



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YJW
Title : Crystal Structure Of Quinupristin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-15
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

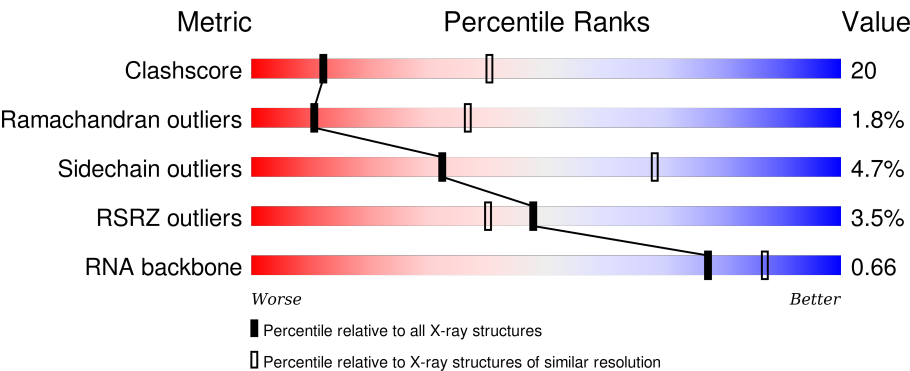
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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 $\leq 5\%$. 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	<div><div>%</div><div>53%35%6%6%</div></div>
2	1	57	<div><div>65%33%</div></div>
3	2	50	<div><div>4%46%46%8%</div></div>
4	3	92	<div><div>%55%45%</div></div>
5	4	8	<div><div>88%13%</div></div>

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Mol	Chain	Length	Quality of chain
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	
30	X	92	

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Mol	Chain	Length	Quality of chain
31	Y	241	
32	Z	83	

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	7	8064	-	-	-	X
34	K	7	8401	-	-	-	X
35	NA	8	8502	-	-	-	X
35	NA	8	8503	-	-	-	X
35	NA	8	8521	-	-	-	X
35	NA	8	8525	-	-	-	X
35	NA	8	8527	-	-	-	X
35	NA	8	8529	-	-	-	X
35	NA	8	8531	-	-	-	X
35	NA	8	8532	-	-	-	X
35	NA	8	8535	-	-	-	X
35	NA	8	8553	-	-	-	X
35	NA	8	8556	-	-	-	X
35	NA	8	8559	-	-	-	X
35	NA	8	8561	-	-	-	X
35	NA	8	8562	-	-	-	X
35	NA	8	8565	-	-	-	X
35	NA	8	8568	-	-	-	X
35	NA	8	8569	-	-	-	X
35	NA	8	8571	-	-	-	X
35	NA	8	8572	-	-	-	X
35	NA	8	8573	-	-	-	X
35	NA	8	8574	-	-	-	X
35	NA	8	8577	-	-	-	X
35	NA	8	8578	-	-	-	X
35	NA	8	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	8	8812	-	-	X	-
36	CL	8	8815	-	-	-	X
36	CL	N	8807	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99111 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
1	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 55229667
0	2099	A	G	ENGINEERED	GB 55229667
0	2587	OMU	U	MODIFIED RESIDUE	GB 55229667
0	2588	OMG	G	MODIFIED RESIDUE	GB 55229667
0	2619	UR3	U	MODIFIED RESIDUE	GB 55229667
0	2621	PSU	U	MODIFIED RESIDUE	GB 55229667

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L2P.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L3P.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L4E.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L5P.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L6P.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

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

- Molecule 13 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13P.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	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 18 is a protein called 50S RIBOSOMAL PROTEIN L15P.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18P.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18E.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19E.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21E.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22P.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24P.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24E.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29P.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30P.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32E.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	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 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	7	110	Total	Mg	0	0
			110	110		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	7	2	Total	K	0	0
			2	2		

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

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	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	8	74	Total Na 74 74	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	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	8	10	Total Cl 10 10	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

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5874	Total	O	0	0
			5874	5874		
38	1	59	Total	O	0	0
			59	59		
38	2	46	Total	O	0	0
			46	46		
38	3	67	Total	O	0	0
			67	67		
38	4	2	Total	O	0	0
			2	2		
38	9	141	Total	O	0	0
			141	141		
38	A	119	Total	O	0	0
			119	119		
38	B	144	Total	O	0	0
			144	144		
38	C	176	Total	O	0	0
			176	176		
38	D	48	Total	O	0	0
			48	48		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	E	42	Total 42	O 42	0	0
38	F	26	Total 26	O 26	0	0
38	G	20	Total 20	O 20	0	0
38	H	67	Total 67	O 67	0	0
38	I	9	Total 9	O 9	0	0
38	J	56	Total 56	O 56	0	0
38	K	60	Total 60	O 60	0	0
38	L	80	Total 80	O 80	0	0
38	M	125	Total 125	O 125	0	0
38	N	60	Total 60	O 60	0	0
38	O	44	Total 44	O 44	0	0
38	P	70	Total 70	O 70	0	0
38	Q	48	Total 48	O 48	0	0
38	R	82	Total 82	O 82	0	0
38	S	33	Total 33	O 33	0	0
38	T	39	Total 39	O 39	0	0
38	U	29	Total 29	O 29	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	27	Total 27	O 27	0	0
38	Y	100	Total 100	O 100	0	0

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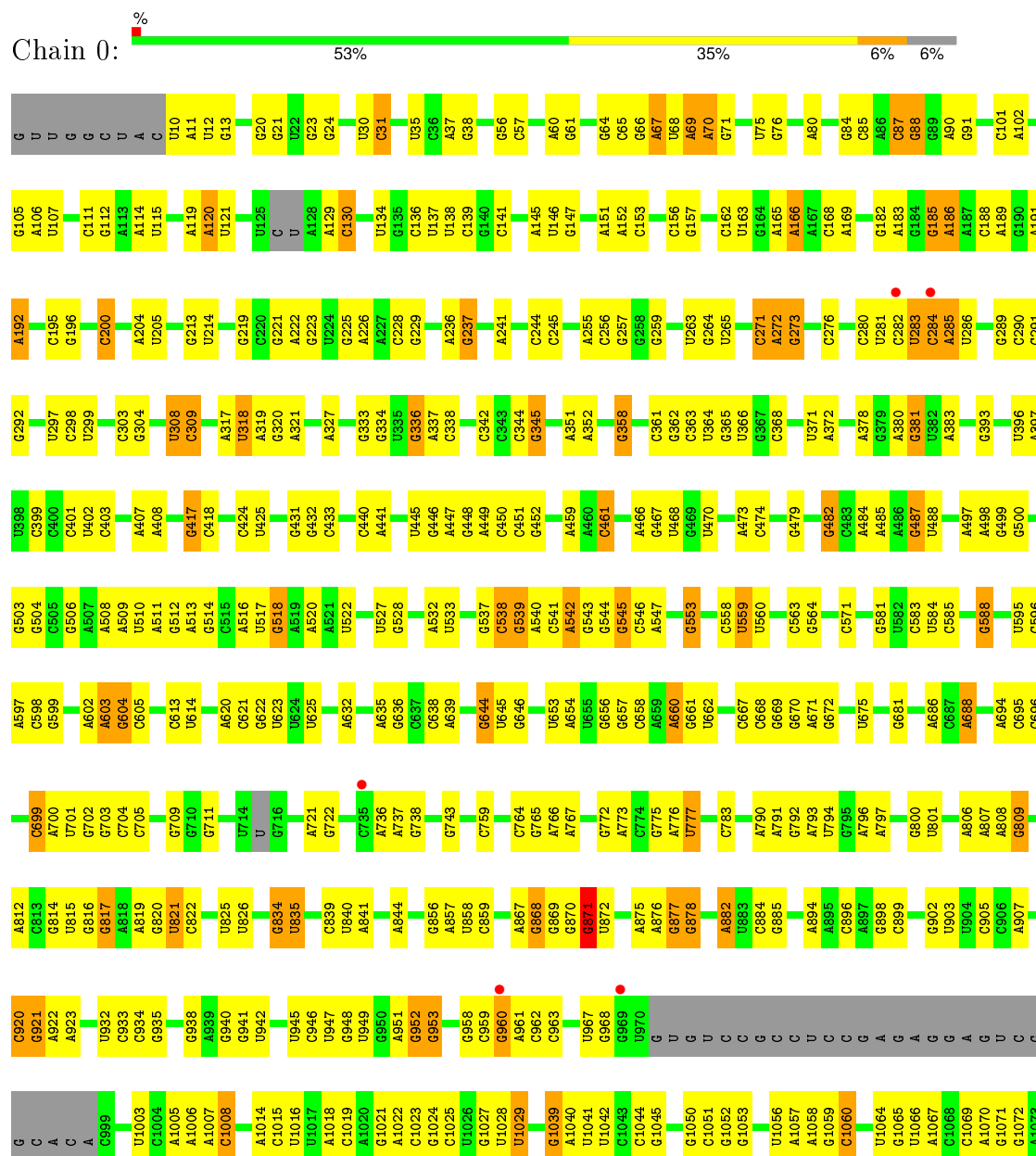
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	35	Total	O	0	0
			35	35		

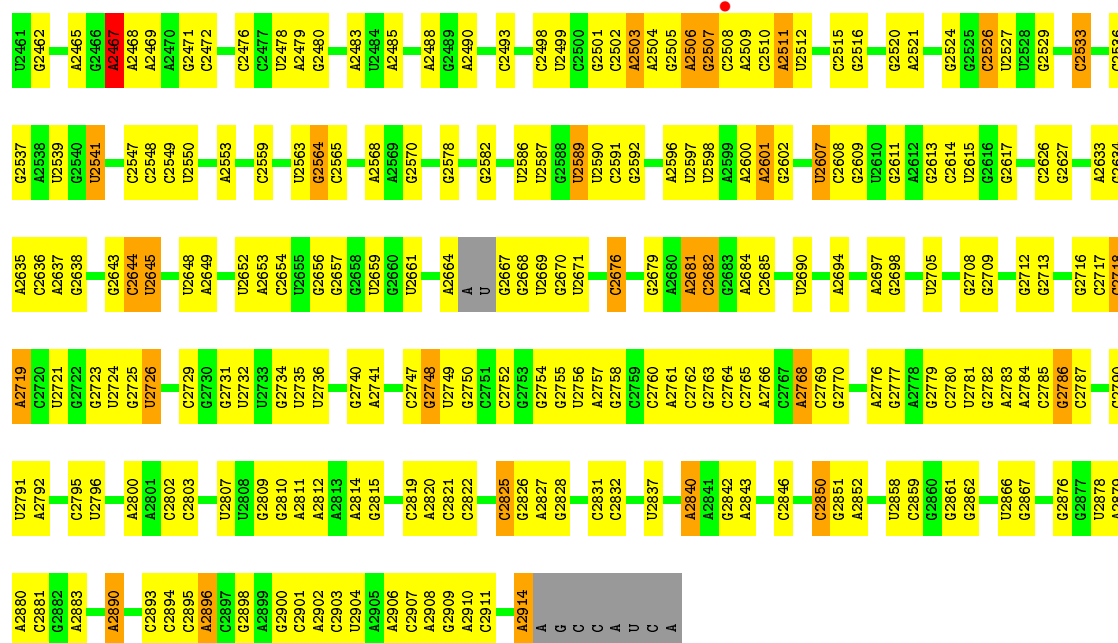
3 Residue-property plots

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

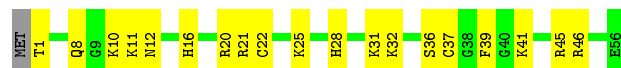


A2369	G2272	C	G	C2035	C1940	U1825	C1735	G1636	G1535	C1439	A1348	A1242	A1173	G1074
A2370	C2273	A	U	C2036	A1941	C1826	A1736	A1637	C1536	U1440	C1348	C1243	A1174	A1081
G2371	G2274	G	C	C2037	C1942	A1829	U1741	U1638	C1537	A1441	C1352	U1244	G1175	
A2372	G2275	A	C	A2038	C1943	C1830	G1742	A1641	G1543	U1442	G1353	C1245	C1176	A1086
U2373	U2276	C	C	C2039	G1946	G1834	G1743	A1642	U1544	U1446	G1354	A1246	A1177	G1087
	U2277	A	G	C2040	G1947	U1835	G1744	C1643	C1545		C1355	C1250	G1178	A1088
U2377	C2281	C	G	G2044	G1948	G1836	U1748	A1653	A1559	C1450	C1360	C1251	U1180	
U2378	U2282	A	U	G2050	G1949	U1838	U1749	U1654	U	C1451		C1251	A1181	A1097
A2380	A2291	G	U	C2050	G1950	U1839	C1750	U1561	U1461		G1363	G1260	A1098	
C2381	U2297	G	G	G2053	A1840	G1751	G1751	G1655	C1462		C1366	A1261	C1183	G1099
A2382	U2297	C	A	A2054	C1841	G1752	G1752	A1656	G1562				C1184	
G2383	A2055	A	A	A2055	A1845	G1753	G1753	A1657	C1563		U1266	U1266	U1185	C1102
U2384	U2064	A	G	A2055	C	A1754	A1754	A1658	C1564			G1267	C1186	
G2385	C2065	U	G	U2064	U	A1755	A1755	A1659	G1571			G1268	U1187	U1109
U2386	C2065	U	A	C2065	G1849	U1761	C1768	G1666	A1572			G1269	C1188	G1110
A2301	G2072	C	U	G2072	C1853	C1762	C1763	A1667	A1573			U1279	A1189	U1111
U2302	A2074	A	G	A2074	G1854	U1766	U1766	U1668	C1574			C1273	G1190	G1112
A2303	G2073	C	G	G2073	C1855	C1767	C1767	U1669	A1580				A1191	
	A2074	C	G	A2074	C1856	U1767	U1767	A1670	A1581				U1192	U1116
C2309	A2081	C	U	A2081	C1862	C1768	C1768	C1674	C1483			C1277	A1192	
G2312	G2312	C	A	A2081	G1863	C1769	C1769	G1484	C1484			U1278	A1193	U1117
C2313	C2313	G	G	C2087	U1964	U1770	U1770	G1585	C1585			G1289	A1194	A1118
C2315	C2315	C	A	C2088	U1966	U1771	U1771	G1586	G1586			G1290	G1195	G1119
G2316	A2089	G	U	A2089	U1967	C1772	C1772	U1587	U1488			G1291	G1196	U1120
C2317	G2090	G	G	G2090	A1968	C1773	C1773	G1588	G1489			U1292	A1197	G1121
U2320	G2091	U	C	G2091	A1969	G1774	G1774	G1589	G1490			G1293	A1202	C1129
A2321	A2096	A	U	A2096	G1970	U1775	U1775	G1592	A1493			G1294	G1203	U1130
	A2096	U	U	A2096	G1971	A1778	A1778	G1593	A1494			G1295	G1204	G1131
G2324	A2100	C	U	A2100	U1972	A1779	A1779	C1594	A1399				U1205	A1132
U2325	A2101	G	A	A2101	A1973	U1783	U1783	C1595	A1400			G1299	U1206	G1137
G2326	G2102	C	C	G2102	C1975	U1784	U1784	U1596	A1406			U1304	A1207	G1138
	A2103	G	G	A2103	G1976	G1785	G1785	A1597	A1407			U1305	C1208	U1139
C2329	C2104	G	G	C2104	U1977	C1786	C1786	U1599	A1408			U1306	C1209	C1140
	G2110	G	U	G2110	A1978	U1788	U1788	G1600	G1409			A1307	G1211	
C2335	G2111	U	G	G2111	U1979	G1789	G1789	G1603	A1413			A1308	G1212	A1150
G2336	A2112	C	A	A2112	U1980	C1790	C1790	U1503	A1414			U1314	C1213	G1151
G2337	G2113	C	C	G2113	U1996	U1791	U1791	A1504	A1415			U1315	G1214	A1154
A2338	C2114	C	C	C2114	A1997	A1797	A1797	U1506	U1506			G1315	A1215	G1155
	U2115	C	C	U2115	G2000	G1798	G1798	G1614	C1513			G1316	G1217	C1157
C2338	U2116	G	G	U2116	G2001	C1799	C1799	A1615	C1514			G1325		G1158
A	U2120	C	C	A	G2002	G1926	G1926	A1616	C1515				G1226	G1159
C	G2121	C	G	C	C2003	C1928	C1928	G1617	A1516			A1328	C1227	G1160
	G2128	U	U	U2004	A1919	G1804	G1804	G1618	C1517			U1422	G1228	A1161
		A	A	G2005	G1925	G1805	G1805	G1619	A1518			G1331	C1229	G1162
		G	G	G2005	G1926	G1806	G1806	C1620	A1518			G1332		G1163
	U2133	C	C	U2008	G1927	C1810	C1810	U1624	U1524			U1333	A1232	U1164
	G2134	G	G	A2011	U1724	A1811	A1811	U1625	G1525			C1334	A1233	G1165
	G2136	G	G	U2012	C1928	G1819	G1819	A1626	A1526			C1335	U1234	A1166
A	G2136	G	G	A1930	G1929	G1820	G1820	A1627	A1527				G1235	G1167
C	A	C	C	A1931	A1931	G1821	G1821	G1627	A1528			G1340	U1236	C1168
C	C	C	C	A1931	A1931	G1822	G1822	G1633	G1529			A1341	U1237	U1169
U	U2032	A	A	U2032	C1935	G1823	G1823	G1634	A1533			C1342	U1170	G1171
G	U2034	C	C	U2034	C1936	G1824	G1824	G1635	C1534			C1343	G1238	G1172



• Molecule 2: 50S RIBOSOMAL PROTEIN L37E

Chain 1: 65% 33%



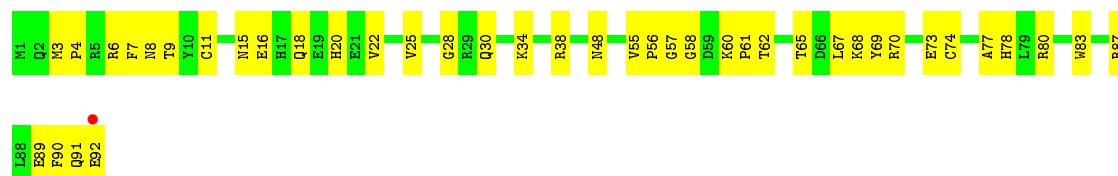
• Molecule 3: 50S RIBOSOMAL PROTEIN L39E

Chain 2: 4% 46% 46% 8%



• Molecule 4: 50S RIBOSOMAL PROTEIN L44E

Chain 3: % 55% 45%

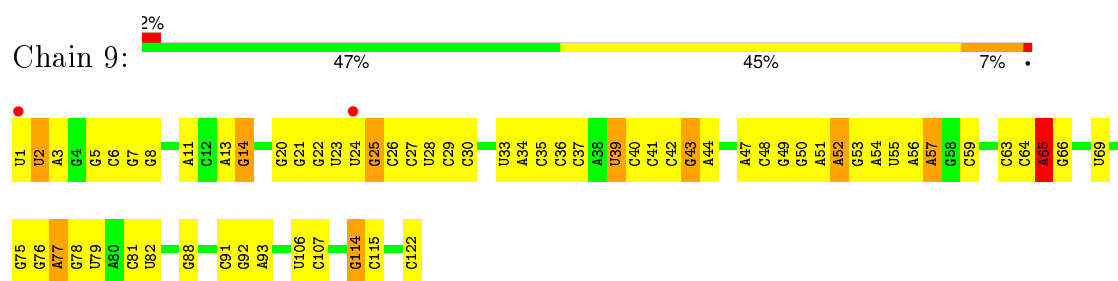


• Molecule 5: QUINUPRISTIN

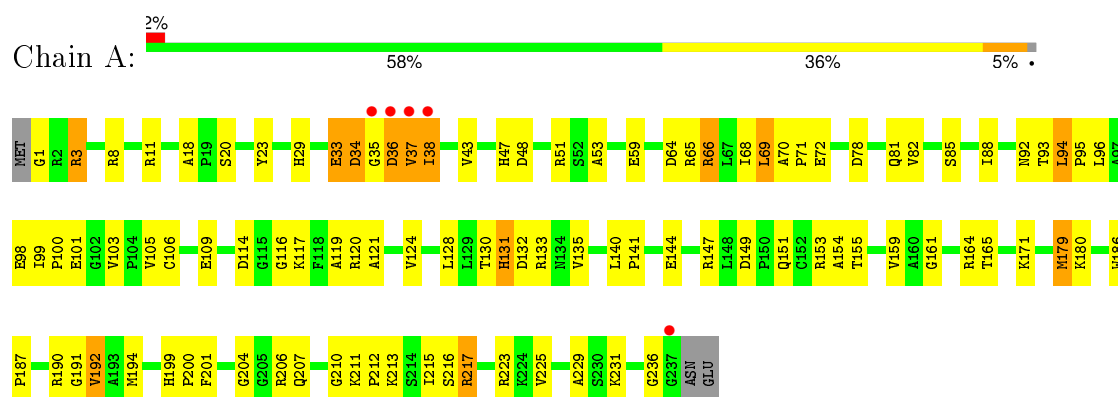
Chain 4: 88% 13%



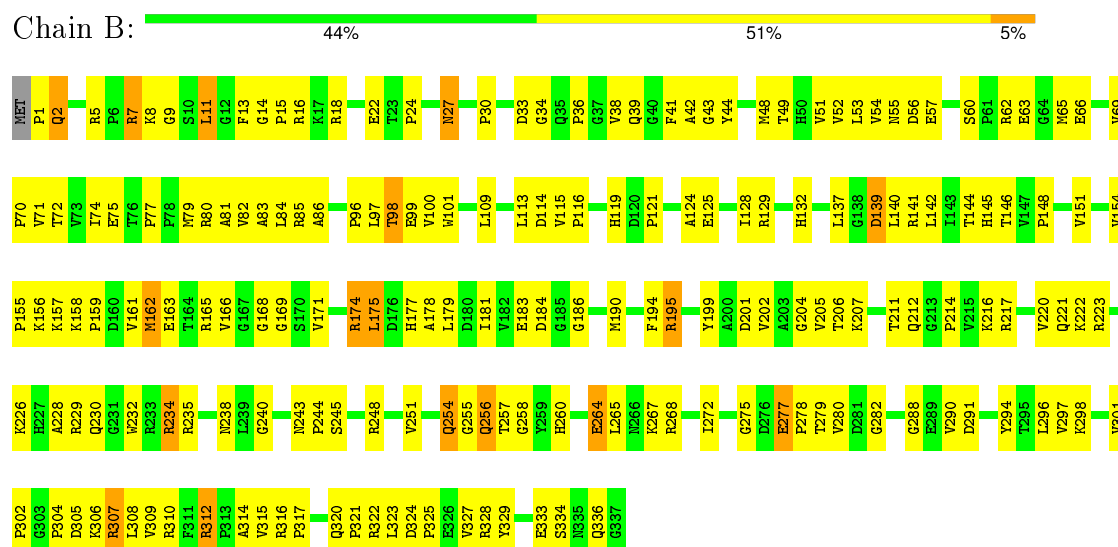
• Molecule 6: 5S RIBOSOMAL RNA



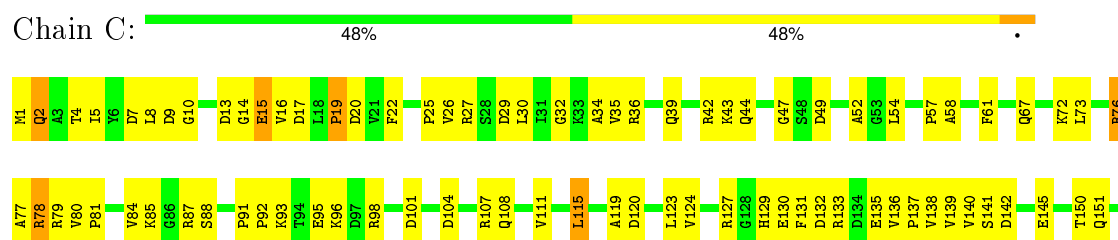
• Molecule 7: 50S RIBOSOMAL PROTEIN L2P

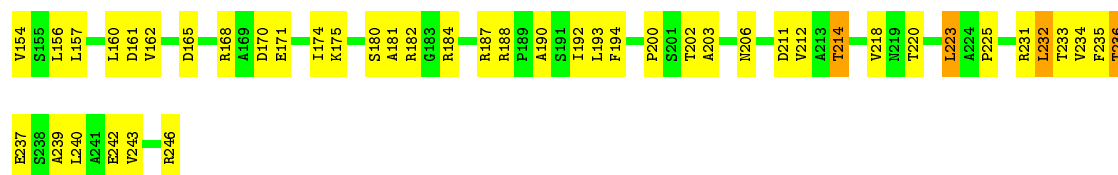


• Molecule 8: 50S RIBOSOMAL PROTEIN L3P

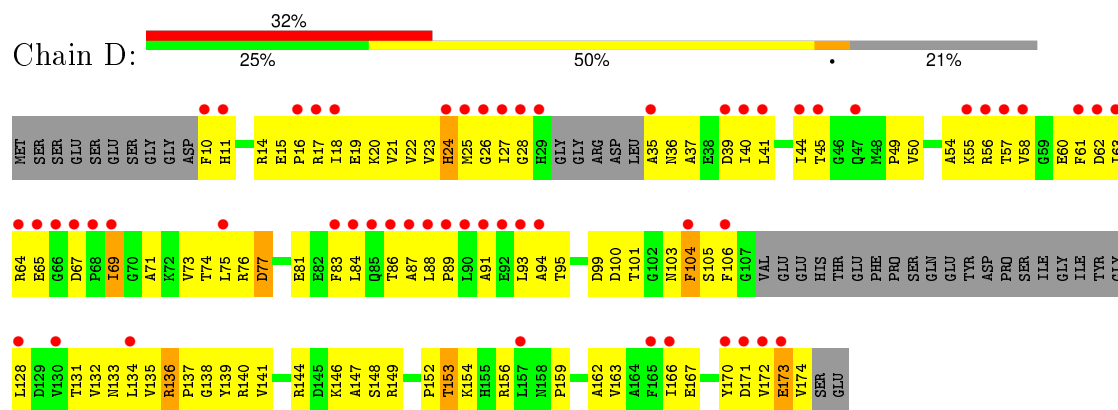


• Molecule 9: 50S RIBOSOMAL PROTEIN L4E

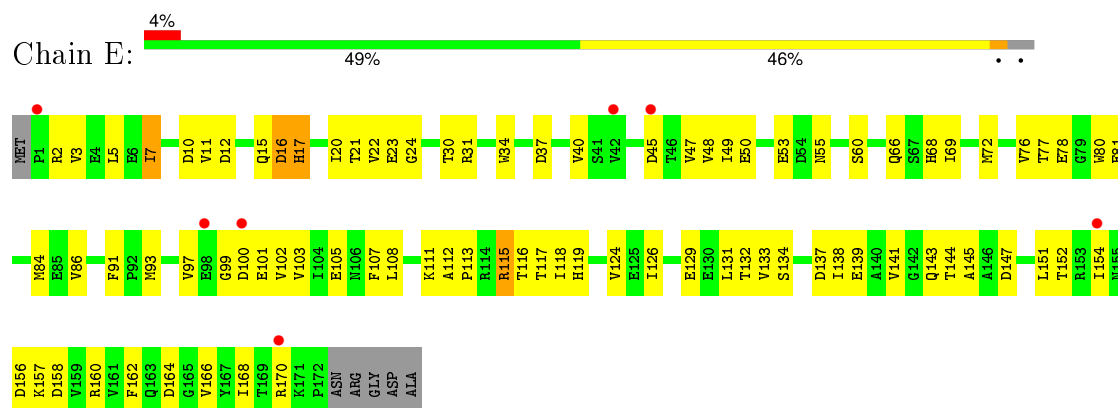




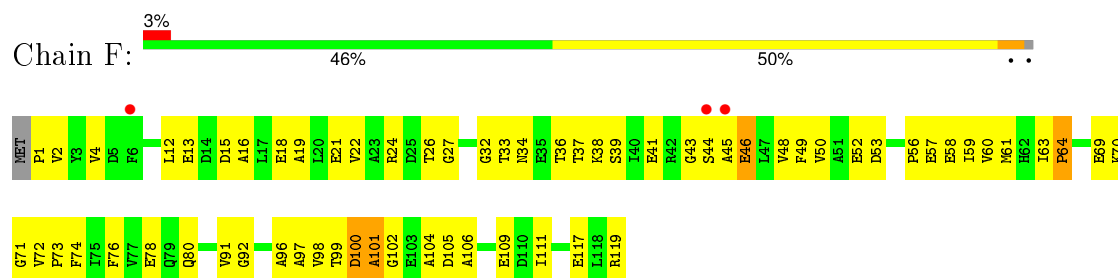
• Molecule 10: 50S RIBOSOMAL PROTEIN L5P



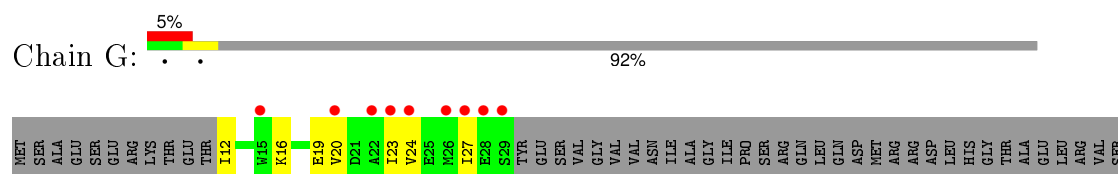
• Molecule 11: 50S RIBOSOMAL PROTEIN L6P

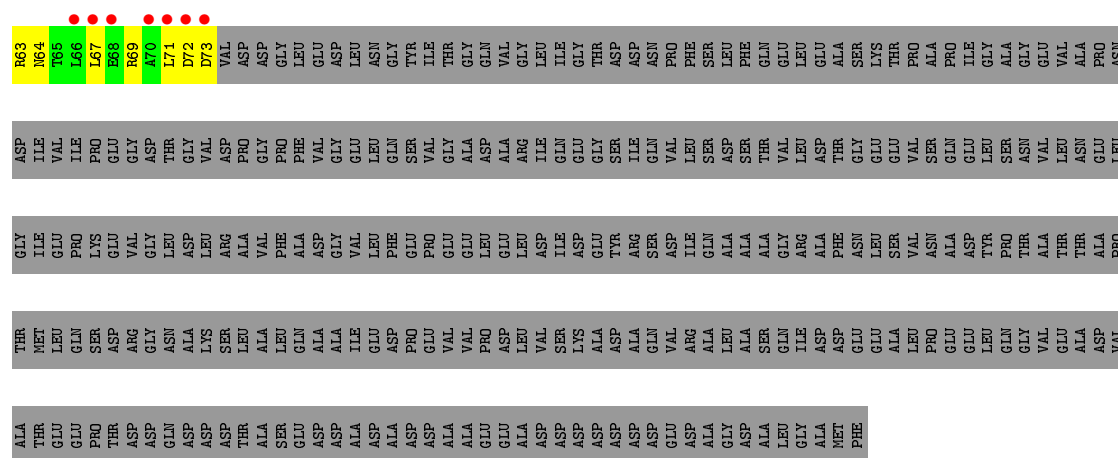


• Molecule 12: 50S RIBOSOMAL PROTEIN L7AE

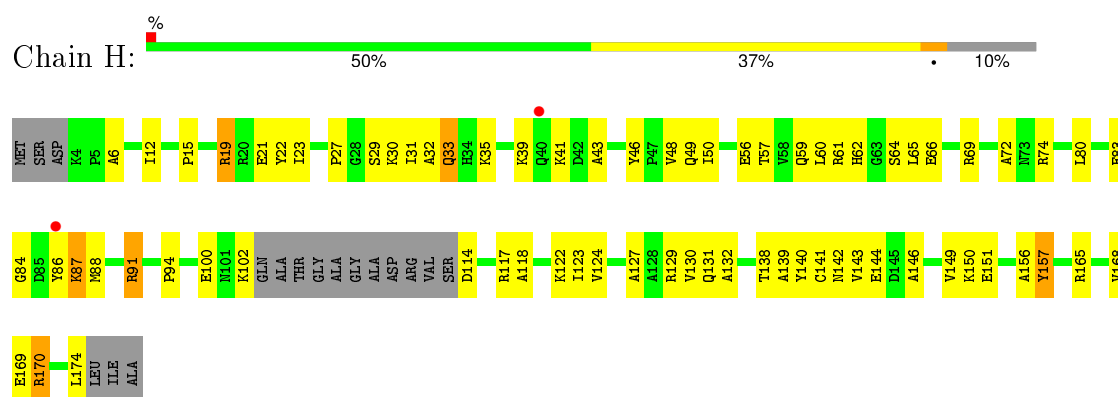


• Molecule 13: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

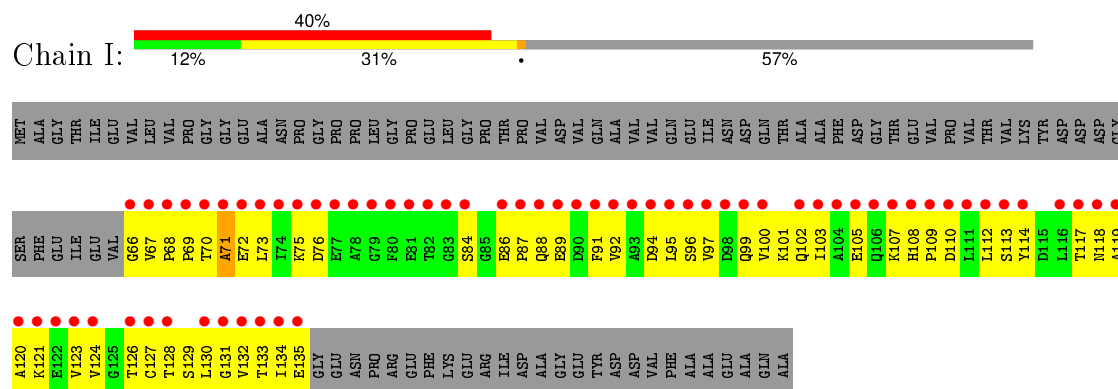




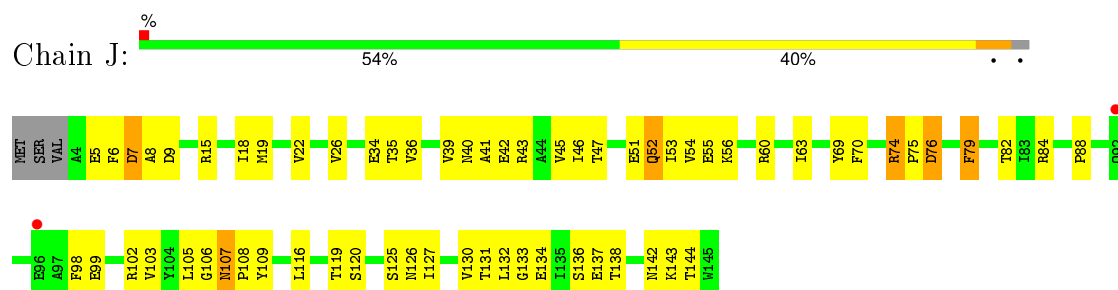
- Molecule 14: 50S RIBOSOMAL PROTEIN L10E



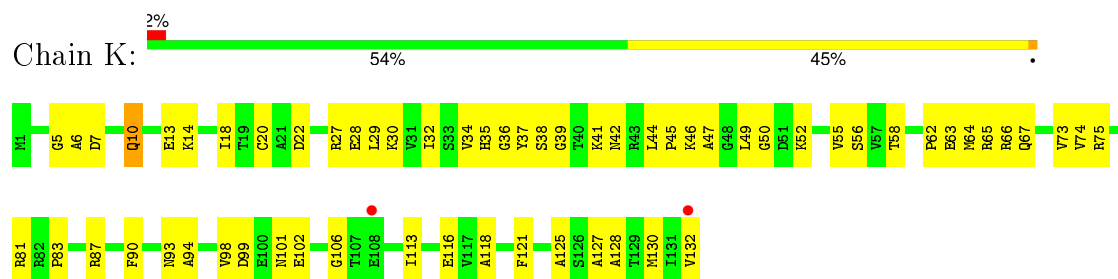
● Molecule 15: 50S RIBOSOMAL PROTEIN L11P



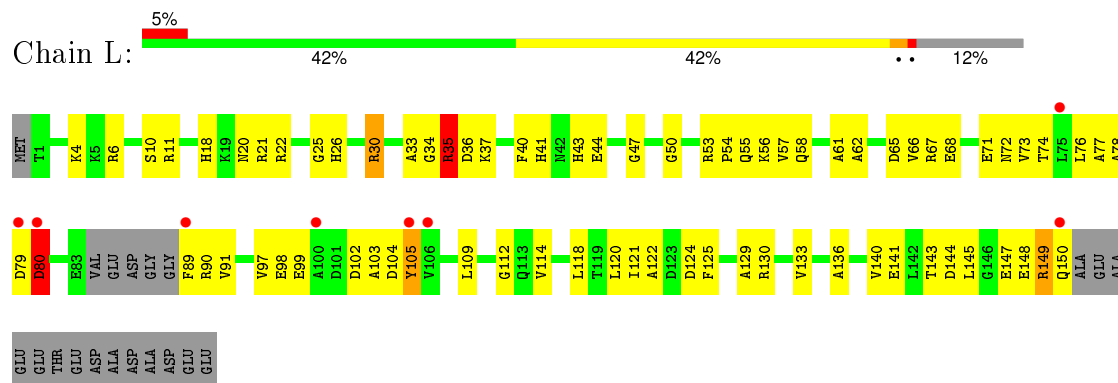
- Molecule 16: 50S RIBOSOMAL PROTEIN L13P



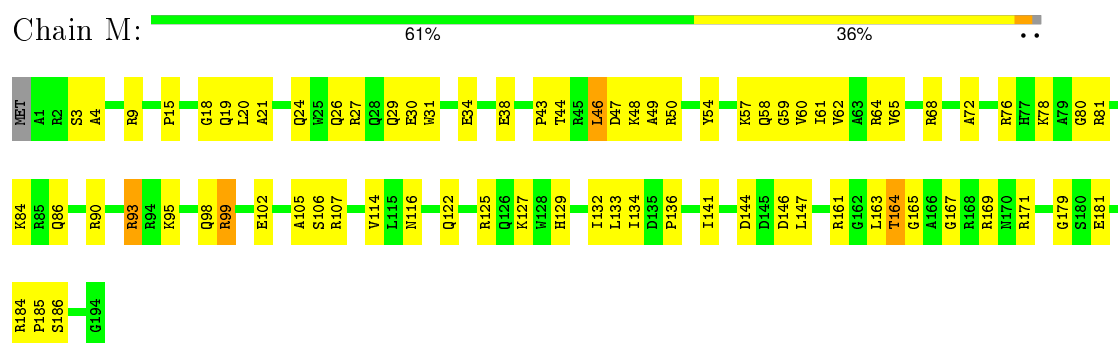
- Molecule 17: 50S RIBOSOMAL PROTEIN L14P



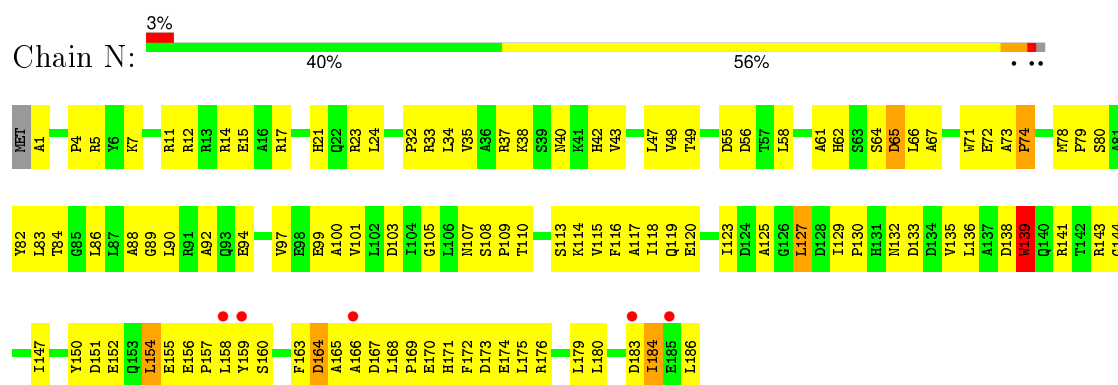
- Molecule 18: 50S RIBOSOMAL PROTEIN L15P



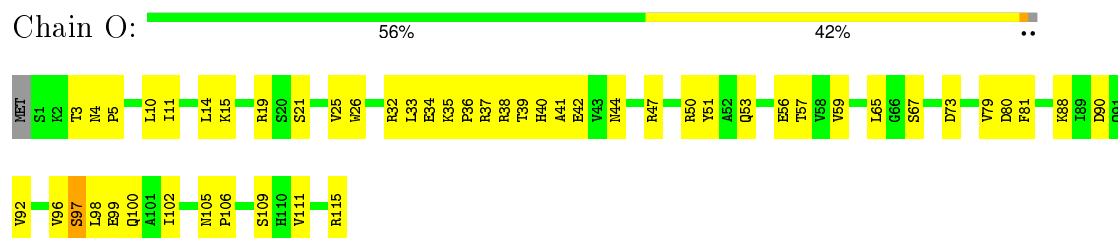
- Molecule 19: 50S RIBOSOMAL PROTEIN L15E



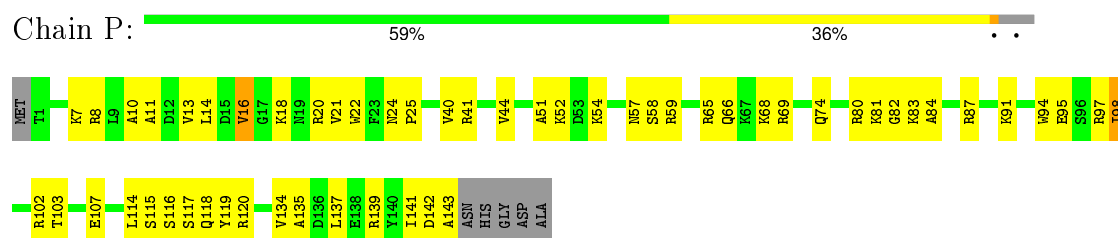
- Molecule 20: 50S RIBOSOMAL PROTEIN L18P



