



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 02:59 pm GMT

PDB ID : 1VQ7  
Title : The structure of the transition state analogue "DCA" bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

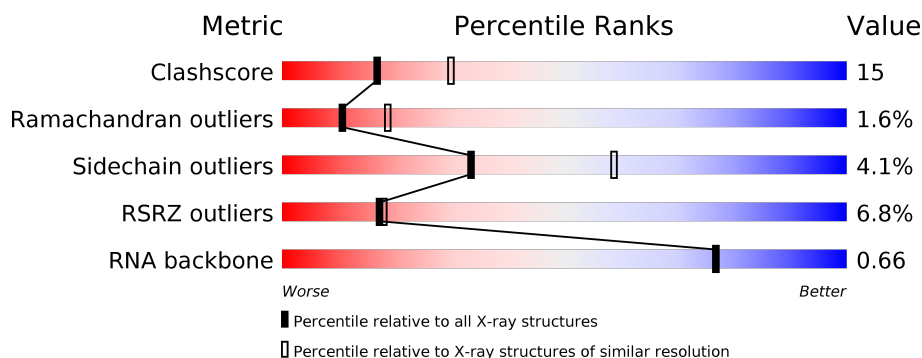
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)
RNA backbone	2636	1092 (2.90-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>28%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>8%</div> <div></div> </div> </div>
3	4	8	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>
4	A	240	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div></div> </div> </div>
5	B	338	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>44%</div> <div>5%</div> </div> </div>
6	C	246	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

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Mol	Chain	Length	Quality of chain
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	O	8092	-	-	-	X
35	NA	S	9112	-	-	-	X

## 2 Entry composition

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

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 38 is water.

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

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

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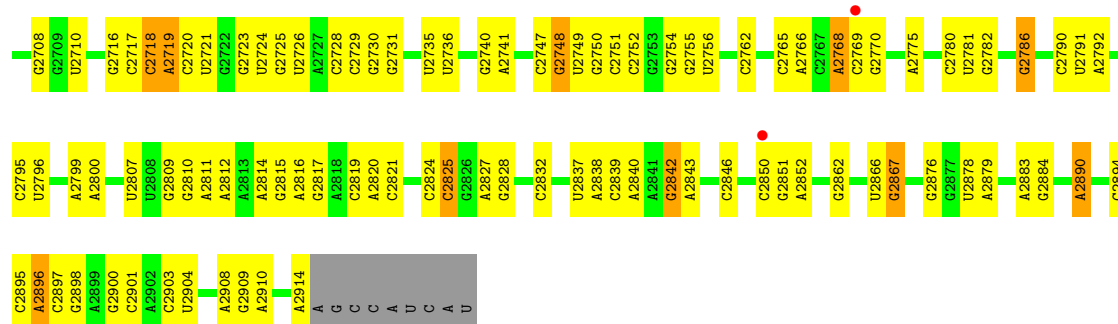
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	2	40	Total 40	O 40	0	0
38	3	74	Total 74	O 74	0	0
38	I	9	Total 9	O 9	0	0



U2587	G2379	A2274	C	C	C2035	G1923	C1798	A1711	G1592	C1462	C1342	A1232	A1161
G2588	A2382	G2275	A	A	C2036	G1929	G1799	A1712	C1594	A1463	C1343	A1233	G1162
U2589	A2382	C2281	C	C	A2039	G1929	G1805	G1713	C1595	G1351	G1351	G1235	U1164
G2477	G2386	U2282	A	U	U2043	A1942	G1806	G1714	U1596	A1470	A1352	G1236	G1165
U2478	U2387	A2291	G	G	G2044	C1943	A1811	C1715	A1597	A1471	C1353	U1237	A1166
G2480	C2388	A2291	U	U	U	G1948	U1817	A1717	A1598	C1472	G1354	G1239	G1167
A2483	A2401	A2300	A	A	G2053	G1949	A1815	U1722	G1603	C1474	C1360	A1242	U1169
U2607	A2402	A2301	A	C	A2054	G1950	A1815	U1722	A1604	C1477	C1360	A1242	U1170
C2608	C2403	A2302	A	A	A2055	G1951	G1820	U1724	G1605	A1478	C1363	C1243	A1171
A2488	C2309	C2309	U	C	C2061	A	A	C1725	C1613	C1477	C1363	C1243	G1172
G2489	A2408	A2311	C	A	A2062	A	U1825	U1724	G1614	A1478	C1363	C1243	G1172
A2490	A2311	A2311	C	U	U2063	C	C1826	G1730	G1614	A1482	C1370	U1244	A1174
C2493	G2412	G2312	C	G	U2064	U	A1829	C1731	U1624	C1483	C1371	A1246	G1175
A2413	A2414	G2314	C	A	U2067	A	A1829	A1732	U1625	A1484	A1372	C1250	G1176
U2499	A2415	G2316	C	U	A2067	U	C1830	A1733	A1626	A1485	A1375	C1251	A1177
G2501	G2418	C2317	C	G	A2068	G	C1834	C1734	G1634	C1496	G1376	C1268	G1178
C2502	U2419	C2317	U	G	G2072	A	U1835	G1739	U1635	G1269	C1377	U1270	U1180
A2503	G2420	C2317	C	A	G2073	C	A1840	U1740	G1636	A1181	U1380	U1270	A1181
G2504	G2421	A2321	G	A	A2074	C	A1840	U1741	A1637	U1500	U1380	C1273	C1183
C2505	U2422	A2321	U	C	G2075	U1964	A1845	A1742	A1637	U1503	G1386	C1273	C1184
A2506	G2423	C2325	G	C	U2076	G1970	A1845	G1743	A1641	A1504	G1387	U1279	U1185
G2507	U2424	C2326	A	A	C2077	A1971	U1846	G1744	A1642	A1504	G1387	U1279	U1185
U2508	A2424	C2326	C	C	U2078	G1971	A1847	G1745	A1642	A1505	C1393	A1287	U1187
A2509	G2425	A2327	U	A	G2079	U1972	G1848	A1746	U1654	U1506	A1393	A1287	U1187
G2510	G2426	U2328	C	U	G2080	A1973	G1849	A1747	U1655	A1515	C1395	U1288	A1188
C2511	C2427	C2329	C	C	A2081	U1973	G1849	A1747	A1655	A1515	C1395	C1289	A1189
U2512	G2428	U2330	C	C	C2081	G1976	G1855	G1751	A1656	C1516	C1396	A1294	G1190
A2521	U2435	G2333	C	C	G2090	U1977	C1856	G1752	A1657	U1524	A1406	A1191	A1192
U2524	G2333	C2333	A	A	G2091	A1978	C1856	G1752	A1658	G1525	A1407	G1299	A1193
G2525	G2438	C2335	G	G	G2092	G1979	C1856	A1753	C1666	A1526	A1407	G1300	A1194
C2526	C2439	G2336	U	U	G2093	U1980	A1667	A1755	A1667	A1527	A1413	G1195	C1196
U2527	G2443	G2337	C	C	G2094	U1985	G1867	C1762	U1668	A1528	A1414	U1304	C1196
A	C2443	C2338	C	C	A2096	U1985	G1868	G1762	U1668	G1529	G1415	C1305	G1197
C2533	U2444	A	C	C	C2096	C1993	U1874	U1766	C1675	U1530	G1416	U1306	U1198
G2533	U2445	C	C	C	A2101	G1996	U1874	U1766	C1676	G1417	G1417	A1197	A1199
C2534	G2446	A	C	C	G2102	U1996	G1877	A1767	U1677	U1531	A1307	A1307	A1201
U2535	G2446	G	C	C	C2105	U1996	G1877	A1767	A1678	G1535	U1418	A1308	C1201
G2451	G2452	A	C	C	G2106	U2004	G1878	C1768	C1679	G1536	U1419	A1309	A1202
G2452	A2345	A	G	G	C2105	G2005	C1880	C1769	C1679	C1537	C1420	U1310	G1203
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C2542	A2456	C2346	C	C	G2110	U2008	C1882	A1776	G1683	U1544	C1423	G1312	C1204
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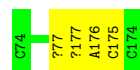




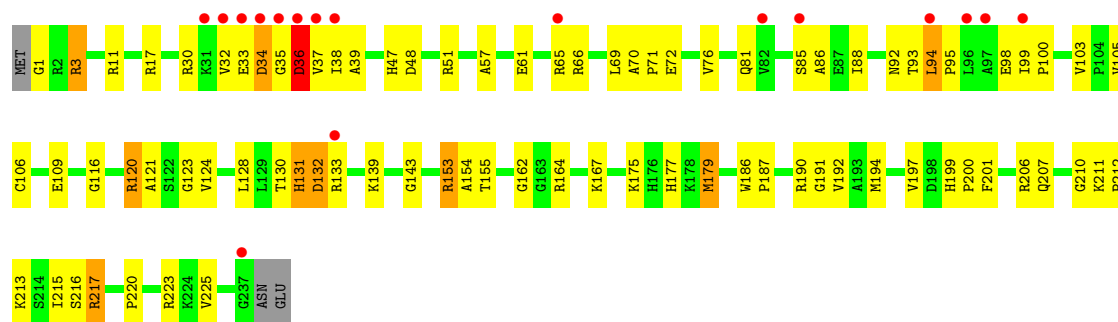
• Molecule 2: 5S ribosomal RNA



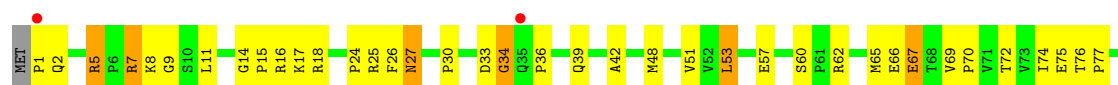
• Molecule 3: 5'-R(\*CP\*CP\*(5AA)P\*(2OP)P\*(PAE)P\*AP\*C\*C)-3'

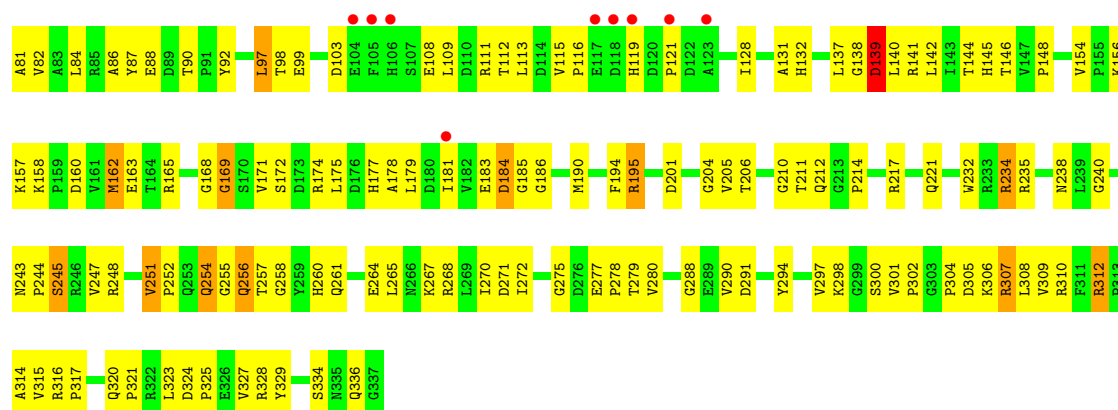


• Molecule 4: 50S ribosomal protein L2P

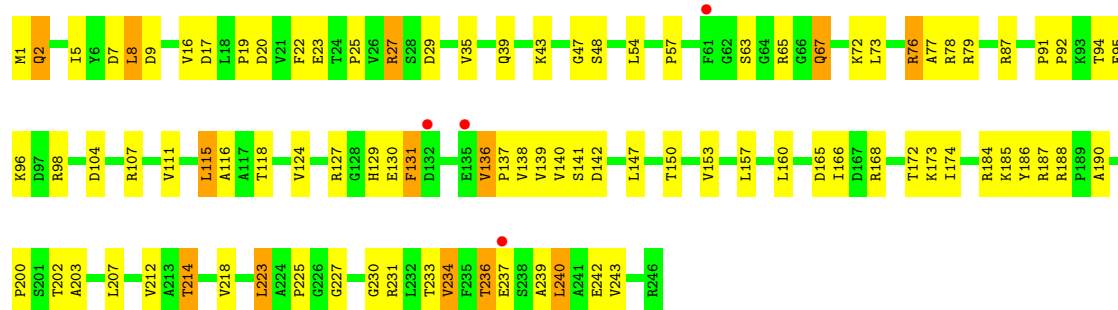


• Molecule 5: 50S ribosomal protein L3P

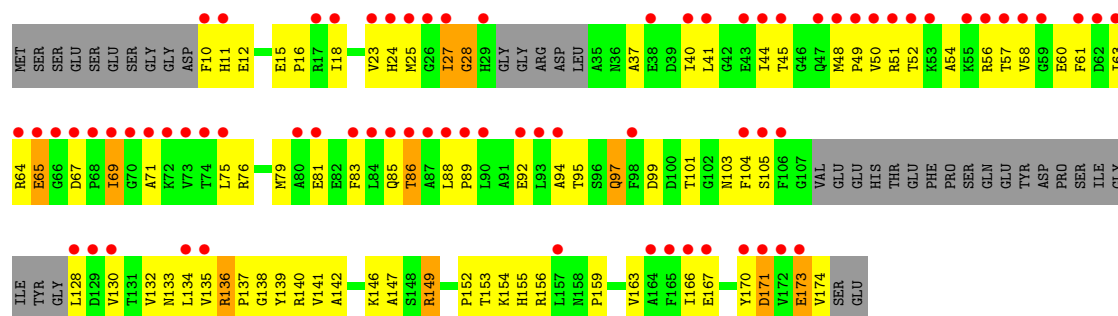




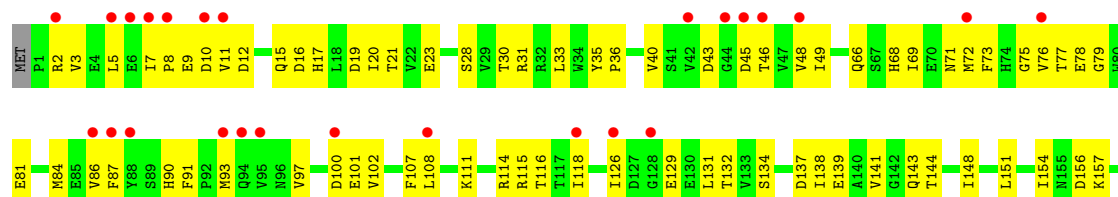
• Molecule 6: 50S ribosomal protein L4E

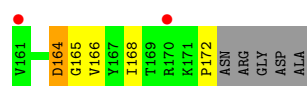


• Molecule 7: 50S ribosomal protein L5P

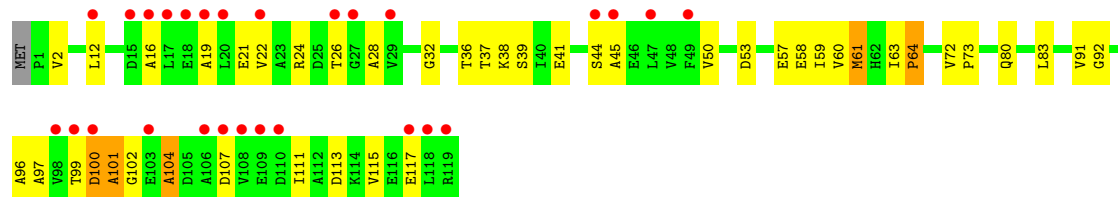


• Molecule 8: 50S ribosomal protein L6P

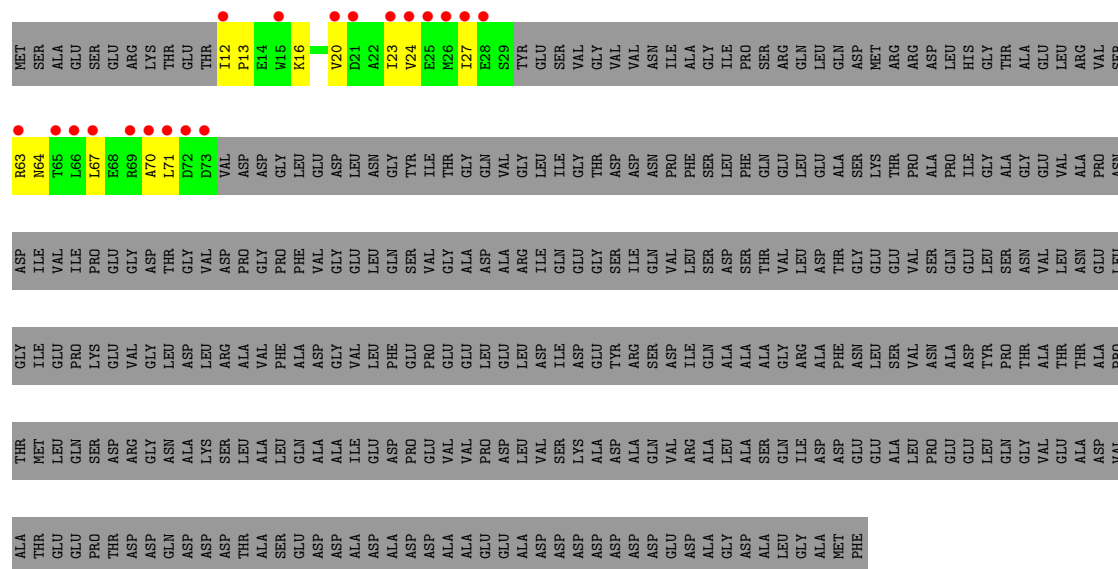




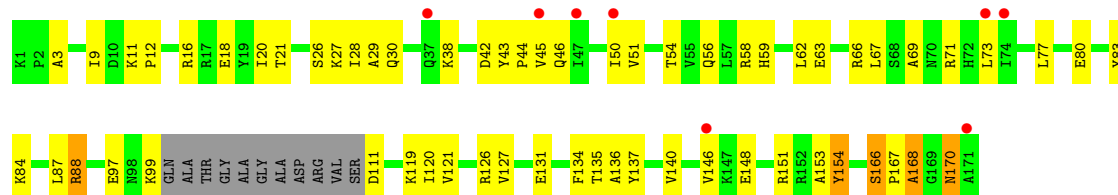
• Molecule 9: 50S ribosomal protein L7AE



• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

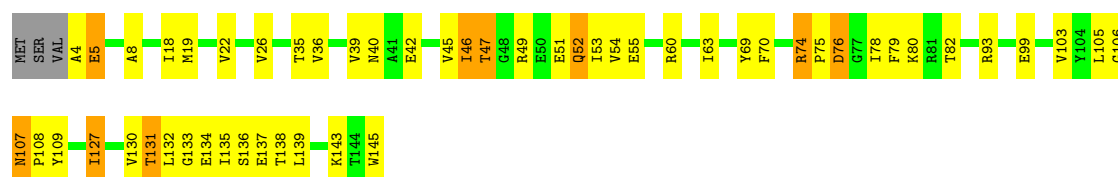


• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

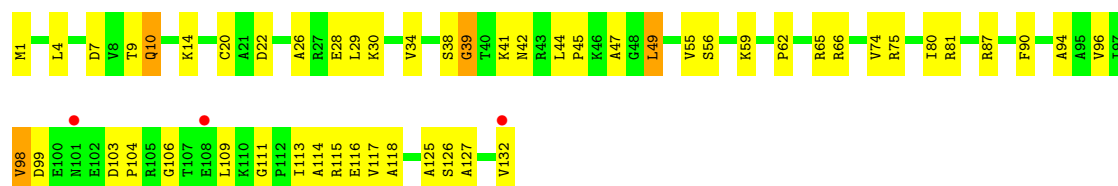


• Molecule 12: 50S ribosomal protein L13P

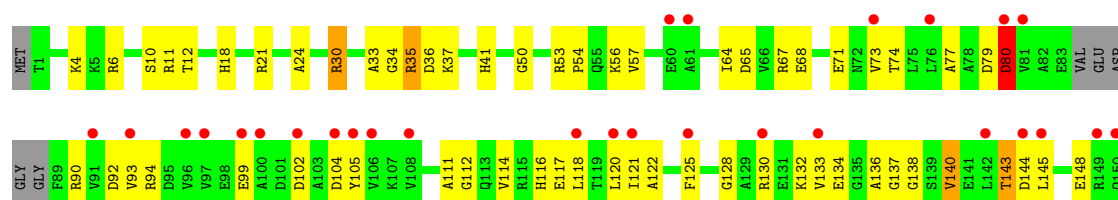




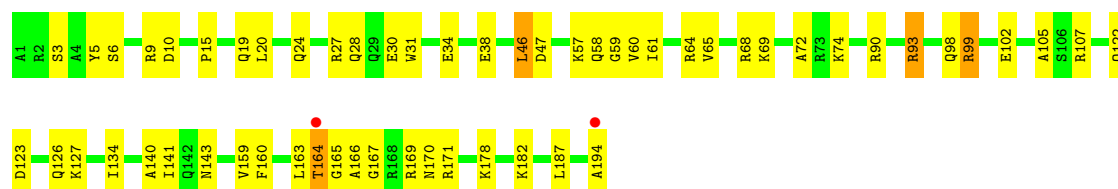
• Molecule 13: 50S ribosomal protein L14P



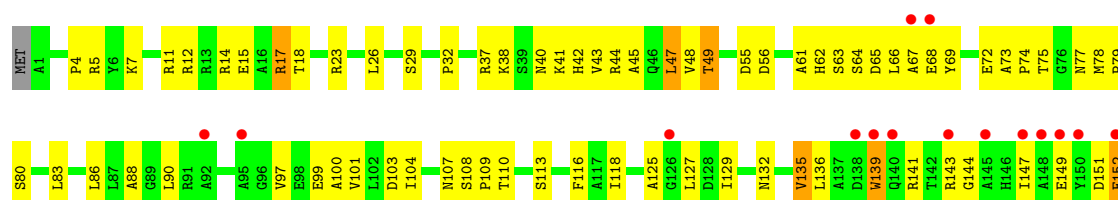
• Molecule 14: 50S ribosomal protein L15P



• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P





- Molecule 17: 50S ribosomal protein L18e



- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

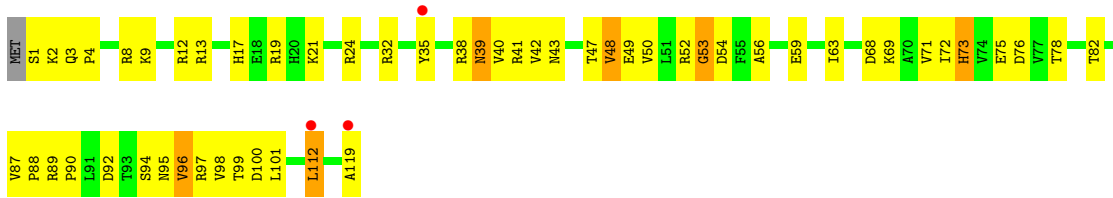


- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

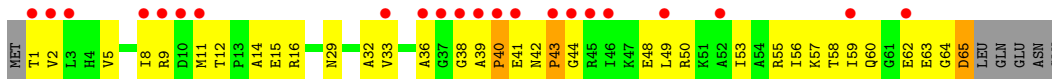




- Molecule 23: 50S ribosomal protein L24E



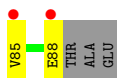
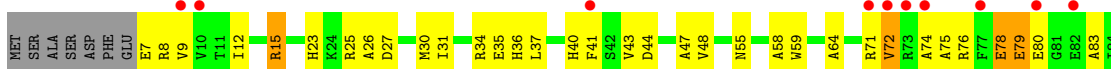
- Molecule 24: 50S ribosomal protein L29P



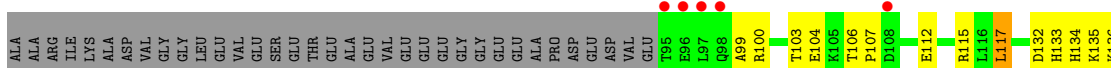
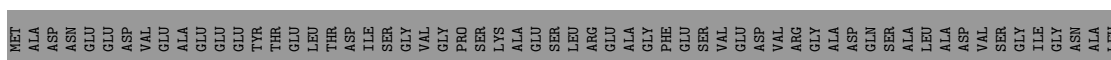
- Molecule 25: 50S ribosomal protein L30P

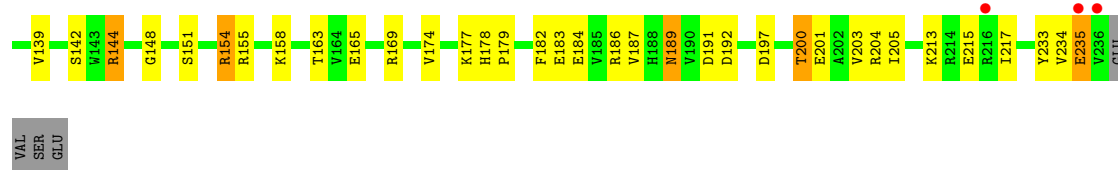


- Molecule 26: 50S ribosomal protein L31e

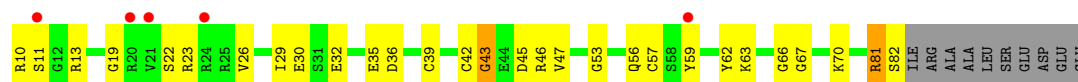


- Molecule 27: 50S ribosomal protein L32E

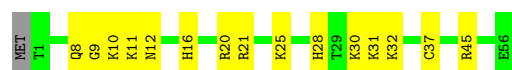




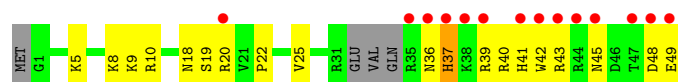
- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.15Å 300.13Å 573.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 89.0 (49.61-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.86 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.244 0.193 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, OMG, CL, NA, K, CD, 5AA, PAE, OMU, UR3, 2OP, 1MA, PSU

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

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

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

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

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

There are no bond length outliers.

All (24) bond angle outliers are listed below:

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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (57) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	791	A	Sidechain
1	0	795	G	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	882	A	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
2	9	3087	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	813	0
2	9	2600	0	1326	57	0
3	4	130	0	77	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	167	0
6	C	1859	0	1816	100	0
7	D	1094	0	1085	85	0
8	E	1357	0	1266	84	0
9	F	890	0	843	43	0
10	G	240	0	231	14	0
11	H	1266	0	1268	64	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	57	0
14	L	1118	0	1076	53	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5809	0	0	103	0
38	1	53	0	0	2	0
38	2	40	0	0	3	0
38	3	74	0	0	4	0
38	4	8	0	0	1	0
38	9	137	0	0	5	0
38	A	119	0	0	13	0
38	B	153	0	0	15	0
38	C	168	0	0	12	0
38	D	47	0	0	10	0
38	E	43	0	0	7	0
38	F	23	0	0	3	0
38	G	18	0	0	2	0
38	H	65	0	0	4	0
38	I	9	0	0	2	0
38	J	51	0	0	4	0
38	K	58	0	0	6	0
38	L	82	0	0	12	0
38	M	116	0	0	5	0
38	N	63	0	0	10	0
38	O	42	0	0	3	0
38	P	64	0	0	3	0
38	Q	51	0	0	3	0
38	R	84	0	0	3	0
38	S	30	0	0	1	0
38	T	42	0	0	2	0
38	U	29	0	0	2	0
38	V	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	68	0	0	2	0
38	X	27	0	0	2	0
38	Y	96	0	0	5	0
38	Z	32	0	0	2	0
All	All	99063	0	59977	2271	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.28	1.16
5:B:62:ARG:HA	5:B:65:MET:HE3	1.29	1.14
1:O:156:C:H5''	15:M:171:ARG:HD3	1.29	1.14
1:O:1160:G:H5'	1:O:1161:A:H5'	1.20	1.11
1:O:1242:A:H5'	12:J:82:THR:HG23	1.34	1.09
6:C:236:THR:HG22	6:C:239:ALA:H	1.16	1.08
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.30	1.08
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.34	1.07
1:O:1119:G:H2'	12:J:52:GLN:NE2	1.72	1.04
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.21	1.04
1:O:1751:G:H2'	1:O:1752:G:H5''	1.40	1.01
2:9:3076:G:H3'	2:9:3077:A:H5''	1.38	1.01
20:R:39:THR:HG22	20:R:42:GLU:H	1.26	1.00
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.40	1.00
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.76	1.00
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.40	1.00
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.77	0.99
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.42	0.99
1:O:2717:C:H2'	1:O:2718:C:H5''	1.46	0.98
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.45	0.97
13:K:10:GLN:H	13:K:10:GLN:NE2	1.61	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	1.10	0.97
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.47	0.96
7:D:154:LYS:HD2	7:D:154:LYS:H	1.29	0.96
1:O:871:G:C8	1:O:871:G:H5'	2.02	0.94
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.50	0.94
13:K:10:GLN:N	13:K:10:GLN:HE21	1.65	0.94
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.49	0.93
1:O:1187:U:HO2'	1:O:1189:A:H2	1.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.93
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.51	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.32	0.92
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.35	0.92
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.52	0.92
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.11	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.92
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.52	0.91
12:J:131:THR:HG22	12:J:134:GLU:H	1.34	0.91
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.11	0.91
1:0:541:C:H2'	1:0:542:A:H5''	1.53	0.91
6:C:1:MET:HG2	6:C:2:GLN:H	1.33	0.91
15:M:164:THR:HG22	15:M:167:GLY:H	1.33	0.91
1:0:2717:C:C2'	1:0:2718:C:H5''	2.01	0.90
1:0:1835:U:H5	1:0:1840:A:N7	1.69	0.90
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.90
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.53	0.90
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.54	0.89
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.89
1:0:542:A:H5'	1:0:542:A:H8	1.37	0.89
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.52	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	1.01	0.89
1:0:1701:A:H4'	1:0:1702:U:H5''	1.55	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.88	0.89
1:0:1372:A:H3'	38:0:7406:HOH:O	1.72	0.89
1:0:21:G:H5'	20:R:2:ILE:HA	1.55	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.88
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.74	0.87
16:N:144:GLY:O	16:N:147:ILE:HG22	1.74	0.87
5:B:248:ARG:O	5:B:251:VAL:HG12	1.73	0.87
1:0:1160:G:C5'	1:0:1161:A:H5'	2.05	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.75	0.86
26:X:30:MET:HE1	26:X:55:ASN:HA	1.57	0.86
1:0:870:G:H2'	1:0:871:G:H5''	1.55	0.86
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.24	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.24	0.85
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.34	0.85
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.58	0.85
1:0:1159:G:H21	1:0:1189:A:H8	1.26	0.84

