
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.64	0.79
1:0:1751:G:H2'	1:0:1752:G:H5"	1.64	0.79
4:A:191:GLY:HA2	4:A:194:MET:CE	2.11	0.79
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.64	0.79
7:D:57:THR:HG23	7:D:63:ILE:HA	1.63	0.79
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.65	0.79
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.84	0.78
1:0:2054:A:N3	20:R:128:ARG:NH2	2.31	0.78
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.66	0.78
1:0:1160:G:C5'	1:0:1161:A:H5'	2.14	0.78
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.45	0.78
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.65	0.78
1:0:2541:U:H4'	1:0:2542:C:OP1	1.82	0.78
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.77
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.64	0.77
1:0:1116:U:HO2'	1:0:1118:A:H2	0.81	0.77
1:0:281:U:H2'	1:0:282:C:O4'	1.84	0.77
1:0:289:G:H22	1:0:363:A:H2	1.31	0.77
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.67	0.77
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.15	0.77
1:0:288:A:H61	1:0:364:C:H42	1.30	0.77
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.15	0.77
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.19	0.77
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.67	0.77
1:0:871:G:C8	1:0:871:G:C5'	2.69	0.76
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.01	0.76
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.67	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.76
18:P:115:SER:OG	18:P:118:GLN:HG3	1.85	0.76
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.13	0.76
6:C:236:THR:CG2	6:C:239:ALA:H	1.98	0.76
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.51	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.49	0.76
11:H:27:LYS:H	11:H:59:HIS:HD2	1.33	0.76
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.66	0.76
1:0:541:C:C2'	1:0:542:A:H5"	2.16	0.76
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.76
29:1:25:LYS:HD2	30:2:49:GLU:H	1.51	0.76
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.23	0.76
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.66	0.75
25:W:88:THR:HG22	25:W:89:ASP:H	1.50	0.75
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.86	0.75
2:9:3014:G:H8	2:9:3014:G:H5'	1.51	0.75
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.68	0.75
16:N:80:SER:HB2	39:N:9333:HOH:O	1.87	0.75
1:0:1603:A:H5'	1:0:1605:G:O4'	1.87	0.75
25:W:122:ARG:NH2	25:W:154:ARG:HG2	2.02	0.75
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.69	0.75
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.86	0.75
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.32	0.75
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.85	0.74
11:H:21:THR:O	11:H:120:ILE:HD12	1.87	0.74
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.69	0.74
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.02	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.00	0.74
1:0:1159:G:H21	1:0:1189:A:H8	1.35	0.74
1:0:2506:A:O2'	1:0:2507:G:H8	1.69	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.17	0.74
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.74
1:0:481:U:H5"	39:0:6187:HOH:O	1.87	0.74
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.68	0.73
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.03	0.73
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.18	0.73
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.69	0.73
18:P:115:SER:H	18:P:118:GLN:NE2	1.85	0.73
1:0:2534:C:H1'	39:0:4094:HOH:O	1.89	0.73
1:0:470:U:O2'	29:1:16:HIS:HD2	1.72	0.73
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.19	0.73
24:V:39:ALA:N	24:V:40:PRO:HD2	2.04	0.73
5:B:16:ARG:NH1	39:B:9613:HOH:O	2.22	0.73
1:0:560:C:H42	1:0:597:A:H61	1.35	0.72
1:0:111:C:O2'	29:1:20:ARG:HG2	1.89	0.72
1:0:1118:A:H62	1:0:1244:U:H3	1.37	0.72
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.54	0.72
1:0:2533:C:H5'	1:0:2533:C:H6	1.54	0.72
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.19	0.72
1:0:559:U:H5'	1:0:559:U:H6	1.54	0.72
1:0:1562:C:H42	1:0:2738:G:H1	1.37	0.72
1:0:545:G:H8	1:0:545:G:H5'	1.54	0.72
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.38	0.72
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.72	0.72
25:W:88:THR:HG22	25:W:89:ASP:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:17:ARG:HD3	39:Z:9220:HOH:O	1.89	0.72
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.70	0.71
25:W:52:VAL:HG22	25:W:53:ALA:H	1.55	0.71
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.05	0.71
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.71
1:0:1701:A:H4'	1:0:1702:U:H5"	1.73	0.71
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.55	0.71
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.72	0.71
1:0:870:G:C2'	1:0:871:G:H5"	2.20	0.71
7:D:99:ASP:HB2	7:D:103:ASN:H	1.54	0.71
1:0:1700:C:H5"	1:0:1701:A:OP2	1.91	0.71
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.72	0.71
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.72	0.71
5:B:179:LEU:O	5:B:183:GLU:HG2	1.89	0.71
4:A:199:HIS:CD2	4:A:201:PHE:H	2.07	0.71
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.09	0.71
1:0:2468:A:H61	31:3:48:ASN:HD21	1.38	0.71
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.04	0.71
2:9:3051:A:H5'	16:N:160:SER:HB3	1.71	0.71
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.54	0.71
1:0:544:G:H2'	1:0:545:G:H5"	1.72	0.71
9:F:37:THR:O	9:F:41:GLU:HG3	1.91	0.70
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.55	0.70
17:O:32:ARG:HD3	17:O:32:ARG:O	1.91	0.70
2:9:3039:U:H1'	2:9:3044:A:N6	2.05	0.70
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.90	0.70
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.72	0.70
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.91	0.70
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.73	0.70
25:W:80:ASP:O	25:W:84:VAL:HG23	1.90	0.70
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.72	0.70
4:A:48:ASP:HB3	39:A:9596:HOH:O	1.90	0.70
1:0:1593:C:OP1	18:P:117:SER:HB3	1.91	0.70
39:0:7918:HOH:O	5:B:211:THR:HG21	1.91	0.70
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.73	0.70
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.90	0.70
1:0:282:C:O2'	1:0:283:U:H5'	1.90	0.70
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.22	0.70
1:0:1206:U:H5'	1:0:1206:U:H6	1.57	0.69
5:B:51:VAL:HG23	5:B:329:TYR:O	1.92	0.69
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2073:G:OP2	1:0:2490:A:H5'	1.93	0.69
22:T:26:THR:HA	22:T:39:ASN:HB3	1.74	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.69
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.75	0.69
24:V:12:THR:HG22	24:V:15:GLU:CG	2.21	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.23	0.69
9:F:96:ALA:HA	39:F:3111:HOH:O	1.91	0.69
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.74	0.69
30:2:20:ARG:HG3	30:2:39:ARG:HH21	1.57	0.69
5:B:162:MET:CE	5:B:310:ARG:HD3	2.22	0.69
11:H:170:ASN:N	11:H:170:ASN:HD22	1.91	0.69
1:0:2005:G:H3'	1:0:2005:G:OP2	1.92	0.69
1:0:2491:G:H1'	39:0:7359:HOH:O	1.91	0.69
39:0:6651:HOH:O	30:2:20:ARG:HB3	1.93	0.69
1:0:2749:U:H5'	39:0:8460:HOH:O	1.92	0.69
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.74	0.69
1:0:1166:A:H1'	1:0:1192:A:C2	2.28	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.07	0.69
1:0:282:C:H1'	1:0:368:C:N4	2.07	0.69
1:0:1165:G:H4'	1:0:1174:A:O2'	1.93	0.69
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.27	0.69
10:G:12:ILE:N	10:G:13:PRO:HD3	2.08	0.69
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.75	0.69
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.93	0.69
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.69
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.06	0.69
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.91	0.69
1:0:1474:C:C6	1:0:1474:C:H5'	2.27	0.69
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.56	0.68
4:A:35:GLY:O	4:A:36:ASP:HB3	1.92	0.68
32:I:87:THR:HG22	32:I:88:GLY:H	1.58	0.68
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.73	0.68
1:0:2291:A:C8	1:0:2309:C:H5'	2.28	0.68
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.73	0.68
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.23	0.68
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.75	0.68
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.57	0.68
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.68
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.75	0.68
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.68
7:D:170:TYR:O	7:D:171:ASP:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.76	0.68
1:0:1377:C:H6	1:0:1377:C:H5'	1.58	0.68
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.07	0.68
27:Y:144:ARG:CZ	39:Y:9404:HOH:O	2.42	0.68
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.22	0.68
1:0:280:C:H2'	1:0:281:U:O4'	1.94	0.68
4:A:51:ARG:HB2	39:A:9596:HOH:O	1.91	0.68
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.93	0.68
12:J:45:VAL:HG23	12:J:130:VAL:O	1.94	0.68
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.22	0.68
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.68
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.59	0.68
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.24	0.68
1:0:1878:G:H1'	39:0:6641:HOH:O	1.93	0.68
1:0:506:G:H22	1:0:509:A:H5"	1.58	0.68
1:0:1175:G:H1'	1:0:1193:A:H2'	1.74	0.67
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.74	0.67
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.25	0.67
1:0:2851:G:H2'	1:0:2852:A:H5'	1.75	0.67
3:4:176:A:O4'	3:4:175:C:H2'	1.94	0.67
1:0:796:A:HO2'	28:Z:10:ARG:N	1.91	0.67
1:0:380:A:OP2	15:M:9:ARG:HD2	1.95	0.67
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.16	0.67
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.59	0.67
1:0:121:U:OP2	30:2:10:ARG:NH2	2.27	0.67
8:E:34:TRP:O	12:J:127:ILE:HD11	1.94	0.67
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.58	0.67
5:B:254:GLN:HG2	5:B:255:GLY:N	2.09	0.67
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.77	0.67
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.25	0.67
25:W:139:GLY:O	25:W:141:HIS:HD2	1.77	0.67
1:0:541:C:H2'	1:0:542:A:C5'	2.25	0.67
1:0:1116:U:H3	1:0:1246:A:H62	1.42	0.67
1:0:709:G:O2'	17:O:25:VAL:HG12	1.93	0.67
39:0:7000:HOH:O	27:Y:141:THR:HG23	1.94	0.67
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.09	0.67
24:V:56:ILE:O	24:V:60:GLN:HG3	1.95	0.67
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.30	0.67
2:9:3013:A:O2'	2:9:3014:G:H5"	1.94	0.67
30:2:18:ASN:ND2	30:2:40:ARG:H	1.88	0.66
11:H:166:SER:CB	11:H:167:PRO:HD3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:89:SER:HB3	32:I:97:VAL:HG23	1.77	0.66
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.08	0.66
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.96	0.66
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.93	0.66
27:Y:165:GLU:HB3	39:Y:9387:HOH:O	1.94	0.66
14:L:133:VAL:HA	39:L:9471:HOH:O	1.94	0.66
6:C:107:ARG:NE	39:C:9258:HOH:O	2.28	0.66
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.30	0.66
1:0:93:C:H5"	24:V:1:THR:HB	1.76	0.66
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.95	0.66
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.61	0.66
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.66
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.74	0.66
1:0:1184:C:H1'	39:0:7928:HOH:O	1.95	0.66
1:0:2908:A:H2'	1:0:2909:G:O4'	1.96	0.66
2:9:3020:G:O2'	2:9:3021:G:H5'	1.96	0.66
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.76	0.65
1:0:1189:A:H1'	1:0:1209:C:O4'	1.96	0.65
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.11	0.65
39:0:4349:HOH:O	22:T:9:LYS:HD3	1.97	0.65
1:0:1666:C:O2'	1:0:1667:A:H5"	1.95	0.65
25:W:48:VAL:HG12	25:W:48:VAL:O	1.95	0.65
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.11	0.65
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.65
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.11	0.65
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.77	0.65
4:A:33:GLU:O	4:A:34:ASP:HB2	1.96	0.65
1:0:2578:G:H5'	1:0:2578:G:H8	1.61	0.65
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.62	0.65
1:0:960:G:H4'	39:0:7894:HOH:O	1.97	0.65
32:I:87:THR:HG22	32:I:88:GLY:N	2.12	0.65
1:0:2878:U:H2'	1:0:2879:A:O4'	1.95	0.65
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.65
29:1:25:LYS:HD2	30:2:49:GLU:N	2.12	0.65
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.65
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.27	0.65
2:9:3056:A:C2'	2:9:3057:A:H5"	2.27	0.65
15:M:164:THR:HG22	15:M:166:ALA:H	1.60	0.65
4:A:33:GLU:CD	4:A:33:GLU:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:O2'	1:0:418:C:H4'	1.97	0.65
14:L:143:THR:HG22	14:L:144:ASP:N	2.12	0.65
1:0:1160:G:H5'	1:0:1161:A:C5'	2.22	0.65
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.97	0.65
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.79	0.65
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.27	0.65
2:9:3069:U:OP1	16:N:4:PRO:HG3	1.97	0.65
25:W:125:HIS:CD2	25:W:127:GLY:H	2.11	0.64
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.79	0.64
1:0:877:G:H5'	1:0:878:G:OP1	1.96	0.64
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.79	0.64
1:0:1666:C:H2'	1:0:1667:A:H5'	1.79	0.64
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.27	0.64
1:0:220:C:H1'	39:0:6292:HOH:O	1.96	0.64
1:0:381:G:H5"	39:M:9377:HOH:O	1.96	0.64
29:1:10:LYS:HG3	39:1:9488:HOH:O	1.96	0.64
12:J:19:MET:CE	12:J:132:LEU:HD11	2.27	0.64
1:0:1182:C:H1'	1:0:1192:A:H8	1.61	0.64
1:0:1299:G:O6	14:L:6:ARG:HD3	1.98	0.64
1:0:2586:U:H3	1:0:2592:G:H22	1.45	0.64
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.27	0.64
1:0:1973:A:H5'	1:0:1973:A:C8	2.31	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.97	0.64
23:U:14:GLU:O	23:U:17:THR:HB	1.97	0.64
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.12	0.64
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.97	0.64
7:D:135:VAL:HG22	7:D:136:ARG:H	1.62	0.64
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.80	0.64
16:N:164:ASP:CG	16:N:167:ASP:HA	2.17	0.64
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.79	0.64
6:C:115:LEU:O	6:C:118:THR:HB	1.97	0.64
39:0:9974:HOH:O	29:1:1:THR:HA	1.97	0.64
25:W:13:MET:CE	25:W:17:ILE:HG22	2.27	0.64
1:0:2426:G:H1'	39:0:6612:HOH:O	1.96	0.64
4:A:179:MET:HG2	4:A:186:TRP:CB	2.27	0.64
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.98	0.64
8:E:68:HIS:O	8:E:72:MET:HG3	1.98	0.63
1:0:1183:C:N4	1:0:1184:C:H41	1.95	0.63
1:0:338:C:H4'	6:C:174:ILE:CD1	2.28	0.63
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.81	0.63
32:I:106:LYS:O	32:I:110:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.97	0.63
2:9:3014:G:C8	2:9:3014:G:H5'	2.32	0.63
1:0:544:G:C2'	1:0:545:G:H5"	2.28	0.63
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.33	0.63
1:0:69:A:H5'	1:0:69:A:C8	2.34	0.63
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.63
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.63	0.63
11:H:154:TYR:HB2	39:H:9555:HOH:O	1.97	0.63
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.65	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.98	0.63
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.28	0.63
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.79	0.63
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.63	0.63
1:0:2661:U:H3	1:0:2812:A:H62	1.47	0.63
1:0:2748:G:H2'	39:0:8000:HOH:O	1.98	0.63
1:0:1201:C:H2'	1:0:1202:A:H5'	1.79	0.63
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.64	0.63
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.98	0.63
20:R:9:ASP:O	20:R:13:THR:HB	1.99	0.63
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.32	0.63
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.64	0.63
1:0:447:A:P	22:T:1:SER:HB2	2.39	0.63
5:B:212:GLN:CB	5:B:257:THR:HG21	2.15	0.63
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.62	0.63
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.81	0.63
1:0:2346:C:O2'	7:D:52:THR:HG21	1.97	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	1.99	0.62
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.62	0.62
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.81	0.62
12:J:74:ARG:O	12:J:78:ILE:HG12	1.99	0.62
5:B:125:GLU:O	5:B:129:ARG:HG3	2.00	0.62
6:C:242:GLU:HG3	39:C:9185:HOH:O	1.99	0.62
1:0:291:C:H2'	1:0:292:G:O4'	1.99	0.62
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.81	0.62
22:T:71:VAL:HG12	22:T:72:ILE:N	2.13	0.62
32:I:113:HIS:N	32:I:114:PRO:HD2	2.14	0.62
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.82	0.62
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.14	0.62
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.82	0.62
11:H:76:GLU:O	11:H:77:LEU:HD23	1.99	0.62
11:H:166:SER:HB2	11:H:167:PRO:CD	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2507:G:H2'	1:0:2510:C:H42	1.64	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.62	0.62
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.86	0.62
18:P:115:SER:N	18:P:118:GLN:HE21	1.91	0.62
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.29	0.62
1:0:558:C:C2'	1:0:559:U:H5"	2.30	0.62
14:L:143:THR:HG22	14:L:144:ASP:H	1.64	0.62
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.79	0.62
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.98	0.62
1:0:834:G:H4'	1:0:835:U:OP2	2.00	0.62
21:S:77:VAL:O	21:S:80:ARG:HG2	1.99	0.62
12:J:75:PRO:HD3	12:J:136:SER:OG	1.99	0.62
4:A:179:MET:HA	4:A:179:MET:CE	2.29	0.62
12:J:39:VAL:HG13	12:J:106:GLY:O	2.00	0.62
1:0:263:U:O4'	9:F:59:ILE:HD13	1.98	0.62
24:V:12:THR:HG23	24:V:14:ALA:H	1.64	0.62
32:I:99:ASP:OD1	32:I:138:THR:HB	2.00	0.62
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.07	0.62
10:G:24:VAL:O	10:G:28:GLU:HB2	1.99	0.62
1:0:2064:U:H5'	1:0:2652:U:O3'	2.00	0.62
22:T:47:THR:HB	22:T:100:ASP:HB3	1.80	0.62
1:0:1119:G:H22	1:0:1246:A:H2	1.43	0.62
1:0:516:A:H5'	39:0:6187:HOH:O	2.00	0.62
1:0:138:U:H5"	1:0:139:C:OP2	2.00	0.62
17:O:97:SER:OG	17:O:100:GLN:HG3	2.00	0.62
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.62
2:9:3029:C:H2'	2:9:3030:C:H5'	1.82	0.61
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.29	0.61
1:0:2064:U:H5'	1:0:2652:U:H4'	1.80	0.61
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.64	0.61
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.00	0.61
1:0:553:G:P	27:Y:204:ARG:HH22	2.22	0.61
7:D:154:LYS:HD2	7:D:154:LYS:H	1.65	0.61
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.81	0.61
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.35	0.61
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.46	0.61
7:D:50:VAL:O	7:D:71:ALA:HA	2.00	0.61
6:C:132:ASP:HB3	39:C:9165:HOH:O	1.98	0.61
6:C:236:THR:HG21	39:C:9177:HOH:O	1.99	0.61
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.82	0.61
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.81	0.61
31:3:65:THR:CG2	31:3:67:LEU:HG	2.30	0.61
1:0:1730:G:H5'	1:0:1731:C:C5	2.35	0.61
9:F:60:VAL:HG12	9:F:60:VAL:O	2.00	0.61
4:A:36:ASP:HB2	4:A:83:GLY:HA3	1.81	0.61
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.66	0.61
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.66	0.61
5:B:297:VAL:HB	39:B:9602:HOH:O	2.00	0.61
17:O:21:SER:OG	17:O:106:PRO:HB2	1.99	0.61
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.83	0.61
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.61
1:0:120:A:H5'	29:1:20:ARG:HH21	1.66	0.61
1:0:757:C:OP1	14:L:27:ARG:HD2	2.00	0.61
1:0:316:A:H5'	22:T:54:ASP:OD2	1.99	0.61
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.34	0.61
1:0:272:A:H5'	1:0:273:G:OP2	1.99	0.61
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.31	0.61
1:0:1209:C:H2'	1:0:1210:G:H8	1.66	0.61
1:0:1205:U:H2'	1:0:1206:U:H5"	1.81	0.61
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.15	0.61
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.00	0.61
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.73	0.61
5:B:40:GLY:HA3	39:B:9642:HOH:O	2.00	0.61
5:B:62:ARG:HA	5:B:65:MET:HE3	1.82	0.61
1:0:2718:C:H6	1:0:2718:C:H5'	1.66	0.61
16:N:115:VAL:HG22	39:N:9352:HOH:O	2.00	0.61
1:0:2073:G:H5"	39:0:4416:HOH:O	2.00	0.61
1:0:2807:U:P	5:B:27:ASN:HD21	2.24	0.61
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.01	0.61
39:0:8062:HOH:O	31:3:60:LYS:HG3	2.01	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.61
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.11	0.61
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.30	0.61
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.35	0.61
5:B:62:ARG:HA	5:B:65:MET:CE	2.30	0.61
5:B:81:ALA:O	5:B:186:GLY:HA3	2.01	0.61
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.01	0.61
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.16	0.61
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.00	0.61
1:0:244:C:OP2	9:F:38:LYS:HE3	2.02	0.60
1:0:12:U:H2'	1:0:13:G:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:110:THR:HB	16:N:113:SER:OG	2.01	0.60
30:2:41:HIS:HD2	30:2:44:ARG:H	1.48	0.60
1:0:775:G:OP1	29:1:16:HIS:HE1	1.84	0.60
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.36	0.60
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.66	0.60
1:0:506:G:H22	1:0:509:A:H5'	1.67	0.60
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.82	0.60
1:0:558:C:O2'	1:0:559:U:H5"	2.02	0.60
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.66	0.60
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.65	0.60
7:D:172:VAL:HG12	7:D:173:GLU:N	2.16	0.60
6:C:236:THR:H	6:C:239:ALA:HB3	1.67	0.60
1:0:2851:G:H4'	5:B:157:LYS:NZ	2.16	0.60
1:0:558:C:H2'	1:0:559:U:C5'	2.31	0.60
26:X:25:ARG:HD3	26:X:64:ALA:O	2.01	0.60
1:0:123:U:H5'	39:0:7153:HOH:O	2.00	0.60
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.49	0.60
1:0:797:A:C4'	28:Z:10:ARG:N	2.64	0.60
1:0:681:G:N3	1:0:681:G:H5'	2.17	0.60
16:N:169:PRO:O	16:N:172:PHE:HB3	2.02	0.60
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.84	0.60
5:B:238:ASN:HD22	5:B:240:GLY:N	1.93	0.60
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.64	0.60
1:0:2502:C:H2'	1:0:2503:A:H5'	1.84	0.60
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.31	0.60
1:0:2533:C:C6	1:0:2533:C:H5'	2.35	0.60
20:R:39:THR:HG22	20:R:107:GLU:O	2.00	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.02	0.59
1:0:1206:U:H2'	1:0:1207:A:O4'	2.02	0.59
1:0:69:A:H5'	1:0:69:A:H8	1.67	0.59
39:0:7365:HOH:O	15:M:178:LYS:HB2	2.02	0.59
39:0:3157:HOH:O	18:P:81:LYS:HG2	2.02	0.59
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	0.59
8:E:15:GLN:HG2	8:E:19:ASP:O	2.02	0.59
1:0:902:G:N7	14:L:18:HIS:HD2	2.00	0.59
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.66	0.59
15:M:164:THR:HG22	15:M:166:ALA:N	2.16	0.59
13:K:115:ARG:HG3	13:K:116:GLU:N	2.17	0.59
1:0:485:A:N3	1:0:487:G:H5"	2.17	0.59
1:0:949:U:H4'	19:Q:95:GLU:HA	1.82	0.59
1:0:1426:C:H2'	39:0:3210:HOH:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:55:VAL:HG12	13:K:56:SER:N	2.17	0.59
15:M:57:LYS:HE2	15:M:140:ALA:O	2.02	0.59
26:X:31:ILE:O	26:X:35:GLU:HG3	2.02	0.59
12:J:52:GLN:HG3	12:J:53:ILE:N	2.16	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.01	0.59
1:0:289:G:N2	1:0:363:A:H2	2.00	0.59
28:Z:10:ARG:HA	39:Z:9214:HOH:O	2.02	0.59
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.68	0.59
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.36	0.59
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.83	0.59
1:0:1595:G:O2'	1:0:1596:U:H5'	2.02	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.59
1:0:2565:C:H4'	39:0:5400:HOH:O	2.03	0.59