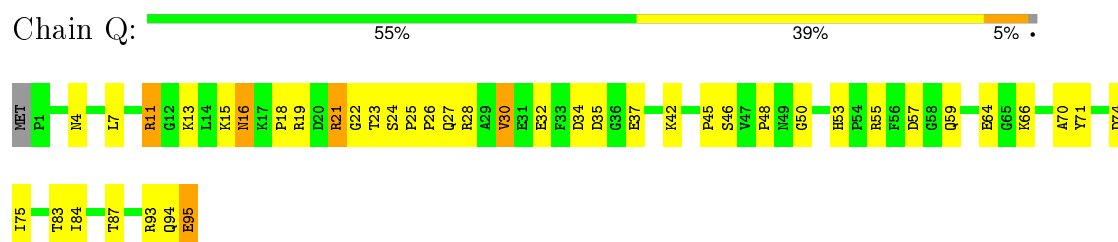
- Molecule 21: 50S RIBOSOMAL PROTEIN L18E



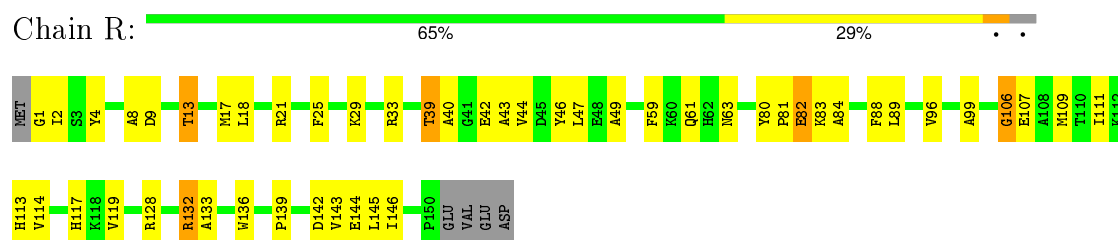
• Molecule 22: 50S RIBOSOMAL PROTEIN L19E



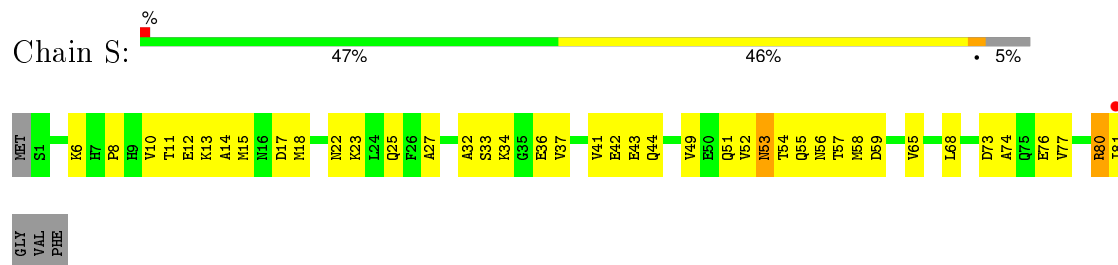
• Molecule 23: 50S RIBOSOMAL PROTEIN L21E



• Molecule 24: 50S RIBOSOMAL PROTEIN L22P

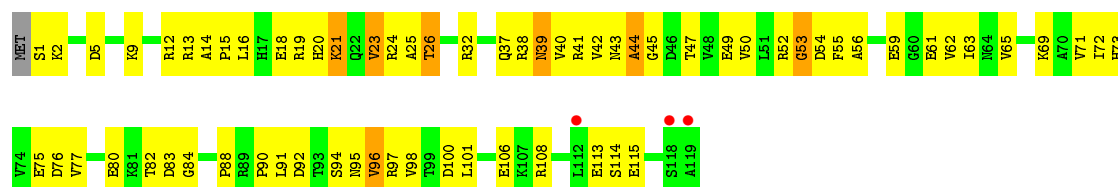


• Molecule 25: 50S RIBOSOMAL PROTEIN L23P

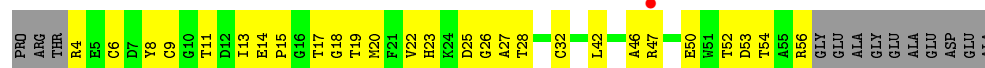


• Molecule 26: 50S RIBOSOMAL PROTEIN L24P

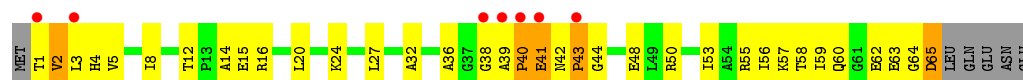




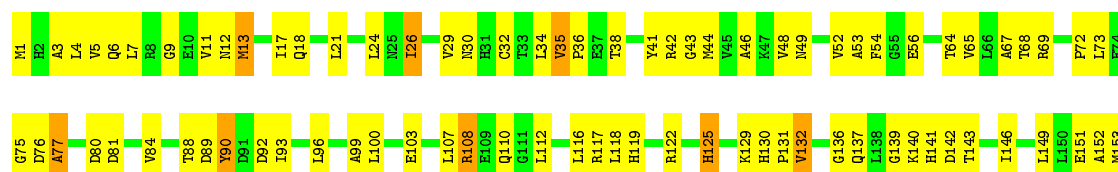
• Molecule 27: 50S RIBOSOMAL PROTEIN L24E



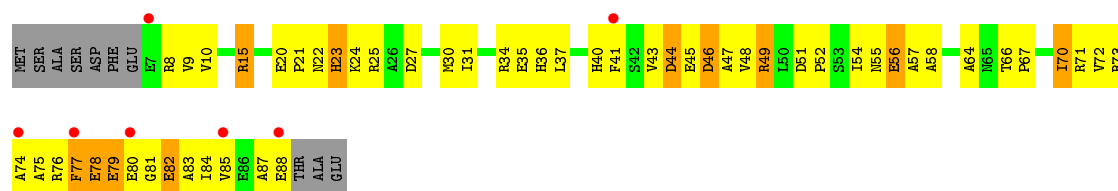
• Molecule 28: 50S RIBOSOMAL PROTEIN L29P



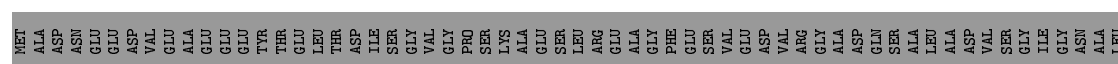
• Molecule 29: 50S RIBOSOMAL PROTEIN L30P

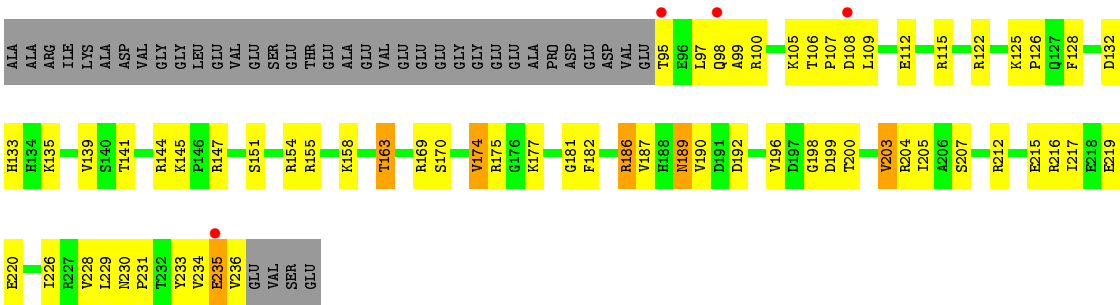


• Molecule 30: 50S RIBOSOMAL PROTEIN L31E

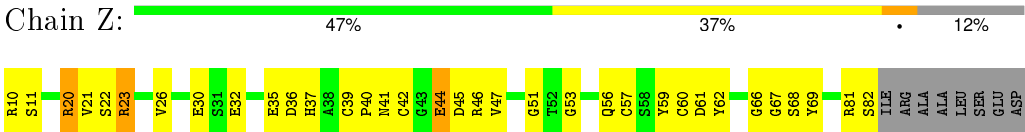


• Molecule 31: 50S RIBOSOMAL PROTEIN L32E





• Molecule 32: 50S RIBOSOMAL PROTEIN L37AE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.69Å 299.78Å 573.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.90 49.95 – 2.89	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.98-2.90) 83.4 (49.95-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.223 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 335760 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99111	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, DBB, CD, 1MA, UR3, OMU, 004, MHV, MHW, MHT, MHU, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.37	0/65957	0.69	13/102867 (0.0%)
2	1	0.38	0/438	0.61	0/578
3	2	0.34	0/401	0.56	0/529
4	3	0.37	0/771	0.57	0/1024
5	4	1.63	0/13	1.38	0/15
6	9	0.35	0/2904	0.69	1/4526 (0.0%)
7	A	0.33	0/1786	0.65	0/2408
8	B	0.33	0/2690	0.63	0/3652
9	C	0.36	0/1884	0.63	0/2551
10	D	0.32	0/1111	0.56	0/1498
11	E	0.33	0/1382	0.58	0/1880
12	F	0.33	0/901	0.57	0/1224
13	G	0.30	0/241	0.48	0/324
14	H	0.34	0/1302	0.64	0/1743
15	I	0.31	0/526	0.55	0/716
16	J	0.35	0/1136	0.59	0/1530
17	K	0.35	0/1001	0.67	0/1347
18	L	0.32	0/1130	0.63	0/1509
19	M	0.34	0/1582	0.60	0/2117
20	N	0.30	0/1474	0.64	0/1999
21	O	0.34	0/874	0.60	0/1181
22	P	0.33	0/1147	0.54	0/1528
23	Q	0.35	0/749	0.66	0/1005
24	R	0.34	0/1172	0.63	0/1578
25	S	0.34	0/648	0.59	0/875
26	T	0.32	0/958	0.61	0/1289
27	U	0.32	0/417	0.58	0/562
28	V	0.29	0/502	0.55	0/675
29	W	0.36	0/1219	0.62	0/1655
30	X	0.33	0/664	0.61	0/895
31	Y	0.35	0/1146	0.62	0/1536
32	Z	0.35	0/589	0.67	0/787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98715	0.67	14/147603 (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	20
6	9	0	1
29	W	0	1
All	All	0	22

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	C1'-O4'-C4'	-6.45	104.74	109.90
1	0	1942	A	C5'-C4'-C3'	6.01	125.61	116.00
1	0	871	G	C5'-C4'-O4'	-5.83	102.10	109.10
1	0	2291	A	N9-C1'-C2'	5.68	121.39	114.00
1	0	2726	U	N1-C1'-C2'	5.63	121.33	114.00
6	9	39	U	N1-C1'-C2'	5.52	121.18	114.00
1	0	1819	G	C5'-C4'-C3'	5.43	124.69	116.00
1	0	2313	C	C5'-C4'-O4'	5.37	115.55	109.10
1	0	1120	U	C5'-C4'-C3'	-5.29	107.54	116.00
1	0	841	A	C1'-O4'-C4'	-5.28	105.68	109.90
1	0	1971	G	N9-C1'-C2'	5.16	120.71	114.00
1	0	2467	A	C1'-O4'-C4'	-5.12	105.81	109.90
1	0	1165	G	C1'-O4'-C4'	-5.09	105.83	109.90
1	0	2313	C	C1'-O4'-C4'	-5.01	105.89	109.90

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1377	C	Sidechain
1	0	1430	G	Sidechain
1	0	1653	A	Sidechain
1	0	1829	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2607	U	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
6	9	65	A	Sidechain
29	W	90	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	59020	0	29811	1125	0
2	1	431	0	426	27	0
3	2	396	0	413	30	0
4	3	755	0	728	38	0
5	4	73	0	64	1	0
6	9	2599	0	1325	72	0
7	A	1753	0	1766	116	0
8	B	2625	0	2533	203	0
9	C	1859	0	1816	140	0
10	D	1094	0	1085	111	0
11	E	1357	0	1266	79	0
12	F	890	0	843	56	0
13	G	240	0	231	19	0
14	H	1282	0	1292	88	0
15	I	519	0	500	62	0
16	J	1120	0	1098	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	992	0	1031	72	0
18	L	1118	0	1076	82	0
19	M	1558	0	1566	82	0
20	N	1445	0	1401	145	0
21	O	865	0	873	48	0
22	P	1136	0	1123	57	0
23	Q	735	0	729	45	0
24	R	1149	0	1122	59	0
25	S	641	0	605	39	0
26	T	950	0	923	71	0
27	U	410	0	364	35	0
28	V	499	0	511	43	0
29	W	1196	0	1137	116	0
30	X	654	0	653	59	0
31	Y	1130	0	1133	69	0
32	Z	578	0	539	24	0
33	3	1	0	0	0	0
33	7	110	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	7	2	0	0	0	0
35	8	74	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	3	1	0	0	0	0
36	8	10	0	0	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	M	1	0	0	0	0
36	N	1	0	0	2	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5874	0	0	198	0
38	1	59	0	0	8	0
38	2	46	0	0	5	0
38	3	67	0	0	11	0
38	4	2	0	0	0	0
38	9	141	0	0	9	0
38	A	119	0	0	19	0
38	B	144	0	0	20	0
38	C	176	0	0	37	0
38	D	48	0	0	22	0
38	E	42	0	0	11	0
38	F	26	0	0	5	0
38	G	20	0	0	2	0
38	H	67	0	0	15	0
38	I	9	0	0	3	0
38	J	56	0	0	4	0
38	K	60	0	0	11	0
38	L	80	0	0	20	0
38	M	125	0	0	12	0
38	N	60	0	0	11	0
38	O	44	0	0	7	0
38	P	70	0	0	5	0
38	Q	48	0	0	7	0
38	R	82	0	0	6	0
38	S	33	0	0	5	0
38	T	39	0	0	8	0
38	U	29	0	0	3	0
38	V	13	0	0	3	0
38	W	69	0	0	12	0
38	X	27	0	0	6	0
38	Y	100	0	0	15	0
38	Z	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	99111	0	59983	2986	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 20.