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2468:A:H61	31:3:48:ASN:HD21	1.37	0.70
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.22	0.70
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.74	0.70
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.74	0.70
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.07	0.70
5:B:139:ASP:HB2	5:B:165:ARG:HE	1.56	0.69
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.72	0.69
1:O:1667:A:C8	1:O:1667:A:H5'	2.24	0.69
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.72	0.69
20:R:44:VAL:O	20:R:48:GLU:HG3	1.92	0.69
25:W:38:THR:HG22	25:W:39:ASP:H	1.58	0.69
38:O:7097:HOH:O	15:M:178:LYS:HB2	1.91	0.69
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.58	0.69
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.27	0.69
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.40	0.69
4:A:223:ARG:HG3	38:A:9398:HOH:O	1.91	0.69
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.73	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.91	0.69
1:O:338:C:H4'	6:C:174:ILE:CD1	2.23	0.69
20:R:9:ASP:O	20:R:13:THR:HB	1.92	0.69
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.58	0.69
1:O:1184:C:H1'	38:O:7669:HOH:O	1.92	0.69
9:F:38:LYS:NZ	15:M:3:SER:HA	2.08	0.69
21:S:57:THR:HG22	21:S:59:ASP:N	2.07	0.69
27:Y:117:LEU:HD12	27:Y:174:VAL:HG13	1.75	0.69
1:O:1166:A:H1'	1:O:1192:A:C2	2.29	0.68
1:O:1206:U:H6	1:O:1206:U:H5'	1.58	0.68
1:O:1116:U:H3	1:O:1246:A:H62	1.39	0.68
1:O:870:G:C2'	1:O:871:G:H5''	2.23	0.68
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.74	0.68
9:F:91:VAL:HG12	9:F:92:GLY:N	2.08	0.68
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.08	0.68
30:2:41:HIS:N	30:2:45:ASN:HD22	1.88	0.68
4:A:199:HIS:HD2	4:A:201:PHE:H	1.38	0.68
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.76	0.68
1:O:1666:C:O2'	1:O:1667:A:H5''	1.93	0.68
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.24	0.68
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.19	0.68
1:O:2502:C:H2'	1:O:2503:A:H5'	1.75	0.68
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.59	0.68
1:O:1236:A:C8	12:J:63:ILE:HD11	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.76	0.67
1:0:1474:C:C6	1:0:1474:C:H5'	2.22	0.67
1:0:2533:C:C6	1:0:2533:C:H5'	2.28	0.67
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.74	0.67
4:A:121:ALA:O	4:A:124:VAL:HG22	1.93	0.67
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.77	0.67
18:P:103:THR:HA	18:P:106:ARG:NH1	2.09	0.67
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.67
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.77	0.67
17:O:32:ARG:HD3	17:O:32:ARG:O	1.94	0.67
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.24	0.67
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.95	0.67
1:0:317:A:H5''	22:T:52:ARG:HD2	1.76	0.67
4:A:179:MET:HA	4:A:179:MET:CE	2.25	0.67
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.09	0.67
1:0:2768:A:H2'	1:0:2769:C:O4'	1.94	0.67
1:0:558:C:C2'	1:0:559:U:H5''	2.25	0.67
20:R:39:THR:HG22	20:R:42:GLU:N	2.05	0.67
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.59	0.67
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.77	0.66
1:0:1634:G:H3'	38:0:4200:HOH:O	1.94	0.66
1:0:542:A:H5'	1:0:542:A:C8	2.26	0.66
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.60	0.66
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.28	0.66
6:C:236:THR:CG2	6:C:239:ALA:H	2.00	0.66
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.66
16:N:169:PRO:O	16:N:172:PHE:HB3	1.96	0.66
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.56	0.66
1:0:560:C:H42	1:0:597:A:H61	1.42	0.66
1:0:1118:A:H3'	1:0:1118:A:H8	1.61	0.66
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.77	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.61	0.66
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.78	0.66
1:0:681:G:N3	1:0:681:G:H5'	2.11	0.66
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.11	0.66
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.77	0.66
1:0:506:G:H22	1:0:509:A:H5''	1.61	0.66
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.96	0.66
19:Q:26:PRO:O	19:Q:30:VAL:HG23	1.95	0.66
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.10	0.65
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.44	0.65

