



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 11:30 AM EDT

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

<https://www.wwpdb.org/validation/2017/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:

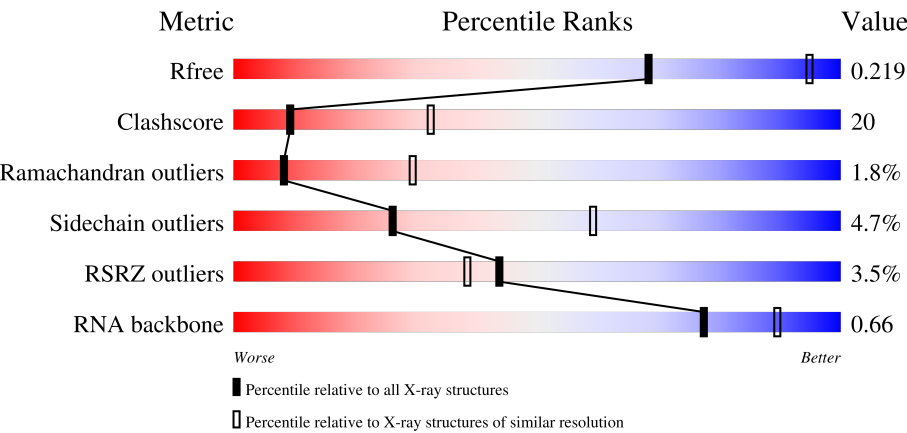
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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></div><div></div><div></div><div></div></div> <div>53%35%6%6%</div>
2	1	57	<div><div></div><div></div><div></div><div></div><div></div></div> <div>65%33%. .</div>
3	2	50	<div><div></div><div></div><div></div><div></div><div></div></div> <div>4%46%46%8%</div>
4	3	92	<div><div></div><div></div><div></div><div></div><div></div></div> <div>55%45%</div>

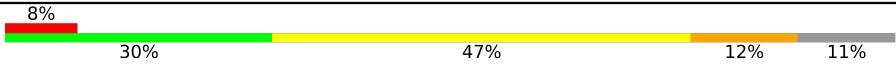


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Mol	Chain	Length	Quality of chain
5	4	8	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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Mol	Chain	Length	Quality of chain
30	X	92	
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
35	NA	0	3120	-	-	-	X
35	NA	0	3134	-	-	-	X
35	NA	0	3174	-	-	-	X
35	NA	0	3175	-	-	-	X
35	NA	0	3183	-	-	-	X
35	NA	9	203	-	-	-	X
35	NA	R	202	-	-	-	X
36	CL	0	3189	-	-	X	-
36	CL	N	201	-	-	X	-

2 Entry composition

There are 39 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 is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	2099	A	G	engineered mutation	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	7	Total	C	N	O	0	0	0
			63	45	8	10			

- 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		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	0	109	Total	Mg	0	0
			109	109		
33	3	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	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	0	74	Total	Na	0	0
			74	74		
35	9	2	Total	Na	0	0
			2	2		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	3	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0

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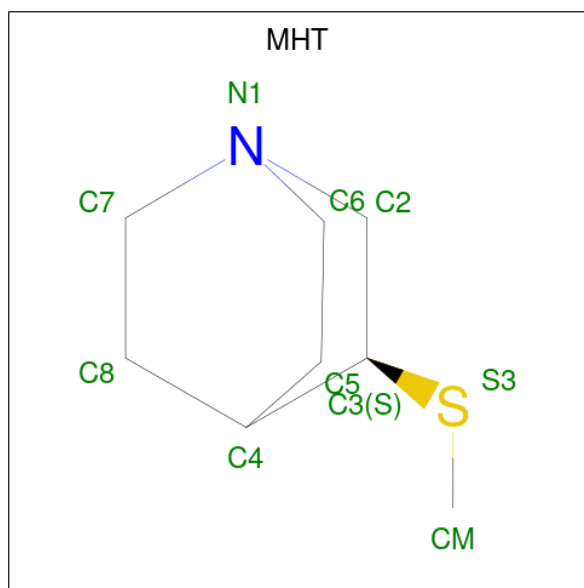
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Y	1	Total	Cl	0	0
			1	1		

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

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

- Molecule 38 is (3S)-3-(methylsulfanyl)-1-azabicyclo[2.2.2]octane (three-letter code: MHT) (formula: C₈H₁₅NS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	S	0	0
			10	8	1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5842	Total 5842	O 5842	0	0
39	1	60	Total 60	O 60	0	0
39	2	49	Total 49	O 49	0	0
39	3	69	Total 69	O 69	0	0
39	4	2	Total 2	O 2	0	0
39	9	143	Total 143	O 143	0	0
39	A	123	Total 123	O 123	0	0
39	B	146	Total 146	O 146	0	0
39	C	185	Total 185	O 185	0	0
39	D	49	Total 49	O 49	0	0
39	E	42	Total 42	O 42	0	0
39	F	26	Total 26	O 26	0	0
39	G	20	Total 20	O 20	0	0
39	H	69	Total 69	O 69	0	0
39	I	9	Total 9	O 9	0	0
39	J	55	Total 55	O 55	0	0
39	K	59	Total 59	O 59	0	0
39	L	82	Total 82	O 82	0	0
39	M	129	Total 129	O 129	0	0
39	N	60	Total 60	O 60	0	0
39	O	42	Total 42	O 42	0	0
39	P	72	Total 72	O 72	0	0

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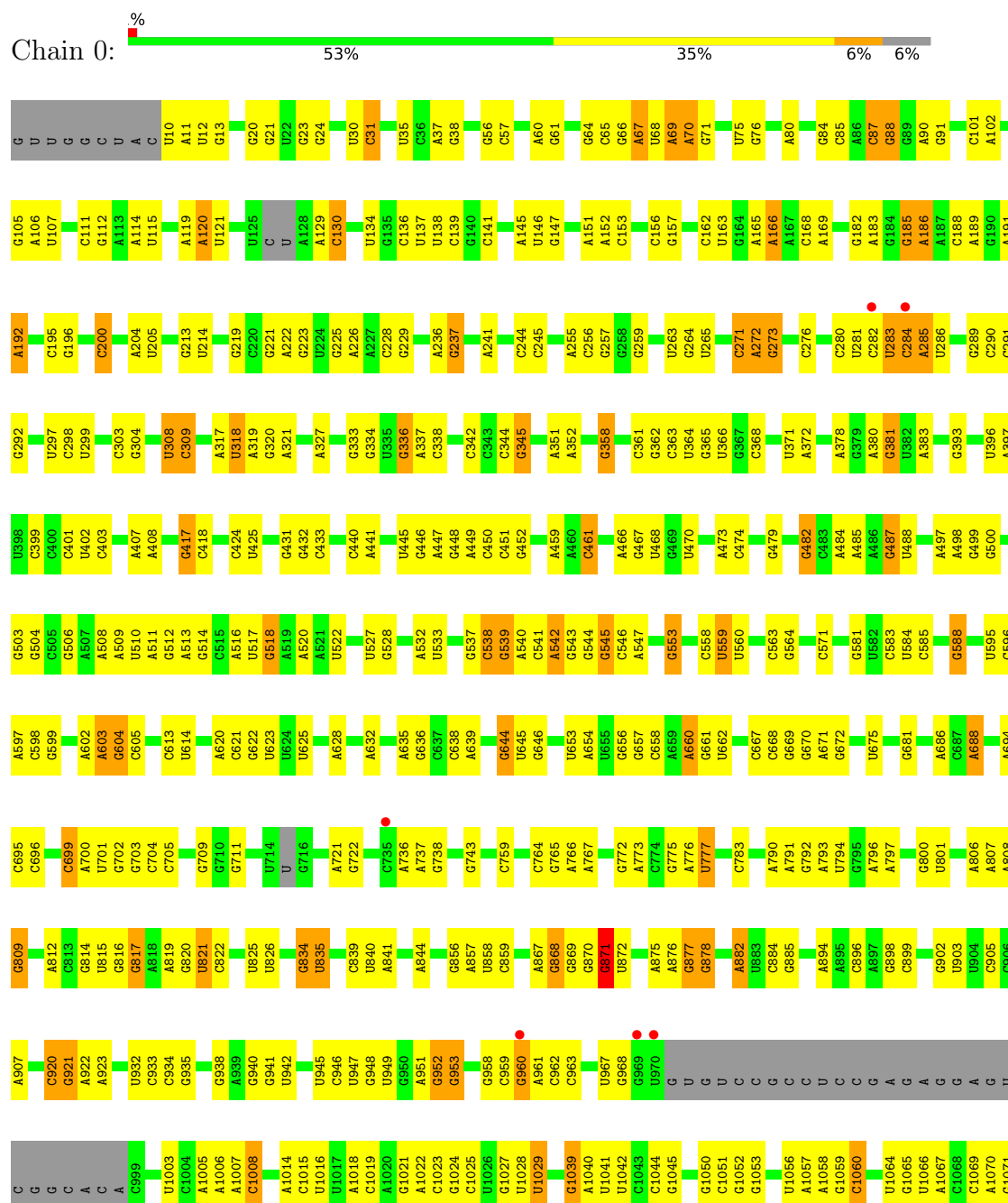
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	48	Total 48	O 48	0	0
39	R	85	Total 85	O 85	0	0
39	S	30	Total 30	O 30	0	0
39	T	39	Total 39	O 39	0	0
39	U	29	Total 29	O 29	0	0
39	V	13	Total 13	O 13	0	0
39	W	69	Total 69	O 69	0	0
39	X	26	Total 26	O 26	0	0
39	Y	101	Total 101	O 101	0	0
39	Z	37	Total 37	O 37	0	0

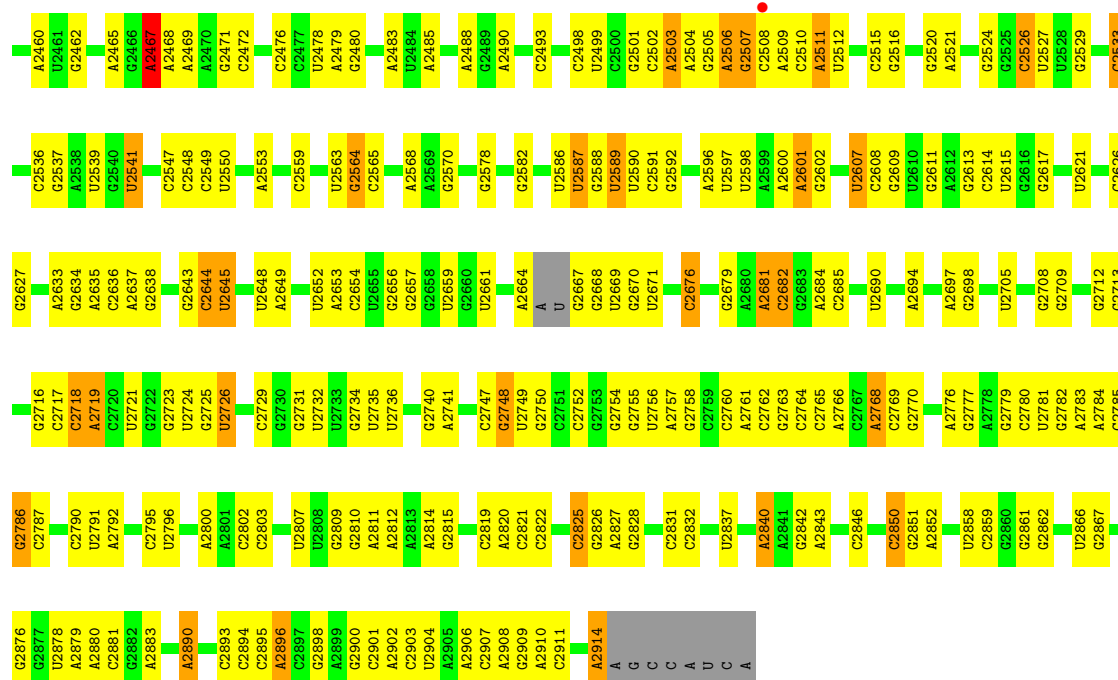
3 Residue-property plots [i](#)

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

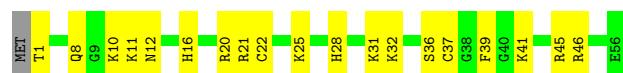
• Molecule 1: 23S RIBOSOMAL RNA



A2364	G2270	C	U	G2033	A1733	A1533	A1437	C1343	G1239	G1072
G2365	G2271	C	G	U2034	C1734	C1534	G1438	A1348	C1242	A1073
A2369	C2272	C	U	C2035	C1735	G1535	U1439	A1349	C1243	G1074
G2370	G2273	C	G	C2036	A1736	A1536	C1439	A1350	A1244	A1081
A2371	G2274	G	C	C2037	U1741	G1543	A1442	A1352	C1245	A1086
G2372	G2275	A	C	A1942	A1742	U1544	U1446	G1354	A1246	G1087
U2373	U2276	C	C	C1943	G1743	C1545	C1451	A1355	C1250	A1088
	U2277	A	C	A1944	G1744	U1546	C1452	C1360	C1251	G1089
		C	C	C1945	U1748	A1559	C1453	C1363	C1260	A1097
		A	U	U1834	C1749	U1554	C1454	C1364	A1261	A1098
		C	G	U1835	U1750	A1555	C1455	C1366	G1266	G1099
		C	U	U1836	C1751	U1556	U1461	C1372	C1267	C1102
		C	U	C1837	G1752	C1557	C1462	A1373	C1268	U1109
		C	C	A1838	A1753	A1558	A1470	C1374	C1269	G1110
		C	C	U1839	G1754	A1559	C1471	C1375	C1273	U1111
		C	C	C1840	U1755	G1560	C1472	A1376	C1277	G1112
		C	C	A1841	U1756	C1561	C1473	C1377	C1278	U1116
		C	C	U1842	C1757	A1562	C1474	C1378	C1279	A1117
		C	C	C1843	U1758	C1563	U1475	C1379	C1280	A1118
		C	C	U1844	C1759	A1564	C1476	C1380	C1281	G1119
		C	C	A1845	U1760	U1565	U1477	C1381	C1282	U1120
		C	C	U1846	C1761	G1566	C1478	C1382	C1283	G1121
		C	C	C1847	U1762	A1567	U1479	C1383	C1284	U1122
		C	C	U1848	C1763	C1568	C1483	C1384	C1285	A1123
		C	C	A1849	U1764	A1569	G1484	C1385	C1286	U1129
		C	C	U1850	C1765	G1570	C1485	C1386	C1287	U1130
		C	C	C1851	U1766	C1571	G1486	C1387	C1288	G1131
		C	C	U1852	C1767	A1572	C1487	C1388	C1289	A1132
		C	C	C1853	U1768	C1573	G1488	C1389	C1290	G1137
		C	C	U1854	C1769	A1574	C1489	C1390	C1291	U1139
		C	C	A1855	U1770	C1575	U1488	C1391	C1292	C1140
		C	C	C1856	C1771	A1576	C1490	C1392	C1293	A1150
		C	C	U1857	U1772	G1577	G1491	C1393	C1294	G1151
		C	C	C1858	G1773	A1578	C1492	C1394	C1295	A1154
		C	C	U1859	U1774	C1579	C1493	C1395	C1296	G1155
		C	C	A1860	C1775	A1580	C1494	C1396	C1297	C1157
		C	C	C1861	U1776	G1581	C1495	C1397	C1298	G1158
		C	C	U1862	C1777	A1582	C1496	C1398	C1299	G1159
		C	C	C1863	U1778	C1583	C1497	C1399	C1300	G1160
		C	C	U1864	C1779	A1584	U1500	C1400	C1301	A1161
		C	C	A1865	U1780	C1585	C1501	C1401	C1302	G1162
		C	C	C1866	C1781	A1586	C1502	C1402	C1303	U1163
		C	C	U1867	U1782	G1587	C1503	C1403	C1304	U1164
		C	C	C1868	C1783	A1588	C1504	C1404	C1305	G1165
		C	C	U1869	U1784	C1589	C1505	C1405	C1306	G1166
		C	C	A1870	C1785	U1590	C1506	C1406	C1307	G1167
		C	C	C1871	U1786	A1591	C1507	C1407	C1308	C1168
		C	C	U1872	C1787	C1592	C1508	C1408	C1309	U1169
		C	C	A1873	U1788	A1593	C1509	C1409	C1310	U1170
		C	C	C1874	G1789	C1594	C1510	C1410	C1311	
		C	C	U1875	U1790	G1595	C1511	C1411	C1312	
		C	C	A1876	C1791	C1596	C1512	C1412	C1313	
		C	C	C1877	U1792	U1597	C1513	C1413	C1314	
		C	C	U1878	C1793	A1598	C1514	C1414	C1315	
		C	C	A1879	U1794	C1599	C1515	C1415	C1316	
		C	C	C1880	C1795	U1600	C1516	C1416	C1317	
		C	C	U1881	U1796	A1601	C1517	C1417	C1318	
		C	C	A1882	C1797	C1602	C1518	C1418	C1319	
		C	C	C1883	U1798	A1603	C1519	C1419	C1320	
		C	C	U1884	C1799	C1604	C1520	C1420	C1321	
		C	C	A1885	U1800	G1605	C1521	C1421	C1322	
		C	C	C1886	C1801	A1606	C1522	C1422	C1323	
		C	C	U1887	U1802	C1607	C1523	C1423	C1324	
		C	C	A1888	C1803	A1608	C1524	C1424	C1325	
		C	C	C1889	G1804	C1609	C1525	C1425	C1326	
		C	C	U1890	U1805	G1610	C1526	C1426	C1327	
		C	C	A1891	C1806	A1611	C1527	C1427	C1328	
		C	C	C1892	U1807	C1612	C1528	C1428	C1329	
		C	C	U1893	C1808	A1613	C1529	C1429	C1330	
		C	C	A1894	U1809	C1614	C1530	C1430	C1331	
		C	C	C1895	C1900	A1615	C1531	C1431	C1332	
		C	C	U1896	U1901	C1616	C1532	C1432	C1333	
		C	C	A1897	C1902	C1617	C1533	C1433	C1334	
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		C	C	C1901	C1906	A1621	C1537	C1437	C1338	
		C	C	U1902	U1907	C1622	C1538	C1438	C1339	
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		C	C	U1905	C1910	A1625	C1541	C1441	C1342	
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		C	C	C1907	C1912	C1627	C1543	C1443	C1344	
		C	C	U1908	U1913	A1628	C1544	C1444	C1345	
		C	C	A1909	C1914	C1629	C1545	C1445	C1346	
		C	C	C1910	U1915	C1630	C1546	C1446	C1347	
		C	C	U1911	C1916	A1631	C1547	C1447	C1348	
		C	C	A1912	U1917	C1632	C1548	C1448	C1349	
		C	C	C1913	C1918	A1633	C1549	C1449	C1350	
		C	C	U1914	U1919	C1634	C1550	C1450	C1351	
		C	C	A1915	C1920	A1635	C1551	C1451	C1352	
		C	C	C1916	U1921	C1636	C1552	C1452	C1353	
		C	C	U1917	C1922	A1637	C1553	C1453	C1354	
		C	C	A1918	U1923	C1638	C1554	C1454	C1355	
		C	C	C1919	C1924	C1639	C1555	C1455	C1356	
		C	C	U1920	U1925	A1640	C1556	C1456	C1357	
		C	C	A1921	G1926	C1641	C1557	C1457	C1358	
		C	C	C1922	U1927	A1642	C1558	C1458	C1359	
		C	C	U1923	C1928	C1643	C1559	C1459	C1360	
		C	C	A1924	U1929	A1644	C1560	C1460	C1361	
		C	C	C1925	C1930	C1645	C1561	C1461	C1362	
		C	C	U1926	A1931	C1646	C1562	C1462	C1363	
		C	C	A1927	C1932	A1647	C1563	C1463	C1364	
		C	C	C1928	U1933	C1648	C1564	C1464	C1365	
		C	C	U1929	C1934	A1649	C1565	C1465	C1366	
		C	C	A1930	U1935	C1650	C1566	C1466	C1367	
		C	C	C1931	C1936	A1651	C1567	C1467	C1368	
		C	C	U1932	U1937	C1652	C1568	C1468	C1369	
		C	C	A1933	C1938	A1653	C1569	C1469	C1370	
		C	C	C1934	U1939	C1654	C1570	C1470	C1371	
		C	C	U1935	C1940	A1655	C1571	C1471	C1372	
		C	C	A1936	U1941	C1656	C1572	C1472	C1373	
		C	C	C1937	C1942	A1657	C1573	C1473	C1374	
		C	C	U1938	U1943	A1658	C1574	C1474	C1375	
		C	C	A1939	C1944	A1659	C1575	C1475	C1376	
		C	C	C1940	U1945	G1560	C1576	C1476	C1377	
		C	C	U1941	C1946	C1561	C1577	C1477	C1378	
		C	C	A1942	U1947	A1562	C1578	C1478	C1379	
		C	C	C1943	G1948	C1563	C1579	C1479	C1380	
		C	C	U1944	U1949	A1564	C1580	C1480	C1381	
		C	C	A1945	C1950	U1565	C1581	C1481	C1382	
		C	C	C1946	U1951	C1566	C1582	C1482	C1383	
		C	C	U1947	C1952	A1567	C1583	C1483	C1384	
		C	C	A1948	U1953	C1568	C1584	C1484	C1385	
		C	C	C1949	C1954	A1569	C1585	C1485	C1386	
		C	C	U1950	U1955	G1560	C1586	C1486	C1387	
		C	C	A1951	C1956	C1561	C1587	C1487	C1388	
		C	C	C1952	U1957	A1562	C1588	C1488	C1389	
		C	C	U1953	C1958	C1563	C1589	C1489	C1390	
		C	C	A1954	U1959	A1564	C1590	C1490	C1391	
		C	C	C1955	C1960	C1565	C1591	C1491	C1392	
		C	C	U1956	U1961	C1566	C1592	C1492	C1393	
		C	C	A1957	C1962	A1567	C1593	C1493	C1394	
		C	C	C1958	U1963	C1568	C1594	C1494	C1395	
		C	C	U1959	C1964	C1569	C1595	C1495	C1396	
		C	C	A1960	U1965	A1569	C1596	C1496	C1397	
		C	C	C1961	C1966	C1570	C1597	C1497	C1398	
		C	C	U1962	U1967	C1571	C1598	C1498	C1399	
		C	C	A1963	C1968	C1572	C1599	C1499	C1400	
		C	C	C1964	U1969	A1573	C1600	C1500	C1401	
		C	C	U1965	C1970	C1574	C1601	C1501	C1402	
		C	C	A1966	U1971	A1575	C1602	C1502	C1403	
		C	C	C1967	C1972	C1576	C1603	C1503	C1404	
		C	C	U1968	U1973	A1577	C1604	C1504	C1405	
		C	C	A1969	C1974	C1578	C1605	C1505	C1406	
		C	C	C1970	U1975	G1579	C1606	C1506	C1407	
		C	C	U1971	C1976	A1580	C1607	C1507	C1408	
		C	C</							



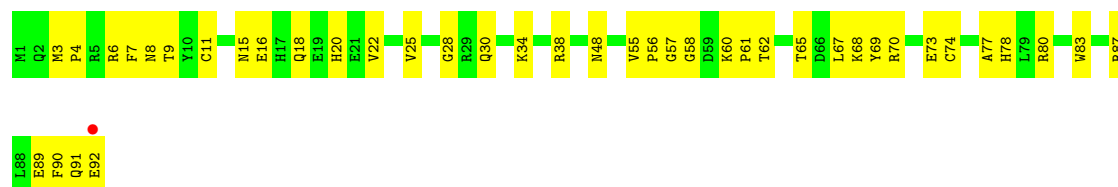
• Molecule 2: 50S RIBOSOMAL PROTEIN L37E



• Molecule 3: 50S RIBOSOMAL PROTEIN L39E



• Molecule 4: 50S RIBOSOMAL PROTEIN L44E

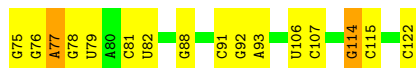
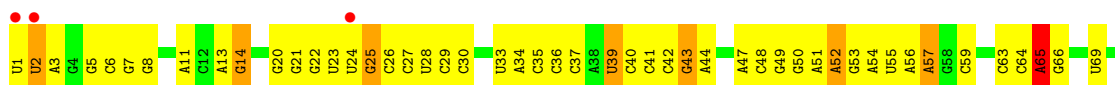


• Molecule 5: QUINUPRISTIN

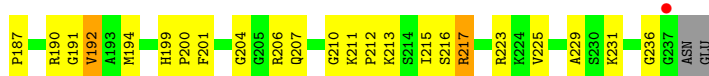
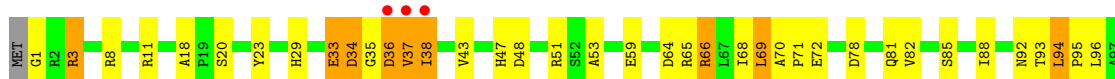




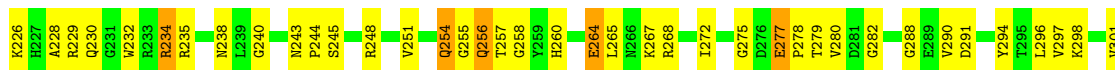
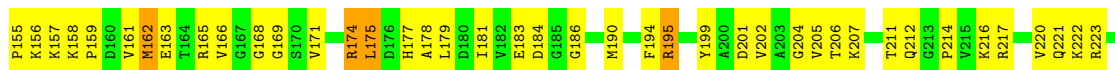
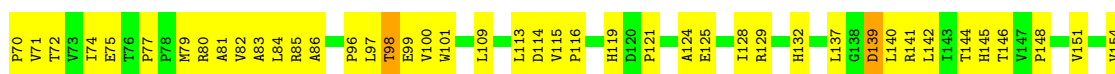
• Molecule 6: 5S RIBOSOMAL RNA



• Molecule 7: 50S RIBOSOMAL PROTEIN L2P

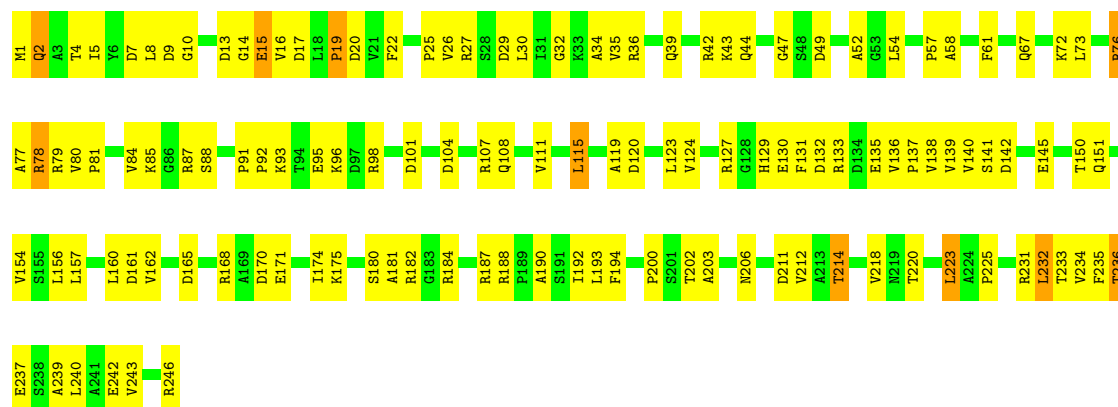


• Molecule 8: 50S RIBOSOMAL PROTEIN L3P

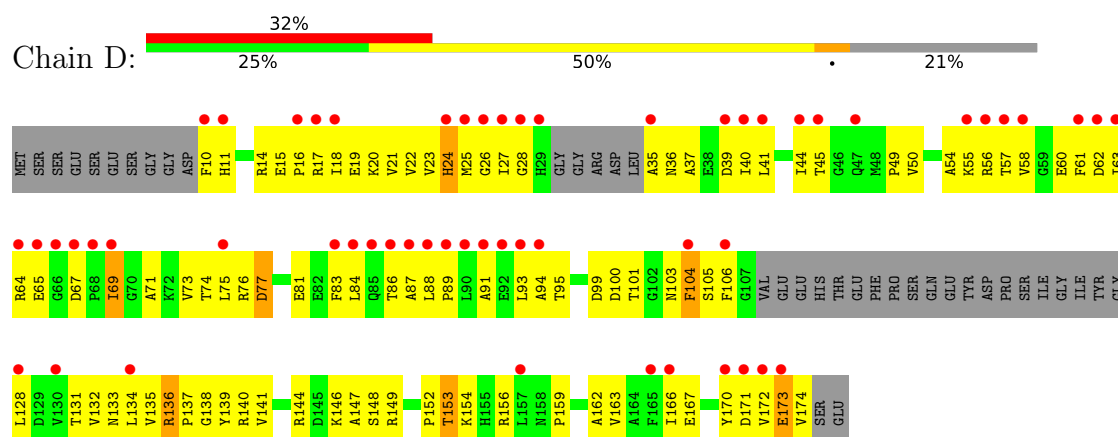


• Molecule 9: 50S RIBOSOMAL PROTEIN L4E

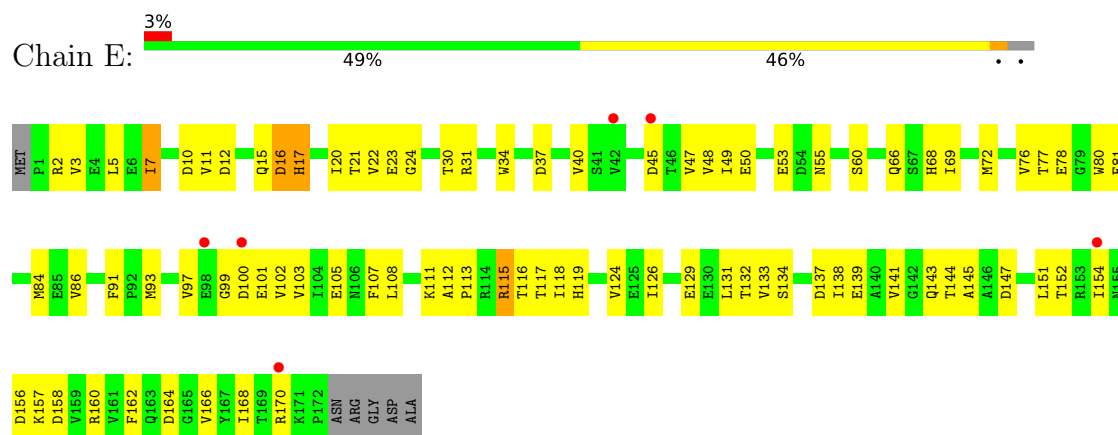




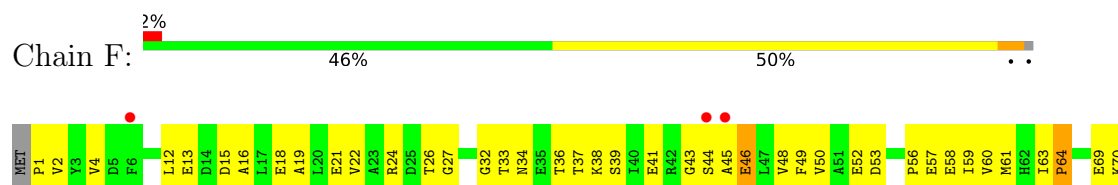
• Molecule 10: 50S RIBOSOMAL PROTEIN L5P



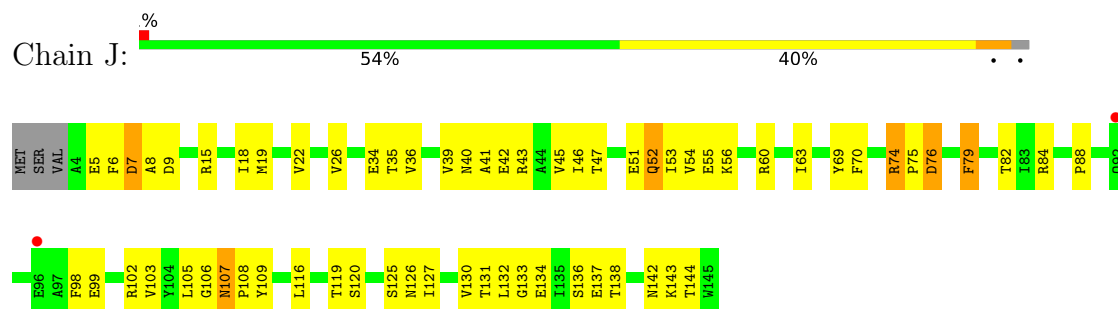
• Molecule 11: 50S RIBOSOMAL PROTEIN L6P



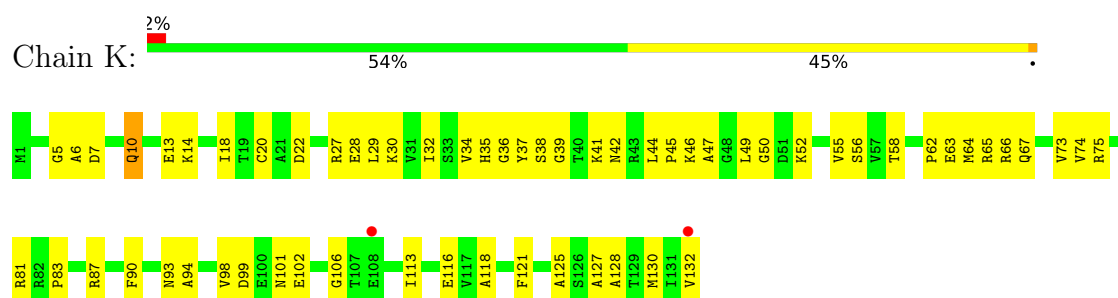
• Molecule 12: 50S RIBOSOMAL PROTEIN L7AE



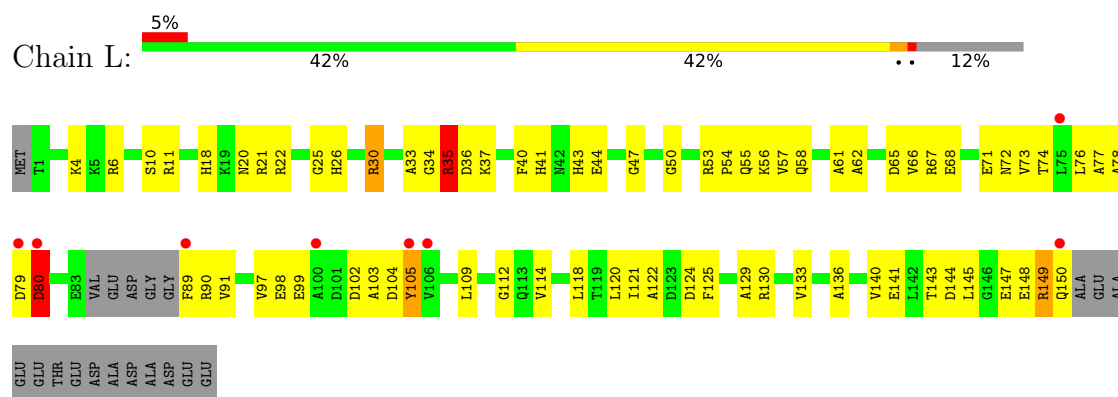
- Molecule 16: 50S RIBOSOMAL PROTEIN L13P



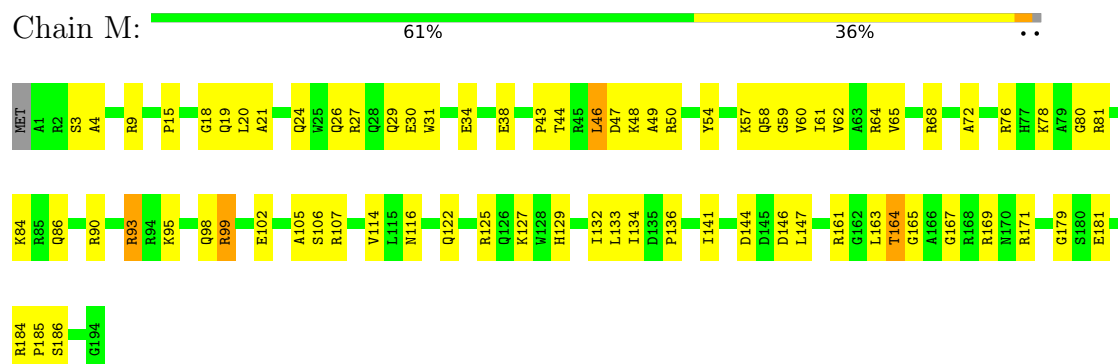
- Molecule 17: 50S RIBOSOMAL PROTEIN L14P



- Molecule 18: 50S RIBOSOMAL PROTEIN L15P

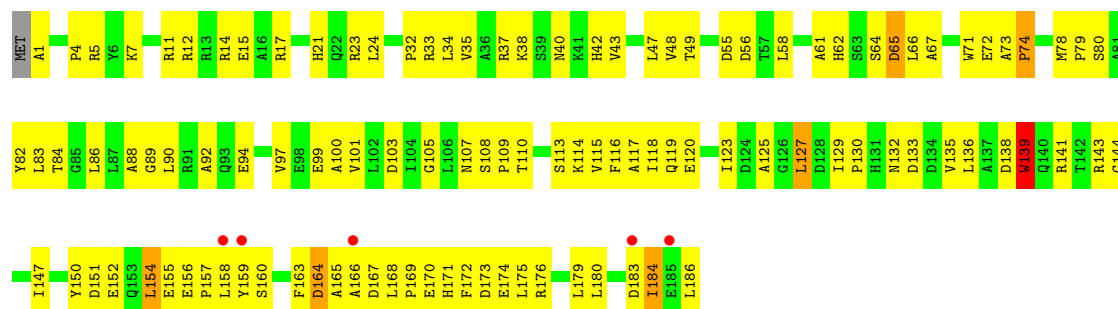


- Molecule 19: 50S RIBOSOMAL PROTEIN L15E



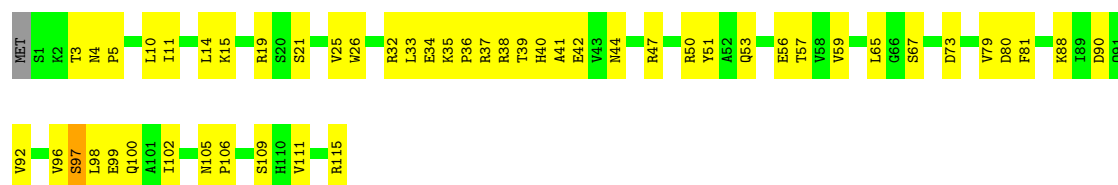
- Molecule 20: 50S RIBOSOMAL PROTEIN L18P





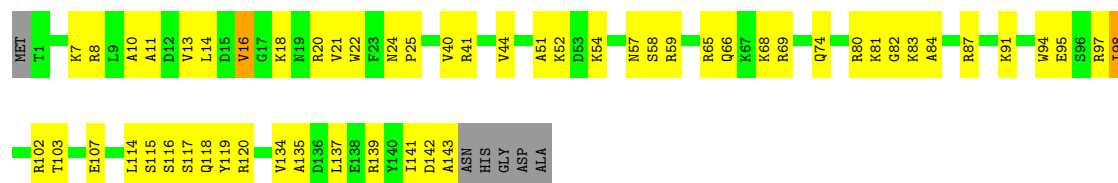
• Molecule 21: 50S RIBOSOMAL PROTEIN L18E

Chain O: 56% 42% ..