All (2986) 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)
6:9:6:C:H5"	20:N:37:ARG:NH1	1.59	1.16
1:0:156:C:H5"	19:M:171:ARG:HD3	1.25	1.15
6:9:6:C:H5"	20:N:37:ARG:HH12	0.97	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.07
1:0:871:G:H8	1:0:871:G:H5'	1.10	1.06
24:R:18:LEU:HB2	24:R:143:VAL:HG12	1.34	1.05
9:C:236:THR:HG22	9:C:239:ALA:H	1.18	1.04
10:D:25:MET:HE3	10:D:37:ALA:HB1	1.33	1.03
10:D:154:LYS:HD2	10:D:154:LYS:H	1.18	1.03
1:0:871:G:C8	1:0:871:G:H5'	1.94	1.02
28:V:12:THR:HG22	28:V:15:GLU:HG3	1.39	1.01
14:H:59:GLN:HE21	14:H:129:ARG:HE	1.08	1.00
9:C:127:ARG:NH2	9:C:225:PRO:HG2	1.76	1.00
14:H:174:LEU:HA	38:H:4067:HOH:O	1.59	0.99
1:0:870:G:H2'	1:0:871:G:H5"	1.41	0.99
8:B:264:GLU:HG2	8:B:267:LYS:HE2	1.41	0.98
1:0:796:A:HO2'	32:Z:10:ARG:N	1.60	0.98
1:0:381:G:H5"	38:O:4940:HOH:O	1.67	0.95
1:0:1119:G:H2'	16:J:52:GLN:NE2	1.80	0.95
15:I:127:CYS:HB3	15:I:132:VAL:HB	1.45	0.95
31:Y:187:VAL:HG23	31:Y:192:ASP:HB2	1.47	0.95
1:0:21:G:H5'	24:R:2:ILE:HA	1.49	0.94
29:W:6:GLN:HB2	29:W:26:ILE:HD12	1.49	0.94
22:P:59:ARG:NH2	22:P:66:GLN:HE22	1.66	0.93
17:K:10:GLN:NE2	17:K:10:GLN:H	1.66	0.93
10:D:134:LEU:HD11	10:D:166:ILE:HD11	1.46	0.93
30:X:72:VAL:HG22	30:X:85:VAL:HG12	1.50	0.93
30:X:37:LEU:HD13	30:X:85:VAL:HG21	1.47	0.92
1:0:1116:U:HO2'	1:0:1118:A:H2	0.92	0.92
1:0:56:G:H5"	28:V:50:ARG:HH12	1.34	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.35	0.92
19:M:164:THR:HG22	19:M:167:GLY:H	1.32	0.92
29:W:4:LEU:HD22	29:W:52:VAL:HG21	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:76:ASP:HA	38:J:4028:HOH:O	1.71	0.91
7:A:35:GLY:O	7:A:36:ASP:HB3	1.70	0.90
29:W:88:THR:HB	38:W:4041:HOH:O	1.69	0.90
1:0:1116:U:H3	1:0:1246:A:H62	1.18	0.90
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.90
32:Z:46:ARG:HD2	32:Z:59:TYR:HB2	1.52	0.90
1:0:1119:G:H2'	16:J:52:GLN:HE22	1.32	0.90
17:K:10:GLN:HE21	17:K:10:GLN:H	0.91	0.90
1:0:1242:A:H5'	16:J:82:THR:HG23	1.54	0.90
1:0:2756:U:H3	1:0:2896:A:H2	1.17	0.90
6:9:14:G:H5'	6:9:14:G:H8	1.36	0.90
17:K:10:GLN:N	17:K:10:GLN:HE21	1.70	0.89
1:0:1751:G:H2'	1:0:1752:G:H5''	1.54	0.89
8:B:62:ARG:HA	8:B:65:MET:HE3	1.53	0.89
17:K:74:VAL:HG11	17:K:113:ILE:HG12	1.53	0.89
1:0:545:G:H8	1:0:545:G:H5'	1.39	0.88
29:W:72:PRO:HG2	29:W:77:ALA:HB3	1.53	0.88
6:9:76:G:H3'	6:9:77:A:H5''	1.54	0.88
1:0:870:G:C2'	1:0:871:G:H5''	2.03	0.88
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.88
14:H:102:LYS:HD3	14:H:122:LYS:HD3	1.56	0.88
29:W:21:LEU:HD13	29:W:26:ILE:HD11	1.56	0.88
26:T:71:VAL:HG11	26:T:90:PRO:HB3	1.56	0.88
9:C:115:LEU:HD21	9:C:243:VAL:HG13	1.56	0.88
21:O:42:GLU:HB2	38:O:4022:HOH:O	1.73	0.88
20:N:47:LEU:HD11	20:N:127:LEU:HD21	1.54	0.88
14:H:59:GLN:NE2	14:H:129:ARG:HE	1.71	0.87
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
16:J:74:ARG:HB3	16:J:74:ARG:HH11	1.37	0.87
1:0:1160:G:C5'	1:0:1161:A:H5'	2.05	0.87
8:B:320:GLN:NE2	8:B:321:PRO:HD2	1.89	0.87
22:P:115:SER:H	22:P:118:GLN:NE2	1.73	0.87
1:0:542:A:H5'	1:0:542:A:H8	1.38	0.86
27:U:9:CYS:HA	27:U:52:THR:HG23	1.57	0.86
38:O:9587:HOH:O	17:K:39:GLY:HA2	1.74	0.86
1:0:200:C:H2'	38:O:4623:HOH:O	1.76	0.86
9:C:1:MET:HG2	9:C:2:GLN:H	1.41	0.86
1:0:962:C:H1'	20:N:5:ARG:HH12	1.38	0.85
1:0:1160:G:H5'	1:0:1161:A:C5'	2.05	0.85
3:2:41:HIS:H	3:2:45:ASN:HD22	1.23	0.85
1:0:877:G:H5'	1:0:878:G:OP1	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:99:ARG:HD2	19:M:167:GLY:HA2	1.58	0.85
9:C:236:THR:HA	38:C:4113:HOH:O	1.76	0.85
29:W:4:LEU:HD23	29:W:54:PHE:HB3	1.56	0.84
14:H:30:LYS:H	14:H:62:HIS:HD2	1.21	0.84
9:C:236:THR:HG22	9:C:239:ALA:N	1.90	0.84
14:H:12:ILE:HD12	14:H:57:THR:HG22	1.57	0.84
26:T:9:LYS:HE3	26:T:13:ARG:NH1	1.92	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.59	0.84
17:K:81:ARG:HB2	17:K:87:ARG:NH1	1.92	0.84
8:B:201:ASP:HB2	8:B:312:ARG:HD2	1.60	0.84
29:W:88:THR:HG22	29:W:89:ASP:H	1.42	0.84
1:0:2291:A:C8	1:0:2309:C:H5'	2.12	0.84
7:A:135:VAL:HG21	7:A:147:ARG:HG2	1.57	0.83
14:H:12:ILE:HG23	14:H:129:ARG:NE	1.91	0.83
14:H:88:MET:HA	14:H:139:ALA:HA	1.59	0.83
17:K:98:VAL:HG13	17:K:102:GLU:HA	1.61	0.83
9:C:236:THR:H	9:C:239:ALA:HB3	1.44	0.83
1:0:558:C:C2'	1:0:559:U:H5''	2.08	0.83
20:N:48:VAL:CG1	20:N:55:ASP:HB3	2.08	0.83
17:K:98:VAL:CG1	17:K:102:GLU:HA	2.09	0.82
19:M:102:GLU:OE1	19:M:164:THR:HG21	1.79	0.82
12:F:53:ASP:OD1	12:F:80:GLN:HB2	1.80	0.82
18:L:79:ASP:HB3	38:L:4056:HOH:O	1.78	0.82
1:0:1679:C:H5'	38:0:7148:HOH:O	1.79	0.82
1:0:1684:A:H1'	3:2:43:ARG:HH22	1.44	0.82
6:9:28:U:H5''	20:N:40:ASN:ND2	1.95	0.82
30:X:30:MET:HE1	30:X:55:ASN:HA	1.61	0.82
1:0:21:G:C5'	24:R:2:ILE:HA	2.10	0.81
1:0:1559:A:H1'	38:0:7406:HOH:O	1.78	0.81
8:B:217:ARG:HG3	8:B:257:THR:HG22	1.62	0.81
38:0:8757:HOH:O	10:D:99:ASP:HA	1.79	0.81
1:0:1878:G:H1'	38:0:8047:HOH:O	1.80	0.81
1:0:506:G:H22	1:0:509:A:C5'	1.93	0.81
6:9:29:C:H2'	6:9:30:C:H5'	1.62	0.81
1:0:282:C:H1'	1:0:368:C:N4	1.95	0.81
1:0:962:C:H1'	20:N:5:ARG:NH1	1.94	0.81
9:C:162:VAL:HG12	9:C:192:ILE:HD11	1.61	0.81
6:9:6:C:C5'	20:N:37:ARG:NH1	2.44	0.81
28:V:12:THR:HG23	28:V:14:ALA:H	1.45	0.80
20:N:37:ARG:HH21	20:N:105:GLY:CA	1.94	0.80
11:E:97:VAL:HG12	38:E:4024:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:162:MET:HE1	8:B:308:LEU:HD21	1.63	0.80
9:C:2:GLN:HB3	38:C:4008:HOH:O	1.81	0.80
1:0:1162:G:H1'	15:I:112:LEU:HD11	1.61	0.80
1:0:1184:C:H1'	38:0:6660:HOH:O	1.82	0.80
38:0:6622:HOH:O	13:G:12:ILE:HA	1.81	0.80
18:L:35:ARG:HH12	18:L:43:HIS:HB3	1.46	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.44	0.80
1:0:544:G:H2'	1:0:545:G:H5''	1.62	0.80
1:0:1835:U:H5	1:0:1840:A:N7	1.80	0.80
4:3:60:LYS:HG3	4:3:61:PRO:HD2	1.65	0.79
8:B:275:GLY:O	8:B:291:ASP:HA	1.82	0.79
29:W:52:VAL:HG22	29:W:53:ALA:H	1.47	0.79
1:0:157:G:H4'	19:M:95:LYS:HE2	1.64	0.79
17:K:81:ARG:HB2	17:K:87:ARG:HH11	1.47	0.79
29:W:13:MET:HE1	29:W:18:GLN:HA	1.64	0.79
17:K:63:GLU:HB2	38:K:4035:HOH:O	1.83	0.79
1:0:2716:G:H5''	8:B:206:THR:HG21	1.63	0.79
20:N:164:ASP:OD1	20:N:167:ASP:HA	1.84	0.79
7:A:100:PRO:HG2	7:A:103:VAL:HG21	1.64	0.78
10:D:57:THR:HG23	10:D:63:ILE:HA	1.64	0.78
24:R:18:LEU:HB2	24:R:143:VAL:CG1	2.14	0.78
10:D:28:GLY:HA2	10:D:69:ILE:HG23	1.63	0.78
23:Q:75:ILE:HD13	23:Q:84:ILE:HD11	1.66	0.78
28:V:56:ILE:O	28:V:60:GLN:HG3	1.84	0.78
14:H:49:GLN:HG3	14:H:140:TYR:CE2	2.19	0.78
22:P:59:ARG:HH22	22:P:66:GLN:HE22	1.28	0.78
1:0:2890:A:H1'	27:U:56:ARG:NH2	1.98	0.78
1:0:1666:C:H2'	1:0:1667:A:H5'	1.66	0.78
1:0:1118:A:H3'	1:0:1118:A:H8	1.48	0.78
28:V:1:THR:HG23	28:V:2:VAL:H	1.49	0.78
16:J:75:PRO:HG2	16:J:105:LEU:HD21	1.65	0.78
1:0:470:U:O2'	2:1:16:HIS:HD2	1.66	0.77
20:N:80:SER:HB2	38:N:4032:HOH:O	1.84	0.77
12:F:46:GLU:OE1	12:F:100:ASP:HA	1.85	0.77
1:0:1244:U:OP1	16:J:18:ILE:HD13	1.85	0.77
22:P:13:VAL:HG21	22:P:41:ARG:HG2	1.66	0.77
15:I:117:THR:HG22	15:I:121:LYS:HE3	1.66	0.77
1:0:506:G:H22	1:0:509:A:H5'	1.50	0.77
1:0:1209:C:H2'	1:0:1210:G:H8	1.48	0.77
1:0:31:C:H2'	38:0:4094:HOH:O	1.84	0.77
12:F:91:VAL:HG12	12:F:92:GLY:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:248:ARG:O	8:B:251:VAL:HG22	1.85	0.77
30:X:71:ARG:HD3	38:X:4024:HOH:O	1.83	0.77
9:C:242:GLU:HG3	38:C:4172:HOH:O	1.83	0.76
1:O:2908:A:H2'	1:O:2909:G:O4'	1.84	0.76
15:I:97:VAL:HG12	15:I:101:LYS:HE3	1.68	0.76
6:9:56:A:H2'	6:9:57:A:H5''	1.66	0.76
14:H:12:ILE:HG23	14:H:129:ARG:CZ	2.15	0.76
1:O:1163:G:H5'	15:I:110:ASP:O	1.85	0.76
1:O:1834:C:H2'	1:O:1840:A:N6	2.00	0.76
12:F:27:GLY:HA3	12:F:101:ALA:O	1.85	0.76
30:X:76:ARG:HH11	30:X:76:ARG:HG3	1.50	0.76
14:H:30:LYS:H	14:H:62:HIS:CD2	2.04	0.76
29:W:64:THR:O	29:W:68:THR:HG22	1.86	0.76
7:A:191:GLY:HA2	7:A:194:MET:HE3	1.65	0.76
29:W:21:LEU:HD21	29:W:48:VAL:HG11	1.68	0.76
1:O:559:U:H5'	1:O:559:U:H6	1.49	0.76
1:O:1834:C:H2'	1:O:1840:A:H62	1.51	0.76
8:B:320:GLN:HE21	8:B:321:PRO:HD2	1.47	0.76
1:O:1701:A:H5'	38:O:7112:HOH:O	1.85	0.76
1:O:2780:C:H1'	11:E:143:GLN:HE21	1.51	0.76
17:K:30:LYS:O	17:K:55:VAL:HG13	1.86	0.76
8:B:140:LEU:HD23	38:B:4056:HOH:O	1.86	0.76
1:O:182:G:H5'	38:O:4559:HOH:O	1.86	0.75
1:O:1293:U:H5'	31:Y:154:ARG:HH21	1.48	0.75
19:M:24:GLN:NE2	19:M:27:ARG:HH11	1.84	0.75
1:O:1118:A:H3'	1:O:1118:A:C8	2.21	0.75
7:A:81:GLN:HB2	7:A:92:ASN:ND2	2.02	0.75
29:W:21:LEU:HD21	29:W:48:VAL:CG1	2.15	0.75
1:O:56:G:H5''	28:V:50:ARG:NH1	2.00	0.75
8:B:86:ALA:HA	38:B:4056:HOH:O	1.85	0.75
12:F:96:ALA:HA	38:F:4009:HOH:O	1.86	0.75
8:B:18:ARG:HG3	8:B:256:GLN:HG3	1.67	0.75
1:O:545:G:C8	1:O:545:G:H5'	2.21	0.75
19:M:164:THR:HG22	19:M:167:GLY:N	2.01	0.75
6:9:14:G:H5'	6:9:14:G:C8	2.20	0.75
1:O:383:A:H4'	38:O:4952:HOH:O	1.86	0.75
20:N:113:SER:HB2	38:N:4044:HOH:O	1.86	0.75
1:O:1474:C:C6	1:O:1474:C:H5'	2.22	0.74
7:A:36:ASP:OD2	7:A:85:SER:HB2	1.87	0.74
8:B:27:ASN:H	8:B:27:ASN:HD22	1.34	0.74
8:B:321:PRO:HA	38:B:4076:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:49:GLN:OE1	14:H:169:GLU:HG3	1.87	0.74
2:1:25:LYS:HD2	3:2:49:GLU:H	1.52	0.74
31:Y:187:VAL:HG23	31:Y:192:ASP:CB	2.17	0.74
16:J:74:ARG:CB	16:J:74:ARG:HH11	1.99	0.74
1:0:10:U:H3'	38:0:5259:HOH:O	1.85	0.74
10:D:99:ASP:HB3	10:D:103:ASN:H	1.52	0.74
1:0:1741:U:H5'	1:0:1742:A:OP1	1.87	0.74
17:K:14:LYS:HB2	17:K:45:PRO:HG2	1.69	0.74
1:0:2364:A:H5''	23:Q:15:LYS:HD3	1.70	0.74
9:C:236:THR:HG21	38:C:4116:HOH:O	1.88	0.74
20:N:48:VAL:HG11	20:N:55:ASP:HB3	1.70	0.74
6:9:48:C:H4'	20:N:141:ARG:NH2	2.03	0.74
4:3:25:VAL:HG22	4:3:68:LYS:HG3	1.68	0.74
16:J:39:VAL:HG13	16:J:106:GLY:O	1.88	0.73
6:9:92:G:H2'	6:9:93:A:C8	2.22	0.73
23:Q:25:PRO:HB2	38:Q:4023:HOH:O	1.88	0.73
1:0:1667:A:H8	1:0:1667:A:H5'	1.54	0.73
29:W:151:GLU:O	29:W:154:ARG:HB3	1.88	0.73
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.73
1:0:2748:G:H2'	38:0:8299:HOH:O	1.89	0.73
1:0:711:G:H1'	38:0:5613:HOH:O	1.87	0.73
18:L:143:THR:HG21	38:L:4069:HOH:O	1.87	0.73
18:L:148:GLU:HA	38:L:4074:HOH:O	1.88	0.73
1:0:544:G:C2'	1:0:545:G:H5''	2.18	0.73
28:V:42:ASN:HB3	38:V:4008:HOH:O	1.88	0.73
1:0:1130:U:H5'	38:0:6587:HOH:O	1.89	0.73
1:0:1884:G:O6	7:A:190:ARG:HD2	1.87	0.73
28:V:12:THR:HG22	28:V:15:GLU:CG	2.19	0.73
1:0:558:C:H2'	1:0:559:U:H5''	1.69	0.73
15:I:96:SER:H	15:I:99:GLN:NE2	1.87	0.73
14:H:62:HIS:HA	14:H:65:LEU:HD23	1.71	0.72
23:Q:75:ILE:CD1	23:Q:84:ILE:HD11	2.18	0.72
20:N:47:LEU:HD13	20:N:97:VAL:HG11	1.69	0.72
16:J:107:ASN:ND2	16:J:109:TYR:H	1.85	0.72
1:0:1603:A:H5'	1:0:1605:G:O4'	1.89	0.72
28:V:39:ALA:N	28:V:40:PRO:HD2	2.05	0.72
24:R:132:ARG:HG2	24:R:133:ALA:N	2.05	0.72
14:H:6:ALA:HA	14:H:61:ARG:HH12	1.53	0.72
20:N:169:PRO:O	20:N:172:PHE:HB3	1.88	0.72
22:P:143:ALA:HA	38:P:4070:HOH:O	1.88	0.72
29:W:132:VAL:HG21	29:W:140:LYS:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:6:ALA:HA	14:H:61:ARG:NH1	2.04	0.72
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.72
8:B:179:LEU:O	8:B:183:GLU:HG2	1.89	0.72
10:D:25:MET:SD	10:D:40:ILE:HD11	2.30	0.72
29:W:52:VAL:HG22	29:W:53:ALA:N	2.05	0.72
29:W:88:THR:HG23	29:W:110:GLN:NE2	2.04	0.72
12:F:58:GLU:OE1	19:M:27:ARG:NH2	2.23	0.72
27:U:47:ARG:HG3	38:U:4026:HOH:O	1.90	0.72
10:D:135:VAL:HG21	10:D:139:TYR:CD1	2.24	0.72
6:9:48:C:H4'	20:N:141:ARG:HH21	1.55	0.71
1:0:1450:C:H4'	1:0:1451:C:OP2	1.88	0.71
1:0:821:U:H2'	1:0:822:C:H6	1.54	0.71
8:B:190:MET:HE2	8:B:194:PHE:CD1	2.25	0.71
31:Y:174:VAL:HG12	31:Y:177:LYS:HD2	1.71	0.71
6:9:54:A:O2'	6:9:55:U:H5'	1.90	0.71
1:0:694:A:H2'	1:0:695:C:H5'	1.72	0.71
14:H:165:ARG:HD3	38:H:4017:HOH:O	1.89	0.71
6:9:114:G:O6	20:N:11:ARG:HD3	1.91	0.71
1:0:2270:G:H4'	7:A:223:ARG:HH12	1.55	0.71
22:P:103:THR:O	22:P:107:GLU:HG3	1.91	0.71
8:B:36:PRO:HA	8:B:168:GLY:HA3	1.73	0.71
9:C:145:GLU:HG3	38:C:4116:HOH:O	1.88	0.71
8:B:212:GLN:HB2	8:B:257:THR:HG21	1.70	0.71
21:O:32:ARG:HD3	21:O:32:ARG:O	1.90	0.71
1:0:2812:A:H2	1:0:2814:A:H62	1.37	0.71
3:2:22:PRO:HG2	3:2:25:VAL:HG23	1.73	0.71
1:0:1819:G:H2'	1:0:1820:G:H4'	1.72	0.71
9:C:142:ASP:OD1	9:C:237:GLU:HB3	1.91	0.71
1:0:2320:U:H4'	1:0:2321:A:O4'	1.90	0.71
1:0:156:C:H5''	19:M:171:ARG:CD	2.15	0.71
14:H:32:ALA:HB3	14:H:69:ARG:HH12	1.54	0.71
10:D:146:LYS:NZ	20:N:107:ASN:HD21	1.89	0.70
20:N:38:LYS:HE2	20:N:107:ASN:ND2	2.05	0.70
1:0:960:G:H4'	38:O:6251:HOH:O	1.90	0.70
9:C:233:THR:HG22	9:C:234:VAL:H	1.56	0.70
29:W:137:GLN:HE21	29:W:141:HIS:HE1	1.38	0.70
1:0:1206:U:H5'	1:0:1206:U:H6	1.56	0.70
16:J:19:MET:HE3	16:J:132:LEU:HD11	1.72	0.70
29:W:6:GLN:HB2	29:W:26:ILE:CD1	2.20	0.70
14:H:59:GLN:HE21	14:H:129:ARG:NE	1.88	0.70
19:M:65:VAL:HG21	19:M:105:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:39:THR:HB	24:R:42:GLU:HG3	1.72	0.70
12:F:2:VAL:HG22	12:F:57:GLU:OE1	1.92	0.70
1:0:259:G:H21	19:M:58:GLN:NE2	1.88	0.70
20:N:61:ALA:HB3	20:N:88:ALA:HB2	1.72	0.70
1:0:1377:C:H6	1:0:1377:C:H5'	1.56	0.70
1:0:814:G:H4'	38:0:5807:HOH:O	1.90	0.70
8:B:162:MET:HE2	8:B:310:ARG:HD3	1.73	0.70
8:B:55:ASN:HB3	8:B:63:GLU:HA	1.74	0.70
18:L:133:VAL:HA	38:L:4073:HOH:O	1.91	0.70
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.70
30:X:72:VAL:HG22	30:X:85:VAL:CG1	2.19	0.70
1:0:2637:A:H5'	38:0:9469:HOH:O	1.91	0.70
25:S:51:GLN:HE21	25:S:53:ASN:HD21	1.40	0.70
16:J:19:MET:HE2	16:J:79:PHE:HA	1.72	0.70
12:F:63:ILE:HB	12:F:64:PRO:HD3	1.72	0.70
27:U:14:GLU:O	27:U:17:THR:HB	1.92	0.70
25:S:42:GLU:HG2	25:S:49:VAL:HG23	1.74	0.70
30:X:78:GLU:HG2	30:X:79:GLU:H	1.56	0.70
22:P:59:ARG:HH22	22:P:66:GLN:NE2	1.89	0.69
7:A:88:ILE:HD13	7:A:100:PRO:HD3	1.72	0.69
9:C:1:MET:HG2	9:C:2:GLN:N	2.07	0.69
24:R:99:ALA:HB1	24:R:109:MET:CE	2.22	0.69
1:0:558:C:H2'	1:0:559:U:C5'	2.21	0.69
17:K:29:LEU:HB3	17:K:55:VAL:HG11	1.73	0.69
16:J:107:ASN:HD22	16:J:107:ASN:C	1.95	0.69
38:0:4887:HOH:O	26:T:53:GLY:HA3	1.92	0.69
7:A:68:ILE:HD11	38:A:4039:HOH:O	1.92	0.69
29:W:88:THR:HG23	29:W:110:GLN:HE21	1.58	0.69
1:0:558:C:O2'	1:0:559:U:H5''	1.92	0.69
30:X:43:VAL:HG11	30:X:82:GLU:HA	1.74	0.69
1:0:2783:A:H3'	38:0:9728:HOH:O	1.93	0.69
1:0:1187:U:H2'	38:0:6670:HOH:O	1.92	0.69
9:C:246:ARG:HD2	38:C:4175:HOH:O	1.93	0.69
1:0:57:C:H5''	38:0:4179:HOH:O	1.93	0.68
32:Z:26:VAL:O	32:Z:30:GLU:HG3	1.93	0.68
18:L:35:ARG:HB2	18:L:35:ARG:NH1	2.08	0.68
15:I:101:LYS:O	15:I:105:GLU:HG3	1.94	0.68
7:A:94:LEU:HG	7:A:99:ILE:HD11	1.75	0.68
24:R:119:VAL:HG21	24:R:142:ASP:CG	2.13	0.68
7:A:200:PRO:HD3	38:A:4109:HOH:O	1.92	0.68
1:0:2506:A:O2'	1:0:2507:G:H8	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:61:MET:HB3	19:M:19:GLN:OE1	1.93	0.68
1:0:2426:G:H1'	38:0:8731:HOH:O	1.92	0.68
11:E:145:ALA:HB1	11:E:168:ILE:HD11	1.76	0.68
15:I:88:GLN:HA	15:I:91:PHE:CE2	2.28	0.68
29:W:5:VAL:HG11	29:W:153:MET:HE3	1.74	0.68
7:A:199:HIS:HD2	7:A:201:PHE:H	1.42	0.68
32:Z:37:HIS:HB2	32:Z:47:VAL:HB	1.75	0.68
32:Z:57:CYS:SG	32:Z:59:TYR:HB3	2.32	0.68
17:K:74:VAL:CG1	17:K:113:ILE:HG12	2.22	0.68
15:I:118:ASN:HA	15:I:121:LYS:HD2	1.75	0.68
27:U:17:THR:HG22	27:U:18:GLY:N	2.07	0.68
8:B:304:PRO:HD2	8:B:307:ARG:HD2	1.76	0.68
1:0:214:U:H5'	38:0:4670:HOH:O	1.92	0.68
1:0:236:A:H4'	1:0:237:G:H5'	1.75	0.68
1:0:399:C:H5'	19:M:179:GLY:O	1.93	0.68
38:0:4801:HOH:O	19:M:58:GLN:HG3	1.93	0.68
24:R:8:ALA:HB1	24:R:13:THR:HG21	1.74	0.68
1:0:447:A:P	26:T:1:SER:HB2	2.34	0.68
7:A:51:ARG:HB2	38:A:4031:HOH:O	1.94	0.68
10:D:25:MET:HE3	10:D:37:ALA:CB	2.20	0.68
29:W:88:THR:HG22	29:W:89:ASP:N	2.08	0.68
7:A:88:ILE:HG22	7:A:88:ILE:O	1.92	0.68
17:K:13:GLU:OE2	17:K:44:LEU:HB2	1.93	0.68
10:D:154:LYS:HD2	10:D:154:LYS:N	2.02	0.68
1:0:1189:A:H1'	1:0:1209:C:O4'	1.94	0.68
1:0:450:C:OP1	9:C:184:ARG:NH2	2.24	0.68
8:B:141:ARG:HD2	8:B:163:GLU:OE2	1.94	0.68
1:0:21:G:H5''	24:R:1:GLY:O	1.95	0.67
29:W:84:VAL:HG12	38:W:4041:HOH:O	1.93	0.67
9:C:61:PHE:HB3	38:C:4050:HOH:O	1.93	0.67
1:0:2533:C:C6	1:0:2533:C:H5'	2.28	0.67
24:R:96:VAL:HG13	24:R:106:GLY:HA3	1.75	0.67
10:D:65:GLU:HA	38:D:4024:HOH:O	1.93	0.67
1:0:1157:C:H2'	1:0:1158:G:H8	1.56	0.67
11:E:137:ASP:OD1	11:E:139:GLU:HB2	1.94	0.67
18:L:136:ALA:HB3	38:L:4073:HOH:O	1.94	0.67
1:0:1417:G:O2'	3:2:11:LEU:HD22	1.94	0.67
8:B:162:MET:CE	8:B:308:LEU:HD21	2.23	0.67
10:D:146:LYS:HZ3	20:N:107:ASN:HD21	1.42	0.67
9:C:132:ASP:HB3	38:C:4107:HOH:O	1.93	0.67
10:D:84:LEU:HA	10:D:87:ALA:HB3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:67:ARG:O	18:L:71:GLU:HG3	1.95	0.67
1:0:1160:G:O2'	1:0:1190:G:H1'	1.95	0.67
1:0:2036:C:O4'	17:K:44:LEU:HG	1.94	0.67
7:A:161:GLY:O	32:Z:68:SER:HB2	1.95	0.67
10:D:159:PRO:O	10:D:163:VAL:HG23	1.94	0.67
2:1:21:ARG:HD2	2:1:37:CYS:SG	2.35	0.67
8:B:140:LEU:HA	38:B:4056:HOH:O	1.94	0.67
16:J:107:ASN:HD21	16:J:109:TYR:HB2	1.60	0.67
1:0:2635:A:O2'	1:0:2636:C:H5'	1.95	0.67
4:3:70:ARG:HG2	4:3:77:ALA:HB2	1.77	0.67
1:0:1654:U:H2'	7:A:47:HIS:HD2	1.59	0.67
19:M:99:ARG:CD	19:M:167:GLY:HA2	2.24	0.67
10:D:146:LYS:NZ	20:N:107:ASN:ND2	2.43	0.67
1:0:111:C:O2'	2:1:20:ARG:HG2	1.94	0.67
1:0:2524:G:H21	1:0:2526:C:N4	1.92	0.67
17:K:34:VAL:HG22	17:K:47:ALA:HB2	1.77	0.67
8:B:139:ASP:HB2	8:B:165:ARG:HE	1.60	0.67
29:W:80:ASP:O	29:W:84:VAL:HG23	1.95	0.67
19:M:78:LYS:HE2	38:M:4053:HOH:O	1.95	0.67
17:K:132:VAL:HG11	27:U:22:VAL:HG22	1.76	0.67
29:W:5:VAL:HG11	29:W:153:MET:CE	2.26	0.66
1:0:542:A:H5'	1:0:542:A:C8	2.27	0.66
1:0:1189:A:H1'	1:0:1209:C:C1'	2.25	0.66
9:C:233:THR:HG22	9:C:234:VAL:N	2.10	0.66
24:R:39:THR:HG23	24:R:107:GLU:O	1.95	0.66
7:A:211:LYS:HB3	7:A:212:PRO:HD2	1.76	0.66
1:0:1790:C:H2'	1:0:1791:U:H6	1.60	0.66
1:0:338:C:H4'	9:C:174:ILE:CD1	2.25	0.66
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.66
7:A:64:ASP:OD1	7:A:66:ARG:HD2	1.95	0.66
20:N:164:ASP:CG	20:N:167:ASP:HA	2.16	0.66
16:J:6:PHE:HB3	16:J:109:TYR:OH	1.94	0.66
1:0:21:G:H4'	24:R:2:ILE:HG22	1.78	0.66
8:B:62:ARG:HA	8:B:65:MET:CE	2.23	0.66
31:Y:151:SER:HB3	31:Y:154:ARG:HB3	1.78	0.66
9:C:180:SER:HB2	38:C:4125:HOH:O	1.94	0.66
14:H:23:ILE:HG23	14:H:123:ILE:HD11	1.77	0.66
1:0:1593:C:OP1	22:P:117:SER:HB3	1.96	0.66
28:V:64:GLY:O	28:V:65:ASP:HB2	1.96	0.66
17:K:28:GLU:HG2	17:K:58:THR:HB	1.78	0.66
11:E:132:THR:HB	38:E:4031:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2508:C:H2'	38:0:9135:HOH:O	1.95	0.66
1:0:1666:C:O2'	1:0:1667:A:H5''	1.95	0.66
21:O:21:SER:OG	21:O:106:PRO:HB2	1.94	0.66
1:0:657:G:OP1	9:C:27:ARG:NH2	2.28	0.66
29:W:129:LYS:HG2	38:W:4056:HOH:O	1.96	0.66
10:D:64:ARG:HB3	10:D:67:ASP:OD2	1.95	0.66
1:0:1121:G:H4'	38:0:6566:HOH:O	1.94	0.66
9:C:139:VAL:HG13	38:C:4171:HOH:O	1.95	0.66
8:B:62:ARG:CA	8:B:65:MET:HE3	2.25	0.66
20:N:34:LEU:HA	20:N:47:LEU:HD23	1.77	0.66
23:Q:26:PRO:O	23:Q:30:VAL:HG23	1.95	0.66
20:N:120:GLU:HG3	20:N:136:LEU:HD13	1.76	0.66
1:0:1007:A:H2'	14:H:22:TYR:CZ	2.31	0.66
20:N:37:ARG:HD3	36:N:8807:CL:CL	2.32	0.66
3:2:22:PRO:HG2	3:2:25:VAL:CG2	2.25	0.66
22:P:65:ARG:HD3	22:P:69:ARG:NH1	2.10	0.66
14:H:49:GLN:HB2	14:H:170:ARG:HD2	1.77	0.66
1:0:1372:A:H3'	38:0:7038:HOH:O	1.95	0.66
17:K:22:ASP:HB2	38:K:4013:HOH:O	1.96	0.66
1:0:1615:A:H4'	38:0:7475:HOH:O	1.95	0.66
7:A:199:HIS:CD2	7:A:201:PHE:H	2.14	0.65
7:A:200:PRO:HG2	7:A:225:VAL:HG21	1.78	0.65
4:3:62:THR:HB	38:3:4046:HOH:O	1.95	0.65
10:D:25:MET:HE1	10:D:41:LEU:HG	1.78	0.65
15:I:120:ALA:O	15:I:124:VAL:HG23	1.96	0.65
1:0:447:A:OP1	26:T:2:LYS:HG2	1.97	0.65
20:N:78:MET:HB2	20:N:79:PRO:HD3	1.78	0.65
1:0:2414:A:H2'	1:0:2415:A:C8	2.29	0.65
1:0:1053:G:OP1	14:H:15:PRO:HG3	1.96	0.65
22:P:134:VAL:O	22:P:137:LEU:HB3	1.95	0.65
14:H:12:ILE:O	14:H:12:ILE:HG22	1.96	0.65
3:2:49:GLU:HB2	38:2:4042:HOH:O	1.94	0.65
1:0:513:A:N3	38:0:5219:HOH:O	2.29	0.65
9:C:5:ILE:HD11	9:C:16:VAL:CG2	2.27	0.65
1:0:541:C:C2'	1:0:542:A:H5''	2.26	0.65
28:V:55:ARG:O	28:V:59:ILE:HG12	1.95	0.65
2:1:46:ARG:HA	38:1:4044:HOH:O	1.96	0.65
24:R:18:LEU:HD12	24:R:143:VAL:HG11	1.78	0.65
27:U:52:THR:HG22	27:U:54:THR:H	1.61	0.65
21:O:47:ARG:HG3	21:O:47:ARG:HH11	1.61	0.65
1:0:645:U:OP2	18:L:4:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:121:ALA:O	7:A:124:VAL:HG22	1.96	0.65
10:D:23:VAL:HG21	10:D:45:THR:HG21	1.77	0.65
27:U:9:CYS:SG	27:U:11:THR:HG23	2.36	0.65
1:O:2850:C:H6	1:O:2850:C:H5'	1.62	0.65
38:O:6656:HOH:O	15:I:87:PRO:HD3	1.96	0.65
10:D:35:ALA:HB1	38:D:4017:HOH:O	1.95	0.65
1:O:447:A:OP2	26:T:1:SER:HB2	1.97	0.65
25:S:77:VAL:O	25:S:80:ARG:HG2	1.97	0.65
23:Q:66:LYS:HB2	23:Q:70:ALA:O	1.97	0.65
16:J:103:VAL:HG12	38:J:4028:HOH:O	1.97	0.65
11:E:118:ILE:HG23	11:E:144:THR:HG21	1.79	0.65
7:A:109:GLU:HG2	7:A:116:GLY:H	1.61	0.65
18:L:22:ARG:HG2	38:L:4026:HOH:O	1.96	0.65
7:A:66:ARG:HH11	7:A:66:ARG:HB2	1.61	0.65
1:O:272:A:H5'	1:O:273:G:OP2	1.96	0.65
21:O:10:LEU:HD13	21:O:99:GLU:HG3	1.79	0.65
38:O:7935:HOH:O	2:I:1:THR:HB	1.96	0.65
11:E:22:VAL:O	11:E:76:VAL:HG11	1.97	0.65
17:K:74:VAL:HG13	17:K:113:ILE:HG23	1.79	0.64
1:O:281:U:H2'	1:O:282:C:O4'	1.97	0.64
18:L:35:ARG:HB2	18:L:35:ARG:HH11	1.61	0.64
10:D:35:ALA:C	10:D:37:ALA:H	1.99	0.64
1:O:2769:C:C2'	1:O:2770:G:H5'	2.27	0.64
11:E:37:ASP:OD1	16:J:125:SER:HB3	1.97	0.64
26:T:24:ARG:HH21	26:T:39:ASN:HD22	1.44	0.64
14:H:146:ALA:O	14:H:149:VAL:HG12	1.98	0.64
29:W:137:GLN:HE21	29:W:141:HIS:CE1	2.15	0.64
20:N:139:TRP:HA	20:N:139:TRP:CE3	2.31	0.64
20:N:67:ALA:HA	20:N:71:TRP:HB3	1.80	0.64
4:3:87:ARG:HD2	4:3:89:GLU:OE2	1.98	0.64
17:K:75:ARG:CZ	38:K:4040:HOH:O	2.45	0.64
11:E:100:ASP:HB2	38:E:4025:HOH:O	1.96	0.64
1:O:709:G:O2'	21:O:25:VAL:HG12	1.97	0.64
19:M:64:ARG:HD2	38:M:4020:HOH:O	1.97	0.64
11:E:20:ILE:HD11	11:E:40:VAL:HG11	1.80	0.64
16:J:54:VAL:HG11	16:J:138:THR:HG21	1.80	0.64
8:B:7:ARG:NH1	8:B:11:LEU:HD22	2.13	0.64
20:N:132:ASN:O	20:N:135:VAL:HG12	1.98	0.64
8:B:314:ALA:HB3	8:B:317:PRO:HG3	1.80	0.64
12:F:34:ASN:HA	19:M:4:ALA:HB2	1.78	0.64
11:E:81:GLU:HG2	11:E:134:SER:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:259:G:H21	19:M:58:GLN:HE22	1.45	0.64
14:H:100:GLU:HB3	14:H:124:VAL:HG11	1.78	0.64
7:A:217:ARG:HG2	7:A:229:ALA:HB2	1.80	0.64
1:0:1116:U:O2'	1:0:1118:A:H2	1.73	0.63
1:0:1119:G:N2	1:0:1246:A:C2	2.64	0.63
1:0:2807:U:P	8:B:27:ASN:HD21	2.21	0.63
1:0:2524:G:H21	1:0:2526:C:H41	1.44	0.63
6:9:20:G:H3'	38:9:4022:HOH:O	1.98	0.63
29:W:90:TYR:N	29:W:90:TYR:CD1	2.65	0.63
8:B:162:MET:HG3	8:B:310:ARG:HD3	1.80	0.63
30:X:37:LEU:CD1	30:X:85:VAL:HG21	2.27	0.63
27:U:46:ALA:HB1	27:U:52:THR:HG21	1.80	0.63
30:X:71:ARG:HB3	30:X:88:GLU:OE1	1.99	0.63
22:P:20:ARG:NH1	22:P:54:LYS:HD3	2.13	0.63
25:S:11:THR:H	25:S:14:ALA:HB3	1.64	0.63
15:I:87:PRO:C	15:I:89:GLU:H	2.02	0.63
16:J:42:GLU:O	16:J:131:THR:HG23	1.99	0.63
29:W:4:LEU:CD2	29:W:54:PHE:HB3	2.25	0.63
20:N:47:LEU:HD12	20:N:92:ALA:HB1	1.78	0.63
26:T:9:LYS:HE3	26:T:13:ARG:CZ	2.27	0.63
1:0:280:C:H2'	1:0:281:U:O4'	1.99	0.63
30:X:76:ARG:O	30:X:77:PHE:HB3	1.97	0.63
11:E:133:VAL:HG12	11:E:141:VAL:HG13	1.80	0.63
18:L:72:ASN:HB2	38:L:4049:HOH:O	1.98	0.63
23:Q:18:PRO:O	23:Q:21:ARG:HB2	1.98	0.63
7:A:211:LYS:HB2	38:A:4100:HOH:O	1.97	0.63
20:N:139:TRP:HA	20:N:139:TRP:HE3	1.63	0.63
30:X:21:PRO:HG2	30:X:24:LYS:HD3	1.81	0.63
18:L:121:ILE:HG12	18:L:141:GLU:HB2	1.79	0.63
8:B:5:ARG:NH1	8:B:8:LYS:HE2	2.14	0.63
1:0:1164:U:OP1	15:I:69:PRO:HA	1.98	0.63
29:W:13:MET:HE3	29:W:17:ILE:HG22	1.81	0.63
1:0:588:G:O6	29:W:154:ARG:NH1	2.32	0.63
1:0:2598:U:H5''	17:K:36:GLY:HA2	1.80	0.63
11:E:2:ARG:HH21	11:E:48:VAL:HG21	1.62	0.63
1:0:1751:G:C2'	1:0:1752:G:H5''	2.29	0.63
14:H:114:ASP:HB2	38:H:4044:HOH:O	1.98	0.63
26:T:43:ASN:ND2	26:T:108:ARG:CZ	2.62	0.63
1:0:1641:A:H2'	1:0:1642:A:H5'	1.81	0.63
1:0:603:A:H5''	1:0:604:G:OP1	1.98	0.63
14:H:49:GLN:HB3	14:H:170:ARG:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H5'	38:0:7834:HOH:O	1.98	0.62
25:S:53:ASN:N	25:S:53:ASN:HD22	1.96	0.62
1:0:338:C:H4'	9:C:174:ILE:HD11	1.81	0.62
1:0:2112:A:H2'	1:0:2113:G:C8	2.34	0.62
7:A:29:HIS:CB	7:A:153:ARG:HH12	2.10	0.62
12:F:38:LYS:NZ	19:M:3:SER:HA	2.13	0.62
29:W:81:ASP:OD1	29:W:92:ASP:HB2	1.99	0.62
16:J:19:MET:HE1	16:J:132:LEU:HD21	1.81	0.62
1:0:2547:C:OP2	8:B:5:ARG:NH1	2.32	0.62
1:0:541:C:H2'	1:0:542:A:C5'	2.29	0.62
14:H:30:LYS:N	14:H:62:HIS:HD2	1.94	0.62
16:J:39:VAL:HG11	16:J:107:ASN:HB2	1.80	0.62
13:G:71:LEU:C	13:G:73:ASP:H	2.01	0.62
1:0:2894:C:O2'	1:0:2895:C:H5'	1.99	0.62
15:I:119:ALA:O	15:I:123:VAL:HG23	2.00	0.62
1:0:2276:U:H5'	38:0:4495:HOH:O	1.99	0.62
8:B:264:GLU:HG2	8:B:267:LYS:CE	2.22	0.62
1:0:1666:C:C2'	1:0:1667:A:H5'	2.30	0.62
1:0:1348:A:H3'	38:0:6958:HOH:O	1.99	0.62
38:3:4033:HOH:O	19:M:84:LYS:HE2	1.98	0.62
7:A:96:LEU:HD22	7:A:128:LEU:HD13	1.80	0.62
15:I:129:SER:O	15:I:130:LEU:HD23	2.00	0.62
16:J:46:ILE:HD11	16:J:53:ILE:CG2	2.29	0.62
6:9:56:A:C2'	6:9:57:A:H5''	2.29	0.62
20:N:58:LEU:N	20:N:58:LEU:HD12	2.15	0.62
1:0:138:U:OP2	1:0:139:C:H5	1.83	0.62
10:D:104:PHE:CE2	10:D:132:VAL:HB	2.35	0.62
22:P:98:ILE:HD12	22:P:102:ARG:NE	2.14	0.62
16:J:130:VAL:HG12	16:J:131:THR:N	2.12	0.62
8:B:162:MET:CE	8:B:310:ARG:HD3	2.29	0.62
12:F:91:VAL:HG12	12:F:92:GLY:H	1.65	0.62
6:9:35:C:H5''	38:9:4047:HOH:O	1.99	0.62
16:J:99:GLU:HA	38:J:4030:HOH:O	1.98	0.62
14:H:57:THR:HA	14:H:130:VAL:O	2.00	0.62
20:N:73:ALA:HB1	20:N:74:PRO:CD	2.30	0.62
14:H:61:ARG:HG3	14:H:61:ARG:HH11	1.63	0.62
25:S:33:SER:OG	25:S:36:GLU:HG3	2.00	0.62
9:C:140:VAL:HB	38:C:4113:HOH:O	2.00	0.62
29:W:4:LEU:HD22	29:W:52:VAL:CG2	2.26	0.62
1:0:1242:A:H5'	16:J:82:THR:CG2	2.28	0.62
28:V:44:GLY:O	28:V:48:GLU:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:21:THR:HG23	11:E:30:THR:OG1	1.99	0.62
8:B:145:HIS:HD2	8:B:146:THR:O	1.83	0.62
1:0:2862:G:H4'	8:B:336:GLN:O	2.00	0.62
1:0:2766:A:H5'	38:0:9708:HOH:O	1.99	0.62
7:A:191:GLY:HA2	7:A:194:MET:CE	2.29	0.62
7:A:211:LYS:HD3	38:A:4101:HOH:O	1.99	0.62
31:Y:235:GLU:H	31:Y:235:GLU:CD	2.02	0.62
19:M:125:ARG:NH1	38:M:4086:HOH:O	2.32	0.62
1:0:1328:A:OP1	31:Y:169:ARG:HD2	2.00	0.62
8:B:41:PHE:HA	8:B:79:MET:HE2	1.80	0.61
1:0:2420:G:O2'	1:0:2421:G:H5'	1.99	0.61
21:O:73:ASP:HA	21:O:92:VAL:O	2.00	0.61
4:3:74:CYS:N	38:3:4056:HOH:O	2.31	0.61
22:P:14:LEU:HD13	22:P:51:ALA:HB2	1.80	0.61
18:L:143:THR:HG22	18:L:144:ASP:N	2.15	0.61
1:0:1717:A:H5''	22:P:54:LYS:HB2	1.82	0.61
22:P:20:ARG:HH12	22:P:54:LYS:HD3	1.64	0.61
17:K:62:PRO:HG3	17:K:65:ARG:HH21	1.65	0.61
29:W:13:MET:CE	29:W:17:ILE:HG22	2.30	0.61
28:V:57:LYS:HA	28:V:60:GLN:HE21	1.65	0.61
6:9:14:G:O2'	20:N:1:ALA:HB2	2.01	0.61
25:S:33:SER:O	25:S:37:VAL:HG23	2.00	0.61
26:T:69:LYS:O	26:T:71:VAL:HG23	2.00	0.61
1:0:541:C:H2'	1:0:542:A:H5''	1.82	0.61
1:0:1234:U:N3	8:B:244:PRO:HB3	2.15	0.61
1:0:2756:U:N3	1:0:2896:A:H2	1.96	0.61
38:0:7521:HOH:O	7:A:165:THR:HG23	2.00	0.61
1:0:621:C:H5'	31:Y:132:ASP:OD2	2.01	0.61
29:W:21:LEU:HB3	29:W:26:ILE:HG12	1.83	0.61
18:L:53:ARG:NH2	18:L:57:VAL:HG12	2.16	0.61
11:E:11:VAL:HG12	11:E:12:ASP:N	2.14	0.61
8:B:202:VAL:HG11	8:B:301:VAL:HG13	1.81	0.61
1:0:2453:G:H3'	38:0:8991:HOH:O	2.01	0.61
4:3:55:VAL:HB	4:3:56:PRO:HD2	1.83	0.61
19:M:30:GLU:O	19:M:34:GLU:HG3	2.01	0.61
18:L:143:THR:HG22	18:L:145:LEU:H	1.66	0.61
9:C:150:THR:HA	9:C:203:ALA:O	2.00	0.61
18:L:61:ALA:HA	38:L:4063:HOH:O	2.01	0.61
29:W:6:GLN:HG2	29:W:29:VAL:HA	1.82	0.61
14:H:49:GLN:HG3	14:H:140:TYR:CD2	2.35	0.61
1:0:602:A:O2'	1:0:605:C:H4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1919:A:H4'	38:0:8115:HOH:O	1.99	0.61
9:C:188:ARG:HD3	38:C:4149:HOH:O	2.00	0.61
26:T:55:PHE:CD2	26:T:77:VAL:HG13	2.35	0.61
1:0:2472:C:O2'	1:0:2634:G:H4'	2.00	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.61
29:W:65:VAL:CG1	29:W:116:LEU:HD13	2.30	0.61
1:0:2036:C:C1'	17:K:44:LEU:HG	2.30	0.61
8:B:294:TYR:HE2	38:B:4127:HOH:O	1.82	0.61
9:C:78:ARG:HH11	9:C:78:ARG:HG3	1.66	0.61
12:F:26:THR:HG21	12:F:102:GLY:C	2.21	0.61
38:0:7726:HOH:O	8:B:254:GLN:HG3	2.00	0.60
38:0:9855:HOH:O	27:U:56:ARG:HD3	2.01	0.60
2:1:25:LYS:HE2	38:2:4044:HOH:O	2.00	0.60
1:0:2004:U:H4'	38:0:8225:HOH:O	2.00	0.60
1:0:1544:U:H2'	1:0:1545:C:H6	1.66	0.60
13:G:27:ILE:HD13	13:G:71:LEU:HD23	1.82	0.60
8:B:195:ARG:HG2	8:B:323:LEU:HD22	1.82	0.60
1:0:660:A:H4'	1:0:661:G:O5'	2.01	0.60
1:0:308:U:C4	1:0:342:C:H1'	2.36	0.60
1:0:794:U:H3	1:0:819:A:H61	1.49	0.60
8:B:154:VAL:HG12	8:B:156:LYS:HG2	1.83	0.60
8:B:80:ARG:HD3	38:B:4070:HOH:O	2.02	0.60
24:R:111:ILE:HG23	24:R:145:LEU:HD11	1.83	0.60
16:J:133:GLY:O	16:J:137:GLU:HG3	2.00	0.60
8:B:74:ILE:HG13	38:B:4036:HOH:O	2.00	0.60
15:I:84:SER:HB3	15:I:92:VAL:CG2	2.32	0.60
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.60
6:9:13:A:O2'	6:9:14:G:H5''	2.01	0.60
16:J:26:VAL:HG13	16:J:36:VAL:HG11	1.82	0.60
1:0:2445:U:H2'	1:0:2446:G:C8	2.37	0.60
24:R:47:LEU:HB2	24:R:89:LEU:HD21	1.83	0.60
14:H:23:ILE:HG23	14:H:123:ILE:CD1	2.31	0.60
26:T:43:ASN:HD22	26:T:108:ARG:NH2	1.98	0.60
8:B:66:GLU:OE1	8:B:328:ARG:HD2	2.00	0.60
26:T:73:HIS:HD2	26:T:88:PRO:HG3	1.66	0.60
11:E:3:VAL:HG22	11:E:49:ILE:HB	1.81	0.60
16:J:45:VAL:HG23	16:J:130:VAL:O	2.00	0.60
19:M:164:THR:HG23	19:M:165:GLY:N	2.15	0.60
1:0:544:G:C3'	1:0:545:G:H5''	2.32	0.60
1:0:470:U:O2'	2:1:16:HIS:CD2	2.53	0.60
1:0:1205:U:H2'	1:0:1206:U:C5'	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:217:ARG:HG3	8:B:257:THR:CG2	2.30	0.60
16:J:75:PRO:HG2	16:J:105:LEU:CD2	2.32	0.60
15:I:108:HIS:N	15:I:109:PRO:HD2	2.16	0.60
1:O:1130:U:H2'	1:O:1131:G:O4'	2.01	0.60
26:T:52:ARG:HB2	26:T:95:ASN:HB3	1.82	0.60
11:E:107:PHE:CE2	11:E:108:LEU:HD13	2.37	0.60
22:P:8:ARG:HG3	38:P:4006:HOH:O	2.02	0.60
19:M:15:PRO:HA	19:M:20:LEU:HD23	1.84	0.60
31:Y:189:ASN:ND2	31:Y:192:ASP:H	2.00	0.60
8:B:312:ARG:HD3	8:B:315:VAL:HG13	1.82	0.60
20:N:15:GLU:OE1	20:N:17:ARG:HD2	2.02	0.60
4:3:65:THR:HG23	4:3:67:LEU:HG	1.84	0.60
1:O:1058:A:H2'	1:O:1060:C:H5''	1.84	0.60
26:T:24:ARG:HH21	26:T:39:ASN:ND2	1.99	0.60
1:O:1768:C:H2'	1:O:1769:C:O4'	2.02	0.60
1:O:2248:C:H3'	38:O:8565:HOH:O	2.01	0.60
1:O:1400:C:H4'	30:X:56:GLU:HG2	1.83	0.60
31:Y:105:LYS:HE2	31:Y:198:GLY:O	2.02	0.60
7:A:36:ASP:O	7:A:38:ILE:N	2.34	0.59
17:K:34:VAL:HG21	17:K:46:LYS:O	2.02	0.59
1:O:2112:A:H2'	1:O:2113:G:H8	1.67	0.59
29:W:125:HIS:HE1	38:W:4003:HOH:O	1.85	0.59
19:M:133:LEU:O	19:M:134:ILE:HD13	2.01	0.59
23:Q:94:GLN:O	23:Q:95:GLU:HB2	2.02	0.59
28:V:12:THR:CG2	28:V:15:GLU:HG3	2.23	0.59
28:V:39:ALA:C	28:V:41:GLU:H	2.05	0.59
13:G:23:ILE:O	13:G:27:ILE:HG13	2.02	0.59
38:9:4056:HOH:O	20:N:147:ILE:HD12	2.01	0.59
20:N:154:LEU:C	20:N:156:GLU:H	2.05	0.59
1:O:2382:A:H5'	38:O:8814:HOH:O	2.01	0.59
26:T:71:VAL:HG11	26:T:90:PRO:CB	2.30	0.59
30:X:43:VAL:HG22	30:X:76:ARG:NH1	2.17	0.59
1:O:820:G:C5	7:A:171:LYS:HB2	2.38	0.59
20:N:179:LEU:HA	20:N:184:ILE:HD12	1.84	0.59
1:O:1379:A:H1'	38:O:7059:HOH:O	2.01	0.59
1:O:2679:G:H2'	1:O:2681:A:OP2	2.03	0.59
20:N:37:ARG:CZ	38:N:4040:HOH:O	2.49	0.59
6:9:28:U:H5''	20:N:40:ASN:HD21	1.66	0.59
16:J:107:ASN:HD22	16:J:109:TYR:H	1.50	0.59
8:B:57:GLU:O	8:B:63:GLU:HB3	2.03	0.59
18:L:30:ARG:NH2	38:L:4029:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2827:A:H2'	1:0:2828:G:O4'	2.02	0.59
18:L:114:VAL:HG11	38:L:4073:HOH:O	2.02	0.59
21:O:38:ARG:NH1	38:O:4017:HOH:O	2.35	0.59
1:0:90:A:H2'	1:0:91:G:O4'	2.03	0.59
13:G:16:LYS:O	13:G:20:VAL:HG23	2.02	0.59
22:P:80:ARG:HG2	22:P:87:ARG:CZ	2.33	0.59
7:A:43:VAL:HG21	7:A:59:GLU:HG3	1.84	0.59
26:T:41:ARG:HG2	26:T:41:ARG:HH11	1.66	0.59
20:N:47:LEU:HD12	20:N:92:ALA:CB	2.32	0.59
20:N:73:ALA:HB1	20:N:74:PRO:HD2	1.85	0.59
30:X:25:ARG:HD3	30:X:64:ALA:O	2.03	0.59
1:0:583:C:H2'	1:0:584:U:C6	2.38	0.59
1:0:407:A:H5'	38:0:5006:HOH:O	2.03	0.59
8:B:85:ARG:NH1	38:B:4043:HOH:O	2.35	0.59
12:F:91:VAL:CG1	12:F:92:GLY:N	2.66	0.59
1:0:2521:A:OP2	14:H:6:ALA:HB3	2.02	0.59
26:T:43:ASN:HD22	26:T:108:ARG:CZ	2.16	0.59
28:V:5:VAL:HG23	38:V:4002:HOH:O	2.02	0.59
7:A:37:VAL:HG22	38:A:4027:HOH:O	2.02	0.59
18:L:35:ARG:NH1	18:L:43:HIS:HB3	2.17	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
14:H:168:VAL:HG13	38:H:4022:HOH:O	2.02	0.59
12:F:69:GLU:O	12:F:70:LYS:HG2	2.03	0.59
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.59
19:M:134:ILE:HG23	19:M:141:ILE:HD13	1.84	0.59
14:H:72:ALA:HB2	14:H:156:ALA:HB2	1.85	0.59
9:C:107:ARG:NE	38:C:4095:HOH:O	2.23	0.59
8:B:125:GLU:O	8:B:129:ARG:HG3	2.01	0.59
1:0:1477:C:H5'	1:0:1868:G:C5'	2.33	0.59
21:O:41:ALA:HA	38:O:4021:HOH:O	2.02	0.59
18:L:62:ALA:HB2	18:L:103:ALA:CB	2.33	0.59
1:0:1835:U:C5	1:0:1840:A:N7	2.68	0.58
30:X:76:ARG:NH1	30:X:76:ARG:HG3	2.18	0.58
20:N:38:LYS:HD2	20:N:114:LYS:HE3	1.83	0.58
1:0:2559:C:H4'	38:0:9749:HOH:O	2.02	0.58
18:L:144:ASP:HA	18:L:147:GLU:HG3	1.84	0.58
27:U:4:ARG:N	38:U:4001:HOH:O	2.35	0.58
29:W:35:VAL:HG23	29:W:41:TYR:CD2	2.38	0.58
19:M:80:GLY:O	19:M:81:ARG:HD2	2.02	0.58
24:R:39:THR:HB	24:R:42:GLU:CG	2.33	0.58
9:C:246:ARG:NH1	9:C:246:ARG:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:512:G:O3'	1:0:513:A:H8	1.86	0.58
31:Y:141:THR:HG23	38:Y:4048:HOH:O	2.01	0.58
22:P:135:ALA:HB1	22:P:139:ARG:HH12	1.67	0.58
20:N:86:LEU:O	20:N:90:LEU:HG	2.03	0.58
1:0:547:A:H3'	38:0:5294:HOH:O	2.02	0.58
31:Y:234:VAL:HG12	31:Y:235:GLU:N	2.18	0.58
22:P:7:LYS:HD3	22:P:21:VAL:CG2	2.33	0.58
11:E:10:ASP:HA	38:E:4004:HOH:O	2.03	0.58
1:0:1213:C:O2'	1:0:1214:G:H5'	2.03	0.58
10:D:44:ILE:HG23	10:D:45:THR:HG23	1.85	0.58
1:0:1189:A:H1'	1:0:1209:C:H1'	1.86	0.58
1:0:2852:A:H5''	38:0:9823:HOH:O	2.03	0.58
1:0:1191:A:H2'	1:0:1193:A:H5'	1.86	0.58
1:0:2831:C:H2'	1:0:2832:C:H5'	1.84	0.58
10:D:163:VAL:HA	38:D:4046:HOH:O	2.03	0.58
1:0:2721:U:H4'	17:K:87:ARG:HG3	1.86	0.58
8:B:217:ARG:CG	8:B:257:THR:HG22	2.32	0.58
1:0:506:G:H22	1:0:509:A:H5''	1.66	0.58
1:0:2073:G:OP2	1:0:2490:A:H5'	2.04	0.58
14:H:31:ILE:HA	14:H:66:GLU:OE1	2.04	0.58
1:0:1157:C:H2'	1:0:1158:G:C8	2.36	0.58
1:0:603:A:H1'	1:0:605:C:C2	2.38	0.58
1:0:138:U:H5''	1:0:139:C:OP2	2.04	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
8:B:238:ASN:HD22	8:B:240:GLY:H	1.52	0.58
1:0:2904:U:H4'	30:X:8:ARG:NH1	2.19	0.58
10:D:91:ALA:HB1	38:D:4032:HOH:O	2.03	0.58
28:V:1:THR:HG23	28:V:2:VAL:N	2.19	0.58
38:0:8128:HOH:O	7:A:213:LYS:HB2	2.04	0.58
1:0:656:G:OP2	21:O:37:ARG:HD2	2.04	0.58
8:B:74:ILE:HD13	8:B:309:VAL:HG21	1.86	0.58
1:0:1097:A:H5''	29:W:125:HIS:NE2	2.19	0.58
1:0:1596:U:H2'	1:0:1598:A:OP2	2.03	0.58
7:A:33:GLU:O	7:A:34:ASP:HB2	2.04	0.58
1:0:1118:A:H62	1:0:1244:U:H3	1.51	0.58
1:0:962:C:H5''	38:0:6258:HOH:O	2.03	0.58
1:0:1790:C:H2'	1:0:1791:U:C6	2.37	0.58
1:0:1060:C:H6	1:0:1060:C:H5'	1.68	0.58
1:0:1862:C:H1'	38:0:8002:HOH:O	2.03	0.58
10:D:41:LEU:HA	10:D:44:ILE:HG22	1.86	0.58
38:0:4093:HOH:O	26:T:9:LYS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:134:ILE:HG22	15:I:135:GLU:N	2.18	0.58
18:L:130:ARG:HA	38:L:4072:HOH:O	2.04	0.58
24:R:99:ALA:HB1	24:R:109:MET:HE3	1.83	0.58
20:N:86:LEU:HD12	20:N:125:ALA:HB2	1.85	0.58
18:L:41:HIS:CD2	18:L:41:HIS:H	2.20	0.58
16:J:52:GLN:HG3	16:J:53:ILE:N	2.19	0.58
31:Y:187:VAL:HB	38:Y:4077:HOH:O	2.02	0.58
1:0:281:U:H3'	38:0:4839:HOH:O	2.04	0.58
1:0:1375:A:C2'	1:0:1376:G:H5'	2.34	0.58
12:F:16:ALA:HA	12:F:111:ILE:HD13	1.86	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.57
9:C:5:ILE:HD11	9:C:16:VAL:HG23	1.85	0.57
29:W:88:THR:HG23	29:W:110:GLN:HB3	1.84	0.57
1:0:1189:A:H3'	38:0:6663:HOH:O	2.03	0.57
2:1:25:LYS:O	2:1:25:LYS:HG2	2.04	0.57
1:0:407:A:H3'	38:0:5008:HOH:O	2.04	0.57
1:0:1266:U:H4'	31:Y:115:ARG:HH21	1.69	0.57
10:D:58:VAL:CG1	10:D:60:GLU:HG2	2.34	0.57
1:0:2755:G:H1'	38:0:9684:HOH:O	2.03	0.57
1:0:1667:A:H2'	1:0:1668:U:C6	2.39	0.57
1:0:2434:A:O3'	4:3:28:GLY:HA3	2.04	0.57
1:0:482:G:H4'	1:0:508:A:N1	2.19	0.57
23:Q:28:ARG:HG2	38:Q:4023:HOH:O	2.03	0.57
38:0:9150:HOH:O	14:H:61:ARG:HG3	2.03	0.57
1:0:2812:A:H2	1:0:2814:A:N6	2.01	0.57
31:Y:234:VAL:HG12	31:Y:235:GLU:H	1.69	0.57
20:N:154:LEU:HD11	20:N:157:PRO:HA	1.86	0.57
1:0:2135:A:O2'	1:0:2136:G:H5'	2.03	0.57
1:0:1015:C:H2'	1:0:1016:U:C6	2.39	0.57
10:D:50:VAL:O	10:D:71:ALA:HA	2.04	0.57
26:T:16:LEU:HA	26:T:19:ARG:HG3	1.86	0.57
1:0:2361:A:H5'	1:0:2361:A:H8	1.69	0.57
1:0:517:U:H2'	1:0:518:G:H5'	1.86	0.57
14:H:12:ILE:HD12	14:H:57:THR:CG2	2.33	0.57
29:W:21:LEU:HD22	29:W:26:ILE:CD1	2.34	0.57
1:0:1878:G:C1'	38:0:8047:HOH:O	2.45	0.57
22:P:18:LYS:HE2	38:P:4006:HOH:O	2.04	0.57
1:0:2270:G:H4'	7:A:223:ARG:NH1	2.18	0.57
9:C:19:PRO:HG2	9:C:22:PHE:CD1	2.39	0.57
31:Y:220:GLU:HG3	38:Y:4092:HOH:O	2.02	0.57
31:Y:95:THR:N	31:Y:236:VAL:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2243:C:H5''	38:0:8560:HOH:O	2.03	0.57
1:0:12:U:H2'	1:0:13:G:H5'	1.86	0.57
16:J:19:MET:CE	16:J:132:LEU:HD11	2.35	0.57
30:X:47:ALA:HB1	30:X:82:GLU:HB3	1.86	0.57
1:0:2055:A:H4'	24:R:132:ARG:NH2	2.19	0.57
12:F:50:VAL:HG13	12:F:60:VAL:HG11	1.87	0.57
22:P:7:LYS:HD3	22:P:21:VAL:HG22	1.86	0.57
1:0:2064:U:H5'	1:0:2652:U:H4'	1.86	0.57
15:I:117:THR:O	15:I:121:LYS:HG3	2.04	0.57
1:0:1741:U:O2'	1:0:2723:G:H4'	2.05	0.57
1:0:2365:G:H4'	23:Q:45:PRO:O	2.03	0.57
20:N:151:ASP:O	20:N:154:LEU:HB2	2.05	0.57
1:0:669:G:O2'	1:0:670:G:H5'	2.05	0.57
8:B:119:HIS:O	8:B:121:PRO:HD3	2.05	0.57
1:0:958:G:H2'	1:0:959:C:C6	2.38	0.57
1:0:1504:A:H5'	38:0:7330:HOH:O	2.03	0.57
38:0:6925:HOH:O	31:Y:186:ARG:HD2	2.02	0.57
10:D:49:PRO:HA	10:D:73:VAL:HG22	1.87	0.57
1:0:1120:U:H5'	1:0:1121:G:OP2	2.04	0.57
13:G:23:ILE:HD13	13:G:67:LEU:HD23	1.86	0.57
22:P:135:ALA:HB1	22:P:139:ARG:NH1	2.19	0.57
3:2:20:ARG:HG3	3:2:21:VAL:H	1.70	0.57
31:Y:106:THR:HG23	31:Y:107:PRO:HD2	1.85	0.57
3:2:41:HIS:HD2	3:2:44:ARG:H	1.53	0.57
8:B:132:HIS:HB2	8:B:137:LEU:HD22	1.87	0.57
19:M:24:GLN:HE21	19:M:27:ARG:HH11	1.52	0.57
1:0:2548:C:OP2	8:B:5:ARG:NH2	2.38	0.57
1:0:2276:U:H2'	1:0:2277:U:C6	2.39	0.57
4:3:73:GLU:HB3	38:3:4056:HOH:O	2.05	0.57
18:L:80:ASP:HB2	18:L:90:ARG:O	2.04	0.57
30:X:51:ASP:OD2	30:X:52:PRO:HD2	2.05	0.57
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.57
1:0:1209:C:H2'	1:0:1210:G:C8	2.36	0.57
1:0:1205:U:H2'	1:0:1206:U:H5'	1.86	0.57
1:0:585:C:H5''	38:0:5344:HOH:O	2.05	0.57
24:R:33:ARG:HD2	38:R:4027:HOH:O	2.04	0.57
9:C:98:ARG:NH1	38:C:4084:HOH:O	2.36	0.57
1:0:899:C:H5'	38:0:6098:HOH:O	2.04	0.57
7:A:48:ASP:HB3	38:A:4031:HOH:O	2.04	0.56
12:F:38:LYS:HZ3	19:M:3:SER:HA	1.70	0.56
10:D:88:LEU:HB2	10:D:89:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:775:G:OP1	2:1:16:HIS:HE1	1.89	0.56
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.56
1:0:2846:C:H4'	8:B:156:LYS:HB3	1.86	0.56
1:0:583:C:H2'	1:0:584:U:H6	1.69	0.56
7:A:105:VAL:CG1	7:A:154:ALA:HB1	2.35	0.56
21:O:53:GLN:HG2	21:O:56:GLU:OE1	2.06	0.56
8:B:305:ASP:O	8:B:306:LYS:HB2	2.05	0.56
15:I:67:VAL:HG13	15:I:68:PRO:HD2	1.86	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
20:N:35:VAL:HG13	38:N:4040:HOH:O	2.04	0.56
9:C:236:THR:O	9:C:239:ALA:N	2.39	0.56
22:P:59:ARG:NH2	22:P:66:GLN:NE2	2.45	0.56
1:0:2780:C:C1'	11:E:143:GLN:HE21	2.17	0.56
1:0:2769:C:H2'	1:0:2770:G:H5'	1.87	0.56
14:H:66:GLU:HA	38:H:4025:HOH:O	2.06	0.56
7:A:94:LEU:HG	7:A:99:ILE:CD1	2.35	0.56
4:3:3:MET:HG3	4:3:4:PRO:HD2	1.86	0.56
4:3:3:MET:O	4:3:90:PHE:HA	2.04	0.56
8:B:71:VAL:HG11	8:B:296:LEU:HB3	1.86	0.56
1:0:2667:G:H1'	1:0:2914:A:N3	2.21	0.56
17:K:87:ARG:NE	38:K:4044:HOH:O	2.39	0.56
15:I:100:VAL:HG11	15:I:124:VAL:CG2	2.34	0.56
15:I:124:VAL:HG13	15:I:134:ILE:HD11	1.88	0.56
1:0:2812:A:H1'	38:0:5263:HOH:O	2.05	0.56
1:0:681:G:N3	1:0:681:G:H5'	2.20	0.56
1:0:945:U:O2'	29:W:43:GLY:HA3	2.04	0.56
1:0:292:G:H2'	1:0:358:G:N2	2.20	0.56
1:0:1183:C:N4	1:0:1184:C:H41	2.03	0.56
29:W:54:PHE:CZ	29:W:140:LYS:HB2	2.40	0.56
15:I:124:VAL:O	15:I:124:VAL:HG12	2.04	0.56
20:N:24:LEU:HD13	23:Q:26:PRO:HB3	1.87	0.56
20:N:49:THR:HG22	20:N:56:ASP:HB2	1.87	0.56
16:J:22:VAL:O	16:J:26:VAL:HG23	2.05	0.56
1:0:871:G:C8	1:0:871:G:C5'	2.80	0.56
20:N:163:PHE:O	20:N:164:ASP:O	2.23	0.56
32:Z:22:SER:O	32:Z:26:VAL:HG23	2.05	0.56
1:0:644:G:N3	1:0:644:G:H5'	2.20	0.56
18:L:55:GLN:HA	18:L:58:GLN:HE21	1.70	0.56
1:0:2565:C:H4'	38:0:9260:HOH:O	2.05	0.56
9:C:156:LEU:O	9:C:160:LEU:HG	2.05	0.56
1:0:2401:A:H5'	38:0:8867:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:36:ASN:HB3	3:2:39:ARG:HG3	1.88	0.56
9:C:119:ALA:HA	9:C:136:VAL:O	2.05	0.56
11:E:116:THR:HG22	11:E:151:LEU:HD22	1.88	0.56
1:0:870:G:H2'	1:0:871:G:C5'	2.27	0.56
1:0:1701:A:H5''	1:0:1702:U:H3'	1.86	0.56
1:0:2505:G:O2'	1:0:2506:A:H5'	2.05	0.56
11:E:2:ARG:HE	11:E:48:VAL:HG13	1.69	0.56
7:A:128:LEU:HG	38:A:4046:HOH:O	2.05	0.56
8:B:154:VAL:CG1	8:B:156:LYS:HG2	2.36	0.56
1:0:1972:U:H2'	1:0:1973:A:C5'	2.36	0.56
1:0:1461:U:H2'	1:0:1462:C:C6	2.41	0.56
8:B:54:VAL:HB	38:B:4033:HOH:O	2.05	0.56
1:0:1398:G:H2'	1:0:1399:A:C8	2.41	0.56
18:L:26:HIS:HB2	38:L:4024:HOH:O	2.06	0.56
11:E:69:ILE:HA	11:E:72:MET:CE	2.36	0.56
29:W:26:ILE:O	29:W:26:ILE:HG13	2.06	0.56
28:V:39:ALA:N	28:V:40:PRO:CD	2.69	0.56
24:R:39:THR:HG22	24:R:42:GLU:H	1.70	0.56
7:A:109:GLU:HG2	7:A:116:GLY:N	2.21	0.56
8:B:7:ARG:HG2	8:B:7:ARG:HH11	1.70	0.56
4:3:15:ASN:ND2	38:3:4006:HOH:O	2.39	0.56
12:F:13:GLU:OE2	12:F:78:GLU:HG2	2.06	0.56
1:0:1677:U:OP2	3:2:8:LYS:NZ	2.38	0.56
1:0:1180:U:H2'	1:0:1181:A:C8	2.41	0.56
27:U:11:THR:HG22	27:U:53:ASP:OD2	2.06	0.56
14:H:43:ALA:HB1	14:H:140:TYR:CE2	2.41	0.56
15:I:105:GLU:HA	15:I:108:HIS:NE2	2.20	0.56
1:0:2769:C:H2'	1:0:2770:G:O4'	2.06	0.56
7:A:51:ARG:NH1	7:A:120:ARG:O	2.39	0.56
19:M:78:LYS:HD3	38:M:4052:HOH:O	2.06	0.56
1:0:1029:U:O2'	1:0:1273:C:OP1	2.23	0.56
23:Q:11:ARG:HD3	38:Q:4012:HOH:O	2.06	0.56
1:0:797:A:C4'	32:Z:10:ARG:N	2.69	0.55
15:I:97:VAL:CG1	15:I:101:LYS:HE3	2.35	0.55
6:9:56:A:O2'	10:D:14:ARG:HD3	2.06	0.55
1:0:272:A:H3'	38:0:4830:HOH:O	2.05	0.55
8:B:314:ALA:CB	8:B:317:PRO:HG3	2.36	0.55
6:9:34:A:H2'	6:9:35:C:O4'	2.06	0.55
1:0:24:G:N2	1:0:518:G:H1'	2.21	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
29:W:34:LEU:HD12	29:W:100:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2488:A:H1'	38:0:9096:HOH:O	2.05	0.55
29:W:88:THR:HG22	29:W:90:TYR:HD1	1.70	0.55
8:B:27:ASN:N	8:B:27:ASN:HD22	1.98	0.55
1:0:2256:G:O2'	1:0:2257:G:H5'	2.05	0.55
9:C:88:SER:O	9:C:91:PRO:HD3	2.06	0.55
1:0:1434:A:H2'	1:0:1436:C:C5	2.41	0.55
16:J:130:VAL:CG1	16:J:131:THR:N	2.69	0.55
1:0:2507:G:H2'	1:0:2510:C:H42	1.71	0.55
1:0:188:C:H5''	19:M:163:LEU:HD21	1.88	0.55
6:9:33:U:H2'	38:9:4042:HOH:O	2.06	0.55
23:Q:13:LYS:NZ	38:Q:4010:HOH:O	2.37	0.55
1:0:1116:U:H3	1:0:1246:A:N6	1.95	0.55
30:X:47:ALA:HB1	30:X:82:GLU:CB	2.37	0.55
1:0:2779:G:H21	11:E:143:GLN:NE2	2.03	0.55
24:R:44:VAL:HG13	24:R:89:LEU:HD22	1.89	0.55
38:0:7452:HOH:O	22:P:117:SER:HB2	2.06	0.55
1:0:2681:A:H4'	1:0:2682:C:H5'	1.88	0.55
11:E:68:HIS:O	11:E:72:MET:HG3	2.07	0.55
1:0:671:A:O2'	1:0:672:G:H2'	2.07	0.55
31:Y:155:ARG:NH1	38:Y:4062:HOH:O	2.37	0.55
8:B:265:LEU:HD21	8:B:316:ARG:HD3	1.88	0.55
1:0:1787:C:H4'	1:0:2883:A:O4'	2.05	0.55
25:S:57:THR:HG22	25:S:59:ASP:H	1.70	0.55
17:K:18:ILE:HG22	17:K:93:ASN:HB2	1.88	0.55
3:2:40:ARG:HG3	3:2:45:ASN:HB2	1.88	0.55
20:N:110:THR:HB	20:N:113:SER:OG	2.05	0.55
1:0:656:G:H5'	21:O:3:THR:HB	1.88	0.55
6:9:1:U:H4'	6:9:3:A:OP1	2.06	0.55
1:0:2904:U:H4'	30:X:8:ARG:HH12	1.71	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.36	0.55
1:0:1380:U:H5'	38:0:7060:HOH:O	2.05	0.55
1:0:1845:A:OP2	7:A:190:ARG:NH1	2.39	0.55
14:H:168:VAL:CG1	38:H:4022:HOH:O	2.54	0.55
1:0:1730:G:H5''	1:0:1731:C:C6	2.42	0.55
20:N:64:SER:C	20:N:66:LEU:H	2.10	0.55
1:0:380:A:OP2	19:M:9:ARG:HD2	2.07	0.55
17:K:98:VAL:HG11	17:K:102:GLU:HA	1.88	0.55
6:9:39:U:H1'	6:9:44:A:H61	1.71	0.55
25:S:6:LYS:HB2	25:S:27:ALA:O	2.06	0.55
25:S:43:GLU:HB3	38:S:4014:HOH:O	2.06	0.55
10:D:37:ALA:O	10:D:40:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1165:G:H1'	1:0:1174:A:H1'	1.88	0.55
11:E:2:ARG:HE	11:E:48:VAL:CG1	2.20	0.55
28:V:16:ARG:NH2	28:V:63:GLU:HG3	2.22	0.55
26:T:50:VAL:HG12	26:T:56:ALA:HA	1.88	0.55
1:0:488:U:H2'	38:0:5191:HOH:O	2.07	0.55
6:9:75:G:H1	6:9:106:U:H3	1.55	0.55
19:M:122:GLN:OE1	19:M:127:LYS:HE2	2.07	0.55
3:2:40:ARG:HG3	3:2:45:ASN:CB	2.37	0.55
10:D:54:ALA:HB2	10:D:69:ILE:HD12	1.88	0.55
1:0:814:G:H2'	1:0:815:U:C6	2.41	0.55
20:N:49:THR:HG22	20:N:58:LEU:HD11	1.89	0.55
24:R:145:LEU:HD12	24:R:146:ILE:H	1.72	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.42	0.55
12:F:21:GLU:O	12:F:24:ARG:HG2	2.06	0.55
23:Q:64:GLU:HG3	23:Q:74:ASP:OD2	2.06	0.55
1:0:703:G:O2'	1:0:704:C:H5'	2.07	0.55
1:0:1528:A:H2'	1:0:1529:G:O4'	2.06	0.55
10:D:40:ILE:HG13	10:D:41:LEU:N	2.22	0.55
29:W:110:GLN:NE2	29:W:110:GLN:HA	2.22	0.55
29:W:90:TYR:CE2	29:W:99:ALA:HB2	2.42	0.55
22:P:13:VAL:HG13	22:P:14:LEU:N	2.22	0.55
12:F:56:PRO:CG	19:M:44:THR:HA	2.37	0.55
27:U:17:THR:CG2	27:U:18:GLY:N	2.70	0.55
2:1:1:THR:HA	38:1:4002:HOH:O	2.07	0.55