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.32	0.59
1:0:1183:C:H2'	39:0:6764:HOH:O	2.03	0.59
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.84	0.59
23:U:17:THR:HG22	23:U:18:GLY:N	2.18	0.59
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.31	0.59
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.85	0.59
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.59
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.03	0.59
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.59
14:L:73:VAL:HG23	14:L:74:THR:H	1.68	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.84	0.59
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.68	0.59
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.59
1:0:1766:U:O2	1:0:1778:A:H5'	2.03	0.59
17:O:73:ASP:HA	17:O:92:VAL:O	2.03	0.58
25:W:130:HIS:O	25:W:136:GLY:HA3	2.04	0.58
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.86	0.58
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.99	0.58
25:W:52:VAL:HG22	25:W:53:ALA:N	2.17	0.58
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.58
1:0:1201:C:H5"	39:0:6753:HOH:O	2.03	0.58
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.58
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.85	0.58
30:2:18:ASN:HD21	30:2:40:ARG:N	1.92	0.58
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.33	0.58
11:H:30:GLN:H	11:H:66:ARG:NH1	2.02	0.58
1:0:2333:G:P	7:D:56:ARG:HH22	2.26	0.58
8:E:7:ILE:HG22	8:E:45:ASP:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:139:VAL:HG13	39:C:9248:HOH:O	2.04	0.58
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.69	0.58
1:0:1119:G:H8	12:J:52:GLN:NE2	2.01	0.58
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.32	0.58
4:A:26:ASP:O	4:A:26:ASP:OD1	2.22	0.58
1:0:1119:G:H8	12:J:52:GLN:HE22	1.52	0.58
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.58
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.86	0.58
5:B:72:THR:HB	39:B:9602:HOH:O	2.04	0.58
1:0:441:A:H1'	1:0:442:A:N7	2.18	0.58
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.04	0.58
12:J:19:MET:HE1	12:J:132:LEU:CD2	2.32	0.58
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.34	0.58
1:0:1189:A:H3'	39:0:8221:HOH:O	2.04	0.58
1:0:2591:C:H2'	1:0:2592:G:O4'	2.03	0.58
32:I:92:PRO:C	32:I:94:GLU:H	2.06	0.58
6:C:236:THR:HG22	6:C:239:ALA:CB	2.34	0.58
11:H:27:LYS:N	11:H:59:HIS:HD2	2.00	0.58
5:B:102:THR:HG21	5:B:182:VAL:O	2.04	0.58
24:V:64:GLY:O	24:V:65:ASP:HB2	2.03	0.58
23:U:17:THR:CG2	23:U:18:GLY:N	2.67	0.58
1:0:1189:A:O2'	1:0:1208:C:H2'	2.04	0.57
5:B:305:ASP:O	5:B:306:LYS:HB2	2.04	0.57
17:O:39:THR:O	17:O:115:ARG:NH2	2.37	0.57
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.85	0.57
32:I:102:VAL:O	32:I:106:LYS:HG3	2.04	0.57
1:0:475:G:H5'	6:C:73:LEU:HD23	1.86	0.57
7:D:25:MET:CE	7:D:41:LEU:HG	2.29	0.57
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.94	0.57
15:M:115:LEU:HD13	15:M:116:ASN:HB2	1.86	0.57
1:0:737:A:H2'	1:0:738:G:O4'	2.04	0.57
1:0:1462:C:H2'	1:0:1463:A:C8	2.40	0.57
23:U:52:THR:HG22	23:U:54:THR:N	2.19	0.57
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.87	0.57
1:0:447:A:OP2	22:T:1:SER:HB2	2.05	0.57
1:0:1943:C:H4'	4:A:211:LYS:O	2.04	0.57
1:0:962:C:H1'	16:N:5:ARG:NH1	2.20	0.57
1:0:656:G:OP2	17:O:37:ARG:HD2	2.05	0.57
11:H:158:THR:HB	11:H:159:PRO:HD3	1.87	0.57
21:S:57:THR:HG22	21:S:59:ASP:H	1.70	0.57
18:P:9:LEU:O	18:P:13:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:40:VAL:HG22	22:T:41:ARG:N	2.20	0.57
1:0:710:G:H5'	17:O:25:VAL:CG1	2.35	0.57
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.03	0.57
16:N:132:ASN:O	16:N:135:VAL:HG12	2.04	0.57
1:0:2643:G:H5"	39:0:4516:HOH:O	2.05	0.57
1:0:2644:C:O2'	1:0:2645:U:H5'	2.04	0.57
1:0:1634:G:H3'	39:0:4484:HOH:O	2.02	0.57
12:J:19:MET:HE1	12:J:132:LEU:HD11	1.87	0.57
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.18	0.57
1:0:90:A:H2'	1:0:91:G:O4'	2.04	0.57
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.34	0.57
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.34	0.57
1:0:475:G:OP1	6:C:73:LEU:HD22	2.04	0.57
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.05	0.57
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.70	0.57
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.87	0.56
1:0:1625:U:H4'	39:0:5235:HOH:O	2.03	0.56
32:I:138:THR:HG22	32:I:139:ILE:H	1.69	0.56
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.56
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.56
1:0:2103:A:H8	1:0:2103:A:H5'	1.70	0.56
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.19	0.56
32:I:75:THR:OG1	32:I:112:LYS:HE2	2.05	0.56
32:I:138:THR:HG22	32:I:139:ILE:N	2.20	0.56
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.38	0.56
6:C:16:VAL:HG12	6:C:17:ASP:H	1.70	0.56
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.23	0.56
1:0:1878:G:O2'	1:0:1879:U:OP2	2.23	0.56
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.41	0.56
1:0:2645:U:OP2	1:0:2645:U:C6	2.58	0.56
5:B:145:HIS:HD2	5:B:146:THR:O	1.89	0.56
13:K:125:ALA:C	13:K:127:ALA:H	2.08	0.56
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.70	0.56
1:0:2649:A:H5'	1:0:2649:A:H8	1.69	0.56
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.87	0.56
1:0:1159:G:H1	1:0:1208:C:H42	1.53	0.56
1:0:1701:A:H4'	1:0:1702:U:C5'	2.35	0.56
32:I:129:VAL:O	32:I:129:VAL:HG12	2.05	0.56
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.41	0.56
1:0:343:C:O2'	1:0:344:C:H5'	2.05	0.56
15:M:107:ARG:NH1	39:M:9384:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:99:ASP:HB3	7:D:101:THR:H	1.71	0.56
1:0:1552:G:N2	1:0:1634:G:H1'	2.20	0.56
22:T:89:ARG:HG3	22:T:89:ARG:O	2.06	0.56
1:0:1333:U:H2'	1:0:1334:C:C6	2.41	0.56
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.35	0.56
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.06	0.56
1:0:88:G:H2'	1:0:89:G:C8	2.40	0.56
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.06	0.56
1:0:2795:C:O2'	1:0:2796:U:H5'	2.06	0.56
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.88	0.56
1:0:2505:G:O2'	1:0:2506:A:H5'	2.06	0.56
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.71	0.56
4:A:105:VAL:HG12	4:A:106:CYS:N	2.21	0.56
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.41	0.56
18:P:40:VAL:O	18:P:44:VAL:HG23	2.06	0.56
1:0:1979:G:O2'	1:0:1980:U:OP1	2.21	0.56
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.21	0.56
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.21	0.56
27:Y:154:ARG:HH11	27:Y:154:ARG:HB3	1.71	0.56
1:0:248:A:H5'	1:0:249:G:OP2	2.06	0.56
15:M:60:VAL:C	15:M:61:ILE:HD12	2.26	0.56
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.41	0.55
1:0:185:G:H4'	1:0:186:A:H4'	1.87	0.55
1:0:1555:G:H4'	1:0:1630:A:H2	1.71	0.55
1:0:1118:A:H8	1:0:1119:G:H5"	1.71	0.55
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.06	0.55
9:F:57:GLU:O	9:F:61:MET:HG3	2.07	0.55
1:0:2837:U:H2'	39:0:7329:HOH:O	2.06	0.55
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.88	0.55
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.18	0.55
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.87	0.55
5:B:156:LYS:HE2	39:B:9627:HOH:O	2.05	0.55
13:K:23:ASN:HD21	13:K:107:THR:HB	1.71	0.55
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.06	0.55
1:0:894:A:N1	6:C:87:ARG:NH2	2.54	0.55
1:0:2866:U:H4'	1:0:2867:G:H5'	1.87	0.55
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.89	0.55
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.22	0.55
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.88	0.55
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.21	0.55
16:N:162:ASP:HA	39:N:9329:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.55
32:I:75:THR:HA	32:I:112:LYS:NZ	2.22	0.55
1:0:1187:U:O2'	1:0:1189:A:H2	1.90	0.55
7:D:138:GLY:N	39:D:7597:HOH:O	2.38	0.55
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.54	0.55
11:H:170:ASN:N	11:H:170:ASN:ND2	2.52	0.55
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.06	0.55
5:B:185:GLY:HA2	39:B:9630:HOH:O	2.07	0.55
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.18	0.55
2:9:3054:A:H2	39:9:3535:HOH:O	1.88	0.55
5:B:85:ARG:NH1	39:B:9631:HOH:O	2.39	0.55
1:0:2827:A:H2'	1:0:2828:G:O4'	2.07	0.55
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.05	0.55
22:T:71:VAL:HG13	22:T:91:LEU:O	2.07	0.55
12:J:47:THR:HG22	12:J:48:GLY:N	2.22	0.55
7:D:59:GLY:O	7:D:61:PHE:N	2.40	0.55
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.07	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
11:H:63:GLU:HA	39:H:9544:HOH:O	2.07	0.55
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.89	0.55
13:K:75:ARG:HD3	13:K:112:PRO:O	2.06	0.55
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.89	0.55
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.88	0.55
9:F:91:VAL:CG1	9:F:92:GLY:H	2.07	0.55
32:I:75:THR:HG22	32:I:79:ILE:HD11	1.88	0.55
1:0:2896:A:N3	1:0:2896:A:H2'	2.23	0.55
29:1:25:LYS:CD	30:2:49:GLU:H	2.20	0.55
4:A:89:ALA:HB3	39:A:9613:HOH:O	2.07	0.55
22:T:115:GLU:HG3	22:T:116:ASP:N	2.22	0.55
6:C:140:VAL:HB	39:C:9251:HOH:O	2.04	0.54
20:R:106:GLY:HA2	20:R:109:MET:CE	2.36	0.54
29:1:25:LYS:HE2	39:2:7213:HOH:O	2.07	0.54
7:D:103:ASN:ND2	7:D:134:LEU:H	2.04	0.54
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.06	0.54
1:0:162:C:H2'	1:0:163:U:H5'	1.89	0.54
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.42	0.54
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.70	0.54
18:P:103:THR:O	18:P:107:GLU:HG3	2.06	0.54
1:0:1406:A:H4'	1:0:1407:A:H5"	1.89	0.54
2:9:3064:C:H2'	2:9:3065:A:H5'	1.89	0.54
9:F:107:ASP:O	9:F:111:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:C2’	1:0:2770:G:H5’	2.37	0.54
1:0:830:G:O2’	1:0:831:U:H5’	2.08	0.54
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.89	0.54
1:0:1163:G:H2’	1:0:1164:U:C5	2.42	0.54
1:0:2480:G:H3’	39:0:4767:HOH:O	2.08	0.54
32:I:102:VAL:HG23	32:I:140:GLU:O	2.08	0.54
1:0:1667:A:C8	1:0:1667:A:H5’	2.35	0.54
1:0:1268:C:O2’	27:Y:169:ARG:HB2	2.08	0.54
1:0:656:G:H5’	17:O:3:THR:HB	1.90	0.54
21:S:57:THR:HG22	21:S:59:ASP:N	2.22	0.54
1:0:1838:U:O2’	1:0:2644:C:H5’	2.08	0.54
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.90	0.54
2:9:3050:G:H5”	16:N:159:TYR:HE1	1.73	0.54
2:9:3057:A:C8	7:D:141:VAL:HG21	2.42	0.54
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.37	0.54
1:0:2563:U:H2’	1:0:2565:C:O5’	2.08	0.54
18:P:16:VAL:HG12	18:P:17:GLY:N	2.21	0.54
1:0:1687:C:O2	29:1:9:GLY:HA2	2.08	0.54
26:X:43:VAL:HG12	26:X:44:ASP:N	2.22	0.54
1:0:1666:C:H2’	1:0:1667:A:C5’	2.37	0.54
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.89	0.54
15:M:182:LYS:O	15:M:194:ALA:HB2	2.08	0.54
10:G:20:VAL:O	10:G:24:VAL:HG23	2.08	0.54
6:C:79:ARG:O	6:C:87:ARG:HG2	2.07	0.54
20:R:44:VAL:O	20:R:48:GLU:HG3	2.08	0.54
1:0:2364:A:H5”	19:Q:15:LYS:HD3	1.88	0.54
1:0:2481:G:H5”	39:0:5116:HOH:O	2.07	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.90	0.54
25:W:26:ILE:O	25:W:26:ILE:HG13	2.07	0.54
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.90	0.54
6:C:246:ARG:NH1	39:C:9173:HOH:O	2.39	0.54
1:0:2649:A:H5’	1:0:2649:A:C8	2.43	0.54
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.40	0.54
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.89	0.54
32:I:139:ILE:HG22	32:I:140:GLU:N	2.22	0.54
1:0:1751:G:C2’	1:0:1752:G:H5”	2.36	0.54
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.72	0.54
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.23	0.54
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.08	0.54
1:0:475:G:C5’	6:C:73:LEU:HD23	2.38	0.54
5:B:96:PRO:HG3	39:B:9631:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.90	0.54
28:Z:30:GLU:HG2	28:Z:33:MET:HE3	1.89	0.54
6:C:218:VAL:HG12	39:C:9225:HOH:O	2.07	0.54
4:A:36:ASP:C	4:A:38:ILE:H	2.11	0.54
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.90	0.54
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.08	0.54
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.90	0.54
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.54
30:2:41:HIS:CD2	30:2:44:ARG:H	2.26	0.53
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.23	0.53
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.92	0.53
2:9:3049:G:O2'	2:9:3050:G:H5'	2.07	0.53
7:D:135:VAL:HG22	7:D:136:ARG:N	2.23	0.53
1:0:545:G:C8	1:0:545:G:H5'	2.41	0.53
7:D:166:ILE:HB	39:D:6326:HOH:O	2.08	0.53
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.43	0.53
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.08	0.53
1:0:926:A:H5'	14:L:39:GLU:OE2	2.08	0.53
32:I:128:VAL:C	32:I:130:GLY:H	2.11	0.53
1:0:171:C:OP2	15:M:84:LYS:HG3	2.08	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.09	0.53
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.89	0.53
1:0:2032:U:H2'	1:0:2033:G:C5'	2.37	0.53
1:0:1120:U:H5"	1:0:1120:U:C6	2.43	0.53
14:L:80:ASP:HB2	14:L:90:ARG:O	2.08	0.53
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.91	0.53
1:0:1878:G:H4'	39:0:4700:HOH:O	2.08	0.53
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.23	0.53
6:C:214:THR:HG23	39:C:9238:HOH:O	2.09	0.53
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.90	0.53
1:0:2015:A:H2'	1:0:2016:U:O4'	2.08	0.53
1:0:1878:G:O2'	1:0:1879:U:C6	2.59	0.53
1:0:1789:G:O6	18:P:73:HIS:HE1	1.91	0.53
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.44	0.53
1:0:299:U:H5'	39:0:7810:HOH:O	2.08	0.53
1:0:308:U:H5'	22:T:97:ARG:NH2	2.23	0.53
12:J:130:VAL:HG12	12:J:131:THR:N	2.24	0.53
1:0:1384:C:H5'	26:X:30:MET:HG2	1.89	0.53
17:O:25:VAL:HG23	17:O:26:TRP:N	2.24	0.53
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.09	0.53
13:K:30:LYS:O	13:K:55:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.07	0.53
8:E:69:ILE:HA	8:E:72:MET:CE	2.39	0.53
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.38	0.53
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.90	0.53
1:0:625:U:H5"	1:0:1044:C:N4	2.24	0.53
6:C:25:PRO:HG2	39:C:9122:HOH:O	2.08	0.53
24:V:29:ASN:O	24:V:33:VAL:HG23	2.09	0.53
1:0:870:G:OP2	4:A:3:ARG:HD3	2.09	0.53
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.39	0.53
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.91	0.53
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.91	0.53
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.05	0.53
8:E:15:GLN:NE2	8:E:40:VAL:O	2.41	0.53
1:0:1205:U:C2'	1:0:1206:U:H5"	2.38	0.53
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.09	0.53
1:0:1730:G:C5'	1:0:1731:C:C6	2.92	0.53
9:F:46:GLU:O	9:F:73:PRO:HD2	2.08	0.53
7:D:172:VAL:HG12	7:D:173:GLU:H	1.74	0.53
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.91	0.53
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
1:0:1981:A:H1'	1:0:1983:C:N4	2.24	0.53
1:0:449:A:N7	6:C:43:LYS:HG2	2.23	0.53
39:0:7264:HOH:O	16:N:4:PRO:HD2	2.08	0.53
8:E:11:VAL:HG12	8:E:12:ASP:N	2.23	0.53
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.90	0.53
17:O:87:THR:O	17:O:91:GLN:HG3	2.08	0.53
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.23	0.53
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.08	0.53
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.44	0.52
1:0:137:U:H2'	1:0:139:C:C5	2.44	0.52
1:0:1730:G:H5"	1:0:1731:C:H6	1.75	0.52
5:B:148:PRO:HB3	5:B:156:LYS:HG2	1.90	0.52
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.39	0.52
1:0:1942:A:H3'	39:0:7817:HOH:O	2.08	0.52
1:0:653:C:H2'	1:0:654:A:C8	2.44	0.52
1:0:151:A:H2'	1:0:152:A:O4'	2.09	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.52
39:0:6869:HOH:O	4:A:205:GLY:HA3	2.09	0.52
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.41	0.52
6:C:2:GLN:HB3	39:C:9188:HOH:O	2.07	0.52
26:X:20:GLU:HG3	26:X:21:PRO:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.09	0.52
1:0:603:A:H5"	1:0:604:G:OP1	2.08	0.52
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.10	0.52
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.07	0.52
1:0:95:A:H5"	1:0:97:G:O4'	2.10	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.74	0.52
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.08	0.52
39:9:5071:HOH:O	16:N:23:ARG:HD3	2.09	0.52
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.22	0.52
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.89	0.52
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.19	0.52
7:D:13:MET:HA	7:D:137:PRO:HG2	1.91	0.52
12:J:70:PHE:CG	12:J:70:PHE:O	2.63	0.52
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.90	0.52
4:A:223:ARG:NE	39:A:9561:HOH:O	2.41	0.52
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.08	0.52
1:0:2769:C:H2'	1:0:2770:G:O4'	2.09	0.52
18:P:64:GLU:HG2	39:P:163:HOH:O	2.09	0.52
25:W:149:LEU:HG	25:W:153:MET:CE	2.40	0.52
15:M:24:GLN:O	15:M:28:GLN:HG3	2.10	0.52
1:0:1119:G:N2	1:0:1246:A:N1	2.57	0.52
12:J:42:GLU:O	12:J:131:THR:HG23	2.10	0.52
5:B:41:PHE:CG	5:B:79:MET:HE2	2.44	0.52
1:0:2320:U:H4'	1:0:2321:A:O4'	2.10	0.52
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.58	0.52
39:0:9697:HOH:O	5:B:214:PRO:HD2	2.09	0.52
1:0:164:G:H4'	14:L:30:ARG:HD3	1.91	0.52
2:9:3049:G:H5"	39:9:4707:HOH:O	2.09	0.52
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.09	0.52
25:W:4:LEU:O	25:W:32:CYS:HA	2.09	0.52
25:W:5:VAL:O	25:W:52:VAL:HG23	2.09	0.52
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.36	0.52
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.90	0.52
1:0:316:A:N3	1:0:336:G:O2'	2.40	0.52
1:0:2824:C:H5"	1:0:2825:C:H5'	1.91	0.52
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.10	0.52
4:A:105:VAL:HG13	4:A:155:THR:O	2.10	0.52
1:0:2072:G:H4'	39:0:4390:HOH:O	2.10	0.52
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.92	0.52
1:0:241:A:C2	1:0:378:A:H4'	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:72:ASN:HB2	39:L:9479:HOH:O	2.10	0.52
1:0:470:U:O2'	29:1:16:HIS:CD2	2.60	0.52
1:0:2419:U:H5"	1:0:2420:G:H5'	1.91	0.52
4:A:94:LEU:N	4:A:94:LEU:HD23	2.25	0.52
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.10	0.52
13:K:14:LYS:HG3	13:K:32:ILE:O	2.09	0.52
7:D:25:MET:CE	7:D:37:ALA:HB1	2.38	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.40	0.52
24:V:39:ALA:C	24:V:41:GLU:H	2.13	0.52
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.25	0.52
39:0:6800:HOH:O	27:Y:158:LYS:HD3	2.10	0.52
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.09	0.52
2:9:3004:G:H21	16:N:44:ARG:NH1	2.08	0.52
1:0:2748:G:H1'	39:0:8436:HOH:O	2.09	0.51
4:A:36:ASP:O	4:A:38:ILE:N	2.43	0.51
1:0:380:A:H2'	39:0:7710:HOH:O	2.10	0.51
1:0:848:C:H5'	39:0:7752:HOH:O	2.10	0.51
1:0:1250:C:O2'	1:0:1251:C:H5'	2.10	0.51
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.76	0.51
1:0:2769:C:O2'	1:0:2770:G:H5'	2.10	0.51
14:L:97:VAL:HG12	14:L:98:GLU:O	2.10	0.51
14:L:148:GLU:HB2	39:L:9487:HOH:O	2.09	0.51
1:0:2815:G:N7	12:J:80:LYS:NZ	2.56	0.51
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.93	0.51
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.12	0.51
10:G:12:ILE:N	10:G:13:PRO:CD	2.73	0.51
4:A:164:ARG:CZ	39:A:9577:HOH:O	2.58	0.51
1:0:1441:G:O2'	1:0:1442:A:H5'	2.10	0.51
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.10	0.51
1:0:2717:C:O2'	1:0:2718:C:H5"	2.10	0.51
1:0:524:A:H5"	20:R:29:LYS:HD3	1.92	0.51
1:0:1164:U:OP1	32:I:74:PRO:HA	2.10	0.51
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.44	0.51
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.39	0.51
1:0:2103:A:C8	1:0:2103:A:H5'	2.45	0.51
1:0:926:A:O2'	14:L:41:HIS:HD2	1.94	0.51
4:A:210:GLY:N	39:A:9576:HOH:O	2.42	0.51
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.93	0.51
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.26	0.51
2:9:3114:G:O6	16:N:11:ARG:HD3	2.11	0.51
7:D:94:ALA:HA	7:D:174:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2508:C:H2'	39:0:7246:HOH:O	2.10	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.44	0.51
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.92	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.92	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.30	0.51
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.39	0.51
22:T:40:VAL:HG22	22:T:41:ARG:H	1.75	0.51
1:0:2779:G:H21	8:E:143:GLN:NE2	2.08	0.51
2:9:3064:C:C2'	2:9:3065:A:H5'	2.39	0.51
1:0:1503:U:H2'	1:0:1504:A:O4'	2.09	0.51
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.10	0.51
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.43	0.51
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.93	0.51
17:O:98:LEU:O	17:O:102:ILE:HG13	2.11	0.51
1:0:317:A:OP1	22:T:52:ARG:O	2.29	0.51
5:B:17:LYS:O	5:B:260:HIS:HD2	1.93	0.51
1:0:2414:A:H2'	1:0:2415:A:C8	2.46	0.51
6:C:154:VAL:O	6:C:158:GLU:HG3	2.11	0.51
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.30	0.51
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.92	0.51
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.41	0.51
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.46	0.51
31:3:3:MET:O	31:3:90:PHE:HA	2.11	0.51
25:W:119:HIS:HD2	25:W:120:PRO:O	1.94	0.51
2:9:3024:U:H3'	2:9:3025:G:H5'	1.92	0.51
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.38	0.51
7:D:25:MET:SD	7:D:40:ILE:HD11	2.51	0.51
39:9:4707:HOH:O	16:N:147:ILE:HB	2.11	0.51
12:J:130:VAL:HG12	12:J:131:THR:H	1.76	0.51
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.92	0.51
23:U:49:LEU:HG	39:U:3805:HOH:O	2.10	0.51
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.09	0.51
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.75	0.51
22:T:61:GLU:HG3	39:T:3851:HOH:O	2.11	0.51
1:0:542:A:H2'	1:0:543:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2541:U:O2	3:4:77:HFA:HA	2.10	0.50
1:0:2726:U:O2	1:0:2749:U:O5'	2.28	0.50
14:L:145:LEU:O	14:L:145:LEU:HD23	2.11	0.50
32:I:112:LYS:C	32:I:114:PRO:HD2	2.31	0.50
7:D:56:ARG:N	39:D:6752:HOH:O	2.44	0.50
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
1:0:2541:U:H5'	39:0:3027:HOH:O	2.11	0.50
2:9:3051:A:H5'	16:N:160:SER:CB	2.39	0.50
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.41	0.50
1:0:969:G:H1	1:0:999:C:H42	1.58	0.50
4:A:109:GLU:HG2	4:A:116:GLY:N	2.26	0.50
1:0:196:G:H2'	39:0:7154:HOH:O	2.10	0.50
26:X:7:GLU:HA	26:X:74:ALA:O	2.11	0.50
32:I:100:LEU:O	32:I:139:ILE:HG23	2.10	0.50
14:L:129:ALA:O	14:L:133:VAL:HG23	2.11	0.50
16:N:11:ARG:O	16:N:15:GLU:HG3	2.11	0.50
5:B:41:PHE:CG	5:B:190:MET:HE3	2.46	0.50
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.80	0.50
1:0:2361:A:H2'	1:0:2362:A:C8	2.45	0.50
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.75	0.50
1:0:558:C:H2'	1:0:559:U:H5"	1.92	0.50
6:C:236:THR:HA	39:C:9251:HOH:O	2.10	0.50
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.41	0.50
12:J:131:THR:HG22	12:J:134:GLU:H	1.75	0.50
1:0:2883:A:H2'	1:0:2884:G:O4'	2.12	0.50
1:0:1626:A:H2'	1:0:1627:G:O4'	2.11	0.50
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.87	0.50
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.76	0.50
1:0:1166:A:H61	1:0:1180:U:H3	1.59	0.50
1:0:1527:A:H1'	1:0:1528:A:C8	2.47	0.50
39:0:3173:HOH:O	25:W:119:HIS:HE1	1.94	0.50
4:A:135:VAL:HG11	4:A:147:ARG:NH1	2.27	0.50
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.92	0.50
21:S:33:SER:O	21:S:37:VAL:HG23	2.12	0.50
1:0:1476:A:O2'	1:0:1477:C:H5'	2.12	0.50
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.26	0.50
15:M:78:LYS:HD3	39:M:9447:HOH:O	2.11	0.50
14:L:35:ARG:HD3	14:L:35:ARG:C	2.32	0.50
4:A:53:ALA:HB3	39:A:9596:HOH:O	2.12	0.50
12:J:45:VAL:HG22	12:J:46:ILE:N	2.26	0.50
21:S:57:THR:HG22	21:S:58:MET:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1406:A:H4'	1:0:1407:A:C5'	2.41	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.93	0.50
18:P:141:ILE:C	18:P:143:ALA:H	2.15	0.50
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.22	0.50
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.93	0.50