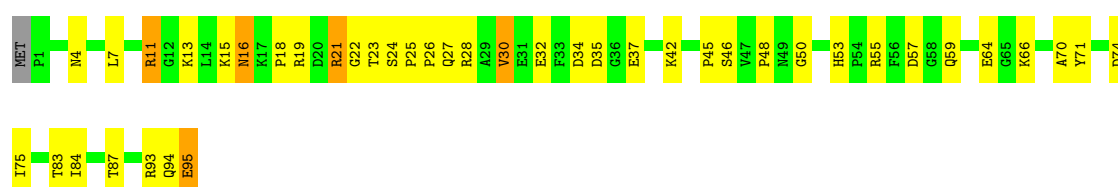
• Molecule 22: 50S RIBOSOMAL PROTEIN L19E

Chain P: 59% 36% ..



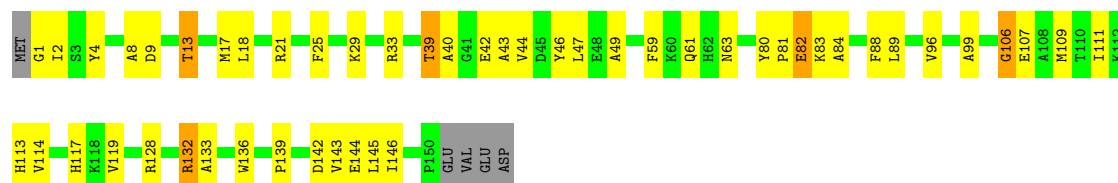
• Molecule 23: 50S RIBOSOMAL PROTEIN L21E

Chain Q: 55% 39% 5% .

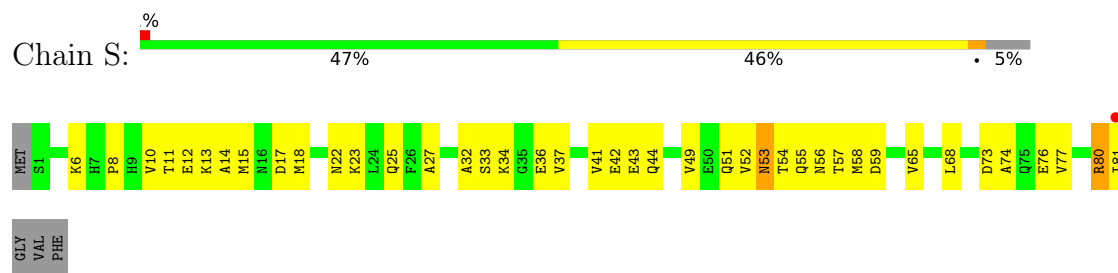


• Molecule 24: 50S RIBOSOMAL PROTEIN L22P

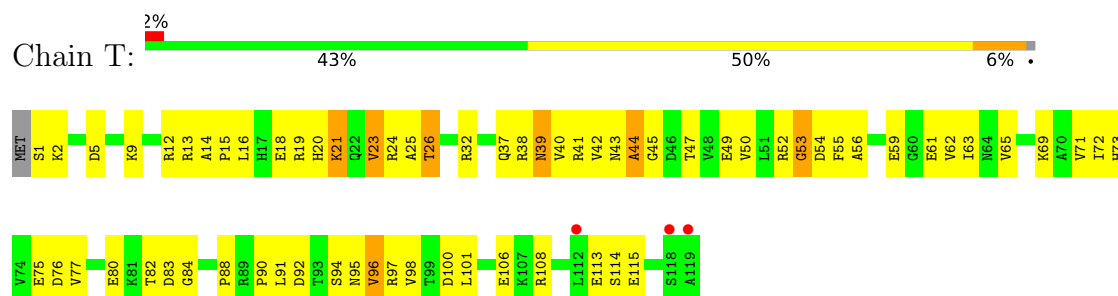
Chain R: 65% 29% ..



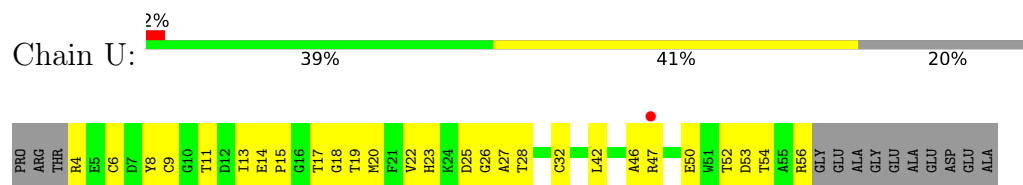
• Molecule 25: 50S RIBOSOMAL PROTEIN L23P



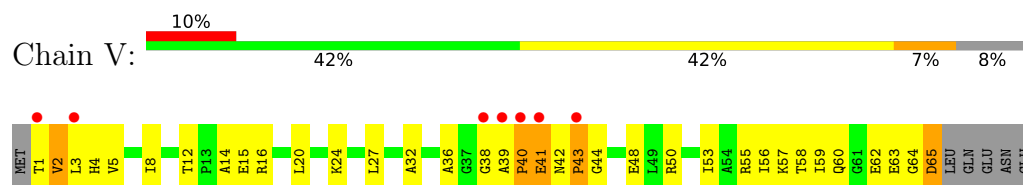
• Molecule 26: 50S RIBOSOMAL PROTEIN L24P



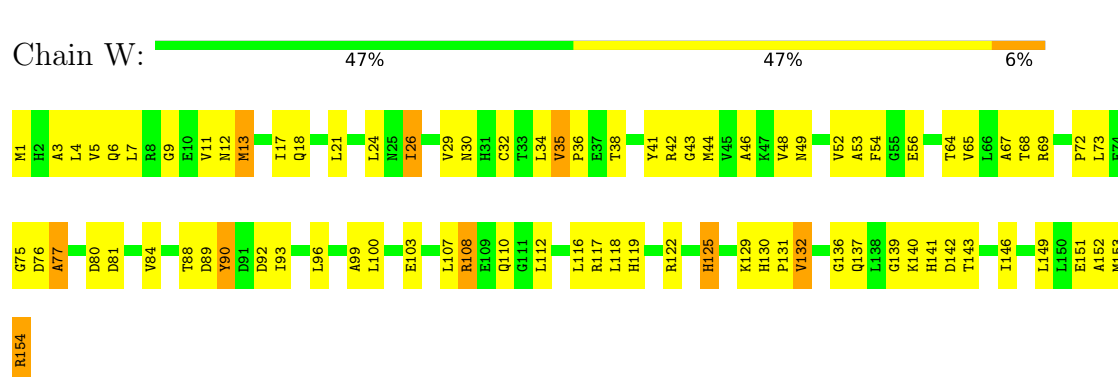
• Molecule 27: 50S RIBOSOMAL PROTEIN L24E



• Molecule 28: 50S RIBOSOMAL PROTEIN L29P

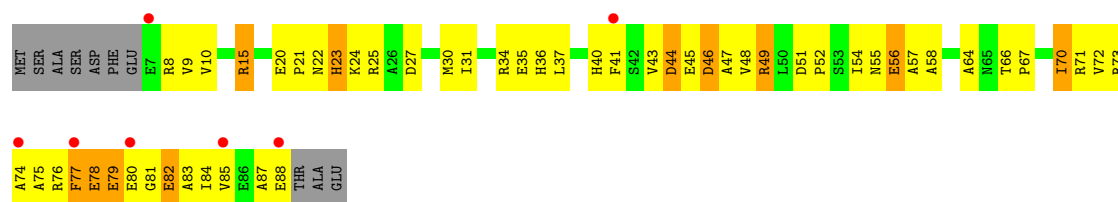


• Molecule 29: 50S RIBOSOMAL PROTEIN L30P

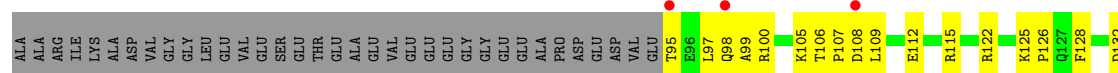
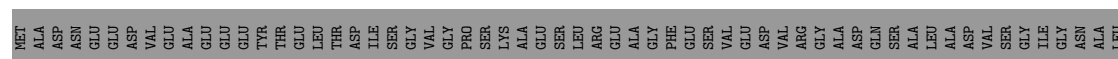
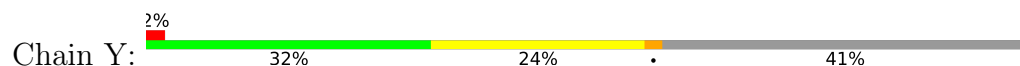


• Molecule 30: 50S RIBOSOMAL PROTEIN L31E





- 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 0.171 , 0.219	Depositor DCC
R_{free} test set	3279 reflections (0.98%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	63	0	50	0	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	0	109	0	0	0	0
33	3	1	0	0	0	0
33	4	1	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	0	2	0	0	0	0
35	0	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	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	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	4	10	0	14	1	0
39	0	5842	0	0	196	0
39	1	60	0	0	8	0
39	2	49	0	0	5	0
39	3	69	0	0	11	0
39	4	2	0	0	0	0
39	9	143	0	0	9	0
39	A	123	0	0	19	0
39	B	146	0	0	20	0
39	C	185	0	0	37	0
39	D	49	0	0	22	0
39	E	42	0	0	11	0
39	F	26	0	0	5	0
39	G	20	0	0	2	0
39	H	69	0	0	15	0
39	I	9	0	0	3	0
39	J	55	0	0	4	0
39	K	59	0	0	11	0
39	L	82	0	0	21	0
39	M	129	0	0	12	0
39	N	60	0	0	11	0
39	O	42	0	0	7	0
39	P	72	0	0	5	0
39	Q	48	0	0	7	0
39	R	85	0	0	6	0
39	S	30	0	0	5	0
39	T	39	0	0	8	0
39	U	29	0	0	3	0
39	V	13	0	0	3	0
39	W	69	0	0	12	0
39	X	26	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Y	101	0	0	16	0
39	Z	37	0	0	2	0
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:H5'	1:0:871:G:H8	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:H	10:D:154:LYS:HD2	1.18	1.03
1:0:871:G:H5'	1:0:871:G:C8	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	39:H:369: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''	39:0:4902: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:H	17:K:10:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:J:76:ASP:HA	39: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	39: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
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
17:K:10:GLN:H	17:K:10:GLN:HE21	0.91	0.90
6:9:14:G:H5'	6:9:14:G:H8	1.36	0.90
17:K:10:GLN:HE21	17:K:10:GLN:N	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:H5'	1:0:545:G:H8	1.39	0.88
6:9:76:G:H3'	6:9:77:A:H5''	1.54	0.88
29:W:72:PRO:HG2	29:W:77:ALA:HB3	1.53	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
9:C:115:LEU:HD21	9:C:243:VAL:HG13	1.56	0.88
26:T:71:VAL:HG11	26:T:90:PRO:HB3	1.56	0.88
29:W:21:LEU:HD13	29:W:26:ILE:HD11	1.56	0.88
20:N:47:LEU:HD11	20:N:127:LEU:HD21	1.54	0.88
21:O:42:GLU:HB2	39:O:4021:HOH:O	1.73	0.88
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
14:H:59:GLN:NE2	14:H:129:ARG:HE	1.71	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
39:O:9537:HOH:O	17:K:39:GLY:HA2	1.74	0.86
1:0:200:C:H2'	39:O:4592: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:M:99:ARG:HD2	19:M:167:GLY:HA2	1.58	0.85
9:C:236:THR:HA	39:C:522: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
1:0:1701:A:H4'	1:0:1702:U:H5''	1.59	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
17:K:81:ARG:HB2	17:K:87:ARG:NH1	1.92	0.84
26:T:9:LYS:HE3	26:T:13:ARG:NH1	1.92	0.84
8:B:201:ASP:HB2	8:B:312:ARG:HD2	1.60	0.84
1:0:2291:A:C8	1:0:2309:C:H5'	2.12	0.84
29:W:88:THR:HG22	29:W:89:ASP:H	1.42	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	39:L:358:HOH:O	1.78	0.82
1:0:1679:C:H5'	39:0:7104: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'	39:0:7360:HOH:O	1.78	0.81
39:0:8709:HOH:O	10:D:99:ASP:HA	1.79	0.81
8:B:217:ARG:HG3	8:B:257:THR:HG22	1.62	0.81
1:0:1878:G:H1'	39:0:8000:HOH:O	1.80	0.81
1:0:506:G:H22	1:0:509:A:C5'	1.93	0.81
1:0:282:C:H1'	1:0:368:C:N4	1.95	0.81
6:9:29:C:H2'	6:9:30:C:H5'	1.62	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