11:E:69:ILE:HA	11:E:72:MET:HE2	1.88	0.55
30:X:70:ILE:HG23	30:X:70:ILE:O	2.07	0.55
1:0:2504:A:H4'	14:H:74:ARG:HH11	1.72	0.55
9:C:200:PRO:HB3	9:C:212:VAL:HG23	1.88	0.55
28:V:12:THR:HG23	28:V:14:ALA:N	2.18	0.54
1:0:136:C:H2'	1:0:137:U:O4'	2.08	0.54
27:U:14:GLU:OE1	27:U:15:PRO:HD2	2.07	0.54
20:N:176:ARG:O	20:N:180:LEU:HD13	2.07	0.54
1:0:284:C:H4'	1:0:285:A:O5'	2.08	0.54
9:C:162:VAL:HG13	9:C:232:LEU:HD21	1.87	0.54
8:B:43:GLY:O	8:B:308:LEU:HD12	2.06	0.54
1:0:308:U:H5'	1:0:309:C:OP1	2.07	0.54
1:0:595:U:H2'	1:0:596:C:H6	1.72	0.54
1:0:1291:A:H2	38:0:6820:HOH:O	1.89	0.54
1:0:1056:U:H2'	1:0:1057:A:O4'	2.07	0.54
9:C:236:THR:O	9:C:237:GLU:C	2.45	0.54
31:Y:189:ASN:HD22	31:Y:189:ASN:C	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:102:LYS:HG3	38:H:4039:HOH:O	2.06	0.54
12:F:46:GLU:O	12:F:73:PRO:HD2	2.06	0.54
1:0:1544:U:H2'	1:0:1545:C:C6	2.42	0.54
1:0:1537:C:H1'	38:0:7382:HOH:O	2.07	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.54
24:R:111:ILE:HG23	24:R:145:LEU:CD1	2.37	0.54
1:0:947:U:H2'	1:0:948:G:H8	1.71	0.54
31:Y:99:ALA:HB2	31:Y:233:TYR:CE2	2.43	0.54
1:0:1535:G:H2'	1:0:1536:C:C6	2.43	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.33	0.54
31:Y:235:GLU:CD	31:Y:235:GLU:N	2.60	0.54
7:A:164:ARG:NE	38:A:4052:HOH:O	2.39	0.54
31:Y:163:THR:HG23	38:Y:4068:HOH:O	2.06	0.54
23:Q:53:HIS:ND1	23:Q:55:ARG:HB2	2.23	0.54
29:W:21:LEU:HD21	29:W:48:VAL:HG13	1.90	0.54
1:0:484:A:N1	1:0:506:G:H4'	2.22	0.54
28:V:4:HIS:HB3	38:V:4003:HOH:O	2.08	0.54
29:W:65:VAL:HA	29:W:68:THR:CG2	2.38	0.54
1:0:2634:G:OP2	7:A:204:GLY:N	2.38	0.54
9:C:78:ARG:HG3	9:C:78:ARG:NH1	2.23	0.54
29:W:34:LEU:CD1	29:W:100:LEU:HD13	2.38	0.54
10:D:10:PHE:CG	10:D:11:HIS:N	2.75	0.54
1:0:2411:C:H4'	38:0:8894:HOH:O	2.06	0.54
10:D:174:VAL:HG12	38:D:4048:HOH:O	2.07	0.54
9:C:129:HIS:CE1	9:C:231:ARG:HA	2.43	0.54
22:P:97:ARG:HD2	38:P:4050:HOH:O	2.08	0.54
15:I:130:LEU:HA	38:I:4002:HOH:O	2.06	0.54
27:U:52:THR:CG2	27:U:54:THR:HB	2.37	0.54
27:U:9:CYS:HA	27:U:52:THR:CG2	2.33	0.54
8:B:254:GLN:HG2	8:B:255:GLY:N	2.22	0.54
10:D:135:VAL:HG22	10:D:136:ARG:N	2.23	0.54
38:0:4379:HOH:O	31:Y:212:ARG:HD2	2.08	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.07	0.54
1:0:1714:C:O2'	1:0:1715:C:H5'	2.08	0.54
7:A:194:MET:HE1	7:A:199:HIS:HB2	1.90	0.54
10:D:65:GLU:HG3	38:D:4024:HOH:O	2.07	0.54
1:0:1942:A:H3'	38:0:8126:HOH:O	2.07	0.54
20:N:154:LEU:O	20:N:155:GLU:HB3	2.07	0.54
8:B:238:ASN:ND2	8:B:240:GLY:H	2.05	0.54
1:0:2256:G:C2'	1:0:2257:G:H5'	2.38	0.54
1:0:2787:C:H5	38:0:9730:HOH:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1151:G:OP1	13:G:63:ARG:NH1	2.41	0.54
24:R:25:PHE:CE2	24:R:29:LYS:HE2	2.43	0.54
1:0:553:G:H5'	38:0:5304:HOH:O	2.07	0.54
15:I:94:ASP:OD1	15:I:133:THR:HB	2.08	0.54
20:N:170:GLU:O	20:N:174:GLU:HG3	2.08	0.54
8:B:41:PHE:CD1	8:B:79:MET:HE2	2.43	0.54
8:B:55:ASN:CB	8:B:63:GLU:HA	2.37	0.54
1:0:447:A:O2'	1:0:448:G:H5'	2.08	0.54
14:H:50:ILE:HD12	14:H:149:VAL:HG11	1.90	0.54
1:0:2111:G:H1'	38:0:5718:HOH:O	2.08	0.54
7:A:82:VAL:HG13	7:A:93:THR:HB	1.88	0.54
28:V:58:THR:O	28:V:62:GLU:HG3	2.08	0.54
38:0:4862:HOH:O	26:T:38:ARG:NH1	2.41	0.54
1:0:1118:A:C8	1:0:1118:A:C3'	2.85	0.53
29:W:3:ALA:O	29:W:54:PHE:HA	2.08	0.53
22:P:10:ALA:HA	22:P:13:VAL:HG12	1.89	0.53
11:E:80:TRP:O	11:E:134:SER:HA	2.07	0.53
17:K:55:VAL:HG12	17:K:56:SER:N	2.22	0.53
9:C:34:ALA:HB3	9:C:220:THR:HG21	1.90	0.53
8:B:223:ARG:HG3	8:B:232:TRP:O	2.08	0.53
1:0:461:C:N3	1:0:479:G:H5'	2.23	0.53
1:0:1166:A:H1'	1:0:1192:A:C2	2.42	0.53
1:0:2717:C:O2'	1:0:2718:C:H5''	2.07	0.53
38:0:9758:HOH:O	8:B:27:ASN:HB3	2.08	0.53
1:0:907:A:H4'	1:0:1328:A:C2	2.43	0.53
12:F:19:ALA:O	12:F:22:VAL:HG22	2.08	0.53
17:K:125:ALA:C	17:K:127:ALA:H	2.10	0.53
32:Z:36:ASP:HB3	32:Z:45:ASP:HB3	1.88	0.53
1:0:553:G:O4'	1:0:1325:G:H5'	2.06	0.53
6:9:56:A:C3'	6:9:57:A:H5''	2.37	0.53
10:D:94:ALA:HA	10:D:174:VAL:O	2.08	0.53
24:R:82:GLU:HG3	24:R:83:LYS:N	2.22	0.53
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.53
38:0:9709:HOH:O	8:B:298:LYS:HD3	2.09	0.53
8:B:2:GLN:HA	38:B:4003:HOH:O	2.07	0.53
1:0:2840:A:OP1	8:B:211:THR:HG23	2.08	0.53
1:0:1086:A:C6	29:W:11:VAL:HG11	2.44	0.53
1:0:920:C:H5''	1:0:921:G:O5'	2.08	0.53
29:W:107:LEU:O	29:W:112:LEU:HB2	2.07	0.53
1:0:902:G:N7	18:L:18:HIS:HD2	2.06	0.53
1:0:1242:A:OP2	16:J:60:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1735:C:OP2	8:B:234:ARG:HG3	2.09	0.53
8:B:41:PHE:CZ	8:B:79:MET:HG3	2.44	0.53
8:B:139:ASP:HB2	8:B:165:ARG:NE	2.23	0.53
1:0:1973:A:H2'	1:0:1974:G:O4'	2.09	0.53
31:Y:99:ALA:HB2	31:Y:233:TYR:CZ	2.43	0.53
11:E:158:ASP:OD1	11:E:160:ARG:HB2	2.08	0.53
1:0:1393:A:H2'	1:0:1394:C:C6	2.44	0.53
1:0:2044:G:OP1	30:X:23:HIS:HE1	1.91	0.53
26:T:49:GLU:OE2	26:T:97:ARG:NH1	2.42	0.53
18:L:149:ARG:O	18:L:150:GLN:HB2	2.08	0.53
1:0:2784:A:H1'	11:E:60:SER:OG	2.07	0.53
6:9:64:C:C2'	6:9:65:A:H5'	2.38	0.53
8:B:199:TYR:CE2	8:B:268:ARG:HB2	2.43	0.53
20:N:37:ARG:HH11	20:N:37:ARG:HG3	1.74	0.53
1:0:1160:G:HO2'	1:0:1190:G:H1'	1.72	0.53
32:Z:11:SER:HB3	32:Z:23:ARG:HB2	1.91	0.53
8:B:51:VAL:CG2	8:B:327:VAL:HG13	2.38	0.53
1:0:1595:G:O2'	1:0:1596:U:H5'	2.07	0.53
1:0:192:A:H5'	38:0:4600:HOH:O	2.08	0.53
31:Y:145:LYS:O	31:Y:147:ARG:HG2	2.09	0.53
1:0:2478:U:H2'	1:0:2479:A:C8	2.44	0.53
10:D:154:LYS:H	10:D:154:LYS:CD	1.97	0.53
29:W:4:LEU:O	29:W:32:CYS:HA	2.09	0.53
17:K:74:VAL:HG12	17:K:75:ARG:HG3	1.91	0.53
1:0:1419:U:H2'	1:0:1685:A:C2	2.44	0.53
6:9:28:U:H2'	6:9:29:C:C6	2.44	0.53
1:0:1173:A:H4'	1:0:1174:A:C8	2.44	0.53
12:F:57:GLU:O	12:F:61:MET:HG3	2.09	0.53
8:B:51:VAL:HG23	8:B:329:TYR:O	2.09	0.53
1:0:1120:U:H5''	1:0:1120:U:C6	2.43	0.53
19:M:61:ILE:CG2	19:M:62:VAL:N	2.72	0.53
1:0:2589:U:H2'	1:0:2590:U:C6	2.44	0.53
29:W:143:THR:N	38:W:4064:HOH:O	2.42	0.53
16:J:46:ILE:HD11	16:J:53:ILE:HG23	1.91	0.53
20:N:89:GLY:O	20:N:92:ALA:HB3	2.08	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
8:B:144:THR:HB	38:B:4058:HOH:O	2.09	0.53
4:3:70:ARG:NH1	4:3:77:ALA:HB2	2.24	0.53
7:A:65:ARG:O	7:A:66:ARG:HG3	2.09	0.53
11:E:24:GLY:HA3	11:E:76:VAL:HB	1.91	0.53
1:0:1973:A:H8	1:0:1973:A:H5'	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1375:A:O2'	1:0:1376:G:H5'	2.09	0.53
19:M:61:ILE:HA	38:M:4025:HOH:O	2.08	0.53
1:0:2050:G:H5''	24:R:80:TYR:O	2.09	0.53
38:0:5207:HOH:O	26:T:82:THR:HA	2.09	0.53
9:C:214:THR:HG21	38:C:4156:HOH:O	2.08	0.53
11:E:53:GLU:HB3	11:E:55:ASN:ND2	2.24	0.53
8:B:16:ARG:NH1	38:B:4013:HOH:O	2.41	0.53
20:N:37:ARG:HH21	20:N:105:GLY:HA2	1.72	0.53
29:W:149:LEU:HG	29:W:153:MET:HE2	1.91	0.53
9:C:115:LEU:HD13	9:C:223:LEU:HD21	1.90	0.53
17:K:7:ASP:OD2	17:K:81:ARG:NH2	2.42	0.53
10:D:63:ILE:HG13	10:D:64:ARG:N	2.24	0.53
12:F:91:VAL:CG1	12:F:92:GLY:H	2.21	0.53
1:0:2441:U:H4'	18:L:53:ARG:HD2	1.91	0.53
18:L:66:VAL:HG23	18:L:67:ARG:N	2.22	0.53
9:C:27:ARG:HG2	9:C:30:LEU:HD12	1.91	0.53
1:0:1014:A:H2'	1:0:1015:C:H5'	1.91	0.53
18:L:104:ASP:O	18:L:105:TYR:HB3	2.08	0.53
1:0:1634:G:H2'	1:0:1635:U:C6	2.44	0.53
16:J:46:ILE:HD11	16:J:53:ILE:HG21	1.90	0.53
6:9:29:C:C2'	6:9:30:C:H5'	2.36	0.53
1:0:282:C:H2'	1:0:283:U:O4'	2.09	0.53
20:N:171:HIS:CE1	38:N:4031:HOH:O	2.62	0.53
10:D:144:ARG:O	10:D:148:SER:HB3	2.08	0.53
8:B:139:ASP:CB	8:B:165:ARG:HE	2.22	0.53
20:N:49:THR:CG2	20:N:58:LEU:HD11	2.39	0.53
1:0:2564:G:OP2	1:0:2565:C:H5''	2.09	0.53
25:S:57:THR:HG22	25:S:59:ASP:N	2.23	0.53
6:9:69:U:OP1	20:N:4:PRO:HG3	2.09	0.53
21:O:50:ARG:HD2	21:O:51:TYR:CE1	2.43	0.53
8:B:56:ASP:OD1	8:B:322:ARG:HB3	2.08	0.53
1:0:2326:C:H4'	1:0:2412:G:H4'	1.91	0.53
12:F:39:SER:HB3	12:F:45:ALA:HB2	1.91	0.53
1:0:1525:G:H5'	1:0:1526:A:OP2	2.09	0.53
29:W:149:LEU:HG	29:W:153:MET:CE	2.39	0.53
29:W:52:VAL:CG2	29:W:53:ALA:H	2.20	0.53
10:D:166:ILE:HB	38:D:4046:HOH:O	2.08	0.53
1:0:558:C:C2'	1:0:559:U:C5'	2.82	0.53
13:G:63:ARG:O	13:G:67:LEU:HG	2.09	0.53
13:G:71:LEU:O	13:G:73:ASP:N	2.42	0.53
38:0:4878:HOH:O	9:C:188:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:289:G:O2'	1:0:290:C:H5'	2.09	0.53
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.53
38:K:4043:HOH:O	27:U:20:MET:HE1	2.08	0.53
1:0:812:A:H1'	38:0:5806:HOH:O	2.08	0.53
11:E:84:MET:HG2	11:E:168:ILE:HA	1.90	0.52
1:0:2598:U:O2	1:0:2600:A:H8	1.92	0.52
1:0:244:C:OP2	12:F:38:LYS:HE3	2.09	0.52
4:3:56:PRO:N	38:3:4043:HOH:O	2.42	0.52
8:B:84:LEU:HD23	8:B:142:LEU:HD23	1.89	0.52
1:0:2831:C:C2'	1:0:2832:C:H5'	2.39	0.52
6:9:8:G:H4'	23:Q:27:GLN:NE2	2.24	0.52
10:D:35:ALA:HB2	38:D:4015:HOH:O	2.10	0.52
29:W:48:VAL:HG12	29:W:48:VAL:O	2.09	0.52
1:0:1734:C:OP1	8:B:234:ARG:HD3	2.09	0.52
15:I:133:THR:HG22	15:I:134:ILE:N	2.24	0.52
1:0:2601:A:N1	17:K:38:SER:HB2	2.24	0.52
17:K:62:PRO:HG3	17:K:65:ARG:NH2	2.23	0.52
4:3:83:TRP:HA	38:3:4063:HOH:O	2.09	0.52
9:C:107:ARG:NH2	38:C:4095:HOH:O	2.41	0.52
7:A:33:GLU:OE1	7:A:33:GLU:N	2.41	0.52
10:D:95:THR:OG1	10:D:174:VAL:HG22	2.10	0.52
1:0:1495:C:H1'	1:0:1573:A:H1'	1.92	0.52
29:W:142:ASP:HB2	38:W:4066:HOH:O	2.09	0.52
29:W:88:THR:HG21	29:W:96:LEU:HD13	1.90	0.52
19:M:134:ILE:O	19:M:136:PRO:HD3	2.09	0.52
6:9:39:U:H1'	6:9:44:A:N6	2.24	0.52
10:D:76:ARG:O	10:D:77:ASP:HB2	2.08	0.52
10:D:10:PHE:CD1	10:D:11:HIS:N	2.77	0.52
1:0:1634:G:H3'	38:0:7496:HOH:O	2.08	0.52
1:0:1946:C:H1'	38:0:8137:HOH:O	2.08	0.52
1:0:538:C:H5''	1:0:539:G:C8	2.44	0.52
9:C:127:ARG:HG2	9:C:127:ARG:HH11	1.73	0.52
1:0:1118:A:H8	1:0:1119:G:H5''	1.73	0.52
27:U:52:THR:HG22	27:U:54:THR:N	2.24	0.52
1:0:2781:U:H2'	1:0:2782:G:H5'	1.91	0.52
12:F:50:VAL:CG1	12:F:60:VAL:HG11	2.39	0.52
10:D:18:ILE:HD13	10:D:84:LEU:CD1	2.40	0.52
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.52
9:C:214:THR:HG23	38:C:4173:HOH:O	2.09	0.52
1:0:2802:C:H2'	1:0:2803:C:C6	2.44	0.52
1:0:255:A:H2'	1:0:256:C:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:177:HIS:O	8:B:181:ILE:HG13	2.09	0.52
1:O:1805:G:H2'	1:O:1806:G:H8	1.73	0.52
1:O:816:G:C6	1:O:817:G:N1	2.77	0.52
20:N:167:ASP:O	20:N:168:LEU:HD23	2.10	0.52
7:A:179:MET:HG2	7:A:186:TRP:CG	2.45	0.52
28:V:39:ALA:O	28:V:41:GLU:N	2.42	0.52
21:O:25:VAL:HG23	21:O:26:TRP:N	2.24	0.52
1:O:60:A:H5'	3:2:19:SER:OG	2.09	0.52
11:E:116:THR:CG2	11:E:151:LEU:HD22	2.39	0.52
1:O:120:A:N3	1:O:120:A:H2'	2.25	0.52
1:O:1304:U:H2'	1:O:1305:C:C6	2.44	0.52
12:F:105:ASP:O	12:F:109:GLU:HB2	2.09	0.52
1:O:2740:G:H2'	1:O:2741:A:O4'	2.08	0.52
8:B:307:ARG:HB2	8:B:307:ARG:HH11	1.75	0.52
9:C:7:ASP:OD2	9:C:9:ASP:HB2	2.09	0.52
14:H:141:CYS:HB2	38:H:4029:HOH:O	2.08	0.52
1:O:1087:G:H4'	1:O:1088:A:OP1	2.09	0.52
1:O:1015:C:H2'	1:O:1016:U:H6	1.74	0.52
38:O:6254:HOH:O	20:N:4:PRO:HD2	2.10	0.52
1:O:88:G:H5'	1:O:88:G:H8	1.75	0.52
21:O:57:THR:O	21:O:111:VAL:HG23	2.10	0.52
1:O:474:C:O3'	9:C:73:LEU:HD21	2.10	0.52
19:M:99:ARG:HD2	19:M:167:GLY:CA	2.37	0.52
29:W:89:ASP:HB2	29:W:90:TYR:CE1	2.44	0.52
8:B:248:ARG:NH2	38:B:4109:HOH:O	2.42	0.52
1:O:2781:U:H1'	11:E:139:GLU:OE2	2.10	0.52
16:J:107:ASN:ND2	16:J:109:TYR:N	2.57	0.52
20:N:61:ALA:CB	20:N:88:ALA:HB2	2.39	0.52
15:I:88:GLN:NE2	15:I:128:THR:HG21	2.25	0.52
28:V:64:GLY:O	28:V:65:ASP:CB	2.57	0.52
1:O:317:A:H5''	26:T:52:ARG:HD2	1.92	0.52
1:O:1730:G:H5''	1:O:1731:C:H6	1.74	0.52
8:B:260:HIS:HE1	38:B:4116:HOH:O	1.91	0.52
1:O:790:A:H2'	1:O:791:A:O4'	2.10	0.52
20:N:47:LEU:CD1	20:N:97:VAL:HG11	2.39	0.52
11:E:137:ASP:O	11:E:141:VAL:HG23	2.10	0.52
3:2:48:ASP:O	3:2:49:GLU:HB2	2.09	0.52
16:J:107:ASN:HD22	16:J:108:PRO:N	2.06	0.52
8:B:205:VAL:O	8:B:307:ARG:NE	2.43	0.52
1:O:236:A:H4'	1:O:237:G:OP1	2.09	0.52
26:T:1:SER:HA	38:T:4001:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:67:VAL:CG1	15:I:68:PRO:HD2	2.40	0.52
32:Z:60:CYS:O	32:Z:61:ASP:HB2	2.09	0.52
1:O:581:G:H5'	38:O:5339:HOH:O	2.09	0.52
21:O:115:ARG:NH1	38:O:4043:HOH:O	2.41	0.52
16:J:131:THR:HG22	16:J:133:GLY:N	2.24	0.52
31:Y:189:ASN:HA	31:Y:217:ILE:HD11	1.90	0.52
10:D:64:ARG:CD	10:D:67:ASP:HB3	2.40	0.52
1:O:1287:A:O4'	29:W:117:ARG:HD3	2.09	0.52
20:N:43:VAL:HG13	20:N:118:ILE:HD11	1.92	0.52
25:S:25:GLN:HG2	25:S:65:VAL:HG22	1.92	0.52
8:B:195:ARG:HD2	8:B:324:ASP:OD1	2.10	0.52
10:D:58:VAL:HG12	10:D:60:GLU:HG2	1.92	0.52
9:C:10:GLY:HA2	9:C:160:LEU:HD21	1.91	0.52
29:W:56:GLU:O	29:W:143:THR:HG23	2.10	0.52
1:O:1947:G:N2	1:O:1966:U:C2	2.78	0.52
1:O:1979:G:H2'	38:O:8174:HOH:O	2.09	0.52
26:T:18:GLU:O	26:T:21:LYS:HG3	2.09	0.52
6:9:51:A:H5'	20:N:160:SER:HB3	1.90	0.52
10:D:128:LEU:HD23	10:D:128:LEU:O	2.10	0.52
30:X:49:ARG:HG2	30:X:84:ILE:HG23	1.92	0.52
1:O:2768:A:O2'	1:O:2769:C:H5'	2.10	0.51
7:A:192:VAL:HB	38:A:4077:HOH:O	2.10	0.51
1:O:2600:A:H2'	1:O:2601:A:O4'	2.11	0.51
8:B:96:PRO:HG3	38:B:4043:HOH:O	2.10	0.51
7:A:105:VAL:HG11	7:A:154:ALA:HB1	1.91	0.51
1:O:2785:C:H4'	1:O:2786:G:OP2	2.11	0.51
8:B:109:LEU:HG	8:B:113:LEU:HD12	1.93	0.51
1:O:485:A:N3	1:O:487:G:H5''	2.25	0.51
16:J:126:ASN:ND2	38:J:4050:HOH:O	2.42	0.51
30:X:66:THR:HG23	30:X:67:PRO:HD2	1.92	0.51
1:O:1446:U:H2'	25:S:55:GLN:NE2	2.25	0.51
22:P:116:SER:O	22:P:119:TYR:HB3	2.09	0.51
1:O:2840:A:H3'	38:O:9796:HOH:O	2.10	0.51
21:O:59:VAL:CG2	21:O:111:VAL:HG21	2.39	0.51
32:Z:56:GLN:HA	32:Z:62:TYR:O	2.10	0.51
19:M:72:ALA:HB2	19:M:93:ARG:HG2	1.93	0.51
12:F:36:THR:HG23	12:F:97:ALA:HB2	1.91	0.51
30:X:74:ALA:HB2	30:X:85:VAL:HG13	1.92	0.51
19:M:27:ARG:NH2	19:M:44:THR:HG23	2.25	0.51
1:O:814:G:H2'	1:O:815:U:H6	1.74	0.51
9:C:19:PRO:HG2	9:C:22:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:37:A:H2'	1:0:38:G:C8	2.45	0.51
1:0:195:C:H5''	38:M:4116:HOH:O	2.09	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.92	0.51
26:T:80:GLU:HG2	38:T:4027:HOH:O	2.10	0.51
1:0:2724:U:H2'	1:0:2725:G:O4'	2.09	0.51
1:0:2570:G:H5''	38:0:9272:HOH:O	2.09	0.51
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.51
1:0:2769:C:O2'	1:0:2770:G:H5'	2.11	0.51
8:B:41:PHE:CE1	8:B:79:MET:HG3	2.45	0.51
18:L:57:VAL:O	18:L:57:VAL:HG12	2.11	0.51
7:A:65:ARG:C	7:A:66:ARG:HG3	2.31	0.51
1:0:1641:A:C2'	1:0:1642:A:H5'	2.40	0.51
17:K:118:ALA:HA	17:K:125:ALA:HB2	1.92	0.51
1:0:1335:C:OP2	31:Y:207:SER:HB3	2.11	0.51
18:L:77:ALA:HB3	38:L:4054:HOH:O	2.11	0.51
17:K:75:ARG:O	17:K:93:ASN:HA	2.10	0.51
38:0:6622:HOH:O	13:G:12:ILE:HG23	2.10	0.51
1:0:2634:G:H3'	38:0:9464:HOH:O	2.10	0.51
13:G:20:VAL:O	13:G:24:VAL:HG23	2.10	0.51
26:T:106:GLU:HG3	38:T:4035:HOH:O	2.10	0.51
2:1:45:ARG:HD2	38:1:4042:HOH:O	2.11	0.51
29:W:38:THR:HG22	38:W:4020:HOH:O	2.10	0.51
10:D:22:VAL:HG22	10:D:74:THR:HG22	1.92	0.51
11:E:126:ILE:HB	11:E:131:LEU:HD23	1.92	0.51
25:S:22:ASN:ND2	25:S:68:LEU:HB2	2.25	0.51
10:D:35:ALA:C	10:D:37:ALA:N	2.64	0.51
38:0:9708:HOH:O	8:B:267:LYS:HD3	2.11	0.51
9:C:235:PHE:HE2	9:C:243:VAL:HG21	1.76	0.51
20:N:23:ARG:NH1	38:N:4013:HOH:O	2.42	0.51
1:0:285:A:C2	1:0:368:C:H4'	2.46	0.51
12:F:32:GLY:N	38:F:4009:HOH:O	2.43	0.51
28:V:42:ASN:N	28:V:43:PRO:HD3	2.25	0.51
1:0:960:G:H3'	1:0:960:G:N3	2.25	0.51
26:T:49:GLU:HB3	26:T:59:GLU:HG3	1.92	0.51
32:Z:53:GLY:HA2	32:Z:67:GLY:O	2.11	0.51
1:0:2719:A:C2	8:B:70:PRO:HG3	2.46	0.51
11:E:34:TRP:HB3	38:E:4012:HOH:O	2.10	0.51
9:C:47:GLY:HA2	9:C:92:PRO:HB2	1.92	0.51
29:W:29:VAL:O	29:W:30:ASN:HB2	2.10	0.51
15:I:105:GLU:HA	15:I:108:HIS:CE1	2.46	0.51
14:H:61:ARG:HG3	14:H:61:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:O2'	1:0:856:G:H4'	2.11	0.51
21:O:47:ARG:HG3	21:O:47:ARG:NH1	2.25	0.51
11:E:7:ILE:HD11	11:E:11:VAL:C	2.31	0.51
1:0:1024:G:H4'	29:W:41:TYR:OH	2.10	0.51
1:0:2325:U:O2'	1:0:2411:C:H1'	2.09	0.51
1:0:1634:G:H2'	1:0:1635:U:H6	1.76	0.51
8:B:258:GLY:H	8:B:260:HIS:CE1	2.28	0.51
12:F:15:ASP:O	12:F:18:GLU:HB2	2.10	0.51
1:0:1226:G:O2'	1:0:1227:C:H5'	2.10	0.51
1:0:2081:A:H4'	16:J:69:TYR:CE1	2.46	0.51
1:0:1786:C:OP1	22:P:74:GLN:HG2	2.11	0.51
1:0:451:C:O2'	1:0:452:G:H5'	2.11	0.51
1:0:1667:A:C8	1:0:1667:A:H5'	2.41	0.51
7:A:94:LEU:HD12	7:A:98:GLU:HB2	1.92	0.51
30:X:25:ARG:NH1	38:X:4013:HOH:O	2.44	0.51
1:0:721:A:H5''	21:O:51:TYR:CE2	2.46	0.51
1:0:2326:C:H4'	1:0:2412:G:C4'	2.40	0.51
10:D:101:THR:O	10:D:101:THR:HG22	2.11	0.51
1:0:168:C:H6	1:0:168:C:O5'	1.93	0.51
29:W:21:LEU:HB3	29:W:26:ILE:CG1	2.41	0.51
14:H:102:LYS:HD3	14:H:122:LYS:CD	2.35	0.51
1:0:877:G:C5'	1:0:878:G:OP1	2.56	0.51
23:Q:75:ILE:HA	38:Q:4038:HOH:O	2.10	0.51
8:B:137:LEU:HD21	8:B:140:LEU:HD21	1.92	0.51
28:V:38:GLY:O	28:V:41:GLU:HG3	2.11	0.51
15:I:91:PHE:HD2	15:I:131:GLY:HA2	1.75	0.51
9:C:79:ARG:O	9:C:87:ARG:HG2	2.11	0.51
38:O:7658:HOH:O	22:P:81:LYS:HG2	2.10	0.51
1:0:1112:G:H1	1:0:1251:C:H42	1.56	0.51
10:D:40:ILE:HG23	38:D:4018:HOH:O	2.10	0.51
1:0:1666:C:O2'	1:0:1667:A:C5'	2.59	0.51
10:D:135:VAL:HG22	10:D:136:ARG:H	1.76	0.51
1:0:2812:A:C2	1:0:2814:A:N6	2.76	0.51
1:0:814:G:H1'	38:O:5809:HOH:O	2.09	0.51
1:0:1654:U:H2'	7:A:47:HIS:CD2	2.44	0.51
11:E:105:GLU:HG2	11:E:113:PRO:HB3	1.93	0.51
27:U:25:ASP:OD2	27:U:26:GLY:N	2.44	0.51
7:A:100:PRO:HG2	7:A:103:VAL:CG2	2.37	0.50
15:I:113:SER:HB2	15:I:118:ASN:HB2	1.93	0.50
10:D:140:ARG:O	10:D:144:ARG:HG2	2.11	0.50
7:A:194:MET:CE	7:A:199:HIS:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:38:GLY:C	28:V:40:PRO:HD2	2.31	0.50
20:N:49:THR:CG2	20:N:56:ASP:HB2	2.41	0.50
31:Y:112:GLU:CD	31:Y:115:ARG:NH1	2.64	0.50
38:O:8333:HOH:O	24:R:139:PRO:HD2	2.11	0.50
1:O:1003:U:H4'	14:H:91:ARG:O	2.10	0.50
1:O:282:C:O2'	1:O:283:U:H5'	2.12	0.50
10:D:146:LYS:HZ3	20:N:107:ASN:ND2	2.08	0.50
8:B:81:ALA:O	8:B:186:GLY:HA3	2.10	0.50
1:O:2361:A:H5''	38:O:8773:HOH:O	2.09	0.50
18:L:97:VAL:HG12	18:L:98:GLU:O	2.10	0.50
1:O:2582:G:O3'	17:K:41:LYS:HA	2.11	0.50
38:O:9027:HOH:O	18:L:37:LYS:HE2	2.11	0.50
1:O:2467:A:O2'	1:O:2468:A:H2'	2.12	0.50
1:O:2005:G:OP2	1:O:2005:G:H3'	2.11	0.50
1:O:2387:U:H2'	1:O:2388:C:C6	2.46	0.50
18:L:73:VAL:HG23	18:L:74:THR:N	2.26	0.50
23:Q:21:ARG:HG2	23:Q:22:GLY:H	1.76	0.50
1:O:2506:A:O2'	1:O:2507:G:C8	2.62	0.50
1:O:1594:C:OP2	22:P:120:ARG:HD2	2.11	0.50
9:C:7:ASP:C	9:C:9:ASP:H	2.15	0.50
1:O:1279:U:H2'	1:O:1279:U:O2	2.12	0.50
1:O:2114:C:O2'	1:O:2115:U:H5'	2.11	0.50
1:O:449:A:N7	9:C:43:LYS:HG2	2.26	0.50
1:O:69:A:H5'	1:O:69:A:C8	2.46	0.50
1:O:1761:U:H5''	22:P:83:LYS:HA	1.93	0.50
1:O:2424:U:H1'	23:Q:7:LEU:HD12	1.94	0.50
1:O:527:U:H2'	1:O:528:G:C8	2.46	0.50
11:E:77:THR:OG1	11:E:78:GLU:N	2.44	0.50
1:O:1441:G:O2'	1:O:1442:A:H5'	2.11	0.50
32:Z:42:CYS:SG	32:Z:44:GLU:HB2	2.51	0.50
17:K:75:ARG:HH21	17:K:94:ALA:CB	2.25	0.50
1:O:545:G:H8	1:O:545:G:C5'	2.19	0.50
1:O:383:A:H5'	38:O:5032:HOH:O	2.11	0.50
26:T:26:THR:HA	26:T:39:ASN:HB3	1.93	0.50
7:A:105:VAL:HG12	7:A:106:CYS:N	2.25	0.50
1:O:61:G:OP1	3:2:17:GLN:HG2	2.11	0.50
8:B:199:TYR:HE2	8:B:268:ARG:HB2	1.76	0.50
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.93	0.50
9:C:7:ASP:O	9:C:9:ASP:N	2.43	0.50
1:O:941:G:O2'	1:O:942:U:H5'	2.11	0.50
1:O:2252:A:C5	1:O:2253:G:H1'	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:109:LEU:HA	38:Y:4015:HOH:O	2.11	0.50
20:N:37:ARG:CD	36:N:8807:CL:CL	2.96	0.50
17:K:81:ARG:HG2	17:K:81:ARG:HH11	1.76	0.50
29:W:65:VAL:HG12	29:W:116:LEU:HD13	1.93	0.50
18:L:73:VAL:HG11	18:L:118:LEU:HD21	1.93	0.50
1:0:764:C:H2'	1:0:765:G:O4'	2.11	0.50
1:0:1421:C:H2'	1:0:1422:U:H6	1.76	0.50
1:0:1684:A:O2'	1:0:1685:A:H5''	2.11	0.50
1:0:290:C:O2'	1:0:291:C:H5'	2.12	0.50
8:B:48:MET:HG2	8:B:72:THR:HA	1.94	0.50
1:0:2694:A:H4'	11:E:91:PHE:HE1	1.76	0.50
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.50
11:E:103:VAL:HG22	11:E:115:ARG:HB3	1.94	0.50
1:0:1711:A:O2'	1:0:1712:A:H5'	2.12	0.50
1:0:2072:G:C6	1:0:2533:C:H1'	2.47	0.50
16:J:107:ASN:C	16:J:107:ASN:ND2	2.63	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.94	0.50
9:C:200:PRO:HB3	9:C:212:VAL:CG2	2.41	0.50
1:0:522:U:O2'	1:0:1366:C:H5'	2.11	0.50
6:9:88:G:OP1	29:W:130:HIS:NE2	2.41	0.50
20:N:43:VAL:O	20:N:84:THR:HG21	2.12	0.50
1:0:1527:A:H1'	1:0:1528:A:C8	2.46	0.50
1:0:466:A:H2'	1:0:467:G:O4'	2.12	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
1:0:1853:C:OP1	7:A:231:LYS:HG3	2.11	0.50
25:S:81:ILE:HG12	38:S:4031:HOH:O	2.12	0.50
19:M:46:LEU:O	19:M:50:ARG:HG3	2.12	0.50
15:I:134:ILE:HG22	15:I:135:GLU:H	1.77	0.50
7:A:66:ARG:HH11	7:A:66:ARG:CB	2.24	0.50
17:K:28:GLU:OE2	17:K:58:THR:HG21	2.12	0.50
1:0:1543:G:N1	1:0:1641:A:OP2	2.36	0.50
24:R:113:HIS:O	24:R:145:LEU:HD12	2.12	0.50
29:W:35:VAL:HG22	29:W:36:PRO:O	2.12	0.50
1:0:517:U:C2'	1:0:518:G:H5'	2.42	0.50
1:0:2671:U:H5''	8:B:161:VAL:O	2.12	0.50
26:T:47:THR:HB	26:T:100:ASP:HB3	1.94	0.50
12:F:99:THR:O	12:F:99:THR:HG23	2.12	0.50
1:0:2878:U:H2'	1:0:2879:A:O4'	2.12	0.50
1:0:64:G:H2'	1:0:65:C:O4'	2.12	0.50
1:0:1855:G:H8	7:A:144:GLU:OE2	1.94	0.50
19:M:169:ARG:NH1	38:M:4109:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1201:C:H5''	38:O:6673:HOH:O	2.12	0.49
11:E:11:VAL:CG1	11:E:12:ASP:N	2.75	0.49
15:I:84:SER:HB3	15:I:92:VAL:HG21	1.94	0.49
38:9:4056:HOH:O	20:N:147:ILE:HB	2.12	0.49
1:O:653:U:H5''	38:O:4017:HOH:O	2.11	0.49
26:T:40:VAL:HG22	26:T:41:ARG:N	2.27	0.49
10:D:58:VAL:HB	10:D:62:ASP:HB3	1.94	0.49
1:O:195:C:H2'	1:O:196:G:H5'	1.94	0.49
1:O:1333:U:H2'	1:O:1334:C:C6	2.46	0.49
18:L:73:VAL:HG23	18:L:74:THR:H	1.77	0.49
1:O:1102:C:H5	38:O:6526:HOH:O	1.94	0.49
1:O:821:U:H2'	1:O:822:C:C6	2.41	0.49
19:M:65:VAL:CG2	19:M:105:ALA:HB2	2.41	0.49
9:C:246:ARG:HH11	9:C:246:ARG:HB3	1.77	0.49
1:O:656:G:H3'	21:O:37:ARG:HH12	1.77	0.49
1:O:596:C:H2'	1:O:597:A:H8	1.77	0.49
1:O:119:A:H2'	1:O:120:A:H5''	1.94	0.49
1:O:790:A:H1'	1:O:1710:A:H2'	1.94	0.49
1:O:1762:C:H2'	1:O:1763:C:H6	1.77	0.49
1:O:571:C:H6	1:O:571:C:O5'	1.94	0.49
13:G:64:ASN:HD22	13:G:64:ASN:N	2.10	0.49
1:O:598:C:H2'	1:O:599:G:H8	1.76	0.49
1:O:2371:G:H5'	38:O:8792:HOH:O	2.11	0.49
1:O:1118:A:C8	1:O:1119:G:H5''	2.46	0.49
29:W:76:ASP:O	29:W:77:ALA:C	2.49	0.49
1:O:559:U:H2'	1:O:560:U:O4'	2.12	0.49
18:L:133:VAL:HB	38:L:4072:HOH:O	2.12	0.49
1:O:1942:A:O2'	1:O:1943:C:H5'	2.11	0.49
13:G:71:LEU:C	13:G:73:ASP:N	2.65	0.49
1:O:702:G:O2'	1:O:703:G:H5'	2.12	0.49
18:L:89:PHE:N	38:L:4055:HOH:O	2.44	0.49
2:1:22:CYS:HA	38:1:4040:HOH:O	2.11	0.49
31:Y:126:PRO:HG2	31:Y:128:PHE:CE1	2.47	0.49
1:O:1307:A:H2'	1:O:1308:A:C8	2.46	0.49
16:J:79:PHE:HB3	16:J:103:VAL:HG11	1.94	0.49
9:C:107:ARG:O	9:C:111:VAL:HG23	2.11	0.49
1:O:1778:A:H2'	1:O:1779:A:H5'	1.95	0.49
1:O:595:U:H2'	1:O:596:C:C6	2.47	0.49
26:T:38:ARG:HH11	26:T:38:ARG:HG3	1.77	0.49
14:H:91:ARG:HH11	14:H:138:THR:CB	2.24	0.49
14:H:80:LEU:O	14:H:84:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:189:A:OP1	19:M:171:ARG:NH2	2.45	0.49
10:D:25:MET:CE	10:D:41:LEU:HG	2.42	0.49
20:N:34:LEU:HD13	20:N:47:LEU:HD21	1.95	0.49
28:V:1:THR:O	28:V:3:LEU:N	2.45	0.49
29:W:122:ARG:NH2	29:W:154:ARG:OXT	2.43	0.49
15:I:95:LEU:HA	15:I:99:GLN:OE1	2.12	0.49
1:0:820:G:C6	7:A:171:LYS:HB2	2.48	0.49
1:0:1715:C:H1'	22:P:57:ASN:HD21	1.77	0.49
1:0:2265:U:H2'	1:0:2266:A:C8	2.48	0.49
14:H:94:PRO:HA	14:H:127:ALA:O	2.13	0.49
1:0:1069:C:H2'	1:0:1070:A:O4'	2.13	0.49
21:O:14:LEU:HD23	21:O:102:ILE:HD11	1.93	0.49
1:0:2668:G:H2'	1:0:2669:U:C6	2.48	0.49
1:0:1181:A:H2'	1:0:1182:C:H5'	1.94	0.49
1:0:2533:C:H6	1:0:2533:C:C5'	2.22	0.49
20:N:73:ALA:N	38:N:4031:HOH:O	2.45	0.49
18:L:145:LEU:C	18:L:145:LEU:HD23	2.32	0.49
8:B:329:TYR:CE2	27:U:15:PRO:HG2	2.48	0.49
20:N:151:ASP:CG	20:N:165:ALA:O	2.51	0.49
10:D:93:LEU:HD23	38:D:4032:HOH:O	2.12	0.49
1:0:1375:A:H2'	1:0:1376:G:H5'	1.92	0.49
1:0:67:A:H5''	1:0:69:A:C8	2.48	0.49
1:0:2764:C:H2'	1:0:2765:C:H6	1.76	0.49
23:Q:32:GLU:HA	23:Q:71:TYR:OH	2.12	0.49
1:0:1039:G:H2'	1:0:1040:A:O4'	2.12	0.49
20:N:5:ARG:HG3	23:Q:18:PRO:HB3	1.94	0.49
18:L:43:HIS:O	18:L:44:GLU:C	2.51	0.49
12:F:100:ASP:O	12:F:101:ALA:O	2.31	0.49
30:X:78:GLU:HG2	30:X:79:GLU:N	2.27	0.49
1:0:1416:G:H2'	1:0:1417:G:H5'	1.93	0.49
1:0:2526:C:O2'	1:0:2527:U:H5'	2.13	0.49
1:0:1593:C:C6	22:P:120:ARG:HD3	2.47	0.49
25:S:57:THR:C	25:S:59:ASP:H	2.16	0.49
1:0:903:U:OP2	18:L:11:ARG:NH1	2.44	0.49
1:0:1633:C:H5''	1:0:1634:G:OP1	2.13	0.49
1:0:1825:U:O2'	1:0:1826:C:H5'	2.13	0.49
19:M:181:GLU:OE1	19:M:181:GLU:N	2.37	0.49
1:0:1316:G:H1'	1:0:1340:G:N2	2.28	0.49
1:0:130:C:H2'	38:O:4412:HOH:O	2.12	0.49
1:0:1783:A:O2'	1:0:1784:U:H5'	2.12	0.49
7:A:18:ALA:O	7:A:20:SER:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:151:GLN:O	9:C:154:VAL:HB	2.13	0.49
9:C:237:GLU:HB2	38:C:4114:HOH:O	2.13	0.49
29:W:88:THR:CG2	29:W:89:ASP:H	2.20	0.49
1:0:2896:A:H5''	38:0:9860:HOH:O	2.11	0.49
26:T:71:VAL:CG1	26:T:90:PRO:HB3	2.36	0.49
9:C:2:GLN:HB3	38:C:4006:HOH:O	2.13	0.49
1:0:1559:A:OP2	1:0:1559:A:H8	1.95	0.49
20:N:143:ARG:HA	20:N:172:PHE:CD2	2.48	0.49
1:0:694:A:C2'	1:0:695:C:H5'	2.41	0.49
1:0:2837:U:H1'	8:B:307:ARG:HH12	1.77	0.49
1:0:1200:A:H1'	38:0:6678:HOH:O	2.13	0.49
1:0:834:G:H3'	1:0:835:U:H4'	1.95	0.49
1:0:1497:G:H4'	1:0:1627:G:O2'	2.13	0.49
1:0:1236:A:C8	16:J:63:ILE:HD11	2.48	0.49
18:L:125:PHE:CZ	18:L:140:VAL:HG13	2.47	0.49
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.49
1:0:1119:G:H22	1:0:1246:A:H2	1.55	0.49
22:P:114:LEU:HA	22:P:118:GLN:NE2	2.28	0.49
1:0:2636:C:H3'	38:0:9469:HOH:O	2.12	0.49
7:A:153:ARG:NH1	7:A:153:ARG:HB2	2.28	0.49
1:0:2468:A:H61	4:3:48:ASN:HD21	1.60	0.49
1:0:2312:G:H2'	1:0:2313:C:H5'	1.94	0.49
1:0:1771:U:H5'	32:Z:20:ARG:HH21	1.76	0.49
10:D:138:GLY:N	38:D:4044:HOH:O	2.36	0.49
15:I:87:PRO:HD3	38:I:4009:HOH:O	2.13	0.49
7:A:153:ARG:CB	7:A:153:ARG:HH11	2.26	0.49
1:0:654:A:OP2	21:O:38:ARG:HD3	2.12	0.49
31:Y:107:PRO:HB3	31:Y:182:PHE:CD2	2.48	0.49
1:0:705:C:H2'	1:0:705:C:O2	2.13	0.49
29:W:38:THR:O	29:W:42:ARG:HB2	2.13	0.49
1:0:1299:G:O6	18:L:6:ARG:HD3	2.13	0.49
1:0:635:A:H2'	1:0:636:G:H5''	1.94	0.49
20:N:37:ARG:HE	20:N:105:GLY:HA3	1.78	0.48
32:Z:10:ARG:HA	38:Z:4016:HOH:O	2.11	0.48
1:0:2896:A:OP1	30:X:15:ARG:NH1	2.46	0.48
9:C:157:LEU:HD11	9:C:194:PHE:HZ	1.78	0.48
1:0:2578:G:C8	1:0:2578:G:H5'	2.43	0.48
18:L:20:ASN:O	18:L:22:ARG:N	2.46	0.48
11:E:20:ILE:CD1	11:E:40:VAL:HG11	2.42	0.48
4:3:65:THR:HB	4:3:83:TRP:H	1.77	0.48
38:0:8002:HOH:O	7:A:11:ARG:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:66:THR:CG2	30:X:67:PRO:HD2	2.44	0.48
1:0:130:C:H5'	38:0:4367:HOH:O	2.13	0.48
24:R:59:PHE:HZ	24:R:81:PRO:HG3	1.77	0.48
1:0:932:U:H2'	1:0:933:C:C6	2.47	0.48
1:0:226:A:H1'	1:0:393:G:C5	2.48	0.48
17:K:121:PHE:HB3	38:K:4052:HOH:O	2.12	0.48
1:0:1811:A:C2	1:0:2752:C:H1'	2.48	0.48
14:H:12:ILE:HG12	14:H:59:GLN:HG2	1.94	0.48
38:0:6512:HOH:O	29:W:119:HIS:HE1	1.96	0.48
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.48
16:J:75:PRO:HD3	16:J:136:SER:OG	2.13	0.48
13:G:19:GLU:O	13:G:23:ILE:HG13	2.14	0.48
22:P:98:ILE:HD13	22:P:98:ILE:O	2.13	0.48
1:0:396:U:H1'	38:0:4988:HOH:O	2.12	0.48
20:N:64:SER:O	20:N:66:LEU:N	2.46	0.48
1:0:808:A:C5	1:0:809:G:H1'	2.48	0.48
19:M:164:THR:CG2	19:M:167:GLY:H	2.15	0.48
8:B:255:GLY:O	8:B:257:THR:HG23	2.14	0.48
14:H:41:LYS:HD3	14:H:46:TYR:OH	2.12	0.48
7:A:186:TRP:CG	7:A:187:PRO:HA	2.48	0.48
1:0:2598:U:O2	1:0:2600:A:C8	2.66	0.48
18:L:62:ALA:HB2	18:L:103:ALA:HB2	1.95	0.48
1:0:1762:C:H4'	38:0:7814:HOH:O	2.13	0.48
21:O:14:LEU:CD2	21:O:102:ILE:HD11	2.42	0.48
18:L:6:ARG:NH2	38:L:4004:HOH:O	2.45	0.48
1:0:777:U:O2'	2:1:11:LYS:HG2	2.13	0.48
8:B:171:VAL:O	8:B:175:LEU:HB2	2.12	0.48
14:H:57:THR:HG23	14:H:131:GLN:HA	1.94	0.48
14:H:59:GLN:NE2	14:H:129:ARG:NE	2.52	0.48
3:2:41:HIS:HB3	3:2:44:ARG:HB2	1.96	0.48
1:0:1874:U:OP1	7:A:51:ARG:HD2	2.12	0.48
9:C:132:ASP:CB	38:C:4107:HOH:O	2.58	0.48
4:3:56:PRO:HA	38:3:4043:HOH:O	2.13	0.48
1:0:1277:C:OP2	21:O:19:ARG:NH1	2.47	0.48
1:0:1909:A:N1	1:0:2128:G:H1'	2.27	0.48
1:0:776:A:OP1	2:1:28:HIS:HE1	1.96	0.48
1:0:87:C:H2'	3:2:28:LYS:O	2.13	0.48
1:0:2359:G:H3'	38:0:8775:HOH:O	2.12	0.48
19:M:26:GLN:O	19:M:29:GLN:HB2	2.14	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.47	0.48
29:W:11:VAL:O	29:W:12:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1278:A:H4'	1:0:1279:U:C4	2.48	0.48
1:0:2314:G:C2'	1:0:2315:C:H5'	2.42	0.48
30:X:46:ASP:OD2	30:X:46:ASP:N	2.45	0.48
21:O:44:ASN:OD1	21:O:65:LEU:HB2	2.13	0.48
19:M:98:GLN:HB2	19:M:129:HIS:NE2	2.28	0.48
15:I:73:LEU:HD12	15:I:107:LYS:NZ	2.29	0.48
11:E:5:LEU:HD21	11:E:66:GLN:HG3	1.95	0.48
1:0:2659:U:H5''	38:0:9542:HOH:O	2.13	0.48
20:N:37:ARG:HH21	20:N:105:GLY:N	2.12	0.48
22:P:142:ASP:O	22:P:143:ALA:O	2.30	0.48
20:N:116:PHE:HB3	20:N:136:LEU:HD23	1.95	0.48
1:0:2754:G:O2'	1:0:2755:G:H5'	2.14	0.48
1:0:1787:C:OP1	22:P:68:LYS:HE2	2.13	0.48
9:C:151:GLN:HB3	38:C:4118:HOH:O	2.13	0.48
1:0:84:G:O2'	1:0:85:C:H5'	2.13	0.48
1:0:228:C:H2'	1:0:229:G:H5'	1.94	0.48
19:M:54:TYR:HB2	19:M:132:ILE:HD13	1.95	0.48
1:0:722:G:H22	1:0:938:G:P	2.37	0.48
1:0:541:C:H2'	1:0:542:A:H5'	1.94	0.48
18:L:129:ALA:O	18:L:133:VAL:HG23	2.14	0.48
1:0:1007:A:H2'	14:H:22:TYR:OH	2.14	0.48
8:B:83:ALA:HB2	8:B:101:TRP:CD2	2.49	0.48
23:Q:93:ARG:HH11	23:Q:93:ARG:HG3	1.79	0.48
1:0:1051:C:H2'	1:0:1052:G:O4'	2.14	0.48
17:K:99:ASP:OD1	17:K:101:ASN:N	2.47	0.48
12:F:4:VAL:HG13	12:F:76:PHE:CE1	2.48	0.48
1:0:553:G:H3'	38:0:5310:HOH:O	2.14	0.48
1:0:2291:A:N9	1:0:2309:C:H5'	2.29	0.48
15:I:100:VAL:HG11	15:I:124:VAL:HG22	1.96	0.48
25:S:52:VAL:C	25:S:53:ASN:HD22	2.17	0.48
1:0:596:C:H2'	1:0:597:A:C8	2.48	0.48
1:0:101:C:H2'	1:0:102:A:C8	2.49	0.48
17:K:35:HIS:HB2	17:K:52:LYS:O	2.14	0.48
4:3:34:LYS:HE2	38:3:4020:HOH:O	2.13	0.48
9:C:26:VAL:HG21	9:C:123:LEU:HD11	1.96	0.48
19:M:184:ARG:HG3	19:M:185:PRO:HA	1.96	0.48
1:0:351:A:O2'	1:0:352:A:H5'	2.13	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.14	0.48
1:0:1638:U:H5'	38:0:7499:HOH:O	2.14	0.48
10:D:67:ASP:O	10:D:69:ILE:HG13	2.13	0.48
30:X:71:ARG:HD2	38:X:4027:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1882:C:OP1	7:A:192:VAL:HG23	2.14	0.48
24:R:132:ARG:NH2	38:R:4075:HOH:O	2.46	0.48
13:G:67:LEU:O	13:G:71:LEU:HG	2.13	0.48
1:O:1477:C:H5'	1:O:1868:G:H5'	1.96	0.48
31:Y:115:ARG:NE	38:Y:4021:HOH:O	2.47	0.48
24:R:82:GLU:HG3	24:R:83:LYS:H	1.79	0.48
11:E:34:TRP:HA	38:E:4013:HOH:O	2.13	0.48
1:O:1524:U:OP1	1:O:1524:U:H4'	2.14	0.48
1:O:105:G:O2'	1:O:106:A:H5'	2.14	0.48
1:O:1018:A:H4'	23:Q:59:GLN:NE2	2.29	0.48
1:O:1041:U:H2'	1:O:1042:U:H5'	1.96	0.48
21:O:88:LYS:HB3	38:O:4028:HOH:O	2.13	0.48
1:O:2456:A:H5'	38:O:8994:HOH:O	2.14	0.48
1:O:2281:C:H2'	1:O:2282:U:H5'	1.95	0.48
32:Z:32:GLU:HA	32:Z:35:GLU:HG3	1.96	0.48
15:I:118:ASN:HA	15:I:121:LYS:CD	2.43	0.48
8:B:27:ASN:H	8:B:27:ASN:ND2	2.06	0.48
9:C:27:ARG:NH1	9:C:29:ASP:OD1	2.43	0.48
11:E:118:ILE:HD13	11:E:124:VAL:HG23	1.95	0.48
20:N:184:ILE:HG23	20:N:184:ILE:O	2.14	0.48
1:O:1150:A:C2	13:G:20:VAL:HG21	2.49	0.48
19:M:9:ARG:HG3	38:M:4033:HOH:O	2.14	0.48
8:B:268:ARG:NH2	8:B:325:PRO:HG3	2.29	0.48
1:O:1470:A:OP1	19:M:93:ARG:HD2	2.14	0.48
1:O:667:C:H2'	1:O:668:C:H6	1.79	0.48
31:Y:144:ARG:CZ	38:Y:4050:HOH:O	2.62	0.48
21:O:105:ASN:HD21	21:O:109:SER:H	1.62	0.48
17:K:37:TYR:HD2	38:K:4016:HOH:O	1.97	0.48
26:T:92:ASP:OD1	26:T:94:SER:HB3	2.14	0.48
1:O:2617:G:H4'	38:O:9406:HOH:O	2.14	0.48
38:O:6494:HOH:O	29:W:9:GLY:HA3	2.13	0.48
31:Y:133:HIS:HD2	38:Y:4039:HOH:O	1.96	0.48
27:U:52:THR:HG22	27:U:54:THR:HB	1.95	0.47
8:B:80:ARG:O	8:B:82:VAL:HG23	2.14	0.47
1:O:644:G:H1'	38:O:5476:HOH:O	2.12	0.47
1:O:68:U:O2'	1:O:69:A:H5''	2.14	0.47
18:L:125:PHE:CE1	18:L:140:VAL:HG13	2.49	0.47
1:O:825:U:H5''	1:O:826:U:OP1	2.14	0.47
1:O:1008:C:H5''	14:H:19:ARG:HH12	1.78	0.47
1:O:1406:A:H5'	1:O:1407:A:C8	2.48	0.47
1:O:134:U:C2	1:O:145:A:C2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2729:C:H4'	1:0:2893:C:O2	2.14	0.47
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
1:0:2735:U:H2'	1:0:2736:U:C6	2.48	0.47
1:0:533:U:H3'	38:0:5265:HOH:O	2.14	0.47
28:V:12:THR:HB	28:V:15:GLU:OE2	2.14	0.47
31:Y:187:VAL:CG1	31:Y:205:ILE:HA	2.43	0.47
20:N:48:VAL:HG12	20:N:55:ASP:HB3	1.90	0.47
8:B:212:GLN:OE1	8:B:216:LYS:HD3	2.13	0.47
16:J:6:PHE:O	16:J:8:ALA:N	2.47	0.47
23:Q:23:THR:HG22	23:Q:24:SER:N	2.29	0.47
29:W:69:ARG:HD2	29:W:117:ARG:O	2.14	0.47
8:B:301:VAL:HG13	8:B:302:PRO:HD2	1.96	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
12:F:78:GLU:HG3	38:F:4017:HOH:O	2.14	0.47
1:0:69:A:H5'	1:0:69:A:H8	1.78	0.47
31:Y:144:ARG:NE	38:Y:4050:HOH:O	2.46	0.47
9:C:104:ASP:O	9:C:108:GLN:HG3	2.14	0.47
1:0:1948:G:H2'	1:0:1949:G:O4'	2.14	0.47
12:F:37:THR:O	12:F:41:GLU:HG3	2.14	0.47
1:0:1581:A:H61	1:0:1614:G:H1'	1.78	0.47
1:0:2002:C:H2'	1:0:2003:U:H5'	1.95	0.47
1:0:2100:A:H5'	38:0:8464:HOH:O	2.14	0.47
29:W:6:GLN:CB	29:W:26:ILE:HD12	2.34	0.47
20:N:7:LYS:HE3	23:Q:21:ARG:O	2.15	0.47
17:K:87:ARG:HB2	27:U:19:THR:HG23	1.95	0.47
15:I:108:HIS:N	15:I:109:PRO:CD	2.77	0.47
17:K:32:ILE:HD11	17:K:56:SER:HB3	1.96	0.47
8:B:36:PRO:HG3	8:B:169:GLY:H	1.77	0.47
6:9:3:A:H2'	38:9:4029:HOH:O	2.14	0.47
6:9:34:A:H8	6:9:34:A:O5'	1.96	0.47
8:B:1:PRO:O	8:B:2:GLN:HB2	2.13	0.47
1:0:766:A:HO2'	1:0:767:A:H8	1.62	0.47
38:0:7728:HOH:O	8:B:214:PRO:HD2	2.14	0.47
6:9:76:G:C3'	6:9:77:A:H5''	2.35	0.47
1:0:1840:A:H4'	1:0:1841:C:O5'	2.14	0.47
18:L:143:THR:CG2	18:L:144:ASP:N	2.77	0.47
1:0:1173:A:H2	38:0:6677:HOH:O	1.96	0.47
24:R:99:ALA:CB	24:R:109:MET:HE3	2.45	0.47
9:C:246:ARG:NH2	38:C:4174:HOH:O	2.42	0.47
20:N:67:ALA:HA	20:N:71:TRP:CB	2.44	0.47
1:0:2388:C:H2'	1:0:2389:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2241:C:O2'	1:0:2242:U:H5'	2.14	0.47
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.47
8:B:30:PRO:HB2	8:B:39:GLN:NE2	2.28	0.47
20:N:37:ARG:NH2	20:N:105:GLY:CA	2.70	0.47
29:W:139:GLY:O	29:W:141:HIS:CD2	2.67	0.47
1:0:2353:A:O2'	20:N:7:LYS:HB3	2.14	0.47
1:0:1735:C:O2'	1:0:1736:A:H5'	2.13	0.47
1:0:213:G:N2	1:0:225:G:H2'	2.30	0.47
2:1:21:ARG:HD2	2:1:39:PHE:HB2	1.97	0.47
21:O:26:TRP:HA	21:O:26:TRP:CE3	2.49	0.47
11:E:16:ASP:O	11:E:17:HIS:HB2	2.14	0.47
24:R:114:VAL:HA	24:R:144:GLU:O	2.14	0.47
14:H:142:ASN:O	14:H:144:GLU:N	2.47	0.47
1:0:1154:A:H2'	1:0:1155:G:C8	2.49	0.47
1:0:1044:C:H5''	38:0:6141:HOH:O	2.15	0.47
1:0:2520:G:H5'	14:H:64:SER:OG	2.15	0.47
7:A:8:ARG:HG2	38:A:4009:HOH:O	2.13	0.47
1:0:363:C:O2'	1:0:364:U:H5'	2.15	0.47
15:I:87:PRO:CB	15:I:129:SER:C	2.83	0.47
14:H:12:ILE:HG12	14:H:59:GLN:CG	2.45	0.47
10:D:64:ARG:HD3	10:D:67:ASP:HB3	1.96	0.47
1:0:2780:C:H2'	1:0:2781:U:C6	2.50	0.47
16:J:39:VAL:CG1	16:J:107:ASN:HB2	2.45	0.47
9:C:233:THR:CG2	9:C:234:VAL:H	2.26	0.47
27:U:13:ILE:HG12	27:U:32:CYS:HB3	1.96	0.47
38:0:8124:HOH:O	7:A:236:GLY:HA3	2.14	0.47
30:X:80:GLU:HG2	30:X:80:GLU:O	2.14	0.47
10:D:23:VAL:HG21	10:D:45:THR:CG2	2.43	0.47
1:0:1116:U:O2'	1:0:1118:A:C2	2.56	0.47
30:X:43:VAL:HG12	30:X:44:ASP:N	2.30	0.47
11:E:81:GLU:HG2	11:E:134:SER:CB	2.44	0.47
1:0:2365:G:P	23:Q:15:LYS:HG3	2.54	0.47
16:J:39:VAL:HG12	16:J:40:ASN:ND2	2.29	0.47
6:9:91:C:H2'	6:9:92:G:O4'	2.15	0.47
20:N:11:ARG:HG3	20:N:14:ARG:NH1	2.29	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.40	0.47
1:0:1416:G:C2'	1:0:1417:G:H5'	2.44	0.47
1:0:657:G:H2'	1:0:658:C:C6	2.50	0.47
17:K:106:GLY:HA3	38:K:4013:HOH:O	2.14	0.47
16:J:54:VAL:CG1	16:J:138:THR:HG21	2.45	0.47
26:T:43:ASN:C	26:T:45:GLY:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:15:PRO:HA	19:M:20:LEU:CD2	2.45	0.47
1:0:946:C:O2'	1:0:947:U:H5'	2.15	0.47
19:M:61:ILE:HG22	19:M:62:VAL:N	2.28	0.47
1:0:101:C:H2'	1:0:102:A:H8	1.80	0.47
1:0:2281:C:C2'	1:0:2282:U:H5'	2.45	0.47
1:0:625:U:H5''	1:0:1044:C:N4	2.29	0.47
14:H:86:TYR:CD1	14:H:86:TYR:C	2.88	0.47
1:0:2607:U:H4'	38:0:9356:HOH:O	2.14	0.47
4:3:30:GLN:NE2	38:3:4016:HOH:O	2.43	0.47
31:Y:108:ASP:N	31:Y:108:ASP:OD1	2.48	0.47
26:T:42:VAL:CG1	26:T:62:VAL:HG21	2.44	0.47
8:B:52:VAL:O	8:B:53:LEU:HD12	2.15	0.47
20:N:100:ALA:O	20:N:129:ILE:HG23	2.15	0.47
3:2:31:ARG:NH1	38:2:4023:HOH:O	2.48	0.47
3:2:35:ARG:HB2	38:2:4028:HOH:O	2.15	0.47
20:N:94:GLU:HG3	20:N:186:LEU:HD12	1.96	0.47
1:0:563:C:H2'	1:0:564:G:O4'	2.15	0.47
9:C:127:ARG:HG2	9:C:127:ARG:NH1	2.30	0.47
8:B:304:PRO:HD2	8:B:307:ARG:CD	2.43	0.47
22:P:16:VAL:CG1	22:P:20:ARG:CZ	2.93	0.47
1:0:2597:U:H2'	1:0:2598:U:H5'	1.96	0.47
1:0:949:U:H4'	23:Q:95:GLU:HA	1.97	0.47
1:0:2064:U:H5'	1:0:2652:U:O3'	2.15	0.47
7:A:164:ARG:CZ	38:A:4052:HOH:O	2.62	0.47
18:L:78:ALA:N	38:L:4054:HOH:O	2.48	0.47
1:0:2114:C:OP1	7:A:1:GLY:HA2	2.15	0.47
1:0:1236:A:C2'	1:0:1237:U:H5'	2.45	0.47
1:0:876:A:H2'	1:0:876:A:N3	2.29	0.47
21:O:96:VAL:HG13	21:O:100:GLN:OE1	2.14	0.47
1:0:2656:G:O2'	1:0:2657:G:H5'	2.15	0.47
19:M:164:THR:HB	38:M:4105:HOH:O	2.13	0.47
28:V:1:THR:O	28:V:4:HIS:CE1	2.68	0.47
8:B:132:HIS:HB2	8:B:137:LEU:CD2	2.45	0.47
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.47
1:0:1205:U:H2'	1:0:1206:U:H5''	1.97	0.47
7:A:211:LYS:CB	38:A:4100:HOH:O	2.60	0.47
7:A:153:ARG:HH11	7:A:153:ARG:HB2	1.80	0.47
17:K:65:ARG:HD3	38:K:4033:HOH:O	2.15	0.47
10:D:91:ALA:HB2	10:D:106:PHE:CD2	2.50	0.47
11:E:31:ARG:HH12	11:E:68:HIS:CE1	2.33	0.47
25:S:57:THR:HG22	25:S:58:MET:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:598:C:H2'	1:0:599:G:C8	2.50	0.47
14:H:117:ARG:O	14:H:118:ALA:C	2.53	0.47
1:0:2324:G:N2	1:0:2377:U:H1'	2.30	0.47
19:M:146:ASP:O	19:M:147:LEU:HD23	2.15	0.47
8:B:24:PRO:CG	8:B:204:GLY:HA2	2.45	0.47
18:L:65:ASP:HA	18:L:109:LEU:O	2.14	0.47
18:L:68:GLU:HB2	38:L:4048:HOH:O	2.15	0.47
16:J:41:ALA:O	16:J:132:LEU:HD12	2.15	0.47
20:N:72:GLU:HB3	20:N:171:HIS:HE1	1.80	0.47
14:H:48:VAL:HA	14:H:170:ARG:O	2.15	0.47
2:1:1:THR:HG21	38:1:4005:HOH:O	2.15	0.47
20:N:154:LEU:CD1	20:N:157:PRO:HA	2.44	0.47
1:0:704:C:H2'	1:0:705:C:H6	1.80	0.47
26:T:44:ALA:HA	26:T:62:VAL:HG12	1.95	0.47
8:B:124:ALA:O	8:B:128:ILE:HG13	2.14	0.47
1:0:2541:U:H5'	1:0:2611:G:O6	2.15	0.47
1:0:327:A:N3	9:C:206:ASN:ND2	2.63	0.47
1:0:2900:G:H2'	1:0:2901:C:O4'	2.15	0.47
10:D:86:THR:HG23	38:D:4030:HOH:O	2.14	0.47
17:K:49:LEU:HA	17:K:73:VAL:HG12	1.97	0.47
1:0:2596:A:H2	36:8:8812:CL:CL	2.35	0.47
1:0:558:C:H2'	1:0:559:U:H5'	1.93	0.46
10:D:141:VAL:HG13	10:D:144:ARG:HH21	1.80	0.46
11:E:81:GLU:HA	11:E:133:VAL:O	2.15	0.46
12:F:56:PRO:HG2	19:M:44:THR:HA	1.97	0.46
1:0:1603:A:C5'	1:0:1605:G:H5'	2.45	0.46
7:A:94:LEU:N	7:A:94:LEU:HD23	2.29	0.46
8:B:83:ALA:HA	8:B:100:VAL:O	2.15	0.46
8:B:84:LEU:HB3	8:B:100:VAL:HB	1.98	0.46
3:2:20:ARG:CG	3:2:21:VAL:N	2.79	0.46
2:1:45:ARG:HB3	38:1:4042:HOH:O	2.14	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.15	0.46
1:0:2314:G:O2'	1:0:2315:C:H5'	2.15	0.46
17:K:49:LEU:HD23	17:K:50:GLY:N	2.30	0.46
16:J:51:GLU:O	16:J:55:GLU:HG3	2.15	0.46
1:0:1064:U:H2'	1:0:1065:G:C8	2.50	0.46
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.46
1:0:870:G:OP2	7:A:3:ARG:HD3	2.15	0.46
20:N:47:LEU:HD23	20:N:47:LEU:HA	1.71	0.46
1:0:2039:A:H4'	1:0:2760:C:O2'	2.16	0.46
28:V:1:THR:CG2	28:V:2:VAL:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:69:ARG:NH2	38:W:4068:HOH:O	2.45	0.46
8:B:41:PHE:HB3	8:B:190:MET:HE1	1.97	0.46
9:C:133:ARG:NE	9:C:138:VAL:HG22	2.30	0.46
21:O:26:TRP:HB2	38:O:4009:HOH:O	2.14	0.46
4:3:55:VAL:HB	4:3:56:PRO:CD	2.45	0.46
18:L:55:GLN:HA	18:L:58:GLN:NE2	2.30	0.46
1:0:2501:G:H1'	38:0:9124:HOH:O	2.16	0.46
17:K:64:MET:HA	17:K:67:GLN:HE21	1.81	0.46
30:X:54:ILE:O	30:X:57:ALA:HB3	2.15	0.46
1:0:152:A:O2'	1:0:153:C:H5'	2.15	0.46
1:0:2644:C:O2'	1:0:2645:U:OP1	2.29	0.46
1:0:806:A:H2'	1:0:807:A:O4'	2.15	0.46
1:0:1625:U:H4'	38:0:7488:HOH:O	2.15	0.46
10:D:152:PRO:O	10:D:156:ARG:HG2	2.15	0.46
9:C:140:VAL:HG12	9:C:141:SER:N	2.30	0.46
1:0:553:G:P	31:Y:204:ARG:HH22	2.38	0.46
29:W:80:ASP:HB2	38:W:4039:HOH:O	2.15	0.46
31:Y:177:LYS:HD3	31:Y:181:GLY:O	2.15	0.46
21:O:26:TRP:HA	21:O:26:TRP:HE3	1.79	0.46
30:X:22:ASN:O	30:X:25:ARG:HG3	2.15	0.46
17:K:66:ARG:HH11	17:K:66:ARG:HG2	1.81	0.46
7:A:37:VAL:HG13	38:A:4028:HOH:O	2.14	0.46
12:F:43:GLY:C	12:F:45:ALA:H	2.18	0.46
8:B:109:LEU:CG	8:B:113:LEU:HD12	2.46	0.46
1:0:1333:U:H2'	1:0:1334:C:H6	1.80	0.46
1:0:2656:G:C2'	1:0:2657:G:H5'	2.45	0.46
10:D:167:GLU:HA	10:D:171:ASP:OD1	2.15	0.46
11:E:170:ARG:NH2	38:E:4042:HOH:O	2.48	0.46
8:B:77:PRO:HG2	8:B:151:VAL:CG2	2.45	0.46
17:K:5:GLY:O	17:K:83:PRO:HD3	2.16	0.46
14:H:151:GLU:HG3	38:H:4057:HOH:O	2.15	0.46
26:T:113:GLU:O	26:T:114:SER:C	2.53	0.46
1:0:1168:C:H5	38:0:6638:HOH:O	1.98	0.46
31:Y:205:ILE:HB	31:Y:230:ASN:HD21	1.80	0.46
1:0:31:C:H4'	38:0:4093:HOH:O	2.16	0.46
6:9:56:A:H1'	10:D:14:ARG:HG2	1.97	0.46
11:E:145:ALA:HB1	11:E:168:ILE:CD1	2.44	0.46
15:I:133:THR:HG22	15:I:134:ILE:H	1.79	0.46
15:I:96:SER:H	15:I:99:GLN:CD	2.18	0.46
19:M:57:LYS:NZ	19:M:144:ASP:OD2	2.38	0.46
1:0:2505:G:H8	38:0:9129:HOH:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2820:A:H2'	1:0:2821:C:C6	2.50	0.46
20:N:179:LEU:HA	20:N:184:ILE:CD1	2.44	0.46
1:0:1762:C:H2'	1:0:1763:C:C6	2.51	0.46
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.46
1:0:106:A:H2'	1:0:107:U:O4'	2.15	0.46
8:B:24:PRO:HD3	38:B:4023:HOH:O	2.14	0.46
32:Z:51:GLY:HA3	38:Z:4024:HOH:O	2.15	0.46
7:A:140:LEU:HB3	7:A:141:PRO:HD2	1.96	0.46
1:0:1515:A:H2'	1:0:1516:U:C6	2.50	0.46
1:0:541:C:C2'	1:0:542:A:C5'	2.92	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
19:M:61:ILE:N	19:M:61:ILE:HD12	2.30	0.46
17:K:130:MET:SD	27:U:25:ASP:O	2.73	0.46
30:X:80:GLU:N	38:X:4026:HOH:O	2.48	0.46
17:K:64:MET:HA	17:K:67:GLN:NE2	2.31	0.46
31:Y:216:ARG:CD	38:Y:4088:HOH:O	2.63	0.46
1:0:1483:C:O2'	1:0:1484:G:H5'	2.14	0.46
29:W:67:ALA:HB2	29:W:93:ILE:HD13	1.98	0.46
1:0:336:G:O6	26:T:54:ASP:N	2.48	0.46
31:Y:196:VAL:CG1	31:Y:226:ILE:HD13	2.45	0.46
1:0:1185:U:H5'	38:0:6660:HOH:O	2.14	0.46
10:D:41:LEU:HA	10:D:44:ILE:CG2	2.45	0.46
29:W:4:LEU:HD23	29:W:54:PHE:CB	2.39	0.46
20:N:115:VAL:HG22	38:N:4044:HOH:O	2.15	0.46
14:H:69:ARG:HB3	38:H:4025:HOH:O	2.14	0.46
12:F:50:VAL:HG21	12:F:63:ILE:HG21	1.97	0.46
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.46
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.46
4:3:11:CYS:HB2	4:3:20:HIS:CE1	2.50	0.46
19:M:31:TRP:CD1	19:M:64:ARG:NH1	2.84	0.46
1:0:1976:G:H5''	38:0:8161:HOH:O	2.15	0.46
1:0:1422:U:H4'	38:0:7154:HOH:O	2.14	0.46
1:0:2455:A:H2'	1:0:2456:A:O4'	2.16	0.46
1:0:121:U:OP2	3:2:10:ARG:NH2	2.48	0.46
38:0:5875:HOH:O	8:B:229:ARG:HD2	2.14	0.46
9:C:120:ASP:O	9:C:124:VAL:HG23	2.16	0.46
15:I:102:GLN:HA	15:I:105:GLU:OE2	2.15	0.46
10:D:146:LYS:HZ1	20:N:107:ASN:ND2	2.14	0.46
14:H:50:ILE:HD12	14:H:149:VAL:CG1	2.45	0.46
11:E:15:GLN:HG3	11:E:20:ILE:HG12	1.98	0.46
38:0:5281:HOH:O	31:Y:135:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:200:PRO:HA	38:C:4143:HOH:O	2.16	0.46
1:0:1614:G:H2'	38:0:7429:HOH:O	2.14	0.46
26:T:61:GLU:N	38:T:4021:HOH:O	2.40	0.46
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.46
38:0:9654:HOH:O	22:P:58:SER:HB3	2.15	0.46
1:0:2708:G:H2'	1:0:2709:G:O4'	2.16	0.46
1:0:2549:C:H2'	1:0:2550:U:O4'	2.16	0.46
1:0:1619:G:H2'	1:0:1620:C:O4'	2.16	0.46
1:0:622:G:O2'	1:0:623:U:H5'	2.16	0.46
26:T:25:ALA:O	26:T:39:ASN:CB	2.64	0.46
1:0:2004:U:H2'	1:0:2004:U:O2	2.15	0.46
6:9:64:C:H2'	6:9:65:A:H5'	1.97	0.46
1:0:894:A:C2	9:C:87:ARG:NH2	2.84	0.46
26:T:61:GLU:HG3	38:T:4018:HOH:O	2.15	0.46
28:V:24:LYS:O	28:V:27:LEU:HB3	2.16	0.46
1:0:1471:A:H2'	1:0:1472:C:C6	2.49	0.46
29:W:1:MET:HB2	29:W:103:GLU:HG2	1.97	0.46
1:0:545:G:H2'	1:0:546:C:O4'	2.16	0.46
1:0:962:C:C1'	20:N:5:ARG:NH1	2.73	0.46
1:0:1878:G:O2'	1:0:1879:U:OP2	2.34	0.46
1:0:1450:C:O2'	1:0:1493:A:H2'	2.15	0.46
1:0:1120:U:H6	1:0:1120:U:H5''	1.81	0.46
25:S:32:ALA:HA	25:S:36:GLU:OE1	2.16	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.46	0.46
1:0:2453:G:H4'	18:L:50:GLY:C	2.36	0.46
8:B:80:ARG:HA	8:B:186:GLY:O	2.16	0.46
1:0:2831:C:H2'	1:0:2832:C:C5'	2.45	0.46
38:9:4011:HOH:O	23:Q:27:GLN:HB2	2.16	0.46
1:0:2002:C:C2'	1:0:2003:U:H5'	2.45	0.46
31:Y:216:ARG:HD3	38:Y:4088:HOH:O	2.15	0.46
1:0:699:C:C2	1:0:743:G:N2	2.84	0.46
1:0:417:G:P	38:0:5015:HOH:O	2.73	0.46
12:F:117:GLU:C	12:F:119:ARG:H	2.18	0.46
1:0:2717:C:OP1	8:B:207:LYS:HG3	2.16	0.46
1:0:1878:G:H5''	38:0:8029:HOH:O	2.16	0.46
1:0:960:G:H8	38:0:6250:HOH:O	1.98	0.46
8:B:55:ASN:CG	8:B:63:GLU:HA	2.36	0.46
7:A:130:THR:N	38:A:4046:HOH:O	2.48	0.46
1:0:661:G:C5	1:0:686:A:C2	3.04	0.46
26:T:32:ARG:NH1	26:T:38:ARG:HH12	2.14	0.46
26:T:82:THR:C	26:T:84:GLY:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1804:A:H2'	1:0:1805:G:C8	2.51	0.46
10:D:128:LEU:HB2	38:D:4034:HOH:O	2.15	0.46
1:0:37:A:H2'	1:0:38:G:H8	1.80	0.46
7:A:101:GLU:OE2	7:A:131:HIS:HB2	2.16	0.46
31:Y:122:ARG:NH2	38:Y:4025:HOH:O	2.49	0.46
30:X:31:ILE:O	30:X:35:GLU:HG3	2.16	0.46
23:Q:4:ASN:ND2	38:Q:4004:HOH:O	2.49	0.46
1:0:675:U:O2'	9:C:42:ARG:NH1	2.49	0.46