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.63
2:9:3029:C:C2'	2:9:3030:C:H5'	2.29	0.63
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.79	0.63
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.29	0.63
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.47	0.63
1:0:1641:A:H2'	1:0:1642:A:H5'	1.80	0.62
12:J:107:ASN:HD22	12:J:108:PRO:N	1.97	0.62
26:X:25:ARG:HD3	26:X:64:ALA:O	1.99	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.30	0.62
8:E:15:GLN:HG2	8:E:19:ASP:O	1.99	0.62
10:G:64:ASN:N	10:G:64:ASN:HD22	1.95	0.62
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.00	0.62
2:9:3014:G:H5'	2:9:3014:G:C8	2.33	0.62
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.80	0.62
11:H:170:ASN:HD22	11:H:170:ASN:N	1.96	0.62
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.81	0.62
1:0:88:G:H5'	1:0:88:G:H8	1.65	0.62
7:D:136:ARG:HD2	7:D:155:HIS:O	1.99	0.62
9:F:19:ALA:O	9:F:22:VAL:HG22	1.98	0.62
16:N:32:PRO:HD2	16:N:99:GLU:O	1.99	0.62
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.81	0.62
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.29	0.62
1:0:544:G:H2'	1:0:545:G:H5''	1.82	0.62
1:0:1053:G:OP1	11:H:12:PRO:HG3	1.99	0.62
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.99	0.62
25:W:122:ARG:CG	25:W:122:ARG:HH11	2.12	0.62
1:0:2534:C:H1'	38:O:3802:HOH:O	1.99	0.62
1:0:2824:C:H5''	1:0:2825:C:H5'	1.81	0.62
7:D:50:VAL:O	7:D:71:ALA:HA	2.00	0.62
10:G:16:LYS:O	10:G:20:VAL:HG23	1.99	0.62
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.99	0.62
1:0:2896:A:H5''	38:O:6350:HOH:O	2.00	0.62
38:O:7630:HOH:O	22:T:9:LYS:HB2	1.99	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:138:U:H5''	1:0:139:C:OP2	2.00	0.62
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.15	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.62
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.30	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
1:0:2256:G:H2'	1:0:2257:G:C5'	2.29	0.61
1:0:447:A:O2'	1:0:448:G:H5'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:O2'	1:0:559:U:H5''	2.00	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.65	0.61
1:0:2717:C:H2'	1:0:2718:C:C5'	2.27	0.61
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.81	0.61
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.98	0.61
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.81	0.61
24:V:1:THR:HG23	24:V:2:VAL:N	2.15	0.61
1:0:1120:U:H5''	1:0:1120:U:C6	2.35	0.61
32:I:138:THR:HG22	32:I:139:ILE:N	2.15	0.61
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.30	0.61
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.15	0.61
27:Y:144:ARG:CZ	38:Y:8201:HOH:O	2.48	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
6:C:1:MET:HG2	6:C:2:GLN:N	2.10	0.61
7:D:163:VAL:HA	38:D:6326:HOH:O	2.01	0.61
7:D:25:MET:CE	7:D:41:LEU:HG	2.30	0.61
32:I:99:ASP:OD1	32:I:138:THR:HB	2.00	0.61
1:0:506:G:H22	1:0:509:A:H5'	1.66	0.61
4:A:33:GLU:O	4:A:34:ASP:HB2	1.98	0.61
7:D:23:VAL:O	7:D:23:VAL:HG23	2.01	0.61
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.61
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.97	0.61
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.66	0.61
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.99	0.61
1:0:2248:C:H3'	38:0:5712:HOH:O	2.01	0.61
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.01	0.61
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.82	0.61
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.31	0.61
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.83	0.61
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.00	0.61
1:0:316:A:H5'	22:T:54:ASP:OD2	2.01	0.61
4:A:179:MET:HG2	4:A:186:TRP:CB	2.31	0.61
1:0:1943:C:H4'	4:A:211:LYS:O	2.01	0.61
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.82	0.61
8:E:93:MET:HE1	8:E:165:GLY:N	2.15	0.61
8:E:9:GLU:HG3	8:E:10:ASP:N	2.16	0.61
11:H:63:GLU:HA	38:H:9178:HOH:O	2.00	0.61
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.15	0.61
1:0:1741:U:O2'	1:0:2723:G:H4'	2.01	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.61
8:E:7:ILE:HG22	8:E:45:ASP:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:9:ILE:O	11:H:9:ILE:HG22	2.01	0.61
4:A:192:VAL:HG13	38:A:9356:HOH:O	2.00	0.61
12:J:133:GLY:O	12:J:137:GLU:HG3	2.01	0.61
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.31	0.61
19:Q:53:HIS:CE1	19:Q:55:ARG:HG3	2.35	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.32	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.82	0.60
1:O:558:C:H2'	1:O:559:U:C5'	2.30	0.60
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.34	0.60
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.83	0.60
16:N:110:THR:HB	16:N:113:SER:OG	2.02	0.60
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.60
1:O:1717:A:H5''	18:P:54:LYS:HB2	1.83	0.60
1:O:2716:G:H5''	5:B:206:THR:HG21	1.84	0.60
38:O:3594:HOH:O	13:K:9:THR:HA	2.01	0.60
16:N:37:ARG:NE	38:N:9331:HOH:O	2.34	0.60
1:O:2346:C:O5'	1:O:2346:C:H6	1.85	0.60
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.33	0.60
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.16	0.60
1:O:121:U:OP2	30:2:10:ARG:NH2	2.28	0.60
29:1:10:LYS:HG3	38:1:2979:HOH:O	2.01	0.60
7:D:153:THR:O	7:D:156:ARG:HB2	2.01	0.60
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.01	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
1:O:1667:A:H2'	1:O:1668:U:C6	2.37	0.60
1:O:475:G:H5'	6:C:73:LEU:HD23	1.84	0.60
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.84	0.60
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.84	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.02	0.60
14:L:143:THR:HG22	14:L:144:ASP:N	2.17	0.60
1:O:541:C:H2'	1:O:542:A:C5'	2.28	0.60
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
1:O:1878:G:H1'	38:O:6371:HOH:O	2.02	0.60
8:E:23:GLU:HG2	8:E:28:SER:CB	2.31	0.60
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.31	0.60
23:U:52:THR:CG2	23:U:54:THR:HB	2.32	0.60
25:W:88:THR:HG22	25:W:89:ASP:N	2.16	0.60
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.84	0.60
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.02	0.60
1:O:474:C:O3'	6:C:73:LEU:HD21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:151:ASP:O	16:N:154:LEU:HB2	2.01	0.60
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.84	0.60
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.37	0.59
21:S:56:ASN:O	30:2:8:LYS:NZ	2.34	0.59
13:K:115:ARG:HB3	13:K:132:VAL:OXT	2.02	0.59
20:R:132:ARG:HG2	20:R:133:ALA:N	2.17	0.59
1:O:1080:C:H4'	1:O:1081:A:OP1	2.01	0.59
1:O:2241:C:O2'	1:O:2242:U:H5'	2.01	0.59
7:D:154:LYS:H	7:D:154:LYS:CD	2.06	0.59
1:O:1119:G:OP2	12:J:49:ARG:HD3	2.02	0.59
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.82	0.59
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.84	0.59
1:O:2414:A:H2'	1:O:2415:A:C8	2.37	0.59
1:O:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
1:O:316:A:N3	1:O:336:G:O2'	2.35	0.59
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.84	0.59
1:O:20:G:H21	20:R:117:HIS:HD2	1.49	0.59
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.85	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.31	0.59
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.03	0.59
6:C:115:LEU:O	6:C:118:THR:HB	2.03	0.59
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.01	0.59
5:B:140:LEU:HD23	38:B:9384:HOH:O	2.02	0.59
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.85	0.59
18:P:103:THR:O	18:P:107:GLU:HG3	2.02	0.59
1:O:1973:A:H5'	1:O:1973:A:H8	1.68	0.59
1:O:247:A:H2'	38:O:4229:HOH:O	2.03	0.59
38:O:7658:HOH:O	5:B:211:THR:HG21	2.01	0.59
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.83	0.59
1:O:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.59
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.35	0.59
13:K:55:VAL:HG12	13:K:56:SER:N	2.18	0.59
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.84	0.59
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.33	0.59
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.32	0.59
1:O:1462:C:H2'	1:O:1463:A:C8	2.38	0.59
1:O:2898:G:H4'	5:B:288:GLY:HA2	1.84	0.59
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.38	0.59
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.02	0.59
12:J:130:VAL:HG12	12:J:131:THR:N	2.17	0.59
16:N:154:LEU:HD12	16:N:156:GLU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.67	0.59
1:0:1666:C:C2'	1:0:1667:A:H5''	2.33	0.59
1:0:1834:C:H2'	1:0:1840:A:N6	2.17	0.59
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.59
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.02	0.59
1:0:775:G:OP1	29:1:16:HIS:HE1	1.85	0.59
4:A:199:HIS:CD2	4:A:201:PHE:H	2.19	0.59
6:C:16:VAL:HG12	6:C:17:ASP:H	1.66	0.59
1:0:289:G:N2	1:0:363:A:H2	1.99	0.59
5:B:177:HIS:O	5:B:181:ILE:HG13	2.02	0.59
5:B:238:ASN:HD22	5:B:240:GLY:N	1.94	0.59
12:J:99:GLU:HA	38:J:9370:HOH:O	2.02	0.59
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.58
38:0:5498:HOH:O	13:K:39:GLY:HA2	2.02	0.58
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.84	0.58
9:F:58:GLU:HA	9:F:61:MET:HE2	1.85	0.58
25:W:149:LEU:HG	25:W:153:MET:CE	2.33	0.58
1:0:1189:A:H1'	1:0:1209:C:C1'	2.34	0.58
8:E:69:ILE:HA	8:E:72:MET:HE3	1.84	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58
1:0:1118:A:H8	1:0:1119:G:H5''	1.68	0.58
1:0:1527:A:H1'	1:0:1528:A:C8	2.39	0.58
1:0:2541:U:H5'	38:0:9722:HOH:O	2.04	0.58
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.18	0.58
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.19	0.58
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.58
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.58
1:0:2710:U:H1'	38:0:7817:HOH:O	2.03	0.58
1:0:2601:A:N1	13:K:38:SER:HB2	2.19	0.58
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.04	0.58
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.03	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.85	0.58
29:1:25:LYS:HG3	30:2:49:GLU:H	1.69	0.58
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.06	0.58
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.84	0.58
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.03	0.58
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.39	0.58
1:0:553:G:P	27:Y:204:ARG:HH22	2.26	0.58
1:0:1766:U:O2	1:0:1778:A:H5'	2.03	0.58
5:B:81:ALA:O	5:B:186:GLY:HA3	2.04	0.58
5:B:98:THR:CG2	5:B:99:GLU:H	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.85	0.58
17:O:105:ASN:HD21	17:O:109:SER:H	1.48	0.58
25:W:108:ARG:HE	25:W:114:PRO:CG	2.15	0.58
1:O:1741:U:H5'	1:O:1742:A:OP1	2.04	0.58
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.17	0.58
1:O:1182:C:H1'	1:O:1192:A:H8	1.68	0.58
16:N:47:LEU:HD12	16:N:97:VAL:HG11	1.86	0.58
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.03	0.58
1:O:1086:A:C6	25:W:11:VAL:HG11	2.38	0.58
1:O:1120:U:H6	1:O:1120:U:H5''	1.69	0.57
1:O:2488:A:H2	38:O:7489:HOH:O	1.87	0.57
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.68	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.86	0.57
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.86	0.57
1:O:2361:A:H8	1:O:2361:A:H5'	1.69	0.57
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.04	0.57
7:D:64:ARG:HB3	7:D:67:ASP:OD2	2.04	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.30	0.57
1:O:1189:A:H3'	38:O:7875:HOH:O	2.03	0.57
4:A:36:ASP:C	4:A:38:ILE:H	2.06	0.57
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.69	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.04	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.85	0.57
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.34	0.57
3:4:77:2OP:HA	3:4:177:PAE:O2	2.04	0.57
2:9:3020:G:O2'	2:9:3021:G:H5'	2.05	0.57
6:C:95:GLU:OE1	6:C:95:GLU:N	2.34	0.57
8:E:81:GLU:HG2	8:E:134:SER:CB	2.31	0.57
11:H:97:GLU:HB3	11:H:121:VAL:HG11	1.87	0.57
12:J:8:ALA:HA	12:J:35:THR:HG22	1.84	0.57
16:N:80:SER:HB2	38:N:9333:HOH:O	2.05	0.57
1:O:1625:U:H4'	38:O:4961:HOH:O	2.03	0.57
1:O:656:G:OP2	17:O:37:ARG:HD2	2.05	0.57
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.03	0.57
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.34	0.57
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.57
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.29	0.57
1:O:1441:G:O2'	1:O:1442:A:H5'	2.04	0.57
1:O:2505:G:O2'	1:O:2506:A:H5'	2.04	0.57
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.85	0.57
16:N:155:GLU:O	16:N:156:GLU:HG3	2.04	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.34	0.57
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.87	0.57
5:B:62:ARG:HA	5:B:65:MET:CE	2.19	0.57
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.87	0.57
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.04	0.57
1:O:1500:U:P	18:P:41:ARG:HH22	2.28	0.57
1:O:1596:U:H2'	1:O:1598:A:OP2	2.05	0.57
6:C:16:VAL:HG12	6:C:17:ASP:N	2.20	0.57
6:C:168:ARG:NH2	6:C:190:ALA:O	2.38	0.57
6:C:25:PRO:HG2	38:C:9122:HOH:O	2.04	0.57
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.86	0.57
32:I:92:PRO:O	32:I:94:GLU:HG3	2.05	0.57
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.86	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.25	0.57
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.20	0.57
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.70	0.57
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.39	0.57
25:W:13:MET:CE	25:W:17:ILE:HG22	2.34	0.57
1:O:503:G:H2'	1:O:504:G:H8	1.69	0.57
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.35	0.57
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.38	0.57
13:K:74:VAL:HG21	13:K:96:VAL:HG23	1.85	0.57
1:O:1010:C:H4'	16:N:4:PRO:HB2	1.86	0.56
1:O:848:C:H5'	38:O:7487:HOH:O	2.04	0.56
23:U:9:CYS:CA	23:U:52:THR:HG23	2.32	0.56
1:O:2649:A:H5'	1:O:2649:A:C8	2.40	0.56
1:O:902:G:N7	14:L:18:HIS:HD2	2.03	0.56
26:X:31:ILE:O	26:X:35:GLU:HG3	2.04	0.56
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.06	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.53	0.56
26:X:30:MET:CE	26:X:55:ASN:HA	2.32	0.56
31:3:3:MET:O	31:3:90:PHE:HA	2.05	0.56
31:3:73:GLU:HB3	38:3:9360:HOH:O	2.05	0.56
8:E:15:GLN:NE2	8:E:40:VAL:O	2.37	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.34	0.56
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.70	0.56
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.05	0.56
11:H:27:LYS:N	11:H:59:HIS:HD2	2.01	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.35	0.56
1:0:2420:G:O2'	1:0:2421:G:H5'	2.06	0.56
12:J:76:ASP:HA	38:J:9365:HOH:O	2.05	0.56
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.20	0.56
2:9:3051:A:H5'	16:N:160:SER:CB	2.32	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.56
1:0:449:A:N7	6:C:43:LYS:HG2	2.21	0.56
16:N:72:GLU:HG2	16:N:72:GLU:O	2.06	0.56
18:P:115:SER:H	18:P:118:GLN:NE2	1.86	0.56
1:0:2301:A:H5''	1:0:2302:A:H5'	1.87	0.56
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.36	0.56
25:W:52:VAL:HG22	25:W:53:ALA:N	2.20	0.56
25:W:59:GLN:HE22	25:W:98:PHE:HB2	1.69	0.56
1:0:1677:U:OP2	30:2:8:LYS:NZ	2.37	0.56
1:0:2769:C:H2'	1:0:2770:G:H5'	1.88	0.56
7:D:86:THR:C	7:D:89:PRO:HD2	2.26	0.56
1:0:2748:G:H2'	38:0:7739:HOH:O	2.05	0.56
5:B:16:ARG:NH1	38:B:9422:HOH:O	2.38	0.56
8:E:137:ASP:O	8:E:141:VAL:HG23	2.06	0.56
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.36	0.56