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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
11:E:97:VAL:HG12	39:E:4024:HOH:O	1.81	0.80
20:N:37:ARG:HH21	20:N:105:GLY:CA	1.94	0.80
1:0:1162:G:H1'	15:I:112:LEU:HD11	1.61	0.80
9:C:2:GLN:HB3	39:C:417:HOH:O	1.81	0.80
1:0:1184:C:H1'	39:0:6617:HOH:O	1.82	0.80
39:0:6579: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
17:K:63:GLU:HB2	39:K:4034:HOH:O	1.83	0.79
29:W:13:MET:HE1	29:W:18:GLN:HA	1.64	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
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
24:R:18:LEU:HB2	24:R:143:VAL:CG1	2.14	0.78
14:H:49:GLN:HG3	14:H:140:TYR:CE2	2.19	0.78
28:V:56:ILE:O	28:V:60:GLN:HG3	1.84	0.78
1:0:2890:A:H1'	27:U:56:ARG:NH2	1.98	0.78
22:P:59:ARG:HH22	22:P:66:GLN:HE22	1.28	0.78
1:0:1666:C:H2'	1:0:1667:A:H5'	1.66	0.78
1:0:1118:A:H8	1:0:1118:A:H3'	1.48	0.78
16:J:75:PRO:HG2	16:J:105:LEU:HD21	1.65	0.78
28:V:1:THR:HG23	28:V:2:VAL:H	1.49	0.78
1:0:470:U:O2'	2:1:16:HIS:HD2	1.66	0.77
12:F:46:GLU:OE1	12:F:100:ASP:HA	1.85	0.77
20:N:80:SER:HB2	39:N:4032:HOH:O	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:31:C:H2'	39:0:4091:HOH:O	1.84	0.77
12:F:91:VAL:HG12	12:F:92:GLY:N	2.00	0.77
8:B:248:ARG:O	8:B:251:VAL:HG22	1.85	0.77
30:X:71:ARG:HD3	39:X:4023:HOH:O	1.83	0.77
9:C:242:GLU:HG3	39:C:581:HOH:O	1.83	0.76
1:0:2908:A:H2'	1:0:2909:G:O4'	1.84	0.76
6:9:56:A:H2'	6:9:57:A:H5''	1.66	0.76
15:I:97:VAL:HG12	15:I:101:LYS:HE3	1.68	0.76
14:H:12:ILE:HG23	14:H:129:ARG:CZ	2.15	0.76
1:0:1163:G:H5'	15:I:110:ASP:O	1.85	0.76
1:0:1834:C:H2'	1:0:1840: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
7:A:191:GLY:HA2	7:A:194:MET:HE3	1.65	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
1:0:559:U:H6	1:0:559:U:H5'	1.49	0.76
1:0:1834:C:H2'	1:0:1840:A:H62	1.51	0.76
29:W:21:LEU:HD21	29:W:48:VAL:HG11	1.68	0.76
1:0:1701:A:H5'	39:0:7068:HOH:O	1.85	0.76
1:0:2780:C:H1'	11:E:143:GLN:HE21	1.51	0.76
8:B:140:LEU:HD23	39:B:559:HOH:O	1.86	0.76
8:B:320:GLN:HE21	8:B:321:PRO:HD2	1.47	0.76
17:K:30:LYS:O	17:K:55:VAL:HG13	1.86	0.76
1:0:182:G:H5'	39:0:4531:HOH:O	1.86	0.75
1:0:1293: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
1:0:1118:A:H3'	1:0:1118:A:C8	2.21	0.75
7:A:81:GLN:HB2	7:A:92:ASN:ND2	2.02	0.75
1:0:56:G:H5''	28:V:50:ARG:NH1	2.00	0.75
8:B:86:ALA:HA	39:B:559:HOH:O	1.85	0.75
12:F:96:ALA:HA	39:F:4009:HOH:O	1.86	0.75
29:W:21:LEU:HD21	29:W:48:VAL:CG1	2.15	0.75
8:B:18:ARG:HG3	8:B:256:GLN:HG3	1.67	0.75
1:0:545:G:H5'	1:0:545:G:C8	2.21	0.75
6:9:14:G:H5'	6:9:14:G:C8	2.20	0.75
19:M:164:THR:HG22	19:M:167:GLY:N	2.01	0.75
1:0:383:A:H4'	39:0:4914:HOH:O	1.86	0.75
20:N:113:SER:HB2	39:N:4044:HOH:O	1.86	0.75
1:0:1474:C:H5'	1:0:1474:C:C6	2.22	0.74
7:A:36:ASP:OD2	7:A:85:SER:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:27:ASN:HD22	8:B:27:ASN:H	1.34	0.74
8:B:321:PRO:HA	39:B:578:HOH:O	1.88	0.74
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
16:J:74:ARG:HH11	16:J:74:ARG:CB	1.99	0.74
31:Y:187:VAL:HG23	31:Y:192:ASP:CB	2.17	0.74
1:0:10:U:H3'	39:0:5221:HOH:O	1.85	0.74
1:0:1741:U:H5'	1:0:1742:A:OP1	1.87	0.74
10:D:99:ASP:HB3	10:D:103:ASN:H	1.52	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
4:3:25:VAL:HG22	4:3:68:LYS:HG3	1.68	0.74
6:9:48:C:H4'	20:N:141:ARG:NH2	2.03	0.74
9:C:236:THR:HG21	39:C:525:HOH:O	1.88	0.74
20:N:48:VAL:HG11	20:N:55:ASP:HB3	1.70	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	39:Q:223:HOH:O	1.88	0.73
1:0:711:G:H1'	39:0:5573:HOH:O	1.87	0.73
1:0:1667:A:H5'	1:0:1667:A:H8	1.54	0.73
1:0:2748:G:H2'	39:0:8252:HOH:O	1.89	0.73
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.73
29:W:151:GLU:O	29:W:154:ARG:HB3	1.88	0.73
18:L:143:THR:HG21	39:L:371:HOH:O	1.87	0.73
18:L:148:GLU:HA	39:L:376: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	39:V:4008:HOH:O	1.88	0.73
1:0:1130:U:H5'	39:0:6544:HOH:O	1.89	0.73
1:0:1884:G:O6	7:A:190:ARG:HD2	1.87	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
28:V:12:THR:HG22	28:V:15:GLU:CG	2.19	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
1:0:1603:A:H5'	1:0:1605:G:O4'	1.89	0.72
16:J:107:ASN:ND2	16:J:109:TYR:H	1.85	0.72
20:N:47:LEU:HD13	20:N:97:VAL:HG11	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:143:ALA:HA	39:P:272:HOH:O	1.88	0.72
1:O:1165:G:H4'	1:O:1174:A:O2'	1.89	0.72
14:H:6:ALA:HA	14:H:61:ARG:NH1	2.04	0.72
29:W:132:VAL:HG21	29:W:140:LYS:O	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
12:F:58:GLU:OE1	19:M:27:ARG:NH2	2.23	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
10:D:135:VAL:HG21	10:D:139:TYR:CD1	2.24	0.72
27:U:47:ARG:HG3	39:U:8826:HOH:O	1.90	0.72
1:O:1450:C:H4'	1:O:1451:C:OP2	1.88	0.71
6:9:48:C:H4'	20:N:141:ARG:HH21	1.55	0.71
1:O:821:U:H2'	1:O: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
1:O:694:A:H2'	1:O:695:C:H5'	1.72	0.71
6:9:54:A:O2'	6:9:55:U:H5'	1.90	0.71
6:9:114:G:O6	20:N:11:ARG:HD3	1.91	0.71
14:H:165:ARG:HD3	39:H:319:HOH:O	1.89	0.71
1:O:2270:G:H4'	7:A:223:ARG:HH12	1.55	0.71
8:B:36:PRO:HA	8:B:168:GLY:HA3	1.73	0.71
22:P:103:THR:O	22:P:107:GLU:HG3	1.91	0.71
1:O:2812:A:H2	1:O:2814:A:H62	1.37	0.71
8:B:212:GLN:HB2	8:B:257:THR:HG21	1.70	0.71
9:C:145:GLU:HG3	39:C:525:HOH:O	1.88	0.71
21:O:32:ARG:O	21:O:32:ARG:HD3	1.90	0.71
3:2:22:PRO:HG2	3:2:25:VAL:HG23	1.73	0.71
1:O:1819:G:H2'	1:O:1820:G:H4'	1.72	0.71
1:O:2320:U:H4'	1:O:2321:A:O4'	1.90	0.71
9:C:142:ASP:OD1	9:C:237:GLU:HB3	1.91	0.71
1:O: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
1:O:960:G:H4'	39:O:6208:HOH:O	1.90	0.70
9:C:233:THR:HG22	9:C:234:VAL:H	1.56	0.70
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:O:1206:U:H5'	1:O:1206:U:H6	1.56	0.70
29:W:137:GLN:HE21	29:W:141:HIS:HE1	1.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:259:G:H21	19:M:58:GLN:NE2	1.88	0.70
12:F:2:VAL:HG22	12:F:57:GLU:OE1	1.92	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
24:R:39:THR:HB	24:R:42:GLU:HG3	1.72	0.70
1:0:814:G:H4'	39:0:5765:HOH:O	1.90	0.70
1:0:1377:C:H5'	1:0:1377:C:H6	1.56	0.70
20:N:61:ALA:HB3	20:N:88:ALA:HB2	1.72	0.70
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.70
8:B:55:ASN:HB3	8:B:63:GLU:HA	1.74	0.70
8:B:162:MET:HE2	8:B:310:ARG:HD3	1.73	0.70
18:L:133:VAL:HA	39:L:375:HOH:O	1.91	0.70
1:0:2637:A:H5'	39:0:9419:HOH:O	1.91	0.70
25:S:51:GLN:HE21	25:S:53:ASN:HD21	1.40	0.70
30:X:72:VAL:HG22	30:X:85:VAL:CG1	2.19	0.70
12:F:63:ILE:HB	12:F:64:PRO:HD3	1.72	0.70
16:J:19:MET:HE2	16:J:79:PHE:HA	1.72	0.70
25:S:42:GLU:HG2	25:S:49:VAL:HG23	1.74	0.70
27:U:14:GLU:O	27:U:17:THR:HB	1.92	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
39:0:4849:HOH:O	26:T:53:GLY:HA3	1.92	0.69
7:A:68:ILE:HD11	39:A:443:HOH:O	1.92	0.69
16:J:107:ASN:C	16:J:107:ASN:HD22	1.95	0.69
17:K:29:LEU:HB3	17:K:55:VAL:HG11	1.73	0.69
1:0:558:C:O2'	1:0:559:U:H5''	1.92	0.69
1:0:2783:A:H3'	39:0:9678:HOH:O	1.93	0.69
29:W:88:THR:HG23	29:W:110:GLN:HE21	1.58	0.69
30:X:43:VAL:HG11	30:X:82:GLU:HA	1.74	0.69
1:0:1187:U:H2'	39:0:6627:HOH:O	1.92	0.69
9:C:246:ARG:HD2	39:C:584:HOH:O	1.93	0.69
1:0:57:C:H5''	39:0:4173:HOH:O	1.93	0.68
32:Z:26:VAL:O	32:Z:30:GLU:HG3	1.93	0.68
7:A:94:LEU:HG	7:A:99:ILE:HD11	1.75	0.68
15:I:101:LYS:O	15:I:105:GLU:HG3	1.94	0.68
18:L:35:ARG:HB2	18:L:35:ARG:NH1	2.08	0.68
24:R:119:VAL:HG21	24:R:142:ASP:CG	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2506:A:O2'	1:0:2507:G:H8	1.75	0.68
7:A:200:PRO:HD3	39:A:513:HOH:O	1.92	0.68
1:0:2426:G:H1'	39:0:8683:HOH:O	1.92	0.68
12:F:61:MET:HB3	19:M:19:GLN:OE1	1.93	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
7:A:199:HIS:HD2	7:A:201:PHE:H	1.42	0.68
29:W:5:VAL:HG11	29:W:153:MET:HE3	1.74	0.68
32:Z:37:HIS:HB2	32:Z:47:VAL:HB	1.75	0.68
1:0:214:U:H5'	39:0:4638: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
8:B:304:PRO:HD2	8:B:307:ARG:HD2	1.76	0.68
15:I:118:ASN:HA	15:I:121:LYS:HD2	1.75	0.68
17:K:74:VAL:CG1	17:K:113:ILE:HG12	2.22	0.68
27:U:17:THR:HG22	27:U:18:GLY:N	2.07	0.68
32:Z:57:CYS:SG	32:Z:59:TYR:HB3	2.32	0.68
1:0:447:A:P	26:T:1:SER:HB2	2.34	0.68
39:0:4764:HOH:O	19:M:58:GLN:HG3	1.93	0.68
7:A:51:ARG:HB2	39:A:435:HOH:O	1.94	0.68
24:R:8:ALA:HB1	24:R:13:THR:HG21	1.74	0.68
7:A:88:ILE:O	7:A:88:ILE:HG22	1.92	0.68
10:D:25:MET:HE3	10:D:37:ALA:CB	2.20	0.68
17:K:13:GLU:OE2	17:K:44:LEU:HB2	1.93	0.68
29:W:88:THR:HG22	29:W:89:ASP:N	2.08	0.68
1:0:450:C:OP1	9:C:184:ARG:NH2	2.24	0.68
1:0:1189:A:H1'	1:0:1209:C:O4'	1.94	0.68
8:B:141:ARG:HD2	8:B:163:GLU:OE2	1.94	0.68
10:D:154:LYS:HD2	10:D:154:LYS:N	2.02	0.68
1:0:21:G:H5''	24:R:1:GLY:O	1.95	0.67
9:C:61:PHE:HB3	39:C:459:HOH:O	1.93	0.67
29:W:84:VAL:HG12	39:W:4041:HOH:O	1.93	0.67
1:0:1157:C:H2'	1:0:1158:G:H8	1.56	0.67
1:0:2533:C:H5'	1:0:2533:C:C6	2.28	0.67
10:D:65:GLU:HA	39:D:225:HOH:O	1.93	0.67
24:R:96:VAL:HG13	24:R:106:GLY:HA3	1.75	0.67
1:0:1417:G:O2'	3:2:11:LEU:HD22	1.94	0.67
11:E:137:ASP:OD1	11:E:139:GLU:HB2	1.94	0.67
18:L:136:ALA:HB3	39:L:375:HOH:O	1.94	0.67
8:B:162:MET:CE	8:B:308:LEU:HD21	2.23	0.67
9:C:132:ASP:HB3	39:C:516:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:84:LEU:HA	10:D:87:ALA:HB3	1.74	0.67
10:D:146:LYS:HZ3	20:N:107:ASN:HD21	1.42	0.67
18:L:67:ARG:O	18:L:71:GLU:HG3	1.95	0.67
1:O:1160:G:O2'	1:O:1190:G:H1'	1.95	0.67
1:O: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
2:1:21:ARG:HD2	2:1:37:CYS:SG	2.35	0.67
10:D:159:PRO:O	10:D:163:VAL:HG23	1.94	0.67
1:O:1654:U:H2'	7:A:47:HIS:HD2	1.59	0.67
1:O:2635:A:O2'	1:O:2636:C:H5'	1.95	0.67
4:3:70:ARG:HG2	4:3:77:ALA:HB2	1.77	0.67
8:B:140:LEU:HA	39:B:559:HOH:O	1.94	0.67
16:J:107:ASN:HD21	16:J:109:TYR:HB2	1.60	0.67
1:O:111:C:O2'	2:1:20:ARG:HG2	1.94	0.67
1:O:2524:G:H21	1:O:2526:C:N4	1.92	0.67
8:B:139:ASP:HB2	8:B:165:ARG:HE	1.60	0.67
10:D:146:LYS:NZ	20:N:107:ASN:ND2	2.43	0.67
17:K:34:VAL:HG22	17:K:47:ALA:HB2	1.77	0.67
19:M:99:ARG:CD	19:M:167:GLY:HA2	2.24	0.67
17:K:132:VAL:HG11	27:U:22:VAL:HG22	1.76	0.67
19:M:78:LYS:HE2	39:M:358:HOH:O	1.95	0.67
29:W:80:ASP:O	29:W:84:VAL:HG23	1.95	0.67
1:O:338:C:H4'	9:C:174:ILE:CD1	2.25	0.66
1:O:542:A:H5'	1:O:542:A:C8	2.27	0.66
1:O:1189:A:H1'	1:O:1209:C:C1'	2.25	0.66
1:O:1790:C:H2'	1:O:1791:U:H6	1.60	0.66
7:A:211:LYS:HB3	7:A:212:PRO:HD2	1.76	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
29:W:5:VAL:HG11	29:W:153:MET:CE	2.26	0.66
1:O:871:G:H8	1:O:871:G:C5'	1.99	0.66
7:A:64:ASP:OD1	7:A:66:ARG:HD2	1.95	0.66
16:J:6:PHE:HB3	16:J:109:TYR:OH	1.94	0.66
20:N:164:ASP:CG	20:N:167:ASP:HA	2.16	0.66
1:O:21:G:H4'	24:R:2:ILE:HG22	1.78	0.66
1:O:1593:C:OP1	22:P:117:SER:HB3	1.96	0.66
8:B:62:ARG:HA	8:B:65:MET:CE	2.23	0.66
9:C:180:SER:HB2	39:C:534:HOH:O	1.94	0.66
11:E:132:THR:HB	39:E:4031:HOH:O	1.95	0.66
14:H:23:ILE:HG23	14:H:123:ILE:HD11	1.77	0.66
17:K:28:GLU:HG2	17:K:58:THR:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:64:GLY:O	28:V:65:ASP:HB2	1.96	0.66
31:Y:151:SER:HB3	31:Y:154:ARG:HB3	1.78	0.66
1:O:2508:C:H2'	39:O:9086:HOH:O	1.95	0.66
1:O:657:G:OP1	9:C:27:ARG:NH2	2.28	0.66
1:O:1666:C:O2'	1:O:1667:A:H5''	1.95	0.66
21:O:21:SER:OG	21:O:106:PRO:HB2	1.94	0.66
29:W:129:LYS:HG2	39:W:4056:HOH:O	1.96	0.66
1:O:1121:G:H4'	39:O:6523:HOH:O	1.94	0.66
9:C:139:VAL:HG13	39:C:580:HOH:O	1.95	0.66
10:D:64:ARG:HB3	10:D:67:ASP:OD2	1.95	0.66
1:O:1007:A:H2'	14:H:22:TYR:CZ	2.31	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
20:N:120:GLU:HG3	20:N:136:LEU:HD13	1.76	0.66
23:Q:26:PRO:O	23:Q:30:VAL:HG23	1.95	0.66
3:2:22:PRO:HG2	3:2:25:VAL:CG2	2.25	0.66
20:N:37:ARG:HD3	36:N:201:CL:CL	2.32	0.66
22:P:65:ARG:HD3	22:P:69:ARG:NH1	2.10	0.66
1:O:1372:A:H3'	39:O:6994:HOH:O	1.95	0.66
1:O:1615:A:H4'	39:O:7429:HOH:O	1.95	0.66
14:H:49:GLN:HB2	14:H:170:ARG:HD2	1.77	0.66
17:K:22:ASP:HB2	39:K:4013:HOH:O	1.96	0.66
4:3:62:THR:HB	39:3:248:HOH:O	1.95	0.65
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
1:O:447:A:OP1	26:T:2:LYS:HG2	1.97	0.65
1:O:1053:G:OP1	14:H:15:PRO:HG3	1.96	0.65
1:O:2414:A:H2'	1:O:2415:A:C8	2.29	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
20:N:78:MET:HB2	20:N:79:PRO:HD3	1.78	0.65
22:P:134:VAL:O	22:P:137:LEU:HB3	1.95	0.65
1:O:513:A:N3	39:O:5181:HOH:O	2.29	0.65
3:2:49:GLU:HB2	39:2:145:HOH:O	1.94	0.65
14:H:12:ILE:O	14:H:12:ILE:HG22	1.96	0.65
1:O:541:C:C2'	1:O:542:A:H5''	2.26	0.65
2:1:46:ARG:HA	39:1:246:HOH:O	1.96	0.65
9:C:5:ILE:HD11	9:C:16:VAL:CG2	2.27	0.65
28:V:55:ARG:O	28:V:59:ILE:HG12	1.95	0.65
1:O:645:U:OP2	18:L:4:LYS:HE2	1.96	0.65
7:A:121:ALA:O	7:A:124:VAL:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:47:ARG:HH11	21:O:47:ARG:HG3	1.61	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
1:O:2850:C:H6	1:O:2850:C:H5'	1.62	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:447:A:OP2	26:T:1:SER:HB2	1.97	0.65
39:O:6613:HOH:O	15:I:87:PRO:HD3	1.96	0.65
10:D:35:ALA:HB1	39:D:218:HOH:O	1.95	0.65
23:Q:66:LYS:HB2	23:Q:70:ALA:O	1.97	0.65
25:S:77:VAL:O	25:S:80:ARG:HG2	1.97	0.65
7:A:109:GLU:HG2	7:A:116:GLY:H	1.61	0.65
11:E:118:ILE:HG23	11:E:144:THR:HG21	1.79	0.65
16:J:103:VAL:HG12	39:J:4028:HOH:O	1.97	0.65
18:L:22:ARG:HG2	39:L:329:HOH:O	1.96	0.65
1:O:272:A:H5'	1:O:273:G:OP2	1.96	0.65
7:A:66:ARG:HH11	7:A:66:ARG:HB2	1.61	0.65
21:O:10:LEU:HD13	21:O:99:GLU:HG3	1.79	0.65
39:O:7889:HOH:O	2:1:1:THR:HB	1.96	0.65
11:E:22:VAL:O	11:E:76:VAL:HG11	1.97	0.65
1:O:281:U:H2'	1:O:282:C:O4'	1.97	0.64
17:K:74:VAL:HG13	17:K:113:ILE:HG23	1.79	0.64
18:L:35:ARG:HB2	18:L:35:ARG:HH11	1.61	0.64
1:O:2769:C:C2'	1:O:2770:G:H5'	2.27	0.64
10:D:35:ALA:C	10:D:37:ALA:H	1.99	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
4:3:87:ARG:HD2	4:3:89:GLU:OE2	1.98	0.64
20:N:67:ALA:HA	20:N:71:TRP:HB3	1.80	0.64
20:N:139:TRP:HA	20:N:139:TRP:CE3	2.31	0.64
29:W:137:GLN:HE21	29:W:141:HIS:CE1	2.15	0.64
17:K:75:ARG:CZ	39:K:4039:HOH:O	2.45	0.64
1:O:709:G:O2'	21:O:25:VAL:HG12	1.97	0.64
11:E:100:ASP:HB2	39:E:4025:HOH:O	1.96	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
19:M:64:ARG:HD2	39:M:325:HOH:O	1.97	0.64
8:B:7:ARG:NH1	8:B:11:LEU:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:132:ASN:O	20:N:135:VAL:HG12	1.98	0.64
1:O:259:G:H21	19:M:58:GLN:HE22	1.45	0.64
7:A:217:ARG:HG2	7:A:229:ALA:HB2	1.80	0.64
11:E:81:GLU:HG2	11:E:134:SER:HB3	1.79	0.64
14:H:100:GLU:HB3	14:H:124:VAL:HG11	1.78	0.64
1:O:1116:U:O2'	1:O:1118:A:H2	1.73	0.63
1:O:1119:G:N2	1:O:1246:A:C2	2.64	0.63
1:O:2524:G:H21	1:O:2526:C:H41	1.44	0.63
1:O:2807:U:P	8:B:27:ASN:HD21	2.21	0.63
6:9:20:G:H3'	39:9:323:HOH:O	1.98	0.63
8:B:162:MET:HG3	8:B:310:ARG:HD3	1.80	0.63
29:W:90:TYR:N	29:W:90:TYR:CD1	2.65	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
27:U:46:ALA:HB1	27:U:52:THR:HG21	1.80	0.63
30:X:37:LEU:CD1	30:X:85:VAL:HG21	2.27	0.63
30:X:71:ARG:HB3	30:X:88:GLU:OE1	1.99	0.63
1:O:280:C:H2'	1:O:281:U:O4'	1.99	0.63
11:E:133:VAL:HG12	11:E:141:VAL:HG13	1.80	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
18:L:72:ASN:HB2	39:L:351:HOH:O	1.98	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
29:W:4:LEU:CD2	29:W:54:PHE:HB3	2.25	0.63
30:X:76:ARG:O	30:X:77:PHE:HB3	1.97	0.63
7:A:211:LYS:HB2	39:A:504:HOH:O	1.97	0.63
18:L:121:ILE:HG12	18:L:141:GLU:HB2	1.79	0.63
20:N:139:TRP:HA	20:N:139:TRP:HE3	1.63	0.63
23:Q:18:PRO:O	23:Q:21:ARG:HB2	1.98	0.63
30:X:21:PRO:HG2	30:X:24:LYS:HD3	1.81	0.63
8:B:5:ARG:NH1	8:B:8:LYS:HE2	2.14	0.63
1:O:588:G:O6	29:W:154:ARG:NH1	2.32	0.63
1:O:1164:U:OP1	15:I:69:PRO:HA	1.98	0.63
1:O: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
29:W:13:MET:HE3	29:W:17:ILE:HG22	1.81	0.63
1:O:1751:G:C2'	1:O:1752:G:H5''	2.29	0.63
14:H:114:ASP:HB2	39:H:346:HOH:O	1.98	0.63
26:T:43:ASN:ND2	26:T:108:ARG:CZ	2.62	0.63
1:O:603:A:H5''	1:O:604:G:OP1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1641:A:H2'	1:0:1642:A:H5'	1.81	0.63
1:0:338:C:H4'	9:C:174:ILE:HD11	1.81	0.62
1:0:1819:G:H5'	39:0:7788:HOH:O	1.98	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
14:H:49:GLN:HB3	14:H:170:ARG:HG3	1.80	0.62
25:S:53:ASN:HD22	25:S:53:ASN:N	1.96	0.62
29:W:81:ASP:OD1	29:W:92:ASP:HB2	1.99	0.62
1:0:2547:C:OP2	8:B:5:ARG:NH1	2.32	0.62
16:J:19:MET:HE1	16:J:132:LEU:HD21	1.81	0.62
1:0:541:C:H2'	1:0:542:A:C5'	2.29	0.62
13:G:71:LEU:C	13:G:73:ASP:H	2.01	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
1:0:2276:U:H5'	39:0:4469:HOH:O	1.99	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
1:0:1348:A:H3'	39:0:6915:HOH:O	1.99	0.62
1:0:1666:C:C2'	1:0:1667:A:H5'	2.30	0.62
39:3:235: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
8:B:264:GLU:HG2	8:B:267:LYS:CE	2.22	0.62
1:0:138:U:OP2	1:0:139:C:H5	1.83	0.62
6:9:56:A:C2'	6:9:57:A:H5''	2.29	0.62
10:D:104:PHE:CE2	10:D:132:VAL:HB	2.35	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
20:N:58:LEU:N	20:N:58:LEU:HD12	2.15	0.62
22:P:98:ILE:HD12	22:P:102:ARG:NE	2.14	0.62
6:9:35:C:H5''	39:9:348:HOH:O	1.99	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
16:J:99:GLU:HA	39:J:4030:HOH:O	1.98	0.62
16:J:130:VAL:HG12	16:J:131:THR:N	2.12	0.62
14:H:57:THR:HA	14:H:130:VAL:O	2.00	0.62
14:H:61:ARG:HH11	14:H:61:ARG:HG3	1.63	0.62
20:N:73:ALA:HB1	20:N:74:PRO:CD	2.30	0.62
25:S:33:SER:OG	25:S:36:GLU:HG3	2.00	0.62
1:0:1242:A:H5'	16:J:82:THR:CG2	2.28	0.62
1:0:2862:G:H4'	8:B:336:GLN:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:145:HIS:HD2	8:B:146:THR:O	1.83	0.62
9:C:140:VAL:HB	39:C:522:HOH:O	2.00	0.62
11:E:21:THR:HG23	11:E:30:THR:OG1	1.99	0.62
28:V:44:GLY:O	28:V:48:GLU:HG2	1.99	0.62
29:W:4:LEU:HD22	29:W:52:VAL:CG2	2.26	0.62
1:O:1328:A:OP1	31:Y:169:ARG:HD2	2.00	0.62
1:O:2766:A:H5'	39:O:9658: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	39:A:505:HOH:O	1.99	0.62
19:M:125:ARG:NH1	39:M:390:HOH:O	2.32	0.62
31:Y:235:GLU:CD	31:Y:235:GLU:H	2.02	0.62
1:O:2420:G:O2'	1:O:2421:G:H5'	1.99	0.61
4:3:74:CYS:N	39:3:258:HOH:O	2.31	0.61
8:B:41:PHE:HA	8:B:79:MET:HE2	1.80	0.61
21:O:73:ASP:HA	21:O:92:VAL:O	2.00	0.61
1:O:1717:A:H5''	22:P:54:LYS:HB2	1.82	0.61
17:K:62:PRO:HG3	17:K:65:ARG:HH21	1.65	0.61
18:L:143:THR:HG22	18:L:144:ASP:N	2.15	0.61
22:P:14:LEU:HD13	22:P:51:ALA:HB2	1.80	0.61
22:P:20:ARG:HH12	22:P:54:LYS:HD3	1.64	0.61
28:V:57:LYS:HA	28:V:60:GLN:HE21	1.65	0.61
29:W:13:MET:CE	29:W:17:ILE:HG22	2.30	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
1:O:541:C:H2'	1:O:542:A:H5''	1.82	0.61
1:O:1234:U:N3	8:B:244:PRO:HB3	2.15	0.61
26:T:69:LYS:O	26:T:71:VAL:HG23	2.00	0.61
1:O:621:C:H5'	31:Y:132:ASP:OD2	2.01	0.61
1:O:2756:U:N3	1:O:2896:A:H2	1.96	0.61
39:O:7475:HOH:O	7:A:165:THR:HG23	2.00	0.61
1:O:2453:G:H3'	39:O:8942:HOH:O	2.01	0.61
4:3:55:VAL:HB	4:3:56:PRO:HD2	1.83	0.61
8:B:202:VAL:HG11	8:B:301:VAL:HG13	1.81	0.61
11:E:11:VAL:HG12	11:E:12:ASP:N	2.14	0.61
18:L:53:ARG:NH2	18:L:57:VAL:HG12	2.16	0.61
19:M:30:GLU:O	19:M:34:GLU:HG3	2.01	0.61
29:W:21:LEU:HB3	29:W:26:ILE:HG12	1.83	0.61
9:C:150:THR:HA	9:C:203:ALA:O	2.00	0.61
18:L:61:ALA:HA	39:L:365:HOH:O	2.01	0.61
18:L:143:THR:HG22	18:L:145:LEU:H	1.66	0.61
1:O:602:A:O2'	1:O: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'	39:0:8068:HOH:O	1.99	0.61
1:0:2472:C:O2'	1:0:2634:G:H4'	2.00	0.61
9:C:188:ARG:HD3	39:C:558:HOH:O	2.00	0.61
14:H:49:GLN:HG3	14:H:140:TYR:CD2	2.35	0.61
26:T:55:PHE:CD2	26:T:77:VAL:HG13	2.35	0.61
29:W:6:GLN:HG2	29:W:29:VAL:HA	1.82	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.61
1:0:2036:C:C1'	17:K:44:LEU:HG	2.30	0.61
8:B:294:TYR:HE2	39:B:629: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
29:W:65:VAL:CG1	29:W:116:LEU:HD13	2.30	0.61
1:0:1544:U:H2'	1:0:1545:C:H6	1.66	0.60
1:0:2004:U:H4'	39:0:8178:HOH:O	2.00	0.60
39:0:7680:HOH:O	8:B:254:GLN:HG3	2.00	0.60
39:0:9805:HOH:O	27:U:56:ARG:HD3	2.01	0.60
2:1:25:LYS:HE2	39:2:147:HOH:O	2.00	0.60
1:0:308:U:C4	1:0:342:C:H1'	2.36	0.60
1:0:660:A:H4'	1:0:661:G:O5'	2.01	0.60
1:0:794:U:H3	1:0:819:A:H61	1.49	0.60
8:B:80:ARG:HD3	39:B:572:HOH:O	2.02	0.60
8:B:154:VAL:HG12	8:B:156:LYS:HG2	1.83	0.60
8:B:195:ARG:HG2	8:B:323:LEU:HD22	1.82	0.60
13:G:27:ILE:HD13	13:G:71:LEU:HD23	1.82	0.60
24:R:111:ILE:HG23	24:R:145:LEU:HD11	1.83	0.60
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.60
8:B:74:ILE:HG13	39:B:539:HOH:O	2.00	0.60
15:I:84:SER:HB3	15:I:92:VAL:CG2	2.32	0.60
16:J:133:GLY:O	16:J:137:GLU:HG3	2.00	0.60
1:0:2445:U:H2'	1:0:2446:G:C8	2.37	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
8:B:66:GLU:OE1	8:B:328:ARG:HD2	2.00	0.60
11:E:3:VAL:HG22	11:E:49:ILE:HB	1.81	0.60
14:H:23:ILE:HG23	14:H:123:ILE:CD1	2.31	0.60
24:R:47:LEU:HB2	24:R:89:LEU:HD21	1.83	0.60
26:T:43:ASN:HD22	26:T:108:ARG:NH2	1.98	0.60
26:T:73:HIS:HD2	26:T:88:PRO:HG3	1.66	0.60
1:0:470:U:O2'	2:1:16:HIS:CD2	2.53	0.60
1:0:544:G:C3'	1:0:545:G:H5''	2.32	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)
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
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.60
8:B:217:ARG:HG3	8:B:257:THR:CG2	2.30	0.60
15:I:108:HIS:N	15:I:109:PRO:HD2	2.16	0.60
16:J:75:PRO:HG2	16:J:105:LEU:CD2	2.32	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
19:M:15:PRO:HA	19:M:20:LEU:HD23	1.84	0.60
22:P:8:ARG:HG3	39:P:208:HOH:O	2.02	0.60
1:0:1058:A:H2'	1:0:1060:C:H5''	1.84	0.60
4:3:65:THR:HG23	4:3:67:LEU:HG	1.84	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
31:Y:189:ASN:ND2	31:Y:192:ASP:H	2.00	0.60
1:0:1400:C:H4'	30:X:56:GLU:HG2	1.83	0.60
1:0:1768:C:H2'	1:0:1769:C:O4'	2.02	0.60
1:0:2248:C:H3'	39:0:8518:HOH:O	2.01	0.60
26:T:24:ARG:HH21	26:T:39:ASN:ND2	1.99	0.60
31:Y:105:LYS:HE2	31:Y:198:GLY:O	2.02	0.60
1:0:2112:A:H2'	1:0:2113:G:H8	1.67	0.59
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
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
29:W:125:HIS:HE1	39:W:4003:HOH:O	1.85	0.59
1:0:2382:A:H5'	39:0:8765:HOH:O	2.01	0.59
39:9:357:HOH:O	20:N:147:ILE:HD12	2.01	0.59
13:G:23:ILE:O	13:G:27:ILE:HG13	2.02	0.59
20:N:154:LEU:C	20:N:156:GLU:H	2.05	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
1:0:820: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
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
1:0:1379:A:H1'	39:0:7015:HOH:O	2.01	0.59
1:0:2679:G:H2'	1:0:2681:A:OP2	2.03	0.59
1:0:2827:A:H2'	1:0:2828:G:O4'	2.02	0.59
6:9:28:U:H5''	20:N:40:ASN:HD21	1.66	0.59
8:B:57:GLU:O	8:B:63:GLU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:107:ASN:HD22	16:J:109:TYR:H	1.50	0.59
18:L:30:ARG:NH2	39:L:332:HOH:O	2.35	0.59
20:N:37:ARG:CZ	39:N:4040:HOH:O	2.49	0.59
1:O:90:A:H2'	1:O:91:G:O4'	2.03	0.59
7:A:43:VAL:HG21	7:A:59:GLU:HG3	1.84	0.59
13:G:16:LYS:O	13:G:20:VAL:HG23	2.02	0.59
18:L:114:VAL:HG11	39:L:375:HOH:O	2.02	0.59
21:O:38:ARG:NH1	39:O:4017:HOH:O	2.35	0.59
22:P:80:ARG:HG2	22:P:87:ARG:CZ	2.33	0.59
26:T:41:ARG:HG2	26:T:41:ARG:HH11	1.66	0.59
1:O:407:A:H5'	39:O:4968:HOH:O	2.03	0.59
1:O:583:C:H2'	1:O:584:U:C6	2.38	0.59
8:B:85:ARG:NH1	39:B:546:HOH:O	2.35	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:O:2521:A:OP2	14:H:6:ALA:HB3	2.02	0.59
7:A:37:VAL:HG22	39:A:431:HOH:O	2.02	0.59
12:F:91:VAL:CG1	12:F:92:GLY:N	2.66	0.59
26:T:43:ASN:HD22	26:T:108:ARG:CZ	2.16	0.59
28:V:5:VAL:HG23	39:V:4002:HOH:O	2.02	0.59
1:O:2851:G:O2'	1:O:2852:A:H5'	2.03	0.59
12:F:69:GLU:O	12:F:70:LYS:HG2	2.03	0.59
14:H:168:VAL:HG13	39:H:324:HOH:O	2.02	0.59
18:L:35:ARG:NH1	18:L:43:HIS:HB3	2.17	0.59
1:O:1377:C:H5'	1:O:1377:C:C6	2.38	0.59
1:O:1477:C:H5'	1:O:1868:G:C5'	2.33	0.59
8:B:125:GLU:O	8:B:129:ARG:HG3	2.01	0.59
9:C:107:ARG:NE	39:C:504:HOH:O	2.23	0.59
14:H:72:ALA:HB2	14:H:156:ALA:HB2	1.85	0.59
18:L:62:ALA:HB2	18:L:103:ALA:CB	2.33	0.59
19:M:134:ILE:HG23	19:M:141:ILE:HD13	1.84	0.59
21:O:41:ALA:HA	39:O:4020:HOH:O	2.02	0.59
1:O:1835:U:C5	1:O:1840:A:N7	2.68	0.58
1:O:2559:C:H4'	39:O:9699:HOH:O	2.02	0.58
20:N:38:LYS:HD2	20:N:114:LYS:HE3	1.83	0.58
30:X:76:ARG:HG3	30:X:76:ARG:NH1	2.18	0.58
18:L:144:ASP:HA	18:L:147:GLU:HG3	1.84	0.58
19:M:80:GLY:O	19:M:81:ARG:HD2	2.02	0.58
27:U:4:ARG:N	39:U:8801:HOH:O	2.35	0.58
29:W:35:VAL:HG23	29:W:41:TYR:CD2	2.38	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
1:0:547:A:H3'	39:0:5256:HOH:O	2.02	0.58
9:C:246:ARG:HB3	9:C:246:ARG:NH1	2.18	0.58
20:N:86:LEU:O	20:N:90:LEU:HG	2.03	0.58
22:P:135:ALA:HB1	22:P:139:ARG:HH12	1.67	0.58
24:R:39:THR:HB	24:R:42:GLU:CG	2.33	0.58
31:Y:141:THR:HG23	39:Y:449:HOH:O	2.01	0.58
1:0:1213:C:O2'	1:0:1214:G:H5'	2.03	0.58
11:E:10:ASP:HA	39:E:4004:HOH:O	2.03	0.58
22:P:7:LYS:HD3	22:P:21:VAL:CG2	2.33	0.58
31:Y:234:VAL:HG12	31:Y:235:GLU:N	2.18	0.58
1:0:1189:A:H1'	1:0:1209:C:H1'	1.86	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
1:0:2852:A:H5''	39:0:9773:HOH:O	2.03	0.58
10:D:44:ILE:HG23	10:D:45:THR:HG23	1.85	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
1:0:506:G:H22	1:0:509:A:H5''	1.66	0.58
1:0:603:A:H1'	1:0:605:C:C2	2.38	0.58
1:0:1157:C:H2'	1:0:1158:G:C8	2.36	0.58
1:0:2073:G:OP2	1:0:2490:A:H5'	2.04	0.58
1:0:2721:U:H4'	17:K:87:ARG:HG3	1.86	0.58
1:0:2904:U:H4'	30:X:8:ARG:NH1	2.19	0.58
8:B:217:ARG:CG	8:B:257:THR:HG22	2.32	0.58
8:B:238:ASN:HD22	8:B:240:GLY:H	1.52	0.58
10:D:91:ALA:HB1	39:D:233:HOH:O	2.03	0.58
10:D:163:VAL:HA	39:D:247:HOH:O	2.03	0.58
14:H:31:ILE:HA	14:H:66:GLU:OE1	2.04	0.58
1:0:656:G:OP2	21:O:37:ARG:HD2	2.04	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
39:0:8081:HOH:O	7:A:213:LYS:HB2	2.04	0.58
7:A:33:GLU:O	7:A:34:ASP:HB2	2.04	0.58
8:B:74:ILE:HD13	8:B:309:VAL:HG21	1.86	0.58
28:V:1:THR:HG23	28:V:2:VAL:N	2.19	0.58
1:0:962:C:H5''	39:0:6215:HOH:O	2.03	0.58
1:0:1060:C:H6	1:0:1060:C:H5'	1.68	0.58
1:0:1118:A:H62	1:0:1244:U:H3	1.51	0.58
1:0:1790:C:H2'	1:0:1791:U:C6	2.37	0.58
1:0:1862:C:H1'	39:0:7955:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:4090:HOH:O	26:T:9:LYS:HB2	2.04	0.58
10:D:41:LEU:HA	10:D:44:ILE:HG22	1.86	0.58
15:I:134:ILE:HG22	15:I:135:GLU:N	2.18	0.58
18:L:41:HIS:H	18:L:41:HIS:CD2	2.20	0.58
18:L:130:ARG:HA	39:L:374:HOH:O	2.04	0.58
20:N:86:LEU:HD12	20:N:125:ALA:HB2	1.85	0.58
24:R:99:ALA:HB1	24:R:109:MET:HE3	1.83	0.58
1:O:281:U:H3'	39:O:4801:HOH:O	2.04	0.58
1:O:1375:A:C2'	1:O:1376:G:H5'	2.34	0.58
12:F:16:ALA:HA	12:F:111:ILE:HD13	1.86	0.58
16:J:52:GLN:HG3	16:J:53:ILE:N	2.19	0.58
31:Y:187:VAL:HB	39:Y:478:HOH:O	2.02	0.58
1:O:407:A:H3'	39:O:4970:HOH:O	2.04	0.57
1:O:1182:C:H1'	1:O:1192:A:H8	1.69	0.57
1:O:1189:A:H3'	39:O:6620:HOH:O	2.03	0.57
1:O:1266:U:H4'	31:Y:115:ARG:HH21	1.69	0.57
1:O:2755:G:H1'	39:O:9634:HOH:O	2.03	0.57
2:1:25:LYS:O	2:1:25:LYS:HG2	2.04	0.57
9:C:5:ILE:HD11	9:C:16:VAL:HG23	1.85	0.57
10:D:58:VAL:CG1	10:D:60:GLU:HG2	2.34	0.57
29:W:88:THR:HG23	29:W:110:GLN:HB3	1.84	0.57
1:O:482:G:H4'	1:O:508:A:N1	2.19	0.57
1:O:1667:A:H2'	1:O:1668:U:C6	2.39	0.57
1:O:2434:A:O3'	4:3:28:GLY:HA3	2.04	0.57
1:O:517:U:H2'	1:O:518:G:H5'	1.86	0.57
1:O:1015:C:H2'	1:O:1016:U:C6	2.39	0.57
1:O:2135:A:O2'	1:O:2136:G:H5'	2.03	0.57
1:O:2361:A:H5'	1:O:2361:A:H8	1.69	0.57
1:O:2812:A:H2	1:O:2814:A:N6	2.01	0.57
39:O:9100:HOH:O	14:H:61:ARG:HG3	2.03	0.57
10:D:50:VAL:O	10:D:71:ALA:HA	2.04	0.57
20:N:154:LEU:HD11	20:N:157:PRO:HA	1.86	0.57
23:Q:28:ARG:HG2	39:Q:223:HOH:O	2.03	0.57
26:T:16:LEU:HA	26:T:19:ARG:HG3	1.86	0.57
31:Y:234:VAL:HG12	31:Y:235:GLU:H	1.69	0.57
1:O:1878:G:C1'	39:O:8000:HOH:O	2.45	0.57
14:H:12:ILE:HD12	14:H:57:THR:CG2	2.33	0.57
22:P:18:LYS:HE2	39:P:208:HOH:O	2.04	0.57
29:W:21:LEU:HD22	29:W:26:ILE:CD1	2.34	0.57
1:O:12:U:H2'	1:O:13:G:H5'	1.86	0.57
1:O:2243:C:H5''	39:O:8513:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O: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:95:THR:N	31:Y:236:VAL:O	2.36	0.57
31:Y:220:GLU:HG3	39:Y:493:HOH:O	2.02	0.57
1:O:2055:A:H4'	24:R:132:ARG:NH2	2.19	0.57
1:O:2064:U:H5'	1:O:2652:U:H4'	1.86	0.57
12:F:50:VAL:HG13	12:F:60:VAL:HG11	1.87	0.57
16:J:19:MET:CE	16:J:132:LEU:HD11	2.35	0.57
22:P:7:LYS:HD3	22:P:21:VAL:HG22	1.86	0.57
30:X:47:ALA:HB1	30:X:82:GLU:HB3	1.86	0.57
1:O:669:G:O2'	1:O:670:G:H5'	2.05	0.57
1:O:958:G:H2'	1:O:959:C:C6	2.38	0.57
1:O:1504:A:H5'	39:O:7284:HOH:O	2.03	0.57
1:O:1741:U:O2'	1:O:2723:G:H4'	2.05	0.57
1:O:2365:G:H4'	23:Q:45:PRO:O	2.03	0.57
39:O:6882:HOH:O	31:Y:186:ARG:HD2	2.02	0.57
8:B:119:HIS:O	8:B:121:PRO:HD3	2.05	0.57
15:I:117:THR:O	15:I:121:LYS:HG3	2.04	0.57
20:N:151:ASP:O	20:N:154:LEU:HB2	2.05	0.57
1:O:1120:U:H5'	1:O:1121:G:OP2	2.04	0.57
3:2:20:ARG:HG3	3:2:21:VAL:H	1.70	0.57
10:D:49:PRO:HA	10:D:73:VAL:HG22	1.87	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
31:Y:106:THR:HG23	31:Y:107:PRO:HD2	1.85	0.57
1:O:2276:U:H2'	1:O:2277:U:C6	2.39	0.57
1:O:2548:C:OP2	8:B:5:ARG:NH2	2.38	0.57
3:2:41:HIS:HD2	3:2:44:ARG:H	1.53	0.57
4:3:73:GLU:HB3	39:3:258:HOH:O	2.05	0.57
8:B:132:HIS:HB2	8:B:137:LEU:HD22	1.87	0.57
18:L:80:ASP:HB2	18:L:90:ARG:O	2.04	0.57
19:M:24:GLN:HE21	19:M:27:ARG:HH11	1.52	0.57
30:X:51:ASP:OD2	30:X:52:PRO:HD2	2.05	0.57
1:O:585:C:H5''	39:O:5306:HOH:O	2.05	0.57
1:O:899:C:H5'	39:O:6055:HOH:O	2.04	0.57
1:O:1205:U:H2'	1:O:1206:U:H5'	1.86	0.57
1:O:1209:C:H2'	1:O:1210:G:C8	2.36	0.57
1:O:2718:C:H6	1:O:2718:C:H5'	1.70	0.57
9:C:98:ARG:NH1	39:C:493:HOH:O	2.36	0.57
24:R:33:ARG:HD2	39:R:331:HOH:O	2.04	0.57
7:A:48:ASP:HB3	39:A:435:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:88:LEU:HB2	10:D:89:PRO:HD3	1.86	0.56
12:F:38:LYS:HZ3	19:M:3:SER:HA	1.70	0.56
1:0:583:C:H2'	1:0:584:U:H6	1.69	0.56
1:0:775:G:OP1	2:1:16:HIS:HE1	1.89	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
1:0:2846:C:H4'	8:B:156:LYS:HB3	1.86	0.56
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.56
7:A:105:VAL:CG1	7:A:154:ALA:HB1	2.35	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
21:O:53:GLN:HG2	21:O:56:GLU:OE1	2.06	0.56
1:0:2667:G:H1'	1:0:2914:A:N3	2.21	0.56
1:0:2769:C:H2'	1:0:2770:G:H5'	1.87	0.56
1:0:2780:C:C1'	11:E:143:GLN:HE21	2.17	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
7:A:94:LEU:HG	7:A:99:ILE:CD1	2.35	0.56
8:B:71:VAL:HG11	8:B:296:LEU:HB3	1.86	0.56
9:C:236:THR:O	9:C:239:ALA:N	2.39	0.56
14:H:66:GLU:HA	39:H:327:HOH:O	2.06	0.56
20:N:35:VAL:HG13	39:N:4040:HOH:O	2.04	0.56