38:9:4139:HOH:O	20:N:65:ASP:HB3	2.14	0.46
1:0:1161:A:O5'	1:0:1161:A:H8	1.98	0.45
29:W:88:THR:HG22	29:W:90:TYR:CD1	2.51	0.45
1:0:1071:G:H4'	31:Y:154:ARG:HH22	1.80	0.45
1:0:700:A:C2	18:L:71:GLU:HG2	2.51	0.45
9:C:84:VAL:O	9:C:85:LYS:HB2	2.15	0.45
6:9:5:G:O2'	6:9:6:C:H5'	2.17	0.45
10:D:23:VAL:O	10:D:23:VAL:HG23	2.16	0.45
3:2:41:HIS:CD2	3:2:44:ARG:H	2.33	0.45
18:L:91:VAL:CG1	18:L:120:LEU:HD23	2.47	0.45
1:0:1603:A:H5'	1:0:1605:G:C4'	2.46	0.45
9:C:133:ARG:HG3	9:C:133:ARG:HH11	1.81	0.45
24:R:39:THR:HB	24:R:42:GLU:CD	2.36	0.45
26:T:73:HIS:HD2	26:T:88:PRO:CG	2.27	0.45
19:M:134:ILE:CG2	19:M:141:ILE:HD13	2.46	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.45
1:0:2802:C:H2'	1:0:2803:C:H6	1.81	0.45
1:0:169:A:H1'	4:3:48:ASN:ND2	2.32	0.45
1:0:130:C:H1'	38:0:4369:HOH:O	2.16	0.45
18:L:122:ALA:HB3	18:L:125:PHE:CZ	2.52	0.45
1:0:932:U:H2'	1:0:933:C:H6	1.81	0.45
7:A:132:ASP:OD1	7:A:133:ARG:N	2.49	0.45
1:0:2335:C:H2'	1:0:2336:G:C8	2.51	0.45
1:0:245:C:H2'	38:0:4774:HOH:O	2.16	0.45
15:I:87:PRO:HB3	15:I:129:SER:C	2.36	0.45
22:P:98:ILE:HD12	22:P:102:ARG:CZ	2.46	0.45
31:Y:132:ASP:OD1	31:Y:135:LYS:HD2	2.16	0.45
31:Y:112:GLU:OE1	31:Y:112:GLU:HA	2.17	0.45
8:B:280:VAL:CG1	8:B:334:SER:HA	2.46	0.45
11:E:86:VAL:CG1	11:E:129:GLU:HA	2.46	0.45
6:9:6:C:O2'	20:N:33:ARG:NH2	2.46	0.45
38:0:4096:HOH:O	26:T:9:LYS:CD	2.64	0.45
25:S:73:ASP:OD1	25:S:76:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:149:VAL:HG13	38:H:4056:HOH:O	2.16	0.45
1:0:2895:C:H2'	38:0:9863:HOH:O	2.17	0.45
8:B:82:VAL:HG12	8:B:101:TRP:CE3	2.51	0.45
20:N:151:ASP:OD1	20:N:154:LEU:HD13	2.16	0.45
9:C:111:VAL:HB	38:C:4097:HOH:O	2.15	0.45
8:B:75:GLU:C	8:B:77:PRO:HD3	2.37	0.45
20:N:42:HIS:CG	20:N:62:HIS:HE1	2.35	0.45
8:B:38:VAL:HA	8:B:166:VAL:HG22	1.99	0.45
15:I:87:PRO:C	15:I:89:GLU:N	2.68	0.45
22:P:115:SER:O	22:P:116:SER:C	2.54	0.45
1:0:1733:A:H4'	8:B:212:GLN:HA	1.99	0.45
29:W:117:ARG:HB3	29:W:117:ARG:HH11	1.82	0.45
1:0:1450:C:C4'	1:0:1451:C:OP2	2.62	0.45
20:N:11:ARG:O	20:N:15:GLU:HG3	2.15	0.45
24:R:96:VAL:O	24:R:99:ALA:HB3	2.16	0.45
2:1:36:SER:O	2:1:46:ARG:HD3	2.16	0.45
1:0:2421:G:H3'	1:0:2422:U:H5''	1.97	0.45
20:N:144:GLY:O	20:N:147:ILE:CG2	2.65	0.45
31:Y:112:GLU:OE2	31:Y:115:ARG:NH1	2.50	0.45
8:B:305:ASP:O	8:B:306:LYS:CB	2.64	0.45
1:0:2335:C:H2'	1:0:2336:G:H8	1.81	0.45
1:0:2053:G:H4'	24:R:136:TRP:CE2	2.52	0.45
1:0:1496:A:H5'	1:0:1572:A:H1'	1.98	0.45
1:0:166:A:N7	18:L:25:GLY:HA2	2.31	0.45
21:O:11:ILE:HD13	21:O:34:GLU:HG3	1.98	0.45
1:0:264:G:H1'	1:0:265:U:H5	1.81	0.45
9:C:14:GLY:O	9:C:15:GLU:HB3	2.16	0.45
38:0:6740:HOH:O	16:J:46:ILE:HA	2.16	0.45
1:0:2353:A:H4'	1:0:2354:A:O5'	2.16	0.45
1:0:962:C:H2'	1:0:963:C:H5'	1.99	0.45
1:0:285:A:H2'	1:0:286:U:O4'	2.17	0.45
20:N:110:THR:HB	20:N:113:SER:HG	1.81	0.45
8:B:329:TYR:HE2	27:U:15:PRO:HG2	1.82	0.45
1:0:1942:A:H4'	38:0:8128:HOH:O	2.16	0.45
1:0:907:A:H4'	1:0:1328:A:N1	2.31	0.45
7:A:165:THR:O	7:A:165:THR:HG22	2.16	0.45
1:0:60:A:O2'	1:0:61:G:H5'	2.17	0.45
1:0:2001:G:O2'	1:0:2002:C:H5'	2.16	0.45
16:J:127:ILE:HG22	36:J:8801:CL:CL	2.54	0.45
1:0:839:C:O2'	5:4:8:MHT:H7	2.15	0.45
1:0:1139:U:H2'	1:0:1140:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2104:C:O2	1:0:2485:A:N1	2.49	0.45
1:0:1186:C:H42	1:0:1190:G:H22	1.63	0.45
24:R:18:LEU:HD22	24:R:21:ARG:NE	2.32	0.45
16:J:74:ARG:NH1	16:J:76:ASP:HB2	2.32	0.45
18:L:91:VAL:HB	38:L:4056:HOH:O	2.16	0.45
1:0:281:U:O2'	1:0:282:C:H5'	2.17	0.45
20:N:72:GLU:HG2	20:N:72:GLU:O	2.17	0.45
1:0:2910:A:H5''	38:0:9872:HOH:O	2.17	0.45
1:0:821:U:H5''	38:0:5828:HOH:O	2.15	0.45
20:N:38:LYS:HE2	20:N:107:ASN:HD21	1.80	0.45
1:0:2511:A:H5'	1:0:2511:A:H8	1.82	0.45
1:0:958:G:H2'	1:0:959:C:H6	1.82	0.45
1:0:2478:U:H2'	1:0:2479:A:H8	1.82	0.45
9:C:57:PRO:HD2	9:C:73:LEU:HD22	1.98	0.45
1:0:2266:A:OP2	19:M:90:ARG:NH2	2.50	0.45
24:R:114:VAL:HG13	24:R:114:VAL:O	2.17	0.45
8:B:24:PRO:HG2	8:B:204:GLY:HA2	1.98	0.45
1:0:1625:U:H5''	38:0:7487:HOH:O	2.16	0.45
1:0:2498:C:O2'	1:0:2499:U:H5'	2.16	0.45
1:0:2690:U:O2'	11:E:111:LYS:HE3	2.17	0.45
1:0:858:U:H2'	1:0:859:C:H6	1.82	0.45
1:0:2515:C:H2'	1:0:2516:G:O4'	2.16	0.45
10:D:21:VAL:HA	10:D:131:THR:O	2.17	0.45
19:M:18:GLY:O	19:M:21:ALA:HB3	2.16	0.45
1:0:146:U:O2'	1:0:147:G:H5'	2.17	0.45
1:0:1872:C:H2'	7:A:23:TYR:HD1	1.82	0.45
8:B:14:GLY:HA2	8:B:15:PRO:C	2.37	0.45
1:0:297:U:H2'	1:0:298:C:C6	2.51	0.45
9:C:165:ASP:O	9:C:168:ARG:HB3	2.17	0.45
1:0:1183:C:H41	1:0:1192:A:H5'	1.81	0.45
29:W:21:LEU:HD22	29:W:26:ILE:HD13	1.98	0.45
20:N:72:GLU:H	20:N:171:HIS:CE1	2.34	0.45
30:X:73:ARG:HB2	30:X:88:GLU:OE2	2.17	0.45
9:C:29:ASP:HB2	21:O:3:THR:HG22	1.98	0.45
26:T:24:ARG:NH2	26:T:39:ASN:HD22	2.14	0.45
30:X:20:GLU:OE1	30:X:21:PRO:HD2	2.17	0.45
20:N:144:GLY:O	20:N:147:ILE:HG22	2.16	0.45
21:O:96:VAL:HG12	21:O:97:SER:N	2.31	0.45
9:C:130:GLU:HA	9:C:130:GLU:OE1	2.17	0.45
26:T:75:GLU:O	26:T:76:ASP:HB2	2.16	0.45
22:P:40:VAL:O	22:P:44:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:45:GLU:HG3	38:X:4018:HOH:O	2.16	0.45
1:0:1903:U:O2'	1:0:1904:A:C8	2.69	0.45
17:K:75:ARG:HE	17:K:94:ALA:HB3	1.82	0.45
1:0:558:C:HO2'	1:0:559:U:H5''	1.81	0.45
6:9:30:C:OP1	10:D:137:PRO:O	2.34	0.45
8:B:79:MET:HE1	38:B:4058:HOH:O	2.16	0.45
20:N:12:ARG:HH21	20:N:17:ARG:HD3	1.80	0.45
9:C:133:ARG:HD2	38:C:4109:HOH:O	2.15	0.45
7:A:29:HIS:HB3	7:A:153:ARG:HH12	1.82	0.45
11:E:11:VAL:HG13	11:E:23:GLU:O	2.16	0.45
1:0:2361:A:H2'	1:0:2362:A:O4'	2.17	0.45
26:T:38:ARG:NH1	26:T:38:ARG:HG3	2.31	0.45
2:1:28:HIS:HB3	2:1:31:LYS:HB2	1.99	0.45
12:F:1:PRO:H3	12:F:4:VAL:CG2	2.30	0.45
1:0:2032:U:O2'	1:0:2033:G:H5''	2.16	0.45
1:0:2054:A:C2	24:R:128:ARG:NH2	2.85	0.45
1:0:1588:G:C6	1:0:1589:G:N1	2.84	0.45
1:0:1414:A:H2'	1:0:1415:G:O4'	2.17	0.45
19:M:47:ASP:CG	19:M:48:LYS:N	2.71	0.45
1:0:1624:A:H5'	1:0:1626:A:O4'	2.16	0.45
1:0:1261:A:H4'	38:0:6496:HOH:O	2.17	0.45
26:T:71:VAL:HG12	26:T:72:ILE:N	2.32	0.45
9:C:235:PHE:CE2	9:C:243:VAL:HG21	2.52	0.45
1:0:1500:U:P	22:P:41:ARG:HH22	2.40	0.45
1:0:2782:G:O6	1:0:2790:C:H5''	2.16	0.45
2:1:25:LYS:HD2	3:2:49:GLU:N	2.25	0.45
29:W:154:ARG:HE	29:W:154:ARG:HB3	1.64	0.45
12:F:50:VAL:CG2	12:F:63:ILE:HG21	2.47	0.45
1:0:657:G:H2'	1:0:658:C:H6	1.81	0.45
1:0:1268:C:H2'	1:0:1269:G:H8	1.82	0.45
8:B:297:VAL:HB	38:B:4036:HOH:O	2.17	0.45
1:0:902:G:N7	18:L:18:HIS:CD2	2.85	0.45
12:F:43:GLY:O	12:F:45:ALA:N	2.46	0.45
1:0:363:C:H2'	1:0:364:U:C6	2.52	0.45
1:0:1940:C:H4'	38:0:8126:HOH:O	2.16	0.44
26:T:55:PHE:CG	26:T:77:VAL:HG13	2.51	0.44
1:0:1175:G:H1'	1:0:1193:A:H2'	1.99	0.44
1:0:2256:G:H2'	1:0:2257:G:H5'	1.98	0.44
10:D:128:LEU:C	10:D:128:LEU:HD23	2.37	0.44
12:F:48:VAL:CG2	12:F:74:PHE:HB3	2.47	0.44
9:C:54:LEU:HD23	9:C:79:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1761:U:H4'	22:P:82:GLY:O	2.18	0.44
19:M:49:ALA:C	19:M:54:TYR:HB3	2.38	0.44
1:0:2054:A:N3	24:R:128:ARG:NH2	2.65	0.44
1:0:1659:A:H2'	1:0:1660:G:O4'	2.16	0.44
1:0:1028:U:H1'	38:0:6313:HOH:O	2.17	0.44
1:0:2614:C:O2'	1:0:2615:U:H5'	2.17	0.44
25:S:13:LYS:HE2	38:S:4006:HOH:O	2.17	0.44
30:X:75:ALA:O	30:X:83:ALA:HA	2.17	0.44
29:W:7:LEU:CD1	29:W:53:ALA:HB2	2.48	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.44
9:C:246:ARG:NE	38:C:4174:HOH:O	2.39	0.44
1:0:1940:C:H1'	38:0:8121:HOH:O	2.17	0.44
1:0:2821:C:H4'	8:B:116:PRO:HB3	1.99	0.44
8:B:84:LEU:HD23	8:B:142:LEU:CD2	2.46	0.44
8:B:98:THR:HG22	8:B:99:GLU:H	1.81	0.44
20:N:86:LEU:HD21	20:N:180:LEU:CD1	2.47	0.44
1:0:24:G:H22	1:0:518:G:H1'	1.82	0.44
18:L:124:ASP:OD1	18:L:149:ARG:NH2	2.50	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.44
20:N:119:GLN:O	20:N:123:ILE:HG13	2.17	0.44
38:0:4619:HOH:O	18:L:56:LYS:HA	2.16	0.44
1:0:2712:G:O2'	1:0:2713:G:H5'	2.18	0.44
8:B:217:ARG:CD	8:B:257:THR:HG22	2.47	0.44
9:C:131:PHE:CD2	9:C:232:LEU:HD22	2.52	0.44
28:V:42:ASN:O	28:V:44:GLY:N	2.50	0.44
9:C:246:ARG:NH1	38:C:4175:HOH:O	2.49	0.44
8:B:7:ARG:CD	8:B:9:GLY:O	2.65	0.44
19:M:125:ARG:HD3	38:M:4086:HOH:O	2.16	0.44
8:B:240:GLY:HA3	38:B:4106:HOH:O	2.17	0.44
24:R:29:LYS:HD3	38:R:4028:HOH:O	2.17	0.44
24:R:33:ARG:NH2	38:R:4028:HOH:O	2.50	0.44
3:2:19:SER:O	3:2:36:ASN:ND2	2.51	0.44
18:L:10:SER:O	18:L:11:ARG:HB3	2.18	0.44
11:E:126:ILE:HB	11:E:131:LEU:CD2	2.48	0.44
1:0:1909:A:H2'	1:0:1910:A:C8	2.53	0.44
1:0:1490:G:H4'	1:0:1533:A:OP1	2.17	0.44
1:0:2911:C:H3'	38:0:9873:HOH:O	2.16	0.44
20:N:23:ARG:NH2	20:N:55:ASP:OD1	2.50	0.44
6:9:114:G:H2'	6:9:115:C:C6	2.53	0.44
38:C:4133:HOH:O	26:T:2:LYS:HE2	2.17	0.44
18:L:67:ARG:HB2	18:L:112:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:15:MET:O	25:S:18:MET:HB3	2.18	0.44
31:Y:133:HIS:HA	31:Y:139:VAL:HG12	1.98	0.44
1:0:2344:G:N3	1:0:2344:G:H2'	2.33	0.44
30:X:10:VAL:HG11	30:X:36:HIS:HE1	1.82	0.44
29:W:46:ALA:O	29:W:49:ASN:HB2	2.17	0.44
9:C:72:LYS:HG2	9:C:77:ALA:HA	1.98	0.44
1:0:499:G:O2'	1:0:500:G:H5'	2.16	0.44
6:9:52:A:H2'	6:9:53:G:O4'	2.18	0.44
16:J:45:VAL:HG22	16:J:46:ILE:N	2.33	0.44
29:W:26:ILE:O	29:W:26:ILE:CG1	2.64	0.44
16:J:19:MET:CE	16:J:132:LEU:HD21	2.47	0.44
10:D:27:ILE:HB	10:D:69:ILE:O	2.17	0.44
1:0:2055:A:H4'	24:R:132:ARG:HH21	1.82	0.44
8:B:42:ALA:HB3	8:B:79:MET:SD	2.57	0.44
24:R:39:THR:O	24:R:40:ALA:C	2.55	0.44
10:D:56:ARG:N	38:D:4024:HOH:O	2.50	0.44
14:H:114:ASP:N	38:H:4042:HOH:O	2.50	0.44
8:B:336:GLN:NE2	38:B:4141:HOH:O	2.49	0.44
8:B:243:ASN:HA	8:B:244:PRO:C	2.38	0.44
8:B:142:LEU:HD21	8:B:178:ALA:HB1	2.00	0.44
38:0:8004:HOH:O	7:A:11:ARG:HG2	2.18	0.44
1:0:380:A:H2'	38:0:4939:HOH:O	2.15	0.44
19:M:60:VAL:C	19:M:61:ILE:HD12	2.37	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.17	0.44
22:P:83:LYS:HG3	22:P:84:ALA:H	1.81	0.44
11:E:162:PHE:CD1	11:E:162:PHE:N	2.85	0.44
1:0:2038:A:H5''	8:B:222:LYS:HG3	1.99	0.44
1:0:1019:C:H5'	38:0:6294:HOH:O	2.16	0.44
1:0:401:C:H2'	1:0:402:U:C6	2.53	0.44
1:0:1137:G:H1'	38:0:6605:HOH:O	2.17	0.44
6:9:42:C:H5'	6:9:43:G:OP2	2.17	0.44
1:0:1478:U:H2'	1:0:1479:G:H8	1.82	0.44
12:F:106:ALA:HB3	38:F:4024:HOH:O	2.18	0.44
1:0:797:A:H5'	32:Z:10:ARG:N	2.32	0.44
7:A:36:ASP:C	7:A:38:ILE:H	2.20	0.44
7:A:38:ILE:HA	7:A:38:ILE:HD13	1.85	0.44
10:D:140:ARG:N	38:D:4039:HOH:O	2.49	0.44
20:N:170:GLU:HA	20:N:173:ASP:OD2	2.18	0.44
18:L:54:PRO:HG2	18:L:57:VAL:CG2	2.47	0.44
1:0:2637:A:H5'	38:0:9472:HOH:O	2.16	0.44
7:A:53:ALA:HB3	38:A:4031:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:115:VAL:HA	8:B:116:PRO:HD3	1.75	0.44
31:Y:219:GLU:HG3	31:Y:220:GLU:N	2.32	0.44
1:0:2064:U:H4'	1:0:2653:A:OP1	2.17	0.44
1:0:1730:G:C5'	1:0:1731:C:C6	3.01	0.44
8:B:221:GLN:HE22	17:K:42:ASN:ND2	2.16	0.44
9:C:39:GLN:O	9:C:43:LYS:HD3	2.18	0.44
1:0:1421:C:O2'	1:0:1422:U:H5'	2.17	0.44
10:D:153:THR:O	10:D:156:ARG:HB2	2.17	0.44
30:X:36:HIS:CE1	30:X:40:HIS:CD2	3.06	0.44
11:E:154:ILE:HD11	11:E:157:LYS:HE2	1.99	0.44
1:0:1025:C:P	29:W:108:ARG:NH1	2.91	0.44
1:0:1517:C:O2'	1:0:1518:A:H5'	2.18	0.44
28:V:20:LEU:HD11	28:V:53:ILE:HG23	1.99	0.44
1:0:1181:A:C2'	1:0:1182:C:H5'	2.47	0.44
10:D:41:LEU:CA	10:D:44:ILE:HG22	2.46	0.44
29:W:4:LEU:HD23	29:W:4:LEU:HA	1.77	0.44
27:U:9:CYS:CA	27:U:52:THR:HG23	2.36	0.44
15:I:91:PHE:HA	15:I:131:GLY:CA	2.48	0.44
30:X:22:ASN:C	30:X:24:LYS:H	2.21	0.44
1:0:1234:U:C4	8:B:244:PRO:HB3	2.53	0.44
25:S:57:THR:CG2	25:S:58:MET:N	2.80	0.44
6:9:106:U:O5'	6:9:106:U:H6	2.01	0.44
1:0:271:C:H41	1:0:378:A:H2	1.63	0.44
1:0:185:G:H4'	1:0:186:A:OP1	2.17	0.44
1:0:2858:U:H2'	1:0:2859:C:C6	2.52	0.44
10:D:15:GLU:HA	10:D:16:PRO:HD3	1.88	0.44
19:M:76:ARG:HG2	19:M:76:ARG:HH11	1.81	0.44
17:K:27:ARG:HD2	38:K:4015:HOH:O	2.18	0.44
1:0:2268:C:H2'	1:0:2269:C:C6	2.53	0.44
1:0:1180:U:H4'	15:I:86:GLU:HG2	2.00	0.44
31:Y:187:VAL:CG2	31:Y:192:ASP:HB2	2.33	0.44
1:0:545:G:C8	1:0:545:G:C5'	2.99	0.44
1:0:559:U:C5'	1:0:559:U:H6	2.27	0.44
1:0:2072:G:H3'	1:0:2073:G:C5'	2.48	0.44
10:D:140:ARG:HG3	10:D:140:ARG:HH11	1.82	0.44
15:I:134:ILE:C	15:I:135:GLU:HG3	2.38	0.44
20:N:143:ARG:NH1	20:N:173:ASP:OD1	2.50	0.44
9:C:133:ARG:HE	9:C:138:VAL:HG22	1.83	0.44
1:0:2506:A:N6	1:0:2511:A:O2'	2.48	0.44
4:3:69:TYR:HB2	4:3:78:HIS:CE1	2.53	0.44
1:0:658:C:O2'	1:0:662:U:OP1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:63:ARG:N	38:G:4014:HOH:O	2.50	0.44
17:K:62:PRO:CG	17:K:65:ARG:HH21	2.31	0.44
26:T:96:VAL:HG13	26:T:97:ARG:N	2.33	0.44
8:B:69:VAL:HA	8:B:70:PRO:HD3	1.84	0.44
3:2:35:ARG:HG2	38:2:4029:HOH:O	2.17	0.44
1:0:1754:A:H2'	1:0:1755:A:O4'	2.18	0.44
1:0:1584:C:O2'	1:0:1585:C:H5'	2.17	0.44
12:F:49:PHE:HE1	12:F:98:VAL:HG23	1.83	0.44
1:0:1437:A:O2'	1:0:1438:G:H5'	2.18	0.44
1:0:163:U:O3'	1:0:896:C:H4'	2.17	0.44
6:9:11:A:P	23:Q:19:ARG:HH21	2.40	0.44
30:X:41:PHE:CZ	30:X:74:ALA:HB3	2.53	0.44
4:3:20:HIS:HA	4:3:70:ARG:O	2.18	0.44
1:0:2819:C:O4'	8:B:96:PRO:HB2	2.18	0.44
1:0:736:A:H2'	1:0:737:A:O4'	2.18	0.44
1:0:858:U:H2'	1:0:859:C:C6	2.52	0.44
4:3:16:GLU:HG3	4:3:18:GLN:HE21	1.82	0.44
7:A:70:ALA:HA	7:A:71:PRO:HD3	1.80	0.44
21:O:80:ASP:OD1	21:O:81:PHE:N	2.50	0.44
1:0:1386:G:O2'	1:0:1387:G:H5'	2.18	0.44
1:0:1513:C:O2'	1:0:1514:C:H5'	2.17	0.44
31:Y:100:ARG:NH1	31:Y:215:GLU:HA	2.33	0.44
32:Z:10:ARG:HG3	32:Z:11:SER:N	2.33	0.43
10:D:166:ILE:HD12	38:D:4046:HOH:O	2.17	0.43
26:T:9:LYS:CE	26:T:13:ARG:NH1	2.73	0.43
28:V:4:HIS:O	28:V:8:ILE:HG13	2.18	0.43
7:A:223:ARG:HG3	38:A:4110:HOH:O	2.17	0.43
9:C:218:VAL:N	38:C:4174:HOH:O	2.50	0.43
1:0:2524:G:N2	1:0:2526:C:H41	2.12	0.43
25:S:76:GLU:HB3	38:S:4032:HOH:O	2.18	0.43
19:M:59:GLY:HA3	19:M:141:ILE:CD1	2.47	0.43
1:0:2433:A:H2'	1:0:2434:A:C8	2.52	0.43
31:Y:182:PHE:HD2	31:Y:200:THR:O	2.01	0.43
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.43
1:0:485:A:O2'	1:0:487:G:H5'	2.18	0.43
1:0:35:U:H5'	9:C:47:GLY:O	2.18	0.43
17:K:41:LYS:O	17:K:42:ASN:HB2	2.18	0.43
1:0:1415:G:H5'	2:1:12:ASN:O	2.18	0.43
1:0:952:G:N3	1:0:2302:A:H2'	2.33	0.43
1:0:844:A:C6	1:0:882:A:C5	3.06	0.43
1:0:2866:U:H4'	1:0:2867:G:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H8	16:J:52:GLN:HE22	1.66	0.43
10:D:64:ARG:HD3	10:D:67:ASP:CB	2.48	0.43
1:0:1174:A:C5	1:0:1201:C:H4'	2.52	0.43
24:R:9:ASP:O	24:R:13:THR:HG22	2.17	0.43
26:T:25:ALA:O	26:T:39:ASN:HB2	2.18	0.43
25:S:14:ALA:HA	25:S:25:GLN:NE2	2.33	0.43
19:M:34:GLU:HB3	19:M:38:GLU:HG3	1.99	0.43
1:0:688:A:N7	18:L:65:ASP:OD2	2.51	0.43
14:H:83:GLU:HA	38:H:4028:HOH:O	2.18	0.43
1:0:2809:G:H2'	1:0:2810:G:O4'	2.18	0.43
9:C:44:GLN:HA	38:C:4030:HOH:O	2.18	0.43
12:F:33:THR:HG21	12:F:59:ILE:O	2.17	0.43
1:0:2274:A:H1'	19:M:86:GLN:NE2	2.33	0.43
2:1:10:LYS:HG3	38:1:4010:HOH:O	2.18	0.43
10:D:39:ASP:HB2	38:D:4018:HOH:O	2.18	0.43
38:0:8295:HOH:O	8:B:216:LYS:HA	2.18	0.43
1:0:2091:G:O3'	8:B:235:ARG:HD3	2.17	0.43
1:0:1207:A:N6	38:0:6685:HOH:O	2.51	0.43
14:H:27:PRO:HD3	14:H:123:ILE:HG22	2.01	0.43
4:3:56:PRO:CA	38:3:4043:HOH:O	2.66	0.43
1:0:256:C:H2'	1:0:257:G:O4'	2.18	0.43
9:C:168:ARG:NH2	9:C:190:ALA:O	2.51	0.43
21:O:35:LYS:HB3	21:O:36:PRO:HD2	2.00	0.43
22:P:22:TRP:CH2	22:P:24:ASN:HA	2.53	0.43
1:0:1839:A:H5'	1:0:2643:G:H4'	2.00	0.43
1:0:2460:A:H5''	4:3:58:GLY:O	2.18	0.43
16:J:84:ARG:HB2	16:J:98:PHE:CE1	2.53	0.43
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.13	0.43
1:0:1119:G:H8	16:J:52:GLN:NE2	2.16	0.43
29:W:5:VAL:O	29:W:52:VAL:HG23	2.18	0.43
11:E:84:MET:HE1	11:E:133:VAL:HG21	2.01	0.43
16:J:39:VAL:HG11	16:J:107:ASN:CB	2.47	0.43
29:W:122:ARG:HG3	29:W:152:ALA:O	2.18	0.43
1:0:2521:A:P	14:H:6:ALA:HB3	2.59	0.43
8:B:190:MET:HG2	8:B:272:ILE:CG2	2.48	0.43
9:C:133:ARG:NH2	38:C:4108:HOH:O	2.50	0.43
4:3:22:VAL:HG11	4:3:67:LEU:HD13	2.00	0.43
6:9:106:U:O2'	6:9:107:C:H5'	2.19	0.43
1:0:793:A:H5''	22:P:83:LYS:HG2	1.99	0.43
19:M:184:ARG:CG	19:M:185:PRO:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:667:C:H2'	1:0:668:C:C6	2.54	0.43
1:0:2443:C:H1'	18:L:56:LYS:HE3	2.00	0.43
1:0:1517:C:O2	1:0:1670:A:C2	2.71	0.43
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.43
1:0:1674:C:P	25:S:34:LYS:HG3	2.59	0.43
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.43
29:W:24:LEU:HD21	29:W:44:MET:SD	2.58	0.43
7:A:149:ASP:OD1	7:A:151:GLN:HB2	2.17	0.43
24:R:46:TYR:O	24:R:49:ALA:HB3	2.17	0.43
10:D:81:GLU:C	10:D:83:PHE:H	2.22	0.43
7:A:215:ILE:HG13	7:A:216:SER:N	2.33	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
1:0:1718:G:O2'	1:0:1719:G:H5'	2.19	0.43
1:0:299:U:H5'	38:0:5064:HOH:O	2.19	0.43
19:M:99:ARG:NH1	38:M:4071:HOH:O	2.49	0.43
20:N:163:PHE:O	20:N:164:ASP:OD1	2.36	0.43
16:J:108:PRO:HG2	16:J:109:TYR:CD1	2.54	0.43
9:C:175:LYS:HD3	9:C:184:ARG:O	2.19	0.43
8:B:84:LEU:O	8:B:99:GLU:HA	2.18	0.43
1:0:2609:G:N2	8:B:238:ASN:HD21	2.17	0.43
1:0:2299:G:C6	1:0:2300:A:C6	3.07	0.43
1:0:922:A:N7	1:0:2281:C:H5'	2.34	0.43
1:0:1478:U:H2'	1:0:1479:G:C8	2.53	0.43
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.43
1:0:2861:G:H4'	8:B:282:GLY:N	2.34	0.43
23:Q:35:ASP:OD1	23:Q:35:ASP:N	2.51	0.43
1:0:165:A:H5''	18:L:33:ALA:HB2	2.01	0.43
30:X:34:ARG:NH1	30:X:48:VAL:O	2.40	0.43
1:0:2906:A:H5'	1:0:2907:C:O4'	2.18	0.43
25:S:8:PRO:HD2	28:V:32:ALA:HA	2.00	0.43
1:0:613:C:H2'	1:0:614:U:H6	1.83	0.43
1:0:1617:C:C4	1:0:1643:C:H4'	2.53	0.43
30:X:30:MET:CE	30:X:58:ALA:HB3	2.48	0.43
30:X:30:MET:CE	30:X:55:ASN:HA	2.39	0.43
1:0:1735:C:H5'	8:B:235:ARG:NH2	2.34	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.36	0.43
15:I:99:GLN:O	15:I:103:ILE:HG13	2.18	0.43
30:X:78:GLU:CG	30:X:79:GLU:H	2.28	0.43
25:S:80:ARG:NH1	38:S:4032:HOH:O	2.51	0.43
6:9:3:A:H2	6:9:21:G:N3	2.17	0.43
1:0:1641:A:H2'	1:0:1642:A:C5'	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:107:PHE:CZ	11:E:152:THR:HB	2.53	0.43
10:D:173:GLU:OE1	10:D:174:VAL:HG23	2.19	0.43
12:F:48:VAL:HG12	12:F:97:ALA:CB	2.48	0.43
1:0:69:A:C2'	1:0:70:A:OP2	2.67	0.43
1:0:1102:C:H4'	38:0:6527:HOH:O	2.18	0.43
1:0:1052:G:N3	1:0:1052:G:H2'	2.33	0.43
31:Y:133:HIS:HA	31:Y:139:VAL:CG1	2.48	0.43
27:U:6:CYS:C	27:U:8:TYR:H	2.22	0.43
24:R:84:ALA:O	24:R:88:PHE:HD1	2.01	0.43
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.43
1:0:1123:A:C2	1:0:1129:C:H4'	2.54	0.43
10:D:24:HIS:CE1	10:D:26:GLY:H	2.37	0.43
17:K:6:ALA:HB3	17:K:116:GLU:HG2	2.01	0.43
1:0:1845:A:O3'	7:A:187:PRO:HB2	2.19	0.43
9:C:194:PHE:HA	9:C:234:VAL:HG13	2.01	0.43
25:S:11:THR:O	25:S:15:MET:HG2	2.18	0.43
25:S:18:MET:HG3	25:S:74:ALA:HB1	2.00	0.43
7:A:95:PRO:HA	7:A:153:ARG:HA	1.99	0.43
1:0:1477:C:H5'	1:0:1868:G:H5''	2.01	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.18	0.43
9:C:136:VAL:HA	9:C:137:PRO:C	2.38	0.43
11:E:47:VAL:HG11	11:E:69:ILE:HD13	2.00	0.43
7:A:164:ARG:HA	32:Z:69:TYR:CE1	2.54	0.43
1:0:1421:C:H2'	1:0:1422:U:C6	2.52	0.43
23:Q:93:ARG:NH1	23:Q:93:ARG:HG3	2.33	0.43
1:0:1427:A:H61	1:0:1440:U:C1'	2.30	0.43
1:0:297:U:H2'	1:0:298:C:H6	1.82	0.43
1:0:2761:A:C4	1:0:2763:G:C8	3.07	0.43
8:B:157:LYS:O	8:B:159:PRO:HD3	2.18	0.43
1:0:1066:U:H2'	1:0:1067:A:C8	2.54	0.43
1:0:2731:G:H2'	1:0:2732:U:O4'	2.18	0.43
17:K:30:LYS:C	17:K:55:VAL:HG13	2.37	0.43
1:0:1603:A:H5''	1:0:1604:G:H3'	2.00	0.43
9:C:233:THR:CG2	9:C:234:VAL:N	2.78	0.43
11:E:2:ARG:HG3	11:E:50:GLU:HB3	2.00	0.43
1:0:396:U:OP2	4:3:38:ARG:HD2	2.19	0.43
1:0:1925:G:O2'	1:0:1926:G:H5'	2.19	0.43
20:N:108:SER:HA	20:N:109:PRO:HD3	1.82	0.43
1:0:1506:U:H6	1:0:1506:U:H5'	1.83	0.43
18:L:34:GLY:C	18:L:36:ASP:H	2.22	0.43
6:9:59:C:H4'	38:9:4063:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:10:VAL:HG11	28:V:36:ALA:HA	2.00	0.43
19:M:107:ARG:NH1	38:M:4074:HOH:O	2.49	0.43
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.43
10:D:14:ARG:NH1	38:D:4008:HOH:O	2.50	0.43
12:F:56:PRO:HG2	19:M:43:PRO:O	2.18	0.43
14:H:69:ARG:HD3	38:H:4025:HOH:O	2.19	0.43
8:B:22:GLU:HA	8:B:205:VAL:HG21	2.01	0.43
26:T:37:GLN:HB3	38:T:4017:HOH:O	2.19	0.43
8:B:278:PRO:HD3	8:B:294:TYR:CE2	2.54	0.43
1:0:1213:C:C2'	1:0:1214:G:H5'	2.49	0.43
1:0:2754:G:HO2'	1:0:2755:G:H5'	1.82	0.43
8:B:13:PHE:O	8:B:16:ARG:HD2	2.19	0.43
6:9:8:G:H4'	23:Q:27:GLN:HE21	1.84	0.43
1:0:1571:G:H1'	1:0:1627:G:N2	2.34	0.43
1:0:468:U:H3'	38:0:5139:HOH:O	2.18	0.43
15:I:126:THR:O	15:I:126:THR:HG22	2.19	0.43
1:0:968:G:H1'	14:H:35:LYS:HD2	2.00	0.43
1:0:1600:G:H4'	38:0:7457:HOH:O	2.17	0.43
26:T:71:VAL:HG13	26:T:91:LEU:O	2.19	0.43
1:0:2712:G:H5'	38:0:9587:HOH:O	2.18	0.43
6:9:29:C:H2'	6:9:30:C:C5'	2.43	0.43
14:H:49:GLN:CB	14:H:170:ARG:HG3	2.46	0.43
14:H:49:GLN:HB3	14:H:170:ARG:CG	2.48	0.43
12:F:46:GLU:N	38:F:4011:HOH:O	2.52	0.43
30:X:76:ARG:O	30:X:77:PHE:CB	2.64	0.43
14:H:6:ALA:CA	14:H:61:ARG:HH12	2.26	0.43
21:O:32:ARG:HD3	21:O:32:ARG:C	2.39	0.43
27:U:17:THR:HG22	27:U:18:GLY:H	1.84	0.43
1:0:213:G:O2'	1:0:214:U:OP2	2.37	0.43
7:A:105:VAL:HG13	7:A:155:THR:O	2.18	0.43
1:0:2764:C:H2'	1:0:2765:C:C6	2.53	0.43
1:0:1314:U:H5''	1:0:1316:G:O4'	2.18	0.43
1:0:2120:U:H2'	1:0:2121:G:O4'	2.19	0.43
20:N:82:TYR:CD2	20:N:82:TYR:C	2.92	0.43
1:0:2898:G:H4'	8:B:288:GLY:HA2	2.00	0.43
10:D:20:LYS:HA	10:D:75:LEU:O	2.19	0.43
26:T:14:ALA:HA	26:T:15:PRO:HD3	1.93	0.43
24:R:4:TYR:CE1	24:R:17:MET:HE2	2.53	0.43
1:0:361:C:H2'	1:0:362:G:O4'	2.19	0.43
29:W:140:LYS:C	29:W:141:HIS:HD2	2.23	0.42
30:X:15:ARG:HB3	30:X:15:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:115:LEU:HD21	9:C:243:VAL:CG1	2.36	0.42
1:O:1702:U:H1'	38:O:7398:HOH:O	2.20	0.42
17:K:98:VAL:HG13	17:K:102:GLU:CA	2.40	0.42
20:N:158:LEU:C	20:N:159:TYR:HD1	2.22	0.42
29:W:69:ARG:HG3	29:W:118:LEU:HD23	2.01	0.42
15:I:95:LEU:O	15:I:134:ILE:HG23	2.18	0.42
20:N:114:LYS:O	20:N:117:ALA:HB3	2.19	0.42
11:E:132:THR:O	11:E:132:THR:HG23	2.19	0.42
21:O:25:VAL:HG23	21:O:26:TRP:CE3	2.54	0.42
6:9:3:A:OP2	6:9:25:G:N2	2.52	0.42
21:O:14:LEU:HG	21:O:102:ILE:HD11	2.00	0.42
1:O:1427:A:N6	1:O:1440:U:H1'	2.34	0.42
1:O:2402:A:H1'	38:O:8877:HOH:O	2.19	0.42
38:O:6201:HOH:O	21:O:39:THR:HB	2.18	0.42
1:O:1289:C:O2'	1:O:1290:G:H5'	2.19	0.42
9:C:95:GLU:CD	9:C:95:GLU:H	2.23	0.42
31:Y:97:LEU:C	31:Y:98:GLN:HG2	2.39	0.42
1:O:1849:G:H1'	1:O:2011:A:N1	2.34	0.42
1:O:1929:G:H1'	38:O:8119:HOH:O	2.18	0.42
27:U:23:HIS:HB2	27:U:27:ALA:HB3	2.00	0.42
9:C:16:VAL:HG21	9:C:237:GLU:OE1	2.19	0.42
28:V:12:THR:HG22	28:V:15:GLU:H	1.83	0.42
26:T:65:VAL:HG22	26:T:72:ILE:HG22	2.01	0.42
20:N:48:VAL:HG11	20:N:55:ASP:CB	2.46	0.42
6:9:26:C:O2'	6:9:27:C:H5'	2.19	0.42
1:O:2039:A:OP2	8:B:234:ARG:NH2	2.52	0.42
28:V:1:THR:O	28:V:2:VAL:C	2.56	0.42
1:O:960:G:H2'	1:O:960:G:N3	2.33	0.42
1:O:111:C:H2'	1:O:112:G:O4'	2.19	0.42
6:9:44:A:O4'	10:D:76:ARG:NE	2.48	0.42
9:C:35:VAL:HG23	9:C:220:THR:HG22	2.01	0.42
19:M:46:LEU:HD22	19:M:50:ARG:HD2	2.00	0.42
21:O:105:ASN:HD21	21:O:109:SER:N	2.16	0.42
10:D:81:GLU:C	10:D:83:PHE:N	2.72	0.42
16:J:15:ARG:NH1	16:J:43:ARG:NH1	2.67	0.42
15:I:71:ALA:O	15:I:75:LYS:HG3	2.19	0.42
1:O:2815:G:C5	16:J:102:ARG:HG2	2.54	0.42
31:Y:229:LEU:O	31:Y:231:PRO:HD3	2.19	0.42
1:O:553:G:P	31:Y:204:ARG:NH2	2.92	0.42
29:W:21:LEU:HD22	29:W:26:ILE:HD11	2.00	0.42
29:W:48:VAL:HG12	29:W:52:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:35:ARG:O	18:L:40:PHE:HA	2.19	0.42
8:B:63:GLU:HG3	8:B:63:GLU:O	2.19	0.42
18:L:66:VAL:CG2	18:L:67:ARG:N	2.83	0.42
7:A:66:ARG:NH1	7:A:66:ARG:CB	2.83	0.42
11:E:31:ARG:NH1	38:E:4034:HOH:O	2.52	0.42
8:B:175:LEU:C	8:B:175:LEU:CD2	2.88	0.42
1:O:87:C:C2	3:2:30:ASP:OD2	2.72	0.42
26:T:63:ILE:HD11	26:T:75:GLU:HB2	2.01	0.42
21:O:79:VAL:O	21:O:80:ASP:HB2	2.19	0.42
1:O:1123:A:C6	1:O:1238:C:H5'	2.54	0.42
4:3:91:GLN:O	4:3:92:GLU:HB2	2.20	0.42
10:D:19:GLU:HG3	38:D:4009:HOH:O	2.19	0.42
38:O:5377:HOH:O	31:Y:158:LYS:HD3	2.18	0.42
1:O:953:G:H2'	38:O:6232:HOH:O	2.19	0.42
1:O:221:G:H2'	1:O:222:A:C8	2.53	0.42
9:C:49:ASP:HB3	9:C:52:ALA:HB2	2.00	0.42
29:W:48:VAL:CG1	29:W:48:VAL:O	2.67	0.42
8:B:320:GLN:NE2	8:B:321:PRO:CD	2.72	0.42
1:O:2090:G:H2'	1:O:2091:G:C8	2.54	0.42
28:V:39:ALA:C	28:V:41:GLU:N	2.72	0.42
1:O:694:A:H4'	1:O:2441:U:OP1	2.20	0.42
10:D:55:LYS:O	10:D:56:ARG:HB2	2.19	0.42
4:3:69:TYR:CZ	4:3:80:ARG:HD2	2.55	0.42
8:B:278:PRO:HD3	8:B:294:TYR:CZ	2.53	0.42
1:O:2445:U:H2'	1:O:2446:G:H8	1.79	0.42
20:N:154:LEU:HG	20:N:155:GLU:N	2.34	0.42
1:O:2653:A:H2'	1:O:2654:C:C6	2.55	0.42
1:O:1805:G:H2'	1:O:1806:G:C8	2.53	0.42
1:O:1772:C:H5'	1:O:1773:G:C5	2.55	0.42
31:Y:108:ASP:OD1	31:Y:199:ASP:HB3	2.19	0.42
1:O:162:C:H2'	1:O:163:U:H5'	2.02	0.42
1:O:2676:C:H4'	16:J:70:PHE:CE1	2.54	0.42
10:D:36:ASN:C	38:D:4021:HOH:O	2.57	0.42
1:O:503:G:H2'	1:O:504:G:H8	1.83	0.42
1:O:2842:G:H2'	1:O:2843:A:H5'	2.01	0.42
1:O:1163:G:N2	38:I:4004:HOH:O	2.49	0.42
15:I:87:PRO:O	15:I:89:GLU:HG3	2.19	0.42
1:O:541:C:O2'	1:O:542:A:H5''	2.20	0.42
29:W:122:ARG:HH11	29:W:122:ARG:HG3	1.84	0.42
27:U:14:GLU:HA	27:U:15:PRO:HD2	1.94	0.42
21:O:25:VAL:CG2	21:O:26:TRP:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:65:ARG:O	17:K:66:ARG:HB2	2.19	0.42
12:F:70:LYS:C	12:F:72:VAL:H	2.22	0.42
1:0:2502:C:H2'	1:0:2503:A:H5'	2.01	0.42
8:B:223:ARG:O	8:B:228:ALA:HB2	2.20	0.42
24:R:59:PHE:O	24:R:63:ASN:HB3	2.19	0.42
1:0:1041:U:H4'	1:0:1295:G:H5'	2.01	0.42
1:0:1935:C:H2'	1:0:1936:C:H6	1.84	0.42
1:0:303:C:H2'	1:0:304:G:O4'	2.20	0.42
4:3:8:ASN:O	4:3:9:THR:HB	2.19	0.42
22:P:91:LYS:O	22:P:95:GLU:HG3	2.20	0.42
1:0:20:G:H21	24:R:117:HIS:HD2	1.66	0.42
1:0:1183:C:O2	1:0:1183:C:H2'	2.19	0.42
16:J:52:GLN:HG3	16:J:53:ILE:H	1.83	0.42
29:W:119:HIS:O	29:W:153:MET:HB3	2.19	0.42
29:W:65:VAL:HG11	29:W:116:LEU:HD13	2.02	0.42
1:0:1874:U:P	7:A:51:ARG:HD2	2.59	0.42
1:0:318:U:O2'	1:0:338:C:H2'	2.19	0.42
17:K:28:GLU:HG2	17:K:58:THR:CB	2.47	0.42
8:B:277:GLU:N	8:B:278:PRO:CD	2.83	0.42
1:0:396:U:C1'	38:0:4988:HOH:O	2.66	0.42
24:R:4:TYR:N	38:R:4004:HOH:O	2.53	0.42
16:J:34:GLU:HA	16:J:34:GLU:OE1	2.19	0.42
7:A:69:LEU:HD11	7:A:159:VAL:HG13	2.01	0.42
9:C:16:VAL:HG12	9:C:17:ASP:N	2.35	0.42
1:0:1798:C:H1'	22:P:66:GLN:OE1	2.20	0.42
14:H:29:SER:HA	14:H:62:HIS:CD2	2.55	0.42
20:N:74:PRO:HG2	20:N:159:TYR:CZ	2.55	0.42
10:D:54:ALA:HB2	10:D:69:ILE:CD1	2.48	0.42
1:0:1666:C:H2'	1:0:1667:A:H8	1.84	0.42
30:X:9:VAL:HG22	30:X:88:GLU:OE2	2.20	0.42
6:9:55:U:H4'	6:9:56:A:C8	2.55	0.42
23:Q:24:SER:HB3	23:Q:28:ARG:HH21	1.83	0.42
7:A:223:ARG:O	7:A:223:ARG:HG2	2.20	0.42
14:H:32:ALA:C	14:H:33:GLN:HG3	2.38	0.42
14:H:146:ALA:O	14:H:150:LYS:HG3	2.19	0.42
1:0:1268:C:O2'	31:Y:169:ARG:HB2	2.20	0.42
1:0:2820:A:OP1	8:B:98:THR:HG23	2.18	0.42
1:0:2822:C:O2'	1:0:2827:A:H4'	2.19	0.42
26:T:41:ARG:NH1	26:T:41:ARG:HG2	2.33	0.42
24:R:29:LYS:CD	38:R:4031:HOH:O	2.68	0.42
10:D:172:VAL:HG12	10:D:173:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2115:U:H2'	1:0:2116:U:C6	2.54	0.42
31:Y:125:LYS:HB2	31:Y:126:PRO:HD2	2.01	0.42
2:1:8:GLN:HE22	2:1:11:LYS:NZ	2.18	0.42
21:O:96:VAL:CG1	21:O:97:SER:N	2.83	0.42
7:A:72:GLU:HG3	32:Z:66:GLY:HA2	2.02	0.42
1:0:431:G:O2'	1:0:432:G:H5'	2.20	0.42
1:0:1186:C:H5''	38:0:6662:HOH:O	2.20	0.42
10:D:23:VAL:CG2	10:D:73:VAL:HB	2.49	0.42
1:0:963:C:O2	1:0:1005:A:N1	2.53	0.42
28:V:1:THR:C	28:V:3:LEU:N	2.73	0.42
30:X:81:GLY:O	30:X:82:GLU:HB3	2.20	0.42
20:N:143:ARG:NH1	20:N:173:ASP:OD2	2.52	0.42
1:0:1201:C:H2'	1:0:1202:A:H5'	2.02	0.42
24:R:145:LEU:HD12	24:R:146:ILE:N	2.34	0.42
11:E:101:GLU:HB2	11:E:116:THR:O	2.19	0.42
1:0:474:C:O3'	9:C:73:LEU:CD2	2.67	0.42
1:0:1334:C:H2'	1:0:1335:C:H6	1.84	0.42
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.42
1:0:1743:G:H2'	1:0:1744:G:O4'	2.19	0.42
1:0:951:A:H5''	23:Q:42:LYS:HD3	2.02	0.42
1:0:2087:C:O2'	1:0:2088:C:H5'	2.20	0.42
23:Q:16:ASN:HB2	38:Q:4014:HOH:O	2.19	0.42
1:0:1181:A:H2'	1:0:1182:C:C5'	2.49	0.42
1:0:962:C:C2'	1:0:963:C:H5'	2.50	0.42
6:9:27:C:H2'	6:9:28:U:O4'	2.20	0.42
6:9:57:A:C8	10:D:141:VAL:HG21	2.54	0.42
1:0:1377:C:H2'	1:0:1723:G:O6	2.20	0.42
4:3:69:TYR:O	4:3:77:ALA:HA	2.20	0.42
18:L:72:ASN:O	18:L:76:LEU:HG	2.20	0.42
30:X:25:ARG:HG2	38:X:4012:HOH:O	2.20	0.42
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.42
26:T:73:HIS:CD2	26:T:88:PRO:CG	3.03	0.42
20:N:151:ASP:HB3	38:N:4054:HOH:O	2.19	0.42
11:E:101:GLU:HB3	11:E:117:THR:HA	2.01	0.42
12:F:52:GLU:OE1	12:F:78:GLU:OE1	2.38	0.42
1:0:69:A:H2'	1:0:70:A:OP2	2.19	0.42
1:0:2133:U:H4'	1:0:2134:G:C5'	2.49	0.42
10:D:170:TYR:O	10:D:171:ASP:HB3	2.20	0.42
1:0:1903:U:O2'	1:0:1904:A:N7	2.51	0.42
29:W:73:LEU:HA	29:W:73:LEU:HD12	1.73	0.42
24:R:61:GLN:HB2	24:R:61:GLN:HE21	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:934:C:H2'	1:0:935:G:C8	2.54	0.42
1:0:2237:G:H1'	38:0:8553:HOH:O	2.19	0.42
8:B:226:LYS:O	8:B:230:GLN:HG2	2.20	0.42
31:Y:170:SER:OG	31:Y:175:ARG:HG3	2.19	0.42
4:3:6:ARG:O	4:3:7:PHE:HB3	2.20	0.42
11:E:119:HIS:HE1	11:E:147:ASP:OD2	2.02	0.42
1:0:2353:A:H1'	23:Q:21:ARG:HH12	1.85	0.42
4:3:11:CYS:HB2	4:3:20:HIS:NE2	2.34	0.42
1:0:1943:C:O4'	7:A:212:PRO:HA	2.20	0.42
1:0:2846:C:OP1	8:B:158:LYS:HD3	2.19	0.42
1:0:1422:U:H2'	1:0:1423:C:C6	2.54	0.42
1:0:1018:A:H4'	23:Q:59:GLN:HE22	1.85	0.42
1:0:1838:U:O4'	1:0:2644:C:C2	2.73	0.42
1:0:967:U:O2	14:H:35:LYS:HE3	2.19	0.42
1:0:432:G:O2'	1:0:433:C:H5'	2.20	0.42
1:0:183:A:H1'	19:M:161:ARG:NH1	2.35	0.42
1:0:2096:A:C8	1:0:2539:U:C2	3.07	0.42
1:0:1169:U:H3	1:0:1177:A:H61	1.68	0.42
1:0:1163:G:H2'	1:0:1164:U:C5	2.54	0.41
9:C:140:VAL:CG1	9:C:141:SER:N	2.82	0.41
16:J:46:ILE:CG1	16:J:46:ILE:O	2.67	0.41
17:K:113:ILE:HD12	17:K:128:ALA:CB	2.49	0.41
10:D:99:ASP:CB	10:D:103:ASN:HB2	2.50	0.41
6:9:47:A:C2	6:9:48:C:C2	3.07	0.41
7:A:192:VAL:HG12	7:A:207:GLN:HB3	2.01	0.41
24:R:40:ALA:O	24:R:44:VAL:HG23	2.19	0.41
19:M:57:LYS:HG2	19:M:58:GLN:H	1.85	0.41
8:B:145:HIS:CD2	8:B:146:THR:O	2.68	0.41
1:0:2456:A:H1'	38:0:8995:HOH:O	2.20	0.41
1:0:2134:G:N2	1:0:2242:U:C2	2.89	0.41
1:0:2443:C:O3'	18:L:56:LYS:HE3	2.20	0.41
23:Q:16:ASN:HD22	23:Q:16:ASN:HA	1.60	0.41
9:C:32:GLY:O	9:C:36:ARG:HB2	2.20	0.41
14:H:56:GLU:HA	14:H:132:ALA:HB2	2.02	0.41
2:1:41:LYS:NZ	38:1:4034:HOH:O	2.53	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.20	0.41
1:0:424:C:H2'	1:0:425:U:C6	2.55	0.41
1:0:333:G:O2'	1:0:334:G:H5'	2.20	0.41
20:N:21:HIS:HB3	38:N:4011:HOH:O	2.19	0.41
9:C:236:THR:CG2	9:C:239:ALA:H	2.08	0.41
24:R:43:ALA:O	24:R:47:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:83:LEU:HD13	20:N:175:LEU:HD23	2.02	0.41
1:0:80:A:H5''	26:T:41:ARG:CZ	2.50	0.41
3:2:36:ASN:HB3	3:2:39:ARG:NE	2.34	0.41
8:B:221:GLN:HE22	17:K:42:ASN:HD22	1.68	0.41
23:Q:32:GLU:O	23:Q:93:ARG:NH2	2.53	0.41
1:0:1050:G:C6	1:0:1051:C:C4	3.08	0.41
38:K:4017:HOH:O	36:8:8812:CL:CL	2.59	0.41
1:0:2303:A:H4'	38:0:8692:HOH:O	2.20	0.41
14:H:157:TYR:CD1	14:H:157:TYR:C	2.93	0.41
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.41
1:0:1968:A:H2'	1:0:1969:A:C8	2.55	0.41
10:D:40:ILE:O	10:D:44:ILE:HG22	2.20	0.41
16:J:56:LYS:HE2	16:J:60:ARG:NH2	2.35	0.41
14:H:43:ALA:O	14:H:170:ARG:NH1	2.53	0.41
29:W:117:ARG:CB	29:W:117:ARG:NH1	2.83	0.41
1:0:1197:G:H1'	1:0:1203:G:N2	2.35	0.41
1:0:2511:A:H2'	1:0:2512:U:O4'	2.20	0.41
9:C:27:ARG:NH2	21:O:4:ASN:ND2	2.68	0.41
21:O:4:ASN:HA	21:O:5:PRO:HD3	1.84	0.41
7:A:217:ARG:CG	7:A:217:ARG:HH11	2.33	0.41
6:9:2:U:OP2	6:9:3:A:H5'	2.21	0.41
1:0:2064:U:H2'	1:0:2065:C:H6	1.84	0.41
9:C:93:LYS:O	9:C:98:ARG:NH2	2.52	0.41
12:F:21:GLU:O	12:F:24:ARG:CG	2.67	0.41
1:0:1948:G:N2	1:0:1965:C:H1'	2.34	0.41
1:0:876:A:C2'	1:0:876:A:N3	2.84	0.41
20:N:62:HIS:HB3	20:N:65:ASP:OD1	2.21	0.41
21:O:33:LEU:HA	21:O:40:HIS:NE2	2.36	0.41
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.55	0.41
1:0:638:C:H2'	1:0:639:A:C8	2.56	0.41
16:J:131:THR:HG22	16:J:134:GLU:H	1.84	0.41
29:W:21:LEU:CD1	29:W:26:ILE:HD11	2.40	0.41
22:P:59:ARG:HG2	22:P:59:ARG:HH11	1.85	0.41
10:D:159:PRO:O	10:D:162:ALA:HB3	2.21	0.41
38:0:4096:HOH:O	26:T:9:LYS:HD3	2.19	0.41
17:K:20:CYS:HB2	17:K:29:LEU:HG	2.02	0.41
20:N:114:LYS:O	20:N:118:ILE:HG13	2.21	0.41
1:0:1206:U:H2'	1:0:1207:A:O4'	2.20	0.41
25:S:73:ASP:O	25:S:77:VAL:HG23	2.20	0.41
26:T:39:ASN:ND2	38:T:4017:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:5:ARG:HH11	8:B:8:LYS:HE2	1.83	0.41
25:S:37:VAL:O	25:S:41:VAL:HG23	2.20	0.41
11:E:7:ILE:HG22	11:E:45:ASP:O	2.20	0.41
8:B:154:VAL:HA	8:B:155:PRO:HD3	1.81	0.41
20:N:155:GLU:O	20:N:156:GLU:HG3	2.20	0.41
1:O:903:U:O4	18:L:18:HIS:HB2	2.20	0.41
14:H:91:ARG:NH1	14:H:138:THR:OG1	2.53	0.41
1:O:1771:U:O2'	1:O:1773:G:N7	2.51	0.41
1:O:1472:C:O5'	1:O:1472:C:H6	2.03	0.41
1:O:30:U:OP2	9:C:181:ALA:HB2	2.19	0.41
16:J:116:LEU:HB2	16:J:119:THR:HG21	2.02	0.41
20:N:32:PRO:HD2	20:N:99:GLU:O	2.20	0.41
6:9:81:C:O2'	6:9:82:U:H5'	2.20	0.41
20:N:163:PHE:CZ	20:N:171:HIS:ND1	2.88	0.41
14:H:41:LYS:O	14:H:87:LYS:HE2	2.20	0.41
1:O:820:G:H5'	1:O:821:U:H5'	2.02	0.41
9:C:218:VAL:HG12	38:C:4174:HOH:O	2.20	0.41
15:I:88:GLN:HE21	15:I:128:THR:HG21	1.85	0.41
6:9:20:G:O2'	6:9:21:G:H5'	2.20	0.41
1:O:1112:G:H1	1:O:1251:C:N4	2.18	0.41
1:O:1041:U:C2'	1:O:1042:U:H5'	2.51	0.41
1:O:2866:U:C4	27:U:50:GLU:HB3	2.55	0.41
13:G:69:ARG:NH1	38:G:4016:HOH:O	2.53	0.41
1:O:646:G:H5''	9:C:96:LYS:HD2	2.03	0.41
9:C:13:ASP:O	9:C:13:ASP:OD1	2.39	0.41
1:O:2697:A:H2'	1:O:2698:G:O4'	2.19	0.41
1:O:320:G:H2'	1:O:321:A:C8	2.55	0.41
31:Y:203:VAL:HG12	31:Y:228:VAL:HG22	2.00	0.41
17:K:55:VAL:CG1	17:K:56:SER:N	2.83	0.41
1:O:1819:G:H2'	1:O:1820:G:C5'	2.51	0.41
8:B:114:ASP:O	8:B:115:VAL:C	2.59	0.41
1:O:1972:U:C2'	1:O:1973:A:C5'	2.99	0.41
22:P:18:LYS:O	22:P:21:VAL:HG13	2.20	0.41
1:O:11:A:H5'	1:O:12:U:OP2	2.20	0.41
1:O:595:U:O2'	1:O:596:C:H5'	2.21	0.41
16:J:88:PRO:HA	36:J:8802:CL:CL	2.58	0.41
11:E:166:VAL:HG12	38:E:4041:HOH:O	2.20	0.41
1:O:2271:G:H2'	1:O:2271:G:N3	2.35	0.41
1:O:2568:A:O5'	1:O:2568:A:H8	2.03	0.41
1:O:1216:G:O2'	1:O:1217:G:H5'	2.21	0.41
9:C:211:ASP:HB3	38:C:4166:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:210:GLY:HA3	38:A:4086:HOH:O	2.19	0.41
31:Y:190:VAL:HG23	38:Y:4081:HOH:O	2.20	0.41
29:W:131:PRO:HB2	38:W:4057:HOH:O	2.21	0.41
1:0:2471:G:N3	1:0:2633:A:H2	2.19	0.41
1:0:2392:C:H4'	38:0:8831:HOH:O	2.19	0.41
1:0:1166:A:H61	1:0:1180:U:H3	1.69	0.41
28:V:12:THR:CG2	28:V:15:GLU:H	2.34	0.41
8:B:60:SER:C	8:B:62:ARG:H	2.24	0.41
1:0:283:U:C5	1:0:284:C:N3	2.88	0.41
28:V:42:ASN:N	28:V:43:PRO:CD	2.83	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.55	0.41
9:C:139:VAL:CG1	38:C:4171:HOH:O	2.62	0.41
22:P:11:ALA:HB2	22:P:18:LYS:HA	2.03	0.41
20:N:147:ILE:O	20:N:150:TYR:HB3	2.20	0.41
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.41
1:0:2502:C:H2'	1:0:2503:A:O4'	2.20	0.41
2:1:28:HIS:CD2	2:1:31:LYS:HG3	2.55	0.41
1:0:2000:G:O2'	1:0:2001:G:H5'	2.21	0.41
8:B:280:VAL:HG13	8:B:333:GLU:O	2.19	0.41
21:O:11:ILE:O	21:O:15:LYS:HG3	2.20	0.41
22:P:24:ASN:HA	22:P:25:PRO:HD3	1.90	0.41
1:0:440:C:O2'	1:0:441:A:H5'	2.19	0.41
1:0:940:G:C5	1:0:1027:G:C2	3.09	0.41
1:0:75:U:H2'	1:0:76:G:C8	2.55	0.41
15:I:70:THR:O	15:I:72:GLU:N	2.53	0.41
1:0:783:C:OP1	7:A:180:LYS:HE3	2.21	0.41
23:Q:50:GLY:HA3	23:Q:87:THR:OG1	2.21	0.41
1:0:2297:U:H1'	38:0:8720:HOH:O	2.19	0.41
20:N:37:ARG:HH11	20:N:37:ARG:CG	2.31	0.41
1:0:1181:A:H5'	15:I:89:GLU:OE2	2.19	0.41
32:Z:10:ARG:CG	32:Z:11:SER:H	2.33	0.41
10:D:17:ARG:NH2	38:D:4039:HOH:O	2.52	0.41
29:W:65:VAL:HA	29:W:68:THR:HG22	2.02	0.41
20:N:115:VAL:HG13	38:N:4043:HOH:O	2.20	0.41
1:0:1882:C:H5''	7:A:192:VAL:HG21	2.03	0.41
10:D:147:ALA:HA	20:N:15:GLU:O	2.21	0.41
1:0:2661:U:H3	1:0:2812:A:H62	1.67	0.41
8:B:195:ARG:NE	8:B:323:LEU:HD13	2.36	0.41
1:0:948:G:C6	1:0:949:U:C4	3.08	0.41
1:0:1477:C:H4'	1:0:1868:G:OP1	2.20	0.41
1:0:1926:G:H2'	1:0:1927:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:63:C:O2'	6:9:64:C:H5'	2.21	0.41
14:H:117:ARG:HB3	38:H:4045:HOH:O	2.20	0.41
1:0:241:A:C2	1:0:378:A:H4'	2.56	0.41
26:T:98:VAL:HG11	26:T:101:LEU:HD23	2.01	0.41
6:9:49:G:O2'	6:9:50:G:H5'	2.21	0.41
16:J:142:ASN:O	16:J:144:THR:N	2.54	0.41
20:N:33:ARG:HD2	20:N:103:ASP:OD2	2.20	0.41
31:Y:204:ARG:HA	31:Y:230:ASN:OD1	2.20	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.41
14:H:60:LEU:O	14:H:65:LEU:HD21	2.21	0.41
11:E:99:GLY:N	38:E:4024:HOH:O	2.53	0.41
8:B:162:MET:HG3	8:B:310:ARG:NH1	2.36	0.41
30:X:43:VAL:HG12	30:X:47:ALA:HB3	2.03	0.41
1:0:1883:U:C2'	1:0:1884:G:H5'	2.51	0.41
1:0:2851:G:H2'	1:0:2902:A:H61	1.85	0.41
11:E:72:MET:HA	38:E:4032:HOH:O	2.21	0.41
1:0:1787:C:O2'	1:0:1788:U:H5'	2.21	0.41
8:B:13:PHE:CD1	8:B:13:PHE:N	2.89	0.41
1:0:539:G:H2'	1:0:540:A:C8	2.56	0.41
1:0:473:A:O2'	1:0:474:C:H5'	2.21	0.41
1:0:2388:C:H5'	23:Q:83:THR:O	2.20	0.41
1:0:2694:A:H4'	11:E:91:PHE:CE1	2.55	0.41
2:1:28:HIS:O	2:1:32:LYS:N	2.47	0.41
1:0:1904:A:H2'	1:0:1905:U:O4'	2.20	0.41
15:I:70:THR:C	15:I:72:GLU:N	2.74	0.41
9:C:20:ASP:HB2	38:C:4011:HOH:O	2.20	0.41
7:A:206:ARG:NH1	38:A:4094:HOH:O	2.54	0.41
1:0:2329:C:O2'	1:0:2330:U:H5'	2.21	0.41
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:1501:A:H4'	38:O:7326:HOH:O	2.20	0.41
26:T:12:ARG:NH1	38:T:4007:HOH:O	2.50	0.41
26:T:20:HIS:O	26:T:23:VAL:HG23	2.21	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
1:0:772:G:H2'	1:0:773:A:O4'	2.20	0.41
1:0:2384:U:H5''	38:O:5634:HOH:O	2.21	0.41
16:J:45:VAL:HA	16:J:130:VAL:O	2.21	0.41
29:W:21:LEU:CD2	29:W:48:VAL:HG11	2.46	0.41
30:X:30:MET:HE2	30:X:58:ALA:HB3	2.03	0.41
18:L:148:GLU:HG3	38:L:4075:HOH:O	2.20	0.41
1:0:137:U:OP1	1:0:259:G:O2'	2.39	0.41
9:C:180:SER:C	9:C:182:ARG:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:38:LYS:HZ1	19:M:3:SER:HA	1.86	0.41
11:E:107:PHE:CD2	11:E:108:LEU:HD13	2.56	0.41
1:0:1761:U:H2'	1:0:1762:C:C6	2.55	0.41
1:0:2644:C:O2'	1:0:2645:U:H5'	2.21	0.41
11:E:154:ILE:HG23	11:E:154:ILE:O	2.20	0.41
9:C:25:PRO:HG2	38:C:4013:HOH:O	2.21	0.41
19:M:106:SER:HB2	19:M:114:VAL:CG2	2.51	0.41
25:S:44:GLN:HA	25:S:44:GLN:OE1	2.21	0.41
1:0:1951:G:N2	38:O:8146:HOH:O	2.54	0.41
1:0:1748:U:C5	1:0:1749:U:C4	3.09	0.41
9:C:80:VAL:HA	9:C:81:PRO:HD3	1.88	0.41
1:0:344:C:H2'	1:0:345:G:O4'	2.21	0.41
1:0:1996:U:O2'	1:0:1997:A:H5'	2.20	0.41
1:0:1355:A:H5''	38:Y:4052:HOH:O	2.21	0.41
15:I:127:CYS:CB	15:I:132:VAL:HB	2.34	0.40
7:A:36:ASP:C	7:A:38:ILE:N	2.74	0.40
1:0:2591:C:H2'	1:0:2592:G:O4'	2.21	0.40
20:N:166:ALA:O	20:N:167:ASP:HB2	2.21	0.40
14:H:87:LYS:O	14:H:140:TYR:HD1	2.04	0.40
30:X:76:ARG:NH1	30:X:76:ARG:CG	2.83	0.40
8:B:27:ASN:N	8:B:27:ASN:ND2	2.67	0.40
22:P:141:ILE:O	22:P:143:ALA:N	2.49	0.40
1:0:1174:A:H5'	38:O:6637:HOH:O	2.21	0.40
1:0:2507:G:H2'	1:0:2510:C:N4	2.36	0.40
20:N:58:LEU:N	20:N:58:LEU:CD1	2.83	0.40
15:I:66:GLY:O	15:I:67:VAL:C	2.58	0.40
1:0:1783:A:C2'	1:0:1784:U:H5'	2.51	0.40
1:0:2734:G:O2'	1:0:2735:U:H5'	2.20	0.40
1:0:1235:G:OP2	1:0:2550:U:H4'	2.21	0.40
1:0:1413:A:H2'	1:0:1414:A:O4'	2.20	0.40
25:S:34:LYS:HG2	25:S:54:THR:HG23	2.03	0.40
1:0:1363:G:OP1	9:C:76:ARG:NH2	2.54	0.40
1:0:2338:G:H1'	10:D:105:SER:OG	2.20	0.40
1:0:2431:C:H5'	18:L:47:GLY:HA2	2.02	0.40
1:0:800:G:H2'	1:0:801:U:C6	2.57	0.40
1:0:1074:G:H4'	1:0:1260:G:C6	2.56	0.40
32:Z:39:CYS:HA	32:Z:40:PRO:HD3	1.92	0.40
27:U:28:THR:HB	38:U:4014:HOH:O	2.20	0.40
27:U:52:THR:HG21	27:U:54:THR:HB	2.02	0.40
1:0:1702:U:H5'	38:O:7666:HOH:O	2.20	0.40
1:0:1733:A:C2	1:0:1734:C:H1'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:138:ILE:HG23	11:E:139:GLU:N	2.35	0.40
29:W:154:ARG:C	38:W:4068:HOH:O	2.59	0.40
18:L:144:ASP:CA	18:L:147:GLU:HG3	2.51	0.40
1:0:1883:U:O2'	1:0:1884:G:H5'	2.21	0.40
7:A:190:ARG:NH2	7:A:207:GLN:OE1	2.54	0.40
1:0:694:A:H2'	1:0:695:C:C5'	2.45	0.40
9:C:138:VAL:O	9:C:234:VAL:HA	2.21	0.40
24:R:119:VAL:HG12	24:R:119:VAL:O	2.21	0.40
6:9:1:U:C4'	6:9:3:A:OP1	2.70	0.40
1:0:1058:A:H2'	1:0:1060:C:C5'	2.51	0.40
26:T:96:VAL:CG1	26:T:97:ARG:N	2.84	0.40
1:0:263:U:O4'	12:F:59:ILE:HD13	2.21	0.40
1:0:1674:C:OP2	25:S:34:LYS:HE3	2.22	0.40
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.40
6:9:81:C:C2'	6:9:82:U:H5'	2.50	0.40
1:0:1822:A:O2'	1:0:1823:G:H5'	2.21	0.40
15:I:114:TYR:CD1	15:I:114:TYR:N	2.89	0.40
16:J:9:ASP:H	16:J:35:THR:HB	1.86	0.40
9:C:4:THR:HB	9:C:135:GLU:OE1	2.21	0.40
1:0:2684:A:H2'	1:0:2685:C:C6	2.56	0.40
1:0:1586:G:O2'	1:0:1587:U:H5'	2.20	0.40
23:Q:46:SER:O	23:Q:48:PRO:HD3	2.22	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:2385:G:H2'	1:0:2386:U:C6	2.57	0.40
1:0:1164:U:H3	1:0:1192:A:H2	1.69	0.40
24:R:18:LEU:HD12	24:R:143:VAL:CG1	2.47	0.40
22:P:59:ARG:HD3	38:P:4024:HOH:O	2.20	0.40
3:2:40:ARG:HG2	3:2:40:ARG:HH11	1.85	0.40
18:L:91:VAL:HG13	18:L:120:LEU:HD23	2.04	0.40
1:0:1197:G:N2	38:0:6673:HOH:O	2.52	0.40
1:0:821:U:H1'	38:0:5831:HOH:O	2.21	0.40
18:L:54:PRO:HG2	18:L:57:VAL:HG21	2.03	0.40
25:S:53:ASN:N	25:S:53:ASN:ND2	2.67	0.40
1:0:1306:U:OP1	9:C:184:ARG:HD2	2.21	0.40
6:9:2:U:OP2	6:9:2:U:H4'	2.22	0.40
1:0:1268:C:H2'	1:0:1269:G:C8	2.57	0.40
7:A:105:VAL:HG11	7:A:154:ALA:CB	2.51	0.40
1:0:2255:A:O2'	1:0:2256:G:H5'	2.21	0.40
1:0:1976:G:H1'	1:0:2005:G:N2	2.37	0.40
27:U:6:CYS:HA	27:U:13:ILE:HD11	2.03	0.40
1:0:365:G:C6	1:0:366:U:C4	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:276:C:O5'	1:0:276:C:H6	2.04	0.40
8:B:44:TYR:OH	8:B:148:PRO:HG3	2.22	0.40
29:W:75:GLY:HA3	38:W:4031:HOH:O	2.21	0.40
1:0:2705:U:O4'	11:E:112:ALA:HB2	2.21	0.40
1:0:1342:C:C2'	1:0:1343:C:H5'	2.52	0.40
1:0:1810:C:H1'	27:U:42:LEU:HD22	2.04	0.40
1:0:2757:A:H2'	1:0:2758:G:O4'	2.20	0.40
10:D:135:VAL:HG23	38:D:4038:HOH:O	2.21	0.40
8:B:41:PHE:HB3	8:B:190:MET:CE	2.50	0.40
8:B:36:PRO:HB3	8:B:174:ARG:HA	2.03	0.40
20:N:71:TRP:CE3	20:N:175:LEU:CD2	3.05	0.40
31:Y:186:ARG:HG2	31:Y:186:ARG:HH11	1.86	0.40
7:A:105:VAL:CG1	7:A:106:CYS:N	2.84	0.40
3:2:8:LYS:NZ	25:S:56:ASN:O	2.50	0.40
8:B:265:LEU:CD2	8:B:316:ARG:HD3	2.50	0.40
29:W:130:HIS:O	29:W:136:GLY:HA3	2.21	0.40
13:G:64:ASN:N	13:G:64:ASN:ND2	2.70	0.40
1:0:402:U:H2'	1:0:403:C:C6	2.56	0.40
9:C:193:LEU:HA	9:C:211:ASP:O	2.21	0.40
38:0:8879:HOH:O	23:Q:50:GLY:HA2	2.21	0.40
1:0:459:A:H4'	38:0:5107:HOH:O	2.21	0.40
8:B:279:THR:OG1	8:B:290:VAL:O	2.35	0.40
6:9:36:C:H2'	6:9:37:C:O4'	2.22	0.40
17:K:75:ARG:HG2	17:K:90:PHE:CD2	2.56	0.40
1:0:962:C:H2'	1:0:963:C:C5'	2.52	0.40
6:9:28:U:H5''	20:N:40:ASN:HD22	1.81	0.40
1:0:1500:U:OP2	22:P:41:ARG:NH2	2.55	0.40
30:X:43:VAL:CG2	30:X:76:ARG:NH1	2.83	0.40
19:M:24:GLN:HE22	19:M:27:ARG:HH11	1.67	0.40
8:B:51:VAL:HG21	8:B:327:VAL:HG13	2.02	0.40
9:C:78:ARG:HD3	38:C:4063:HOH:O	2.22	0.40
1:0:2435:U:OP1	4:3:28:GLY:HA3	2.22	0.40
9:C:160:LEU:O	9:C:161:ASP:HB2	2.22	0.40
8:B:214:PRO:C	8:B:220:VAL:HG22	2.42	0.40
9:C:170:ASP:O	9:C:171:GLU:HG3	2.22	0.40
7:A:114:ASP:HB2	7:A:117:LYS:HE2	2.02	0.40
11:E:93:MET:HB2	11:E:93:MET:HE2	1.90	0.40
1:0:2776:A:H2'	1:0:2777:G:O4'	2.21	0.40
23:Q:34:ASP:O	23:Q:37:GLU:HG3	2.21	0.40
1:0:2529:G:H5'	38:0:9170:HOH:O	2.22	0.40
25:S:17:ASP:HB3	25:S:23:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:78:G:O2'	6:9:79:U:OP2	2.40	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	
2	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
4	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	17	51
5	4	2/8 (25%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	203 (86%)	28 (12%)	4 (2%)	11	38
8	B	335/338 (99%)	294 (88%)	36 (11%)	5 (2%)	13	42
9	C	244/246 (99%)	218 (89%)	21 (9%)	5 (2%)	9	33
10	D	134/177 (76%)	92 (69%)	39 (29%)	3 (2%)	8	31
11	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	30	67
12	F	117/120 (98%)	100 (86%)	12 (10%)	5 (4%)	3	13
13	G	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	4	15
14	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	10	35
15	I	68/162 (42%)	50 (74%)	16 (24%)	2 (3%)	6	23
16	J	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	9	32
17	K	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
18	L	141/165 (86%)	113 (80%)	24 (17%)	4 (3%)	6	24
19	M	192/195 (98%)	175 (91%)	17 (9%)	0	100	100
20	N	184/187 (98%)	154 (84%)	21 (11%)	9 (5%)	3	10
21	O	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	21	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	P	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
23	Q	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	17	51
24	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	26	63
25	S	79/85 (93%)	68 (86%)	11 (14%)	0	100	100
26	T	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	7	26
27	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
28	V	63/71 (89%)	53 (84%)	6 (10%)	4 (6%)	2	5
29	W	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	26	63
30	X	80/92 (87%)	66 (82%)	9 (11%)	5 (6%)	2	5
31	Y	140/241 (58%)	133 (95%)	7 (5%)	0	100	100
32	Z	71/83 (86%)	54 (76%)	14 (20%)	3 (4%)	3	13
All	All	3707/4445 (83%)	3245 (88%)	397 (11%)	65 (2%)	11	37