1:0:119:A:H2'	1:0:120:A:H5"	1.93	0.50
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.76	0.50
20:R:114:VAL:HA	20:R:144:GLU:O	2.12	0.50
1:0:1299:G:H5'	39:0:4657:HOH:O	2.11	0.50
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.12	0.50
1:0:2768:A:O2'	1:0:2769:C:H5'	2.12	0.50
39:0:4807:HOH:O	30:2:38:LYS:HE3	2.12	0.50
1:0:407:A:H2'	1:0:408:A:C8	2.47	0.50
32:I:80:LYS:HD3	32:I:86:GLU:O	2.12	0.50
1:0:793:A:H5"	18:P:83:LYS:HG2	1.94	0.50
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.10	0.50
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.12	0.50
32:I:113:HIS:N	32:I:114:PRO:CD	2.75	0.49
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.49
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.49
24:V:1:THR:CG2	24:V:2:VAL:H	2.14	0.49
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.42	0.49
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.32	0.49
1:0:603:A:H1'	1:0:605:C:C2	2.47	0.49
1:0:204:A:C2'	1:0:205:U:H5'	2.42	0.49
1:0:432:G:O2'	1:0:433:C:H5'	2.12	0.49
5:B:254:GLN:HG3	39:B:9532:HOH:O	2.12	0.49
5:B:264:GLU:CG	5:B:267:LYS:HE2	2.36	0.49
2:9:3039:U:HO2'	2:9:3042:C:H5	1.52	0.49
25:W:65:VAL:HA	25:W:68:THR:HG22	1.93	0.49
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.94	0.49
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.49
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.43	0.49
1:0:2456:A:H2'	1:0:2457:U:C6	2.48	0.49
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.11	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.23	0.49
6:C:246:ARG:NE	39:C:9225:HOH:O	2.35	0.49
1:0:960:G:N3	1:0:960:G:H2'	2.25	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.45	0.49
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.42	0.49
7:D:36:ASN:HA	39:D:7500:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.12	0.49
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.77	0.49
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.76	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.90	0.49
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.95	0.49
1:0:794:U:H3	1:0:819:A:H61	1.59	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
25:W:64:THR:O	25:W:68:THR:HG22	2.13	0.49
11:H:76:GLU:C	11:H:77:LEU:HD23	2.33	0.49
1:0:920:C:H5"	1:0:921:G:O5'	2.13	0.49
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.95	0.49
24:V:12:THR:HG23	24:V:14:ALA:N	2.26	0.49
25:W:88:THR:CG2	25:W:89:ASP:H	2.20	0.49
1:0:2852:A:H5"	39:0:5781:HOH:O	2.13	0.49
1:0:1163:G:H5'	32:I:115:ASP:O	2.12	0.49
6:C:98:ARG:NH1	39:C:9158:HOH:O	2.46	0.49
1:0:1946:C:H2'	1:0:1971:G:C8	2.48	0.49
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.49
2:9:3041:C:C6	7:D:50:VAL:HG21	2.47	0.49
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.49
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.95	0.49
1:0:2568:A:H2'	1:0:2569:A:O4'	2.13	0.49
10:G:64:ASN:N	10:G:64:ASN:HD22	2.09	0.49
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.93	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.95	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.61	0.49
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.76	0.49
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.92	0.49
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.93	0.49
27:Y:212:ARG:HD2	39:Y:9395:HOH:O	2.12	0.49
1:0:1666:C:C2'	1:0:1667:A:H5"	2.43	0.49
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.26	0.49
1:0:625:U:H5'	39:0:3785:HOH:O	2.13	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.42	0.49
9:F:21:GLU:O	9:F:24:ARG:HG3	2.13	0.49
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.93	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.12	0.49
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.27	0.49
1:0:1218:U:H2'	1:0:1219:U:H6	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.13	0.49
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.94	0.49
1:0:155:C:OP2	15:M:188:ARG:HD3	2.12	0.49
1:0:1172:G:H1'	39:0:5534:HOH:O	2.13	0.49
1:0:462:A:C2	30:2:37:HIS:HB3	2.48	0.49
1:0:1198:U:H2'	1:0:1200:A:OP2	2.12	0.49
12:J:76:ASP:HA	39:J:5907:HOH:O	2.13	0.48
1:0:1209:C:H2'	1:0:1210:G:C8	2.47	0.48
11:H:30:GLN:H	11:H:66:ARG:HH11	1.59	0.48
11:H:63:GLU:O	11:H:67:LEU:HB2	2.13	0.48
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.78	0.48
1:0:2768:A:H2'	1:0:2769:C:O4'	2.13	0.48
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.95	0.48
1:0:500:G:H21	20:R:98:ASN:HD21	1.60	0.48
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.48
1:0:1119:G:C8	12:J:52:GLN:NE2	2.81	0.48
2:9:3006:C:H5"	16:N:37:ARG:HE	1.78	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.14	0.48
1:0:1753:C:O2	5:B:229:ARG:NH2	2.40	0.48
1:0:2626:C:H2'	1:0:2627:G:C8	2.48	0.48
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.13	0.48
1:0:1717:A:H5"	18:P:54:LYS:HB2	1.94	0.48
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.43	0.48
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.46	0.48
1:0:1667:A:H2'	1:0:1668:U:C6	2.48	0.48
26:X:41:PHE:O	26:X:43:VAL:HG23	2.13	0.48
5:B:301:VAL:HG11	5:B:309:VAL:HG11	1.95	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.13	0.48
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.95	0.48
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.34	0.48
1:0:21:G:H4'	20:R:2:ILE:HG22	1.93	0.48
4:A:194:MET:CE	4:A:199:HIS:HB2	2.42	0.48
29:1:25:LYS:HG3	30:2:49:GLU:H	1.78	0.48
1:0:1192:A:H3'	1:0:1193:A:H5'	1.95	0.48
1:0:447:A:O2'	1:0:448:G:H5'	2.14	0.48
31:3:65:THR:HG22	31:3:67:LEU:HG	1.95	0.48
8:E:6:GLU:HA	8:E:46:THR:HG22	1.94	0.48
1:0:629:A:H2'	1:0:630:A:O4'	2.14	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
25:W:122:ARG:NH1	25:W:152:ALA:O	2.46	0.48
1:0:1183:C:H5	1:0:1192:A:OP1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:12:ILE:HD12	39:G:692:HOH:O	2.13	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.48	0.48
5:B:41:PHE:HA	5:B:79:MET:CE	2.43	0.48
1:0:2866:U:C4	23:U:50:GLU:HB3	2.49	0.48
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.48
15:M:98:GLN:O	15:M:102:GLU:HG3	2.13	0.48
1:0:588:G:O6	25:W:154:ARG:NH1	2.47	0.48
22:T:23:VAL:HG23	22:T:41:ARG:HG3	1.94	0.48
17:O:25:VAL:HG23	17:O:26:TRP:H	1.79	0.48
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.66	0.48
1:0:932:U:H2'	1:0:933:C:C6	2.49	0.48
2:9:3091:C:H2'	2:9:3092:G:O4'	2.13	0.48
20:R:132:ARG:CZ	39:R:9497:HOH:O	2.61	0.48
4:A:206:ARG:NH1	39:A:9499:HOH:O	2.47	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.49	0.48
1:0:447:A:OP1	22:T:2:LYS:HG2	2.14	0.48
10:G:16:LYS:O	10:G:20:VAL:HG23	2.14	0.48
23:U:9:CYS:O	23:U:52:THR:HG23	2.12	0.48
6:C:233:THR:HG22	6:C:234:VAL:N	2.28	0.48
22:T:19:ARG:HD3	22:T:67:LEU:O	2.14	0.48
12:J:88:PRO:O	12:J:94:GLY:HA3	2.14	0.48
1:0:622:G:P	27:Y:148:GLY:HA3	2.53	0.48
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.25	0.48
1:0:2748:G:H8	39:0:8000:HOH:O	1.95	0.48
15:M:61:ILE:N	15:M:61:ILE:HD12	2.28	0.48
1:0:1745:G:H22	1:0:2033:G:H5'	1.79	0.48
25:W:11:VAL:O	25:W:12:ASN:HB2	2.13	0.48
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.79	0.48
6:C:168:ARG:NH2	6:C:190:ALA:O	2.47	0.48
1:0:450:C:OP1	6:C:184:ARG:NH2	2.44	0.48
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.48
3:4:176:A:OP1	3:4:175:C:H5"	2.14	0.48
2:9:3008:G:O6	16:N:11:ARG:NH1	2.45	0.48
1:0:474:C:O3'	6:C:73:LEU:HD21	2.13	0.48
14:L:149:ARG:O	14:L:150:GLN:HB2	2.13	0.48
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.49	0.48
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.27	0.48
6:C:118:THR:O	6:C:136:VAL:HG13	2.13	0.48
1:0:136:C:H2'	1:0:137:U:O4'	2.13	0.48
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.14	0.48
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.48
15:M:69:LYS:O	15:M:73:ARG:NH2	2.44	0.48
5:B:238:ASN:ND2	5:B:240:GLY:H	1.99	0.47
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.41	0.47
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.94	0.47
6:C:246:ARG:CB	6:C:246:ARG:HH11	2.27	0.47
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.29	0.47
1:0:1462:C:H2'	1:0:1463:A:H8	1.78	0.47
18:P:98:ILE:O	18:P:98:ILE:HD13	2.14	0.47
31:3:91:GLN:O	31:3:92:GLU:HB2	2.14	0.47
1:0:883:U:H2'	1:0:883:U:O2	2.14	0.47
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.95	0.47
12:J:39:VAL:CG1	12:J:40:ASN:N	2.76	0.47
16:N:154:LEU:HG	16:N:155:GLU:H	1.79	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.14	0.47
2:9:3012:C:H5'	2:9:3070:U:O4'	2.15	0.47
1:0:1168:C:H5"	32:I:87:THR:CG2	2.45	0.47
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.47	0.47
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.96	0.47
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.44	0.47
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.17	0.47
5:B:16:ARG:NH2	39:B:9555:HOH:O	2.41	0.47
12:J:131:THR:HG22	12:J:133:GLY:N	2.30	0.47
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.49	0.47
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.14	0.47
16:N:183:ASP:O	16:N:184:ILE:O	2.33	0.47
31:3:3:MET:HB2	31:3:88:LEU:HD11	1.97	0.47
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.44	0.47
14:L:57:VAL:HG12	14:L:57:VAL:O	2.14	0.47
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.44	0.47
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.14	0.47
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.96	0.47
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.97	0.47
1:0:2265:U:H2'	1:0:2266:A:C8	2.50	0.47
27:Y:133:HIS:HD2	39:Y:9377:HOH:O	1.97	0.47
1:0:1736:A:H1'	39:0:8130:HOH:O	2.15	0.47
6:C:16:VAL:HG12	6:C:17:ASP:N	2.29	0.47
25:W:108:ARG:HE	25:W:114:PRO:CG	2.27	0.47
1:0:2769:C:H2'	1:0:2770:G:C5'	2.44	0.47
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.50	0.47
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.96	0.47
1:0:1025:C:H5'	25:W:23:MET:O	2.15	0.47
26:X:34:ARG:NH1	26:X:48:VAL:O	2.47	0.47
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.79	0.47
15:M:58:GLN:HG3	39:M:9414:HOH:O	2.12	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
2:9:3002:U:OP2	2:9:3003:A:H5'	2.14	0.47
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.47
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.15	0.47
1:0:1972:U:H2'	1:0:1973:A:H5'	1.97	0.47
1:0:93:C:H5"	24:V:1:THR:CB	2.43	0.47
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.61	0.47
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.96	0.47
1:0:2676:C:H6	1:0:2676:C:H5"	1.79	0.47
1:0:797:A:O4'	28:Z:10:ARG:N	2.47	0.47
5:B:62:ARG:CA	5:B:65:MET:HE3	2.44	0.47
16:N:154:LEU:O	16:N:155:GLU:CB	2.63	0.47
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.97	0.47
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.49	0.47
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.13	0.47
1:0:2329:C:O2'	1:0:2330:U:H5'	2.15	0.47
1:0:286:U:H2'	1:0:287:C:C6	2.50	0.47
24:V:8:ILE:HA	24:V:11:MET:CE	2.44	0.47
2:9:3049:G:C2'	2:9:3050:G:H5'	2.45	0.47
20:R:29:LYS:NZ	39:R:9452:HOH:O	2.47	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.73	0.47
1:0:1211:G:O2'	1:0:1212:C:H5'	2.15	0.47
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.50	0.47
1:0:2911:C:O2'	1:0:2912:C:H5'	2.15	0.47
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.14	0.47
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.47
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.48	0.47
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.45	0.47
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.40	0.47
12:J:45:VAL:CG2	12:J:129:PHE:CD1	2.98	0.47
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.45	0.47
31:3:22:VAL:HG11	31:3:67:LEU:HD13	1.97	0.47
1:0:1778:A:H2'	1:0:1779:A:H5'	1.96	0.47
1:0:204:A:H2'	1:0:205:U:H5'	1.96	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.15	0.47
1:0:27:U:H2'	1:0:28:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.47
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.50	0.47
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.49	0.47
26:X:66:THR:HG22	26:X:67:PRO:O	2.14	0.47
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.45	0.47
1:0:392:U:H5"	15:M:193:LYS:HB3	1.96	0.47
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.45	0.47
1:0:1234:U:N3	5:B:244:PRO:HB3	2.30	0.47
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.47
1:0:2712:G:H5'	39:K:4183:HOH:O	2.15	0.46
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.97	0.46
1:0:407:A:H5'	39:0:6549:HOH:O	2.14	0.46
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.15	0.46
5:B:321:PRO:HG3	39:B:9597:HOH:O	2.15	0.46
39:0:5296:HOH:O	16:N:21:HIS:HD2	1.98	0.46
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.50	0.46
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.15	0.46
7:D:99:ASP:N	7:D:103:ASN:O	2.43	0.46
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.46
1:0:710:G:H5'	17:O:25:VAL:HG13	1.98	0.46
1:0:1441:G:H1'	39:0:8302:HOH:O	2.15	0.46
1:0:2443:C:H5'	14:L:57:VAL:HG21	1.97	0.46
1:0:2435:U:H1'	39:0:5974:HOH:O	2.15	0.46
1:0:1252:A:H2'	1:0:1253:C:O4'	2.15	0.46
8:E:97:VAL:HG12	39:E:4191:HOH:O	2.15	0.46
8:E:35:TYR:HB2	39:E:5715:HOH:O	2.16	0.46
4:A:34:ASP:OD1	4:A:35:GLY:N	2.48	0.46
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.16	0.46
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.98	0.46
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.97	0.46
1:0:1477:C:H5'	1:0:1868:G:C5'	2.45	0.46
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.97	0.46
15:M:68:ARG:HD3	15:M:68:ARG:O	2.15	0.46
7:D:25:MET:HE1	7:D:37:ALA:O	2.14	0.46
32:I:131:THR:O	32:I:135:LEU:HG	2.16	0.46
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.95	0.46
6:C:162:VAL:HG13	6:C:192:ILE:HD11	1.97	0.46
1:0:1182:C:H1'	1:0:1192:A:C8	2.47	0.46
4:A:33:GLU:OE1	4:A:33:GLU:N	2.38	0.46
1:0:797:A:H4'	28:Z:10:ARG:N	2.30	0.46
5:B:41:PHE:HA	5:B:79:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:292:G:H2'	1:0:358:G:N2	2.30	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.50	0.46
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.97	0.46
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.46	0.46
1:0:666:A:H2'	1:0:667:C:O4'	2.15	0.46
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.50	0.46
5:B:171:VAL:HG23	5:B:172:SER:N	2.31	0.46
30:2:39:ARG:HG2	39:2:3143:HOH:O	2.16	0.46
1:0:1268:C:O2'	1:0:1269:G:H5'	2.15	0.46
1:0:249:G:O2'	1:0:250:C:H5'	2.15	0.46
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.45	0.46
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.16	0.46
22:T:53:GLY:HA3	39:T:6384:HOH:O	2.14	0.46
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.48	0.46
1:0:1118:A:C8	1:0:1119:G:H5"	2.50	0.46
8:E:69:ILE:HA	8:E:72:MET:HE2	1.97	0.46
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.98	0.46
1:0:2064:U:H4'	1:0:2653:A:OP1	2.15	0.46
7:D:173:GLU:HG3	7:D:174:VAL:N	2.31	0.46
1:0:1044:C:H5"	39:0:9648:HOH:O	2.16	0.46
25:W:142:ASP:HB3	25:W:145:GLY:H	1.81	0.46
4:A:207:GLN:O	4:A:208:HIS:HB3	2.15	0.46
1:0:1299:G:N2	39:0:5251:HOH:O	2.49	0.46
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.31	0.46
1:0:285:A:H2'	1:0:286:U:O4'	2.16	0.46
1:0:1615:A:H5'	39:0:4766:HOH:O	2.15	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.31	0.46
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.80	0.46
26:X:72:VAL:CG2	26:X:85:VAL:HG12	2.44	0.46
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.56	0.46
15:M:164:THR:CG2	15:M:165:GLY:N	2.78	0.46
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.15	0.46
7:D:62:ASP:HA	39:D:4233:HOH:O	2.16	0.46
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.16	0.46
4:A:88:ILE:HG22	4:A:88:ILE:O	2.16	0.46
11:H:116:ALA:O	11:H:117:PHE:C	2.55	0.46
24:V:42:ASN:O	24:V:44:GLY:N	2.49	0.46
13:K:55:VAL:CG1	13:K:56:SER:N	2.78	0.46
1:0:2851:G:O3'	5:B:157:LYS:NZ	2.46	0.46
14:L:114:VAL:HB	39:L:9471:HOH:O	2.15	0.46
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1755:A:H2'	1:0:1756:G:O4'	2.16	0.46
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.30	0.46
1:0:177:A:H2'	1:0:178:U:O4'	2.16	0.46
1:0:189:A:OP1	15:M:171:ARG:NH2	2.49	0.46
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.46	0.46
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.46	0.46
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.80	0.46
5:B:16:ARG:NE	39:B:9555:HOH:O	2.34	0.46
7:D:65:GLU:HG3	39:D:6752:HOH:O	2.15	0.46
1:0:2415:A:N3	16:N:26:LEU:HD13	2.30	0.46
1:0:1171:A:H2'	1:0:1172:G:H5'	1.97	0.46
11:H:47:ILE:HG21	39:H:9541:HOH:O	2.14	0.46
1:0:1926:G:H2'	1:0:1927:A:C8	2.51	0.46
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.16	0.46
4:A:121:ALA:O	4:A:124:VAL:HG22	2.16	0.46
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.98	0.45
1:0:1603:A:H5"	1:0:1605:G:H5'	1.97	0.45
5:B:221:GLN:NE2	13:K:42:ASN:HD22	2.07	0.45
1:0:834:G:H3'	1:0:835:U:H4'	1.99	0.45
1:0:2032:U:H2'	1:0:2033:G:H5'	1.97	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.35	0.45
1:0:92:G:H4'	24:V:44:GLY:HA3	1.98	0.45
1:0:65:C:O2'	1:0:66:G:H5'	2.16	0.45
2:9:3052:A:H2'	2:9:3053:G:O4'	2.16	0.45
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.82	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.49	0.45
20:R:114:VAL:HG13	20:R:114:VAL:O	2.16	0.45
14:L:136:ALA:HB3	39:L:9471:HOH:O	2.16	0.45
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.51	0.45
25:W:105:THR:HA	25:W:109:GLU:OE1	2.16	0.45
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.45
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.45
6:C:133:ARG:NH1	39:C:9213:HOH:O	2.49	0.45
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.32	0.45
1:0:820:G:O2'	1:0:856:G:H4'	2.16	0.45
2:9:3050:G:H5"	16:N:159:TYR:CE1	2.52	0.45
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.45
2:9:3114:G:H2'	2:9:3115:C:C6	2.51	0.45
27:Y:115:ARG:NE	39:Y:9350:HOH:O	2.49	0.45
8:E:66:GLN:O	8:E:70:GLU:HG3	2.16	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2299:G:O6	19:Q:1:PRO:HA	2.17	0.45
5:B:84:LEU:HD13	5:B:84:LEU:O	2.17	0.45
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.59	0.45
2:9:3076:G:C3'	2:9:3077:A:H5"	2.30	0.45
1:0:2717:C:H5'	5:B:302:PRO:HA	1.97	0.45
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.45
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.45
39:0:9644:HOH:O	14:L:30:ARG:HD2	2.17	0.45
4:A:135:VAL:HG11	4:A:147:ARG:HH12	1.81	0.45
1:0:1947:G:H2'	1:0:1948:G:H8	1.81	0.45
1:0:1525:G:H5'	1:0:1526:A:OP2	2.17	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.16	0.45
1:0:2906:A:H5'	1:0:2907:C:O4'	2.16	0.45
16:N:155:GLU:O	16:N:156:GLU:HG3	2.16	0.45
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.49	0.45
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.45
15:M:74:LYS:HG2	15:M:75:ARG:N	2.31	0.45
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.52	0.45
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.46	0.45
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.17	0.45
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.17	0.45
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.98	0.45
1:0:1724:U:H5"	39:0:4327:HOH:O	2.16	0.45
4:A:201:PHE:HB3	39:A:9621:HOH:O	2.15	0.45
1:0:288:A:H2'	1:0:289:G:C8	2.51	0.45
39:9:5851:HOH:O	16:N:38:LYS:HD3	2.16	0.45
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.98	0.45
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.99	0.45
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.52	0.45
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.98	0.45
1:0:2316:G:OP1	1:0:2317:C:H1'	2.16	0.45
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.45	0.45
1:0:2748:G:OP1	1:0:2749:U:H5"	2.17	0.45
1:0:137:U:OP1	1:0:259:G:O2'	2.35	0.45
2:9:3054:A:O2'	2:9:3055:U:H5'	2.17	0.45
1:0:2568:A:H5"	1:0:2702:A:O2'	2.16	0.45
22:T:78:THR:HB	22:T:87:VAL:O	2.17	0.45
13:K:99:ASP:OD1	13:K:101:ASN:N	2.49	0.45
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.52	0.45
16:N:72:GLU:HG2	16:N:72:GLU:O	2.16	0.45
5:B:254:GLN:NE2	39:B:9589:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.98	0.45
1:0:1185:U:H2'	1:0:1186:C:C6	2.51	0.45
1:0:2907:C:H2'	1:0:2908:A:O4'	2.17	0.45
4:A:99:ILE:O	4:A:131:HIS:CE1	2.70	0.45
9:F:99:THR:O	9:F:100:ASP:HB2	2.17	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.99	0.45
1:0:2681:A:H4'	1:0:2682:C:H5'	1.99	0.45
1:0:2252:A:C5	1:0:2253:G:H1'	2.51	0.45
11:H:45:VAL:HA	11:H:167:PRO:O	2.17	0.44
27:Y:155:ARG:NH1	39:Y:9352:HOH:O	2.49	0.44
5:B:215:VAL:HB	5:B:234:ARG:NH1	2.26	0.44
2:9:3029:C:C2'	2:9:3030:C:H5'	2.47	0.44
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.99	0.44
1:0:1942:A:H5'	4:A:233:THR:HB	1.98	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.65	0.44
1:0:1573:A:H2'	1:0:1574:C:O4'	2.16	0.44
1:0:1773:G:C8	28:Z:16:ALA:HA	2.50	0.44
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.32	0.44
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.97	0.44
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.98	0.44
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.99	0.44
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.18	0.44
1:0:1120:U:H6	1:0:1120:U:H5"	1.82	0.44
16:N:82:TYR:HE1	16:N:120:GLU:HG2	1.82	0.44
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.44
1:0:1748:U:H4'	39:0:7981:HOH:O	2.16	0.44
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.44
6:C:150:THR:HA	6:C:203:ALA:O	2.17	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.44
7:D:163:VAL:HA	39:D:6326:HOH:O	2.17	0.44
4:A:51:ARG:HH21	4:A:55:VAL:HG23	1.83	0.44
8:E:23:GLU:HG2	8:E:28:SER:CB	2.46	0.44
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.82	0.44
8:E:84:MET:HE3	8:E:131:LEU:HD13	1.99	0.44
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.55	0.44
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.52	0.44
23:U:20:MET:CG	23:U:28:THR:HG23	2.47	0.44
6:C:236:THR:HG22	6:C:239:ALA:HB2	1.99	0.44
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.53	0.44
25:W:5:VAL:O	25:W:52:VAL:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:58:GLU:HG3	9:F:61:MET:CE	2.47	0.44
11:H:58:ARG:O	11:H:62:LEU:HD22	2.18	0.44
1:0:1163:G:H5"	32:I:115:ASP:HB3	1.99	0.44
1:0:1878:G:O2'	1:0:1879:U:C5	2.63	0.44
11:H:56:GLN:NE2	11:H:93:GLN:HG2	2.31	0.44
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.47	0.44
25:W:29:VAL:O	25:W:30:ASN:HB2	2.18	0.44
1:0:1768:C:H2'	1:0:1769:C:O4'	2.17	0.44
1:0:1226:G:H5'	39:0:5101:HOH:O	2.18	0.44
1:0:426:G:H2'	1:0:427:C:O4'	2.18	0.44
1:0:821:U:H2'	1:0:822:C:H6	1.82	0.44
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.17	0.44
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.00	0.44
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.44
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.15	0.44
1:0:2346:C:H4'	7:D:52:THR:CG2	2.48	0.44
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.49	0.44
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.18	0.44
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.44
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.44
1:0:2003:U:H4'	1:0:2004:U:H5	1.83	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.50	0.44
30:2:20:ARG:NE	30:2:39:ARG:NH2	2.66	0.44
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.18	0.44
1:0:488:U:O2'	22:T:82:THR:HG21	2.17	0.44
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.98	0.44
6:C:219:ASN:O	6:C:222:ASP:OD1	2.36	0.44
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.52	0.44
1:0:564:G:H1'	39:0:6825:HOH:O	2.16	0.44
9:F:102:GLY:O	9:F:103:GLU:HB2	2.18	0.44
1:0:461:C:N3	1:0:479:G:H5'	2.33	0.44
1:0:2478:U:O2'	1:0:2479:A:H5'	2.18	0.44
9:F:60:VAL:O	9:F:60:VAL:CG1	2.66	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
4:A:36:ASP:CB	4:A:83:GLY:HA3	2.45	0.44