22:P:59:ARG:NH2	22:P:66:GLN:NE2	2.45	0.56
1:0:292:G:H2'	1:0:358:G:N2	2.20	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
1:0:2812:A:H1'	39:O:5225:HOH:O	2.05	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
17:K:87:ARG:NE	39:K:4043:HOH:O	2.39	0.56
1:0:1183:C:N4	1:0:1184:C:H41	2.03	0.56
15:I:124:VAL:O	15:I:124:VAL:HG12	2.04	0.56
16:J:22:VAL:O	16:J:26:VAL:HG23	2.05	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
29:W:54:PHE:CZ	29:W:140:LYS:HB2	2.40	0.56
1:0:644:G:H5'	1:0:644:G:N3	2.20	0.56
1:0:871:G:C8	1:0:871:G:C5'	2.80	0.56
1:0:2401:A:H5'	39:O:8818:HOH:O	2.06	0.56
1:0:2565:C:H4'	39:O:9210:HOH:O	2.05	0.56
9:C:156:LEU:O	9:C:160:LEU:HG	2.05	0.56
18:L:55:GLN:HA	18:L:58:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:1398:G:H2'	1:0:1399:A:C8	2.41	0.56
1:0:1461:U:H2'	1:0:1462:C:C6	2.41	0.56
1:0:1701:A:H5''	1:0:1702:U:H3'	1.86	0.56
1:0:1972:U:H2'	1:0:1973:A:C5'	2.36	0.56
1:0:2505:G:O2'	1:0:2506:A:H5'	2.05	0.56
7:A:128:LEU:HG	39:A:450:HOH:O	2.05	0.56
8:B:54:VAL:HB	39:B:536:HOH:O	2.05	0.56
8:B:154:VAL:CG1	8:B:156:LYS:HG2	2.36	0.56
11:E:2:ARG:HE	11:E:48:VAL:HG13	1.69	0.56
11:E:69:ILE:HA	11:E:72:MET:CE	2.36	0.56
18:L:26:HIS:HB2	39:L:327:HOH:O	2.06	0.56
1:0:1677:U:OP2	3:2:8:LYS:NZ	2.38	0.56
4:3:15:ASN:ND2	39:3:208:HOH:O	2.39	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
12:F:13:GLU:OE2	12:F:78:GLU:HG2	2.06	0.56
24:R:39:THR:HG22	24:R:42:GLU:H	1.70	0.56
28:V:39:ALA:N	28:V:40:PRO:CD	2.69	0.56
29:W:26:ILE:O	29:W:26:ILE:HG13	2.06	0.56
1:0:1029:U:O2'	1:0:1273:C:OP1	2.23	0.56
1:0:1180:U:H2'	1:0:1181:A:C8	2.41	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
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
19:M:78:LYS:HD3	39:M:357:HOH:O	2.06	0.56
23:Q:11:ARG:HD3	39:Q:213:HOH:O	2.06	0.56
27:U:11:THR:HG22	27:U:53:ASP:OD2	2.06	0.56
1:0:24:G:N2	1:0:518:G:H1'	2.21	0.55
1:0:272:A:H3'	39:0:4792:HOH:O	2.05	0.55
1:0:797:A:C4'	32:Z:10:ARG:N	2.69	0.55
1:0:2488:A:H1'	39:0:9047:HOH:O	2.05	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
6:9:34:A:H2'	6:9:35:C:O4'	2.06	0.55
6:9:56:A:O2'	10:D:14:ARG:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:314:ALA:CB	8:B:317:PRO:HG3	2.36	0.55
15:I:97:VAL:CG1	15:I:101:LYS:HE3	2.35	0.55
29:W:34:LEU:HD12	29:W:100:LEU:HD13	1.88	0.55
1:O:1434:A:H2'	1:O:1436:C:C5	2.41	0.55
1:O:2256:G:O2'	1:O:2257:G:H5'	2.05	0.55
8:B:27:ASN:HD22	8:B:27:ASN:N	1.98	0.55
9:C:88:SER:O	9:C:91:PRO:HD3	2.06	0.55
29:W:88:THR:HG22	29:W:90:TYR:HD1	1.70	0.55
1:O:188:C:H5''	19:M:163:LEU:HD21	1.88	0.55
1:O:2507:G:H2'	1:O:2510:C:H42	1.71	0.55
6:9:33:U:H2'	39:9:343:HOH:O	2.06	0.55
16:J:130:VAL:CG1	16:J:131:THR:N	2.69	0.55
23:Q:13:LYS:NZ	39:Q:211:HOH:O	2.37	0.55
1:O:671:A:O2'	1:O:672:G:H2'	2.07	0.55
1:O:1116:U:H3	1:O:1246:A:N6	1.95	0.55
1:O:1787:C:H4'	1:O:2883:A:O4'	2.05	0.55
1:O:2681:A:H4'	1:O:2682:C:H5'	1.88	0.55
1:O:2779:G:H21	11:E:143:GLN:NE2	2.03	0.55
39:O:7406:HOH:O	22:P:117:SER:HB2	2.06	0.55
8:B:265:LEU:HD21	8:B:316:ARG:HD3	1.88	0.55
11:E:68:HIS:O	11:E:72:MET:HG3	2.07	0.55
24:R:44:VAL:HG13	24:R:89:LEU:HD22	1.89	0.55
25:S:57:THR:HG22	25:S:59:ASP:H	1.70	0.55
30:X:47:ALA:HB1	30:X:82:GLU:CB	2.37	0.55
31:Y:155:ARG:NH1	39:Y:463:HOH:O	2.37	0.55
1:O:656:G:H5'	21:O:3:THR:HB	1.88	0.55
1:O:1380:U:H5'	39:O:7016:HOH:O	2.05	0.55
1:O:2502:C:C2'	1:O:2503:A:H5'	2.36	0.55
1:O:2904:U:H4'	30:X:8:ARG:HH12	1.71	0.55
3:2:40:ARG:HG3	3:2:45:ASN:HB2	1.88	0.55
6:9:1:U:H4'	6:9:3:A:OP1	2.06	0.55
17:K:18:ILE:HG22	17:K:93:ASN:HB2	1.88	0.55
20:N:110:THR:HB	20:N:113:SER:OG	2.05	0.55
1:O:380:A:OP2	19:M:9:ARG:HD2	2.07	0.55
1:O:1730:G:H5''	1:O:1731:C:C6	2.42	0.55
1:O:1845:A:OP2	7:A:190:ARG:NH1	2.39	0.55
14:H:168:VAL:CG1	39:H:324:HOH:O	2.54	0.55
20:N:64:SER:C	20:N:66:LEU:H	2.10	0.55
6:9:39:U:H1'	6:9:44:A:H61	1.71	0.55
17:K:98:VAL:HG11	17:K:102:GLU:HA	1.88	0.55
25:S:6:LYS:HB2	25:S:27:ALA:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:43:GLU:HB3	39:S:4013:HOH:O	2.06	0.55
1:0:488:U:H2'	39:0:5153:HOH:O	2.07	0.55
1:0:1165:G:H1'	1:0:1174:A:H1'	1.88	0.55
6:9:75:G:H1	6:9:106:U:H3	1.55	0.55
10:D:37:ALA:O	10:D:40:ILE:HG12	2.07	0.55
11:E:2:ARG:HE	11:E:48:VAL:CG1	2.20	0.55
19:M:122:GLN:OE1	19:M:127:LYS:HE2	2.07	0.55
26:T:50:VAL:HG12	26:T:56:ALA:HA	1.88	0.55
28:V:16:ARG:NH2	28:V:63:GLU:HG3	2.22	0.55
1:0:703:G:O2'	1:0:704:C:H5'	2.07	0.55
1:0:814:G:H2'	1:0:815:U:C6	2.41	0.55
1:0:1528:A:H2'	1:0:1529:G:O4'	2.06	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.42	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
12:F:21:GLU:O	12:F:24:ARG:HG2	2.06	0.55
20:N:49:THR:HG22	20:N:58:LEU:HD11	1.89	0.55
23:Q:64:GLU:HG3	23:Q:74:ASP:OD2	2.06	0.55
24:R:145:LEU:HD12	24:R:146:ILE:H	1.72	0.55
1:0:2504:A:H4'	14:H:74:ARG:HH11	1.72	0.55
2:1:1:THR:HA	39:1:204:HOH:O	2.07	0.55
9:C:200:PRO:HB3	9:C:212:VAL:HG23	1.88	0.55
10:D:40:ILE:HG13	10:D:41:LEU:N	2.22	0.55
11:E:69:ILE:HA	11:E:72:MET:HE2	1.88	0.55
12:F:56:PRO:CG	19:M:44:THR:HA	2.37	0.55
22:P:13:VAL:HG13	22:P:14:LEU:N	2.22	0.55
27:U:17:THR:CG2	27:U:18:GLY:N	2.70	0.55
29:W:90:TYR:CE2	29:W:99:ALA:HB2	2.42	0.55
29:W:110:GLN:NE2	29:W:110:GLN:HA	2.22	0.55
30:X:70:ILE:HG23	30:X:70:ILE:O	2.07	0.55
1:0:136:C:H2'	1:0:137:U:O4'	2.08	0.54
20:N:176:ARG:O	20:N:180:LEU:HD13	2.07	0.54
27:U:14:GLU:OE1	27:U:15:PRO:HD2	2.07	0.54
28:V:12:THR:HG23	28:V:14:ALA:N	2.18	0.54
1:0:284:C:H4'	1:0:285:A:O5'	2.08	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
1:0:1056:U:H2'	1:0:1057:A:O4'	2.07	0.54
1:0:1291:A:H2	39:0:6777:HOH:O	1.89	0.54
8:B:43:GLY:O	8:B:308:LEU:HD12	2.06	0.54
9:C:162:VAL:HG13	9:C:232:LEU:HD21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1537:C:H1'	39:0:7336:HOH:O	2.07	0.54
1:0:1544:U:H2'	1:0:1545:C:C6	2.42	0.54
9:C:236:THR:O	9:C:237:GLU:C	2.45	0.54
12:F:46:GLU:O	12:F:73:PRO:HD2	2.06	0.54
14:H:102:LYS:HG3	39:H:341:HOH:O	2.06	0.54
31:Y:189:ASN:C	31:Y:189:ASN:HD22	2.09	0.54
1:0:947:U:H2'	1:0:948:G:H8	1.71	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.54
1:0:1535:G:H2'	1:0:1536:C:C6	2.43	0.54
24:R:111:ILE:HG23	24:R:145:LEU:CD1	2.37	0.54
31:Y:99:ALA:HB2	31:Y:233:TYR:CE2	2.43	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.33	0.54
7:A:164:ARG:NE	39:A:456:HOH:O	2.39	0.54
23:Q:53:HIS:ND1	23:Q:55:ARG:HB2	2.23	0.54
31:Y:163:THR:HG23	39:Y:469:HOH:O	2.06	0.54
31:Y:235:GLU:CD	31:Y:235:GLU:N	2.60	0.54
1:0:484:A:N1	1:0:506:G:H4'	2.22	0.54
1:0:2411:C:H4'	39:0:8845:HOH:O	2.06	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
9:C:129:HIS:CE1	9:C:231:ARG:HA	2.43	0.54
10:D:10:PHE:CG	10:D:11:HIS:N	2.75	0.54
10:D:174:VAL:HG12	39:D:249:HOH:O	2.07	0.54
22:P:97:ARG:HD2	39:P:252:HOH:O	2.08	0.54
28:V:4:HIS:HB3	39:V:4003:HOH:O	2.08	0.54
29:W:21:LEU:HD21	29:W:48:VAL:HG13	1.90	0.54
29:W:34:LEU:CD1	29:W:100:LEU:HD13	2.38	0.54
29:W:65:VAL:HA	29:W:68:THR:CG2	2.38	0.54
1:0:1714:C:O2'	1:0:1715:C:H5'	2.08	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.07	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
15:I:130:LEU:HA	39:I:4002:HOH:O	2.06	0.54
27:U:9:CYS:HA	27:U:52:THR:CG2	2.33	0.54
27:U:52:THR:CG2	27:U:54:THR:HB	2.37	0.54
31:Y:212:ARG:HD2	39:Y:402:HOH:O	2.08	0.54
1:0:1942:A:H3'	39:0:8079:HOH:O	2.07	0.54
1:0:2256:G:C2'	1:0:2257:G:H5'	2.38	0.54
1:0:2787:C:H5	39:0:9680:HOH:O	1.90	0.54
7:A:194:MET:HE1	7:A:199:HIS:HB2	1.90	0.54
8:B:238:ASN:ND2	8:B:240:GLY:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:65:GLU:HG3	39:D:225:HOH:O	2.07	0.54
20:N:154:LEU:O	20:N:155:GLU:HB3	2.07	0.54
1:O: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:O:447:A:O2'	1:O:448:G:H5'	2.08	0.54
1:O:553:G:H5'	39:O:5266:HOH:O	2.07	0.54
1:O:2111:G:H1'	39:O:5678:HOH:O	2.08	0.54
39:O:4824:HOH:O	26:T:38:ARG:NH1	2.41	0.54
7:A:82:VAL:HG13	7:A:93:THR:HB	1.88	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
14:H:50:ILE:HD12	14:H:149:VAL:HG11	1.90	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
28:V:58:THR:O	28:V:62:GLU:HG3	2.08	0.54
1:O:461:C:N3	1:O:479:G:H5'	2.23	0.53
1:O:1118:A:C8	1:O:1118:A:C3'	2.85	0.53
8:B:223:ARG:HG3	8:B:232:TRP:O	2.08	0.53
9:C:34:ALA:HB3	9:C:220:THR:HG21	1.90	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
22:P:10:ALA:HA	22:P:13:VAL:HG12	1.89	0.53
29:W:3:ALA:O	29:W:54:PHE:HA	2.08	0.53
1:O:907:A:H4'	1:O:1328:A:C2	2.43	0.53
1:O:1166:A:H1'	1:O:1192:A:C2	2.42	0.53
1:O:2717:C:O2'	1:O:2718:C:H5''	2.07	0.53
39:O:9708:HOH:O	8:B:27:ASN:HB3	2.08	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:O:553:G:O4'	1:O:1325:G:H5'	2.06	0.53
1:O:902:G:N7	18:L:18:HIS:HD2	2.06	0.53
1:O:920:C:H5''	1:O:921:G:O5'	2.08	0.53
1:O:1086:A:C6	29:W:11:VAL:HG11	2.44	0.53
1:O:2670:G:O2'	1:O:2671:U:H5'	2.08	0.53
1:O:2840:A:OP1	8:B:211:THR:HG23	2.08	0.53
39:O:9659:HOH:O	8:B:298:LYS:HD3	2.09	0.53
6:9:56:A:C3'	6:9:57:A:H5''	2.37	0.53
8:B:2:GLN:HA	39:B:506:HOH:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:107:LEU:O	29:W:112:LEU:HB2	2.07	0.53
1:O:1242:A:OP2	16:J:60:ARG:NH2	2.41	0.53
1:O:1393:A:H2'	1:O:1394:C:C6	2.44	0.53
1:O:1735:C:OP2	8:B:234:ARG:HG3	2.09	0.53
1:O:1973:A:H2'	1:O:1974:G:O4'	2.09	0.53
1:O:2044:G:OP1	30:X:23:HIS:HE1	1.91	0.53
1:O: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: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
8:B:199:TYR:CE2	8:B:268:ARG:HB2	2.43	0.53
11:E:158:ASP:OD1	11:E:160:ARG:HB2	2.08	0.53
18:L:149:ARG:O	18:L:150:GLN:HB2	2.08	0.53
26:T:49:GLU:OE2	26:T:97:ARG:NH1	2.42	0.53
31:Y:99:ALA:HB2	31:Y:233:TYR:CZ	2.43	0.53
1:O:192:A:H5'	39:O:4570:HOH:O	2.08	0.53
1:O:1160:G:HO2'	1:O:1190:G:H1'	1.72	0.53
1:O:1595:G:O2'	1:O:1596:U:H5'	2.07	0.53
1:O:2478:U:H2'	1:O:2479:A:C8	2.44	0.53
8:B:51:VAL:CG2	8:B:327:VAL:HG13	2.38	0.53
20:N:37:ARG:HG3	20:N:37:ARG:HH11	1.74	0.53
31:Y:145:LYS:O	31:Y:147:ARG:HG2	2.09	0.53
32:Z:11:SER:HB3	32:Z:23:ARG:HB2	1.91	0.53
1:O:1120:U:H5''	1:O:1120:U:C6	2.43	0.53
1:O:1173:A:H4'	1:O:1174:A:C8	2.44	0.53
1:O:1419:U:H2'	1:O:1685:A:C2	2.44	0.53
1:O:2589:U:H2'	1:O:2590:U:C6	2.44	0.53
6:9:28:U:H2'	6:9:29:C:C6	2.44	0.53
8:B:51:VAL:HG23	8:B:329:TYR:O	2.09	0.53
10:D:154:LYS:H	10:D:154:LYS:CD	1.97	0.53
12:F:57:GLU:O	12:F:61:MET:HG3	2.09	0.53
17:K:74:VAL:HG12	17:K:75:ARG:HG3	1.91	0.53
19:M:61:ILE:CG2	19:M:62:VAL:N	2.72	0.53
29:W:4:LEU:O	29:W:32:CYS:HA	2.09	0.53
29:W:143:THR:N	39:W:4064:HOH:O	2.42	0.53
1:O:1375:A:O2'	1:O:1376:G:H5'	2.09	0.53
1:O:1973:A:H5'	1:O:1973:A:H8	1.74	0.53
1:O:2050:G:H5''	24:R:80:TYR:O	2.09	0.53
1:O:2769:C:H2'	1:O:2770:G:C5'	2.39	0.53
39:O:5169:HOH:O	26:T:82:THR:HA	2.09	0.53
4:3:70:ARG:NH1	4:3:77:ALA:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:65:ARG:O	7:A:66:ARG:HG3	2.09	0.53
8:B:16:ARG:NH1	39:B:516:HOH:O	2.41	0.53
8:B:144:THR:HB	39:B:561:HOH:O	2.09	0.53
9:C:214:THR:HG21	39:C:565:HOH:O	2.08	0.53
11:E:24:GLY:HA3	11:E:76:VAL:HB	1.91	0.53
11:E:53:GLU:HB3	11:E:55:ASN:ND2	2.24	0.53
16:J:46:ILE:HD11	16:J:53:ILE:HG23	1.91	0.53
19:M:61:ILE:HA	39:M:330:HOH:O	2.08	0.53
20:N:89:GLY:O	20:N:92:ALA:HB3	2.08	0.53
1:0:1014:A:H2'	1:0:1015:C:H5'	1.91	0.53
1:0:1634:G:H2'	1:0:1635:U:C6	2.44	0.53
1:0:2441:U:H4'	18:L:53:ARG:HD2	1.91	0.53
9:C:27:ARG:HG2	9:C:30:LEU:HD12	1.91	0.53
9:C:115:LEU:HD13	9:C:223:LEU:HD21	1.90	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
17:K:7:ASP:OD2	17:K:81:ARG:NH2	2.42	0.53
18:L:66:VAL:HG23	18:L:67:ARG:N	2.22	0.53
18:L:104:ASP:O	18:L:105:TYR:HB3	2.08	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
1:0:282:C:H2'	1:0:283:U:O4'	2.09	0.53
1:0:1525:G:H5'	1:0:1526:A:OP2	2.09	0.53
1:0:2326:C:H4'	1:0:2412:G:H4'	1.91	0.53
1:0:2564:G:OP2	1:0:2565:C:H5''	2.09	0.53
6:9:29:C:C2'	6:9:30:C:H5'	2.36	0.53
6:9:69:U:OP1	20:N:4:PRO:HG3	2.09	0.53
8:B:56:ASP:OD1	8:B:322:ARG:HB3	2.08	0.53
8:B:139:ASP:CB	8:B:165:ARG:HE	2.22	0.53
10:D:144:ARG:O	10:D:148:SER:HB3	2.08	0.53
12:F:39:SER:HB3	12:F:45:ALA:HB2	1.91	0.53
16:J:46:ILE:HD11	16:J:53:ILE:HG21	1.90	0.53
20:N:49:THR:CG2	20:N:58:LEU:HD11	2.39	0.53
20:N:171:HIS:CE1	39:N:4031:HOH:O	2.62	0.53
21:O:50:ARG:HD2	21:O:51:TYR:CE1	2.43	0.53
25:S:57:THR:HG22	25:S:59:ASP:N	2.23	0.53
1:0:289:G:O2'	1:0:290:C:H5'	2.09	0.53
1:0:558:C:C2'	1:0:559:U:C5'	2.82	0.53
1:0:812:A:H1'	39:0:5764:HOH:O	2.08	0.53
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.53
39:0:4840: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)
10:D:166:ILE:HB	39:D:247:HOH:O	2.08	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
39:K:4042:HOH:O	27:U:20:MET:HE1	2.08	0.53
29:W:52:VAL:CG2	29:W:53:ALA:H	2.20	0.53
29:W:149:LEU:HG	29:W:153:MET:CE	2.39	0.53
1:0:244:C:OP2	12:F:38:LYS:HE3	2.09	0.52
1:0:2598:U:O2	1:0:2600:A:H8	1.92	0.52
1:0:2831:C:C2'	1:0:2832:C:H5'	2.39	0.52
4:3:56:PRO:N	39:3:245:HOH:O	2.42	0.52
6:9:8:G:H4'	23:Q:27:GLN:NE2	2.24	0.52
8:B:84:LEU:HD23	8:B:142:LEU:HD23	1.89	0.52
11:E:84:MET:HG2	11:E:168:ILE:HA	1.90	0.52
1:0:1495:C:H1'	1:0:1573:A:H1'	1.92	0.52
1:0:1734:C:OP1	8:B:234:ARG:HD3	2.09	0.52
1:0:2601:A:N1	17:K:38:SER:HB2	2.24	0.52
4:3:83:TRP:HA	39:3:265:HOH:O	2.09	0.52
7:A:33:GLU:OE1	7:A:33:GLU:N	2.41	0.52
9:C:107:ARG:NH2	39:C:504:HOH:O	2.41	0.52
10:D:35:ALA:HB2	39:D:216:HOH:O	2.10	0.52
10:D:95:THR:OG1	10:D:174:VAL:HG22	2.10	0.52
15:I:133:THR:HG22	15:I:134:ILE:N	2.24	0.52
17:K:62:PRO:HG3	17:K:65:ARG:NH2	2.23	0.52
29:W:48:VAL:O	29:W:48:VAL:HG12	2.09	0.52
29:W:142:ASP:HB2	39:W:4066:HOH:O	2.09	0.52
1:0:538:C:H5''	1:0:539:G:C8	2.44	0.52
1:0:1634:G:H3'	39:0:7450:HOH:O	2.08	0.52
1:0:1946:C:H1'	39:0:8090:HOH:O	2.08	0.52
6:9:39:U:H1'	6:9:44:A:N6	2.24	0.52
10:D:10:PHE:CD1	10:D:11:HIS:N	2.77	0.52
10:D:76:ARG:O	10:D:77:ASP:HB2	2.08	0.52
19:M:134:ILE:O	19:M:136:PRO:HD3	2.09	0.52
29:W:88:THR:HG21	29:W:96:LEU:HD13	1.90	0.52
1:0:255:A:H2'	1:0:256:C:O4'	2.09	0.52
1:0:816:G:C6	1:0:817:G:N1	2.77	0.52
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.52
1:0:1118:A:H8	1:0:1119:G:H5''	1.73	0.52
1:0:1805:G:H2'	1:0:1806:G:H8	1.73	0.52
1:0:2781:U:H2'	1:0:2782:G:H5'	1.91	0.52
1:0:2802:C:H2'	1:0:2803:C:C6	2.44	0.52
8:B:177:HIS:O	8:B:181:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:127:ARG:HG2	9:C:127:ARG:HH11	1.73	0.52
9:C:214:THR:HG23	39:C:582:HOH:O	2.09	0.52
10:D:18:ILE:HD13	10:D:84:LEU:CD1	2.40	0.52
12:F:50:VAL:CG1	12:F:60:VAL:HG11	2.39	0.52
27:U:52:THR:HG22	27:U:54:THR:N	2.24	0.52
1:0:60:A:H5'	3:2:19:SER:OG	2.09	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
1:0:1304:U:H2'	1:0:1305:C:C6	2.44	0.52
1:0:2740:G:H2'	1:0:2741:A:O4'	2.08	0.52
7:A:179:MET:HG2	7:A:186:TRP:CG	2.45	0.52
11:E:116:THR:CG2	11:E:151:LEU:HD22	2.39	0.52
12:F:105:ASP:O	12:F:109:GLU:HB2	2.09	0.52
20:N:167:ASP:O	20:N:168:LEU:HD23	2.10	0.52
21:O:25:VAL:HG23	21:O:26:TRP:N	2.24	0.52
28:V:39:ALA:O	28:V:41:GLU:N	2.42	0.52
1:0:1087:G:H4'	1:0:1088:A:OP1	2.09	0.52
8:B:307:ARG:HH11	8:B:307:ARG:HB2	1.75	0.52
9:C:7:ASP:OD2	9:C:9:ASP:HB2	2.09	0.52
14:H:141:CYS:HB2	39:H:331:HOH:O	2.08	0.52
1:0:88:G:H8	1:0:88:G:H5'	1.75	0.52
1:0:474:C:O3'	9:C:73:LEU:HD21	2.10	0.52
1:0:1015:C:H2'	1:0:1016:U:H6	1.74	0.52
39:O:6211:HOH:O	20:N:4:PRO:HD2	2.10	0.52
21:O:57:THR:O	21:O:111:VAL:HG23	2.10	0.52
1:0:317:A:H5''	26:T:52:ARG:HD2	1.92	0.52
1:0:790:A:H2'	1:0:791:A:O4'	2.10	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.52
1:0:2781:U:H1'	11:E:139:GLU:OE2	2.10	0.52
8:B:248:ARG:NH2	39:B:611:HOH:O	2.42	0.52
8:B:260:HIS:HE1	39:B:618:HOH:O	1.91	0.52
15:I:88:GLN:NE2	15:I:128:THR:HG21	2.25	0.52
16:J:107:ASN:ND2	16:J:109:TYR:N	2.57	0.52
19:M:99:ARG:HD2	19:M:167:GLY:CA	2.37	0.52
20:N:61:ALA:CB	20:N:88:ALA:HB2	2.39	0.52
28:V:64:GLY:O	28:V:65:ASP:CB	2.57	0.52
29:W:89:ASP:HB2	29:W:90:TYR:CE1	2.44	0.52
1:0:236:A:H4'	1:0:237:G:OP1	2.09	0.52
1:0:581:G:H5'	39:O:5301:HOH:O	2.09	0.52
3:2:48:ASP:O	3:2:49:GLU:HB2	2.09	0.52
8:B:205:VAL:O	8:B:307:ARG:NE	2.43	0.52
11:E:137:ASP:O	11:E:141:VAL:HG23	2.10	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
16:J:107:ASN:HD22	16:J:108:PRO:N	2.06	0.52
20:N:47:LEU:CD1	20:N:97:VAL:HG11	2.39	0.52
21:O:115:ARG:NH1	39:O:4041:HOH:O	2.41	0.52
26:T:1:SER:HA	39:T:4001:HOH:O	2.08	0.52
32:Z:60:CYS:O	32:Z:61:ASP:HB2	2.09	0.52
1:O:1287:A:O4'	29:W:117:ARG:HD3	2.09	0.52
1:O:1947:G:N2	1:O:1966:U:C2	2.78	0.52
1:O:1979:G:H2'	39:O:8127:HOH:O	2.09	0.52
6:9:51:A:H5'	20:N:160:SER:HB3	1.90	0.52
8:B:195:ARG:HD2	8:B:324:ASP:OD1	2.10	0.52
9:C:10:GLY:HA2	9:C:160:LEU:HD21	1.91	0.52
10:D:58:VAL:HG12	10:D:60:GLU:HG2	1.92	0.52
10:D:64:ARG:CD	10:D:67:ASP:HB3	2.40	0.52
10:D:128:LEU:O	10:D:128:LEU:HD23	2.10	0.52
16:J:131:THR:HG22	16:J:133:GLY:N	2.24	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
26:T:18:GLU:O	26:T:21:LYS:HG3	2.09	0.52
29:W:56:GLU:O	29:W:143:THR:HG23	2.10	0.52
30:X:49:ARG:HG2	30:X:84:ILE:HG23	1.92	0.52
31:Y:189:ASN:HA	31:Y:217:ILE:HD11	1.90	0.52
1:O:485:A:N3	1:O:487:G:H5''	2.25	0.51
1:O:1446:U:H2'	25:S:55:GLN:NE2	2.25	0.51
1:O:2600:A:H2'	1:O:2601:A:O4'	2.11	0.51
1:O:2768:A:O2'	1:O:2769:C:H5'	2.10	0.51
1:O:2785:C:H4'	1:O:2786:G:OP2	2.11	0.51
7:A:105:VAL:HG11	7:A:154:ALA:HB1	1.91	0.51
7:A:192:VAL:HB	39:A:481:HOH:O	2.10	0.51
8:B:96:PRO:HG3	39:B:546:HOH:O	2.10	0.51
8:B:109:LEU:HG	8:B:113:LEU:HD12	1.93	0.51
16:J:126:ASN:ND2	39:J:4050:HOH:O	2.42	0.51
30:X:66:THR:HG23	30:X:67:PRO:HD2	1.92	0.51
1:O:2840:A:H3'	39:O:9746:HOH:O	2.10	0.51
12:F:36:THR:HG23	12:F:97:ALA:HB2	1.91	0.51
19:M:72:ALA:HB2	19:M:93:ARG:HG2	1.93	0.51
21:O:59:VAL:CG2	21:O:111:VAL:HG21	2.39	0.51
22:P:116:SER:O	22:P:119:TYR:HB3	2.09	0.51
32:Z:56:GLN:HA	32:Z:62:TYR:O	2.10	0.51
1:O:37:A:H2'	1:O:38:G:C8	2.45	0.51
1:O:195:C:H5''	39:M:420:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:814:G:H2'	1:0:815:U:H6	1.74	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.92	0.51
1:0:2570:G:H5''	39:0:9222:HOH:O	2.09	0.51
1:0:2724:U:H2'	1:0:2725:G:O4'	2.09	0.51
9:C:19:PRO:HG2	9:C:22:PHE:CE1	2.45	0.51
19:M:27:ARG:NH2	19:M:44:THR:HG23	2.25	0.51
26:T:80:GLU:HG2	39:T:4027:HOH:O	2.10	0.51
30:X:74:ALA:HB2	30:X:85:VAL:HG13	1.92	0.51
1:0:1335:C:OP2	31:Y:207:SER:HB3	2.11	0.51
1:0:1641:A:C2'	1:0:1642:A:H5'	2.40	0.51
1:0:2769:C:O2'	1:0:2770:G:H5'	2.11	0.51
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.51
7:A:65:ARG:C	7:A:66:ARG:HG3	2.31	0.51
8:B:41:PHE:CE1	8:B:79:MET:HG3	2.45	0.51
17:K:118:ALA:HA	17:K:125:ALA:HB2	1.92	0.51
18:L:57:VAL:HG12	18:L:57:VAL:O	2.11	0.51
18:L:77:ALA:HB3	39:L:356:HOH:O	2.11	0.51
1:0:2634:G:H3'	39:0:9414:HOH:O	2.10	0.51
39:0:6579:HOH:O	13:G:12:ILE:HG23	2.10	0.51
2:1:45:ARG:HD2	39:1:244:HOH:O	2.11	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
13:G:20:VAL:O	13:G:24:VAL:HG23	2.10	0.51
17:K:75:ARG:O	17:K:93:ASN:HA	2.10	0.51
25:S:22:ASN:ND2	25:S:68:LEU:HB2	2.25	0.51
26:T:106:GLU:HG3	39:T:4035:HOH:O	2.10	0.51
29:W:38:THR:HG22	39:W:4020:HOH:O	2.10	0.51
1:0:285:A:C2	1:0:368:C:H4'	2.46	0.51
1:0:960:G:H3'	1:0:960:G:N3	2.25	0.51
1:0:2719:A:C2	8:B:70:PRO:HG3	2.46	0.51
39:0:9658:HOH:O	8:B:267:LYS:HD3	2.11	0.51
9:C:47:GLY:HA2	9:C:92:PRO:HB2	1.92	0.51
9:C:235:PHE:HE2	9:C:243:VAL:HG21	1.76	0.51
10:D:35:ALA:C	10:D:37:ALA:N	2.64	0.51
11:E:34:TRP:HB3	39:E:4012:HOH:O	2.10	0.51
12:F:32:GLY:N	39:F:4009:HOH:O	2.43	0.51
20:N:23:ARG:NH1	39:N:4013:HOH:O	2.42	0.51
26:T:49:GLU:HB3	26:T:59:GLU:HG3	1.92	0.51
28:V:42:ASN:N	28:V:43:PRO:HD3	2.25	0.51
32:Z:53:GLY:HA2	32:Z:67:GLY:O	2.11	0.51
1:0:451:C:O2'	1:0:452:G:H5'	2.11	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
1:0:1024:G:H4'	29:W:41:TYR:OH	2.10	0.51
1:0:1226:G:O2'	1:0:1227:C:H5'	2.10	0.51
1:0:1634:G:H2'	1:0:1635:U:H6	1.76	0.51
1:0:1786:C:OP1	22:P:74:GLN:HG2	2.11	0.51
1:0:2081:A:H4'	16:J:69:TYR:CE1	2.46	0.51
1:0:2325:U:O2'	1:0:2411:C:H1'	2.09	0.51
8:B:258:GLY:H	8:B:260:HIS:CE1	2.28	0.51
11:E:7:ILE:HD11	11:E:11:VAL:C	2.31	0.51
12:F:15:ASP:O	12:F:18:GLU:HB2	2.10	0.51
14:H:61:ARG:NH1	14:H:61:ARG:HG3	2.26	0.51
15:I:105:GLU:HA	15:I:108:HIS:CE1	2.46	0.51
21:O:47:ARG:HG3	21:O:47:ARG:NH1	2.25	0.51
29:W:29:VAL:O	29:W:30:ASN:HB2	2.10	0.51
1:0:168:C:O5'	1:0:168:C:H6	1.93	0.51
1:0:721:A:H5''	21:O:51:TYR:CE2	2.46	0.51
1:0:1667:A:H5'	1:0:1667:A:C8	2.41	0.51
1:0:2326:C:H4'	1:0:2412:G:C4'	2.40	0.51
7:A:94:LEU:HD12	7:A:98:GLU:HB2	1.92	0.51
10:D:101:THR:O	10:D:101:THR:HG22	2.11	0.51
30:X:25:ARG:NH1	39:X:4012:HOH:O	2.44	0.51
1:0:877:G:C5'	1:0:878:G:OP1	2.56	0.51
1:0:1112:G:H1	1:0:1251:C:H42	1.56	0.51
39:O:7612:HOH:O	22:P:81:LYS:HG2	2.10	0.51
8:B:137:LEU:HD21	8:B:140:LEU:HD21	1.92	0.51
9:C:79:ARG:O	9:C:87:ARG:HG2	2.11	0.51
14:H:102:LYS:HD3	14:H:122:LYS:CD	2.35	0.51
15:I:91:PHE:HD2	15:I:131:GLY:HA2	1.75	0.51
23:Q:75:ILE:HA	39:Q:238:HOH:O	2.10	0.51
28:V:38:GLY:O	28:V:41:GLU:HG3	2.11	0.51
29:W:21:LEU:HB3	29:W:26:ILE:CG1	2.41	0.51
1:0:814:G:H1'	39:O:5767:HOH:O	2.09	0.51
1:0:1654:U:H2'	7:A:47:HIS:CD2	2.44	0.51
1:0:1666:C:O2'	1:0:1667:A:C5'	2.59	0.51
1:0:2812:A:C2	1:0:2814:A:N6	2.76	0.51
10:D:40:ILE:HG23	39:D:219:HOH:O	2.10	0.51
10:D:135:VAL:HG22	10:D:136:ARG:H	1.76	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
1:0:1003:U:H4'	14:H:91:ARG:O	2.10	0.50
39:O:8286:HOH:O	24:R:139:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:100:PRO:HG2	7:A:103:VAL:CG2	2.37	0.50
7:A:194:MET:CE	7:A:199:HIS:HB2	2.41	0.50
10:D:140:ARG:O	10:D:144:ARG:HG2	2.11	0.50
15:I:113:SER:HB2	15:I:118:ASN:HB2	1.93	0.50
20:N:49:THR:CG2	20:N:56:ASP:HB2	2.41	0.50
28:V:38:GLY:C	28:V:40:PRO:HD2	2.31	0.50
31:Y:112:GLU:CD	31:Y:115:ARG:NH1	2.64	0.50
1:O:282:C:O2'	1:O:283:U:H5'	2.12	0.50
1:O:2005:G:H3'	1:O:2005:G:OP2	2.11	0.50
1:O:2361:A:H5''	39:O:8725:HOH:O	2.09	0.50
1:O:2387:U:H2'	1:O:2388:C:C6	2.46	0.50
1:O:2467:A:O2'	1:O:2468:A:H2'	2.12	0.50
1:O:2582:G:O3'	17:K:41:LYS:HA	2.11	0.50
39:O:8978:HOH:O	18:L:37:LYS:HE2	2.11	0.50
8:B:81:ALA:O	8:B:186:GLY:HA3	2.10	0.50
10:D:146:LYS:HZ3	20:N:107:ASN:ND2	2.08	0.50
18:L:73:VAL:HG23	18:L:74:THR:N	2.26	0.50
18:L:97:VAL:HG12	18:L:98:GLU:O	2.10	0.50
1:O:69:A:H5'	1:O:69:A:C8	2.46	0.50
1:O:449:A:N7	9:C:43:LYS:HG2	2.26	0.50
1:O:527:U:H2'	1:O:528:G:C8	2.46	0.50
1:O:1279:U:O2	1:O:1279:U:H2'	2.12	0.50
1:O:1441:G:O2'	1:O:1442:A:H5'	2.11	0.50
1:O:1594:C:OP2	22:P:120:ARG:HD2	2.11	0.50
1:O:1761:U:H5''	22:P:83:LYS:HA	1.93	0.50
1:O:2114:C:O2'	1:O:2115:U:H5'	2.11	0.50
1:O:2424:U:H1'	23:Q:7:LEU:HD12	1.94	0.50
1:O:2506:A:O2'	1:O:2507:G:C8	2.62	0.50
9:C:7:ASP:C	9:C:9:ASP:H	2.15	0.50
11:E:77:THR:OG1	11:E:78:GLU:N	2.44	0.50
23:Q:21:ARG:HG2	23:Q:22:GLY:H	1.76	0.50
32:Z:42:CYS:SG	32:Z:44:GLU:HB2	2.51	0.50
1:O:61:G:OP1	3:2:17:GLN:HG2	2.11	0.50
1:O:383:A:H5'	39:O:4994:HOH:O	2.11	0.50
1:O:545:G:H8	1:O:545:G:C5'	2.19	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
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.93	0.50
7:A:105:VAL:HG12	7:A:106:CYS:N	2.25	0.50
8:B:199:TYR:HE2	8:B:268:ARG:HB2	1.76	0.50
9:C:7:ASP:O	9:C:9:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:75:ARG:HH21	17:K:94:ALA:CB	2.25	0.50
26:T:26:THR:HA	26:T:39:ASN:HB3	1.93	0.50
31:Y:109:LEU:HA	39:Y:417:HOH:O	2.11	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
17:K:81:ARG:HH11	17:K:81:ARG:HG2	1.76	0.50
18:L:73:VAL:HG11	18:L:118:LEU:HD21	1.93	0.50
20:N:37:ARG:CD	36:N:201:CL:CL	2.96	0.50
29:W:65:VAL:HG12	29:W:116:LEU:HD13	1.93	0.50
1:0:290:C:O2'	1:0:291:C:H5'	2.12	0.50
1:0:1684:A:O2'	1:0:1685:A:H5''	2.11	0.50
1:0:1711:A:O2'	1:0:1712:A:H5'	2.12	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
8:B:48:MET:HG2	8:B:72:THR:HA	1.94	0.50
11:E:103:VAL:HG22	11:E:115:ARG:HB3	1.94	0.50
1:0:522:U:O2'	1:0:1366:C:H5'	2.11	0.50
1:0:2072:G:C6	1:0:2533:C:H1'	2.47	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.94	0.50
6:9:88:G:OP1	29:W:130:HIS:NE2	2.41	0.50
9:C:200:PRO:HB3	9:C:212:VAL:CG2	2.41	0.50
16:J:107:ASN:ND2	16:J:107:ASN:C	2.63	0.50
1:0:466:A:H2'	1:0:467:G:O4'	2.12	0.50
1:0:1527:A:H1'	1:0:1528:A:C8	2.46	0.50
1:0:1853:C:OP1	7:A:231:LYS:HG3	2.11	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
19:M:46:LEU:O	19:M:50:ARG:HG3	2.12	0.50
20:N:43:VAL:O	20:N:84:THR:HG21	2.12	0.50
25:S:81:ILE:HG12	39:S:4028:HOH:O	2.12	0.50
1:0:64:G:H2'	1:0:65:C:O4'	2.12	0.50
1:0:517:U:C2'	1:0:518:G:H5'	2.42	0.50
1:0:1543:G:N1	1:0:1641:A:OP2	2.36	0.50
1:0:1855:G:H8	7:A:144:GLU:OE2	1.94	0.50
1:0:2671:U:H5''	8:B:161:VAL:O	2.12	0.50
1:0:2878:U:H2'	1:0:2879:A:O4'	2.12	0.50
7:A:66:ARG:HH11	7:A:66:ARG:CB	2.24	0.50
12:F:99:THR:HG23	12:F:99:THR:O	2.12	0.50
15:I:134:ILE:HG22	15:I:135:GLU:H	1.77	0.50
17:K:28:GLU:OE2	17:K:58:THR:HG21	2.12	0.50
19:M:169:ARG:NH1	39:M:413:HOH:O	2.43	0.50
24:R:113:HIS:O	24:R:145:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:47:THR:HB	26:T:100:ASP:HB3	1.94	0.50
29:W:35:VAL:HG22	29:W:36:PRO:O	2.12	0.50
1:0:195:C:H2'	1:0:196:G:H5'	1.94	0.49
1:0:653:U:H5''	39:O:4017:HOH:O	2.11	0.49
1:0:1102:C:H5	39:O:6483:HOH:O	1.94	0.49
1:0:1201:C:H5''	39:O:6630:HOH:O	2.12	0.49
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.49
39:9:357:HOH:O	20:N:147:ILE:HB	2.12	0.49
10:D:58:VAL:HB	10:D:62:ASP:HB3	1.94	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
18:L:73:VAL:HG23	18:L:74:THR:H	1.77	0.49
26:T:40:VAL:HG22	26:T:41:ARG:N	2.27	0.49
1:0:119:A:H2'	1:0:120:A:H5''	1.94	0.49
1:0:571:C:O5'	1:0:571:C:H6	1.94	0.49
1:0:596:C:H2'	1:0:597:A:H8	1.77	0.49
1:0:598:C:H2'	1:0:599:G:H8	1.76	0.49
1:0:656:G:H3'	21:O:37:ARG:HH12	1.77	0.49
1:0:790:A:H1'	1:0:1710:A:H2'	1.94	0.49
1:0:821:U:H2'	1:0:822:C:C6	2.41	0.49
1:0:1762:C:H2'	1:0:1763:C:H6	1.77	0.49
1:0:2371:G:H5'	39:O:8744:HOH:O	2.11	0.49
9:C:246:ARG:HB3	9:C:246:ARG:HH11	1.77	0.49
13:G:64:ASN:HD22	13:G:64:ASN:N	2.10	0.49
19:M:65:VAL:CG2	19:M:105:ALA:HB2	2.41	0.49
1:0:559:U:H2'	1:0:560:U:O4'	2.12	0.49
1:0:702:G:O2'	1:0:703:G:H5'	2.12	0.49
1:0:1118:A:C8	1:0:1119:G:H5''	2.46	0.49
1:0:1307:A:H2'	1:0:1308:A:C8	2.46	0.49
1:0:1942:A:O2'	1:0:1943:C:H5'	2.11	0.49
2:1:22:CYS:HA	39:1:242:HOH:O	2.11	0.49
13:G:71:LEU:C	13:G:73:ASP:N	2.65	0.49
18:L:89:PHE:N	39:L:357:HOH:O	2.44	0.49
18:L:133:VAL:HB	39:L:374:HOH:O	2.12	0.49
29:W:76:ASP:O	29:W:77:ALA:C	2.49	0.49
31:Y:126:PRO:HG2	31:Y:128:PHE:CE1	2.47	0.49
1:0:595:U:H2'	1:0:596:C:C6	2.47	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.95	0.49
9:C:107:ARG:O	9:C:111:VAL:HG23	2.11	0.49
14:H:80:LEU:O	14:H:84:GLY:HA3	2.13	0.49
14:H:91:ARG:HH11	14:H:138:THR:CB	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:79:PHE:HB3	16:J:103:VAL:HG11	1.94	0.49
26:T:38:ARG:HG3	26:T:38:ARG:HH11	1.77	0.49
1:0:189:A:OP1	19:M:171:ARG:NH2	2.45	0.49
1:0:820:G:C6	7:A:171:LYS:HB2	2.48	0.49
1:0:1069:C:H2'	1:0:1070:A:O4'	2.13	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
1:0:2668:G:H2'	1:0:2669:U:C6	2.48	0.49
10:D:25:MET:CE	10:D:41:LEU:HG	2.42	0.49
14:H:94:PRO:HA	14:H:127:ALA:O	2.13	0.49
15:I:95:LEU:HA	15:I:99:GLN:OE1	2.12	0.49
20:N:34:LEU:HD13	20:N:47:LEU:HD21	1.95	0.49
21:O:14:LEU:HD23	21:O:102:ILE:HD11	1.93	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
1:0:67:A:H5''	1:0:69:A:C8	2.48	0.49
1:0:1039:G:H2'	1:0:1040:A:O4'	2.12	0.49
1:0:1181:A:H2'	1:0:1182:C:H5'	1.94	0.49
1:0:1375:A:H2'	1:0:1376:G:H5'	1.92	0.49
1:0:2533:C:H6	1:0:2533:C:C5'	2.22	0.49
1:0:2764:C:H2'	1:0:2765:C:H6	1.76	0.49
8:B:329:TYR:CE2	27:U:15:PRO:HG2	2.48	0.49
10:D:93:LEU:HD23	39:D:233:HOH:O	2.12	0.49
18:L:145:LEU:HD23	18:L:145:LEU:C	2.32	0.49
20:N:73:ALA:N	39:N:4031:HOH:O	2.45	0.49
20:N:151:ASP:CG	20:N:165:ALA:O	2.51	0.49
23:Q:32:GLU:HA	23:Q:71:TYR:OH	2.12	0.49
1:0:130:C:H2'	39:0:4389:HOH:O	2.12	0.49
1:0:903:U:OP2	18:L:11:ARG:NH1	2.44	0.49
1:0:1316:G:H1'	1:0:1340:G:N2	2.28	0.49
1:0:1416:G:H2'	1:0:1417:G:H5'	1.93	0.49
1:0:1593:C:C6	22:P:120:ARG:HD3	2.47	0.49
1:0:1633:C:H5''	1:0:1634:G:OP1	2.13	0.49
1:0:1783:A:O2'	1:0:1784:U:H5'	2.12	0.49
1:0:1825:U:O2'	1:0:1826:C:H5'	2.13	0.49
1:0:2526:C:O2'	1:0:2527:U:H5'	2.13	0.49
7:A:18:ALA:O	7:A:20:SER:N	2.42	0.49
9:C:151:GLN:O	9:C:154:VAL:HB	2.13	0.49
12:F:100:ASP:O	12:F:101:ALA:O	2.31	0.49
18:L:43:HIS:O	18:L:44:GLU:C	2.51	0.49
19:M:181:GLU:OE1	19:M:181:GLU:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:5:ARG:HG3	23:Q:18:PRO:HB3	1.94	0.49
25:S:57:THR:C	25:S:59:ASP:H	2.16	0.49
30:X:78:GLU:HG2	30:X:79:GLU:N	2.27	0.49
1:0:694:A:C2'	1:0:695:C:H5'	2.41	0.49
1:0:834:G:H3'	1:0:835:U:H4'	1.95	0.49
1:0:1200:A:H1'	39:0:6635:HOH:O	2.13	0.49
1:0:1236:A:C8	16:J:63:ILE:HD11	2.48	0.49
1:0:1497:G:H4'	1:0:1627:G:O2'	2.13	0.49
1:0:1559:A:OP2	1:0:1559:A:H8	1.95	0.49
1:0:2837:U:H1'	8:B:307:ARG:HH12	1.77	0.49
1:0:2896:A:H5''	39:0:9810:HOH:O	2.11	0.49
9:C:2:GLN:HB3	39:C:415:HOH:O	2.13	0.49
9:C:237:GLU:HB2	39:C:523:HOH:O	2.13	0.49
18:L:125:PHE:CZ	18:L:140:VAL:HG13	2.47	0.49
20:N:143:ARG:HA	20:N:172:PHE:CD2	2.48	0.49
26:T:71:VAL:CG1	26:T:90:PRO:HB3	2.36	0.49
29:W:88:THR:CG2	29:W:89:ASP:H	2.20	0.49
1:0:1119:G:H22	1:0:1246:A:H2	1.55	0.49
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.49
1:0:1771:U:H5'	32:Z:20:ARG:HH21	1.76	0.49
1:0:2312:G:H2'	1:0:2313:C:H5'	1.94	0.49
1:0:2468:A:H61	4:3:48:ASN:HD21	1.60	0.49
1:0:2636:C:H3'	39:0:9419:HOH:O	2.12	0.49
7:A:153:ARG:HB2	7:A:153:ARG:NH1	2.28	0.49
10:D:138:GLY:N	39:D:245:HOH:O	2.36	0.49
22:P:114:LEU:HA	22:P:118:GLN:NE2	2.28	0.49
1:0:635:A:H2'	1:0:636:G:H5''	1.94	0.49
1:0:654:A:OP2	21:O:38:ARG:HD3	2.12	0.49
1:0:705:C:O2	1:0:705:C:H2'	2.13	0.49
1:0:1299:G:O6	18:L:6:ARG:HD3	2.13	0.49
7:A:153:ARG:CB	7:A:153:ARG:HH11	2.26	0.49
15:I:87:PRO:HD3	39:I:4009:HOH:O	2.13	0.49
29:W:38:THR:O	29:W:42:ARG:HB2	2.13	0.49
31:Y:107:PRO:HB3	31:Y:182:PHE:CD2	2.48	0.49
1:0:130:C:H5'	39:0:4351:HOH:O	2.13	0.48
1:0:226:A:H1'	1:0:393:G:C5	2.48	0.48
1:0:932:U:H2'	1:0:933:C:C6	2.47	0.48
1:0:1811:A:C2	1:0:2752:C:H1'	2.48	0.48
1:0:2578:G:H5'	1:0:2578:G:C8	2.43	0.48
1:0:2896:A:OP1	30:X:15:ARG:NH1	2.46	0.48
39:0:7955: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)
4:3:65:THR:HB	4:3:83:TRP:H	1.77	0.48
9:C:157:LEU:HD11	9:C:194:PHE:HZ	1.78	0.48
11:E:20:ILE:CD1	11:E:40:VAL:HG11	2.42	0.48
17:K:121:PHE:HB3	39:K:4051:HOH:O	2.12	0.48