11:H:170:ASN:ND2	11:H:170:ASN:N	2.53	0.56
22:T:41:ARG:NH1	22:T:42:VAL:O	2.38	0.56
9:F:38:LYS:HZ1	15:M:3:SER:HA	1.68	0.56
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.70	0.56
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.20	0.56
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.69	0.56
1:0:1211:G:O2'	1:0:1212:C:H5'	2.05	0.55
1:0:709:G:O2'	17:O:25:VAL:HG12	2.07	0.55
2:9:3049:G:O2'	2:9:3050:G:H5'	2.05	0.55
1:0:475:G:C5'	6:C:73:LEU:HD23	2.37	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.36	0.55
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.05	0.55
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.35	0.55
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.30	0.55
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.35	0.55
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.36	0.55
1:0:2036:C:O4'	13:K:44:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:60:VAL:C	15:M:61:ILE:HD12	2.26	0.55
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.52	0.55
38:O:6997:HOH:O	16:N:4:PRO:HD2	2.06	0.55
21:S:77:VAL:O	21:S:80:ARG:HG2	2.06	0.55
24:V:39:ALA:O	24:V:41:GLU:N	2.33	0.55
26:X:78:GLU:HG2	26:X:79:GLU:N	2.21	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.04	0.55
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.05	0.55
5:B:98:THR:CG2	5:B:99:GLU:N	2.70	0.55
9:F:22:VAL:HG21	9:F:104:ALA:HB2	1.89	0.55
2:9:3054:A:O2'	2:9:3055:U:H5'	2.07	0.55
38:O:5127:HOH:O	12:J:47:THR:HB	2.06	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.06	0.55
7:D:138:GLY:N	38:D:7597:HOH:O	2.39	0.55
8:E:132:THR:O	8:E:132:THR:HG23	2.05	0.55
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.42	0.55
1:O:1058:A:H2'	1:O:1060:C:H5''	1.89	0.55
1:O:1418:U:OP1	30:2:42:TRP:HB3	2.06	0.55
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.87	0.55
1:O:282:C:H1'	1:O:368:C:H42	1.68	0.55
1:O:704:C:H2'	1:O:705:C:H6	1.71	0.55
6:C:138:VAL:O	6:C:234:VAL:HA	2.07	0.55
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.36	0.55
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.88	0.55
9:F:37:THR:O	9:F:41:GLU:HG3	2.07	0.55
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.87	0.55
1:O:1123:A:C6	1:O:1238:C:H5'	2.41	0.55
6:C:236:THR:HA	38:C:9249:HOH:O	2.06	0.55
38:O:5728:HOH:O	10:G:12:ILE:HA	2.05	0.55
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.72	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.63	0.55
25:W:46:ALA:O	25:W:49:ASN:HB2	2.06	0.55
25:W:65:VAL:CA	25:W:68:THR:HG22	2.35	0.55
1:O:1185:U:H2'	1:O:1186:C:C6	2.41	0.55
1:O:2718:C:H6	1:O:2718:C:H5'	1.72	0.55
1:O:644:G:N3	1:O:644:G:H5'	2.21	0.55
5:B:103:ASP:HB2	38:B:9399:HOH:O	2.06	0.55
16:N:86:LEU:O	16:N:90:LEU:HG	2.07	0.55
27:Y:155:ARG:NH1	38:Y:8144:HOH:O	2.40	0.55
1:O:1441:G:H1'	38:O:7960:HOH:O	2.06	0.55
1:O:263:U:O4'	9:F:59:ILE:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:135:VAL:HG22	7:D:136:ARG:H	1.71	0.55
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.88	0.55
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.42	0.55
1:O:1333:U:H2'	1:O:1334:C:C6	2.42	0.54
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.42	0.54
2:9:3028:U:H5''	16:N:40:ASN:HD21	1.72	0.54
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.89	0.54
20:R:29:LYS:NZ	38:R:9338:HOH:O	2.40	0.54
20:R:39:THR:HB	20:R:42:GLU:CD	2.27	0.54
1:O:1406:A:H4'	1:O:1407:A:H5''	1.89	0.54
1:O:299:U:H5'	38:O:7544:HOH:O	2.08	0.54
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.90	0.54
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.42	0.54
20:R:39:THR:HB	20:R:42:GLU:CG	2.37	0.54
1:O:56:G:H5''	24:V:50:ARG:NH1	2.22	0.54
25:W:125:HIS:CD2	25:W:127:GLY:H	2.25	0.54
1:O:2270:G:H4'	4:A:223:ARG:NH1	2.20	0.54
1:O:2780:C:H1'	8:E:143:GLN:NE2	2.22	0.54
8:E:9:GLU:HG3	8:E:10:ASP:H	1.73	0.54
12:J:135:ILE:O	12:J:139:LEU:HG	2.07	0.54
14:L:148:GLU:HA	38:L:9369:HOH:O	2.07	0.54
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.23	0.54
1:O:870:G:OP2	4:A:3:ARG:HD3	2.08	0.54
5:B:14:GLY:HA3	38:B:9415:HOH:O	2.08	0.54
5:B:86:ALA:HA	38:B:9384:HOH:O	2.07	0.54
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.72	0.54
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.10	0.54
1:O:1352:A:N1	6:C:48:SER:HB3	2.23	0.54
1:O:380:A:H2'	38:O:7443:HOH:O	2.07	0.54
15:M:24:GLN:O	15:M:28:GLN:HG3	2.07	0.54
1:O:1666:C:H2'	1:O:1667:A:C5'	2.38	0.54
1:O:2055:A:H4'	20:R:132:ARG:NH2	2.23	0.54
1:O:2251:G:H2'	1:O:2252:A:C8	2.43	0.54
1:O:65:C:O2'	1:O:66:G:H5'	2.07	0.54
1:O:2815:G:N7	12:J:80:LYS:NZ	2.55	0.54
1:O:1451:C:H5'	1:O:1505:U:H3	1.73	0.54
1:O:558:C:H2'	1:O:559:U:H5'	1.89	0.54
1:O:797:A:H4'	28:Z:10:ARG:N	2.23	0.54
5:B:144:THR:HG22	5:B:145:HIS:N	2.23	0.54
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.07	0.54
1:O:1477:C:H5'	1:O:1868:G:C5'	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2054:A:C2	20:R:128:ARG:NH2	2.72	0.54
1:0:669:G:O2'	1:0:670:G:H5'	2.08	0.54
1:0:462:A:C2	30:2:37:HIS:HB3	2.43	0.54
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.90	0.54
5:B:82:VAL:HG12	5:B:82:VAL:O	2.08	0.54
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.89	0.54
25:W:11:VAL:O	25:W:12:ASN:HB2	2.08	0.54
1:0:625:U:H5''	1:0:1044:C:N4	2.23	0.53
1:0:1667:A:H2'	1:0:1668:U:H6	1.72	0.53
1:0:2769:C:O2'	1:0:2770:G:H5'	2.09	0.53
2:9:3107:C:H2'	2:9:3108:C:C6	2.43	0.53
7:D:159:PRO:O	7:D:163:VAL:HG23	2.08	0.53
12:J:45:VAL:HG22	12:J:46:ILE:N	2.23	0.53
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.53
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.08	0.53
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.53
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.41	0.53
1:0:1679:C:H5'	38:0:9641:HOH:O	2.07	0.53
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.72	0.53
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.90	0.53
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.43	0.53
5:B:84:LEU:HD23	5:B:178:ALA:HB1	1.90	0.53
7:D:170:TYR:O	7:D:171:ASP:HB3	2.08	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.09	0.53
1:0:2467:A:O2'	1:0:2468:A:H2'	2.09	0.53
1:0:396:U:OP2	31:3:38:ARG:HD2	2.08	0.53
38:0:7567:HOH:O	4:A:177:HIS:HE1	1.91	0.53
5:B:27:ASN:H	5:B:27:ASN:HD22	1.57	0.53
6:C:140:VAL:HB	38:C:9249:HOH:O	2.08	0.53
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.89	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.89	0.53
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.90	0.53
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.53
1:0:2565:C:H4'	38:0:5126:HOH:O	2.08	0.53
1:0:2769:C:H2'	1:0:2770:G:O4'	2.08	0.53
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.90	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
7:D:154:LYS:HD2	7:D:154:LYS:N	2.12	0.53
8:E:81:GLU:O	8:E:172:PRO:HD3	2.08	0.53
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.91	0.53
1:0:475:G:OP1	6:C:73:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:H2'	1:0:559:U:H5''	1.90	0.53
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.07	0.53
38:0:9935:HOH:O	9:F:38:LYS:HE2	2.08	0.53
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.90	0.53
32:I:96:PHE:HA	32:I:136:GLY:CA	2.39	0.53
25:W:1:MET:HB2	25:W:103:GLU:HG2	1.89	0.53
1:0:1250:C:O2'	1:0:1251:C:H5'	2.08	0.53
1:0:2748:G:H1'	38:0:8202:HOH:O	2.09	0.53
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.91	0.53
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.53
1:0:517:U:H1'	38:0:7774:HOH:O	2.09	0.53
38:0:7754:HOH:O	31:3:60:LYS:HG3	2.08	0.53
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.91	0.53
14:L:92:ASP:HA	14:L:121:ILE:HB	1.91	0.53
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.37	0.53
1:0:1636:G:O2'	1:0:1637:A:H5'	2.08	0.53
1:0:2241:C:H2'	1:0:2242:U:C6	2.44	0.53
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.42	0.53
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.91	0.53
1:0:441:A:H1'	1:0:442:A:N7	2.24	0.53
1:0:947:U:H2'	1:0:948:G:H8	1.73	0.53
6:C:150:THR:HA	6:C:203:ALA:O	2.09	0.53
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.09	0.53
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.24	0.53
15:M:6:SER:O	15:M:10:ASP:HB2	2.09	0.53
24:V:56:ILE:O	24:V:60:GLN:HG3	2.09	0.53
27:Y:136:LYS:HB3	27:Y:139:VAL:HG23	1.91	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.52
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.08	0.52
5:B:162:MET:CE	5:B:310:ARG:HD3	2.37	0.52
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.39	0.52
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.43	0.52
12:J:130:VAL:HG12	12:J:131:THR:H	1.72	0.52
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.91	0.52
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.38	0.52
18:P:103:THR:HB	38:P:180:HOH:O	2.09	0.52
23:U:33:SER:O	23:U:37:GLU:HG3	2.09	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
25:W:82:GLU:O	25:W:86:GLU:HG3	2.09	0.52
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.74	0.52
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.52
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.52
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.90	0.52
5:B:128:ILE:O	5:B:131:ALA:HB3	2.09	0.52
5:B:258:GLY:H	5:B:260:HIS:CE1	2.27	0.52
6:C:118:THR:O	6:C:136:VAL:HG13	2.08	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.10	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.24	0.52
17:O:39:THR:O	17:O:115:ARG:NH2	2.39	0.52
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.52
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.09	0.52
23:U:17:THR:HG22	23:U:18:GLY:N	2.24	0.52
23:U:52:THR:HG22	23:U:54:THR:HB	1.90	0.52
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.09	0.52
6:C:79:ARG:O	6:C:87:ARG:HG2	2.09	0.52
11:H:21:THR:O	11:H:120:ILE:HD12	2.09	0.52
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.73	0.52
14:L:143:THR:CG2	14:L:144:ASP:N	2.72	0.52
38:O:9851:HOH:O	18:P:81:LYS:HG2	2.09	0.52
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.52
1:0:137:U:H2'	1:0:139:C:C5	2.44	0.52
1:0:1484:G:H2'	38:O:9420:HOH:O	2.08	0.52
1:0:2694:A:H5''	8:E:90:HIS:CE1	2.44	0.52
4:A:105:VAL:HG12	4:A:106:CYS:N	2.24	0.52
5:B:214:PRO:HD2	38:B:9321:HOH:O	2.08	0.52
32:I:113:HIS:N	32:I:114:PRO:HD2	2.24	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52
16:N:132:ASN:O	16:N:135:VAL:HG12	2.10	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.91	0.52
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.43	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.91	0.52
24:V:12:THR:HG23	24:V:14:ALA:N	2.25	0.52
1:0:1923:G:H4'	31:3:31:THR:O	2.09	0.52
1:0:328:U:O4'	6:C:202:THR:HG22	2.10	0.52
1:0:703:G:O2'	1:0:704:C:H5'	2.10	0.52
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.91	0.52
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.91	0.52
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.52
1:0:1537:C:H1'	38:O:6819:HOH:O	2.10	0.52
1:0:1787:C:H2'	1:0:1788:U:H6	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:777:U:O2'	29:1:11:LYS:HG2	2.10	0.52
1:0:2839:C:H4'	5:B:18:ARG:NH2	2.24	0.52
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.40	0.52
1:0:1462:C:H2'	1:0:1463:A:H8	1.74	0.52
1:0:1535:G:H2'	1:0:1536:C:C6	2.45	0.52
38:O:7247:HOH:O	4:A:211:LYS:HG2	2.08	0.52
1:0:2094:G:C4'	5:B:245:SER:HB3	2.36	0.52
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.39	0.52
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.39	0.52
17:O:87:THR:O	17:O:91:GLN:HG3	2.09	0.52
1:0:1482:A:O2'	1:0:1483:C:H5'	2.10	0.52
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.52
30:2:5:LYS:O	30:2:9:LYS:HG3	2.10	0.52
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.10	0.52
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.92	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.73	0.52
2:9:3114:G:O6	16:N:11:ARG:HD3	2.10	0.52
11:H:46:GLN:HG3	11:H:137:TYR:CE2	2.44	0.52
32:I:92:PRO:C	32:I:94:GLU:H	2.13	0.52
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.24	0.52
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.75	0.52
38:O:9868:HOH:O	25:W:119:HIS:HE1	1.93	0.52
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.83	0.52
1:0:1189:A:O2'	1:0:1208:C:H2'	2.09	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.76	0.52
1:0:1741:U:H3'	38:O:3073:HOH:O	2.10	0.52
1:0:2252:A:C5	1:0:2253:G:H1'	2.45	0.52
1:0:2372:A:H2'	1:0:2373:U:C6	2.45	0.52
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.52
1:0:2730:G:O2'	1:0:2731:G:H5'	2.10	0.52
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.90	0.52
11:H:27:LYS:H	11:H:59:HIS:CD2	2.21	0.52
14:L:136:ALA:HB3	38:L:9370:HOH:O	2.09	0.52
1:0:290:C:O2'	1:0:291:C:H5'	2.10	0.51
2:9:3050:G:H2'	2:9:3051:A:C8	2.45	0.51
2:9:3057:A:C8	7:D:141:VAL:HG21	2.45	0.51
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.51
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.92	0.51
14:L:10:SER:O	14:L:12:THR:N	2.41	0.51
20:R:82:GLU:HG3	20:R:83:LYS:N	2.25	0.51
1:0:1130:U:H2'	1:0:1131:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1173:A:H4'	1:0:1174:A:C8	2.45	0.51
1:0:1427:A:H61	1:0:1440:U:H1'	1.76	0.51
1:0:185:G:O3'	1:0:186:A:H4'	2.10	0.51
1:0:188:C:H5''	15:M:163:LEU:HD21	1.92	0.51
29:1:28:HIS:HD2	29:1:30:LYS:H	1.57	0.51
38:0:5678:HOH:O	4:A:164:ARG:CZ	2.58	0.51
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.91	0.51
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.10	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
25:W:122:ARG:NH1	25:W:152:ALA:O	2.43	0.51
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.10	0.51
4:A:35:GLY:O	4:A:36:ASP:CB	2.58	0.51
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.44	0.51
5:B:171:VAL:HG23	5:B:172:SER:N	2.24	0.51
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.11	0.51
1:0:2064:U:H5'	1:0:2652:U:H4'	1.93	0.51
1:0:2090:G:H2'	1:0:2091:G:C8	2.45	0.51
5:B:119:HIS:O	5:B:121:PRO:HD3	2.09	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
12:J:45:VAL:HG23	12:J:130:VAL:O	2.10	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51
13:K:74:VAL:HG13	13:K:113:ILE:HG12	1.91	0.51
14:L:104:ASP:O	14:L:105:TYR:HB3	2.09	0.51
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.43	0.51
25:W:65:VAL:HA	25:W:68:THR:CG2	2.37	0.51
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.93	0.51
6:C:1:MET:HG2	6:C:2:GLN:NE2	2.25	0.51
32:I:131:THR:HG22	32:I:131:THR:O	2.11	0.51
16:N:64:SER:C	16:N:66:LEU:H	2.14	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.40	0.51
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.25	0.51
38:0:7630:HOH:O	22:T:9:LYS:HD2	2.09	0.51
1:0:2526:C:O2'	1:0:2527:U:H5'	2.09	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.10	0.51
32:I:75:THR:HA	32:I:112:LYS:NZ	2.25	0.51
22:T:4:PRO:O	22:T:8:ARG:HG3	2.10	0.51
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.41	0.51
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.10	0.51
1:0:1166:A:H61	1:0:1180:U:H3	1.57	0.51
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.10	0.51
1:0:2720:C:O2	13:K:87:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.09	0.51
2:9:3064:C:H2'	2:9:3065:A:H5'	1.93	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
6:C:236:THR:HG22	6:C:239:ALA:CB	2.41	0.51
7:D:67:ASP:O	7:D:69:ILE:HG13	2.11	0.51