31:3:69:TYR:O	31:3:77:ALA:HA	2.17	0.44
14:L:143:THR:CG2	14:L:144:ASP:N	2.81	0.44
1:0:920:C:H5'	1:0:921:G:C4	2.52	0.44
4:A:232:ARG:NH2	4:A:236:GLY:O	2.43	0.44
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:51:VAL:CG1	11:H:53:GLU:O	2.66	0.44
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.18	0.44
7:D:23:VAL:O	7:D:23:VAL:HG23	2.18	0.44
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.53	0.44
1:0:1884:G:O6	4:A:190:ARG:HD2	2.17	0.44
25:W:13:MET:HE1	25:W:18:GLN:CA	2.41	0.44
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.44
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.39	0.44
16:N:119:GLN:O	16:N:123:ILE:HG13	2.18	0.44
1:0:1130:U:H2'	1:0:1131:G:O4'	2.18	0.44
1:0:1066:U:H2'	1:0:1067:A:C8	2.52	0.44
1:0:1067:A:H5'	39:0:4922:HOH:O	2.17	0.44
17:O:10:LEU:HD13	17:O:99:GLU:HG3	1.99	0.44
16:N:42:HIS:CE1	16:N:75:THR:OG1	2.71	0.44
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.44
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.00	0.44
30:2:41:HIS:N	30:2:45:ASN:HD22	1.99	0.44
26:X:73:ARG:NH1	26:X:88:GLU:HG2	2.33	0.44
32:I:87:THR:CG2	32:I:88:GLY:N	2.81	0.44
4:A:179:MET:HG2	4:A:186:TRP:HB3	1.99	0.44
21:S:56:ASN:O	30:2:8:LYS:NZ	2.44	0.44
1:0:1919:A:H4'	39:0:5415:HOH:O	2.17	0.44
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.18	0.44
5:B:217:ARG:HG3	5:B:257:THR:HB	2.00	0.43
5:B:254:GLN:HG2	5:B:255:GLY:H	1.80	0.43
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.43
15:M:81:ARG:HG3	15:M:85:ARG:HB2	2.00	0.43
4:A:223:ARG:O	4:A:223:ARG:HG2	2.18	0.43
1:0:960:G:N3	1:0:960:G:C2'	2.81	0.43
5:B:41:PHE:HB3	5:B:190:MET:CE	2.48	0.43
16:N:176:ARG:HG3	16:N:180:LEU:HD13	2.00	0.43
9:F:11:ASP:O	9:F:14:ASP:HB2	2.18	0.43
1:0:1422:U:H2'	1:0:1423:C:C6	2.53	0.43
5:B:49:THR:HG22	5:B:280:VAL:CG2	2.48	0.43
5:B:175:LEU:O	5:B:175:LEU:HD23	2.18	0.43
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.17	0.43
1:0:2083:A:N6	12:J:90:LYS:HE2	2.32	0.43
1:0:1588:G:C6	1:0:1589:G:N1	2.87	0.43
1:0:1681:G:H5"	1:0:1682:A:H5'	2.00	0.43
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.83	0.43
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.43
1:0:2506:A:O2'	1:0:2507:G:O5'	2.36	0.43
25:W:65:VAL:HG12	25:W:116:LEU:HD13	2.01	0.43
7:D:149:ARG:HH12	16:N:15:GLU:HA	1.83	0.43
1:0:2032:U:H2'	1:0:2033:G:H5"	1.99	0.43
27:Y:189:ASN:HD22	27:Y:191:ASP:N	2.16	0.43
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.18	0.43
31:3:17:HIS:O	31:3:18:GLN:HG3	2.19	0.43
8:E:81:GLU:HA	8:E:133:VAL:O	2.18	0.43
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.43
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.18	0.43
1:0:2846:C:H4'	39:0:5633:HOH:O	2.18	0.43
1:0:1096:U:O2'	1:0:1097:A:H5'	2.18	0.43
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.48	0.43
1:0:2549:C:OP1	5:B:7:ARG:NH1	2.51	0.43
14:L:73:VAL:HG23	14:L:74:THR:N	2.33	0.43
24:V:5:VAL:HG11	24:V:9:ARG:NH1	2.32	0.43
1:0:185:G:O3'	1:0:186:A:H4'	2.19	0.43
26:X:20:GLU:CG	26:X:21:PRO:HD2	2.47	0.43
1:0:2526:C:H5'	1:0:2526:C:C6	2.53	0.43
14:L:145:LEU:C	14:L:145:LEU:HD23	2.38	0.43
1:0:702:G:O2'	1:0:703:G:H5'	2.18	0.43
25:W:5:VAL:C	25:W:52:VAL:HG23	2.39	0.43
1:0:2533:C:H6	1:0:2533:C:C5'	2.26	0.43
12:J:99:GLU:HA	39:J:7377:HOH:O	2.18	0.43
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.18	0.43
1:0:2323:G:H5'	39:0:7509:HOH:O	2.18	0.43
1:0:1741:U:O2'	1:0:2723:G:H4'	2.18	0.43
1:0:2239:C:H2'	1:0:2240:U:C6	2.54	0.43
39:0:7490:HOH:O	19:Q:9:GLY:HA2	2.17	0.43
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.18	0.43
20:R:84:ALA:O	20:R:88:PHE:HD1	2.02	0.43
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.51	0.43
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.43
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.19	0.43
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.53	0.43
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.19	0.43
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.48	0.43
1:0:1406:A:H5'	1:0:1407:A:C8	2.54	0.43
1:0:2456:A:H2'	1:0:2457:U:H6	1.84	0.43
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.84	0.43
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.19	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.49	0.43
25:W:139:GLY:O	25:W:141:HIS:CD2	2.65	0.43
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.82	0.43
5:B:267:LYS:HE3	5:B:300:SER:O	2.18	0.43
13:K:118:ALA:O	13:K:119:GLN:C	2.56	0.43
4:A:223:ARG:NH1	39:A:9507:HOH:O	2.51	0.43
1:0:338:C:H4'	6:C:174:ILE:HD11	2.01	0.43
22:T:75:GLU:O	22:T:76:ASP:HB2	2.19	0.43
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.48	0.43
15:M:144:ASP:O	15:M:148:SER:HB3	2.19	0.43
1:0:23:G:C6	1:0:24:G:N1	2.87	0.43
1:0:1760:G:H5'	1:0:1818:C:O2'	2.17	0.43
1:0:697:G:H4'	1:0:730:G:O3'	2.18	0.43
32:I:132:CYS:O	32:I:135:LEU:N	2.49	0.43
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.78	0.43
4:A:36:ASP:C	4:A:38:ILE:N	2.71	0.43
5:B:190:MET:CE	5:B:194:PHE:CD1	3.02	0.43
4:A:206:ARG:HH11	4:A:206:ARG:HG3	1.83	0.43
8:E:133:VAL:HG12	8:E:141:VAL:HG13	2.01	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
14:L:10:SER:O	14:L:11:ARG:HB3	2.19	0.43
1:0:522:U:O2'	1:0:1366:C:H5'	2.18	0.43
9:F:101:ALA:HA	39:F:5413:HOH:O	2.18	0.43
1:0:294:C:H2'	1:0:295:C:O4'	2.19	0.43
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.18	0.43
23:U:47:ARG:HG3	39:U:4381:HOH:O	2.18	0.43
1:0:2408:A:H4'	31:3:15:ASN:O	2.19	0.43
13:K:20:CYS:HB2	13:K:29:LEU:HG	2.01	0.43
24:V:11:MET:HB3	24:V:15:GLU:HB2	2.00	0.43
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.48	0.43
2:9:3044:A:O4'	7:D:76:ARG:NE	2.52	0.43
1:0:2072:G:N2	39:0:7359:HOH:O	2.52	0.43
30:2:19:SER:O	30:2:36:ASN:ND2	2.52	0.43
1:0:263:U:C2	9:F:59:ILE:HD12	2.54	0.43
5:B:146:THR:C	5:B:148:PRO:HD3	2.39	0.43
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.49	0.43
1:0:999:C:H2'	1:0:1000:C:O4'	2.19	0.43
5:B:171:VAL:HG23	5:B:172:SER:H	1.84	0.43
16:N:93:GLN:HE21	16:N:127:LEU:CD1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:C5'	2.36	0.42
1:0:2720:C:O2	13:K:87:ARG:NH2	2.52	0.42
20:R:61:GLN:NE2	39:R:9452:HOH:O	2.52	0.42
1:0:1473:U:O2'	1:0:1474:C:H5"	2.19	0.42
29:1:18:LYS:HD3	30:2:10:ARG:HD3	2.01	0.42
4:A:105:VAL:CG1	4:A:106:CYS:N	2.82	0.42
1:0:1163:G:H1	1:0:1184:C:N4	2.17	0.42
1:0:1185:U:H5'	39:0:7928:HOH:O	2.19	0.42
12:J:45:VAL:CG2	12:J:129:PHE:HD1	2.32	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.49	0.42
1:0:1236:A:C8	12:J:63:ILE:HD11	2.54	0.42
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.34	0.42
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.49	0.42
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.99	0.42
20:R:119:VAL:CG1	20:R:119:VAL:O	2.66	0.42
1:0:2690:U:H4'	8:E:111:LYS:HE3	2.01	0.42
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.49	0.42
15:M:159:VAL:HG13	15:M:160:PHE:N	2.34	0.42
1:0:2365:G:H4'	19:Q:45:PRO:O	2.19	0.42
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.42
1:0:2379:G:N3	1:0:2418:G:H2'	2.33	0.42
2:9:3045:A:H4'	7:D:143:LYS:O	2.19	0.42
20:R:69:LYS:HB2	20:R:72:VAL:HG23	2.01	0.42
15:M:64:ARG:HD2	39:M:9392:HOH:O	2.19	0.42
1:0:370:G:O2'	1:0:371:U:H5'	2.19	0.42
8:E:36:PRO:HD3	12:J:127:ILE:CD1	2.43	0.42
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.18	0.42
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.48	0.42
24:V:39:ALA:O	24:V:41:GLU:N	2.47	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
12:J:107:ASN:HD22	12:J:107:ASN:C	2.23	0.42
1:0:138:U:OP2	1:0:139:C:H5	2.02	0.42
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	1.99	0.42
1:0:1044:C:H3'	1:0:1045:G:H5"	2.00	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.72	0.42
8:E:81:GLU:HG2	8:E:134:SER:CB	2.50	0.42
16:N:89:GLY:O	16:N:92:ALA:HB3	2.19	0.42
1:0:1797:A:H2'	1:0:1799:G:O5'	2.19	0.42
1:0:359:U:H3'	39:0:6300:HOH:O	2.18	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.48	0.42
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.42
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.94	0.42
1:0:2032:U:C2'	1:0:2033:G:H5"	2.49	0.42
17:O:29:VAL:HG11	17:O:98:LEU:HD21	2.00	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.42
10:G:63:ARG:HB2	10:G:66:LEU:HG	2.01	0.42
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.42
1:0:645:U:OP2	14:L:4:LYS:HE2	2.19	0.42
1:0:2374:A:H2'	1:0:2375:G:C8	2.54	0.42
25:W:59:GLN:NE2	25:W:97:ALA:HB3	2.34	0.42
6:C:33:LYS:HE2	39:C:9162:HOH:O	2.19	0.42
1:0:21:G:C5'	20:R:2:ILE:HA	2.32	0.42
16:N:110:THR:HB	16:N:113:SER:HG	1.82	0.42
1:0:1162:G:H1'	32:I:117:LEU:CD1	2.46	0.42
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.07	0.42
1:0:903:U:O4	14:L:18:HIS:HB2	2.19	0.42
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.49	0.42
1:0:2820:A:OP1	5:B:98:THR:HG22	2.20	0.42
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.42
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.83	0.42
5:B:321:PRO:HA	39:B:9650:HOH:O	2.18	0.42
1:0:2587:OMU:H2'	1:0:2589:U:H5"	2.00	0.42
1:0:2679:G:H2'	1:0:2681:A:OP2	2.19	0.42
1:0:941:G:C5	1:0:942:U:C4	3.08	0.42
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.49	0.42
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.43	0.42
19:Q:47:VAL:HB	19:Q:90:HIS:CE1	2.55	0.42
1:0:2314:G:C2'	1:0:2315:C:H5'	2.49	0.42
7:D:99:ASP:HB2	7:D:103:ASN:N	2.29	0.42
1:0:1739:G:H1'	1:0:2726:U:O4	2.19	0.42
4:A:223:ARG:CZ	39:A:9561:HOH:O	2.68	0.42
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.49	0.42
13:K:22:ASP:O	13:K:110:LYS:HE3	2.19	0.42
1:0:1020:A:H2'	1:0:1021:G:C8	2.55	0.42
1:0:2784:A:H1'	8:E:60:SER:OG	2.19	0.42
1:0:1714:C:O2'	1:0:1715:C:H5'	2.19	0.42
20:R:82:GLU:O	20:R:86:LYS:HG3	2.20	0.42
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.50	0.42
31:3:48:ASN:ND2	31:3:50:GLY:H	2.18	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:41:PHE:CB	5:B:190:MET:HE3	2.49	0.42
9:F:99:THR:HG23	9:F:99:THR:O	2.20	0.42
1:0:664:U:O4	1:0:681:G:H5"	2.19	0.42
4:A:65:ARG:C	4:A:66:ARG:HG3	2.40	0.42
31:3:16:GLU:HG3	31:3:18:GLN:NE2	2.35	0.42
22:T:48:VAL:HG21	22:T:96:VAL:CG1	2.49	0.42
6:C:153:VAL:O	6:C:157:LEU:HG	2.20	0.42
3:4:74:DCZ:C2'	3:4:75:DC:H5'	2.49	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.02	0.42
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.01	0.42
13:K:113:ILE:HG22	13:K:114:ALA:N	2.34	0.42
32:I:98:ALA:O	32:I:137:VAL:HA	2.19	0.42
1:0:1117:A:C2	1:0:1244:U:C2	3.07	0.42
7:D:57:THR:HG23	7:D:63:ILE:HG22	2.02	0.42
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.49	0.42
4:A:36:ASP:HB2	4:A:83:GLY:CA	2.49	0.42
4:A:179:MET:HG2	4:A:186:TRP:HB2	2.01	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.35	0.42
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.55	0.42
1:0:2898:G:H4'	5:B:288:GLY:HA2	2.01	0.42
1:0:401:C:O2'	15:M:92:THR:HB	2.19	0.42
1:0:1311:G:O6	6:C:173:LYS:HE3	2.19	0.42
2:9:3057:A:H8	7:D:141:VAL:HG21	1.85	0.42
25:W:4:LEU:CD1	25:W:24:LEU:HD13	2.50	0.42
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.40	0.42
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.50	0.42
30:2:20:ARG:CG	30:2:21:VAL:N	2.83	0.42
1:0:2748:G:H4'	1:0:2749:U:H5'	2.01	0.42
1:0:1165:G:O2'	1:0:1174:A:H1'	2.20	0.42
1:0:2547:C:OP2	5:B:5:ARG:NH1	2.53	0.42
1:0:1086:A:C6	25:W:11:VAL:HG11	2.55	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
5:B:280:VAL:HG13	5:B:333:GLU:O	2.19	0.42
1:0:1203:G:O2'	1:0:1204:C:H5'	2.19	0.42
1:0:424:C:H2'	1:0:425:U:C6	2.54	0.42
5:B:294:TYR:HE2	39:B:9644:HOH:O	2.02	0.42
32:I:139:ILE:CG2	32:I:140:GLU:N	2.83	0.42
32:I:79:ILE:HG23	32:I:100:LEU:HD11	2.02	0.42
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	2.02	0.42
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.55	0.42
15:M:107:ARG:CG	15:M:107:ARG:NH1	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:559:U:H2'	1:0:560:C:O4'	2.20	0.42
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.53	0.42
12:J:107:ASN:ND2	12:J:109:TYR:H	2.18	0.42
5:B:277:GLU:N	5:B:278:PRO:CD	2.83	0.42
1:0:2511:A:H2'	1:0:2512:U:O4'	2.20	0.42
1:0:2894:C:O2'	1:0:2895:C:H5'	2.19	0.42
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.51	0.42
1:0:130:C:H2'	39:0:3760:HOH:O	2.19	0.42
1:0:2351:C:H2'	1:0:2352:G:O4'	2.19	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.84	0.42
7:D:60:GLU:O	7:D:61:PHE:C	2.58	0.42
11:H:30:GLN:N	11:H:66:ARG:NH1	2.68	0.42
1:0:12:U:C2'	1:0:13:G:H5'	2.49	0.42
1:0:441:A:H8	1:0:441:A:O5'	2.03	0.42
1:0:2645:U:H1'	39:0:9923:HOH:O	2.19	0.42
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.42
21:S:37:VAL:O	21:S:41:VAL:HG23	2.19	0.42
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.55	0.42
1:0:1482:A:O2'	1:0:1483:C:H5'	2.20	0.42
1:0:1594:C:O2'	1:0:1607:A:H4'	2.19	0.42
14:L:36:ASP:HB2	39:L:9429:HOH:O	2.18	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
1:0:907:A:H2'	1:0:908:A:C8	2.54	0.42
2:9:3076:G:H3'	2:9:3077:A:C5'	2.31	0.41
1:0:1972:U:C2'	1:0:1973:A:H5"	2.50	0.41
2:9:3042:C:H5'	2:9:3043:G:OP2	2.20	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.85	0.41
17:O:26:TRP:N	39:O:3062:HOH:O	2.53	0.41
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.20	0.41
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.53	0.41
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.55	0.41
9:F:117:GLU:C	9:F:119:ARG:N	2.73	0.41
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.50	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.49	0.41
25:W:45:VAL:HG23	25:W:46:ALA:N	2.35	0.41
39:0:4982:HOH:O	4:A:11:ARG:CZ	2.68	0.41
1:0:157:G:H4'	15:M:95:LYS:HE2	2.00	0.41
1:0:2011:A:H4'	1:0:2012:U:O5'	2.20	0.41
26:X:80:GLU:HG2	26:X:80:GLU:O	2.20	0.41
5:B:255:GLY:O	5:B:257:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:75:THR:HG22	32:I:79:ILE:CD1	2.51	0.41
4:A:192:VAL:HG13	39:A:9547:HOH:O	2.19	0.41
7:D:136:ARG:HB3	7:D:137:PRO:HD2	2.01	0.41
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.19	0.41
2:9:3008:G:OP1	16:N:23:ARG:NH1	2.53	0.41
25:W:38:THR:O	25:W:42:ARG:HB2	2.20	0.41
18:P:16:VAL:CG1	18:P:17:GLY:N	2.82	0.41
6:C:133:ARG:HE	6:C:138:VAL:HG22	1.84	0.41
1:0:1947:G:H2'	1:0:1948:G:C8	2.55	0.41
16:N:39:SER:HB3	16:N:42:HIS:H	1.85	0.41
1:0:1741:U:H3'	39:0:3376:HOH:O	2.18	0.41
24:V:43:PRO:O	24:V:46:ILE:HG22	2.20	0.41
1:0:2065:C:O2'	1:0:2066:C:H5'	2.20	0.41
1:0:816:G:H5'	1:0:1598:A:H4'	2.01	0.41
1:0:415:A:O2'	1:0:416:G:H5'	2.21	0.41
10:G:27:ILE:HD13	10:G:71:LEU:HD23	2.02	0.41
1:0:1613:C:H2'	1:0:1614:G:O4'	2.19	0.41
1:0:1076:G:C2	1:0:1084:C:C2	3.08	0.41
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.02	0.41
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.52	0.41
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.35	0.41
7:D:76:ARG:O	7:D:77:ASP:HB2	2.21	0.41
4:A:103:VAL:O	4:A:105:VAL:HG23	2.20	0.41
4:A:69:LEU:HD23	4:A:107:ASN:CG	2.40	0.41
23:U:52:THR:HG22	23:U:55:ALA:H	1.85	0.41
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.56	0.41
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.56	0.41
11:H:83:TYR:C	11:H:83:TYR:CD1	2.93	0.41
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.19	0.41
39:0:6253:HOH:O	13:K:87:ARG:CZ	2.68	0.41
13:K:98:VAL:HG11	13:K:102:GLU:HA	2.02	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
2:9:3092:G:H2'	2:9:3093:A:C8	2.55	0.41
1:0:1149:U:H5"	1:0:1151:G:O4'	2.19	0.41
1:0:56:G:H5"	24:V:50:ARG:NH1	2.35	0.41
12:J:64:GLY:HA3	36:J:9321:CL:CL	2.57	0.41
19:Q:59:GLN:HB3	39:Q:6286:HOH:O	2.20	0.41
31:3:62:THR:HB	39:3:9483:HOH:O	2.20	0.41
1:0:1432:U:H5'	39:0:9820:HOH:O	2.20	0.41
1:0:1099:G:H2'	1:0:1100:G:O4'	2.21	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3107:C:H5	39:9:3167:HOH:O	2.03	0.41
24:V:1:THR:O	24:V:2:VAL:C	2.58	0.41
25:W:108:ARG:CG	25:W:114:PRO:HG3	2.43	0.41
12:J:107:ASN:HD22	12:J:109:TYR:H	1.68	0.41
7:D:172:VAL:CG1	7:D:173:GLU:N	2.82	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.20	0.41
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.55	0.41
1:0:297:U:H1'	39:0:4524:HOH:O	2.20	0.41
1:0:1733:A:H4'	5:B:212:GLN:HA	2.02	0.41
6:C:104:ASP:CA	6:C:107:ARG:HH12	2.12	0.41
15:M:167:GLY:O	15:M:171:ARG:HG3	2.20	0.41
1:0:870:G:C3'	1:0:871:G:H5"	2.51	0.41
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.21	0.41
16:N:38:LYS:HB2	16:N:38:LYS:HE3	1.80	0.41
4:A:36:ASP:O	4:A:36:ASP:OD1	2.38	0.41
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	2.02	0.41
1:0:1555:G:H4'	1:0:1630:A:C2	2.54	0.41
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.03	0.41
1:0:2819:C:O4'	5:B:96:PRO:HB2	2.19	0.41
1:0:2326:U:H4'	1:0:2412:G:H4'	2.02	0.41
5:B:139:ASP:HB3	39:B:9550:HOH:O	2.21	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
7:D:128:LEU:C	7:D:128:LEU:HD23	2.41	0.41
1:0:330:C:H5	6:C:170:ASP:OD2	2.04	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.41
1:0:1909:A:N1	1:0:2128:G:H1'	2.36	0.41
5:B:60:SER:HA	5:B:61:PRO:HD3	1.92	0.41
16:N:67:ALA:C	16:N:69:TYR:H	2.23	0.41
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.55	0.41
1:0:2072:G:C6	1:0:2533:C:H1'	2.56	0.41
20:R:113:HIS:O	20:R:145:LEU:HD12	2.21	0.41
6:C:133:ARG:NE	6:C:135:GLU:O	2.53	0.41
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.21	0.41
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.84	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.77	0.41
4:A:217:ARG:HG3	39:A:9520:HOH:O	2.19	0.41
1:0:2504:A:H2'	1:0:2505:G:O4'	2.21	0.41
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.56	0.41
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.04	0.41
32:I:128:VAL:C	32:I:130:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:93:LYS:O	6:C:98:ARG:NH2	2.54	0.41
1:0:371:U:H2'	1:0:372:A:H8	1.86	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.86	0.41
1:0:889:C:H2'	1:0:890:C:C6	2.56	0.41
28:Z:49:ARG:HB2	28:Z:55:TRP:CZ3	2.56	0.41
16:N:37:ARG:NH2	16:N:105:GLY:HA3	2.35	0.41
8:E:69:ILE:HA	8:E:72:MET:HE3	2.02	0.41
4:A:55:VAL:HG12	4:A:67:LEU:HD22	2.02	0.41
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.84	0.41
1:0:2748:G:H4'	1:0:2749:U:C5'	2.50	0.41
15:M:80:GLY:O	15:M:81:ARG:CD	2.66	0.41
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.85	0.41
1:0:396:U:O2'	1:0:418:C:C4'	2.68	0.41
8:E:11:VAL:HG13	8:E:23:GLU:O	2.20	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.91	0.41
32:I:92:PRO:C	32:I:94:GLU:N	2.73	0.41
6:C:133:ARG:HG3	6:C:133:ARG:HH11	1.85	0.41
9:F:52:GLU:HG3	9:F:77:VAL:O	2.21	0.41
8:E:108:LEU:CD1	8:E:164:ASP:HB2	2.51	0.41
22:T:48:VAL:HG21	22:T:96:VAL:HG13	2.02	0.41
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.56	0.41
1:0:2365:G:H5"	39:Q:6597:HOH:O	2.19	0.41
30:2:5:LYS:O	30:2:9:LYS:HG3	2.20	0.41
1:0:2868:C:H2'	1:0:2869:G:O4'	2.21	0.41
1:0:2102:G:H5"	1:0:2538:A:C2	2.55	0.41
1:0:1794:G:N2	1:0:1796:A:H3'	2.36	0.41
1:0:2453:G:H4'	14:L:50:GLY:C	2.41	0.41
1:0:1008:C:H5"	11:H:16:ARG:HH12	1.86	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.41	0.41
1:0:2398:A:H2'	1:0:2399:G:O4'	2.20	0.41
1:0:2857:C:H2'	1:0:2858:U:C6	2.56	0.41
7:D:167:GLU:C	7:D:169:THR:H	2.24	0.41
12:J:47:THR:CG2	12:J:48:GLY:N	2.84	0.41
30:2:48:ASP:O	30:2:49:GLU:HB2	2.21	0.41
5:B:183:GLU:O	5:B:184:ASP:C	2.60	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.94	0.41
1:0:1181:A:N1	1:0:1192:A:O2'	2.53	0.41
2:9:3001:U:H5"	2:9:3003:A:OP1	2.21	0.41
1:0:2912:C:H2'	1:0:2913:A:O4'	2.21	0.41
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.56	0.41
22:T:85:GLU:CG	22:T:86:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1257:C:H2'	1:0:1258:G:O4'	2.21	0.41
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.21	0.41
11:H:54:THR:O	11:H:55:VAL:HG13	2.20	0.41
1:0:2718:C:H5'	1:0:2718:C:C6	2.51	0.40
12:J:19:MET:HE2	12:J:79:PHE:HA	2.03	0.40
8:E:31:ARG:NH1	39:E:5919:HOH:O	2.53	0.40
20:R:145:LEU:HD12	20:R:146:ILE:N	2.36	0.40
1:0:2820:A:H2'	1:0:2821:C:O4'	2.20	0.40
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.03	0.40
26:X:10:VAL:HG12	26:X:11:THR:N	2.35	0.40
1:0:684:G:H2'	1:0:685:C:C6	2.56	0.40
5:B:112:THR:HG23	5:B:158:LYS:HE3	2.03	0.40
25:W:13:MET:CE	25:W:18:GLN:HA	2.43	0.40
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.40
7:D:65:GLU:HA	39:D:6752:HOH:O	2.21	0.40
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.50	0.40
1:0:2243:C:H5"	39:0:4344:HOH:O	2.22	0.40
4:A:97:ALA:HB2	4:A:150:PRO:HB2	2.03	0.40
11:H:29:ALA:C	11:H:30:GLN:HG3	2.42	0.40
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.56	0.40
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.51	0.40
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.20	0.40
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.48	0.40
25:W:38:THR:CG2	25:W:39:ASP:N	2.84	0.40
25:W:149:LEU:HG	25:W:153:MET:HE1	2.03	0.40
16:N:183:ASP:O	16:N:184:ILE:C	2.59	0.40
1:0:1873:G:H2'	1:0:1874:U:H5'	2.03	0.40
1:0:881:C:H5"	39:0:4234:HOH:O	2.20	0.40
1:0:561:G:O2'	1:0:562:A:H5'	2.21	0.40
1:0:2509:A:H2'	1:0:2510:C:O4'	2.21	0.40
13:K:115:ARG:O	13:K:118:ALA:HB3	2.21	0.40
15:M:59:GLY:C	15:M:141:ILE:HD11	2.41	0.40
4:A:94:LEU:HD12	4:A:98:GLU:HB2	2.02	0.40
13:K:125:ALA:O	13:K:127:ALA:N	2.54	0.40
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.20	0.40
39:0:6200:HOH:O	22:T:68:ASP:HB2	2.20	0.40
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.22	0.40
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.22	0.40
1:0:2445:U:H2'	1:0:2446:G:C8	2.56	0.40
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.86	0.40
1:0:1706:G:OP1	18:P:65:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2507:G:H2'	1:0:2510:C:N4	2.33	0.40
7:D:27:ILE:HG22	7:D:28:GLY:N	2.35	0.40
7:D:57:THR:HG23	7:D:63:ILE:CA	2.41	0.40
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.69	0.40
17:O:23:GLY:C	39:O:3062:HOH:O	2.60	0.40
14:L:6:ARG:NH2	39:L:9441:HOH:O	2.53	0.40
29:1:28:HIS:HD2	29:1:30:LYS:H	1.69	0.40
1:0:1015:C:H2'	1:0:1016:U:C6	2.56	0.40
1:0:1679:C:H5'	39:0:9941:HOH:O	2.22	0.40
1:0:694:A:H2'	1:0:695:C:H5'	2.03	0.40
4:A:171:LYS:NZ	39:A:9514:HOH:O	2.45	0.40
4:A:173:GLY:O	4:A:176:HIS:HB3	2.21	0.40
6:C:124:VAL:HA	6:C:230:GLY:O	2.22	0.40
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.86	0.40
1:0:1386:G:O2'	1:0:1387:G:H5'	2.22	0.40
1:0:2283:G:C6	11:H:113:MET:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	235/240 (98%)	212 (90%)	19 (8%)	4 (2%)	11 6
5	B	335/338 (99%)	316 (94%)	16 (5%)	3 (1%)	21 18
6	C	244/246 (99%)	224 (92%)	20 (8%)	0	100 100
7	D	134/177 (76%)	108 (81%)	14 (10%)	12 (9%)	1 0
8	E	170/178 (96%)	166 (98%)	4 (2%)	0	100 100
9	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	11 6
10	G	25/348 (7%)	25 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	H	156/171 (91%)	143 (92%)	11 (7%)	2 (1%)	15 10
12	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	14 9
13	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	24 21
14	L	141/165 (86%)	123 (87%)	17 (12%)	1 (1%)	26 26
15	M	192/195 (98%)	183 (95%)	9 (5%)	0	100 100
16	N	184/187 (98%)	165 (90%)	13 (7%)	6 (3%)	5 2
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100 100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100 100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
20	R	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	26 26
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100 100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	21 18
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100 100
24	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	5 2
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100 100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100 100
27	Y	140/241 (58%)	140 (100%)	0	0	100 100
28	Z	71/83 (86%)	59 (83%)	8 (11%)	4 (6%)	2 0
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%)	89 (99%)	0	1 (1%)	17 13
32	I	68/162 (42%)	53 (78%)	14 (21%)	1 (2%)	13 8
All	All	3705/4431 (84%)	3451 (93%)	211 (6%)	43 (1%)	16 11