18:L:20:ASN:O	18:L:22:ARG:N	2.46	0.48
20:N:37:ARG:HE	20:N:105:GLY:HA3	1.78	0.48
24:R:59:PHE:HZ	24:R:81:PRO:HG3	1.77	0.48
30:X:66:THR:CG2	30:X:67:PRO:HD2	2.44	0.48
32:Z:10:ARG:HA	39:Z:218:HOH:O	2.11	0.48
1:0:396:U:H1'	39:0:4950:HOH:O	2.12	0.48
1:0:808:A:C5	1:0:809:G:H1'	2.48	0.48
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.48
39:0:6469:HOH:O	29:W:119:HIS:HE1	1.96	0.48
13:G:19:GLU:O	13:G:23:ILE:HG13	2.14	0.48
14:H:12:ILE:HG12	14:H:59:GLN:HG2	1.94	0.48
16:J:75:PRO:HD3	16:J:136:SER:OG	2.13	0.48
20:N:64:SER:O	20:N:66:LEU:N	2.46	0.48
22:P:98:ILE:O	22:P:98:ILE:HD13	2.13	0.48
1:0:777:U:O2'	2:1:11:LYS:HG2	2.13	0.48
1:0:1762:C:H4'	39:0:7768:HOH:O	2.13	0.48
1:0:2598:U:O2	1:0:2600:A:C8	2.66	0.48
7:A:186:TRP:CG	7:A:187:PRO:HA	2.48	0.48
8:B:171:VAL:O	8:B:175:LEU:HB2	2.12	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
18:L:6:ARG:NH2	39:L:308:HOH:O	2.45	0.48
18:L:62:ALA:HB2	18:L:103:ALA:HB2	1.95	0.48
19:M:164:THR:CG2	19:M:167:GLY:H	2.15	0.48
21:O:14:LEU:CD2	21:O:102:ILE:HD11	2.42	0.48
1:0:87:C:H2'	3:2:28:LYS:O	2.13	0.48
1:0:776:A:OP1	2:1:28:HIS:HE1	1.96	0.48
1:0:1277:C:OP2	21:O:19:ARG:NH1	2.47	0.48
1:0:1874:U:OP1	7:A:51:ARG:HD2	2.12	0.48
1:0:1909:A:N1	1:0:2128:G:H1'	2.27	0.48
1:0:2359:G:H3'	39:0:8727:HOH:O	2.12	0.48
3:2:41:HIS:HB3	3:2:44:ARG:HB2	1.96	0.48
4:3:56:PRO:HA	39:3:245:HOH:O	2.13	0.48
9:C:132:ASP:CB	39:C:516:HOH:O	2.58	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
19:M:26:GLN:O	19:M:29:GLN:HB2	2.14	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
1:0:2659:U:H5''	39:0:9492:HOH:O	2.13	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.47	0.48
11:E:5:LEU:HD21	11:E:66:GLN:HG3	1.95	0.48
15:I:73:LEU:HD12	15:I:107:LYS:NZ	2.29	0.48
19:M:98:GLN:HB2	19:M:129:HIS:NE2	2.28	0.48
21:O:44:ASN:OD1	21:O:65:LEU:HB2	2.13	0.48
29:W:11:VAL:O	29:W:12:ASN:HB2	2.13	0.48
30:X:46:ASP:OD2	30:X:46:ASP:N	2.45	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
1:0:722:G:H22	1:0:938:G:P	2.37	0.48
1:0:1787:C:OP1	22:P:68:LYS:HE2	2.13	0.48
1:0:2754:G:O2'	1:0:2755:G:H5'	2.14	0.48
9:C:151:GLN:HB3	39:C:527:HOH:O	2.13	0.48
19:M:54:TYR:HB2	19:M:132:ILE:HD13	1.95	0.48
20:N:37:ARG:HH21	20:N:105:GLY:N	2.12	0.48
20:N:116:PHE:HB3	20:N:136:LEU:HD23	1.95	0.48
22:P:142:ASP:O	22:P:143:ALA:O	2.30	0.48
1:0:541:C:H2'	1:0:542:A:H5'	1.94	0.48
1:0:1007:A:H2'	14:H:22:TYR:OH	2.14	0.48
1:0:1051:C:H2'	1:0:1052:G:O4'	2.14	0.48
8:B:83:ALA:HB2	8:B:101:TRP:CD2	2.49	0.48
12:F:4:VAL:HG13	12:F:76:PHE:CE1	2.48	0.48
17:K:99:ASP:OD1	17:K:101:ASN:N	2.47	0.48
18:L:129:ALA:O	18:L:133:VAL:HG23	2.14	0.48
23:Q:93:ARG:HG3	23:Q:93:ARG:HH11	1.79	0.48
1:0:101:C:H2'	1:0:102:A:C8	2.49	0.48
1:0:351:A:O2'	1:0:352:A:H5'	2.13	0.48
1:0:553:G:H3'	39:0:5272:HOH:O	2.14	0.48
1:0:596:C:H2'	1:0:597:A:C8	2.48	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.14	0.48
1:0:1638:U:H5'	39:0:7453:HOH:O	2.14	0.48
1:0:2291:A:N9	1:0:2309:C:H5'	2.29	0.48
4:3:34:LYS:HE2	39:3:222:HOH:O	2.13	0.48
9:C:26:VAL:HG21	9:C:123:LEU:HD11	1.96	0.48
15:I:100:VAL:HG11	15:I:124:VAL:HG22	1.96	0.48
17:K:35:HIS:HB2	17:K:52:LYS:O	2.14	0.48
19:M:184:ARG:HG3	19:M:185:PRO:HA	1.96	0.48
25:S:52:VAL:C	25:S:53:ASN:HD22	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:105:G:O2'	1:0:106:A:H5'	2.14	0.48
1:0:1018:A:H4'	23:Q:59:GLN:NE2	2.29	0.48
1:0:1041:U:H2'	1:0:1042:U:H5'	1.96	0.48
1:0:1477:C:H5'	1:0:1868:G:H5'	1.96	0.48
1:0:1524:U:OP1	1:0:1524:U:H4'	2.14	0.48
1:0:1882:C:OP1	7:A:192:VAL:HG23	2.14	0.48
1:0:2281:C:H2'	1:0:2282:U:H5'	1.95	0.48
1:0:2456:A:H5'	39:0:8945:HOH:O	2.14	0.48
10:D:67:ASP:O	10:D:69:ILE:HG13	2.13	0.48
11:E:34:TRP:HA	39:E:4013:HOH:O	2.13	0.48
13:G:67:LEU:O	13:G:71:LEU:HG	2.13	0.48
21:O:88:LYS:HB3	39:O:4026:HOH:O	2.13	0.48
24:R:82:GLU:HG3	24:R:83:LYS:H	1.79	0.48
24:R:132:ARG:NH2	39:R:379:HOH:O	2.46	0.48
30:X:71:ARG:HD2	39:X:4026:HOH:O	2.13	0.48
31:Y:115:ARG:NE	39:Y:423:HOH:O	2.47	0.48
32:Z:32:GLU:HA	32:Z:35:GLU:HG3	1.96	0.48
1:0:667:C:H2'	1:0:668:C:H6	1.79	0.48
1:0:1150:A:C2	13:G:20:VAL:HG21	2.49	0.48
1:0:1470:A:OP1	19:M:93:ARG:HD2	2.14	0.48
1:0:2617:G:H4'	39:0:9356:HOH:O	2.14	0.48
39:0:6451:HOH:O	29:W:9:GLY:HA3	2.13	0.48
8:B:27:ASN:H	8:B:27:ASN:ND2	2.06	0.48
8:B:268:ARG:NH2	8:B:325:PRO:HG3	2.29	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
15:I:118:ASN:HA	15:I:121:LYS:CD	2.43	0.48
17:K:37:TYR:HD2	39:K:4016:HOH:O	1.97	0.48
19:M:9:ARG:HG3	39:M:338:HOH:O	2.14	0.48
20:N:184:ILE:HG23	20:N:184:ILE:O	2.14	0.48
21:O:105:ASN:HD21	21:O:109:SER:H	1.62	0.48
26:T:92:ASP:OD1	26:T:94:SER:HB3	2.14	0.48
31:Y:133:HIS:HD2	39:Y:440:HOH:O	1.96	0.48
31:Y:144:ARG:CZ	39:Y:451:HOH:O	2.62	0.48
1:0:68:U:O2'	1:0:69:A:H5''	2.14	0.47
1:0:134:U:C2	1:0:145:A:C2	3.02	0.47
1:0:533:U:H3'	39:0:5227:HOH:O	2.14	0.47
1:0:644:G:H1'	39:0:5437:HOH:O	2.12	0.47
1:0:825:U:H5''	1:0:826:U:OP1	2.14	0.47
1:0:1008:C:H5''	14:H:19:ARG:HH12	1.78	0.47
1:0:1406:A:H5'	1:0:1407:A:C8	2.48	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
1:0:2735:U:H2'	1:0:2736:U:C6	2.48	0.47
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
8:B:80:ARG:O	8:B:82:VAL:HG23	2.14	0.47
18:L:125:PHE:CE1	18:L:140:VAL:HG13	2.49	0.47
27:U:52:THR:HG22	27:U:54:THR:HB	1.95	0.47
1:0:69:A:H5'	1:0:69:A:H8	1.78	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:1581:A:H61	1:0:1614:G:H1'	1.78	0.47
1:0:1948:G:H2'	1:0:1949:G:O4'	2.14	0.47
1:0:2002:C:H2'	1:0:2003:U:H5'	1.95	0.47
1:0:2100:A:H5'	39:0:8417:HOH:O	2.14	0.47
8:B:212:GLN:OE1	8:B:216:LYS:HD3	2.13	0.47
8:B:301:VAL:HG13	8:B:302:PRO:HD2	1.96	0.47
9:C:104:ASP:O	9:C:108:GLN:HG3	2.14	0.47
12:F:37:THR:O	12:F:41:GLU:HG3	2.14	0.47
12:F:78:GLU:HG3	39:F:4017:HOH:O	2.14	0.47
16:J:6:PHE:O	16:J:8:ALA:N	2.47	0.47
20:N:48:VAL:HG12	20:N:55:ASP:HB3	1.90	0.47
23:Q:23:THR:HG22	23:Q:24:SER:N	2.29	0.47
28:V:12:THR:HB	28:V:15:GLU:OE2	2.14	0.47
29:W:69:ARG:HD2	29:W:117:ARG:O	2.14	0.47
31:Y:144:ARG:NE	39:Y:451:HOH:O	2.46	0.47
31:Y:187:VAL:CG1	31:Y:205:ILE:HA	2.43	0.47
1:0:766:A:HO2'	1:0:767:A:H8	1.62	0.47
39:0:7682:HOH:O	8:B:214:PRO:HD2	2.14	0.47
6:9:3:A:H2'	39:9:330:HOH:O	2.14	0.47
6:9:34:A:O5'	6:9:34:A:H8	1.96	0.47
8:B:1:PRO:O	8:B:2:GLN:HB2	2.13	0.47
8:B:36:PRO:HG3	8:B:169:GLY:H	1.77	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
17:K:87:ARG:HB2	27:U:19:THR:HG23	1.95	0.47
20:N:7:LYS:HE3	23:Q:21:ARG:O	2.15	0.47
29:W:6:GLN:CB	29:W:26:ILE:HD12	2.34	0.47
1:0:1173:A:H2	39:0:6634:HOH:O	1.96	0.47
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.47
1:0:1840:A:H4'	1:0:1841:C:O5'	2.14	0.47
1:0:2241:C:O2'	1:0:2242:U:H5'	2.14	0.47
1:0:2388:C:H2'	1:0:2389:U:O4'	2.14	0.47
6:9:76:G:C3'	6:9:77:A:H5''	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:30:PRO:HB2	8:B:39:GLN:NE2	2.28	0.47
9:C:246:ARG:NH2	39:C:583:HOH:O	2.42	0.47
18:L:143:THR:CG2	18:L:144:ASP:N	2.77	0.47
20:N:67:ALA:HA	20:N:71:TRP:CB	2.44	0.47
24:R:99:ALA:CB	24:R:109:MET:HE3	2.45	0.47
1:O:213:G:N2	1:O:225:G:H2'	2.30	0.47
1:O:363:C:O2'	1:O:364:U:H5'	2.15	0.47
1:O:1044:C:H5''	39:O:6098:HOH:O	2.15	0.47
1:O:1154:A:H2'	1:O:1155:G:C8	2.49	0.47
1:O:1735:C:O2'	1:O:1736:A:H5'	2.13	0.47
1:O:2353:A:O2'	20:N:7:LYS:HB3	2.14	0.47
1:O:2520:G:H5'	14:H:64:SER:OG	2.15	0.47
2:1:21:ARG:HD2	2:1:39:PHE:HB2	1.97	0.47
7:A:8:ARG:HG2	39:A:413:HOH:O	2.13	0.47
11:E:16:ASP:O	11:E:17:HIS:HB2	2.14	0.47
14:H:142:ASN:O	14:H:144:GLU:N	2.47	0.47
20:N:37:ARG:NH2	20:N:105:GLY:CA	2.70	0.47
21:O:26:TRP:HA	21:O:26:TRP:CE3	2.49	0.47
24:R:114:VAL:HA	24:R:144:GLU:O	2.14	0.47
29:W:139:GLY:O	29:W:141:HIS:CD2	2.67	0.47
1:O:2780:C:H2'	1:O:2781:U:C6	2.50	0.47
39:O:8077:HOH:O	7:A:236:GLY:HA3	2.14	0.47
9:C:233:THR:CG2	9:C:234:VAL:H	2.26	0.47
10:D:64:ARG:HD3	10:D:67:ASP:HB3	1.96	0.47
14:H:12:ILE:HG12	14:H:59:GLN:CG	2.45	0.47
15:I:87:PRO:CB	15:I:129:SER:C	2.83	0.47
16:J:39:VAL:CG1	16:J:107:ASN:HB2	2.45	0.47
27:U:13:ILE:HG12	27:U:32:CYS:HB3	1.96	0.47
30:X:80:GLU:O	30:X:80:GLU:HG2	2.14	0.47
1:O:101:C:H2'	1:O:102:A:H8	1.80	0.47
1:O:563:C:H2'	1:O:564:G:O4'	2.15	0.47
1:O:625:U:H5''	1:O:1044:C:N4	2.29	0.47
1:O:657:G:H2'	1:O:658:C:C6	2.50	0.47
1:O:946:C:O2'	1:O:947:U:H5'	2.15	0.47
1:O:1116:U:O2'	1:O:1118:A:C2	2.56	0.47
1:O:1416:G:C2'	1:O:1417:G:H5'	2.44	0.47
1:O:1819:G:H2'	1:O:1820:G:C4'	2.40	0.47
1:O:2281:C:C2'	1:O:2282:U:H5'	2.45	0.47
1:O:2365:G:P	23:Q:15:LYS:HG3	2.54	0.47
1:O:2607:U:H4'	39:O:9306:HOH:O	2.14	0.47
3:2:31:ARG:NH1	39:2:127:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:35:ARG:HB2	39:2:132:HOH:O	2.15	0.47
4:3:30:GLN:NE2	39:3:218:HOH:O	2.43	0.47
6:9:91:C:H2'	6:9:92:G:O4'	2.15	0.47
8:B:52:VAL:O	8:B:53:LEU:HD12	2.15	0.47
10:D:23:VAL:HG21	10:D:45:THR:CG2	2.43	0.47
11:E:81:GLU:HG2	11:E:134:SER:CB	2.44	0.47
14:H:86:TYR:C	14:H:86:TYR:CD1	2.88	0.47
16:J:39:VAL:HG12	16:J:40:ASN:ND2	2.29	0.47
16:J:54:VAL:CG1	16:J:138:THR:HG21	2.45	0.47
17:K:106:GLY:HA3	39:K:4013:HOH:O	2.14	0.47
19:M:15:PRO:HA	19:M:20:LEU:CD2	2.45	0.47
19:M:61:ILE:HG22	19:M:62:VAL:N	2.28	0.47
20:N:11:ARG:HG3	20:N:14:ARG:NH1	2.29	0.47
20:N:94:GLU:HG3	20:N:186:LEU:HD12	1.96	0.47
20:N:100:ALA:O	20:N:129:ILE:HG23	2.15	0.47
26:T:42:VAL:CG1	26:T:62:VAL:HG21	2.44	0.47
26:T:43:ASN:C	26:T:45:GLY:H	2.18	0.47
30:X:43:VAL:HG12	30:X:44:ASP:N	2.30	0.47
31:Y:108:ASP:OD1	31:Y:108:ASP:N	2.48	0.47
1:0:876:A:H2'	1:0:876:A:N3	2.29	0.47
1:0:949:U:H4'	23:Q:95:GLU:HA	1.97	0.47
1:0:1236:A:C2'	1:0:1237:U:H5'	2.45	0.47
1:0:2064:U:H5'	1:0:2652:U:O3'	2.15	0.47
1:0:2114:C:OP1	7:A:1:GLY:HA2	2.15	0.47
1:0:2597:U:H2'	1:0:2598:U:H5'	1.96	0.47
1:0:2656:G:O2'	1:0:2657:G:H5'	2.15	0.47
7:A:164:ARG:CZ	39:A:456:HOH:O	2.62	0.47
8:B:304:PRO:HD2	8:B:307:ARG:CD	2.43	0.47
9:C:127:ARG:HG2	9:C:127:ARG:NH1	2.30	0.47
18:L:78:ALA:N	39:L:356:HOH:O	2.48	0.47
21:O:96:VAL:HG13	21:O:100:GLN:OE1	2.14	0.47
22:P:16:VAL:CG1	22:P:20:ARG:CZ	2.93	0.47
1:0:598:C:H2'	1:0:599:G:C8	2.50	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
1:0:2324:G:N2	1:0:2377:U:H1'	2.30	0.47
7:A:153:ARG:HB2	7:A:153:ARG:HH11	1.80	0.47
7:A:211:LYS:CB	39:A:504:HOH:O	2.60	0.47
8:B:24:PRO:CG	8:B:204:GLY:HA2	2.45	0.47
8:B:132:HIS:HB2	8:B:137:LEU:CD2	2.45	0.47
10:D:91:ALA:HB2	10:D:106:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:31:ARG:HH12	11:E:68:HIS:CE1	2.33	0.47
14:H:117:ARG:O	14:H:118:ALA:C	2.53	0.47
17:K:65:ARG:HD3	39:K:4032:HOH:O	2.15	0.47
18:L:65:ASP:HA	18:L:109:LEU:O	2.14	0.47
18:L:68:GLU:HB2	39:L:350:HOH:O	2.15	0.47
19:M:146:ASP:O	19:M:147:LEU:HD23	2.15	0.47
19:M:164:THR:HB	39:M:409:HOH:O	2.13	0.47
25:S:57:THR:HG22	25:S:58:MET:N	2.29	0.47
28:V:1:THR:O	28:V:4:HIS:CE1	2.68	0.47
1:0:327:A:N3	9:C:206:ASN:ND2	2.63	0.47
1:0:704:C:H2'	1:0:705:C:H6	1.80	0.47
1:0:2541:U:H5'	1:0:2611:G:O6	2.15	0.47
1:0:2596:A:H2	36:0:3189:CL:CL	2.35	0.47
1:0:2900:G:H2'	1:0:2901:C:O4'	2.15	0.47
2:1:1:THR:HG21	39:1:207:HOH:O	2.15	0.47
8:B:124:ALA:O	8:B:128:ILE:HG13	2.14	0.47
10:D:86:THR:HG23	39:D:231:HOH:O	2.14	0.47
14:H:48:VAL:HA	14:H:170:ARG:O	2.15	0.47
16:J:41:ALA:O	16:J:132:LEU:HD12	2.15	0.47
17:K:49:LEU:HA	17:K:73:VAL:HG12	1.97	0.47
20:N:72:GLU:HB3	20:N:171:HIS:HE1	1.80	0.47
20:N:154:LEU:CD1	20:N:157:PRO:HA	2.44	0.47
26:T:44:ALA:HA	26:T:62:VAL:HG12	1.95	0.47
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.15	0.46
1:0:558:C:H2'	1:0:559:U:H5'	1.93	0.46
1:0:1064:U:H2'	1:0:1065:G:C8	2.50	0.46
1:0:1603:A:C5'	1:0:1605:G:H5'	2.45	0.46
1:0:2314:G:O2'	1:0:2315:C:H5'	2.15	0.46
2:1:45:ARG:HB3	39:1:244:HOH:O	2.14	0.46
3:2:20:ARG:CG	3:2:21:VAL:N	2.79	0.46
7:A:94:LEU:HD23	7:A:94:LEU:N	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
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
16:J:51:GLU:O	16:J:55:GLU:HG3	2.15	0.46
17:K:49:LEU:HD23	17:K:50:GLY:N	2.30	0.46
1:0:152:A:O2'	1:0:153:C:H5'	2.15	0.46
1:0:806:A:H2'	1:0:807:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:870:G:OP2	7:A:3:ARG:HD3	2.15	0.46
1:0:1625:U:H4'	39:0:7442:HOH:O	2.15	0.46
1:0:2039:A:H4'	1:0:2760:C:O2'	2.16	0.46
1:0:2501:G:H1'	39:0:9075:HOH:O	2.16	0.46
1:0:2644:C:O2'	1:0:2645:U:OP1	2.29	0.46
4:3:55:VAL:HB	4:3:56:PRO:CD	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
10:D:152:PRO:O	10:D:156:ARG:HG2	2.15	0.46
17:K:64:MET:HA	17:K:67:GLN:HE21	1.81	0.46
18:L:55:GLN:HA	18:L:58:GLN:NE2	2.30	0.46
20:N:47:LEU:HD23	20:N:47:LEU:HA	1.71	0.46
21:O:26:TRP:HB2	39:O:4009:HOH:O	2.14	0.46
28:V:1:THR:CG2	28:V:2:VAL:H	2.19	0.46
29:W:69:ARG:NH2	39:W:4068:HOH:O	2.45	0.46
30:X:54:ILE:O	30:X:57:ALA:HB3	2.15	0.46
1:0:553:G:P	31:Y:204:ARG:HH22	2.38	0.46
1:0:1168:C:H5	39:0:6595:HOH:O	1.98	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
7:A:37:VAL:HG13	39:A:432:HOH:O	2.14	0.46
8:B:77:PRO:HG2	8:B:151:VAL:CG2	2.45	0.46
8:B:109:LEU:CG	8:B:113:LEU:HD12	2.46	0.46
9:C:140:VAL:HG12	9:C:141:SER:N	2.30	0.46
10:D:167:GLU:HA	10:D:171:ASP:OD1	2.15	0.46
11:E:170:ARG:NH2	39:E:4042:HOH:O	2.48	0.46
12:F:43:GLY:C	12:F:45:ALA:H	2.18	0.46
14:H:151:GLU:HG3	39:H:359:HOH:O	2.15	0.46
17:K:5:GLY:O	17:K:83:PRO:HD3	2.16	0.46
17:K:66:ARG:HG2	17:K:66:ARG:HH11	1.81	0.46
21:O:26:TRP:HA	21:O:26:TRP:HE3	1.79	0.46
26:T:113:GLU:O	26:T:114:SER:C	2.53	0.46
29:W:80:ASP:HB2	39:W:4039:HOH:O	2.15	0.46
30:X:22:ASN:O	30:X:25:ARG:HG3	2.15	0.46
31:Y:177:LYS:HD3	31:Y:181:GLY:O	2.15	0.46
1:0:31:C:H4'	39:0:4090:HOH:O	2.16	0.46
1:0:106:A:H2'	1:0:107:U:O4'	2.15	0.46
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.46
1:0:1515:A:H2'	1:0:1516:U:C6	2.50	0.46
1:0:1762:C:H2'	1:0:1763:C:C6	2.51	0.46
1:0:2505:G:H8	39:0:9080: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
6:9:56:A:H1'	10:D:14:ARG:HG2	1.97	0.46
7:A:140:LEU:HB3	7:A:141:PRO:HD2	1.96	0.46
8:B:24:PRO:HD3	39:B:526:HOH:O	2.14	0.46
11:E:145:ALA:HB1	11:E:168:ILE:CD1	2.44	0.46
15:I:96:SER:H	15:I:99:GLN:CD	2.18	0.46
15:I:133:THR:HG22	15:I:134:ILE:H	1.79	0.46
19:M:57:LYS:NZ	19:M:144:ASP:OD2	2.38	0.46
20:N:179:LEU:HA	20:N:184:ILE:CD1	2.44	0.46
31:Y:205:ILE:HB	31:Y:230:ASN:HD21	1.80	0.46
32:Z:51:GLY:HA3	39:Z:226:HOH:O	2.15	0.46
1:0:336:G:O6	26:T:54:ASP:N	2.48	0.46
1:0:541:C:C2'	1:0:542:A:C5'	2.92	0.46
1:0:1483:C:O2'	1:0:1484:G:H5'	2.14	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
17:K:64:MET:HA	17:K:67:GLN:NE2	2.31	0.46
17:K:130:MET:SD	27:U:25:ASP:O	2.73	0.46
19:M:61:ILE:HD12	19:M:61:ILE:N	2.30	0.46
29:W:67:ALA:HB2	29:W:93:ILE:HD13	1.98	0.46
30:X:80:GLU:N	39:X:4025:HOH:O	2.48	0.46
31:Y:196:VAL:CG1	31:Y:226:ILE:HD13	2.45	0.46
31:Y:216:ARG:CD	39:Y:489:HOH:O	2.63	0.46
1:0:121:U:OP2	3:2:10:ARG:NH2	2.48	0.46
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.46
1:0:1185:U:H5'	39:0:6617:HOH:O	2.14	0.46
1:0:1422:U:H4'	39:0:7110:HOH:O	2.14	0.46
1:0:1976:G:H5''	39:0:8114:HOH:O	2.15	0.46
1:0:2455:A:H2'	1:0:2456:A:O4'	2.16	0.46
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.46
39:0:5833:HOH:O	8:B:229:ARG:HD2	2.14	0.46
4:3:11:CYS:HB2	4:3:20:HIS:CE1	2.50	0.46
9:C:120:ASP:O	9:C:124:VAL:HG23	2.16	0.46
10:D:41:LEU:HA	10:D:44:ILE:CG2	2.45	0.46
12:F:50:VAL:HG21	12:F:63:ILE:HG21	1.97	0.46
14:H:69:ARG:HB3	39:H:327:HOH:O	2.14	0.46
19:M:31:TRP:CD1	19:M:64:ARG:NH1	2.84	0.46
20:N:115:VAL:HG22	39:N:4044:HOH:O	2.15	0.46
29:W:4:LEU:HD23	29:W:54:PHE:CB	2.39	0.46
1:0:622:G:O2'	1:0:623:U:H5'	2.16	0.46
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.46
1:0:1614:G:H2'	39:0:7383:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1619:G:H2'	1:0:1620:C:O4'	2.16	0.46
1:0:2549:C:H2'	1:0:2550:U:O4'	2.16	0.46
1:0:2708:G:H2'	1:0:2709:G:O4'	2.16	0.46
39:0:5243:HOH:O	31:Y:135:LYS:HE3	2.16	0.46
39:0:9604:HOH:O	22:P:58:SER:HB3	2.15	0.46
9:C:200:PRO:HA	39:C:552:HOH:O	2.16	0.46
10:D:146:LYS:HZ1	20:N:107:ASN:ND2	2.14	0.46
11:E:15:GLN:HG3	11:E:20:ILE:HG12	1.98	0.46
14:H:50:ILE:HD12	14:H:149:VAL:CG1	2.45	0.46
15:I:102:GLN:HA	15:I:105:GLU:OE2	2.15	0.46
26:T:61:GLU:N	39:T:4021:HOH:O	2.40	0.46
1:0:894:A:C2	9:C:87:ARG:NH2	2.84	0.46
1:0:1471:A:H2'	1:0:1472:C:C6	2.49	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
26:T:25:ALA:O	26:T:39:ASN:CB	2.64	0.46
26:T:61:GLU:HG3	39:T:4018:HOH:O	2.15	0.46
28:V:24:LYS:O	28:V:27:LEU:HB3	2.16	0.46
29:W:1:MET:HB2	29:W:103:GLU:HG2	1.97	0.46
1:0:417:G:P	39:0:4977:HOH:O	2.73	0.46
1:0:545:G:H2'	1:0:546:C:O4'	2.16	0.46
1:0:699:C:C2	1:0:743:G:N2	2.84	0.46
1:0:962:C:C1'	20:N:5:ARG:NH1	2.73	0.46
1:0:1120:U:H5''	1:0:1120:U:H6	1.81	0.46
1:0:1450:C:O2'	1:0:1493:A:H2'	2.15	0.46
1:0:1878:G:O2'	1:0:1879:U:OP2	2.34	0.46
1:0:2002:C:C2'	1:0:2003:U:H5'	2.45	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
1:0:2831:C:H2'	1:0:2832:C:C5'	2.45	0.46
39:9:312:HOH:O	23:Q:27:GLN:HB2	2.16	0.46
8:B:80:ARG:HA	8:B:186:GLY:O	2.16	0.46
12:F:117:GLU:C	12:F:119:ARG:H	2.18	0.46
25:S:32:ALA:HA	25:S:36:GLU:OE1	2.16	0.46
31:Y:216:ARG:HD3	39:Y:489:HOH:O	2.15	0.46
1:0:37:A:H2'	1:0:38:G:H8	1.80	0.46
1:0:661:G:C5	1:0:686:A:C2	3.04	0.46
1:0:675:U:O2'	9:C:42:ARG:NH1	2.49	0.46
1:0:960:G:H8	39:0:6207:HOH:O	1.98	0.46
1:0:1804:A:H2'	1:0:1805:G:C8	2.51	0.46
1:0:1878:G:H5''	39:0:7982:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2717:C:OP1	8:B:207:LYS:HG3	2.16	0.46
39:9:440:HOH:O	20:N:65:ASP:HB3	2.14	0.46
7:A:101:GLU:OE2	7:A:131:HIS:HB2	2.16	0.46
7:A:130:THR:N	39:A:450:HOH:O	2.48	0.46
8:B:55:ASN:CG	8:B:63:GLU:HA	2.36	0.46
10:D:128:LEU:HB2	39:D:235:HOH:O	2.15	0.46
23:Q:4:ASN:ND2	39:Q:205:HOH:O	2.49	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
30:X:31:ILE:O	30:X:35:GLU:HG3	2.16	0.46
31:Y:122:ARG:NH2	39:Y:427:HOH:O	2.49	0.46
1:O:700:A:C2	18:L:71:GLU:HG2	2.51	0.45
1:O:1071:G:H4'	31:Y:154:ARG:HH22	1.80	0.45
1:O:1161:A:O5'	1:O:1161:A:H8	1.98	0.45
9:C:84:VAL:O	9:C:85:LYS:HB2	2.15	0.45
29:W:88:THR:HG22	29:W:90:TYR:CD1	2.51	0.45
1:O:130:C:H1'	39:O:4353:HOH:O	2.16	0.45
1:O:169:A:H1'	4:3:48:ASN:ND2	2.32	0.45
1:O:245:C:H2'	39:O:4738:HOH:O	2.16	0.45
1:O:407:A:H2'	1:O:408:A:C8	2.51	0.45
1:O:932:U:H2'	1:O:933:C:H6	1.81	0.45
1:O:1603:A:H5'	1:O:1605:G:C4'	2.46	0.45
1:O:2335:C:H2'	1:O:2336:G:C8	2.51	0.45
1:O:2802:C:H2'	1:O:2803:C:H6	1.81	0.45
3:2:41:HIS:CD2	3:2:44:ARG:H	2.33	0.45
6:9:5:G:O2'	6:9:6:C:H5'	2.17	0.45
7:A:132:ASP:OD1	7:A:133:ARG:N	2.49	0.45
9:C:133:ARG:HH11	9:C:133:ARG:HG3	1.81	0.45
10:D:23:VAL:HG23	10:D:23:VAL:O	2.16	0.45
18:L:91:VAL:CG1	18:L:120:LEU:HD23	2.47	0.45
18:L:122:ALA:HB3	18:L:125:PHE:CZ	2.52	0.45
19:M:134:ILE:CG2	19:M:141:ILE:HD13	2.46	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
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
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:112:GLU:HA	31:Y:112:GLU:OE1	2.17	0.45
31:Y:132:ASP:OD1	31:Y:135:LYS:HD2	2.16	0.45
1:O:2895:C:H2'	39:O:9813:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:4093:HOH:O	26:T:9:LYS:CD	2.64	0.45
6:9:6:C:O2'	20:N:33:ARG:NH2	2.46	0.45
8:B:38:VAL:HA	8:B:166:VAL:HG22	1.99	0.45
8:B:75:GLU:C	8:B:77:PRO:HD3	2.37	0.45
8:B:82:VAL:HG12	8:B:101:TRP:CE3	2.51	0.45
9:C:111:VAL:HB	39:C:506:HOH:O	2.15	0.45
14:H:149:VAL:HG13	39:H:358:HOH:O	2.16	0.45
20:N:42:HIS:CG	20:N:62:HIS:HE1	2.35	0.45
20:N:151:ASP:OD1	20:N:154:LEU:HD13	2.16	0.45
25:S:73:ASP:OD1	25:S:76:GLU:HG3	2.17	0.45
1:O:166:A:N7	18:L:25:GLY:HA2	2.31	0.45
1:O:264:G:H1'	1:O:265:U:H5	1.81	0.45
1:O:1450:C:C4'	1:O:1451:C:OP2	2.62	0.45
1:O:1496:A:H5'	1:O:1572:A:H1'	1.98	0.45
1:O:1733:A:H4'	8:B:212:GLN:HA	1.99	0.45
1:O:2053:G:H4'	24:R:136:TRP:CE2	2.52	0.45
1:O:2335:C:H2'	1:O:2336:G:H8	1.81	0.45
1:O:2421:G:H3'	1:O:2422:U:H5''	1.97	0.45
2:1:36:SER:O	2:1:46:ARG:HD3	2.16	0.45
8:B:305:ASP:O	8:B:306:LYS:CB	2.64	0.45
9:C:14:GLY:O	9:C:15:GLU:HB3	2.16	0.45
15:I:87:PRO:C	15:I:89:GLU:N	2.68	0.45
20:N:11:ARG:O	20:N:15:GLU:HG3	2.15	0.45
20:N:144:GLY:O	20:N:147:ILE:CG2	2.65	0.45
21:O:11:ILE:HD13	21:O:34:GLU:HG3	1.98	0.45
22:P:115:SER:O	22:P:116:SER:C	2.54	0.45
24:R:96:VAL:O	24:R:99:ALA:HB3	2.16	0.45
29:W:117:ARG:HB3	29:W:117:ARG:HH11	1.82	0.45
31:Y:112:GLU:OE2	31:Y:115:ARG:NH1	2.50	0.45
1:O:60:A:O2'	1:O:61:G:H5'	2.17	0.45
1:O:285:A:H2'	1:O:286:U:O4'	2.17	0.45
1:O:839:C:O2'	38:4:101:MHT:H7	2.15	0.45
1:O:907:A:H4'	1:O:1328:A:N1	2.31	0.45
1:O:962:C:H2'	1:O:963:C:H5'	1.99	0.45
1:O:1139:U:H2'	1:O:1140:C:C6	2.52	0.45
1:O:1942:A:H4'	39:O:8081:HOH:O	2.16	0.45
1:O:2001:G:O2'	1:O:2002:C:H5'	2.16	0.45
1:O:2104:C:O2	1:O:2485:A:N1	2.49	0.45
1:O:2353:A:H4'	1:O:2354:A:O5'	2.16	0.45
39:O:6697:HOH:O	16:J:46:ILE:HA	2.16	0.45
7:A:165:THR:O	7:A:165:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:329:TYR:HE2	27:U:15:PRO:HG2	1.82	0.45
16:J:127:ILE:HG22	36:J:202:CL:CL	2.54	0.45
20:N:110:THR:HB	20:N:113:SER:HG	1.81	0.45
1:0:146:U:O2'	1:0:147:G:H5'	2.17	0.45
1:0:281:U:O2'	1:0:282:C:H5'	2.17	0.45
1:0:297:U:H2'	1:0:298:C:C6	2.51	0.45
1:0:821:U:H5''	39:0:5786:HOH:O	2.15	0.45
1:0:858:U:H2'	1:0:859:C:H6	1.82	0.45
1:0:958:G:H2'	1:0:959:C:H6	1.82	0.45
1:0:1186:C:H42	1:0:1190:G:H22	1.63	0.45
1:0:1625:U:H5''	39:0:7441:HOH:O	2.16	0.45
1:0:1872:C:H2'	7:A:23:TYR:HD1	1.82	0.45
1:0:2266:A:OP2	19:M:90:ARG:NH2	2.50	0.45
1:0:2478:U:H2'	1:0:2479:A:H8	1.82	0.45
1:0:2498:C:O2'	1:0:2499:U:H5'	2.16	0.45
1:0:2511:A:H5'	1:0:2511:A:H8	1.82	0.45
1:0:2515:C:H2'	1:0:2516:G:O4'	2.16	0.45
1:0:2690:U:O2'	11:E:111:LYS:HE3	2.17	0.45
1:0:2910:A:H5''	39:0:9822:HOH:O	2.17	0.45
8:B:14:GLY:HA2	8:B:15:PRO:C	2.37	0.45
8:B:24:PRO:HG2	8:B:204:GLY:HA2	1.98	0.45
9:C:57:PRO:HD2	9:C:73:LEU:HD22	1.98	0.45
9:C:165:ASP:O	9:C:168:ARG:HB3	2.17	0.45
10:D:21:VAL:HA	10:D:131:THR:O	2.17	0.45
16:J:74:ARG:NH1	16:J:76:ASP:HB2	2.32	0.45
18:L:91:VAL:HB	39:L:358:HOH:O	2.16	0.45
19:M:18:GLY:O	19:M:21:ALA:HB3	2.16	0.45
20:N:38:LYS:HE2	20:N:107:ASN:HD21	1.80	0.45
20:N:72:GLU:O	20:N:72:GLU:HG2	2.17	0.45
24:R:18:LEU:HD22	24:R:21:ARG:NE	2.32	0.45
24:R:114:VAL:HG13	24:R:114:VAL:O	2.17	0.45
1:0:1183:C:H41	1:0:1192:A:H5'	1.81	0.45
1:0:1903:U:O2'	1:0:1904:A:C8	2.69	0.45
9:C:29:ASP:HB2	21:O:3:THR:HG22	1.98	0.45
9:C:130:GLU:OE1	9:C:130:GLU:HA	2.17	0.45
20:N:72:GLU:H	20:N:171:HIS:CE1	2.34	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
22:P:40:VAL:O	22:P:44:VAL:HG23	2.17	0.45
26:T:24:ARG:NH2	26:T:39:ASN:HD22	2.14	0.45
26:T:75:GLU:O	26:T:76:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:21:LEU:HD22	29:W:26:ILE:HD13	1.98	0.45
30:X:20:GLU:OE1	30:X:21:PRO:HD2	2.17	0.45
30:X:45:GLU:HG3	39:X:4017:HOH:O	2.16	0.45
30:X:73:ARG:HB2	30:X:88:GLU:OE2	2.17	0.45
1:0:558:C:HO2'	1:0:559:U:H5''	1.81	0.45
1:0:1261:A:H4'	39:0:6453:HOH:O	2.17	0.45
1:0:1414:A:H2'	1:0:1415:G:O4'	2.17	0.45
1:0:1588:G:C6	1:0:1589:G:N1	2.84	0.45
1:0:1624:A:H5'	1:0:1626:A:O4'	2.16	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
1:0:2361:A:H2'	1:0:2362:A:O4'	2.17	0.45
2:1:28:HIS:HB3	2:1:31:LYS:HB2	1.99	0.45
6:9:30:C:OP1	10:D:137:PRO:O	2.34	0.45
7:A:29:HIS:HB3	7:A:153:ARG:HH12	1.82	0.45
8:B:79:MET:HE1	39:B:561:HOH:O	2.16	0.45
9:C:133:ARG:HD2	39:C:518:HOH:O	2.15	0.45
11:E:11:VAL:HG13	11:E:23:GLU:O	2.16	0.45
12:F:1:PRO:H3	12:F:4:VAL:CG2	2.30	0.45
17:K:75:ARG:HE	17:K:94:ALA:HB3	1.82	0.45
19:M:47:ASP:CG	19:M:48:LYS:N	2.71	0.45
20:N:12:ARG:HH21	20:N:17:ARG:HD3	1.80	0.45
26:T:38:ARG:NH1	26:T:38:ARG:HG3	2.31	0.45
1:0:363:C:H2'	1:0:364:U:C6	2.52	0.45
1:0:657:G:H2'	1:0:658:C:H6	1.81	0.45
1:0:902:G:N7	18:L:18:HIS:CD2	2.85	0.45
1:0:1268:C:H2'	1:0:1269:G:H8	1.82	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
8:B:297:VAL:HB	39:B:539:HOH:O	2.17	0.45
9:C:235:PHE:CE2	9:C:243:VAL:HG21	2.52	0.45
12:F:43:GLY:O	12:F:45:ALA:N	2.46	0.45
12:F:50:VAL:CG2	12:F:63:ILE:HG21	2.47	0.45
26:T:71:VAL:HG12	26:T:72:ILE:N	2.32	0.45
29:W:154:ARG:HB3	29:W:154:ARG:HE	1.64	0.45
1:0:1028:U:H1'	39:0:6270:HOH:O	2.17	0.44
1:0:1175:G:H1'	1:0:1193:A:H2'	1.99	0.44
1:0:1659:A:H2'	1:0:1660:G:O4'	2.16	0.44
1:0:1761:U:H4'	22:P:82:GLY:O	2.18	0.44
1:0:1940:C:H4'	39:0:8079:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2054:A:N3	24:R:128:ARG:NH2	2.65	0.44
1:0:2256:G:H2'	1:0:2257:G:H5'	1.98	0.44
1:0:2614:C:O2'	1:0:2615:U:H5'	2.17	0.44
9:C:54:LEU:HD23	9:C:79:ARG:HG3	1.99	0.44
10:D:128:LEU:HD23	10:D:128:LEU:C	2.37	0.44
12:F:48:VAL:CG2	12:F:74:PHE:HB3	2.47	0.44
19:M:49:ALA:C	19:M:54:TYR:HB3	2.38	0.44
25:S:13:LYS:HE2	39:S:4005:HOH:O	2.17	0.44
26:T:55:PHE:CG	26:T:77:VAL:HG13	2.51	0.44
30:X:75:ALA:O	30:X:83:ALA:HA	2.17	0.44
1:0:24:G:H22	1:0:518:G:H1'	1.82	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.44
1:0:1940:C:H1'	39:0:8074:HOH:O	2.17	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	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
9:C:246:ARG:NE	39:C:583:HOH:O	2.39	0.44
18:L:56:LYS:HA	39:L:302:HOH:O	2.16	0.44
18:L:124:ASP:OD1	18:L:149:ARG:NH2	2.50	0.44
20:N:86:LEU:HD21	20:N:180:LEU:CD1	2.47	0.44
20:N:119:GLN:O	20:N:123:ILE:HG13	2.17	0.44
29:W:7:LEU:CD1	29:W:53:ALA:HB2	2.48	0.44
1:0:1490:G:H4'	1:0:1533:A:OP1	2.17	0.44
1:0:1909:A:H2'	1:0:1910:A:C8	2.53	0.44
1:0:2712:G:O2'	1:0:2713:G:H5'	2.18	0.44
1:0:2911:C:H3'	39:0:9823:HOH:O	2.16	0.44
3:2:19:SER:O	3:2:36:ASN:ND2	2.51	0.44
8:B:7:ARG:CD	8:B:9:GLY:O	2.65	0.44
8:B:217:ARG:CD	8:B:257:THR:HG22	2.47	0.44
8:B:240:GLY:HA3	39:B:608:HOH:O	2.17	0.44
9:C:131:PHE:CD2	9:C:232:LEU:HD22	2.52	0.44
9:C:246:ARG:NH1	39:C:584:HOH:O	2.49	0.44
11:E:126:ILE:HB	11:E:131:LEU:CD2	2.48	0.44
18:L:10:SER:O	18:L:11:ARG:HB3	2.18	0.44
19:M:125:ARG:HD3	39:M:390:HOH:O	2.16	0.44
24:R:29:LYS:HD3	39:R:332:HOH:O	2.17	0.44
24:R:33:ARG:NH2	39:R:332:HOH:O	2.50	0.44
28:V:42:ASN:O	28:V:44:GLY:N	2.50	0.44
1:0:499:G:O2'	1:0:500:G:H5'	2.16	0.44
1:0:2344:G:H2'	1:0:2344:G:N3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:52:A:H2'	6:9:53:G:O4'	2.18	0.44
6:9:114:G:H2'	6:9:115:C:C6	2.53	0.44
9:C:72:LYS:HG2	9:C:77:ALA:HA	1.98	0.44
39:C:542: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
20:N:23:ARG:NH2	20:N:55:ASP:OD1	2.50	0.44
25:S:15:MET:O	25:S:18:MET:HB3	2.18	0.44
29:W:46:ALA:O	29:W:49:ASN:HB2	2.17	0.44
30:X:10:VAL:HG11	30:X:36:HIS:HE1	1.82	0.44
31:Y:133:HIS:HA	31:Y:139:VAL:HG12	1.98	0.44
1:0:380:A:H2'	39:0:4901:HOH:O	2.15	0.44
1:0:401:C:H2'	1:0:402:U:C6	2.53	0.44
1:0:1019:C:H5'	39:0:6251:HOH:O	2.16	0.44
1:0:1137:G:H1'	39:0:6562:HOH:O	2.17	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.17	0.44
1:0:1478:U:H2'	1:0:1479:G:H8	1.82	0.44
1:0:2038:A:H5''	8:B:222:LYS:HG3	1.99	0.44
1:0:2055:A:H4'	24:R:132:ARG:HH21	1.82	0.44
39:0:7957:HOH:O	7:A:11:ARG:HG2	2.18	0.44
6:9:42:C:H5'	6:9:43:G:OP2	2.17	0.44
8:B:42:ALA:HB3	8:B:79:MET:SD	2.57	0.44
8:B:142:LEU:HD21	8:B:178:ALA:HB1	2.00	0.44
8:B:243:ASN:HA	8:B:244:PRO:C	2.38	0.44
8:B:336:GLN:NE2	39:B:643:HOH:O	2.49	0.44
10:D:27:ILE:HB	10:D:69:ILE:O	2.17	0.44
10:D:56:ARG:N	39:D:225:HOH:O	2.50	0.44
11:E:162:PHE:N	11:E:162:PHE:CD1	2.85	0.44
12:F:106:ALA:HB3	39:F:4024:HOH:O	2.18	0.44
14:H:114:ASP:N	39:H:344:HOH:O	2.50	0.44
16:J:19:MET:CE	16:J:132:LEU:HD21	2.47	0.44
16:J:45:VAL:HG22	16:J:46:ILE:N	2.33	0.44
19:M:60:VAL:C	19:M:61:ILE:HD12	2.37	0.44
22:P:83:LYS:HG3	22:P:84:ALA:H	1.81	0.44
24:R:39:THR:O	24:R:40:ALA:C	2.55	0.44
29:W:26:ILE:O	29:W:26:ILE:CG1	2.64	0.44
1:0:797:A:H5'	32:Z:10:ARG:N	2.32	0.44
1:0:1025:C:P	29:W:108:ARG:NH1	2.91	0.44
1:0:1421:C:O2'	1:0:1422:U:H5'	2.17	0.44
1:0:1517:C:O2'	1:0:1518:A:H5'	2.18	0.44
1:0:1730:G:C5'	1:0:1731:C:C6	3.01	0.44
1:0:2064:U:H4'	1:0:2653:A:OP1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2637:A:H5'	39:0:9422:HOH:O	2.16	0.44
7:A:36:ASP:C	7:A:38:ILE:H	2.20	0.44
7:A:38:ILE:HD13	7:A:38:ILE:HA	1.85	0.44
7:A:53:ALA:HB3	39:A:435:HOH:O	2.17	0.44
8:B:115:VAL:HA	8:B:116:PRO:HD3	1.75	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
10:D:140:ARG:N	39:D:240:HOH:O	2.49	0.44
10:D:153:THR:O	10:D:156:ARG:HB2	2.17	0.44
11:E:154:ILE:HD11	11:E:157:LYS:HE2	1.99	0.44
18:L:54:PRO:HG2	18:L:57:VAL:CG2	2.47	0.44
20:N:170:GLU:HA	20:N:173:ASP:OD2	2.18	0.44
28:V:20:LEU:HD11	28:V:53:ILE:HG23	1.99	0.44
30:X:36:HIS:CE1	30:X:40:HIS:CD2	3.06	0.44
31:Y:219:GLU:HG3	31:Y:220:GLU:N	2.32	0.44
1:0:185:G:H4'	1:0:186:A:OP1	2.17	0.44
1:0:271:C:H41	1:0:378:A:H2	1.63	0.44
1:0:1181:A:C2'	1:0:1182:C:H5'	2.47	0.44
1:0:1234:U:C4	8:B:244:PRO:HB3	2.53	0.44
1:0:2268:C:H2'	1:0:2269:C:C6	2.53	0.44
1:0:2858:U:H2'	1:0:2859:C:C6	2.52	0.44
6:9:106:U:O5'	6:9:106:U:H6	2.01	0.44
10:D:15:GLU:HA	10:D:16:PRO:HD3	1.88	0.44
10:D:41:LEU:CA	10:D:44:ILE:HG22	2.46	0.44
15:I:91:PHE:HA	15:I:131:GLY:CA	2.48	0.44
17:K:27:ARG:HD2	39:K:4015:HOH:O	2.18	0.44
19:M:76:ARG:HG2	19:M:76:ARG:HH11	1.81	0.44
25:S:57:THR:CG2	25:S:58:MET:N	2.80	0.44
27:U:9:CYS:CA	27:U:52:THR:HG23	2.36	0.44
29:W:4:LEU:HD23	29:W:4:LEU:HA	1.77	0.44
30:X:22:ASN:C	30:X:24:LYS:H	2.21	0.44
1:0:163:U:O3'	1:0:896:C:H4'	2.17	0.44
1:0:545:G:C8	1:0:545:G:C5'	2.99	0.44
1:0:559:U:H6	1:0:559:U:C5'	2.27	0.44
1:0:658:C:O2'	1:0:662:U:OP1	2.32	0.44
1:0:1180:U:H4'	15:I:86:GLU:HG2	2.00	0.44
1:0:1437:A:O2'	1:0:1438:G:H5'	2.18	0.44
1:0:1584:C:O2'	1:0:1585:C:H5'	2.17	0.44
1:0:1754:A:H2'	1:0:1755:A:O4'	2.18	0.44
1:0:2072:G:H3'	1:0:2073:G:C5'	2.48	0.44
1:0:2506:A:N6	1:0:2511:A:O2'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:35:ARG:HG2	39:2:133:HOH:O	2.17	0.44
4:3:69:TYR:HB2	4:3:78:HIS:CE1	2.53	0.44
6:9:11:A:P	23:Q:19:ARG:HH21	2.40	0.44
8:B:69:VAL:HA	8:B:70:PRO:HD3	1.84	0.44
9:C:133:ARG:HE	9:C:138:VAL:HG22	1.83	0.44
10:D:140:ARG:HH11	10:D:140:ARG:HG3	1.82	0.44
12:F:49:PHE:HE1	12:F:98:VAL:HG23	1.83	0.44
13:G:63:ARG:N	39:G:4014:HOH:O	2.50	0.44
15:I:134:ILE:C	15:I:135:GLU:HG3	2.38	0.44
17:K:62:PRO:CG	17:K:65:ARG:HH21	2.31	0.44
20:N:143:ARG:NH1	20:N:173:ASP:OD1	2.50	0.44
26:T:96:VAL:HG13	26:T:97:ARG:N	2.33	0.44
31:Y:187:VAL:CG2	31:Y:192:ASP:HB2	2.33	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
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
1:0:2819:C:O4'	8:B:96:PRO:HB2	2.18	0.44
4:3:16:GLU:HG3	4:3:18:GLN:HE21	1.82	0.44
4:3:20:HIS:HA	4:3:70:ARG:O	2.18	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
30:X:41:PHE:CZ	30:X:74:ALA:HB3	2.53	0.44