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
7	A	37	VAL
8	B	184	ASP
9	C	8	LEU
10	D	173	GLU
12	F	101	ALA
20	N	133	ASP
20	N	154	LEU
20	N	164	ASP
20	N	184	ILE
32	Z	20	ARG
32	Z	81	ARG
8	B	139	ASP
12	F	44	SER
13	G	72	ASP
14	H	143	VAL
16	J	143	LYS
18	L	21	ARG
18	L	80	ASP
20	N	65	ASP
26	T	44	ALA
28	V	43	PRO

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Mol	Chain	Res	Type
30	X	70	ILE
8	B	245	SER
9	C	58	ALA
12	F	71	GLY
16	J	7	ASP
20	N	183	ASP
23	Q	21	ARG
26	T	53	GLY
26	T	83	ASP
28	V	41	GLU
29	W	77	ALA
30	X	23	HIS
30	X	77	PHE
30	X	87	ALA
4	3	57	GLY
7	A	119	ALA
9	C	232	LEU
10	D	77	ASP
14	H	19	ARG
14	H	39	LYS
15	I	71	ALA
16	J	5	GLU
18	L	35	ARG
18	L	105	TYR
20	N	74	PRO
32	Z	21	VAL
9	C	15	GLU
11	E	17	HIS
12	F	104	ALA
15	I	76	ASP
20	N	139	TRP
21	O	90	ASP
28	V	40	PRO
30	X	78	GLU
28	V	2	VAL
8	B	34	GLY
24	R	106	GLY
8	B	2	GLN
10	D	69	ILE
7	A	192	VAL
9	C	19	PRO
20	N	130	PRO