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	166	SER
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
4	A	37	VAL

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Mol	Chain	Res	Type
5	B	34	GLY
5	B	169	GLY
7	D	27	ILE
7	D	60	GLU
7	D	137	PRO
7	D	171	ASP
7	D	173	GLU
9	F	101	ALA
11	H	168	ALA
12	J	143	LYS
4	A	132	ASP
5	B	185	GLY
7	D	16	PRO
7	D	28	GLY
7	D	56	ARG
12	J	5	GLU
13	K	126	SER
16	N	164	ASP
16	N	167	ASP
16	N	183	ASP
22	T	53	GLY
24	V	43	PRO
7	D	65	GLU
7	D	97	GLN
28	Z	20	ARG
28	Z	43	GLY
7	D	61	PHE
16	N	155	GLU
4	A	236	GLY
9	F	71	GLY
31	3	56	PRO
32	I	129	VAL
24	V	2	VAL
28	Z	21	VAL
7	D	138	GLY
20	R	81	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	26	27
5	B	282/283 (100%)	261 (93%)	21 (7%)	17	16
6	C	193/193 (100%)	177 (92%)	16 (8%)	14	12
7	D	117/148 (79%)	112 (96%)	5 (4%)	35	41
8	E	152/156 (97%)	148 (97%)	4 (3%)	54	65
9	F	93/94 (99%)	92 (99%)	1 (1%)	80	88
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	127 (96%)	5 (4%)	40	49
12	J	118/121 (98%)	111 (94%)	7 (6%)	24	24
13	K	106/106 (100%)	102 (96%)	4 (4%)	40	49
14	L	113/127 (89%)	109 (96%)	4 (4%)	43	53
15	M	158/159 (99%)	153 (97%)	5 (3%)	46	57
16	N	149/150 (99%)	145 (97%)	4 (3%)	52	63
17	O	93/94 (99%)	92 (99%)	1 (1%)	80	88
18	P	113/117 (97%)	111 (98%)	2 (2%)	66	77
19	Q	79/80 (99%)	76 (96%)	3 (4%)	40	49
20	R	117/122 (96%)	114 (97%)	3 (3%)	54	65
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	40	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	63	73
25	W	130/130 (100%)	126 (97%)	4 (3%)	47	58
26	X	66/74 (89%)	62 (94%)	4 (6%)	23	23
27	Y	120/196 (61%)	108 (90%)	12 (10%)	9	7
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	60	70
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	67
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2971 (96%)	122 (4%)	39	48