11:H:9:ILE:HD12	11:H:54:THR:CG2	2.38	0.51
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.41	0.51
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.51
31:3:62:THR:HB	38:3:9350:HOH:O	2.11	0.51
5:B:254:GLN:NE2	38:B:9395:HOH:O	2.43	0.51
20:R:99:ALA:CB	20:R:109:MET:HE1	2.32	0.51
27:Y:100:ARG:NH1	27:Y:215:GLU:HA	2.26	0.51
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.91	0.51
1:0:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.94	0.51
1:0:1942:A:O2'	1:0:1943:C:H5'	2.11	0.51
1:0:2748:G:H5'	38:0:7739:HOH:O	2.11	0.51
9:F:99:THR:HG23	9:F:99:THR:O	2.11	0.51
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.54	0.51
1:0:2072:G:C6	1:0:2533:C:H1'	2.46	0.51
1:0:2073:G:H5''	38:0:4132:HOH:O	2.11	0.51
1:0:396:U:O2'	1:0:418:C:H4'	2.10	0.51
15:M:164:THR:HG22	15:M:167:GLY:N	2.13	0.51
18:P:115:SER:C	18:P:117:SER:H	2.14	0.51
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.16	0.51
1:0:1733:A:H4'	5:B:212:GLN:HA	1.92	0.50
1:0:1878:G:O2'	1:0:1879:U:OP2	2.29	0.50
1:0:2325:C:H1'	38:0:4453:HOH:O	2.11	0.50
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.50
11:H:28:ILE:HG23	38:H:9178:HOH:O	2.10	0.50
11:H:66:ARG:HD3	38:H:9178:HOH:O	2.11	0.50
14:L:79:ASP:HB3	38:L:9357:HOH:O	2.11	0.50
1:0:156:C:H5''	15:M:171:ARG:CD	2.21	0.50
1:0:200:U:H2'	38:0:3752:HOH:O	2.10	0.50
1:0:2862:G:H4'	5:B:336:GLN:O	2.11	0.50
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.93	0.50
12:J:19:MET:CE	12:J:132:LEU:HD11	2.41	0.50
17:O:25:VAL:HG23	17:O:26:TRP:N	2.26	0.50
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.11	0.50
24:V:58:THR:O	24:V:62:GLU:HG3	2.11	0.50
25:W:1:MET:N	25:W:37:GLU:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.41	0.50
1:0:1427:A:H61	1:0:1440:U:C1'	2.25	0.50
1:0:544:G:C2'	1:0:545:G:H5''	2.40	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.88	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
20:R:114:VAL:HA	20:R:144:GLU:O	2.11	0.50
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.12	0.50
24:V:49:LEU:O	24:V:53:ILE:HG13	2.10	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.46	0.50
1:0:2851:G:C2'	1:0:2852:A:H5'	2.40	0.50
22:T:71:VAL:HG12	22:T:72:ILE:N	2.26	0.50
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.50
1:0:1515:A:H2'	1:0:1516:C:C6	2.46	0.50
1:0:2717:C:O2'	1:0:2718:C:H5''	2.11	0.50
1:0:536:A:H3'	38:0:5332:HOH:O	2.10	0.50
1:0:1185:U:OP1	32:I:126:LYS:HD3	2.11	0.50
16:N:154:LEU:C	16:N:156:GLU:H	2.15	0.50
23:U:44:ARG:HB3	38:U:3805:HOH:O	2.11	0.50
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.94	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
1:0:588:G:O6	25:W:154:ARG:NH1	2.44	0.50
4:A:88:ILE:HG22	4:A:88:ILE:O	2.12	0.50
9:F:101:ALA:HA	38:F:5413:HOH:O	2.11	0.50
38:0:5260:HOH:O	11:H:58:ARG:HG3	2.11	0.50
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.50
1:0:130:C:H2'	38:0:3469:HOH:O	2.11	0.50
1:0:1528:A:H2'	1:0:1529:G:O4'	2.11	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.12	0.50
1:0:424:C:H2'	1:0:425:U:C6	2.46	0.50
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.40	0.50
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.25	0.50
16:N:183:ASP:O	16:N:184:ILE:O	2.28	0.50
25:W:4:LEU:O	25:W:32:CYS:HA	2.11	0.50
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.65	0.50
1:0:1180:U:H4'	32:I:91:GLU:OE2	2.11	0.50
38:0:9535:HOH:O	4:A:11:ARG:HD3	2.12	0.50
1:0:2270:G:C4'	4:A:223:ARG:HH12	2.22	0.50
4:A:36:ASP:CG	4:A:85:SER:HB2	2.30	0.50
5:B:280:VAL:HG13	5:B:334:SER:HA	1.94	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.12	0.50
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:65:VAL:O	25:W:68:THR:HG22	2.12	0.50
1:O:1304:U:H2'	1:O:1305:C:C6	2.47	0.50
1:O:2387:U:H2'	1:O:2388:C:C6	2.47	0.50
1:O:2524:G:H21	1:O:2526:C:H41	1.59	0.50
1:O:951:A:C2'	1:O:952:G:H5'	2.42	0.50
4:A:17:ARG:HD2	38:A:9339:HOH:O	2.12	0.50
4:A:215:ILE:HG13	4:A:216:SER:N	2.27	0.50
5:B:109:LEU:HG	5:B:113:LEU:HD12	1.94	0.50
5:B:148:PRO:HB2	5:B:156:LYS:O	2.12	0.50
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.26	0.50
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.39	0.50
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.92	0.50
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.44	0.50
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.76	0.50
25:W:125:HIS:HD2	25:W:127:GLY:H	1.59	0.50
1:O:343:C:O2'	1:O:344:C:H5'	2.11	0.49
5:B:139:ASP:HB2	5:B:165:ARG:NE	2.24	0.49
6:C:65:ARG:HG3	6:C:67:GLN:HB2	1.93	0.49
1:O:1008:C:H5''	11:H:16:ARG:HH12	1.77	0.49
21:S:37:VAL:O	21:S:41:VAL:HG23	2.12	0.49
26:X:34:ARG:NH1	26:X:48:VAL:O	2.44	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.28	0.49
1:O:1701:A:H5''	1:O:1702:U:H3'	1.95	0.49
1:O:2472:C:O2'	1:O:2634:G:H4'	2.12	0.49
8:E:11:VAL:HG13	8:E:76:VAL:HG21	1.94	0.49
9:F:113:ASP:O	9:F:117:GLU:HG3	2.12	0.49
12:J:107:ASN:HD22	12:J:107:ASN:C	2.15	0.49
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.49
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.94	0.49
1:O:2385:G:H2'	1:O:2386:U:C6	2.48	0.49
1:O:284:C:H4'	1:O:285:A:O5'	2.12	0.49
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.77	0.49
1:O:1150:A:C2	10:G:20:VAL:HG21	2.47	0.49
32:I:139:ILE:HG22	32:I:140:GLU:N	2.27	0.49
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.76	0.49
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.49
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.41	0.49
1:O:2265:U:H2'	1:O:2266:A:C8	2.48	0.49
6:C:111:VAL:HB	38:C:9121:HOH:O	2.11	0.49
12:J:131:THR:HG22	12:J:134:GLU:N	2.16	0.49
2:9:3006:C:C5'	16:N:37:ARG:HH12	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:59:GLN:HE22	25:W:98:PHE:CA	2.25	0.49
1:0:2004:U:H2'	1:0:2004:U:O2	2.12	0.49
1:0:380:A:OP2	15:M:9:ARG:HD2	2.12	0.49
1:0:512:G:O3'	1:0:513:A:H8	1.95	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
20:R:33:ARG:NH1	38:R:9341:HOH:O	2.45	0.49
26:X:43:VAL:CG1	26:X:44:ASP:N	2.74	0.49
1:0:1681:G:H5''	1:0:1682:A:H5'	1.93	0.49
1:0:2681:A:H4'	1:0:2682:C:H5'	1.95	0.49
38:0:3270:HOH:O	31:3:84:ARG:HB2	2.11	0.49
4:A:130:THR:HG22	4:A:131:HIS:O	2.11	0.49
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.95	0.49
27:Y:133:HIS:HD2	38:Y:8170:HOH:O	1.94	0.49
1:0:21:G:H4'	20:R:2:ILE:HG22	1.95	0.49
1:0:2883:A:H2'	1:0:2884:G:O4'	2.13	0.49
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.49
1:0:834:G:H4'	1:0:835:U:OP2	2.13	0.49
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.79	0.49
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.39	0.49
14:L:145:LEU:O	14:L:148:GLU:HG3	2.13	0.49
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.48	0.49
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.26	0.49
1:0:2054:A:H2	20:R:128:ARG:HH22	1.57	0.49
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.76	0.49
1:0:1666:C:H2'	1:0:1667:A:H5'	1.94	0.49
1:0:1697:G:O2'	1:0:1698:U:H5'	2.12	0.49
1:0:177:A:H2'	1:0:178:U:O4'	2.12	0.49
1:0:2821:C:H4'	5:B:116:PRO:HB3	1.95	0.49
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.94	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
7:D:128:LEU:C	7:D:128:LEU:HD23	2.33	0.49
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.48	0.49
13:K:41:LYS:O	13:K:42:ASN:HB2	2.13	0.49
38:0:5799:HOH:O	15:M:58:GLN:HG3	2.13	0.49
38:0:4910:HOH:O	17:O:39:THR:HB	2.13	0.49
1:0:2338:G:H1'	7:D:105:SER:OG	2.12	0.49
1:0:2780:C:H2'	1:0:2781:U:C6	2.48	0.49
2:9:3029:C:H2'	2:9:3030:C:C5'	2.39	0.49
4:A:95:PRO:HA	4:A:153:ARG:HA	1.95	0.49
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.95	0.49
16:N:163:PHE:O	16:N:164:ASP:OD1	2.31	0.49
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.16	0.49
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.43	0.49
1:O:2335:C:H2'	1:O:2336:G:C8	2.48	0.49
1:O:2353:A:H4'	1:O:2354:A:O5'	2.12	0.49
1:O:2756:U:N3	1:O:2896:A:H2	2.08	0.49
6:C:20:ASP:O	6:C:23:GLU:HB2	2.13	0.49
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.28	0.49
11:H:166:SER:CB	11:H:167:PRO:CD	2.82	0.49
15:M:64:ARG:HD2	38:M:9382:HOH:O	2.13	0.49
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.49
1:O:1415:G:H5'	29:1:12:ASN:O	2.12	0.48
2:9:3049:G:H2'	2:9:3050:G:O4'	2.13	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
10:G:64:ASN:N	10:G:64:ASN:ND2	2.60	0.48
12:J:75:PRO:HD3	12:J:136:SER:OG	2.13	0.48
38:O:3957:HOH:O	17:O:3:THR:HG21	2.12	0.48
27:Y:144:ARG:NH1	38:Y:8164:HOH:O	2.45	0.48
1:O:1624:A:H5'	1:O:1626:A:O4'	2.13	0.48
1:O:1904:A:H2'	1:O:1905:U:O4'	2.13	0.48
1:O:485:A:N3	1:O:487:G:H5''	2.28	0.48
31:3:65:THR:HB	31:3:83:TRP:H	1.78	0.48
4:A:93:THR:HG23	4:A:154:ALA:O	2.12	0.48
1:O:2846:C:H4'	5:B:156:LYS:HB3	1.94	0.48
1:O:1734:C:OP1	5:B:234:ARG:HD3	2.13	0.48
5:B:255:GLY:O	5:B:257:THR:HG23	2.13	0.48
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.95	0.48
8:E:21:THR:HG23	8:E:30:THR:OG1	2.12	0.48
14:L:80:ASP:HB2	14:L:90:ARG:O	2.13	0.48
16:N:154:LEU:O	16:N:155:GLU:HB3	2.13	0.48
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.13	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
20:R:113:HIS:O	20:R:145:LEU:HD12	2.13	0.48
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.27	0.48
1:O:820:G:H5'	1:O:821:U:H5'	1.95	0.48
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.34	0.48
18:P:41:ARG:O	18:P:44:VAL:HB	2.13	0.48
1:O:1503:U:H2'	1:O:1504:A:O4'	2.13	0.48
1:O:474:C:O3'	6:C:73:LEU:CD2	2.61	0.48
1:O:90:A:H2'	1:O:91:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.48
4:A:132:ASP:OD1	4:A:133:ARG:N	2.47	0.48
5:B:277:GLU:N	5:B:278:PRO:HD2	2.28	0.48
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.96	0.48
7:D:135:VAL:HG22	7:D:136:ARG:N	2.28	0.48
11:H:167:PRO:O	11:H:168:ALA:HB2	2.13	0.48
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.95	0.48
17:O:35:LYS:O	17:O:40:HIS:NE2	2.47	0.48
21:S:11:THR:O	21:S:15:MET:HG2	2.13	0.48
26:X:75:ALA:O	26:X:83:ALA:HA	2.14	0.48
1:0:638:C:H2'	1:0:639:A:C8	2.48	0.48
30:2:41:HIS:O	30:2:45:ASN:HB2	2.13	0.48
5:B:251:VAL:HG23	5:B:252:PRO:HD2	1.95	0.48
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.43	0.48
6:C:19:PRO:HD2	6:C:240:LEU:HD21	1.95	0.48
14:L:114:VAL:HG11	38:L:9370:HOH:O	2.12	0.48
14:L:134:GLU:HA	14:L:138:GLY:O	2.13	0.48
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.48
16:N:100:ALA:O	16:N:129:ILE:HG23	2.13	0.48
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.13	0.48
38:O:6529:HOH:O	27:Y:158:LYS:HD3	2.13	0.48
1:0:2361:A:H2'	1:0:2362:A:C8	2.47	0.48
1:0:251:C:H5''	15:M:143:ASN:HD22	1.77	0.48
1:0:661:G:C5	1:0:686:A:C2	3.02	0.48
1:0:74:A:H2'	1:0:75:U:C6	2.48	0.48
2:9:3001:U:H5''	2:9:3003:A:OP1	2.14	0.48
8:E:101:GLU:HB2	8:E:116:THR:O	2.13	0.48
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.61	0.48
25:W:7:LEU:CD1	25:W:53:ALA:HB2	2.44	0.48
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.14	0.48
1:0:2073:G:OP2	1:0:2490:A:H5'	2.14	0.48
1:0:545:G:C8	1:0:545:G:H5'	2.40	0.48
31:3:67:LEU:HD21	31:3:88:LEU:CD2	2.43	0.48
32:I:102:VAL:O	32:I:106:LYS:HG3	2.14	0.48
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.95	0.48
14:L:143:THR:HG22	14:L:145:LEU:H	1.79	0.48
14:L:21:ARG:N	38:L:9329:HOH:O	2.46	0.48
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.96	0.48
18:P:16:VAL:CG1	18:P:17:GLY:N	2.76	0.48
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.95	0.48
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:8:ALA:CB	20:R:13:THR:HG21	2.39	0.48
25:W:137:GLN:HG3	25:W:137:GLN:O	2.14	0.48
1:0:1657:A:H2'	1:0:1658:A:C8	2.49	0.48
1:0:1919:A:H4'	38:0:5141:HOH:O	2.13	0.48
1:0:2900:G:H2'	1:0:2901:C:O4'	2.14	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.49	0.48
4:A:105:VAL:HG13	4:A:155:THR:O	2.14	0.48
4:A:210:GLY:HA3	38:A:9383:HOH:O	2.13	0.48
4:A:36:ASP:HB2	4:A:85:SER:H	1.78	0.48
8:E:84:MET:HE3	8:E:131:LEU:HD13	1.94	0.48
16:N:15:GLU:HB3	16:N:17:ARG:CG	2.42	0.48
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.95	0.48
25:W:7:LEU:HD12	25:W:53:ALA:HB2	1.96	0.48
1:0:1119:G:H22	1:0:1246:A:H2	1.52	0.48
1:0:1201:C:H2'	1:0:1202:A:H5'	1.95	0.48
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.48
1:0:2866:U:H4'	1:0:2867:G:H5'	1.94	0.48
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.14	0.48
1:0:1163:G:H2'	1:0:1164:U:C5	2.49	0.48
1:0:2421:G:H4'	38:0:5073:HOH:O	2.14	0.48
1:0:2909:G:H2'	1:0:2910:A:H8	1.79	0.48
4:A:39:ALA:O	4:A:61:GLU:HG3	2.14	0.48
5:B:140:LEU:HD13	5:B:175:LEU:HA	1.95	0.48
5:B:305:ASP:O	5:B:306:LYS:CB	2.61	0.48
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.44	0.48
9:F:58:GLU:HA	9:F:61:MET:HG3	1.95	0.48
10:G:67:LEU:O	10:G:71:LEU:HG	2.13	0.48
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.48	0.48
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.28	0.48
1:0:1086:A:N6	25:W:11:VAL:HG11	2.29	0.47
1:0:189:A:OP1	15:M:171:ARG:NH2	2.47	0.47
1:0:1811:A:C2	1:0:2752:C:H1'	2.49	0.47
1:0:2807:U:P	5:B:27:ASN:HD21	2.36	0.47
1:0:794:U:H3	1:0:819:A:H61	1.63	0.47
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
2:9:3064:C:C2'	2:9:3065:A:H5'	2.43	0.47
4:A:51:ARG:NH1	4:A:120:ARG:O	2.47	0.47
5:B:275:GLY:O	5:B:291:ASP:HA	2.14	0.47
16:N:42:HIS:HB3	16:N:62:HIS:CE1	2.49	0.47
21:S:57:THR:CG2	21:S:58:MET:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:78:GLU:CG	26:X:79:GLU:H	2.24	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
1:0:1805:G:H2'	1:0:1806:G:H8	1.78	0.47
1:0:2078:U:O2'	1:0:2079:G:H5'	2.14	0.47
1:0:2445:U:H2'	1:0:2446:G:C8	2.49	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.14	0.47
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.14	0.47
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.95	0.47
10:G:63:ARG:N	38:G:2569:HOH:O	2.46	0.47
11:H:63:GLU:O	11:H:67:LEU:HB2	2.14	0.47
12:J:8:ALA:HA	12:J:35:THR:CG2	2.44	0.47
1:0:2241:C:H2'	1:0:2242:U:H6	1.79	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2424:U:H1'	19:Q:7:LEU:HD12	1.96	0.47
1:0:2838:A:H2'	1:0:2839:C:C6	2.50	0.47
5:B:140:LEU:HA	38:B:9384:HOH:O	2.14	0.47
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.96	0.47
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.96	0.47
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.27	0.47
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.13	0.47
23:U:9:CYS:HA	23:U:52:THR:CG2	2.38	0.47
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.47
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.14	0.47
1:0:392:U:O2'	15:M:182:LYS:HE2	2.15	0.47
31:3:65:THR:HG21	31:3:83:TRP:CZ3	2.49	0.47
6:C:214:THR:HG23	38:C:9236:HOH:O	2.14	0.47
6:C:237:GLU:HA	38:C:9228:HOH:O	2.13	0.47
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.21	0.47
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.30	0.47
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.96	0.47
15:M:59:GLY:C	15:M:141:ILE:HD11	2.35	0.47
15:M:99:ARG:HD2	15:M:167:GLY:CA	2.35	0.47
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.95	0.47
1:0:1191:A:H2'	1:0:1193:A:H5'	1.96	0.47
1:0:128:A:O2'	1:0:129:A:H5'	2.14	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.59	0.47
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.47	0.47
38:O:3544:HOH:O	32:I:92:PRO:HD2	2.13	0.47
15:M:107:ARG:NH1	38:M:9374:HOH:O	2.48	0.47
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.47
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.74	0.47