31:Y:100:ARG:NH1	31:Y:215:GLU:HA	2.33	0.44
1:0:35:U:H5'	9:C:47:GLY:O	2.18	0.43
1:0:485:A:O2'	1:0:487:G:H5'	2.18	0.43
1:0:844:A:C6	1:0:882:A:C5	3.06	0.43
1:0:952:G:N3	1:0:2302:A:H2'	2.33	0.43
1:0:1415:G:H5'	2:1:12:ASN:O	2.18	0.43
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.43
1:0:2433:A:H2'	1:0:2434:A:C8	2.52	0.43
1:0:2524:G:N2	1:0:2526:C:H41	2.12	0.43
1:0:2866:U:H4'	1:0:2867:G:H5'	2.00	0.43
7:A:223:ARG:HG3	39:A:514:HOH:O	2.17	0.43
9:C:218:VAL:N	39:C:583:HOH:O	2.50	0.43
10:D:166:ILE:HD12	39:D:247:HOH:O	2.17	0.43
17:K:41:LYS:O	17:K:42:ASN:HB2	2.18	0.43
19:M:59:GLY:HA3	19:M:141:ILE:CD1	2.47	0.43
25:S:76:GLU:HB3	39:S:4029:HOH:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:182:PHE:HD2	31:Y:200:THR:O	2.01	0.43
32:Z:10:ARG:HG3	32:Z:11:SER:N	2.33	0.43
1:O:688:A:N7	18:L:65:ASP:OD2	2.51	0.43
1:O:1119:G:H8	16:J:52:GLN:HE22	1.66	0.43
1:O:1174:A:C5	1:O:1201:C:H4'	2.52	0.43
1:O:2274:A:H1'	19:M:86:GLN:NE2	2.33	0.43
1:O:2809:G:H2'	1:O:2810:G:O4'	2.18	0.43
2:1:10:LYS:HG3	39:1:212:HOH:O	2.18	0.43
9:C:44:GLN:HA	39:C:439:HOH:O	2.18	0.43
10:D:64:ARG:HD3	10:D:67:ASP:CB	2.48	0.43
12:F:33:THR:HG21	12:F:59:ILE:O	2.17	0.43
14:H:83:GLU:HA	39:H:330:HOH:O	2.18	0.43
19:M:34:GLU:HB3	19:M:38:GLU:HG3	1.99	0.43
24:R:9:ASP:O	24:R:13:THR:HG22	2.17	0.43
25:S:14:ALA:HA	25:S:25:GLN:NE2	2.33	0.43
26:T:25:ALA:O	26:T:39:ASN:HB2	2.18	0.43
1:O:256:C:H2'	1:O:257:G:O4'	2.18	0.43
1:O:445:U:H2'	1:O:446:G:H8	1.82	0.43
1:O:1207:A:N6	39:O:6642:HOH:O	2.51	0.43
1:O:1839:A:H5'	1:O:2643:G:H4'	2.00	0.43
1:O:2091:G:O3'	8:B:235:ARG:HD3	2.17	0.43
1:O:2460:A:H5''	4:3:58:GLY:O	2.18	0.43
39:O:8248:HOH:O	8:B:216:LYS:HA	2.18	0.43
4:3:56:PRO:CA	39:3:245:HOH:O	2.66	0.43
9:C:168:ARG:NH2	9:C:190:ALA:O	2.51	0.43
10:D:39:ASP:HB2	39:D:219:HOH:O	2.18	0.43
14:H:27:PRO:HD3	14:H:123:ILE:HG22	2.01	0.43
16:J:84:ARG:HB2	16:J:98:PHE:CE1	2.53	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:O:299:U:H5'	39:O:5026:HOH:O	2.19	0.43
1:O:667:C:H2'	1:O:668:C:C6	2.54	0.43
1:O:793:A:H5''	22:P:83:LYS:HG2	1.99	0.43
1:O:1098:A:H2'	1:O:1099:G:O4'	2.17	0.43
1:O:1119:G:N2	1:O:1246:A:H2	2.13	0.43
1:O:1119:G:H8	16:J:52:GLN:NE2	2.16	0.43
1:O:1211:G:H2'	1:O:1212:C:H6	1.83	0.43
1:O:1517:C:O2	1:O:1670:A:C2	2.71	0.43
1:O:1674:C:P	25:S:34:LYS:HG3	2.59	0.43
1:O:1718:G:O2'	1:O:1719:G:H5'	2.19	0.43
1:O:2372:A:H2'	1:O:2373:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2443:C:H1'	18:L:56:LYS:HE3	2.00	0.43
1:0:2521:A:P	14:H:6:ALA:HB3	2.59	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
7:A:149:ASP:OD1	7:A:151:GLN:HB2	2.17	0.43
7:A:215:ILE:HG13	7:A:216:SER:N	2.33	0.43
8:B:190:MET:HG2	8:B:272:ILE:CG2	2.48	0.43
9:C:133:ARG:NH2	39:C:517:HOH:O	2.50	0.43
10:D:81:GLU:C	10:D:83:PHE:H	2.22	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
19:M:184:ARG:CG	19:M:185:PRO:HA	2.49	0.43
24:R:46:TYR:O	24:R:49:ALA:HB3	2.17	0.43
29:W:5:VAL:O	29:W:52:VAL:HG23	2.18	0.43
29:W:24:LEU:HD21	29:W:44:MET:SD	2.58	0.43
29:W:122:ARG:HG3	29:W:152:ALA:O	2.18	0.43
1:0:165:A:H5''	18:L:33:ALA:HB2	2.01	0.43
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.43
1:0:613:C:H2'	1:0:614:U:H6	1.83	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
1:0:1617:C:C4	1:0:1643:C:H4'	2.53	0.43
1:0:2299:G:C6	1:0:2300:A:C6	3.07	0.43
1:0:2609:G:N2	8:B:238:ASN:HD21	2.17	0.43
1:0:2861:G:H4'	8:B:282:GLY:N	2.34	0.43
1:0:2906:A:H5'	1:0:2907:C:O4'	2.18	0.43
8:B:84:LEU:O	8:B:99:GLU:HA	2.18	0.43
9:C:175:LYS:HD3	9:C:184:ARG:O	2.19	0.43
16:J:108:PRO:HG2	16:J:109:TYR:CD1	2.54	0.43
19:M:99:ARG:NH1	39:M:375:HOH:O	2.49	0.43
20:N:163:PHE:O	20:N:164:ASP:OD1	2.36	0.43
23:Q:35:ASP:N	23:Q:35:ASP:OD1	2.51	0.43
25:S:8:PRO:HD2	28:V:32:ALA:HA	2.00	0.43
30:X:34:ARG:NH1	30:X:48:VAL:O	2.40	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.36	0.43
1:0:69:A:C2'	1:0:70:A:OP2	2.67	0.43
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.43
1:0:1052:G:H2'	1:0:1052:G:N3	2.33	0.43
1:0:1102:C:H4'	39:0:6484:HOH:O	2.18	0.43
1:0:1123:A:C2	1:0:1129:C:H4'	2.54	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)
1:O:1735:C:H5'	8:B:235:ARG:NH2	2.34	0.43
6:9:3:A:H2	6:9:21:G:N3	2.17	0.43
10:D:24:HIS:CE1	10:D:26:GLY:H	2.37	0.43
10:D:173:GLU:OE1	10:D:174:VAL:HG23	2.19	0.43
11:E:107:PHE:CZ	11:E:152:THR:HB	2.53	0.43
12:F:48:VAL:HG12	12:F:97:ALA:CB	2.48	0.43
15:I:99:GLN:O	15:I:103:ILE:HG13	2.18	0.43
17:K:6:ALA:HB3	17:K:116:GLU:HG2	2.01	0.43
24:R:84:ALA:O	24:R:88:PHE:HD1	2.01	0.43
25:S:80:ARG:NH1	39:S:4029:HOH:O	2.51	0.43
27:U:6:CYS:C	27:U:8:TYR:H	2.22	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
30:X:78:GLU:CG	30:X:79:GLU:H	2.28	0.43
31:Y:133:HIS:HA	31:Y:139:VAL:CG1	2.48	0.43
1:O:297:U:H2'	1:O:298:C:H6	1.82	0.43
1:O:1023:C:H2'	1:O:1024:G:O4'	2.18	0.43
1:O:1066:U:H2'	1:O:1067:A:C8	2.54	0.43
1:O:1421:C:H2'	1:O:1422:U:C6	2.52	0.43
1:O:1427:A:H61	1:O:1440:U:C1'	2.30	0.43
1:O:1477:C:H5'	1:O:1868:G:H5''	2.01	0.43
1:O:1845:A:O3'	7:A:187:PRO:HB2	2.19	0.43
1:O:2731:G:H2'	1:O:2732:U:O4'	2.18	0.43
1:O:2761:A:C4	1:O:2763:G:C8	3.07	0.43
7:A:95:PRO:HA	7:A:153:ARG:HA	1.99	0.43
7:A:164:ARG:HA	32:Z:69:TYR:CE1	2.54	0.43
8:B:157:LYS:O	8:B:159:PRO:HD3	2.18	0.43
9:C:136:VAL:HA	9:C:137:PRO:C	2.38	0.43
9:C:194:PHE:HA	9:C:234:VAL:HG13	2.01	0.43
11:E:47:VAL:HG11	11:E:69:ILE:HD13	2.00	0.43
23:Q:93:ARG:HG3	23:Q:93:ARG:NH1	2.33	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
1:O:396:U:OP2	4:3:38:ARG:HD2	2.19	0.43
1:O:1506:U:H6	1:O:1506:U:H5'	1.83	0.43
1:O:1603:A:H5''	1:O:1604:G:H3'	2.00	0.43
1:O:1925:G:O2'	1:O:1926:G:H5'	2.19	0.43
6:9:59:C:H4'	39:9:364:HOH:O	2.19	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
17:K:30:LYS:C	17:K:55:VAL:HG13	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:34:GLY:C	18:L:36:ASP:H	2.22	0.43
19:M:107:ARG:NH1	39:M:378:HOH:O	2.49	0.43
20:N:108:SER:HA	20:N:109:PRO:HD3	1.82	0.43
25:S:10:VAL:HG11	28:V:36:ALA:HA	2.00	0.43
1:O:468:U:H3'	39:O:5101:HOH:O	2.18	0.43
1:O:968:G:H1'	14:H:35:LYS:HD2	2.00	0.43
1:O:1213:C:C2'	1:O:1214:G:H5'	2.49	0.43
1:O:1571:G:H1'	1:O:1627:G:N2	2.34	0.43
1:O:1600:G:H4'	39:O:7411:HOH:O	2.17	0.43
1:O:2039:A:H2'	1:O:2040:C:C6	2.54	0.43
1:O:2754:G:HO2'	1:O:2755:G:H5'	1.82	0.43
6:9:8:G:H4'	23:Q:27:GLN:HE21	1.84	0.43
8:B:13:PHE:O	8:B:16:ARG:HD2	2.19	0.43
8:B:22:GLU:HA	8:B:205:VAL:HG21	2.01	0.43
8:B:278:PRO:HD3	8:B:294:TYR:CE2	2.54	0.43
10:D:14:ARG:NH1	39:D:209: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	39:H:327:HOH:O	2.19	0.43
15:I:126:THR:HG22	15:I:126:THR:O	2.19	0.43
26:T:37:GLN:HB3	39:T:4017:HOH:O	2.19	0.43
1:O:213:G:O2'	1:O:214:U:OP2	2.37	0.43
1:O:361:C:H2'	1:O:362:G:O4'	2.19	0.43
1:O:1314:U:H5''	1:O:1316:G:O4'	2.18	0.43
1:O:2120:U:H2'	1:O:2121:G:O4'	2.19	0.43
1:O:2712:G:H5'	39:O:9537:HOH:O	2.18	0.43
1:O:2764:C:H2'	1:O:2765:C:C6	2.53	0.43
1:O:2898:G:H4'	8:B:288:GLY:HA2	2.00	0.43
6:9:29:C:H2'	6:9:30:C:C5'	2.43	0.43
7:A:105:VAL:HG13	7:A:155:THR:O	2.18	0.43
10:D:20:LYS:HA	10:D:75:LEU:O	2.19	0.43
12:F:46:GLU:N	39:F:4011:HOH:O	2.52	0.43
14:H:6:ALA:CA	14:H:61:ARG:HH12	2.26	0.43
14:H:49:GLN:HB3	14:H:170:ARG:CG	2.48	0.43
14:H:49:GLN:CB	14:H:170:ARG:HG3	2.46	0.43
20:N:82:TYR:CD2	20:N:82:TYR:C	2.92	0.43
21:O:32:ARG:HD3	21:O:32:ARG:C	2.39	0.43
24:R:4:TYR:CE1	24:R:17:MET:HE2	2.53	0.43
26:T:14:ALA:HA	26:T:15:PRO:HD3	1.93	0.43
26:T:71:VAL:HG13	26:T:91:LEU:O	2.19	0.43
27:U:17:THR:HG22	27:U:18:GLY:H	1.84	0.43
30:X:76:ARG:O	30:X:77:PHE:CB	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.42
1:0:1427:A:N6	1:0:1440:U:H1'	2.34	0.42
1:0:1702:U:H1'	39:0:7352:HOH:O	2.20	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
1:0:1929:G:H1'	39:0:8072:HOH:O	2.18	0.42
1:0:2402:A:H1'	39:0:8828:HOH:O	2.19	0.42
39:0:6158:HOH:O	21:O:39:THR:HB	2.18	0.42
6:9:3:A:OP2	6:9:25:G:N2	2.52	0.42
9:C:95:GLU:CD	9:C:95:GLU:H	2.23	0.42
9:C:115:LEU:HD21	9:C:243:VAL:CG1	2.36	0.42
11:E:132:THR:HG23	11:E:132:THR:O	2.19	0.42
15:I:95:LEU:O	15:I:134:ILE:HG23	2.18	0.42
17:K:98:VAL:HG13	17:K:102:GLU:CA	2.40	0.42
20:N:114:LYS:O	20:N:117:ALA:HB3	2.19	0.42
20:N:158:LEU:C	20:N:159:TYR:HD1	2.22	0.42
21:O:14:LEU:HG	21:O:102:ILE:HD11	2.00	0.42
21:O:25:VAL:HG23	21:O:26:TRP:CE3	2.54	0.42
27:U:23:HIS:HB2	27:U:27:ALA:HB3	2.00	0.42
29:W:69:ARG:HG3	29:W:118:LEU:HD23	2.01	0.42
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
31:Y:97:LEU:C	31:Y:98:GLN:HG2	2.39	0.42
1:0:111:C:H2'	1:0:112:G:O4'	2.19	0.42
1:0:960:G:N3	1:0:960:G:H2'	2.33	0.42
1:0:2039:A:OP2	8:B:234:ARG:NH2	2.52	0.42
1:0:2815:G:C5	16:J:102:ARG:HG2	2.54	0.42
6:9:26:C:O2'	6:9:27:C:H5'	2.19	0.42
6:9:44:A:O4'	10:D:76:ARG:NE	2.48	0.42
9:C:16:VAL:HG21	9:C:237:GLU:OE1	2.19	0.42
9:C:35:VAL:HG23	9:C:220:THR:HG22	2.01	0.42
10:D:81:GLU:C	10:D:83:PHE:N	2.72	0.42
15:I:71:ALA:O	15:I:75:LYS:HG3	2.19	0.42
16:J:15:ARG:NH1	16:J:43:ARG:NH1	2.67	0.42
19:M:46:LEU:HD22	19:M:50:ARG:HD2	2.00	0.42
20:N:48:VAL:HG11	20:N:55:ASP:CB	2.46	0.42
21:O:105:ASN:HD21	21:O:109:SER:N	2.16	0.42
26:T:65:VAL:HG22	26:T:72:ILE:HG22	2.01	0.42
28:V:1:THR:O	28:V:2:VAL:C	2.56	0.42
28:V:12:THR:HG22	28:V:15:GLU:H	1.83	0.42
31:Y:229:LEU:O	31:Y:231:PRO:HD3	2.19	0.42
1:0:87:C:C2	3:2:30:ASP:OD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:221:G:H2'	1:0:222:A:C8	2.53	0.42
1:0:553:G:P	31:Y:204:ARG:NH2	2.92	0.42
1:0:953:G:H2'	39:0:6189:HOH:O	2.19	0.42
1:0:1123:A:C6	1:0:1238:C:H5'	2.54	0.42
39:0:5339:HOH:O	31:Y:158:LYS:HD3	2.18	0.42
4:3:91:GLN:O	4:3:92:GLU:HB2	2.20	0.42
7:A:66:ARG:CB	7:A:66:ARG:NH1	2.83	0.42
8:B:63:GLU:O	8:B:63:GLU:HG3	2.19	0.42
8:B:175:LEU:C	8:B:175:LEU:CD2	2.88	0.42
9:C:49:ASP:HB3	9:C:52:ALA:HB2	2.00	0.42
10:D:19:GLU:HG3	39:D:210:HOH:O	2.19	0.42
11:E:31:ARG:NH1	39:E:4034:HOH:O	2.52	0.42
18:L:35:ARG:O	18:L:40:PHE:HA	2.19	0.42
18:L:66:VAL:CG2	18:L:67:ARG:N	2.83	0.42
21:O:79:VAL:O	21:O:80:ASP:HB2	2.19	0.42
26:T:63:ILE:HD11	26:T:75:GLU:HB2	2.01	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
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.42
1:0:503:G:H2'	1:0:504:G:H8	1.83	0.42
1:0:694:A:H4'	1:0:2441:U:OP1	2.20	0.42
1:0:1772:C:H5'	1:0:1773:G:C5	2.55	0.42
1:0:1805:G:H2'	1:0:1806:G:C8	2.53	0.42
1:0:2090:G:H2'	1:0:2091:G:C8	2.54	0.42
1:0:2445:U:H2'	1:0:2446:G:H8	1.79	0.42
1:0:2653:A:H2'	1:0:2654:C:C6	2.55	0.42
1:0:2676:C:H4'	16:J:70:PHE:CE1	2.54	0.42
1:0:2842:G:H2'	1:0:2843:A:H5'	2.01	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
8:B:320:GLN:NE2	8:B:321:PRO:CD	2.72	0.42
10:D:36:ASN:C	39:D:222:HOH:O	2.57	0.42
10:D:55:LYS:O	10:D:56:ARG:HB2	2.19	0.42
20:N:154:LEU:HG	20:N:155:GLU:N	2.34	0.42
28:V:39:ALA:C	28:V:41:GLU:N	2.72	0.42
29:W:48:VAL:CG1	29:W:48:VAL:O	2.67	0.42
31:Y:108:ASP:OD1	31:Y:199:ASP:HB3	2.19	0.42
1:0:20:G:H21	24:R:117:HIS:HD2	1.66	0.42
1:0:303:C:H2'	1:0:304:G:O4'	2.20	0.42
1:0:541:C:O2'	1:0:542:A:H5''	2.20	0.42
1:0:1041:U:H4'	1:0:1295:G:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1163:G:N2	39:I:4004:HOH:O	2.49	0.42
1:0:1935:C:H2'	1:0:1936:C:H6	1.84	0.42
1:0:2502:C:H2'	1:0:2503:A:H5'	2.01	0.42
4:3:8:ASN:O	4:3:9:THR:HB	2.19	0.42
8:B:223:ARG:O	8:B:228:ALA:HB2	2.20	0.42
12:F:70:LYS:C	12:F:72:VAL:H	2.22	0.42
15:I:87:PRO:O	15:I:89:GLU:HG3	2.19	0.42
17:K:65:ARG:O	17:K:66:ARG:HB2	2.19	0.42
21:O:25:VAL:CG2	21:O:26:TRP:N	2.81	0.42
22:P:91:LYS:O	22:P:95:GLU:HG3	2.20	0.42
24:R:59:PHE:O	24:R:63:ASN:HB3	2.19	0.42
27:U:14:GLU:HA	27:U:15:PRO:HD2	1.94	0.42
29:W:122:ARG:HG3	29:W:122:ARG:HH11	1.84	0.42
1:0:318:U:O2'	1:0:338:C:H2'	2.19	0.42
1:0:396:U:C1'	39:0:4950:HOH:O	2.66	0.42
1:0:1183:C:O2	1:0:1183:C:H2'	2.19	0.42
1:0:1874:U:P	7:A:51:ARG:HD2	2.59	0.42
7:A:69:LEU:HD11	7:A:159:VAL:HG13	2.01	0.42
8:B:277:GLU:N	8:B:278:PRO:CD	2.83	0.42
16:J:34:GLU:HA	16:J:34:GLU:OE1	2.19	0.42
16:J:52:GLN:HG3	16:J:53:ILE:H	1.83	0.42
17:K:28:GLU:HG2	17:K:58:THR:CB	2.47	0.42
24:R:4:TYR:N	39:R:308:HOH:O	2.53	0.42
29:W:65:VAL:HG11	29:W:116:LEU:HD13	2.02	0.42
29:W:119:HIS:O	29:W:153:MET:HB3	2.19	0.42
1:0:431:G:O2'	1:0:432:G:H5'	2.20	0.42
1:0:1268:C:O2'	31:Y:169:ARG:HB2	2.20	0.42
1:0:1666:C:H2'	1:0:1667:A:H8	1.84	0.42
1:0:1798:C:H1'	22:P:66:GLN:OE1	2.20	0.42
1:0:2115:U:H2'	1:0:2116:U:C6	2.54	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
2:1:8:GLN:HE22	2:1:11:LYS:NZ	2.18	0.42
6:9:55:U:H4'	6:9:56:A:C8	2.55	0.42
7:A:72:GLU:HG3	32:Z:66:GLY:HA2	2.02	0.42
7:A:223:ARG:O	7:A:223:ARG:HG2	2.20	0.42
9:C:16:VAL:HG12	9:C:17:ASP:N	2.35	0.42
10:D:54:ALA:HB2	10:D:69:ILE:CD1	2.48	0.42
10:D:172:VAL:HG12	10:D:173:GLU:N	2.35	0.42
14:H:29:SER:HA	14:H:62:HIS:CD2	2.55	0.42
14:H:32:ALA:C	14:H:33:GLN:HG3	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:146:ALA:O	14:H:150:LYS:HG3	2.19	0.42
20:N:74:PRO:HG2	20:N:159:TYR:CZ	2.55	0.42
21:O:96:VAL:CG1	21:O:97:SER:N	2.83	0.42
23:Q:24:SER:HB3	23:Q:28:ARG:HH21	1.83	0.42
24:R:29:LYS:CD	39:R:335:HOH:O	2.68	0.42
26:T:41:ARG:HG2	26:T:41:ARG:NH1	2.33	0.42
30:X:9:VAL:HG22	30:X:88:GLU:OE2	2.20	0.42
31:Y:125:LYS:HB2	31:Y:126:PRO:HD2	2.01	0.42
1:O:474:C:O3'	9:C:73:LEU:CD2	2.67	0.42
1:O:951:A:H5''	23:Q:42:LYS:HD3	2.02	0.42
1:O:963:C:O2	1:O:1005:A:N1	2.53	0.42
1:O:1186:C:H5''	39:O:6619:HOH:O	2.20	0.42
1:O:1201:C:H2'	1:O:1202:A:H5'	2.02	0.42
1:O:1334:C:H2'	1:O:1335:C:H6	1.84	0.42
1:O:1743:G:H2'	1:O:1744:G:O4'	2.19	0.42
1:O:2087:C:O2'	1:O:2088:C:H5'	2.20	0.42
1:O:2251:G:H2'	1:O:2252:A:C8	2.54	0.42
10:D:23:VAL:CG2	10:D:73:VAL:HB	2.49	0.42
11:E:101:GLU:HB2	11:E:116:THR:O	2.19	0.42
20:N:143:ARG:NH1	20:N:173:ASP:OD2	2.52	0.42
23:Q:16:ASN:HB2	39:Q:215:HOH:O	2.19	0.42
24:R:145:LEU:HD12	24:R:146:ILE:N	2.34	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
1:O:69:A:H2'	1:O:70:A:OP2	2.19	0.42
1:O:934:C:H2'	1:O:935:G:C8	2.54	0.42
1:O:962:C:C2'	1:O:963:C:H5'	2.50	0.42
1:O:1181:A:H2'	1:O:1182:C:C5'	2.49	0.42
1:O:1268:C:O2'	1:O:1269:G:H5'	2.20	0.42
1:O:1377:C:H2'	1:O:1723:G:O6	2.20	0.42
1:O:1903:U:O2'	1:O:1904:A:N7	2.51	0.42
1:O:2133:U:H4'	1:O:2134:G:C5'	2.49	0.42
1:O:2237:G:H1'	39:O:8506:HOH:O	2.19	0.42
4:3:6:ARG:O	4:3:7:PHE:HB3	2.20	0.42
4:3:69:TYR:O	4:3:77:ALA:HA	2.20	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
8:B:226:LYS:O	8:B:230:GLN:HG2	2.20	0.42
10:D:170:TYR:O	10:D:171:ASP:HB3	2.20	0.42
11:E:101:GLU:HB3	11:E:117:THR:HA	2.01	0.42
11:E:119:HIS:HE1	11:E:147:ASP:OD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:52:GLU:OE1	12:F:78:GLU:OE1	2.38	0.42
18:L:72:ASN:O	18:L:76:LEU:HG	2.20	0.42
20:N:151:ASP:HB3	39:N:4054:HOH:O	2.19	0.42
24:R:61:GLN:HE21	24:R:61:GLN:HB2	1.63	0.42
26:T:73:HIS:CD2	26:T:88:PRO:CG	3.03	0.42
29:W:73:LEU:HD12	29:W:73:LEU:HA	1.73	0.42
30:X:25:ARG:HG2	39:X:4011:HOH:O	2.20	0.42
31:Y:170:SER:OG	31:Y:175:ARG:HG3	2.19	0.42
1:O:183:A:H1'	19:M:161:ARG:NH1	2.35	0.42
1:O:432:G:O2'	1:O:433:C:H5'	2.20	0.42
1:O:967:U:O2	14:H:35:LYS:HE3	2.19	0.42
1:O:1018:A:H4'	23:Q:59:GLN:HE22	1.85	0.42
1:O:1169:U:H3	1:O:1177:A:H61	1.68	0.42
1:O:1422:U:H2'	1:O:1423:C:C6	2.54	0.42
1:O:1838:U:O4'	1:O:2644:C:C2	2.73	0.42
1:O:1943:C:O4'	7:A:212:PRO:HA	2.20	0.42
1:O:2096:A:C8	1:O:2539:U:C2	3.07	0.42
1:O:2353:A:H1'	23:Q:21:ARG:HH12	1.85	0.42
1:O:2846:C:OP1	8:B:158:LYS:HD3	2.19	0.42
4:3:11:CYS:HB2	4:3:20:HIS:NE2	2.34	0.42
1:O:333:G:O2'	1:O:334:G:H5'	2.20	0.41
1:O:424:C:H2'	1:O:425:U:C6	2.55	0.41
1:O:1163:G:H2'	1:O:1164:U:C5	2.54	0.41
1:O:1797:A:H2'	1:O:1799:G:O5'	2.20	0.41
1:O:2134:G:N2	1:O:2242:U:C2	2.89	0.41
1:O:2443:C:O3'	18:L:56:LYS:HE3	2.20	0.41
1:O:2456:A:H1'	39:O:8946:HOH:O	2.20	0.41
2:1:41:LYS:NZ	39:1:236:HOH:O	2.53	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
8:B:145:HIS:CD2	8:B:146:THR:O	2.68	0.41
9:C:32:GLY:O	9:C:36:ARG:HB2	2.20	0.41
9:C:140:VAL:CG1	9:C:141:SER:N	2.82	0.41
10:D:99:ASP:CB	10:D:103:ASN:HB2	2.50	0.41
14:H:56:GLU:HA	14:H:132:ALA:HB2	2.02	0.41
16:J:46:ILE:O	16:J:46:ILE:CG1	2.67	0.41
17:K:113:ILE:HD12	17:K:128:ALA:CB	2.49	0.41
19:M:57:LYS:HG2	19:M:58:GLN:H	1.85	0.41
20:N:21:HIS:HB3	39:N:4011:HOH:O	2.19	0.41
23:Q:16:ASN:HD22	23:Q:16:ASN:HA	1.60	0.41
24:R:40:ALA:O	24:R:44:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:80:A:H5''	26:T:41:ARG:CZ	2.50	0.41
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.41
1:0:1050:G:C6	1:0:1051:C:C4	3.08	0.41
1:0:1968:A:H2'	1:0:1969:A:C8	2.55	0.41
1:0:2303:A:H4'	39:0:8645:HOH:O	2.20	0.41
36:0:3189:CL:CL	39:K:4017:HOH:O	2.59	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
9:C:236:THR:CG2	9:C:239:ALA:H	2.08	0.41
14:H:157:TYR:CD1	14:H:157:TYR:C	2.93	0.41
20:N:83:LEU:HD13	20:N:175:LEU:HD23	2.02	0.41
23:Q:32:GLU:O	23:Q:93:ARG:NH2	2.53	0.41
24:R:43:ALA:O	24:R:47:LEU:HG	2.20	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
1:0:876:A:N3	1:0:876:A:C2'	2.84	0.41
1:0:1197:G:H1'	1:0:1203:G:N2	2.35	0.41
1:0:1948:G:N2	1:0:1965:C:H1'	2.34	0.41
1:0:2064:U:H2'	1:0:2065:C:H6	1.84	0.41
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.41
1:0:2511:A:H2'	1:0:2512:U:O4'	2.20	0.41
6:9:2:U:OP2	6:9:3:A:H5'	2.21	0.41
7:A:217:ARG:HH11	7:A:217:ARG:CG	2.33	0.41
9:C:27:ARG:NH2	21:O:4:ASN:ND2	2.68	0.41
9:C:93:LYS:O	9:C:98:ARG:NH2	2.52	0.41
10:D:40:ILE:O	10:D:44:ILE:HG22	2.20	0.41
12:F:21:GLU:O	12:F:24:ARG:CG	2.67	0.41
14:H:43:ALA:O	14:H:170:ARG:NH1	2.53	0.41
16:J:56:LYS:HE2	16:J:60:ARG:NH2	2.35	0.41
20:N:62:HIS:HB3	20:N:65:ASP:OD1	2.21	0.41
21:O:4:ASN:HA	21:O:5:PRO:HD3	1.84	0.41
21:O:33:LEU:HA	21:O:40:HIS:NE2	2.36	0.41
29:W:117:ARG:CB	29:W:117:ARG:NH1	2.83	0.41
1:0:30:U:OP2	9:C:181:ALA:HB2	2.19	0.41
1:0:903:U:O4	18:L:18:HIS:HB2	2.20	0.41
1:0:1206:U:H2'	1:0:1207:A:O4'	2.20	0.41
1:0:1472:C:O5'	1:0:1472:C:H6	2.03	0.41
1:0:1771:U:O2'	1:0:1773:G:N7	2.51	0.41
39:0:4093:HOH:O	26:T:9:LYS:HD3	2.19	0.41
6:9:81:C:O2'	6:9:82:U:H5'	2.20	0.41
8:B:5:ARG:HH11	8:B:8:LYS:HE2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:154:VAL:HA	8:B:155:PRO:HD3	1.81	0.41
10:D:159:PRO:O	10:D:162:ALA:HB3	2.21	0.41
11:E:7:ILE:HG22	11:E:45:ASP:O	2.20	0.41
14:H:91:ARG:NH1	14:H:138:THR:OG1	2.53	0.41
16:J:116:LEU:HB2	16:J:119:THR:HG21	2.02	0.41
16:J:131:THR:HG22	16:J:134:GLU:H	1.84	0.41
17:K:20:CYS:HB2	17:K:29:LEU:HG	2.02	0.41
20:N:32:PRO:HD2	20:N:99:GLU:O	2.20	0.41
20:N:114:LYS:O	20:N:118:ILE:HG13	2.21	0.41
20:N:155:GLU:O	20:N:156:GLU:HG3	2.20	0.41
22:P:59:ARG:HG2	22:P:59:ARG:HH11	1.85	0.41
25:S:37:VAL:O	25:S:41:VAL:HG23	2.20	0.41
25:S:73:ASP:O	25:S:77:VAL:HG23	2.20	0.41
26:T:39:ASN:ND2	39:T:4017:HOH:O	2.54	0.41
29:W:21:LEU:CD1	29:W:26:ILE:HD11	2.40	0.41
1:0:320:G:H2'	1:0:321:A:C8	2.55	0.41
1:0:646:G:H5''	9:C:96:LYS:HD2	2.03	0.41
1:0:820:G:H5'	1:0:821:U:H5'	2.02	0.41
1:0:1041:U:C2'	1:0:1042:U:H5'	2.51	0.41
1:0:1112:G:H1	1:0:1251:C:N4	2.18	0.41
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.41
1:0:2866:U:C4	27:U:50:GLU:HB3	2.55	0.41
6:9:20:G:O2'	6:9:21:G:H5'	2.20	0.41
9:C:13:ASP:OD1	9:C:13:ASP:O	2.39	0.41
9:C:218:VAL:HG12	39:C:583:HOH:O	2.20	0.41
13:G:69:ARG:NH1	39:G:4016:HOH:O	2.53	0.41
14:H:41:LYS:O	14:H:87:LYS:HE2	2.20	0.41
15:I:88:GLN:HE21	15:I:128:THR:HG21	1.85	0.41
20:N:163:PHE:CZ	20:N:171:HIS:ND1	2.88	0.41
31:Y:203:VAL:HG12	31:Y:228:VAL:HG22	2.00	0.41
1:0:11:A:H5'	1:0:12:U:OP2	2.20	0.41
1:0:595:U:O2'	1:0:596:C:H5'	2.21	0.41
1:0:1216:G:O2'	1:0:1217:G:H5'	2.21	0.41
1:0:1819:G:H2'	1:0:1820:G:C5'	2.51	0.41
1:0:1972:U:C2'	1:0:1973:A:C5'	2.99	0.41
1:0:2271:G:N3	1:0:2271:G:H2'	2.35	0.41
1:0:2392:C:H4'	39:0:8782:HOH:O	2.19	0.41
1:0:2471:G:N3	1:0:2633:A:H2	2.19	0.41
1:0:2568:A:H8	1:0:2568:A:O5'	2.03	0.41
7:A:210:GLY:HA3	39:A:490:HOH:O	2.19	0.41
8:B:114:ASP:O	8:B:115:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:211:ASP:HB3	39:C:575:HOH:O	2.21	0.41
11:E:166:VAL:HG12	39:E:4041:HOH:O	2.20	0.41
16:J:88:PRO:HA	36:J:203:CL:CL	2.58	0.41
17:K:55:VAL:CG1	17:K:56:SER:N	2.83	0.41
22:P:18:LYS:O	22:P:21:VAL:HG13	2.20	0.41
29:W:131:PRO:HB2	39:W:4057:HOH:O	2.21	0.41
31:Y:190:VAL:HG23	39:Y:482:HOH:O	2.20	0.41
1:O:75:U:H2'	1:O:76:G:C8	2.55	0.41
1:O:283:U:C5	1:O:284:C:N3	2.88	0.41
1:O:291:C:H2'	1:O:292:G:O4'	2.21	0.41
1:O:440:C:O2'	1:O:441:A:H5'	2.19	0.41
1:O:695:C:H2'	1:O:696:C:C6	2.55	0.41
1:O:783:C:OP1	7:A:180:LYS:HE3	2.21	0.41
1:O:940:G:C5	1:O:1027:G:C2	3.09	0.41
1:O:1166:A:H61	1:O:1180:U:H3	1.69	0.41
1:O:2000:G:O2'	1:O:2001:G:H5'	2.21	0.41
1:O:2297:U:H1'	39:O:8672:HOH:O	2.19	0.41
1:O:2502:C:H2'	1:O:2503:A:O4'	2.20	0.41
2:1:28:HIS:CD2	2:1:31:LYS:HG3	2.55	0.41
8:B:60:SER:C	8:B:62:ARG:H	2.24	0.41
8:B:280:VAL:HG13	8:B:333:GLU:O	2.19	0.41
9:C:139:VAL:CG1	39:C:580:HOH:O	2.62	0.41
15:I:70:THR:O	15:I:72:GLU:N	2.53	0.41
20:N:147:ILE:O	20:N:150:TYR:HB3	2.20	0.41
21:O:11:ILE:O	21:O:15:LYS:HG3	2.20	0.41
22:P:11:ALA:HB2	22:P:18:LYS:HA	2.03	0.41
22:P:24:ASN:HA	22:P:25:PRO:HD3	1.90	0.41
23:Q:50:GLY:HA3	23:Q:87:THR:OG1	2.21	0.41
28:V:12:THR:CG2	28:V:15:GLU:H	2.34	0.41
28:V:42:ASN:N	28:V:43:PRO:CD	2.83	0.41
1:O:241:A:C2	1:O:378:A:H4'	2.56	0.41
1:O:948:G:C6	1:O:949:U:C4	3.08	0.41
1:O:1181:A:H5'	15:I:89:GLU:OE2	2.19	0.41
1:O:1477:C:H4'	1:O:1868:G:OP1	2.20	0.41
1:O:1882:C:H5''	7:A:192:VAL:HG21	2.03	0.41
1:O:1926:G:H2'	1:O:1927:A:H8	1.84	0.41
1:O:2661:U:H3	1:O:2812:A:H62	1.67	0.41
6:9:49:G:O2'	6:9:50:G:H5'	2.21	0.41
6:9:63:C:O2'	6:9:64:C:H5'	2.21	0.41
8:B:195:ARG:NE	8:B:323:LEU:HD13	2.36	0.41
10:D:17:ARG:NH2	39:D:240:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:147:ALA:HA	20:N:15:GLU:O	2.21	0.41
14:H:117:ARG:HB3	39:H:347:HOH:O	2.20	0.41
16:J:142:ASN:O	16:J:144:THR:N	2.54	0.41
20:N:37:ARG:HH11	20:N:37:ARG:CG	2.31	0.41
20:N:115:VAL:HG13	39:N:4043:HOH:O	2.20	0.41
26:T:98:VAL:HG11	26:T:101:LEU:HD23	2.01	0.41
29:W:65:VAL:HA	29:W:68:THR:HG22	2.02	0.41
32:Z:10:ARG:CG	32:Z:11:SER:H	2.33	0.41
1:O:473:A:O2'	1:O:474:C:H5'	2.21	0.41
1:O:539:G:H2'	1:O:540:A:C8	2.56	0.41
1:O:542:A:H2'	1:O:543:G:O4'	2.21	0.41
1:O:772:G:H2'	1:O:773:A:O4'	2.20	0.41
1:O:1501:A:H4'	39:O:7280:HOH:O	2.20	0.41
1:O:1787:C:O2'	1:O:1788:U:H5'	2.21	0.41
1:O:1829:A:H2'	1:O:1830:C:H5'	2.03	0.41
1:O:1883:U:C2'	1:O:1884:G:H5'	2.51	0.41
1:O:1904:A:H2'	1:O:1905:U:O4'	2.20	0.41
1:O:2329:C:O2'	1:O:2330:U:H5'	2.21	0.41
1:O:2384:U:H5''	39:O:5594:HOH:O	2.21	0.41
1:O:2388:C:H5'	23:Q:83:THR:O	2.20	0.41
1:O:2626:C:H2'	1:O:2627:G:C8	2.56	0.41
1:O:2694:A:H4'	11:E:91:PHE:CE1	2.55	0.41
1:O:2851:G:H2'	1:O:2902:A:H61	1.85	0.41
2:I:28:HIS:O	2:I:32:LYS:N	2.47	0.41
7:A:206:ARG:NH1	39:A:498:HOH:O	2.54	0.41
8:B:13:PHE:CD1	8:B:13:PHE:N	2.89	0.41
8:B:162:MET:HG3	8:B:310:ARG:NH1	2.36	0.41
9:C:20:ASP:HB2	39:C:420:HOH:O	2.20	0.41
11:E:72:MET:HA	39:E:4032:HOH:O	2.21	0.41
11:E:99:GLY:N	39:E:4024:HOH:O	2.53	0.41
14:H:60:LEU:O	14:H:65:LEU:HD21	2.21	0.41
15:I:70:THR:C	15:I:72:GLU:N	2.74	0.41
20:N:33:ARG:HD2	20:N:103:ASP:OD2	2.20	0.41
26:T:12:ARG:NH1	39:T:4007:HOH:O	2.50	0.41
26:T:20:HIS:O	26:T:23:VAL:HG23	2.21	0.41
30:X:43:VAL:HG12	30:X:47:ALA:HB3	2.03	0.41
31:Y:204:ARG:HA	31:Y:230:ASN:OD1	2.20	0.41
1:O:137:U:OP1	1:O:259:G:O2'	2.39	0.41
1:O:344:C:H2'	1:O:345:G:O4'	2.21	0.41
1:O:1355:A:H5''	39:Y:453:HOH:O	2.21	0.41
1:O:1748:U:C5	1:O:1749:U:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1761:U:H2'	1:0:1762:C:C6	2.55	0.41
1:0:1951:G:N2	39:0:8099:HOH:O	2.54	0.41
1:0:1996:U:O2'	1:0:1997:A:H5'	2.20	0.41
1:0:2644:C:O2'	1:0:2645:U:H5'	2.21	0.41
9:C:25:PRO:HG2	39:C:422:HOH:O	2.21	0.41
9:C:80:VAL:HA	9:C:81:PRO:HD3	1.88	0.41
9:C:180:SER:C	9:C:182:ARG:H	2.24	0.41
11:E:107:PHE:CD2	11:E:108:LEU:HD13	2.56	0.41
11:E:154:ILE:HG23	11:E:154:ILE:O	2.20	0.41
12:F:38:LYS:HZ1	19:M:3:SER:HA	1.86	0.41
16:J:45:VAL:HA	16:J:130:VAL:O	2.21	0.41
18:L:148:GLU:HG3	39:L:377:HOH:O	2.20	0.41
19:M:106:SER:HB2	19:M:114:VAL:CG2	2.51	0.41
25:S:44:GLN:OE1	25:S:44:GLN:HA	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
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
1:0:1174:A:H5'	39:0:6594:HOH:O	2.21	0.40
1:0:1235:G:OP2	1:0:2550:U:H4'	2.21	0.40
1:0:1363:G:OP1	9:C:76:ARG:NH2	2.54	0.40
1:0:1413:A:H2'	1:0:1414:A:O4'	2.20	0.40
1:0:1783:A:C2'	1:0:1784:U:H5'	2.51	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
1:0:2507:G:H2'	1:0:2510:C:N4	2.36	0.40
1:0:2591:C:H2'	1:0:2592:G:O4'	2.21	0.40
1:0:2734:G:O2'	1:0:2735:U:H5'	2.20	0.40
7:A:36:ASP:C	7:A:38:ILE:N	2.74	0.40
8:B:27:ASN:N	8:B:27:ASN:ND2	2.67	0.40
14:H:87:LYS:O	14:H:140:TYR:HD1	2.04	0.40
15:I:66:GLY:O	15:I:67:VAL:C	2.58	0.40
15:I:127:CYS:CB	15:I:132:VAL:HB	2.34	0.40
20:N:58:LEU:N	20:N:58:LEU:CD1	2.83	0.40
20:N:166:ALA:O	20:N:167:ASP:HB2	2.21	0.40
22:P:141:ILE:O	22:P:143:ALA:N	2.49	0.40
25:S:34:LYS:HG2	25:S:54:THR:HG23	2.03	0.40
27:U:28:THR:HB	39:U:8814:HOH:O	2.20	0.40
30:X:76:ARG:NH1	30:X:76:ARG:CG	2.83	0.40
32:Z:39:CYS:HA	32:Z:40:PRO:HD3	1.92	0.40
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:263:U:O4'	12:F:59:ILE:HD13	2.21	0.40
1:0:694:A:H2'	1:0:695:C:C5'	2.45	0.40
1:0:1058:A:H2'	1:0:1060:C:C5'	2.51	0.40
1:0:1586:G:O2'	1:0:1587:U:H5'	2.20	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:1674:C:OP2	25:S:34:LYS:HE3	2.22	0.40
1:0:1702:U:H5'	39:0:7620:HOH:O	2.20	0.40
1:0:1733:A:C2	1:0:1734:C:H1'	2.56	0.40
1:0:1822:A:O2'	1:0:1823:G:H5'	2.21	0.40
1:0:1883:U:O2'	1:0:1884:G:H5'	2.21	0.40
1:0:2385:G:H2'	1:0:2386:U:C6	2.57	0.40
1:0:2684:A:H2'	1:0:2685:C:C6	2.56	0.40
6:9:1:U:C4'	6:9:3:A:OP1	2.70	0.40
6:9:81:C:C2'	6:9:82:U:H5'	2.50	0.40
7:A:190:ARG:NH2	7:A:207:GLN:OE1	2.54	0.40
9:C:4:THR:HB	9:C:135:GLU:OE1	2.21	0.40
9:C:138:VAL:O	9:C:234:VAL:HA	2.21	0.40
11:E:138:ILE:HG23	11:E:139:GLU:N	2.35	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
18:L:144:ASP:CA	18:L:147:GLU:HG3	2.51	0.40
23:Q:46:SER:O	23:Q:48:PRO:HD3	2.22	0.40
24:R:119:VAL:HG12	24:R:119:VAL:O	2.21	0.40
26:T:96:VAL:CG1	26:T:97:ARG:N	2.84	0.40
27:U:52:THR:HG21	27:U:54:THR:HB	2.02	0.40
29:W:154:ARG:C	39:W:4068:HOH:O	2.59	0.40
1:0:276:C:H6	1:0:276:C:O5'	2.04	0.40
1:0:365:G:C6	1:0:366:U:C4	3.10	0.40
1:0:821:U:H1'	39:0:5789:HOH:O	2.21	0.40
1:0:1164:U:H3	1:0:1192:A:H2	1.69	0.40
1:0:1197:G:N2	39:0:6630:HOH:O	2.52	0.40
1:0:1268:C:H2'	1:0:1269:G:C8	2.57	0.40
1:0:1306:U:OP1	9:C:184:ARG:HD2	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
1:0:1976:G:H1'	1:0:2005:G:N2	2.37	0.40
1:0:2255:A:O2'	1:0:2256:G:H5'	2.21	0.40
1:0:2705:U:O4'	11:E:112:ALA:HB2	2.21	0.40
1:0:2757:A:H2'	1:0:2758:G:O4'	2.20	0.40
3:2:40:ARG:HH11	3:2:40:ARG:HG2	1.85	0.40
6:9:2:U:OP2	6:9:2:U:H4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:105:VAL:HG11	7:A:154:ALA:CB	2.51	0.40
8:B:44:TYR:OH	8:B:148:PRO:HG3	2.22	0.40
18:L:54:PRO:HG2	18:L:57:VAL:HG21	2.03	0.40
18:L:91:VAL:HG13	18:L:120:LEU:HD23	2.04	0.40
22:P:59:ARG:HD3	39:P:226:HOH:O	2.20	0.40
24:R:18:LEU:HD12	24:R:143:VAL:CG1	2.47	0.40
25:S:53:ASN:N	25:S:53:ASN:ND2	2.67	0.40
27:U:6:CYS:HA	27:U:13:ILE:HD11	2.03	0.40
29:W:75:GLY:HA3	39:W:4031:HOH:O	2.21	0.40
1:0:402:U:H2'	1:0:403:C:C6	2.56	0.40
1:0:459:A:H4'	39:0:5069:HOH:O	2.21	0.40
39:0:8830:HOH:O	23:Q:50:GLY:HA2	2.21	0.40
3:2:8:LYS:NZ	25:S:56:ASN:O	2.50	0.40
6:9:36:C:H2'	6:9:37:C:O4'	2.22	0.40
7:A:105:VAL:CG1	7:A:106:CYS:N	2.84	0.40
8:B:36:PRO:HB3	8:B:174:ARG:HA	2.03	0.40
8:B:41:PHE:HB3	8:B:190:MET:CE	2.50	0.40
8:B:265:LEU:CD2	8:B:316:ARG:HD3	2.50	0.40
8:B:279:THR:OG1	8:B:290:VAL:O	2.35	0.40
9:C:193:LEU:HA	9:C:211:ASP:O	2.21	0.40
10:D:135:VAL:HG23	39:D:239:HOH:O	2.21	0.40
13:G:64:ASN:N	13:G:64:ASN:ND2	2.70	0.40
20:N:71:TRP:CE3	20:N:175:LEU:CD2	3.05	0.40
29:W:130:HIS:O	29:W:136:GLY:HA3	2.21	0.40
31:Y:186:ARG:HH11	31:Y:186:ARG:HG2	1.86	0.40
1:0:962:C:H2'	1:0:963:C:C5'	2.52	0.40
1:0:1500:U:OP2	22:P:41:ARG:NH2	2.55	0.40
1:0:2435:U:OP1	4:3:28:GLY:HA3	2.22	0.40
1:0:2529:G:H5'	39:0:9120:HOH:O	2.22	0.40
1:0:2776:A:H2'	1:0:2777:G:O4'	2.21	0.40
6:9:28:U:H5''	20:N:40:ASN:HD22	1.81	0.40
6:9:78:G:O2'	6:9:79:U:OP2	2.40	0.40
7:A:114:ASP:HB2	7:A:117:LYS:HE2	2.02	0.40
8:B:51:VAL:HG21	8:B:327:VAL:HG13	2.02	0.40
8:B:214:PRO:C	8:B:220:VAL:HG22	2.42	0.40
9:C:78:ARG:HD3	39:C:472:HOH:O	2.22	0.40
9:C:160:LEU:O	9:C:161:ASP:HB2	2.22	0.40
9:C:170:ASP:O	9:C:171:GLU:HG3	2.22	0.40
11:E:93:MET:HE2	11:E:93:MET:HB2	1.90	0.40
17:K:75:ARG:HG2	17:K:90:PHE:CD2	2.56	0.40
19:M:24:GLN:HE22	19:M:27:ARG:HH11	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:34:ASP:O	23:Q:37:GLU:HG3	2.21	0.40
25:S:17:ASP:HB3	25:S:23:LYS:HB2	2.03	0.40
30:X:43:VAL:CG2	30:X:76:ARG:NH1	2.83	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%)	14	42
5	4	2/8 (25%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	203 (86%)	28 (12%)	4 (2%)	9	31
8	B	335/338 (99%)	294 (88%)	36 (11%)	5 (2%)	10	34
9	C	244/246 (99%)	218 (89%)	21 (9%)	5 (2%)	7	27
10	D	134/177 (76%)	92 (69%)	39 (29%)	3 (2%)	6	24
11	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	25	58
12	F	117/120 (98%)	100 (86%)	12 (10%)	5 (4%)	2	10
13	G	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	11
14	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	8	28
15	I	68/162 (42%)	50 (74%)	16 (24%)	2 (3%)	4	18
16	J	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	7	26
17	K	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
18	L	141/165 (86%)	113 (80%)	24 (17%)	4 (3%)	5	19
19	M	192/195 (98%)	175 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	N	184/187 (98%)	154 (84%)	21 (11%)	9 (5%)	2	8
21	O	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	17	48
22	P	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
23	Q	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	14	42
24	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	22	54
25	S	79/85 (93%)	68 (86%)	11 (14%)	0	100	100
26	T	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	5	20
27	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
28	V	63/71 (89%)	53 (84%)	6 (10%)	4 (6%)	1	4
29	W	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	22	54
30	X	80/92 (87%)	66 (82%)	9 (11%)	5 (6%)	1	4
31	Y	140/241 (58%)	133 (95%)	7 (5%)	0	100	100
32	Z	71/83 (86%)	54 (76%)	14 (20%)	3 (4%)	3	10
All	All	3707/4445 (83%)	3245 (88%)	397 (11%)	65 (2%)	8	29