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	26	ASP
4	A	33	GLU
4	A	36	ASP
4	A	78	ASP
4	A	94	LEU
4	A	131	HIS
4	A	165	THR
4	A	179	MET
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	28	SER
5	B	33	ASP
5	B	53	LEU
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	190	MET
5	B	195	ARG
5	B	234	ARG
5	B	254	GLN
5	B	257	THR
5	B	265	LEU
5	B	277	GLU
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	202	THR
6	C	214	THR

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Mol	Chain	Res	Type
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	133	ASN
8	E	15	GLN
8	E	102	VAL
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
11	H	84	LYS
11	H	88	ARG
11	H	154	TYR
11	H	159	PRO
11	H	170	ASN
12	J	46	ILE
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
13	K	4	LEU
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	104	ASP
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	26	LEU
16	N	37	ARG

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Mol	Chain	Res	Type
16	N	127	LEU
16	N	139	TRP
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	35	VAL
25	W	76	ASP
25	W	142	ASP
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	72	VAL
26	X	79	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
29	1	47	ASP
30	2	18	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	199	HIS
5	B	27	ASN
5	B	94	GLN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
6	C	163	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	58	GLN
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN

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Mol	Chain	Res	Type
16	N	107	ASN
17	O	100	GLN
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	53	ASN
22	T	7	GLN
22	T	37	GLN
22	T	39	ASN
22	T	43	ASN
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	27	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	119	GLN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	36	ASN

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Mol	Chain	Res	Type
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	232 (8%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	246 (8%)	35 (1%)

All (246) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	21	G
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U

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Mol	Chain	Res	Type
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	735	C
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	846	A

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Mol	Chain	Res	Type
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	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	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
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	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C

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Mol	Chain	Res	Type
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A

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Mol	Chain	Res	Type
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C

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Mol	Chain	Res	Type
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	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2840	A
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G

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Mol	Chain	Res	Type
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1351	G
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C

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Mol	Chain	Res	Type
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2852	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMU	0	2587	1	12,22,23	1.03	2 (16%)	19,31,34	3.13	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.06	1 (5%)	21,38,41	2.54	3 (14%)
1	UR3	0	2619	1	12,22,23	0.93	1 (8%)	16,32,35	0.73	0
1	PSU	0	2621	1	13,21,22	1.65	2 (15%)	18,30,33	6.08	3 (16%)
1	1MA	0	628	1,35	14,25,26	0.93	1 (7%)	15,37,40	1.15	1 (6%)
3	PPU	4	76	1,3	16,26,41	0.70	0	15,38,60	1.23	1 (6%)
3	HFA	4	77	3	11,11,12	1.08	1 (9%)	13,13,15	1.06	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.81	1.48	1.52
1	0	2619	UR3	C6-C5	-2.05	1.33	1.38
1	0	2587	OMU	C6-C5	-2.05	1.33	1.38
1	0	2587	OMU	C4-N3	2.30	1.37	1.33
1	0	628	1MA	C6-N6	2.53	1.33	1.29
1	0	2621	PSU	C4-N3	2.82	1.38	1.33
3	4	77	HFA	OA-CA	2.90	1.49	1.43
1	0	2588	OMG	C6-N1	3.13	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	N1-C2-N3	-21.28	114.75	128.33
1	0	2588	OMG	C5-C6-N1	-8.77	111.59	123.59
1	0	628	1MA	C2-N3-C4	-3.57	110.88	116.40
1	0	2587	OMU	C5-C4-N3	-3.23	114.84	123.12
3	4	77	HFA	CB-CA-C	-2.66	106.71	111.70
1	0	2588	OMG	N3-C2-N1	-2.32	123.92	127.44
1	0	2621	PSU	C6-N1-C2	2.64	119.72	115.47
3	4	76	PPU	C2-N1-C6	3.50	118.89	111.43
1	0	2588	OMG	C6-N1-C2	6.68	125.21	115.94
1	0	2587	OMU	C4-N3-C2	12.96	126.97	114.14
1	0	2621	PSU	C4-N3-C2	13.88	127.24	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	1	0
3	4	77	HFA	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 313 ligands modelled in this entry, 313 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.04	136 (4%) 33 36	23, 45, 88, 147	0
2	9	122/122 (100%)	0.45	7 (5%) 27 30	40, 63, 89, 149	0
3	4	4/8 (50%)	-0.23	0 100 100	40, 45, 47, 48	0
4	A	237/240 (98%)	0.41	14 (5%) 26 28	27, 48, 83, 102	0
5	B	337/338 (99%)	0.26	12 (3%) 46 50	27, 50, 76, 88	0
6	C	246/246 (100%)	0.11	4 (1%) 74 77	24, 45, 68, 79	0
7	D	140/177 (79%)	1.88	45 (32%) 1 0	55, 93, 121, 129	0
8	E	172/178 (96%)	0.46	15 (8%) 13 14	41, 63, 83, 88	0
9	F	119/120 (99%)	0.79	15 (12%) 5 5	46, 69, 94, 106	0
10	G	29/348 (8%)	2.81	19 (65%) 0 0	67, 89, 97, 100	0
11	H	160/171 (93%)	0.56	24 (15%) 3 3	40, 58, 91, 98	0
12	J	142/145 (97%)	0.11	5 (3%) 48 52	34, 47, 69, 90	0
13	K	132/132 (100%)	0.07	4 (3%) 54 58	33, 44, 68, 78	0
14	L	145/165 (87%)	0.67	16 (11%) 7 7	26, 62, 107, 117	0
15	M	194/195 (99%)	0.33	6 (3%) 52 57	32, 44, 60, 69	0
16	N	186/187 (99%)	1.02	38 (20%) 1 1	44, 61, 107, 115	0
17	O	115/116 (99%)	0.30	4 (3%) 48 52	38, 53, 68, 77	0
18	P	143/149 (95%)	0.38	6 (4%) 40 44	36, 50, 63, 75	0
19	Q	95/96 (98%)	0.00	2 (2%) 67 71	37, 46, 61, 72	0
20	R	150/155 (96%)	-0.03	2 (1%) 79 82	30, 43, 62, 71	0
21	S	81/85 (95%)	0.46	6 (7%) 17 18	39, 55, 75, 90	0
22	T	119/120 (99%)	0.74	13 (10%) 7 7	39, 53, 79, 104	0
23	U	53/66 (80%)	0.32	2 (3%) 44 48	40, 50, 69, 78	0
24	V	65/71 (91%)	2.03	20 (30%) 1 0	52, 72, 109, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	0.33	7 (4%) 37 41	37, 49, 69, 78	0
26	X	82/92 (89%)	0.62	9 (10%) 7 7	39, 54, 81, 98	0
27	Y	142/241 (58%)	0.04	8 (5%) 28 31	28, 42, 64, 84	0
28	Z	73/83 (87%)	0.89	15 (20%) 1 1	46, 63, 80, 91	0
29	1	56/57 (98%)	-0.16	0 100 100	28, 33, 40, 48	0
30	2	46/50 (92%)	1.55	12 (26%) 1 1	34, 60, 89, 96	0
31	3	92/92 (100%)	0.29	4 (4%) 39 43	34, 54, 68, 80	0
32	I	70/162 (43%)	6.56	64 (91%) 0 0	105, 117, 137, 138	0
All	All	6650/7483 (88%)	0.34	534 (8%) 15 16	23, 50, 95, 149	0

All (534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	88	GLY	22.9
32	I	71	GLY	18.9
24	V	1	THR	18.8
32	I	133	THR	17.8
32	I	96	PHE	17.4
16	N	166	ALA	16.7
7	D	63	ILE	15.2
32	I	85	PHE	14.0
22	T	119	ALA	12.6
32	I	137	VAL	12.3
7	D	57	THR	12.0
32	I	79	ILE	11.7
32	I	109	ALA	11.2
2	9	3001	U	11.2
32	I	76	ALA	10.9
24	V	39	ALA	10.7
32	I	105	VAL	10.5
32	I	102	VAL	9.9
32	I	91	GLU	9.7
32	I	87	THR	9.6
32	I	93	GLN	9.0
22	T	118	SER	9.0
24	V	40	PRO	9.0
32	I	89	SER	8.8
32	I	121	LEU	8.6
7	D	61	PHE	8.4

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Mol	Chain	Res	Type	RSRZ
32	I	113	HIS	8.3
32	I	136	GLY	8.3
32	I	75	THR	8.3
1	0	497	A	8.0
32	I	118	SER	7.7
32	I	81	ASP	7.7
32	I	129	VAL	7.7
1	0	1951	G	7.6
32	I	77	GLU	7.6
1	0	1199	A	7.5
32	I	97	VAL	7.4
32	I	98	ALA	7.3
30	2	49	GLU	7.3
32	I	138	THR	7.2
32	I	86	GLU	7.2
32	I	83	ALA	7.1
4	A	237	GLY	7.0
32	I	94	GLU	7.0
24	V	43	PRO	6.9
21	S	81	ILE	6.8
1	0	1177	A	6.8
7	D	11	HIS	6.7
1	0	282	C	6.6
16	N	165	ALA	6.5
10	G	23	ILE	6.5
22	T	116	ASP	6.4
32	I	132	CYS	6.4
1	0	999	C	6.4
32	I	78	LEU	6.4
1	0	2769	C	6.4
4	A	37	VAL	6.3
32	I	104	GLN	6.3
32	I	116	LEU	6.3
1	0	1173	A	6.3
2	9	3002	U	6.2
32	I	114	PRO	6.2
16	N	155	GLU	6.2
1	0	735	C	6.1
1	0	272	A	6.1
26	X	88	GLU	6.1
28	Z	11	SER	6.0
10	G	26	MET	6.0