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1060:C:H6	1:0:1060:C:H5'	1.80	0.47
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.47	0.47
1:0:1165:G:O2'	1:0:1174:A:H1'	2.15	0.47
1:0:1687:C:O2	29:1:9:GLY:HA2	2.15	0.47
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.47
1:0:407:A:H2'	1:0:408:A:C8	2.50	0.47
1:0:790:A:H2'	1:0:791:A:O4'	2.15	0.47
4:A:179:MET:HE2	4:A:179:MET:HA	1.96	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
10:G:12:ILE:N	10:G:13:PRO:CD	2.78	0.47
32:I:132:CYS:C	32:I:134:SER:H	2.16	0.47
32:I:133:THR:N	38:I:5371:HOH:O	2.48	0.47
1:0:1787:C:H4'	1:0:2883:A:O4'	2.15	0.47
4:A:51:ARG:HB2	38:A:9402:HOH:O	2.15	0.47
5:B:271:ASP:OD1	5:B:272:ILE:N	2.48	0.47
5:B:48:MET:HG2	5:B:72:THR:HA	1.97	0.47
7:D:166:ILE:HB	38:D:6326:HOH:O	2.13	0.47
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.47
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.45	0.47
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.49	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.50	0.47
1:0:1118:A:C3'	1:0:1118:A:C8	2.94	0.46
1:0:1375:A:H2'	1:0:1376:G:H5'	1.97	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
1:0:1855:G:H4'	1:0:1856:C:O5'	2.15	0.46
1:0:2135:A:O2'	1:0:2136:G:H5'	2.15	0.46
1:0:2613:G:O2'	1:0:2614:C:H5'	2.15	0.46
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.80	0.46
9:F:26:THR:HG21	9:F:102:GLY:C	2.35	0.46
1:0:317:A:OP1	22:T:52:ARG:O	2.33	0.46
23:U:52:THR:HG21	23:U:54:THR:HB	1.96	0.46
24:V:8:ILE:HA	24:V:11:MET:CE	2.44	0.46
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.15	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.15	0.46
1:0:249:G:O2'	1:0:250:C:H5'	2.15	0.46
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.96	0.46
16:N:67:ALA:C	16:N:69:TYR:H	2.17	0.46
1:0:2335:C:H2'	1:0:2336:G:H8	1.81	0.46
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.16	0.46
1:0:656:G:H5'	17:O:3:THR:CG2	2.45	0.46
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:91:GLN:O	31:3:92:GLU:HB2	2.14	0.46
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.50	0.46
1:0:1747:A:C8	13:K:44:LEU:HD13	2.50	0.46
14:L:24:ALA:HB2	14:L:30:ARG:HD2	1.97	0.46
16:N:152:GLU:C	16:N:154:LEU:H	2.17	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.95	0.46
22:T:48:VAL:HG22	22:T:96:VAL:HG13	1.97	0.46
25:W:35:VAL:CG2	25:W:41:TYR:CD2	2.98	0.46
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.56	0.46
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.46
1:0:1413:A:H2'	1:0:1414:A:O4'	2.15	0.46
1:0:1790:C:H2'	1:0:1791:U:H6	1.80	0.46
1:0:2255:A:H2'	1:0:2256:G:O4'	2.16	0.46
1:0:2478:U:O2'	1:0:2479:A:H5'	2.14	0.46
1:0:538:C:H5''	1:0:539:G:C8	2.51	0.46
1:0:571:C:H6	1:0:571:C:O5'	1.98	0.46
1:0:589:U:H2'	1:0:590:A:H8	1.79	0.46
1:0:899:C:H5'	38:0:3511:HOH:O	2.14	0.46
4:A:94:LEU:N	4:A:94:LEU:HD23	2.30	0.46
32:I:98:ALA:O	32:I:137:VAL:HA	2.16	0.46
16:N:164:ASP:OD1	16:N:167:ASP:CA	2.60	0.46
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.16	0.46
1:0:1380:U:O4	1:0:2043:U:H4'	2.16	0.46
1:0:960:G:H3'	1:0:960:G:N3	2.31	0.46
2:9:3039:U:H3'	2:9:3040:C:H5''	1.98	0.46
5:B:157:LYS:HG2	38:B:9467:HOH:O	2.16	0.46
8:E:68:HIS:O	8:E:72:MET:HG3	2.15	0.46
15:M:164:THR:HB	38:M:9319:HOH:O	2.15	0.46
18:P:14:LEU:HD13	18:P:51:ALA:HB2	1.96	0.46
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.16	0.46
23:U:20:MET:CG	23:U:28:THR:HG23	2.46	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
1:0:1342:C:C2'	1:0:1343:C:H5'	2.46	0.46
1:0:2897:C:H2'	1:0:2898:G:H8	1.80	0.46
1:0:949:U:H4'	19:Q:95:GLU:HA	1.97	0.46
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.45	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.46
7:D:37:ALA:O	7:D:40:ILE:HG12	2.16	0.46
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.48	0.46
16:N:108:SER:HA	16:N:109:PRO:HD3	1.72	0.46
25:W:13:MET:HE1	25:W:18:GLN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:83:TRP:CZ3	25:W:112:LEU:HD21	2.51	0.46
1:0:1375:A:C2'	1:0:1376:G:H5'	2.45	0.46
1:0:1530:U:H2'	1:0:1531:U:O4'	2.16	0.46
1:0:2507:G:H2'	1:0:2510:C:H42	1.81	0.46
1:0:241:A:C2	1:0:378:A:H4'	2.51	0.46
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.37	0.46
6:C:147:LEU:HA	38:C:9210:HOH:O	2.15	0.46
7:D:81:GLU:C	7:D:83:PHE:H	2.19	0.46
8:E:77:THR:OG1	8:E:78:GLU:N	2.43	0.46
13:K:49:LEU:HD21	13:K:74:VAL:O	2.16	0.46
22:T:75:GLU:O	22:T:76:ASP:HB2	2.15	0.46
22:T:78:THR:HB	22:T:87:VAL:O	2.16	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.16	0.46
1:0:797:A:O4'	28:Z:10:ARG:N	2.49	0.46
1:0:1181:A:N1	1:0:1192:A:O2'	2.46	0.46
1:0:1309:U:O2'	1:0:1310:U:H5'	2.16	0.46
1:0:2413:A:H2'	1:0:2414:A:O4'	2.15	0.46
1:0:2819:C:H2'	1:0:2820:A:C8	2.50	0.46
1:0:314:G:N2	1:0:316:A:H3'	2.31	0.46
4:A:105:VAL:CG1	4:A:106:CYS:N	2.79	0.46
1:0:1874:U:OP1	4:A:51:ARG:HD2	2.16	0.46
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.46
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.83	0.46
22:T:40:VAL:HG23	22:T:119:ALA:OXT	2.16	0.46
24:V:29:ASN:O	24:V:33:VAL:HG23	2.16	0.46
24:V:57:LYS:HA	24:V:60:GLN:NE2	2.28	0.46
1:0:1168:C:H4'	38:I:5128:HOH:O	2.16	0.46
1:0:1849:G:H1'	1:0:2011:A:N1	2.31	0.46
1:0:2846:C:OP1	5:B:158:LYS:HD2	2.15	0.46
1:0:31:C:H2'	38:O:7883:HOH:O	2.15	0.46
1:0:660:A:H4'	1:0:661:G:O5'	2.16	0.46
14:L:130:ARG:HA	38:L:9356:HOH:O	2.16	0.46
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.31	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.98	0.46
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.36	0.46
1:0:1164:U:H3	1:0:1192:A:H2	1.64	0.46
1:0:1768:C:H2'	1:0:1769:C:O4'	2.15	0.46
5:B:66:GLU:O	5:B:67:GLU:HB2	2.16	0.46
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.97	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:90:PHE:CD1	13:K:90:PHE:N	2.84	0.46
1:0:926:A:O2'	14:L:41:HIS:CD2	2.69	0.46
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.36	0.46
26:X:30:MET:CE	26:X:58:ALA:HB3	2.46	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.45
1:0:1120:U:H5'	1:0:1121:G:OP2	2.15	0.45
1:0:1419:U:H5'	1:0:1420:C:OP2	2.16	0.45
1:0:1825:U:O2'	1:0:1826:C:H5'	2.16	0.45
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
31:3:65:THR:HG23	31:3:67:LEU:HG	1.98	0.45
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.45
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.45
7:D:173:GLU:HG3	7:D:174:VAL:H	1.81	0.45
38:0:3205:HOH:O	12:J:46:ILE:HA	2.15	0.45
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.34	0.45
25:W:90:TYR:N	25:W:90:TYR:CD1	2.84	0.45
1:0:1634:G:H2'	1:0:1635:U:C6	2.51	0.45
1:0:2346:C:O2'	7:D:52:THR:HG21	2.16	0.45
1:0:2795:C:O2'	1:0:2796:U:H5'	2.15	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.16	0.45
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.98	0.45
32:I:132:CYS:C	32:I:134:SER:N	2.69	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
13:K:98:VAL:HG13	13:K:99:ASP:N	2.30	0.45
14:L:117:GLU:HB3	14:L:137:GLY:O	2.17	0.45
22:T:12:ARG:O	22:T:19:ARG:NH2	2.49	0.45
1:0:1139:U:H2'	1:0:1140:C:C6	2.51	0.45
1:0:2379:G:N3	1:0:2418:G:H2'	2.32	0.45
1:0:2563:U:H2'	1:0:2565:C:O5'	2.17	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
5:B:24:PRO:O	5:B:25:ARG:HD3	2.15	0.45
5:B:270:ILE:O	5:B:271:ASP:HB2	2.17	0.45
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.98	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
32:I:97:VAL:HG12	32:I:97:VAL:O	2.16	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.14	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
1:0:292:G:H2'	1:0:358:G:N2	2.31	0.45
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:671:A:O2'	1:0:672:G:H2'	2.17	0.45
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
9:F:32:GLY:N	38:F:3111:HOH:O	2.49	0.45
32:I:101:SER:OG	32:I:104:GLN:HG3	2.16	0.45
32:I:131:THR:O	32:I:135:LEU:HG	2.16	0.45
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.45	0.45
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.52	0.45
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.81	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
25:W:13:MET:HE2	25:W:18:GLN:N	2.31	0.45
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.51	0.45
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.45
1:0:2428:G:N7	31:3:60:LYS:NZ	2.61	0.45
1:0:816:G:C6	1:0:817:G:N1	2.84	0.45
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.97	0.45
32:I:75:THR:CA	32:I:112:LYS:NZ	2.79	0.45
17:O:96:VAL:HA	38:O:4258:HOH:O	2.17	0.45
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.03	0.45
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.99	0.45
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.45
1:0:1118:A:H62	1:0:1244:U:H3	1.63	0.45
1:0:1269:G:H2'	1:0:1270:U:C6	2.52	0.45
1:0:1299:G:N7	14:L:6:ARG:NH1	2.64	0.45
1:0:2508:C:H2'	38:O:6980:HOH:O	2.15	0.45
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.45
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.98	0.45
4:A:211:LYS:NZ	38:A:9415:HOH:O	2.43	0.45
4:A:48:ASP:HB3	38:A:9402:HOH:O	2.15	0.45
5:B:17:LYS:O	5:B:260:HIS:HD2	1.99	0.45
5:B:33:ASP:O	5:B:34:GLY:O	2.34	0.45
8:E:31:ARG:HH12	8:E:68:HIS:CE1	2.35	0.45
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.17	0.45
1:0:21:G:H5''	20:R:2:ILE:HA	1.95	0.45
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.98	0.45
1:0:1595:G:O2'	1:0:1596:U:H5'	2.16	0.45
1:0:1891:G:H1'	1:0:1972:U:C2	2.51	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.17	0.45
31:3:48:ASN:ND2	31:3:50:GLY:H	2.14	0.45
1:0:2101:A:H2'	6:C:63:SER:OG	2.17	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.46	0.45
9:F:91:VAL:CG1	9:F:92:GLY:N	2.79	0.45
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.45
14:L:57:VAL:O	14:L:57:VAL:HG12	2.17	0.45
21:S:30:ASP:HA	21:S:62:LYS:HE3	1.99	0.45
21:S:52:VAL:C	21:S:53:ASN:HD22	2.19	0.45
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.82	0.45
1:O:1477:C:O2'	1:O:1478:U:H5'	2.17	0.45
1:O:2266:A:H2'	1:O:2267:G:C8	2.52	0.45
1:O:820:G:O2'	1:O:856:G:H4'	2.17	0.45
1:O:952:G:N3	1:O:2302:A:H2'	2.32	0.45
1:O:960:G:H2'	1:O:960:G:N3	2.31	0.45
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.82	0.45
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.51	0.45
1:O:2637:A:N6	3:4:176:A:H2'	2.32	0.45
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.51	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
8:E:71:ASN:ND2	8:E:138:ILE:HD13	2.31	0.45
13:K:103:ASP:O	13:K:104:PRO:C	2.56	0.45
38:9:3472:HOH:O	16:N:41:LYS:HD3	2.16	0.45
22:T:48:VAL:HG21	22:T:96:VAL:CG1	2.47	0.45
25:W:132:VAL:C	25:W:134:GLU:H	2.20	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.68	0.45
1:O:1829:A:H2'	1:O:1830:C:H5'	1.99	0.45
1:O:2329:C:O2'	1:O:2330:U:H5'	2.16	0.45
1:O:2401:A:H2'	1:O:2402:A:C8	2.52	0.45
1:O:2541:U:C2	1:O:2620:U:O4	2.69	0.45
1:O:958:G:H2'	1:O:959:C:C6	2.52	0.45
4:A:139:LYS:HE2	4:A:143:GLY:HA2	1.99	0.45
4:A:213:LYS:NZ	38:A:9362:HOH:O	2.46	0.45
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.98	0.45
6:C:240:LEU:O	6:C:240:LEU:HD23	2.17	0.45
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.17	0.45
11:H:45:VAL:HA	11:H:167:PRO:O	2.16	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.81	0.45
38:O:4963:HOH:O	21:S:67:ARG:HD3	2.16	0.45
22:T:71:VAL:CG1	22:T:72:ILE:N	2.79	0.45
26:X:41:PHE:O	26:X:43:VAL:HG23	2.17	0.45
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:165:A:H5''	14:L:33:ALA:HB2	1.99	0.45
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.45
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.45
38:0:5788:HOH:O	5:B:298:LYS:HD3	2.15	0.45
6:C:166:ILE:CD1	6:C:207:LEU:HD13	2.46	0.45
13:K:20:CYS:HB3	13:K:26:ALA:O	2.17	0.45
13:K:66:ARG:HD3	38:K:2777:HOH:O	2.17	0.45
1:0:1058:A:H2'	1:0:1060:C:C5'	2.47	0.44
1:0:1300:G:H1'	38:0:4978:HOH:O	2.17	0.44
1:0:2419:U:H5''	1:0:2420:G:H5'	1.99	0.44
1:0:2435:U:H1'	38:0:5700:HOH:O	2.17	0.44
1:0:291:C:H2'	1:0:292:G:O4'	2.17	0.44
1:0:700:A:C2	14:L:71:GLU:HG2	2.52	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.17	0.44
1:0:2451:G:O2'	31:3:38:ARG:NH2	2.50	0.44
7:D:63:ILE:HG13	7:D:64:ARG:N	2.32	0.44
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.82	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.44
20:R:124:GLY:HA3	20:R:136:TRP:O	2.17	0.44
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.47	0.44
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.99	0.44
1:0:1189:A:H1'	1:0:1209:C:H1'	1.97	0.44
1:0:1329:A:N1	36:0:9313:CL:CL	2.87	0.44
1:0:500:G:H21	20:R:98:ASN:HD21	1.63	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.65	0.44
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.18	0.44
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.83	0.44
7:D:140:ARG:O	7:D:140:ARG:HG2	2.17	0.44
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.99	0.44
32:I:112:LYS:C	32:I:114:PRO:HD2	2.37	0.44
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.99	0.44
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.47	0.44
18:P:108:LEU:HB2	18:P:114:LEU:HD12	2.00	0.44
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.47	0.44
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.85	0.44
21:S:33:SER:OG	21:S:36:GLU:HG3	2.16	0.44
24:V:5:VAL:HG11	24:V:9:ARG:NH1	2.32	0.44
1:0:1495:C:H2'	1:0:1496:G:C8	2.52	0.44
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.44
1:0:2403:C:H3'	38:0:5489:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2821:C:H4'	5:B:116:PRO:CB	2.48	0.44
1:0:447:A:OP1	22:T:2:LYS:HG2	2.17	0.44
1:0:736:A:H2'	1:0:737:A:O4'	2.17	0.44
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.44
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.46	0.44
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.99	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
13:K:106:GLY:HA3	38:K:5264:HOH:O	2.16	0.44
1:0:1183:C:N4	1:0:1184:C:H41	2.15	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.35	0.44
1:0:2894:C:O2'	1:0:2895:C:H5'	2.17	0.44
1:0:396:U:H1'	38:0:7824:HOH:O	2.15	0.44
29:1:28:HIS:O	29:1:32:LYS:N	2.48	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.32	0.44
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.44
7:D:18:ILE:HG12	7:D:134:LEU:CD2	2.47	0.44
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.17	0.44
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.44
1:0:2036:C:C1'	13:K:44:LEU:HG	2.47	0.44
18:P:55:LYS:CG	18:P:56:GLY:N	2.80	0.44
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.05	0.44
1:0:1309:U:C2'	1:0:1310:U:H5'	2.48	0.44
1:0:820:G:H3'	38:0:3359:HOH:O	2.18	0.44
5:B:294:TYR:HE2	38:B:9456:HOH:O	2.01	0.44
9:F:91:VAL:CG1	9:F:92:GLY:H	2.28	0.44
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.00	0.44
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.83	0.44
14:L:92:ASP:OD1	14:L:94:ARG:HB2	2.17	0.44
20:R:114:VAL:HB	20:R:145:LEU:HD13	2.00	0.44
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.99	0.44
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.44
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.44
1:0:1909:A:N1	1:0:2128:G:H1'	2.33	0.44
1:0:2011:A:H4'	1:0:2012:U:O5'	2.18	0.44
1:0:2281:C:C2'	1:0:2282:U:H5'	2.47	0.44
1:0:2542:C:H5''	1:0:2608:C:N4	2.33	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.48	0.44
5:B:138:GLY:O	5:B:139:ASP:C	2.55	0.44
5:B:195:ARG:NH2	5:B:323:LEU:HD13	2.33	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.83	0.44
6:C:153:VAL:O	6:C:157:LEU:HG	2.17	0.44
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.47	0.44
10:G:20:VAL:O	10:G:24:VAL:HG23	2.18	0.44
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.44