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

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Mol	Chain	Res	Type
20	N	65	ASP
26	T	44	ALA
28	V	43	PRO
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

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Mol	Chain	Res	Type
7	A	192	VAL
9	C	19	PRO
20	N	130	PRO
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%)	49	79
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%)	18	48
8	B	282/283 (100%)	264 (94%)	18 (6%)	17	45
9	C	193/193 (100%)	181 (94%)	12 (6%)	18	47
10	D	117/148 (79%)	109 (93%)	8 (7%)	16	42
11	E	152/156 (97%)	146 (96%)	6 (4%)	32	66
12	F	93/94 (99%)	90 (97%)	3 (3%)	39	73
13	G	27/283 (10%)	27 (100%)	0	100	100
14	H	134/145 (92%)	128 (96%)	6 (4%)	27	61
15	I	58/130 (45%)	58 (100%)	0	100	100
16	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
17	K	106/106 (100%)	105 (99%)	1 (1%)	78	93
18	L	113/127 (89%)	107 (95%)	6 (5%)	22	54
19	M	158/159 (99%)	151 (96%)	7 (4%)	28	61
20	N	149/150 (99%)	144 (97%)	5 (3%)	37	71
21	O	93/94 (99%)	90 (97%)	3 (3%)	39	73
22	P	113/117 (97%)	109 (96%)	4 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Q	79/80 (99%)	74 (94%)	5 (6%)	18	46
24	R	117/122 (96%)	113 (97%)	4 (3%)	37	71
25	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
26	T	105/106 (99%)	98 (93%)	7 (7%)	16	43
27	U	44/52 (85%)	44 (100%)	0	100	100
28	V	51/57 (90%)	50 (98%)	1 (2%)	55	82
29	W	130/130 (100%)	122 (94%)	8 (6%)	18	47
30	X	66/74 (89%)	58 (88%)	8 (12%)	5	15
31	Y	120/196 (61%)	114 (95%)	6 (5%)	24	57
32	Z	60/68 (88%)	56 (93%)	4 (7%)	16	43
All	All	3097/3621 (86%)	2952 (95%)	145 (5%)	26	59