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Mol	Chain	Res	Type	RSRZ
1	0	736	A	5.9
30	2	27	LEU	5.9
1	0	2508	C	5.9
26	X	80	GLU	5.8
8	E	45	ASP	5.8
32	I	103	ASP	5.7
32	I	107	GLN	5.7
32	I	111	GLN	5.7
30	2	44	ARG	5.7
1	0	1525	G	5.7
32	I	95	ASP	5.6
24	V	41	GLU	5.6
32	I	126	LYS	5.6
32	I	108	ILE	5.6
1	0	2004	U	5.5
1	0	970	U	5.5
1	0	2645	U	5.5
22	T	82	THR	5.5
1	0	2237	G	5.4
7	D	107	GLY	5.4
30	2	39	ARG	5.4
24	V	38	GLY	5.3
1	0	1172	G	5.3
2	9	3024	U	5.2
32	I	99	ASP	5.1
7	D	170	TYR	5.1
7	D	90	LEU	5.1
1	0	1202	A	5.1
32	I	122	THR	5.1
1	0	280	C	5.1
1	0	288	A	5.0
1	0	1198	U	5.0
1	0	2238	A	5.0
10	G	71	LEU	5.0
32	I	90	GLY	5.0
1	0	2511	A	5.0
1	0	1196	C	5.0
1	0	1965	C	5.0
22	T	117	ASP	4.9
7	D	10	PHE	4.9
1	0	1200	A	4.9
14	L	75	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
7	D	62	ASP	4.8
5	B	1	PRO	4.8
32	I	125	ALA	4.8
2	9	3023	U	4.7
32	I	80	LYS	4.7
7	D	92	GLU	4.7
1	0	960	G	4.6
9	F	117	GLU	4.6
24	V	45	ARG	4.6
1	0	1169	U	4.6
1	0	1171	A	4.6
1	0	10	U	4.5
24	V	37	GLY	4.5
1	0	358	G	4.4
7	D	40	ILE	4.4
10	G	24	VAL	4.4
10	G	27	ILE	4.4
23	U	47	ARG	4.3
32	I	119	TYR	4.3
1	0	285	A	4.3
16	N	154	LEU	4.3
10	G	73	ASP	4.3
1	0	1175	G	4.2
32	I	74	PRO	4.2
26	X	77	PHE	4.2
7	D	66	GLY	4.2
8	E	10	ASP	4.2
6	C	61	PHE	4.2
14	L	91	VAL	4.2
16	N	68	GLU	4.2
1	0	1197	G	4.2
1	0	1176	C	4.2
2	9	3122	C	4.1
7	D	64	ARG	4.1
10	G	69	ARG	4.1
1	0	1948	G	4.1
9	F	25	ASP	4.1
7	D	56	ARG	4.1
19	Q	95	GLU	4.1
32	I	92	PRO	4.1
1	0	1195	G	4.0
16	N	183	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
11	H	37	GLN	4.0
16	N	134	ASP	4.0
1	0	1179	C	4.0
7	D	69	ILE	4.0
4	A	31	LYS	4.0
10	G	22	ALA	4.0
24	V	36	ALA	3.9
27	Y	235	GLU	3.9
9	F	22	VAL	3.9
14	L	81	VAL	3.9
9	F	106	ALA	3.9
1	0	365	G	3.9
12	J	70	PHE	3.9
4	A	35	GLY	3.9
28	Z	20	ARG	3.8
14	L	80	ASP	3.8
30	2	37	HIS	3.8
1	0	1168	C	3.8
32	I	120	ASP	3.8
16	N	185	GLU	3.8
1	0	1206	U	3.8
26	X	85	VAL	3.8
4	A	236	GLY	3.8
22	T	115	GLU	3.8
10	G	25	GLU	3.7
14	L	76	LEU	3.7
1	0	1950	G	3.7
1	0	284	C	3.7
7	D	85	GLN	3.7
1	0	1966	U	3.7
1	0	1203	G	3.7
16	N	37	ARG	3.7
1	0	2344	G	3.7
9	F	119	ARG	3.7
1	0	1178	G	3.7
1	0	2748	G	3.7
11	H	138	CYS	3.7
4	A	133	ARG	3.7
10	G	67	LEU	3.6
1	0	737	A	3.6
32	I	140	GLU	3.6
9	F	118	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
31	3	92	GLU	3.6
1	0	969	G	3.6
16	N	156	GLU	3.6
16	N	163	PHE	3.6
31	3	56	PRO	3.6
1	0	271	C	3.6
10	G	21	ASP	3.5
32	I	135	LEU	3.5
24	V	2	VAL	3.5
1	0	1625	U	3.5
16	N	39	SER	3.5
16	N	152	GLU	3.5
1	0	1192	A	3.5
1	0	1208	C	3.5
30	2	24	TRP	3.5
1	0	1170	U	3.5
16	N	43	VAL	3.4
28	Z	24	ARG	3.4
27	Y	95	THR	3.4
8	E	43	ASP	3.4
1	0	281	U	3.4
9	F	110	ASP	3.4
28	Z	22	SER	3.4
10	G	72	ASP	3.4
7	D	135	VAL	3.4
1	0	1929	G	3.4
1	0	363	A	3.4
1	0	1000	C	3.4
13	K	119	GLN	3.4
1	0	441	A	3.3
28	Z	59	TYR	3.3
28	Z	25	ARG	3.3
32	I	115	ASP	3.3
5	B	134	ALA	3.3
32	I	123	ASN	3.3
1	0	1967	U	3.3
32	I	106	LYS	3.3
1	0	283	U	3.3
1	0	514	G	3.3
1	0	289	G	3.2
1	0	716	G	3.2
25	W	86	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
11	H	171	ALA	3.2
1	0	1174	A	3.2
22	T	112	LEU	3.2
32	I	110	GLU	3.2
8	E	99	GLY	3.2
14	L	148	GLU	3.2
1	0	369	G	3.1
1	0	138	U	3.1
16	N	181	ASP	3.1
11	H	139	ASN	3.1
1	0	1201	C	3.1
11	H	143	ALA	3.1
1	0	1947	G	3.1
1	0	295	C	3.1
1	0	1181	A	3.1
7	D	73	VAL	3.1
16	N	160	SER	3.1
1	0	1165	G	3.1
16	N	184	ILE	3.0
10	G	66	LEU	3.0
16	N	76	GLY	3.0
1	0	2509	A	3.0
15	M	74	LYS	3.0
1	0	362	G	3.0
30	2	35	ARG	3.0
7	D	53	LYS	3.0
1	0	808	A	3.0
1	0	2914	A	3.0
12	J	4	ALA	3.0
7	D	173	GLU	3.0
1	0	279	C	3.0
30	2	26	MET	3.0
1	0	1279	U	3.0
7	D	68	PRO	3.0
14	L	99	GLU	3.0
21	S	76	GLU	3.0
32	I	84	GLY	3.0
30	2	23	ALA	3.0
24	V	8	ILE	3.0
1	0	2507	G	3.0
24	V	10	ASP	2.9
10	G	70	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
31	3	62	THR	2.9
14	L	102	ASP	2.9
8	E	11	VAL	2.9
27	Y	216	ARG	2.9
7	D	86	THR	2.9
30	2	48	ASP	2.9
14	L	77	ALA	2.9
11	H	111	ASP	2.9
1	0	2345	A	2.9
7	D	51	ARG	2.9
7	D	58	VAL	2.9
15	M	132	ILE	2.9
1	0	2825	C	2.9
1	0	1194	A	2.9
10	G	20	VAL	2.8
19	Q	76	VAL	2.8
7	D	134	LEU	2.8
11	H	45	VAL	2.8
4	A	36	ASP	2.8
26	X	7	GLU	2.8
1	0	1189	A	2.8
1	0	1527	A	2.8
16	N	169	PRO	2.8
11	H	35	ARG	2.8
30	2	20	ARG	2.8
7	D	166	ILE	2.8
1	0	128	A	2.8
1	0	370	G	2.8
16	N	172	PHE	2.8
32	I	139	ILE	2.8
16	N	177	GLU	2.8
8	E	100	ASP	2.8
21	S	20	PHE	2.8
7	D	38	GLU	2.8
17	O	23	GLY	2.7
7	D	157	LEU	2.7
22	T	36	GLY	2.7
28	Z	21	VAL	2.7
14	L	100	ALA	2.7
24	V	14	ALA	2.7
11	H	82	ASP	2.7
28	Z	36	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	0	2506	A	2.7
5	B	2	GLN	2.7
32	I	117	LEU	2.7
7	D	81	GLU	2.7
9	F	16	ALA	2.7
1	0	2664	A	2.7
5	B	183	GLU	2.7
7	D	88	LEU	2.7
10	G	12	ILE	2.7
8	E	87	PHE	2.7
1	0	2510	C	2.7
1	0	293	A	2.7
26	X	65	ASN	2.6
8	E	154	ILE	2.6
12	J	110	ASP	2.6
5	B	57	GLU	2.6
1	0	2335	C	2.6
8	E	42	VAL	2.6
17	O	92	VAL	2.6
7	D	44	ILE	2.6
25	W	91	ASP	2.6
8	E	6	GLU	2.6
1	0	1163	G	2.6
2	9	3073	G	2.6
15	M	70	GLY	2.6
1	0	2747	C	2.6
14	L	79	ASP	2.6
25	W	26	ILE	2.6
28	Z	44	GLU	2.6
22	T	35	TYR	2.6
4	A	208	HIS	2.6
28	Z	12	GLY	2.6
16	N	95	ALA	2.6
22	T	77	VAL	2.6
1	0	372	A	2.6
7	D	100	ASP	2.6
14	L	147	GLU	2.6
1	0	1182	C	2.6
13	K	101	ASN	2.6
1	0	1526	A	2.5
9	F	90	GLU	2.5
21	S	70	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
7	D	89	PRO	2.5
11	H	167	PRO	2.5
24	V	6	GLN	2.5
15	M	79	ALA	2.5
4	A	135	VAL	2.5
11	H	140	VAL	2.5
1	0	1981	A	2.5
26	X	71	ARG	2.5
6	C	132	ASP	2.5
18	P	114	LEU	2.5
14	L	44	GLU	2.5
7	D	93	LEU	2.5
16	N	175	LEU	2.5
16	N	164	ASP	2.5
5	B	104	GLU	2.5
32	I	82	GLU	2.5
25	W	52	VAL	2.5
32	I	72	VAL	2.5
1	0	351	G	2.5
1	0	368	C	2.5
2	9	3065	A	2.5
1	0	1964	U	2.5
28	Z	42	CYS	2.5
7	D	55	LYS	2.5
30	2	38	LYS	2.5
4	A	209	PRO	2.5
8	E	48	VAL	2.5
24	V	59	ILE	2.5
1	0	1523	G	2.5
7	D	154	LYS	2.4
32	I	101	SER	2.4
32	I	134	SER	2.4
12	J	5	GLU	2.4
27	Y	96	GLU	2.4
1	0	255	A	2.4
11	H	74	ILE	2.4
1	0	367	G	2.4
26	X	41	PHE	2.4
27	Y	98	GLN	2.4
16	N	2	THR	2.4
24	V	20	LEU	2.4
31	3	41	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
24	V	63	GLU	2.4
16	N	180	LEU	2.4
15	M	75	ARG	2.4
4	A	64	ASP	2.4
7	D	18	ILE	2.4
7	D	26	GLY	2.4
16	N	161	GLY	2.4
1	0	1522	A	2.4
1	0	2890	A	2.4
16	N	147	ILE	2.4
22	T	80	GLU	2.4
14	L	89	PHE	2.4
20	R	150	PRO	2.4
16	N	153	GLN	2.4
7	D	67	ASP	2.3
1	0	129	A	2.3
18	P	18	LYS	2.3
25	W	85	ALA	2.3
7	D	12	GLU	2.3
8	E	127	ASP	2.3
16	N	94	GLU	2.3
1	0	292	G	2.3
1	0	1919	A	2.3
11	H	47	ILE	2.3
5	B	133	GLU	2.3
28	Z	32	GLU	2.3
11	H	21	THR	2.3
8	E	7	ILE	2.3
4	A	85	SER	2.3
7	D	167	GLU	2.3
1	0	805	G	2.3
1	0	2826	G	2.3
5	B	33	ASP	2.3
1	0	2768	A	2.3
4	A	134	ASN	2.3
13	K	118	ALA	2.3
23	U	43	GLY	2.3
16	N	149	GLU	2.3
22	T	33	GLU	2.3
11	H	77	LEU	2.3
9	F	28	ALA	2.3
1	0	1180	U	2.3

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Mol	Chain	Res	Type	RSRZ
5	B	117	GLU	2.3
4	A	206	ARG	2.3
1	0	809	G	2.2
7	D	104	PHE	2.2
18	P	25	PRO	2.2
8	E	98	GLU	2.2
1	0	807	A	2.2
16	N	159	TYR	2.2
21	S	45	TYR	2.2
18	P	67	LYS	2.2
5	B	308	LEU	2.2
11	H	78	GLY	2.2
9	F	11	ASP	2.2
16	N	162	ASP	2.2
18	P	135	ALA	2.2
1	0	2770	G	2.2
1	0	1204	C	2.2
8	E	4	GLU	2.2
16	N	36	ALA	2.2
25	W	28	HIS	2.2
1	0	1524	U	2.2
1	0	1207	A	2.2
1	0	1528	A	2.2
22	T	83	ASP	2.2
7	D	43	GLU	2.2
26	X	10	VAL	2.2
9	F	100	ASP	2.2
1	0	354	A	2.2
28	Z	10	ARG	2.2
1	0	717	C	2.2
6	C	135	GLU	2.2
10	G	68	GLU	2.2
32	I	100	LEU	2.2
7	D	95	THR	2.2
12	J	46	ILE	2.1
25	W	92	ASP	2.1
14	L	130	ARG	2.1
16	N	41	LYS	2.1
13	K	132	VAL	2.1
20	R	96	VAL	2.1
11	H	24	PRO	2.1
14	L	60	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
17	O	20	SER	2.1
1	0	361	C	2.1
5	B	118	ASP	2.1
11	H	39	ASP	2.1
7	D	65	GLU	2.1
10	G	28	GLU	2.1
11	H	79	GLU	2.1
11	H	34	GLY	2.1
1	0	2512	U	2.1
1	0	296	G	2.1
9	F	15	ASP	2.1
10	G	15	TRP	2.1
15	M	54	TYR	2.1
1	0	290	C	2.1
1	0	804	C	2.1
16	N	67	ALA	2.1
16	N	40	ASN	2.1
11	H	141	GLU	2.1
11	H	162	ARG	2.1
24	V	31	ARG	2.1
11	H	42	ASP	2.1
27	Y	236	VAL	2.1
1	0	90	A	2.1
1	0	287	C	2.1
5	B	180	ASP	2.1
28	Z	45	ASP	2.1
9	F	60	VAL	2.1
27	Y	234	VAL	2.1
18	P	108	LEU	2.1
1	0	291	C	2.1
1	0	1562	C	2.1
27	Y	108	ASP	2.1
32	I	112	LYS	2.1
24	V	42	ASN	2.0
28	Z	41	ASN	2.0
11	H	168	ALA	2.0
1	0	1161	A	2.0
24	V	33	VAL	2.0
21	S	78	ALA	2.0
1	0	294	C	2.0
1	0	2239	C	2.0
1	0	352	A	2.0