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Mol	Chain	Res	Type
12	F	64	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	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	42/46 (91%)	41 (98%)	1 (2%)	57	86
4	3	79/79 (100%)	79 (100%)	0	100	100
5	4	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	168 (94%)	11 (6%)	23	56
8	B	282/283 (100%)	264 (94%)	18 (6%)	22	53
9	C	193/193 (100%)	181 (94%)	12 (6%)	23	55
10	D	117/148 (79%)	109 (93%)	8 (7%)	20	49
11	E	152/156 (97%)	146 (96%)	6 (4%)	39	75
12	F	93/94 (99%)	90 (97%)	3 (3%)	46	81
13	G	27/283 (10%)	27 (100%)	0	100	100
14	H	134/145 (92%)	128 (96%)	6 (4%)	34	70
15	I	58/130 (45%)	58 (100%)	0	100	100
16	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
17	K	106/106 (100%)	105 (99%)	1 (1%)	84	96
18	L	113/127 (89%)	107 (95%)	6 (5%)	28	63
19	M	158/159 (99%)	151 (96%)	7 (4%)	35	70
20	N	149/150 (99%)	144 (97%)	5 (3%)	44	79
21	O	93/94 (99%)	90 (97%)	3 (3%)	46	81
22	P	113/117 (97%)	109 (96%)	4 (4%)	43	78
23	Q	79/80 (99%)	74 (94%)	5 (6%)	22	54
24	R	117/122 (96%)	113 (97%)	4 (3%)	44	79
25	S	71/74 (96%)	68 (96%)	3 (4%)	36	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	T	105/106 (99%)	98 (93%)	7 (7%)	20	50
27	U	44/52 (85%)	44 (100%)	0	100	100
28	V	51/57 (90%)	50 (98%)	1 (2%)	63	88
29	W	130/130 (100%)	122 (94%)	8 (6%)	23	55
30	X	66/74 (89%)	58 (88%)	8 (12%)	6	18
31	Y	120/196 (61%)	114 (95%)	6 (5%)	30	65
32	Z	60/68 (88%)	56 (93%)	4 (7%)	20	50
All	All	3097/3621 (86%)	2952 (95%)	145 (5%)	32	68