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

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Mol	Chain	Res	Type
8	B	234	ARG
8	B	254	GLN
8	B	256	GLN
8	B	264	GLU
8	B	277	GLU
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

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Mol	Chain	Res	Type
16	J	7	ASP
16	J	47	THR
16	J	52	GLN
16	J	74	ARG
16	J	76	ASP
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

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Mol	Chain	Res	Type
24	R	132	ARG
25	S	12	GLU
25	S	53	ASN
25	S	80	ARG
26	T	5	ASP
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

Sometimes 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
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

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Mol	Chain	Res	Type
16	J	126	ASN
17	K	10	GLN
17	K	42	ASN
18	L	18	HIS
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

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Mol	Chain	Res	Type
30	X	23	HIS
30	X	36	HIS
31	Y	129	ASN
31	Y	133	HIS
31	Y	134	HIS
31	Y	149	GLN
31	Y	189	ASN

5.3.3 RNA ⓘ

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

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Mol	Chain	Res	Type
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	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

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Mol	Chain	Res	Type
1	0	840	U
1	0	857	A
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	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

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Mol	Chain	Res	Type
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1234	U
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

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Mol	Chain	Res	Type
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	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

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Mol	Chain	Res	Type
1	0	2291	A
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	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

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Mol	Chain	Res	Type
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
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

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Mol	Chain	Res	Type
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
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	35,1	14,22,23	1.06	1 (7%)	14,31,34	1.19	1 (7%)
5	004	4	7	5	9,10,11	2.92	3 (33%)	9,12,14	2.09	3 (33%)
5	DBB	4	3	5	4,5,6	1.05	0	1,5,7	0.24	0
1	1MA	0	628	35,1	15,25,26	0.76	0	15,37,40	1.41	1 (6%)
1	UR3	0	2619	1	14,22,23	0.82	0	15,32,35	0.59	0
5	MHW	4	1	5,33	9,9,10	2.56	4 (44%)	10,11,13	1.22	1 (10%)
5	MHU	4	5	5	14,15,16	2.86	8 (57%)	18,19,21	1.65	5 (27%)
5	MHV	4	6	38,5	7,9,10	2.05	2 (28%)	7,11,13	1.72	2 (28%)
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	20,38,41	2.59	5 (25%)
1	PSU	0	2621	1	17,21,22	1.64	3 (17%)	20,30,33	5.42	4 (20%)

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	35,1	-	0/7/27/28	0/2/2/2
5	004	4	7	5	-	2/4/6/8	0/1/1/1
5	DBB	4	3	5	-	0/3/4/6	-
1	1MA	0	628	35,1	-	0/3/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
5	MHW	4	1	5,33	-	0/2/2/4	0/1/1/1
5	MHU	4	5	5	-	0/9/12/14	0/1/1/1
5	MHV	4	6	38,5	-	0/1/12/14	0/1/1/1
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	004	CB-CA	7.09	1.60	1.52
1	0	2621	PSU	C5-C1'	-5.24	1.47	1.52
5	4	1	MHW	CA-N	4.54	1.42	1.35
5	4	5	MHU	CA-N	4.52	1.55	1.47
5	4	6	MHV	CB-CG	4.38	1.57	1.50
5	4	5	MHU	CE2-CZ	4.18	1.47	1.39
5	4	5	MHU	CD2-CE2	3.96	1.46	1.38
5	4	5	MHU	CB-CA	3.61	1.62	1.54
1	0	2588	OMG	C6-N1	3.56	1.39	1.33
5	4	7	004	CD2-CG2	3.45	1.46	1.38
5	4	1	MHW	CB-CA	3.42	1.46	1.40
5	4	5	MHU	CE1-CZ	3.33	1.45	1.39
5	4	5	MHU	CD1-CG	3.28	1.45	1.38
5	4	1	MHW	CG2-CB	3.24	1.45	1.39
1	0	2587	OMU	C4-N3	3.07	1.38	1.33
5	4	1	MHW	CA-C	2.99	1.51	1.48
1	0	2621	PSU	C4-N3	2.88	1.38	1.33
5	4	5	MHU	CE1-CD1	2.50	1.43	1.38
1	0	2621	PSU	C2-N1	2.43	1.43	1.38
5	4	7	004	CG1-CB	2.42	1.42	1.39
5	4	6	MHV	CD2-CG	2.26	1.55	1.50
1	0	2588	OMG	C8-N7	-2.10	1.31	1.34
5	4	5	MHU	CZ-NZ	2.03	1.42	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.12	114.82	128.43
1	0	2621	PSU	C4-N3-C2	14.34	127.25	115.14
1	0	2588	OMG	C5-C6-N1	-8.58	111.69	123.43
1	0	2621	PSU	C5-C4-N3	-8.24	114.74	125.36
1	0	2588	OMG	C6-N1-C2	5.83	125.20	115.93
1	0	628	1MA	C2-N3-C4	-4.75	110.64	116.58
1	0	2587	OMU	C5-C4-N3	-4.01	114.48	123.31
5	4	7	004	CG2-CB-CA	3.82	126.81	120.65
5	4	5	MHU	CB-CA-N	3.45	116.00	110.65
5	4	7	004	CB-CA-N	-3.42	104.21	112.40
5	4	5	MHU	O-C-CA	-3.19	116.43	124.78
1	0	2588	OMG	C2-N3-C4	-3.07	111.85	115.36
5	4	6	MHV	CB-CA-N	-2.83	106.64	112.50
1	0	2621	PSU	C6-N1-C2	2.64	119.71	115.36
1	0	2588	OMG	N3-C2-N1	-2.52	123.86	127.22
5	4	5	MHU	CG-CB-CA	2.48	117.18	113.63
5	4	5	MHU	CB-CA-C	-2.45	107.00	111.65
5	4	6	MHV	CD2-CE-N	-2.37	104.86	110.03
1	0	2588	OMG	C6-C5-C4	-2.11	118.78	120.80
5	4	5	MHU	CM-N-CA	2.04	120.00	113.64
5	4	7	004	CG1-CB-CA	-2.04	117.36	120.65
5	4	1	MHW	CE-N-CA	2.02	120.17	116.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	4	7	004	C-CA-CB-CG1
5	4	7	004	C-CA-CB-CG2

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	MHT	4	101	5	9,11,11	1.66	3 (33%)	11,15,15	0.56	0

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
38	MHT	4	101	5	-	0/0/20/20	0/3/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	101	MHT	C8-C7	2.54	1.59	1.52
38	4	101	MHT	C5-C6	2.31	1.58	1.52
38	4	101	MHT	C8-C4	2.04	1.57	1.53

There are no bond angle outliers.

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
38	4	101	MHT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.23	37 (1%) 77 77	18, 42, 85, 147	0
2	1	56/57 (98%)	-0.56	0 100 100	23, 28, 34, 41	0
3	2	46/50 (92%)	0.10	2 (4%) 35 31	24, 56, 82, 96	0
4	3	92/92 (100%)	0.02	1 (1%) 80 80	30, 48, 61, 79	0
5	4	2/8 (25%)	-0.11	0 100 100	49, 49, 49, 54	0
6	9	122/122 (100%)	-0.14	3 (2%) 57 55	36, 57, 84, 148	0
7	A	237/240 (98%)	-0.11	4 (1%) 70 69	21, 44, 80, 100	0
8	B	337/338 (99%)	-0.13	0 100 100	23, 50, 76, 86	0
9	C	246/246 (100%)	-0.32	0 100 100	19, 39, 62, 72	0
10	D	140/177 (79%)	1.73	56 (40%) 0 0	47, 94, 117, 125	0
11	E	172/178 (96%)	0.47	6 (3%) 44 38	41, 61, 83, 88	0
12	F	119/120 (99%)	0.35	3 (2%) 57 55	41, 63, 88, 104	0
13	G	29/348 (8%)	2.33	16 (55%) 0 0	71, 87, 95, 96	0
14	H	160/177 (90%)	0.10	2 (1%) 77 77	36, 52, 88, 105	0
15	I	70/162 (43%)	4.05	65 (92%) 0 0	108, 118, 136, 138	0
16	J	142/145 (97%)	-0.08	2 (1%) 75 75	34, 46, 66, 86	0
17	K	132/132 (100%)	-0.22	2 (1%) 73 73	26, 46, 65, 75	0
18	L	145/165 (87%)	0.38	8 (5%) 25 21	22, 60, 100, 114	0
19	M	194/195 (99%)	-0.48	0 100 100	25, 36, 52, 59	0
20	N	186/187 (99%)	0.05	5 (2%) 54 50	34, 58, 100, 110	0
21	O	115/116 (99%)	-0.13	0 100 100	33, 47, 66, 71	0
22	P	143/149 (95%)	-0.03	0 100 100	33, 49, 61, 73	0
23	Q	95/96 (98%)	-0.15	0 100 100	28, 39, 54, 66	0
24	R	150/155 (96%)	-0.20	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%)	0.01	1 (1%) 79 79	37, 52, 71, 79	0
26	T	119/120 (99%)	0.21	3 (2%) 57 55	35, 51, 80, 94	0
27	U	53/66 (80%)	0.08	1 (1%) 66 65	39, 51, 67, 78	0
28	V	65/71 (91%)	0.69	7 (10%) 5 4	46, 66, 105, 112	0
29	W	154/154 (100%)	-0.17	0 100 100	27, 42, 59, 71	0
30	X	82/92 (89%)	0.36	7 (8%) 10 8	38, 55, 76, 96	0
31	Y	142/241 (58%)	-0.10	4 (2%) 53 49	24, 40, 62, 81	0
32	Z	73/83 (87%)	-0.19	0 100 100	39, 53, 69, 87	0
All	All	6648/7489 (88%)	-0.03	235 (3%) 44 38	18, 46, 91, 148	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	I	88	GLN	8.5
15	I	132	VAL	8.5
15	I	128	THR	7.7
15	I	70	THR	7.4
15	I	66	GLY	7.1
10	D	63	ILE	7.0
15	I	104	ALA	6.7
15	I	119	ALA	6.2
28	V	1	THR	6.1
15	I	68	PRO	6.0
15	I	112	LEU	5.9
15	I	118	ASN	5.9
15	I	113	SER	5.9
15	I	106	GLN	5.5
15	I	91	PHE	5.4
15	I	108	HIS	5.4
15	I	74	ILE	5.3
15	I	111	LEU	5.3
15	I	117	THR	5.2
10	D	27	ILE	5.1
10	D	93	LEU	5.1
1	0	1198	U	5.1
15	I	80	PHE	5.0
15	I	79	GLY	5.0
15	I	99	GLN	5.0
1	0	1203	G	5.0

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Mol	Chain	Res	Type	RSRZ
15	I	69	PRO	5.0
1	0	1172	G	4.9
10	D	172	VAL	4.8
10	D	64	ARG	4.8
15	I	110	ASP	4.8
10	D	29	HIS	4.7
10	D	61	PHE	4.6
15	I	127	CYS	4.6
10	D	57	THR	4.6
28	V	39	ALA	4.5
18	L	80	ASP	4.5
15	I	133	THR	4.5
6	9	1	U	4.5
15	I	72	GLU	4.4
15	I	73	LEU	4.4
15	I	97	VAL	4.4
15	I	76	ASP	4.3
10	D	171	ASP	4.3
10	D	18	ILE	4.3
15	I	102	GLN	4.2
30	X	88	GLU	4.2
13	G	23	ILE	4.2
15	I	131	GLY	4.2
7	A	37	VAL	4.1
10	D	88	LEU	4.1
10	D	66	GLY	4.1
15	I	100	VAL	4.1
10	D	26	GLY	4.0
10	D	90	LEU	4.0
15	I	121	LYS	4.0
1	0	1196	C	3.9
15	I	109	PRO	3.9
13	G	26	MET	3.9
10	D	10	PHE	3.9
15	I	67	VAL	3.8
1	0	1202	A	3.8
1	0	1197	G	3.7
10	D	87	ALA	3.7
15	I	135	GLU	3.7
13	G	24	VAL	3.7
13	G	68	GLU	3.7
15	I	71	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
10	D	85	GLN	3.6
10	D	44	ILE	3.6
13	G	27	ILE	3.6
10	D	69	ILE	3.6
1	0	1204	C	3.6
10	D	170	TYR	3.6
15	I	75	LYS	3.5
15	I	103	ILE	3.5
15	I	134	ILE	3.5
15	I	120	ALA	3.5
15	I	107	LYS	3.4
10	D	92	GLU	3.4
13	G	71	LEU	3.4
15	I	98	ASP	3.4
1	0	1199	A	3.4
18	L	106	VAL	3.3
15	I	93	ALA	3.3
1	0	1186	C	3.3
28	V	40	PRO	3.3
10	D	62	ASP	3.3
15	I	130	LEU	3.3
15	I	92	VAL	3.3
1	0	1951	G	3.3
15	I	116	LEU	3.3
15	I	105	GLU	3.2
10	D	84	LEU	3.2
15	I	78	ALA	3.2
1	0	1177	A	3.2
1	0	1169	U	3.2
15	I	95	LEU	3.1
15	I	114	TYR	3.1
27	U	47	ARG	3.1
13	G	73	ASP	3.1
3	2	35	ARG	3.1
10	D	83	PHE	3.1
15	I	96	SER	3.1
1	0	1171	A	3.1
10	D	75	LEU	3.1
10	D	45	THR	3.0
1	0	1170	U	3.0
10	D	134	LEU	3.0
31	Y	95	THR	3.0

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Mol	Chain	Res	Type	RSRZ
10	D	17	ARG	3.0
10	D	89	PRO	3.0
6	9	24	U	3.0
1	0	284	C	3.0
15	I	84	SER	3.0
28	V	38	GLY	2.9
15	I	90	ASP	2.9
26	T	119	ALA	2.9
15	I	94	ASP	2.9
10	D	11	HIS	2.9
10	D	128	LEU	2.9
13	G	70	ALA	2.9
1	0	970	U	2.8
15	I	126	THR	2.8
1	0	2237	G	2.8
10	D	67	ASP	2.8
10	D	25	MET	2.8
30	X	41	PHE	2.8
10	D	58	VAL	2.8
10	D	40	ILE	2.7
7	A	38	ILE	2.7
18	L	105	TYR	2.7
10	D	106	PHE	2.7
15	I	82	THR	2.7
14	H	40	GLN	2.7
31	Y	235	GLU	2.7
10	D	56	ARG	2.7
20	N	183	ASP	2.6
10	D	55	LYS	2.6
7	A	237	GLY	2.6
15	I	124	VAL	2.6
14	H	86	TYR	2.6
1	0	735	C	2.6
30	X	85	VAL	2.6
15	I	86	GLU	2.6
20	N	166	ALA	2.6
13	G	72	ASP	2.5
10	D	35	ALA	2.5
16	J	92	GLN	2.5
11	E	45	ASP	2.5
30	X	80	GLU	2.5
1	0	1195	G	2.5

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Mol	Chain	Res	Type	RSRZ
10	D	104	PHE	2.5
15	I	89	GLU	2.5
10	D	166	ILE	2.5
13	G	15	TRP	2.5
13	G	67	LEU	2.5
25	S	81	ILE	2.5
18	L	79	ASP	2.5
10	D	68	PRO	2.5
1	0	282	C	2.4
20	N	158	LEU	2.4
1	0	2508	C	2.4
13	G	66	LEU	2.4
15	I	77	GLU	2.4
28	V	41	GLU	2.4
1	0	1180	U	2.4
26	T	112	LEU	2.4
10	D	86	THR	2.4
15	I	122	GLU	2.4
30	X	74	ALA	2.4
1	0	1181	A	2.4
12	F	6	PHE	2.3
18	L	150	GLN	2.3
6	9	2	U	2.3
31	Y	108	ASP	2.3
10	D	65	GLU	2.3
10	D	41	LEU	2.3
26	T	118	SER	2.3
10	D	165	PHE	2.3
1	0	1168	C	2.3
1	0	1173	A	2.3
1	0	1200	A	2.3
12	F	44	SER	2.3
1	0	1175	G	2.3
1	0	1185	U	2.3
28	V	43	PRO	2.3
28	V	3	LEU	2.3
1	0	1525	G	2.3
10	D	47	GLN	2.3
15	I	83	GLY	2.2
15	I	87	PRO	2.2
13	G	22	ALA	2.2
30	X	7	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
11	E	170	ARG	2.2
1	0	960	G	2.2
3	2	39	ARG	2.2
1	0	1205	U	2.2
7	A	36	ASP	2.2
16	J	96	GLU	2.2
1	0	2238	A	2.2
18	L	89	PHE	2.2
11	E	100	ASP	2.2
10	D	94	ALA	2.2
18	L	100	ALA	2.2
13	G	29	SER	2.2
1	0	1174	A	2.2
10	D	130	VAL	2.2
20	N	185	GLU	2.2
1	0	969	G	2.1
10	D	39	ASP	2.1
18	L	75	LEU	2.1
10	D	28	GLY	2.1
30	X	77	PHE	2.1
10	D	157	LEU	2.1
10	D	173	GLU	2.1
10	D	16	PRO	2.1
15	I	123	VAL	2.1
17	K	132	VAL	2.1
11	E	154	ILE	2.1
1	0	1190	G	2.1
10	D	24	HIS	2.1
12	F	45	ALA	2.1
11	E	98	GLU	2.1
15	I	81	GLU	2.1
1	0	1130	U	2.1
20	N	159	TYR	2.0
17	K	108	GLU	2.0
1	0	1178	G	2.0
4	3	92	GLU	2.0
11	E	42	VAL	2.0
31	Y	98	GLN	2.0
13	G	28	GLU	2.0
10	D	91	ALA	2.0
13	G	20	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DBB	4	3	6/7	0.94	0.18	51,51,52,53	0
5	MHV	4	6	9/10	0.94	0.18	53,55,59,59	0
5	MHU	4	5	15/16	0.95	0.17	56,59,62,63	0
5	004	4	7	10/11	0.95	0.20	45,48,49,51	0
5	MHW	4	1	9/10	0.96	0.20	46,47,49,50	0
1	1MA	0	628	23/24	0.98	0.15	25,28,31,32	0
1	OMU	0	2587	21/22	0.98	0.15	29,32,37,38	0
1	OMG	0	2588	24/25	0.98	0.14	28,31,34,35	0
1	UR3	0	2619	21/22	0.98	0.13	30,35,39,42	0
1	PSU	0	2621	20/21	0.98	0.14	33,35,37,38	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	3183	1/1	0.09	0.92	81,81,81,81	0
35	NA	0	3174	1/1	0.53	0.47	75,75,75,75	0
35	NA	R	202	1/1	0.60	0.59	75,75,75,75	0
35	NA	0	3134	1/1	0.61	0.61	72,72,72,72	0
35	NA	0	3175	1/1	0.71	0.45	54,54,54,54	0
35	NA	9	203	1/1	0.73	0.70	85,85,85,85	0
35	NA	0	3140	1/1	0.74	0.35	47,47,47,47	0
35	NA	0	3137	1/1	0.76	0.30	81,81,81,81	0
33	MG	0	3105	1/1	0.77	0.26	47,47,47,47	0
35	NA	0	3120	1/1	0.80	0.52	36,36,36,36	0
35	NA	0	3121	1/1	0.80	0.30	50,50,50,50	0
35	NA	0	3141	1/1	0.81	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	C	301	1/1	0.82	0.25	32,32,32,32	0
35	NA	0	3117	1/1	0.83	0.43	56,56,56,56	0
35	NA	0	3170	1/1	0.83	0.35	72,72,72,72	0
35	NA	9	202	1/1	0.84	0.13	31,31,31,31	0
35	NA	0	3147	1/1	0.84	0.25	44,44,44,44	0
33	MG	0	3063	1/1	0.85	0.39	37,37,37,37	0
35	NA	0	3165	1/1	0.85	0.33	60,60,60,60	0
35	NA	0	3156	1/1	0.86	0.28	55,55,55,55	0
33	MG	0	3082	1/1	0.86	0.18	46,46,46,46	0
33	MG	0	3071	1/1	0.87	0.08	55,55,55,55	0
35	NA	0	3184	1/1	0.87	0.15	45,45,45,45	0
33	MG	0	3097	1/1	0.87	0.44	79,79,79,79	0
36	CL	0	3192	1/1	0.87	0.43	88,88,88,88	0
35	NA	0	3173	1/1	0.88	0.23	53,53,53,53	0
35	NA	0	3122	1/1	0.88	0.17	47,47,47,47	0
35	NA	0	3164	1/1	0.88	0.34	75,75,75,75	0
33	MG	0	3050	1/1	0.88	0.19	72,72,72,72	0
35	NA	0	3118	1/1	0.88	0.15	39,39,39,39	0
36	CL	0	3194	1/1	0.88	0.18	58,58,58,58	0
33	MG	0	3108	1/1	0.89	0.11	46,46,46,46	0
35	NA	0	3161	1/1	0.89	0.48	54,54,54,54	0
33	MG	0	3093	1/1	0.89	0.16	45,45,45,45	0
35	NA	0	3138	1/1	0.89	0.31	41,41,41,41	0
33	MG	0	3092	1/1	0.90	0.16	42,42,42,42	0
33	MG	0	3047	1/1	0.90	0.20	62,62,62,62	0
35	NA	H	201	1/1	0.90	0.15	38,38,38,38	0
35	NA	0	3166	1/1	0.90	0.14	35,35,35,35	0
35	NA	0	3160	1/1	0.90	0.47	48,48,48,48	0
33	MG	0	3049	1/1	0.90	0.25	58,58,58,58	0
35	NA	0	3159	1/1	0.91	0.07	49,49,49,49	0
35	NA	0	3171	1/1	0.91	0.36	65,65,65,65	0
35	NA	0	3132	1/1	0.91	0.21	39,39,39,39	0
33	MG	T	201	1/1	0.91	0.11	45,45,45,45	0
33	MG	0	3034	1/1	0.91	0.09	29,29,29,29	0
35	NA	0	3154	1/1	0.91	0.36	40,40,40,40	0
33	MG	0	3051	1/1	0.91	0.12	58,58,58,58	0
36	CL	A	303	1/1	0.91	0.19	58,58,58,58	0
35	NA	0	3167	1/1	0.92	0.51	43,43,43,43	0
35	NA	0	3185	1/1	0.92	0.32	38,38,38,38	0
33	MG	0	3084	1/1	0.92	0.11	49,49,49,49	0
33	MG	0	3066	1/1	0.92	0.07	34,34,34,34	0
35	NA	0	3125	1/1	0.92	0.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	3061	1/1	0.92	0.06	52,52,52,52	0
35	NA	R	201	1/1	0.92	0.10	33,33,33,33	0
33	MG	0	3077	1/1	0.92	0.17	58,58,58,58	0
35	NA	0	3179	1/1	0.92	0.23	64,64,64,64	0
35	NA	0	3181	1/1	0.92	0.31	46,46,46,46	0
33	MG	0	3046	1/1	0.92	0.11	52,52,52,52	0
35	NA	0	3145	1/1	0.93	0.06	55,55,55,55	0
33	MG	0	3101	1/1	0.93	0.08	73,73,73,73	0
35	NA	0	3148	1/1	0.93	0.13	29,29,29,29	0
33	MG	0	3069	1/1	0.93	0.08	56,56,56,56	0
33	MG	0	3087	1/1	0.93	0.29	75,75,75,75	0
35	NA	0	3157	1/1	0.93	0.56	71,71,71,71	0
33	MG	0	3089	1/1	0.93	0.13	47,47,47,47	0
34	K	0	3111	1/1	0.93	0.12	62,62,62,62	0
35	NA	0	3176	1/1	0.93	0.63	60,60,60,60	0
35	NA	0	3114	1/1	0.93	0.20	50,50,50,50	0
35	NA	0	3143	1/1	0.93	0.26	47,47,47,47	0
35	NA	0	3182	1/1	0.93	0.16	40,40,40,40	0
38	MHT	4	101	10/10	0.93	0.22	63,64,65,67	0
33	MG	9	201	1/1	0.94	0.09	53,53,53,53	0
33	MG	K	201	1/1	0.94	0.07	46,46,46,46	0
35	NA	0	3144	1/1	0.94	0.13	44,44,44,44	0
33	MG	0	3060	1/1	0.94	0.08	27,27,27,27	0
35	NA	0	3168	1/1	0.94	0.20	40,40,40,40	0
33	MG	0	3073	1/1	0.94	0.07	28,28,28,28	0
35	NA	0	3130	1/1	0.94	0.42	61,61,61,61	0
33	MG	0	3103	1/1	0.94	0.08	60,60,60,60	0
35	NA	L	201	1/1	0.94	0.71	61,61,61,61	0
35	NA	Q	101	1/1	0.94	0.09	33,33,33,33	0
35	NA	0	3115	1/1	0.94	0.11	29,29,29,29	0
35	NA	0	3135	1/1	0.94	0.31	60,60,60,60	0
35	NA	0	3116	1/1	0.94	0.41	33,33,33,33	0
35	NA	0	3177	1/1	0.94	0.30	58,58,58,58	0
36	CL	0	3195	1/1	0.94	0.27	88,88,88,88	0
33	MG	0	3076	1/1	0.94	0.10	50,50,50,50	0
36	CL	O	202	1/1	0.94	0.18	74,74,74,74	0
33	MG	0	3086	1/1	0.94	0.05	41,41,41,41	0
33	MG	0	3083	1/1	0.95	0.07	25,25,25,25	0
35	NA	0	3139	1/1	0.95	0.17	62,62,62,62	0
35	NA	J	201	1/1	0.95	0.09	61,61,61,61	0
35	NA	0	3123	1/1	0.95	0.12	27,27,27,27	0
33	MG	0	3106	1/1	0.95	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	3126	1/1	0.95	0.10	28,28,28,28	0
35	NA	0	3127	1/1	0.95	0.17	26,26,26,26	0
36	CL	0	3187	1/1	0.95	0.19	57,57,57,57	0
33	MG	0	3094	1/1	0.95	0.10	73,73,73,73	0
33	MG	0	3041	1/1	0.95	0.20	38,38,38,38	0
33	MG	0	3098	1/1	0.95	0.20	48,48,48,48	0
35	NA	0	3150	1/1	0.95	0.09	42,42,42,42	0
36	CL	J	203	1/1	0.95	0.14	63,63,63,63	0
36	CL	L	202	1/1	0.95	0.11	46,46,46,46	0
33	MG	0	3090	1/1	0.95	0.08	41,41,41,41	0
33	MG	0	3001	1/1	0.95	0.07	30,30,30,30	0
33	MG	0	3085	1/1	0.96	0.18	41,41,41,41	0
35	NA	0	3112	1/1	0.96	0.14	21,21,21,21	0
33	MG	0	3035	1/1	0.96	0.05	50,50,50,50	0
33	MG	0	3052	1/1	0.96	0.05	35,35,35,35	0
33	MG	0	3088	1/1	0.96	0.21	48,48,48,48	0
33	MG	0	3008	1/1	0.96	0.04	33,33,33,33	0
33	MG	0	3011	1/1	0.96	0.08	21,21,21,21	0
33	MG	0	3015	1/1	0.96	0.06	38,38,38,38	0
36	CL	0	3191	1/1	0.96	0.12	51,51,51,51	0
33	MG	3	101	1/1	0.96	0.04	40,40,40,40	0
35	NA	0	3163	1/1	0.96	0.21	44,44,44,44	0
33	MG	0	3033	1/1	0.96	0.09	31,31,31,31	0
35	NA	0	3142	1/1	0.96	0.07	26,26,26,26	0
36	CL	J	202	1/1	0.96	0.18	55,55,55,55	0
33	MG	0	3002	1/1	0.96	0.04	26,26,26,26	0
36	CL	J	204	1/1	0.96	0.11	57,57,57,57	0
33	MG	0	3096	1/1	0.96	0.16	49,49,49,49	0
34	K	0	3110	1/1	0.96	0.20	86,86,86,86	0
35	NA	A	302	1/1	0.96	0.16	38,38,38,38	0
33	MG	0	3099	1/1	0.97	0.22	53,53,53,53	0
35	NA	0	3158	1/1	0.97	0.53	43,43,43,43	0
33	MG	0	3010	1/1	0.97	0.07	24,24,24,24	0
35	NA	0	3136	1/1	0.97	0.32	50,50,50,50	0
33	MG	0	3027	1/1	0.97	0.11	40,40,40,40	0
33	MG	0	3045	1/1	0.97	0.08	58,58,58,58	0
33	MG	0	3091	1/1	0.97	0.06	26,26,26,26	0
33	MG	0	3107	1/1	0.97	0.09	49,49,49,49	0
35	NA	0	3119	1/1	0.97	0.09	40,40,40,40	0
35	NA	M	201	1/1	0.97	0.13	30,30,30,30	0
33	MG	0	3065	1/1	0.97	0.10	38,38,38,38	0
33	MG	0	3109	1/1	0.97	0.11	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	3169	1/1	0.97	0.14	35,35,35,35	0
33	MG	0	3056	1/1	0.97	0.09	42,42,42,42	0
36	CL	0	3188	1/1	0.97	0.14	57,57,57,57	0
33	MG	0	3067	1/1	0.97	0.11	41,41,41,41	0
35	NA	0	3146	1/1	0.97	0.12	26,26,26,26	0
36	CL	0	3193	1/1	0.97	0.13	56,56,56,56	0
33	MG	B	401	1/1	0.97	0.09	32,32,32,32	0
33	MG	0	3095	1/1	0.97	0.11	49,49,49,49	0
35	NA	0	3149	1/1	0.97	0.12	35,35,35,35	0
33	MG	0	3068	1/1	0.97	0.09	59,59,59,59	0
35	NA	0	3151	1/1	0.97	0.05	30,30,30,30	0
35	NA	0	3180	1/1	0.97	0.38	45,45,45,45	0
35	NA	0	3153	1/1	0.97	0.14	43,43,43,43	0
36	CL	N	201	1/1	0.97	0.13	57,57,57,57	0
33	MG	0	3058	1/1	0.97	0.06	27,27,27,27	0
36	CL	R	203	1/1	0.97	0.15	43,43,43,43	0
33	MG	0	3059	1/1	0.97	0.14	44,44,44,44	0
33	MG	0	3013	1/1	0.98	0.10	37,37,37,37	0
33	MG	0	3053	1/1	0.98	0.13	48,48,48,48	0
33	MG	4	102	1/1	0.98	0.08	46,46,46,46	0
33	MG	0	3054	1/1	0.98	0.09	24,24,24,24	0
33	MG	A	301	1/1	0.98	0.08	44,44,44,44	0
33	MG	0	3055	1/1	0.98	0.13	40,40,40,40	0
33	MG	0	3014	1/1	0.98	0.07	31,31,31,31	0
33	MG	0	3057	1/1	0.98	0.08	32,32,32,32	0
33	MG	Y	301	1/1	0.98	0.12	34,34,34,34	0
33	MG	0	3006	1/1	0.98	0.05	46,46,46,46	0
33	MG	0	3038	1/1	0.98	0.08	28,28,28,28	0
33	MG	0	3039	1/1	0.98	0.10	33,33,33,33	0
35	NA	0	3113	1/1	0.98	0.26	44,44,44,44	0
33	MG	0	3040	1/1	0.98	0.14	70,70,70,70	0
33	MG	0	3062	1/1	0.98	0.07	51,51,51,51	0
33	MG	0	3016	1/1	0.98	0.11	23,23,23,23	0
35	NA	0	3152	1/1	0.98	0.11	34,34,34,34	0
33	MG	0	3064	1/1	0.98	0.18	96,96,96,96	0
33	MG	0	3043	1/1	0.98	0.06	35,35,35,35	0
35	NA	0	3155	1/1	0.98	0.20	39,39,39,39	0
33	MG	0	3044	1/1	0.98	0.06	37,37,37,37	0
33	MG	0	3017	1/1	0.98	0.05	26,26,26,26	0
35	NA	S	101	1/1	0.98	0.13	10,10,10,10	0
36	CL	0	3186	1/1	0.98	0.16	43,43,43,43	0
33	MG	0	3018	1/1	0.98	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	3021	1/1	0.98	0.10	32,32,32,32	0
36	CL	0	3189	1/1	0.98	0.07	39,39,39,39	0
33	MG	0	3100	1/1	0.98	0.05	35,35,35,35	0
35	NA	0	3124	1/1	0.98	0.12	48,48,48,48	0
35	NA	0	3162	1/1	0.98	0.40	49,49,49,49	0
33	MG	0	3048	1/1	0.98	0.07	48,48,48,48	0
33	MG	0	3025	1/1	0.98	0.03	42,42,42,42	0
36	CL	3	103	1/1	0.98	0.08	53,53,53,53	0
33	MG	0	3104	1/1	0.98	0.06	40,40,40,40	0
36	CL	B	402	1/1	0.98	0.12	40,40,40,40	0
35	NA	0	3128	1/1	0.98	0.13	22,22,22,22	0
33	MG	0	3075	1/1	0.98	0.07	38,38,38,38	0
35	NA	0	3131	1/1	0.98	0.12	39,39,39,39	0
33	MG	0	3012	1/1	0.98	0.07	25,25,25,25	0
35	NA	0	3133	1/1	0.98	0.16	50,50,50,50	0
33	MG	0	3032	1/1	0.98	0.07	40,40,40,40	0
35	NA	0	3172	1/1	0.98	0.13	58,58,58,58	0
36	CL	Y	302	1/1	0.98	0.11	30,30,30,30	0
37	CD	3	102	1/1	0.98	0.05	55,55,55,55	0
37	CD	O	201	1/1	0.98	0.07	70,70,70,70	0
33	MG	0	3081	1/1	0.98	0.16	41,41,41,41	0
33	MG	0	3079	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	3080	1/1	0.99	0.09	65,65,65,65	0
33	MG	0	3004	1/1	0.99	0.07	27,27,27,27	0
33	MG	0	3042	1/1	0.99	0.10	31,31,31,31	0
33	MG	0	3026	1/1	0.99	0.07	19,19,19,19	0
33	MG	0	3009	1/1	0.99	0.07	22,22,22,22	0
33	MG	0	3028	1/1	0.99	0.09	39,39,39,39	0
36	CL	0	3190	1/1	0.99	0.12	46,46,46,46	0
33	MG	0	3029	1/1	0.99	0.08	33,33,33,33	0
33	MG	0	3030	1/1	0.99	0.08	31,31,31,31	0
35	NA	0	3178	1/1	0.99	0.10	29,29,29,29	0
33	MG	0	3031	1/1	0.99	0.08	28,28,28,28	0
35	NA	0	3129	1/1	0.99	0.10	25,25,25,25	0
33	MG	0	3005	1/1	0.99	0.10	27,27,27,27	0
33	MG	0	3019	1/1	0.99	0.05	23,23,23,23	0
33	MG	0	3020	1/1	0.99	0.08	22,22,22,22	0
33	MG	0	3003	1/1	0.99	0.12	31,31,31,31	0
33	MG	0	3070	1/1	0.99	0.06	25,25,25,25	0
33	MG	0	3036	1/1	0.99	0.05	32,32,32,32	0
33	MG	0	3072	1/1	0.99	0.08	47,47,47,47	0
36	CL	M	202	1/1	0.99	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	3037	1/1	0.99	0.07	44,44,44,44	0
33	MG	0	3074	1/1	0.99	0.10	20,20,20,20	0
33	MG	0	3022	1/1	0.99	0.08	36,36,36,36	0
33	MG	0	3023	1/1	0.99	0.06	34,34,34,34	0
37	CD	1	101	1/1	0.99	0.08	56,56,56,56	0
33	MG	0	3024	1/1	0.99	0.06	12,12,12,12	0
33	MG	0	3078	1/1	0.99	0.04	22,22,22,22	0
33	MG	0	3102	1/1	0.99	0.08	23,23,23,23	0
37	CD	U	8701	1/1	1.00	0.08	60,60,60,60	0
37	CD	Z	101	1/1	1.00	0.11	59,59,59,59	0
33	MG	0	3007	1/1	1.00	0.07	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.