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Mol	Chain	Res	Type	RSRZ
17	O	22	GLY	2.0
9	F	99	THR	2.0
16	N	170	GLU	2.0
6	C	63	SER	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	1MA	0	628	23/24	0.98	0.15	-	30,32,34,39	0
1	OMU	0	2587	21/22	0.98	0.11	-	28,35,37,37	0
1	OMG	0	2588	24/25	0.98	0.13	-	28,32,36,37	0
3	PPU	4	76	24/38	0.98	0.10	-	35,39,41,43	0
3	HFA	4	77	11/12	0.97	0.16	-	37,39,42,43	0
1	UR3	0	2619	21/22	0.98	0.12	-	34,37,39,41	0
1	PSU	0	2621	20/21	0.98	0.08	-	28,31,38,39	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	9125	1/1	0.74	1.04	73.44	93,93,93,93	0
35	NA	0	9120	1/1	0.92	0.39	40.62	53,53,53,53	0
34	K	0	9001	1/1	0.82	0.35	32.20	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	9168	1/1	0.76	0.38	29.64	63,63,63,63	0
35	NA	0	9172	1/1	0.88	0.67	28.38	71,71,71,71	0
35	NA	0	9174	1/1	0.71	0.34	18.90	62,62,62,62	0
35	NA	0	9164	1/1	0.77	0.24	16.52	59,59,59,59	0
35	NA	0	9169	1/1	0.58	0.57	15.30	96,96,96,96	0
33	MG	0	8021	1/1	0.93	0.20	14.14	53,53,53,53	0
37	SR	0	9482	1/1	0.98	0.24	11.87	93,93,93,93	0
33	MG	0	8080	1/1	0.94	0.28	11.04	48,48,48,48	0
35	NA	0	9185	1/1	0.66	0.28	9.54	50,50,50,50	0
33	MG	0	8038	1/1	0.99	0.27	9.33	27,27,27,27	0
35	NA	0	9177	1/1	0.86	0.34	9.20	62,62,62,62	0
35	NA	0	9173	1/1	0.74	0.26	7.53	66,66,66,66	0
33	MG	0	8101	1/1	0.79	0.25	7.01	78,78,78,78	0
35	NA	0	9182	1/1	0.70	0.27	6.80	78,78,78,78	0
33	MG	0	8012	1/1	0.98	0.19	6.48	40,40,40,40	0
35	NA	0	9161	1/1	0.94	0.22	6.14	59,59,59,59	0
33	MG	0	8001	1/1	0.96	0.20	6.05	23,23,23,23	0
33	MG	0	8008	1/1	0.99	0.15	5.89	23,23,23,23	0
35	NA	0	9162	1/1	0.94	0.20	5.83	49,49,49,49	0
35	NA	0	9171	1/1	0.81	0.23	5.30	56,56,56,56	0
33	MG	0	8039	1/1	0.94	0.15	4.53	80,80,80,80	0
35	NA	R	9186	1/1	0.83	0.23	4.36	67,67,67,67	0
35	NA	0	9114	1/1	0.96	0.26	4.34	42,42,42,42	0
35	NA	0	9124	1/1	0.91	0.27	3.67	53,53,53,53	0
35	NA	0	9131	1/1	0.97	0.17	3.59	44,44,44,44	0
33	MG	0	8054	1/1	0.94	0.18	3.45	39,39,39,39	0
33	MG	0	8017	1/1	0.85	0.17	3.40	31,31,31,31	0
33	MG	0	8020	1/1	0.95	0.20	3.25	34,34,34,34	0
35	NA	0	9127	1/1	0.80	0.19	3.01	45,45,45,45	0
37	SR	0	9534	1/1	0.99	0.15	3.00	90,90,90,90	0
35	NA	0	9105	1/1	0.98	0.19	2.97	38,38,38,38	0
33	MG	0	8013	1/1	0.91	0.16	2.57	37,37,37,37	0
33	MG	0	8027	1/1	0.95	0.15	2.46	33,33,33,33	0
35	NA	0	9156	1/1	0.96	0.17	2.14	53,53,53,53	0
33	MG	0	8058	1/1	0.86	0.26	2.09	79,79,79,79	0
36	CL	0	9315	1/1	0.96	0.13	2.06	50,50,50,50	0
37	SR	0	9515	1/1	0.98	0.17	1.97	81,81,81,81	0
35	NA	9	9183	1/1	0.83	0.20	1.95	73,73,73,73	0
35	NA	0	9178	1/1	0.93	0.23	1.70	51,51,51,51	0
33	MG	0	8074	1/1	0.98	0.20	1.55	31,31,31,31	0
35	NA	0	9135	1/1	0.98	0.17	1.33	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
36	CL	0	9316	1/1	0.97	0.17	1.18	71,71,71,71	0
33	MG	0	8107	1/1	0.88	0.17	1.04	63,63,63,63	0
35	NA	0	9165	1/1	0.94	0.17	1.04	42,42,42,42	0
35	NA	R	9138	1/1	0.98	0.17	0.93	59,59,59,59	0
35	NA	0	9150	1/1	0.90	0.18	0.70	42,42,42,42	0
37	SR	H	9486	1/1	0.98	0.15	0.69	97,97,97,97	0
36	CL	B	9319	1/1	0.90	0.16	0.67	55,55,55,55	0
33	MG	0	8019	1/1	0.94	0.12	0.54	45,45,45,45	0
35	NA	0	9117	1/1	0.95	0.18	0.53	43,43,43,43	0
33	MG	0	8004	1/1	0.98	0.12	0.45	33,33,33,33	0
37	SR	0	9406	1/1	0.99	0.14	0.41	32,32,32,32	0
35	NA	C	9104	1/1	0.89	0.17	0.39	27,27,27,27	0
37	SR	B	9521	1/1	0.80	0.18	0.33	165,165,165,165	0
35	NA	0	9132	1/1	0.96	0.12	0.17	45,45,45,45	0
33	MG	0	8057	1/1	0.86	0.20	-0.12	69,69,69,69	0
35	NA	M	9147	1/1	0.95	0.17	-0.23	39,39,39,39	0
36	CL	0	9312	1/1	0.99	0.13	-0.24	48,48,48,48	0
37	SR	1	9419	1/1	0.98	0.12	-0.41	41,41,41,41	0
36	CL	M	9318	1/1	0.99	0.17	-0.55	39,39,39,39	0
33	MG	0	8060	1/1	0.97	0.11	-0.59	76,76,76,76	0
33	MG	0	8056	1/1	0.98	0.13	-0.59	46,46,46,46	0
35	NA	0	9139	1/1	0.96	0.12	-0.62	41,41,41,41	0
33	MG	A	8066	1/1	0.94	0.13	-0.81	56,56,56,56	0
37	SR	0	9407	1/1	1.00	0.10	-0.81	41,41,41,41	0
33	MG	A	8065	1/1	0.87	0.14	-0.94	79,79,79,79	0
35	NA	J	9146	1/1	0.98	0.09	-1.01	43,43,43,43	0
36	CL	J	9321	1/1	0.97	0.08	-1.05	57,57,57,57	0
37	SR	L	9409	1/1	1.00	0.10	-1.07	36,36,36,36	0
37	SR	0	9424	1/1	1.00	0.13	-1.13	45,45,45,45	0
37	SR	F	9595	1/1	0.95	0.12	-1.14	99,99,99,99	0
37	SR	0	9532	1/1	0.88	0.10	-1.25	123,123,123,123	0
37	SR	0	9490	1/1	0.93	0.09	-1.36	89,89,89,89	0
33	MG	T	8073	1/1	0.97	0.14	-1.37	40,40,40,40	0
33	MG	0	8096	1/1	0.95	0.10	-1.40	42,42,42,42	0
38	CD	Z	9203	1/1	0.92	0.06	-1.52	57,57,57,57	0
37	SR	0	9450	1/1	0.99	0.06	-1.52	65,65,65,65	0
38	CD	U	9201	1/1	0.99	0.07	-1.61	58,58,58,58	0
37	SR	0	9410	1/1	0.99	0.13	-1.74	36,36,36,36	0
37	SR	0	9455	1/1	0.96	0.07	-1.75	78,78,78,78	0
35	NA	Q	9148	1/1	0.94	0.08	-1.75	48,48,48,48	0
36	CL	3	9304	1/1	0.97	0.09	-1.78	54,54,54,54	0
33	MG	0	8118	1/1	0.95	0.08	-1.82	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	R	9137	1/1	0.95	0.06	-1.90	38,38,38,38	0
37	SR	0	9442	1/1	0.97	0.11	-2.06	59,59,59,59	0
35	NA	0	9166	1/1	0.88	0.07	-2.11	59,59,59,59	0
38	CD	3	9204	1/1	0.99	0.05	-2.15	57,57,57,57	0
33	MG	0	8003	1/1	0.95	0.11	-2.18	33,33,33,33	0
33	MG	0	8032	1/1	0.97	0.09	-2.18	41,41,41,41	0
33	MG	Y	8109	1/1	0.96	0.09	-2.23	38,38,38,38	0
37	SR	A	9436	1/1	1.00	0.06	-2.23	47,47,47,47	0
33	MG	0	8097	1/1	0.98	0.10	-2.27	56,56,56,56	0
35	NA	0	9115	1/1	0.97	0.11	-2.37	36,36,36,36	0
36	CL	O	9308	1/1	0.96	0.10	-2.42	61,61,61,61	0
36	CL	0	9305	1/1	0.97	0.09	-2.44	52,52,52,52	0
37	SR	0	9451	1/1	0.99	0.07	-2.60	62,62,62,62	0
35	NA	0	9123	1/1	0.99	0.08	-2.60	38,38,38,38	0
35	NA	0	9167	1/1	0.89	0.09	-2.61	50,50,50,50	0
37	SR	0	9468	1/1	0.92	0.07	-2.62	108,108,108,108	0
37	SR	0	9504	1/1	0.95	0.06	-2.73	90,90,90,90	0
34	K	0	9002	1/1	0.97	0.07	-2.80	61,61,61,61	0
33	MG	0	8015	1/1	0.99	0.07	-2.96	31,31,31,31	0
37	SR	0	9416	1/1	0.99	0.08	-3.05	45,45,45,45	0
37	SR	3	9439	1/1	0.98	0.06	-3.08	57,57,57,57	0
37	SR	0	9475	1/1	0.92	0.07	-3.30	76,76,76,76	0
38	CD	1	9202	1/1	0.99	0.04	-3.45	50,50,50,50	0
37	SR	0	9444	1/1	0.99	0.04	-3.60	51,51,51,51	0
33	MG	0	8110	1/1	0.98	0.09	-3.66	43,43,43,43	0
35	NA	0	9143	1/1	0.96	0.07	-3.72	36,36,36,36	0
37	SR	0	9428	1/1	1.00	0.03	-3.82	49,49,49,49	0
33	MG	0	8044	1/1	0.96	0.07	-3.86	41,41,41,41	0
37	SR	0	9509	1/1	0.98	0.08	-3.92	84,84,84,84	0
37	SR	0	9506	1/1	0.97	0.06	-3.96	61,61,61,61	0
33	MG	0	8067	1/1	0.98	0.08	-4.01	38,38,38,38	0
37	SR	0	9483	1/1	0.96	0.05	-4.51	68,68,68,68	0
33	MG	0	8112	1/1	0.97	0.07	-4.69	41,41,41,41	0
37	SR	0	9453	1/1	0.98	0.05	-4.85	66,66,66,66	0
33	MG	0	8002	1/1	0.93	0.06	-4.85	45,45,45,45	0
37	SR	0	9498	1/1	0.99	0.03	-4.87	58,58,58,58	0
37	SR	0	9473	1/1	0.99	0.03	-5.26	69,69,69,69	0
37	SR	0	9457	1/1	0.98	0.06	-5.51	56,56,56,56	0
37	SR	0	9456	1/1	0.99	0.04	-9.34	57,57,57,57	0
33	MG	0	8091	1/1	0.97	0.05	-9.63	47,47,47,47	0
35	NA	0	9140	1/1	0.85	0.13	-	55,55,55,55	0
33	MG	0	8117	1/1	0.97	0.18	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	0	9590	1/1	0.93	0.05	-	91,91,91,91	0
33	MG	0	8005	1/1	0.98	0.09	-	28,28,28,28	0
37	SR	0	9420	1/1	0.98	0.14	-	59,59,59,59	0
37	SR	0	9570	1/1	0.98	0.06	-	86,86,86,86	0
37	SR	0	9539	1/1	0.90	0.25	-	134,134,134,134	0
37	SR	0	9464	1/1	0.98	0.05	-	73,73,73,73	0
33	MG	0	8108	1/1	0.69	0.17	-	111,111,111,111	0
37	SR	0	9462	1/1	0.99	0.10	-	64,64,64,64	0
33	MG	0	8084	1/1	0.82	0.34	-	76,76,76,76	0
33	MG	0	8055	1/1	0.48	0.26	-	102,102,102,102	0
33	MG	0	8102	1/1	0.92	0.05	-	61,61,61,61	0
35	NA	0	9116	1/1	0.76	0.22	-	44,44,44,44	0
35	NA	0	9157	1/1	0.70	0.13	-	44,44,44,44	0
37	SR	0	9440	1/1	0.98	0.03	-	69,69,69,69	0
37	SR	0	9405	1/1	0.97	0.07	-	67,67,67,67	0
36	CL	0	9317	1/1	0.97	0.06	-	45,45,45,45	0
33	MG	0	8046	1/1	0.93	0.05	-	41,41,41,41	0
37	SR	0	9477	1/1	0.95	0.06	-	83,83,83,83	0
33	MG	0	8047	1/1	0.87	0.29	-	89,89,89,89	0
33	MG	0	8037	1/1	0.97	0.09	-	37,37,37,37	0
37	SR	0	9417	1/1	0.98	0.09	-	55,55,55,55	0
37	SR	0	9508	1/1	0.98	0.04	-	82,82,82,82	0
33	MG	0	8070	1/1	0.99	0.18	-	27,27,27,27	0
37	SR	0	9459	1/1	0.86	0.06	-	97,97,97,97	0
33	MG	0	8025	1/1	0.87	0.35	-	29,29,29,29	0
37	SR	0	9431	1/1	0.98	0.07	-	61,61,61,61	0
37	SR	9	9503	1/1	0.98	0.07	-	104,104,104,104	0
37	SR	0	9560	1/1	0.97	0.05	-	91,91,91,91	0
37	SR	9	9588	1/1	0.89	0.15	-	126,126,126,126	0
37	SR	0	9469	1/1	0.97	0.05	-	81,81,81,81	0
33	MG	0	8106	1/1	0.97	0.06	-	43,43,43,43	0
35	NA	S	9112	1/1	0.67	0.41	-	68,68,68,68	0
35	NA	0	9128	1/1	0.99	0.09	-	40,40,40,40	0
36	CL	0	9311	1/1	0.96	0.09	-	60,60,60,60	0
37	SR	0	9467	1/1	0.97	0.04	-	74,74,74,74	0
35	NA	0	9158	1/1	0.86	0.31	-	66,66,66,66	0
35	NA	0	9155	1/1	0.96	0.13	-	52,52,52,52	0
37	SR	0	9435	1/1	0.96	0.08	-	67,67,67,67	0
37	SR	0	9452	1/1	0.91	0.18	-	107,107,107,107	0
33	MG	0	8113	1/1	0.89	0.11	-	43,43,43,43	0
35	NA	H	9122	1/1	0.65	0.20	-	80,80,80,80	0
37	SR	0	9421	1/1	0.99	0.05	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8059	1/1	0.80	0.47	-	61,61,61,61	0
33	MG	9	8095	1/1	0.93	0.21	-	49,49,49,49	0
33	MG	0	8104	1/1	0.91	0.12	-	50,50,50,50	0
36	CL	N	9307	1/1	0.89	0.15	-	55,55,55,55	0
37	SR	0	9501	1/1	1.00	0.07	-	64,64,64,64	0
37	SR	R	9418	1/1	0.99	0.12	-	50,50,50,50	0
33	MG	0	8022	1/1	0.71	1.23	-	103,103,103,103	0
33	MG	0	8088	1/1	0.94	0.14	-	36,36,36,36	0
33	MG	0	8114	1/1	0.93	0.40	-	76,76,76,76	0
37	SR	0	9423	1/1	0.99	0.04	-	56,56,56,56	0
37	SR	0	9626	1/1	0.93	0.23	-	114,114,114,114	0
33	MG	0	8045	1/1	0.87	0.31	-	66,66,66,66	0
33	MG	0	8098	1/1	0.95	0.08	-	43,43,43,43	0
37	SR	0	9422	1/1	0.99	0.09	-	52,52,52,52	0
37	SR	0	9454	1/1	0.99	0.05	-	65,65,65,65	0
33	MG	0	8042	1/1	0.82	0.08	-	53,53,53,53	0
33	MG	0	8068	1/1	0.96	0.20	-	46,46,46,46	0
33	MG	K	8069	1/1	0.99	0.28	-	22,22,22,22	0
33	MG	0	8030	1/1	0.99	0.09	-	34,34,34,34	0
37	SR	0	9581	1/1	0.92	0.13	-	106,106,106,106	0
37	SR	0	9461	1/1	0.99	0.04	-	69,69,69,69	0
37	SR	0	9465	1/1	0.94	0.05	-	93,93,93,93	0
33	MG	0	8079	1/1	0.94	0.16	-	30,30,30,30	0
37	SR	0	9430	1/1	0.99	0.09	-	47,47,47,47	0
35	NA	0	9175	1/1	0.96	0.12	-	51,51,51,51	0
33	MG	0	8075	1/1	0.98	0.04	-	37,37,37,37	0
35	NA	0	9179	1/1	0.86	0.33	-	107,107,107,107	0
35	NA	0	9159	1/1	0.96	0.20	-	55,55,55,55	0
36	CL	A	9309	1/1	0.93	0.10	-	57,57,57,57	0
37	SR	0	9443	1/1	0.99	0.06	-	54,54,54,54	0
37	SR	0	9480	1/1	0.97	0.06	-	85,85,85,85	0
33	MG	0	8043	1/1	0.96	0.08	-	49,49,49,49	0
37	SR	0	9495	1/1	0.98	0.08	-	90,90,90,90	0
37	SR	0	9445	1/1	0.99	0.07	-	55,55,55,55	0
38	CD	O	9205	1/1	0.52	0.23	-	183,183,183,183	0
35	NA	0	9106	1/1	0.97	0.10	-	37,37,37,37	0
37	SR	0	9466	1/1	0.97	0.05	-	80,80,80,80	0
37	SR	0	9530	1/1	0.98	0.13	-	66,66,66,66	0
37	SR	0	9449	1/1	0.99	0.06	-	60,60,60,60	0
33	MG	0	8072	1/1	0.94	0.25	-	69,69,69,69	0
37	SR	0	9411	1/1	0.99	0.15	-	42,42,42,42	0
35	NA	0	9141	1/1	0.90	0.09	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	0	9566	1/1	0.96	0.05	-	76,76,76,76	0
33	MG	0	8063	1/1	0.92	0.18	-	60,60,60,60	0
33	MG	0	8028	1/1	0.91	0.14	-	35,35,35,35	0
33	MG	0	8092	1/1	0.90	0.65	-	68,68,68,68	0
35	NA	0	9110	1/1	0.97	0.12	-	44,44,44,44	0
37	SR	0	9413	1/1	0.99	0.10	-	43,43,43,43	0
33	MG	0	8024	1/1	0.42	1.11	-	92,92,92,92	0
37	SR	0	9433	1/1	0.97	0.12	-	64,64,64,64	0
37	SR	A	9497	1/1	0.92	0.09	-	78,78,78,78	0
37	SR	0	9438	1/1	0.99	0.06	-	59,59,59,59	0
33	MG	0	8103	1/1	0.90	0.16	-	63,63,63,63	0
37	SR	0	9547	1/1	0.63	0.77	-	194,194,194,194	0
33	MG	0	8051	1/1	0.92	0.27	-	35,35,35,35	0
33	MG	0	8116	1/1	0.95	0.07	-	49,49,49,49	0
35	NA	0	9160	1/1	0.97	0.09	-	35,35,35,35	0
36	CL	J	9302	1/1	0.99	0.09	-	51,51,51,51	0
37	SR	0	9529	1/1	0.99	0.05	-	89,89,89,89	0
33	MG	0	8041	1/1	0.97	0.12	-	53,53,53,53	0
36	CL	R	9306	1/1	0.98	0.15	-	44,44,44,44	0
37	SR	0	9505	1/1	0.96	0.08	-	79,79,79,79	0
37	SR	0	9414	1/1	0.99	0.09	-	57,57,57,57	0
37	SR	0	9568	1/1	0.98	0.03	-	70,70,70,70	0
33	MG	0	8040	1/1	0.85	0.29	-	69,69,69,69	0
37	SR	0	9429	1/1	0.98	0.07	-	59,59,59,59	0
37	SR	9	9481	1/1	0.99	0.04	-	80,80,80,80	0
37	SR	0	9427	1/1	0.98	0.11	-	50,50,50,50	0
35	NA	0	9170	1/1	0.87	0.54	-	82,82,82,82	0
37	SR	0	9425	1/1	0.99	0.12	-	54,54,54,54	0
37	SR	1	9460	1/1	0.99	0.07	-	47,47,47,47	0
36	CL	0	9303	1/1	0.98	0.12	-	44,44,44,44	0
37	SR	0	9488	1/1	0.99	0.07	-	69,69,69,69	0
33	MG	0	8061	1/1	0.74	0.10	-	60,60,60,60	0
37	SR	0	9426	1/1	0.98	0.04	-	61,61,61,61	0
35	NA	0	9134	1/1	0.97	0.14	-	48,48,48,48	0
33	MG	0	8094	1/1	0.83	0.58	-	92,92,92,92	0
35	NA	0	9129	1/1	0.68	0.22	-	70,70,70,70	0
37	SR	0	9585	1/1	0.96	0.05	-	77,77,77,77	0
37	SR	0	9415	1/1	1.00	0.10	-	50,50,50,50	0
35	NA	0	9181	1/1	0.87	0.17	-	52,52,52,52	0
35	NA	0	9113	1/1	0.92	0.10	-	61,61,61,61	0
37	SR	0	9474	1/1	0.99	0.06	-	57,57,57,57	0
35	NA	0	9108	1/1	0.90	0.14	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8031	1/1	0.96	0.04	-	44,44,44,44	0
36	CL	0	9313	1/1	0.97	0.09	-	51,51,51,51	0
35	NA	0	9101	1/1	0.97	0.24	-	46,46,46,46	0
37	SR	0	9447	1/1	0.96	0.07	-	64,64,64,64	0
37	SR	0	9545	1/1	0.99	0.03	-	70,70,70,70	0
35	NA	0	9152	1/1	0.81	0.23	-	66,66,66,66	0
35	NA	0	9107	1/1	0.95	0.28	-	63,63,63,63	0
37	SR	0	9629	1/1	0.97	0.07	-	71,71,71,71	0
37	SR	A	9437	1/1	0.96	0.11	-	59,59,59,59	0
37	SR	0	9517	1/1	0.93	0.05	-	113,113,113,113	0
37	SR	0	9522	1/1	0.95	0.03	-	103,103,103,103	0
37	SR	0	9601	1/1	0.97	0.06	-	107,107,107,107	0
33	MG	0	8026	1/1	0.99	0.20	-	33,33,33,33	0
37	SR	0	9441	1/1	0.99	0.06	-	62,62,62,62	0
33	MG	0	8036	1/1	0.97	0.19	-	56,56,56,56	0
37	SR	S	9470	1/1	0.97	0.12	-	87,87,87,87	0
33	MG	0	8029	1/1	0.96	0.25	-	35,35,35,35	0
35	NA	0	9126	1/1	0.80	0.31	-	54,54,54,54	0
35	NA	0	9136	1/1	0.94	0.15	-	33,33,33,33	0
35	NA	0	9149	1/1	0.94	0.14	-	42,42,42,42	0
33	MG	0	8089	1/1	0.78	0.17	-	58,58,58,58	0
37	SR	0	9408	1/1	1.00	0.11	-	36,36,36,36	0
33	MG	0	8083	1/1	0.93	0.05	-	50,50,50,50	0
36	CL	0	9314	1/1	0.98	0.14	-	45,45,45,45	0
35	NA	0	9102	1/1	0.94	0.32	-	58,58,58,58	0
35	NA	0	9130	1/1	0.90	0.09	-	44,44,44,44	0
35	NA	0	9154	1/1	0.95	0.14	-	46,46,46,46	0
35	NA	0	9111	1/1	0.87	0.21	-	66,66,66,66	0
36	CL	0	9322	1/1	0.96	0.09	-	53,53,53,53	0
34	K	0	9003	1/1	0.87	0.23	-	80,80,80,80	0
37	SR	0	9432	1/1	0.98	0.13	-	61,61,61,61	0
33	MG	0	8099	1/1	0.94	0.16	-	62,62,62,62	0
37	SR	0	9500	1/1	0.01	0.64	-	179,179,179,179	0
33	MG	0	8115	1/1	0.91	0.12	-	51,51,51,51	0
37	SR	0	9484	1/1	0.87	0.09	-	123,123,123,123	0
33	MG	0	8052	1/1	0.64	0.23	-	88,88,88,88	0
35	NA	0	9163	1/1	0.82	0.12	-	59,59,59,59	0
35	NA	0	9184	1/1	0.76	0.23	-	75,75,75,75	0
36	CL	Y	9320	1/1	0.98	0.08	-	39,39,39,39	0
35	NA	D	9151	1/1	0.78	0.13	-	61,61,61,61	0
33	MG	0	8014	1/1	0.81	0.27	-	78,78,78,78	0
37	SR	0	9446	1/1	0.99	0.09	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	0	9448	1/1	1.00	0.06	-	52,52,52,52	0
37	SR	0	9434	1/1	0.98	0.09	-	60,60,60,60	0
36	CL	J	9301	1/1	0.92	0.08	-	51,51,51,51	0
33	MG	0	8009	1/1	0.96	0.15	-	32,32,32,32	0
33	MG	0	8050	1/1	0.79	0.18	-	74,74,74,74	0
37	SR	0	9537	1/1	0.98	0.07	-	119,119,119,119	0
36	CL	L	9310	1/1	0.96	0.06	-	49,49,49,49	0
33	MG	0	8076	1/1	0.96	0.16	-	56,56,56,56	0
35	NA	0	9118	1/1	0.76	0.44	-	60,60,60,60	0
33	MG	0	8082	1/1	0.80	0.31	-	89,89,89,89	0
37	SR	B	9458	1/1	0.97	0.09	-	68,68,68,68	0
33	MG	0	8093	1/1	0.85	0.13	-	41,41,41,41	0
33	MG	0	8085	1/1	0.87	0.30	-	65,65,65,65	0
37	SR	0	9489	1/1	0.98	0.07	-	80,80,80,80	0
37	SR	0	9478	1/1	0.99	0.07	-	71,71,71,71	0
37	SR	0	9412	1/1	1.00	0.11	-	38,38,38,38	0
33	MG	0	8090	1/1	0.94	0.64	-	84,84,84,84	0

6.5 Other polymers

There are no such residues in this entry.