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	18	ASN
7	A	3	ARG
7	A	33	GLU
7	A	36	ASP
7	A	38	ILE
7	A	66	ARG
7	A	69	LEU
7	A	78	ASP
7	A	94	LEU
7	A	131	HIS
7	A	179	MET
7	A	217	ARG
8	B	7	ARG
8	B	11	LEU
8	B	27	ASN
8	B	33	ASP
8	B	49	THR
8	B	97	LEU
8	B	98	THR
8	B	162	MET
8	B	174	ARG
8	B	175	LEU
8	B	195	ARG
8	B	234	ARG
8	B	254	GLN
8	B	256	GLN
8	B	264	GLU
8	B	277	GLU

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Mol	Chain	Res	Type
8	B	307	ARG
8	B	312	ARG
9	C	2	GLN
9	C	67	GLN
9	C	76	ARG
9	C	78	ARG
9	C	101	ASP
9	C	115	LEU
9	C	187	ARG
9	C	202	THR
9	C	214	THR
9	C	223	LEU
9	C	236	THR
9	C	240	LEU
10	D	24	HIS
10	D	61	PHE
10	D	100	ASP
10	D	104	PHE
10	D	133	ASN
10	D	136	ARG
10	D	149	ARG
10	D	153	THR
11	E	7	ILE
11	E	16	ASP
11	E	102	VAL
11	E	115	ARG
11	E	156	ASP
11	E	164	ASP
12	F	12	LEU
12	F	46	GLU
12	F	100	ASP
14	H	21	GLU
14	H	33	GLN
14	H	87	LYS
14	H	91	ARG
14	H	157	TYR
14	H	170	ARG
16	J	7	ASP
16	J	47	THR
16	J	52	GLN
16	J	74	ARG
16	J	76	ASP

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Mol	Chain	Res	Type
16	J	79	PHE
16	J	107	ASN
16	J	120	SER
17	K	10	GLN
18	L	30	ARG
18	L	35	ARG
18	L	80	ASP
18	L	99	GLU
18	L	102	ASP
18	L	149	ARG
19	M	46	LEU
19	M	68	ARG
19	M	93	ARG
19	M	99	ARG
19	M	116	ASN
19	M	164	THR
19	M	186	SER
20	N	101	VAL
20	N	127	LEU
20	N	138	ASP
20	N	139	TRP
20	N	152	GLU
21	O	67	SER
21	O	97	SER
21	O	98	LEU
22	P	16	VAL
22	P	52	LYS
22	P	94	TRP
22	P	98	ILE
23	Q	11	ARG
23	Q	16	ASN
23	Q	30	VAL
23	Q	57	ASP
23	Q	95	GLU
24	R	13	THR
24	R	39	THR
24	R	82	GLU
24	R	132	ARG
25	S	12	GLU
25	S	53	ASN
25	S	80	ARG
26	T	5	ASP

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Mol	Chain	Res	Type
26	T	21	LYS
26	T	23	VAL
26	T	26	THR
26	T	39	ASN
26	T	96	VAL
26	T	115	GLU
28	V	65	ASP
29	W	13	MET
29	W	26	ILE
29	W	35	VAL
29	W	108	ARG
29	W	125	HIS
29	W	132	VAL
29	W	146	ILE
29	W	154	ARG
30	X	15	ARG
30	X	27	ASP
30	X	44	ASP
30	X	46	ASP
30	X	49	ARG
30	X	56	GLU
30	X	79	GLU
30	X	82	GLU
31	Y	163	THR
31	Y	174	VAL
31	Y	186	ARG
31	Y	189	ASN
31	Y	203	VAL
31	Y	235	GLU
32	Z	23	ARG
32	Z	41	ASN
32	Z	44	GLU
32	Z	82	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	8	GLN
2	1	16	HIS
2	1	28	HIS
3	2	16	ASN
3	2	18	ASN

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Mol	Chain	Res	Type
3	2	41	HIS
3	2	45	ASN
4	3	15	ASN
4	3	30	GLN
4	3	48	ASN
7	A	47	HIS
7	A	92	ASN
7	A	125	ASN
7	A	199	HIS
8	B	27	ASN
8	B	106	HIS
8	B	145	HIS
8	B	238	ASN
8	B	260	HIS
8	B	320	GLN
8	B	332	ASN
9	C	129	HIS
9	C	163	HIS
10	D	47	GLN
10	D	97	GLN
10	D	103	ASN
10	D	133	ASN
11	E	55	ASN
11	E	90	HIS
11	E	119	HIS
11	E	143	GLN
12	F	80	GLN
13	G	17	GLN
13	G	64	ASN
14	H	34	HIS
14	H	59	GLN
14	H	62	HIS
14	H	73	ASN
14	H	148	HIS
15	I	88	GLN
15	I	108	HIS
16	J	52	GLN
16	J	107	ASN
16	J	126	ASN
17	K	10	GLN
17	K	42	ASN
18	L	18	HIS

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Mol	Chain	Res	Type
18	L	41	HIS
18	L	42	ASN
18	L	58	GLN
18	L	116	HIS
19	M	24	GLN
19	M	58	GLN
19	M	137	ASN
19	M	143	ASN
19	M	170	ASN
19	M	190	ASN
20	N	40	ASN
20	N	93	GLN
20	N	107	ASN
21	O	53	GLN
22	P	50	GLN
22	P	66	GLN
22	P	118	GLN
23	Q	16	ASN
23	Q	40	HIS
23	Q	59	GLN
24	R	61	GLN
24	R	94	ASN
24	R	98	ASN
24	R	113	HIS
24	R	123	GLN
25	S	25	GLN
25	S	53	ASN
26	T	39	ASN
26	T	43	ASN
26	T	73	HIS
27	U	39	ASN
27	U	48	ASN
28	V	60	GLN
29	W	87	HIS
29	W	110	GLN
29	W	119	HIS
29	W	125	HIS
29	W	141	HIS
30	X	23	HIS
30	X	36	HIS
31	Y	129	ASN
31	Y	133	HIS

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Mol	Chain	Res	Type
31	Y	134	HIS
31	Y	149	GLN
31	Y	189	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	23 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	261 (9%)	24 (0%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A

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Mol	Chain	Res	Type
1	0	308	U
1	0	309	C
1	0	319	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	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	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	868	G
1	0	869	G

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Mol	Chain	Res	Type
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1234	U

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Mol	Chain	Res	Type
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1562	C
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G

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Mol	Chain	Res	Type
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2320	U
1	0	2321	A

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A

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Mol	Chain	Res	Type
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
6	9	2	U
6	9	7	G
6	9	14	G
6	9	22	G
6	9	23	U
6	9	24	U
6	9	25	G
6	9	40	C
6	9	41	C
6	9	43	G
6	9	52	A
6	9	57	A
6	9	66	G
6	9	77	A
6	9	114	G
6	9	122	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	318	U
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1232	A
1	0	1237	U
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C

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Mol	Chain	Res	Type
1	0	1856	C
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2644	C
1	0	2718	C
1	0	2791	U
6	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1,35	12,22,23	1.07	1 (8%)	19,31,34	3.16	2 (10%)
1	OMG	0	2588	1	17,26,27	1.05	1 (5%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.84	0	16,32,35	0.76	0
1	PSU	0	2621	1	13,21,22	1.67	2 (15%)	18,30,33	6.07	4 (22%)
1	1MA	0	628	1,35	14,25,26	1.02	1 (7%)	15,37,40	1.13	1 (6%)
5	MHW	4	1	33,5	9,9,10	2.52	4 (44%)	8,11,13	1.21	1 (12%)
5	DBB	4	3	5	4,5,6	0.97	0	3,5,7	1.56	1 (33%)
5	MHU	4	5	5	13,15,16	2.77	6 (46%)	15,19,21	1.28	1 (6%)
5	MHV	4	6	5	7,9,10	1.96	2 (28%)	8,11,13	1.58	2 (25%)
5	004	4	7	5	9,10,11	3.13	3 (33%)	10,12,14	2.79	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1,35	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
5	MHW	4	1	33,5	-	0/2/2/4	0/1/1/1
5	DBB	4	3	5	-	0/2/4/6	0/0/0/0
5	MHU	4	5	5	-	0/8/12/14	0/1/1/1
5	MHV	4	6	5	-	0/1/12/14	0/1/1/1
5	004	4	7	5	-	0/4/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.12	1.47	1.52
5	4	6	MHV	CD2-CG	2.27	1.55	1.50
5	4	7	004	CG1-CB	2.39	1.42	1.39
5	4	1	MHW	CA-C	2.46	1.51	1.48
5	4	5	MHU	CE1-CD1	2.53	1.43	1.38
1	0	2621	PSU	C4-N3	2.66	1.38	1.33
1	0	628	1MA	C6-N6	2.76	1.34	1.29
1	0	2587	OMU	C4-N3	2.85	1.38	1.33
5	4	1	MHW	CG2-CB	3.12	1.45	1.39
1	0	2588	OMG	C6-N1	3.31	1.39	1.33
5	4	5	MHU	CE1-CZ	3.34	1.45	1.39
5	4	5	MHU	CD1-CG	3.34	1.45	1.38
5	4	7	004	CD2-CG2	3.55	1.46	1.38
5	4	1	MHW	CB-CA	3.67	1.46	1.40
5	4	5	MHU	CD2-CE2	4.01	1.46	1.38
5	4	6	MHV	CB-CG	4.13	1.57	1.50
5	4	5	MHU	CE2-CZ	4.19	1.47	1.39
5	4	5	MHU	CA-N	4.37	1.55	1.47
5	4	1	MHW	CA-N	4.48	1.42	1.35
5	4	7	004	CB-CA	7.83	1.60	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.18	114.82	128.33
1	0	2588	OMG	C5-C6-N1	-8.70	111.69	123.59
1	0	628	1MA	C2-N3-C4	-3.72	110.64	116.40
5	4	7	004	CB-CA-N	-3.53	104.21	112.54
5	4	5	MHU	O-C-CA	-3.41	116.43	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2587	OMU	C5-C4-N3	-3.37	114.48	123.12
5	4	3	DBB	O-C-CA	-2.69	118.49	125.49
5	4	6	MHV	CD2-CE-N	-2.52	104.86	109.82
5	4	6	MHV	CA-CB-CG	-2.50	109.08	111.87
1	0	2588	OMG	N3-C2-N1	-2.35	123.86	127.44
1	0	2621	PSU	C5-C1'-C2'	-2.04	111.90	115.52
5	4	1	MHW	CE-N-CA	2.13	120.17	116.90
1	0	2621	PSU	C6-N1-C2	2.64	119.71	115.47
5	4	7	004	CG2-CB-CA	3.53	126.81	120.70
5	4	7	004	C-CA-N	6.39	122.99	109.12
1	0	2588	OMG	C6-N1-C2	6.67	125.20	115.94
1	0	2587	OMU	C4-N3-C2	13.13	127.14	114.14
1	0	2621	PSU	C4-N3-C2	13.88	127.25	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.18	33 (1%) 81 78	18, 42, 85, 147	0
2	1	56/57 (98%)	-0.55	0 100 100	23, 28, 34, 41	0
3	2	46/50 (92%)	0.11	2 (4%) 39 32	24, 56, 82, 96	0
4	3	92/92 (100%)	0.03	1 (1%) 82 80	30, 48, 61, 79	0
5	4	2/8 (25%)	-0.10	0 100 100	49, 49, 49, 54	0
6	9	122/122 (100%)	-0.12	2 (1%) 74 72	36, 57, 84, 148	0
7	A	237/240 (98%)	-0.10	5 (2%) 67 62	21, 44, 80, 100	0
8	B	337/338 (99%)	-0.11	0 100 100	23, 50, 76, 86	0
9	C	246/246 (100%)	-0.31	0 100 100	19, 39, 62, 72	0
10	D	140/177 (79%)	1.76	56 (40%) 0 0	47, 94, 117, 125	0
11	E	172/178 (96%)	0.49	7 (4%) 41 34	41, 61, 83, 88	0
12	F	119/120 (99%)	0.37	3 (2%) 61 55	41, 63, 88, 104	0
13	G	29/348 (8%)	2.38	16 (55%) 0 0	71, 87, 95, 96	0
14	H	160/177 (90%)	0.11	2 (1%) 79 78	36, 52, 88, 105	0
15	I	70/162 (43%)	4.12	65 (92%) 0 0	108, 118, 136, 138	0
16	J	142/145 (97%)	-0.06	2 (1%) 78 76	34, 46, 66, 86	0
17	K	132/132 (100%)	-0.21	2 (1%) 76 74	26, 46, 65, 75	0
18	L	145/165 (87%)	0.40	8 (5%) 29 22	22, 60, 100, 114	0
19	M	194/195 (99%)	-0.47	0 100 100	25, 36, 52, 59	0
20	N	186/187 (99%)	0.06	5 (2%) 58 52	34, 58, 100, 110	0
21	O	115/116 (99%)	-0.12	0 100 100	33, 47, 66, 71	0
22	P	143/149 (95%)	-0.02	0 100 100	33, 49, 61, 73	0
23	Q	95/96 (98%)	-0.13	0 100 100	28, 39, 54, 66	0
24	R	150/155 (96%)	-0.19	0 100 100	28, 40, 58, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	S	81/85 (95%)	0.02	1 (1%) 81 78	37, 52, 71, 79	0
26	T	119/120 (99%)	0.23	3 (2%) 61 55	35, 51, 80, 94	0
27	U	53/66 (80%)	0.09	1 (1%) 70 66	39, 51, 67, 78	0
28	V	65/71 (91%)	0.71	7 (10%) 8 4	46, 66, 105, 112	0
29	W	154/154 (100%)	-0.16	0 100 100	27, 42, 59, 71	0
30	X	82/92 (89%)	0.37	7 (8%) 13 8	38, 55, 76, 96	0
31	Y	142/241 (58%)	-0.08	4 (2%) 56 50	24, 40, 62, 81	0
32	Z	73/83 (87%)	-0.18	0 100 100	39, 53, 69, 87	0
All	All	6648/7489 (88%)	0.00	232 (3%) 48 40	18, 46, 91, 148	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	I	88	GLN	8.7
15	I	132	VAL	8.5
15	I	128	THR	7.9
15	I	70	THR	7.5
15	I	66	GLY	7.2
10	D	63	ILE	7.1
15	I	104	ALA	6.6
28	V	1	THR	6.3
15	I	68	PRO	6.2
15	I	118	ASN	6.1
15	I	119	ALA	6.1
15	I	113	SER	6.1
15	I	112	LEU	6.0
15	I	106	GLN	5.6
15	I	91	PHE	5.6
15	I	74	ILE	5.4
15	I	108	HIS	5.4
15	I	111	LEU	5.4
15	I	117	THR	5.3
10	D	27	ILE	5.2
10	D	93	LEU	5.2
15	I	80	PHE	5.1
15	I	99	GLN	5.1
15	I	69	PRO	5.1
1	0	1203	G	5.1
15	I	79	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	0	1172	G	5.0
10	D	172	VAL	4.9
15	I	110	ASP	4.9
10	D	57	THR	4.8
15	I	127	CYS	4.8
10	D	29	HIS	4.7
10	D	61	PHE	4.7
18	L	80	ASP	4.6
15	I	133	THR	4.6
10	D	64	ARG	4.6
28	V	39	ALA	4.5
15	I	72	GLU	4.5
10	D	171	ASP	4.4
15	I	73	LEU	4.4
15	I	76	ASP	4.4
15	I	97	VAL	4.4
15	I	102	GLN	4.3
10	D	18	ILE	4.3
30	X	88	GLU	4.3
13	G	23	ILE	4.2
7	A	37	VAL	4.2
10	D	88	LEU	4.2
10	D	66	GLY	4.2
15	I	131	GLY	4.2
10	D	26	GLY	4.1
1	0	1196	C	4.1
15	I	100	VAL	4.1
15	I	109	PRO	4.1
15	I	121	LYS	4.1
13	G	26	MET	4.0
10	D	90	LEU	4.0
10	D	10	PHE	4.0
15	I	67	VAL	3.9
1	0	1197	G	3.8
15	I	135	GLU	3.8
10	D	85	GLN	3.8
13	G	68	GLU	3.7
13	G	24	VAL	3.7
10	D	44	ILE	3.7
1	0	1204	C	3.7
13	G	27	ILE	3.7
10	D	87	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
10	D	69	ILE	3.6
10	D	170	TYR	3.6
15	I	71	ALA	3.6
15	I	75	LYS	3.6
1	0	1198	U	3.6
15	I	103	ILE	3.5
15	I	134	ILE	3.5
1	0	1202	A	3.5
10	D	92	GLU	3.5
15	I	107	LYS	3.5
15	I	98	ASP	3.5
13	G	71	LEU	3.5
1	0	1186	C	3.4
28	V	40	PRO	3.4
15	I	120	ALA	3.4
10	D	62	ASP	3.4
18	L	106	VAL	3.4
1	0	1951	G	3.3
15	I	105	GLU	3.3
15	I	116	LEU	3.3
15	I	130	LEU	3.3
15	I	92	VAL	3.3
15	I	93	ALA	3.3
10	D	84	LEU	3.2
15	I	114	TYR	3.2
13	G	73	ASP	3.2
15	I	78	ALA	3.2
15	I	95	LEU	3.2
1	0	1199	A	3.2
10	D	45	THR	3.1
10	D	83	PHE	3.1
15	I	96	SER	3.1
10	D	75	LEU	3.1
6	9	1	U	3.1
10	D	89	PRO	3.1
15	I	84	SER	3.1
31	Y	95	THR	3.1
1	0	284	C	3.1
10	D	134	LEU	3.0
15	I	90	ASP	3.0
15	I	94	ASP	3.0
27	U	47	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
28	V	38	GLY	3.0
1	0	1177	A	3.0
3	2	35	ARG	3.0
10	D	11	HIS	2.9
10	D	25	MET	2.9
10	D	67	ASP	2.9
26	T	119	ALA	2.9
1	0	2237	G	2.9
10	D	128	LEU	2.9
15	I	126	THR	2.9
1	0	1171	A	2.9
10	D	17	ARG	2.9
30	X	41	PHE	2.8
13	G	70	ALA	2.8
10	D	58	VAL	2.8
18	L	105	TYR	2.8
20	N	183	ASP	2.8
10	D	40	ILE	2.8
14	H	40	GLN	2.7
31	Y	235	GLU	2.7
7	A	38	ILE	2.7
10	D	106	PHE	2.7
15	I	82	THR	2.7
7	A	237	GLY	2.7
10	D	55	LYS	2.7
15	I	86	GLU	2.7
1	0	735	C	2.7
14	H	86	TYR	2.6
16	J	92	GLN	2.6
15	I	124	VAL	2.6
11	E	45	ASP	2.6
13	G	72	ASP	2.6
30	X	80	GLU	2.6
30	X	85	VAL	2.6
1	0	1195	G	2.6
13	G	15	TRP	2.6
15	I	89	GLU	2.6
18	L	79	ASP	2.6
20	N	166	ALA	2.5
10	D	68	PRO	2.5
1	0	282	C	2.5
10	D	56	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	2508	C	2.5
10	D	35	ALA	2.5
10	D	104	PHE	2.5
15	I	77	GLU	2.5
10	D	166	ILE	2.5
15	I	122	GLU	2.5
13	G	67	LEU	2.5
25	S	81	ILE	2.5
28	V	41	GLU	2.5
10	D	86	THR	2.5
20	N	158	LEU	2.5
13	G	66	LEU	2.5
26	T	112	LEU	2.4
18	L	150	GLN	2.4
31	Y	108	ASP	2.4
10	D	65	GLU	2.4
12	F	44	SER	2.4
1	0	1168	C	2.4
30	X	74	ALA	2.4
1	0	1175	G	2.4
28	V	43	PRO	2.4
26	T	118	SER	2.4
12	F	6	PHE	2.4
10	D	41	LEU	2.3
10	D	47	GLN	2.3
1	0	1525	G	2.3
28	V	3	LEU	2.3
10	D	165	PHE	2.3
15	I	87	PRO	2.3
7	A	36	ASP	2.3
1	0	960	G	2.3
15	I	83	GLY	2.3
16	J	96	GLU	2.3
30	X	7	GLU	2.3
11	E	100	ASP	2.3
20	N	185	GLU	2.3
18	L	89	PHE	2.2
13	G	29	SER	2.2
1	0	969	G	2.2
10	D	39	ASP	2.2
1	0	1181	A	2.2
13	G	22	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	1169	U	2.2
10	D	173	GLU	2.2
10	D	157	LEU	2.2
10	D	16	PRO	2.2
11	E	98	GLU	2.2
10	D	130	VAL	2.2
18	L	75	LEU	2.2
30	X	77	PHE	2.2
18	L	100	ALA	2.2
1	0	1173	A	2.1
1	0	1200	A	2.1
10	D	28	GLY	2.1
1	0	1190	G	2.1
10	D	94	ALA	2.1
15	I	81	GLU	2.1
11	E	170	ARG	2.1
20	N	159	TYR	2.1
17	K	132	VAL	2.1
10	D	24	HIS	2.1
17	K	108	GLU	2.1
1	0	1178	G	2.1
31	Y	98	GLN	2.1
3	2	39	ARG	2.1
4	3	92	GLU	2.1
11	E	154	ILE	2.1
13	G	28	GLU	2.1
15	I	123	VAL	2.1
11	E	42	VAL	2.1
1	0	1170	U	2.1
1	0	2238	A	2.1
12	F	45	ALA	2.1
6	9	24	U	2.0
11	E	1	PRO	2.0
7	A	35	GLY	2.0
13	G	20	VAL	2.0
1	0	1174	A	2.0
1	0	1163	G	2.0
10	D	91	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OMG	0	2588	24/25	0.98	0.14	-	28,31,34,35	0
5	MHW	4	1	9/10	0.96	0.20	-	46,47,49,50	0
1	PSU	0	2621	20/21	0.98	0.14	-	33,35,37,38	0
5	MHV	4	6	9/10	0.94	0.18	-	53,55,59,59	0
1	UR3	0	2619	21/22	0.98	0.13	-	30,35,39,42	0
1	OMU	0	2587	21/22	0.98	0.15	-	29,32,37,38	0
5	DBB	4	3	6/7	0.94	0.18	-	51,51,52,53	0
5	MHU	4	5	15/16	0.95	0.17	-	56,59,62,63	0
1	1MA	0	628	23/24	0.98	0.15	-	25,28,31,32	0
5	004	4	7	10/11	0.95	0.20	-	45,48,49,51	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	8	8574	1/1	0.93	0.64	47.17	60,60,60,60	0
36	CL	8	8815	1/1	0.87	0.43	38.62	88,88,88,88	0
35	NA	8	8521	1/1	0.94	0.42	36.34	61,61,61,61	0
35	NA	8	8582	1/1	0.08	0.93	35.68	81,81,81,81	0
35	NA	9	8583	1/1	0.73	0.71	28.85	85,85,85,85	0
35	NA	8	8556	1/1	0.97	0.53	28.41	43,43,43,43	0
35	NA	8	8562	1/1	0.89	0.34	26.48	75,75,75,75	0
35	NA	8	8527	1/1	0.94	0.31	24.60	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	L	8580	1/1	0.94	0.71	23.86	61,61,61,61	0
35	NA	8	8559	1/1	0.89	0.49	23.55	54,54,54,54	0
35	NA	8	8502	1/1	0.98	0.26	21.86	44,44,44,44	0
35	NA	8	8573	1/1	0.71	0.45	19.98	54,54,54,54	0
35	NA	8	8568	1/1	0.83	0.35	19.33	72,72,72,72	0
33	MG	7	8064	1/1	0.85	0.39	18.80	37,37,37,37	0
35	NA	8	8578	1/1	0.97	0.38	18.17	45,45,45,45	0
35	NA	8	8572	1/1	0.53	0.47	17.36	75,75,75,75	0
35	NA	R	8586	1/1	0.60	0.59	17.05	75,75,75,75	0
35	NA	8	8561	1/1	0.96	0.21	16.92	44,44,44,44	0
35	NA	8	8535	1/1	0.93	0.26	15.24	47,47,47,47	0
35	NA	8	8529	1/1	0.76	0.31	14.98	81,81,81,81	0
35	NA	8	8532	1/1	0.74	0.35	14.43	47,47,47,47	0
35	NA	8	8569	1/1	0.91	0.37	13.90	65,65,65,65	0
35	NA	8	8565	1/1	0.92	0.51	11.86	43,43,43,43	0
35	NA	8	8571	1/1	0.88	0.23	11.50	53,53,53,53	0
35	NA	8	8577	1/1	0.92	0.23	5.43	64,64,64,64	0
35	NA	8	8531	1/1	0.95	0.17	4.76	62,62,62,62	0
35	NA	8	8503	1/1	0.93	0.20	4.70	50,50,50,50	0
34	K	7	8401	1/1	0.96	0.20	4.22	86,86,86,86	0
35	NA	8	8525	1/1	0.97	0.16	3.12	50,50,50,50	0
35	NA	8	8553	1/1	0.98	0.20	2.89	39,39,39,39	0
35	NA	8	8550	1/1	0.97	0.14	1.22	43,43,43,43	0
35	NA	8	8566	1/1	0.94	0.20	0.94	40,40,40,40	0
35	NA	C	8504	1/1	0.82	0.25	0.92	32,32,32,32	0
33	MG	7	8102	1/1	0.96	0.16	0.77	49,49,49,49	0
33	MG	7	8053	1/1	0.98	0.13	0.37	48,48,48,48	0
35	NA	A	8545	1/1	0.96	0.16	0.09	38,38,38,38	0
33	MG	7	8060	1/1	0.97	0.14	-0.23	44,44,44,44	0
36	CL	O	8808	1/1	0.94	0.18	-0.26	74,74,74,74	0
35	NA	8	8564	1/1	0.90	0.14	-0.62	35,35,35,35	0
35	NA	8	8533	1/1	0.81	0.12	-0.81	37,37,37,37	0
36	CL	8	8813	1/1	0.99	0.12	-0.83	46,46,46,46	0
35	NA	8	8514	1/1	0.95	0.12	-0.94	27,27,27,27	0
36	CL	8	8816	1/1	0.97	0.13	-0.99	56,56,56,56	0
37	CD	Z	8703	1/1	1.00	0.11	-1.29	59,59,59,59	0
37	CD	U	8701	1/1	1.00	0.08	-1.41	60,60,60,60	0
36	CL	J	8821	1/1	0.96	0.11	-1.47	57,57,57,57	0
36	CL	B	8819	1/1	0.98	0.12	-1.50	40,40,40,40	0
35	NA	M	8547	1/1	0.97	0.12	-1.64	30,30,30,30	0
35	NA	Q	8548	1/1	0.94	0.09	-1.72	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	8	8517	1/1	0.95	0.10	-1.94	28,28,28,28	0
37	CD	3	8704	1/1	0.98	0.05	-1.98	55,55,55,55	0
36	CL	L	8810	1/1	0.95	0.11	-2.10	46,46,46,46	0
35	NA	R	8537	1/1	0.92	0.09	-2.15	33,33,33,33	0
35	NA	8	8539	1/1	0.97	0.13	-2.29	26,26,26,26	0
34	K	7	8402	1/1	0.93	0.12	-2.34	62,62,62,62	0
35	NA	J	8546	1/1	0.95	0.09	-2.39	61,61,61,61	0
33	MG	Y	8108	1/1	0.98	0.12	-2.47	34,34,34,34	0
35	NA	8	8509	1/1	0.97	0.09	-2.61	40,40,40,40	0
33	MG	7	8074	1/1	0.99	0.06	-2.70	25,25,25,25	0
33	MG	T	8073	1/1	0.91	0.11	-2.77	45,45,45,45	0
36	CL	8	8812	1/1	0.98	0.07	-3.19	39,39,39,39	0
37	CD	1	8702	1/1	0.99	0.08	-3.30	56,56,56,56	0
35	NA	8	8543	1/1	0.95	0.09	-3.37	42,42,42,42	0
33	MG	B	8055	1/1	0.97	0.09	-3.48	32,32,32,32	0
33	MG	7	8017	1/1	0.98	0.05	-3.53	26,26,26,26	0
33	MG	7	8044	1/1	0.98	0.06	-3.58	37,37,37,37	0
33	MG	A	8065	1/1	0.98	0.08	-3.62	44,44,44,44	0
33	MG	3	8078	1/1	0.95	0.04	-3.65	40,40,40,40	0
35	NA	8	8538	1/1	0.94	0.06	-3.66	55,55,55,55	0
35	NA	8	8576	1/1	0.99	0.10	-3.67	29,29,29,29	0
36	CL	M	8818	1/1	0.99	0.08	-3.77	31,31,31,31	0
33	MG	7	8056	1/1	0.98	0.12	-3.90	40,40,40,40	0
33	MG	7	8067	1/1	0.97	0.10	-4.10	38,38,38,38	0
35	NA	8	8544	1/1	0.97	0.05	-4.12	30,30,30,30	0
33	MG	7	8004	1/1	0.99	0.07	-4.19	27,27,27,27	0
33	MG	7	8058	1/1	0.98	0.08	-4.36	32,32,32,32	0
33	MG	7	8003	1/1	0.99	0.12	-4.46	31,31,31,31	0
33	MG	7	8077	1/1	0.95	0.07	-4.69	28,28,28,28	0
33	MG	7	8012	1/1	0.98	0.07	-4.71	25,25,25,25	0
35	NA	8	8505	1/1	0.94	0.11	-4.83	29,29,29,29	0
33	MG	7	8032	1/1	0.98	0.07	-4.90	40,40,40,40	0
33	MG	7	8057	1/1	0.97	0.10	-5.02	42,42,42,42	0
35	NA	8	8523	1/1	0.98	0.12	-5.03	39,39,39,39	0
33	MG	7	8013	1/1	0.98	0.10	-5.08	37,37,37,37	0
33	MG	7	8111	1/1	0.98	0.06	-5.22	40,40,40,40	0
33	MG	7	8015	1/1	0.96	0.06	-5.33	38,38,38,38	0
33	MG	7	8096	1/1	0.94	0.08	-5.35	41,41,41,41	0
33	MG	7	8018	1/1	0.98	0.09	-5.69	34,34,34,34	0
33	MG	7	8020	1/1	0.99	0.08	-5.73	22,22,22,22	0
33	MG	7	8080	1/1	0.98	0.07	-5.79	38,38,38,38	0
33	MG	7	8001	1/1	0.95	0.07	-5.87	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	7	8033	1/1	0.96	0.09	-6.06	31,31,31,31	0
35	NA	8	8520	1/1	0.99	0.10	-6.32	25,25,25,25	0
33	MG	7	8109	1/1	0.99	0.08	-6.39	23,23,23,23	0
33	MG	7	8038	1/1	0.98	0.08	-6.88	28,28,28,28	0
33	MG	7	8101	1/1	0.97	0.11	-7.12	49,49,49,49	0
36	CL	3	8804	1/1	0.98	0.08	-7.27	53,53,53,53	0
33	MG	7	8084	1/1	0.99	0.03	-7.62	42,42,42,42	0
33	MG	7	8052	1/1	0.96	0.05	-7.85	35,35,35,35	0
33	MG	7	8010	1/1	0.97	0.07	-7.93	24,24,24,24	0
33	MG	7	8014	1/1	0.98	0.07	-8.08	31,31,31,31	0
33	MG	7	8008	1/1	0.96	0.04	-8.22	33,33,33,33	0
33	MG	7	8035	1/1	0.96	0.05	-8.25	50,50,50,50	0
33	MG	7	8107	1/1	0.92	0.08	-8.28	73,73,73,73	0
33	MG	7	8002	1/1	0.96	0.04	-8.42	26,26,26,26	0
33	MG	7	8091	1/1	0.94	0.05	-8.51	41,41,41,41	0
33	MG	7	8007	1/1	1.00	0.07	-9.67	12,12,12,12	0
33	MG	7	8019	1/1	0.99	0.05	-10.31	23,23,23,23	0
33	MG	7	8006	1/1	0.98	0.04	-10.69	46,46,46,46	0
33	MG	7	8054	1/1	0.98	0.09	-11.46	24,24,24,24	0
33	MG	7	8088	1/1	0.95	0.07	-20.34	25,25,25,25	0
36	CL	J	8801	1/1	0.96	0.18	-	55,55,55,55	0
35	NA	8	8570	1/1	0.98	0.13	-	58,58,58,58	0
33	MG	7	8094	1/1	0.93	0.13	-	47,47,47,47	0
36	CL	R	8806	1/1	0.97	0.15	-	43,43,43,43	0
33	MG	7	8030	1/1	0.99	0.08	-	31,31,31,31	0
33	MG	7	8029	1/1	0.99	0.08	-	33,33,33,33	0
35	NA	8	8518	1/1	0.95	0.17	-	26,26,26,26	0
33	MG	K	8069	1/1	0.94	0.07	-	46,46,46,46	0
33	MG	7	8093	1/1	0.96	0.21	-	48,48,48,48	0
35	NA	8	8542	1/1	0.97	0.12	-	35,35,35,35	0
33	MG	7	8105	1/1	0.97	0.22	-	53,53,53,53	0
33	MG	7	8042	1/1	0.99	0.10	-	31,31,31,31	0
33	MG	7	8114	1/1	0.97	0.09	-	49,49,49,49	0
36	CL	8	8822	1/1	0.94	0.27	-	88,88,88,88	0
33	MG	7	8090	1/1	0.96	0.18	-	41,41,41,41	0
33	MG	7	8112	1/1	0.77	0.26	-	47,47,47,47	0
35	NA	8	8575	1/1	0.94	0.30	-	58,58,58,58	0
35	NA	8	8506	1/1	0.94	0.41	-	33,33,33,33	0
35	NA	8	8563	1/1	0.85	0.33	-	60,60,60,60	0
33	MG	7	8025	1/1	0.98	0.03	-	42,42,42,42	0
37	CD	O	8705	1/1	0.98	0.08	-	70,70,70,70	0
35	NA	8	8579	1/1	0.92	0.31	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	9	8095	1/1	0.94	0.09	-	53,53,53,53	0
35	NA	8	8519	1/1	0.98	0.13	-	22,22,22,22	0
33	MG	7	8117	1/1	0.98	0.09	-	46,46,46,46	0
35	NA	8	8510	1/1	0.80	0.51	-	36,36,36,36	0
36	CL	J	8802	1/1	0.95	0.14	-	63,63,63,63	0
33	MG	7	8097	1/1	0.97	0.06	-	26,26,26,26	0
33	MG	7	8009	1/1	0.99	0.07	-	22,22,22,22	0
33	MG	7	8099	1/1	0.89	0.16	-	45,45,45,45	0
33	MG	7	8049	1/1	0.90	0.25	-	58,58,58,58	0
35	NA	8	8515	1/1	0.98	0.12	-	48,48,48,48	0
33	MG	7	8087	1/1	0.86	0.18	-	46,46,46,46	0
36	CL	N	8807	1/1	0.97	0.13	-	57,57,57,57	0
33	MG	7	8051	1/1	0.91	0.12	-	58,58,58,58	0
33	MG	7	8040	1/1	0.98	0.13	-	70,70,70,70	0
35	NA	8	8567	1/1	0.97	0.14	-	35,35,35,35	0
33	MG	7	8027	1/1	0.97	0.11	-	40,40,40,40	0
36	CL	8	8811	1/1	0.97	0.14	-	57,57,57,57	0
33	MG	7	8047	1/1	0.90	0.20	-	62,62,62,62	0
33	MG	7	8063	1/1	0.98	0.07	-	51,51,51,51	0
36	CL	A	8809	1/1	0.91	0.19	-	58,58,58,58	0
33	MG	7	8100	1/1	0.95	0.10	-	73,73,73,73	0
33	MG	7	8024	1/1	0.99	0.06	-	12,12,12,12	0
33	MG	7	8081	1/1	0.94	0.10	-	50,50,50,50	0
35	NA	8	8541	1/1	0.93	0.13	-	29,29,29,29	0
33	MG	7	8116	1/1	0.97	0.11	-	20,20,20,20	0
35	NA	8	8540	1/1	0.84	0.25	-	44,44,44,44	0
33	MG	7	8043	1/1	0.98	0.06	-	35,35,35,35	0
33	MG	7	8104	1/1	0.95	0.20	-	48,48,48,48	0
33	MG	7	8115	1/1	0.88	0.11	-	46,46,46,46	0
33	MG	7	8110	1/1	0.95	0.08	-	60,60,60,60	0
35	NA	8	8534	1/1	0.96	0.07	-	26,26,26,26	0
33	MG	7	8066	1/1	0.98	0.18	-	96,96,96,96	0
33	MG	7	8023	1/1	0.99	0.06	-	34,34,34,34	0
35	NA	8	8584	1/1	0.86	0.15	-	45,45,45,45	0
33	MG	7	8076	1/1	0.99	0.08	-	47,47,47,47	0
35	NA	8	8560	1/1	0.98	0.40	-	49,49,49,49	0
35	NA	9	8551	1/1	0.84	0.13	-	31,31,31,31	0
33	MG	7	8083	1/1	0.99	0.04	-	22,22,22,22	0
35	NA	S	8512	1/1	0.98	0.13	-	10,10,10,10	0
33	MG	7	8089	1/1	0.93	0.11	-	49,49,49,49	0
33	MG	7	8046	1/1	0.92	0.11	-	52,52,52,52	0
33	MG	7	8113	1/1	0.95	0.24	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	8	8581	1/1	0.93	0.16	-	40,40,40,40	0
33	MG	7	8070	1/1	0.97	0.11	-	41,41,41,41	0
35	NA	8	8530	1/1	0.89	0.31	-	41,41,41,41	0
35	NA	8	8508	1/1	0.88	0.15	-	39,39,39,39	0
33	MG	7	8011	1/1	0.95	0.08	-	21,21,21,21	0
35	NA	8	8513	1/1	0.88	0.17	-	47,47,47,47	0
33	MG	7	8041	1/1	0.95	0.20	-	38,38,38,38	0
35	NA	8	8552	1/1	0.91	0.36	-	40,40,40,40	0
35	NA	8	8524	1/1	0.91	0.21	-	39,39,39,39	0
33	MG	7	8050	1/1	0.88	0.19	-	72,72,72,72	0
35	NA	8	8549	1/1	0.98	0.11	-	34,34,34,34	0
35	NA	8	8585	1/1	0.92	0.32	-	38,38,38,38	0
36	CL	Y	8820	1/1	0.98	0.11	-	30,30,30,30	0
33	MG	7	8062	1/1	0.92	0.06	-	52,52,52,52	0
33	MG	7	8072	1/1	0.93	0.08	-	56,56,56,56	0
33	MG	7	8037	1/1	0.99	0.07	-	44,44,44,44	0
33	MG	7	8021	1/1	0.98	0.10	-	32,32,32,32	0
33	MG	7	8036	1/1	0.99	0.05	-	32,32,32,32	0
33	MG	7	8034	1/1	0.91	0.09	-	29,29,29,29	0
35	NA	8	8528	1/1	0.97	0.32	-	50,50,50,50	0
35	NA	8	8526	1/1	0.61	0.61	-	72,72,72,72	0
35	NA	8	8507	1/1	0.83	0.43	-	56,56,56,56	0
35	NA	8	8558	1/1	0.90	0.46	-	48,48,48,48	0
33	MG	7	8016	1/1	0.98	0.11	-	23,23,23,23	0
33	MG	7	8061	1/1	0.94	0.08	-	27,27,27,27	0
35	NA	H	8522	1/1	0.90	0.15	-	38,38,38,38	0
33	MG	7	8079	1/1	0.99	0.10	-	20,20,20,20	0
35	NA	8	8516	1/1	0.92	0.25	-	39,39,39,39	0
33	MG	7	8071	1/1	0.97	0.09	-	59,59,59,59	0
33	MG	7	8031	1/1	0.99	0.08	-	28,28,28,28	0
36	CL	8	8817	1/1	0.88	0.17	-	58,58,58,58	0
33	MG	7	8082	1/1	0.92	0.17	-	58,58,58,58	0
33	MG	7	8045	1/1	0.97	0.08	-	58,58,58,58	0
35	NA	8	8511	1/1	0.80	0.30	-	50,50,50,50	0
36	CL	8	8814	1/1	0.96	0.12	-	51,51,51,51	0
33	MG	7	8103	1/1	0.87	0.44	-	79,79,79,79	0
33	MG	7	8098	1/1	0.90	0.16	-	42,42,42,42	0
33	MG	7	8039	1/1	0.98	0.10	-	33,33,33,33	0
35	NA	8	8555	1/1	0.93	0.55	-	71,71,71,71	0
33	MG	7	8026	1/1	0.99	0.07	-	19,19,19,19	0
33	MG	7	8048	1/1	0.98	0.07	-	48,48,48,48	0
33	MG	7	8022	1/1	0.99	0.08	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	7	8106	1/1	0.98	0.05	-	35,35,35,35	0
33	MG	7	8086	1/1	0.98	0.16	-	41,41,41,41	0
35	NA	8	8557	1/1	0.91	0.07	-	49,49,49,49	0
35	NA	8	8536	1/1	0.94	0.13	-	44,44,44,44	0
33	MG	7	8005	1/1	0.99	0.10	-	27,27,27,27	0
33	MG	7	8075	1/1	0.87	0.08	-	55,55,55,55	0
33	MG	7	8085	1/1	0.99	0.09	-	65,65,65,65	0
36	CL	8	8803	1/1	0.98	0.16	-	43,43,43,43	0
33	MG	7	8028	1/1	0.99	0.09	-	39,39,39,39	0
36	CL	8	8805	1/1	0.95	0.19	-	57,57,57,57	0
35	NA	8	8501	1/1	0.96	0.14	-	21,21,21,21	0
33	MG	7	8059	1/1	0.97	0.06	-	27,27,27,27	0
35	NA	8	8554	1/1	0.86	0.29	-	55,55,55,55	0
33	MG	7	8092	1/1	0.93	0.29	-	75,75,75,75	0
33	MG	7	8068	1/1	0.93	0.07	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.