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.82	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.85	0.44
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.18	0.44
1:O:1976:G:H1'	1:O:2005:G:N2	2.33	0.44
1:O:289:G:O2'	1:O:290:C:H5'	2.18	0.44
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.17	0.44
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.17	0.44
12:J:42:GLU:HG3	12:J:145:TRP:CD1	2.53	0.44
16:N:67:ALA:C	16:N:69:TYR:N	2.71	0.44
17:O:96:VAL:HG12	17:O:97:SER:N	2.33	0.44
1:O:1202:A:H2'	1:O:1203:G:H5'	1.99	0.44
1:O:2004:U:H2'	1:O:2005:G:OP1	2.18	0.44
1:O:2243:C:H5''	38:0:4058:HOH:O	2.17	0.44
1:O:2781:U:H2'	1:O:2782:G:H5'	1.99	0.44
1:O:2782:G:O6	1:O:2790:C:H5''	2.17	0.44
1:O:553:G:P	27:Y:204:ARG:NH2	2.90	0.44
1:O:818:A:O2'	28:Z:13:ARG:HD3	2.18	0.44
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.53	0.44
5:B:251:VAL:HG13	38:B:9371:HOH:O	2.18	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.98	0.44
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.44
17:O:24:ALA:O	17:O:28:ASP:HB2	2.18	0.44
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.48	0.44
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.80	0.44
27:Y:177:LYS:HE2	27:Y:183:GLU:OE2	2.17	0.44
1:O:1167:G:O2'	1:O:1168:C:H5'	2.18	0.44
1:O:2504:A:H2'	1:O:2505:G:O4'	2.18	0.44
6:C:7:ASP:C	6:C:9:ASP:H	2.21	0.44
15:M:165:GLY:O	15:M:169:ARG:HG3	2.18	0.44
1:O:100:C:O2	22:T:17:HIS:HB3	2.18	0.43
1:O:1268:C:H2'	1:O:1269:G:H8	1.83	0.43
1:O:1744:G:H2'	1:O:1745:G:H5'	1.98	0.43
1:O:2363:G:O3'	19:Q:11:ARG:NH1	2.51	0.43
1:O:508:A:H2'	1:O:509:A:H5''	2.00	0.43
1:O:585:C:H5''	38:0:5161:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.53	0.43
8:E:7:ILE:HD11	8:E:11:VAL:HG12	2.00	0.43
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.98	0.43
1:0:841:A:OP2	20:R:128:ARG:HD2	2.18	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.17	0.43
1:0:1067:A:H5'	38:0:4650:HOH:O	2.16	0.43
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.43
1:0:1883:U:C2'	1:0:1884:G:H5'	2.48	0.43
1:0:1929:G:H1'	38:0:5438:HOH:O	2.18	0.43
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.33	0.43
6:C:115:LEU:HD21	6:C:243:VAL:CG1	2.38	0.43
32:I:118:SER:HB2	32:I:123:ASN:HB2	2.00	0.43
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.33	0.43
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.51	0.43
23:U:17:THR:CG2	23:U:18:GLY:N	2.81	0.43
28:Z:13:ARG:NH1	38:Z:9219:HOH:O	2.51	0.43
1:0:2015:A:H2'	1:0:2016:U:O4'	2.18	0.43
1:0:2274:A:O2'	1:0:2275:G:H5'	2.18	0.43
1:0:2781:U:C2'	1:0:2782:G:H5'	2.48	0.43
1:0:2775:A:C6	1:0:2799:A:C8	3.06	0.43
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.43
2:9:3042:C:O2	7:D:76:ARG:NH1	2.51	0.43
2:9:3055:U:H4'	2:9:3056:A:C8	2.53	0.43
2:9:3106:C:O2'	2:9:3107:C:H5'	2.18	0.43
5:B:36:PRO:HD3	5:B:169:GLY:H	1.83	0.43
6:C:131:PHE:CD2	6:C:131:PHE:N	2.86	0.43
7:D:142:ALA:HA	7:D:149:ARG:O	2.19	0.43
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.43
11:H:154:TYR:CD1	11:H:154:TYR:C	2.91	0.43
12:J:103:VAL:HG12	38:J:9365:HOH:O	2.19	0.43
16:N:151:ASP:HB3	38:N:9324:HOH:O	2.17	0.43
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.79	0.43
1:0:1268:C:O2'	1:0:1269:G:H5'	2.18	0.43
1:0:2039:A:OP2	5:B:234:ARG:NH2	2.51	0.43
1:0:2438:G:H2'	1:0:2439:C:O4'	2.18	0.43
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
5:B:232:TRP:CD1	5:B:235:ARG:HD2	2.54	0.43
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.00	0.43
18:P:71:TYR:HD2	18:P:73:HIS:CD2	2.36	0.43
23:U:5:GLU:HG3	23:U:10:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:39:ALA:C	24:V:41:GLU:H	2.17	0.43
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.51	0.43
1:0:1423:C:O2'	1:0:1424:A:H5'	2.18	0.43
1:0:1625:U:H5''	38:0:6274:HOH:O	2.18	0.43
3:4:176:A:OP1	3:4:175:C:H5''	2.17	0.43
2:9:3054:A:H2	38:9:3535:HOH:O	2.01	0.43
38:0:4151:HOH:O	11:H:11:LYS:HE2	2.18	0.43
32:I:138:THR:CG2	32:I:139:ILE:H	2.23	0.43
1:0:2890:A:C8	23:U:56:ARG:NE	2.87	0.43
25:W:59:GLN:HE22	25:W:98:PHE:N	2.17	0.43
1:0:1169:U:H2'	1:0:1170:U:O4'	2.18	0.43
1:0:1451:C:H5'	1:0:1505:U:N3	2.34	0.43
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.99	0.43
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.99	0.43
5:B:254:GLN:HG3	38:B:9331:HOH:O	2.17	0.43
5:B:51:VAL:HG22	5:B:53:LEU:CD1	2.49	0.43
7:D:48:MET:HA	7:D:49:PRO:HD3	1.79	0.43
8:E:11:VAL:HG12	8:E:12:ASP:N	2.34	0.43
16:N:147:ILE:HB	38:N:9342:HOH:O	2.19	0.43
16:N:42:HIS:HB3	16:N:62:HIS:HE1	1.82	0.43
22:T:48:VAL:HG22	22:T:97:ARG:C	2.39	0.43
23:U:6:CYS:C	23:U:8:TYR:H	2.22	0.43
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.43
1:0:1119:G:H8	12:J:52:GLN:NE2	2.17	0.43
1:0:2061:C:C2'	1:0:2062:A:H5'	2.49	0.43
1:0:2511:A:H2'	1:0:2512:U:O4'	2.19	0.43
1:0:920:C:H5''	1:0:921:G:O5'	2.19	0.43
6:C:8:LEU:HD13	6:C:147:LEU:HD21	1.99	0.43
7:D:139:TYR:N	38:D:3723:HOH:O	2.51	0.43
7:D:23:VAL:HG11	7:D:83:PHE:CZ	2.54	0.43
8:E:49:ILE:HD11	8:E:69:ILE:HD12	2.01	0.43
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.49	0.43
14:L:145:LEU:O	14:L:145:LEU:HD23	2.19	0.43
15:M:98:GLN:O	15:M:102:GLU:HG3	2.19	0.43
15:M:30:GLU:O	15:M:34:GLU:HG3	2.18	0.43
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.33	0.43
24:V:1:THR:CG2	24:V:2:VAL:N	2.79	0.43
27:Y:165:GLU:HB3	38:Y:8182:HOH:O	2.17	0.43
1:0:645:U:OP2	14:L:4:LYS:CE	2.67	0.43
2:9:3052:A:H8	2:9:3052:A:O5'	2.02	0.43
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:36:ASP:CB	4:A:85:SER:HB2	2.49	0.43
5:B:26:PHE:CE1	5:B:310:ARG:HB3	2.54	0.43
5:B:7:ARG:HD3	5:B:9:GLY:O	2.19	0.43
6:C:98:ARG:NH1	38:C:9154:HOH:O	2.50	0.43
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.18	0.43
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
22:T:40:VAL:HG23	22:T:119:ALA:C	2.38	0.43
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.43
1:O:1206:U:H2'	1:O:1207:A:O4'	2.18	0.43
1:O:2382:A:H5'	38:3:9334:HOH:O	2.18	0.43
2:9:3056:A:C3'	2:9:3057:A:H5''	2.49	0.43
7:D:81:GLU:C	7:D:83:PHE:N	2.72	0.43
18:P:55:LYS:HG2	18:P:56:GLY:N	2.33	0.43
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.01	0.43
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.01	0.43
1:O:1942:A:H3'	38:0:7554:HOH:O	2.19	0.43
1:O:2816:A:H5''	1:O:2817:G:H5'	2.01	0.43
5:B:88:GLU:HB3	5:B:97:LEU:HG	2.00	0.43
15:M:159:VAL:HG13	15:M:160:PHE:N	2.33	0.43
1:O:721:A:H4'	17:O:51:TYR:CD1	2.53	0.43
18:P:40:VAL:O	18:P:44:VAL:HG23	2.19	0.43
18:P:6:GLN:OE1	18:P:6:GLN:N	2.47	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
1:O:1118:A:C8	1:O:1119:G:H5''	2.51	0.42
1:O:1331:A:OP2	27:Y:142:SER:OG	2.27	0.42
1:O:1654:U:H5''	38:0:7627:HOH:O	2.18	0.42
1:O:1942:A:H4'	38:A:9312:HOH:O	2.19	0.42
1:O:2740:G:H2'	1:O:2741:A:O4'	2.19	0.42
1:O:282:C:H2'	1:O:283:U:O4'	2.18	0.42
1:O:969:G:H1	1:O:999:C:H42	1.67	0.42
30:2:19:SER:HB3	38:2:4479:HOH:O	2.19	0.42
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.84	0.42
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.42
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.57	0.42
7:D:57:THR:HG23	7:D:63:ILE:HG22	2.00	0.42
9:F:22:VAL:CG2	9:F:104:ALA:HB2	2.49	0.42
15:M:46:LEU:HG	38:M:9413:HOH:O	2.18	0.42
1:O:1705:C:C5'	18:P:59:ARG:HH12	2.32	0.42
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1377:C:H6	1:0:1377:C:C5'	2.31	0.42
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.42
1:0:544:G:H2'	1:0:545:G:C5'	2.49	0.42
1:0:559:U:H2'	1:0:560:C:O4'	2.19	0.42
1:0:2708:G:N2	13:K:1:MET:O	2.52	0.42
16:N:104:ILE:HG13	16:N:104:ILE:O	2.18	0.42
16:N:44:ARG:HG3	16:N:45:ALA:N	2.34	0.42
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.23	0.42
20:R:25:PHE:CE2	20:R:29:LYS:CE	3.01	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.42
1:0:1711:A:O2'	1:0:1712:A:H5'	2.19	0.42
1:0:2327:A:H2'	1:0:2328:U:O4'	2.19	0.42
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.42
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.42
7:D:101:THR:HG22	38:D:7400:HOH:O	2.19	0.42
8:E:166:VAL:HB	38:E:6341:HOH:O	2.19	0.42
13:K:45:PRO:HB2	38:K:7169:HOH:O	2.18	0.42
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.52	0.42
16:N:149:GLU:O	16:N:152:GLU:HB2	2.19	0.42
38:O:6997:HOH:O	16:N:5:ARG:HB2	2.19	0.42
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.33	0.42
1:0:1205:U:H2'	1:0:1206:U:C5'	2.49	0.42
1:0:1544:U:H2'	1:0:1545:C:H6	1.84	0.42
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
1:0:2499:U:O2'	1:0:2500:C:H5'	2.18	0.42
1:0:2719:A:C2	5:B:70:PRO:HG3	2.54	0.42
2:9:3007:G:H5'	38:N:9345:HOH:O	2.17	0.42
1:0:875:A:C2	4:A:194:MET:SD	3.12	0.42
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.32	0.42
9:F:107:ASP:O	9:F:111:ILE:HG13	2.20	0.42
9:F:83:LEU:HD11	9:F:96:ALA:HB3	2.02	0.42
1:0:1167:G:H4'	32:I:135:LEU:HD22	2.01	0.42
12:J:4:ALA:O	12:J:5:GLU:O	2.37	0.42
15:M:123:ASP:OD1	15:M:126:GLN:HG2	2.19	0.42
20:R:39:THR:CG2	20:R:42:GLU:HG3	2.49	0.42
22:T:47:THR:HG22	22:T:99:THR:OG1	2.19	0.42
1:0:1175:G:H1'	1:0:1193:A:C2'	2.47	0.42
1:0:1427:A:N6	1:0:1440:U:H1'	2.34	0.42
1:0:1773:G:N2	1:0:1774:G:C8	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1785:G:OP1	18:P:76:GLY:HA3	2.20	0.42
1:0:2372:A:H2'	1:0:2373:U:H6	1.84	0.42
1:0:2453:G:H5'	38:0:4985:HOH:O	2.18	0.42
1:0:2728:C:H2'	1:0:2729:C:C6	2.54	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
1:0:969:G:H1	1:0:999:C:N4	2.17	0.42
4:A:200:PRO:HD3	38:A:9319:HOH:O	2.19	0.42
5:B:90:THR:C	5:B:92:TYR:H	2.22	0.42
6:C:107:ARG:NE	38:C:9256:HOH:O	2.27	0.42
6:C:124:VAL:HA	6:C:230:GLY:O	2.18	0.42
8:E:31:ARG:NH1	38:E:5919:HOH:O	2.53	0.42
11:H:38:LYS:HE2	11:H:42:ASP:HB2	2.01	0.42
32:I:92:PRO:C	32:I:94:GLU:N	2.72	0.42
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.02	0.42
16:N:103:ASP:OD1	16:N:103:ASP:C	2.57	0.42
22:T:40:VAL:HA	22:T:119:ALA:O	2.19	0.42
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.01	0.42
25:W:59:GLN:HE22	25:W:98:PHE:CB	2.30	0.42
1:0:196:G:H2'	38:L:9371:HOH:O	2.18	0.42
1:0:2415:A:O2'	16:N:29:SER:HB3	2.19	0.42
1:0:333:G:O2'	1:0:334:G:H5'	2.20	0.42
1:0:581:G:O2'	1:0:582:C:H5'	2.19	0.42
1:0:963:C:O2	1:0:1005:A:N1	2.52	0.42
2:9:3049:G:C2'	2:9:3050:G:H5'	2.50	0.42
2:9:3059:C:H5'	38:9:5233:HOH:O	2.19	0.42
4:A:153:ARG:HD3	38:A:9328:HOH:O	2.18	0.42
4:A:186:TRP:CG	4:A:187:PRO:HA	2.54	0.42
8:E:84:MET:HE3	8:E:148:ILE:HG21	2.02	0.42
12:J:80:LYS:NZ	38:J:9370:HOH:O	2.52	0.42
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.02	0.42
18:P:143:ALA:HA	38:P:190:HOH:O	2.20	0.42
1:0:1185:U:H2'	1:0:1186:C:H6	1.82	0.42
1:0:1562:C:N4	38:0:6127:HOH:O	2.53	0.42
1:0:1587:U:H2'	1:0:1588:G:O4'	2.19	0.42
1:0:970:U:H2'	38:0:6568:HOH:O	2.19	0.42
30:2:36:ASN:O	30:2:39:ARG:HG3	2.19	0.42
1:0:2474:A:N6	3:4:176:A:OP2	2.53	0.42
2:9:3107:C:H2'	2:9:3108:C:H6	1.83	0.42
7:D:56:ARG:N	38:D:6752:HOH:O	2.53	0.42
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.49	0.42
8:E:43:ASP:HA	38:E:5864:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.42
16:N:163:PHE:O	16:N:164:ASP:O	2.38	0.42
16:N:171:HIS:CE1	38:N:9364:HOH:O	2.73	0.42
38:O:4910:HOH:O	17:O:35:LYS:HD3	2.20	0.42
18:P:92:GLU:HA	18:P:95:GLU:OE1	2.20	0.42
1:O:1471:A:H2'	1:O:1472:C:C6	2.55	0.42
1:O:2728:C:H2'	1:O:2729:C:H6	1.83	0.42
1:O:581:G:H5'	38:O:7877:HOH:O	2.19	0.42
1:O:603:A:H4'	1:O:604:G:O5'	2.19	0.42
1:O:462:A:N3	30:2:37:HIS:HB3	2.35	0.42
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.54	0.42
5:B:279:THR:CG2	5:B:280:VAL:N	2.83	0.42
6:C:115:LEU:HD12	6:C:115:LEU:HA	1.92	0.42
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.19	0.42
8:E:107:PHE:CD2	8:E:108:LEU:HD13	2.55	0.42
12:J:22:VAL:O	12:J:26:VAL:HG23	2.20	0.42
13:K:75:ARG:HH21	13:K:94:ALA:CB	2.32	0.42
25:W:84:VAL:HG21	25:W:93:ILE:HG12	2.00	0.42
1:O:1187:U:O2'	1:O:1189:A:H2	1.82	0.42
1:O:2326:U:H4'	1:O:2412:G:C4'	2.50	0.42
1:O:2786:G:H2'	38:O:7404:HOH:O	2.20	0.42
1:O:371:U:H2'	1:O:372:A:H8	1.85	0.42
1:O:484:A:N1	1:O:506:G:H4'	2.35	0.42
1:O:664:U:O4	1:O:681:G:H5''	2.19	0.42
4:A:86:ALA:HB3	4:A:94:LEU:HD13	2.02	0.42
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.50	0.42
5:B:210:GLY:HA2	5:B:256:GLN:NE2	2.35	0.42
6:C:173:LYS:O	6:C:186:TYR:HA	2.20	0.42
1:O:2333:G:P	7:D:56:ARG:HH22	2.42	0.42
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.20	0.42
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.38	0.42
24:V:12:THR:CG2	24:V:15:GLU:H	2.33	0.42
24:V:1:THR:HG22	24:V:48:GLU:OE1	2.20	0.42
1:O:1163:G:N2	38:O:6299:HOH:O	2.53	0.42
1:O:1312:G:OP1	27:Y:213:LYS:NZ	2.46	0.42
1:O:1594:C:O2'	1:O:1595:G:H5'	2.20	0.42
1:O:1684:A:O2'	1:O:1685:A:H5''	2.19	0.42
1:O:2105:C:H2'	1:O:2106:C:C6	2.55	0.42
1:O:2254:G:O2'	1:O:2255:A:H5'	2.20	0.42
1:O:23:G:C6	1:O:24:G:N1	2.88	0.42
1:O:731:U:O2'	1:O:732:C:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.73	0.42
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.42
8:E:31:ARG:NH1	8:E:68:HIS:ND1	2.66	0.42
11:H:50:ILE:HG23	11:H:131:GLU:O	2.20	0.42
14:L:133:VAL:HB	38:L:9356:HOH:O	2.18	0.42
28:Z:81:ARG:O	28:Z:82:SER:C	2.57	0.42
1:0:1878:G:H5''	38:0:3103:HOH:O	2.19	0.41
1:0:2271:G:N3	1:0:2271:G:H2'	2.35	0.41
1:0:569:A:H5''	1:0:587:A:N1	2.35	0.41
4:A:93:THR:HA	4:A:154:ALA:O	2.19	0.41
6:C:140:VAL:HG12	6:C:141:SER:N	2.34	0.41
6:C:35:VAL:HG21	6:C:227:GLY:HA2	2.02	0.41
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.19	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.50	0.41
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.53	0.41
27:Y:134:HIS:CD2	27:Y:134:HIS:H	2.38	0.41
1:0:1028:U:H5'	1:0:1031:G:O4'	2.20	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.87	0.41
1:0:1393:A:H2'	1:0:1394:C:C6	2.55	0.41
1:0:1593:C:O2'	1:0:1594:C:H5'	2.20	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.88	0.41
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.41
5:B:279:THR:HG22	5:B:280:VAL:N	2.35	0.41
13:K:132:VAL:O	13:K:132:VAL:HG12	2.20	0.41
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.20	0.41
15:M:182:LYS:NZ	38:M:9325:HOH:O	2.53	0.41
16:N:181:ASP:O	16:N:184:ILE:HG22	2.20	0.41
25:W:21:LEU:HD21	25:W:48:VAL:HG13	2.01	0.41
1:0:1776:A:C8	1:0:1778:A:O4'	2.73	0.41
1:0:2541:U:O2'	1:0:2542:C:H5'	2.19	0.41
1:0:2754:G:O2'	1:0:2755:G:H5'	2.20	0.41
1:0:2780:C:H2'	1:0:2781:U:H6	1.84	0.41
1:0:288:A:H61	1:0:364:C:H42	1.69	0.41
1:0:705:C:H2'	1:0:705:C:O2	2.20	0.41
29:1:25:LYS:HD2	30:2:49:GLU:N	2.34	0.41
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.20	0.41
4:A:179:MET:HG2	4:A:186:TRP:CG	2.55	0.41
5:B:87:TYR:OH	5:B:163:GLU:OE2	2.27	0.41
5:B:168:GLY:H	5:B:174:ARG:HD2	1.85	0.41
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:53:LEU:HD11	5:B:327:VAL:HG22	2.01	0.41
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.41
32:I:129:VAL:O	32:I:129:VAL:HG12	2.21	0.41
1:O:2269:C:C2'	1:O:2270:G:H5'	2.50	0.41
1:O:2832:C:H5	38:O:7429:HOH:O	2.03	0.41
29:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
5:B:247:VAL:HG13	5:B:251:VAL:HG11	2.03	0.41
12:J:45:VAL:CG2	12:J:46:ILE:N	2.83	0.41
14:L:128:GLY:O	14:L:132:LYS:HG3	2.20	0.41
1:O:2904:U:H4'	26:X:8:ARG:NH1	2.34	0.41
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	2.02	0.41
1:O:1044:C:H5''	38:O:9342:HOH:O	2.21	0.41
1:O:1131:G:C6	1:O:1230:A:C4	3.09	0.41
1:O:1180:U:H2'	1:O:1181:A:O4'	2.21	0.41
1:O:1921:A:O2'	1:O:1922:A:H5'	2.20	0.41
1:O:2072:G:H3'	1:O:2073:G:C5'	2.51	0.41
1:O:2464:C:H5''	1:O:2465:A:OP1	2.20	0.41
1:O:2670:G:O2'	1:O:2671:U:H5'	2.21	0.41
1:O:827:A:H2'	1:O:828:G:O4'	2.20	0.41
31:3:30:GLN:HB3	31:3:30:GLN:HE21	1.61	0.41
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.85	0.41
11:H:80:GLU:HA	38:H:9182:HOH:O	2.20	0.41
14:L:140:VAL:HG12	14:L:140:VAL:O	2.19	0.41
14:L:34:GLY:C	14:L:36:ASP:H	2.24	0.41
16:N:154:LEU:O	16:N:155:GLU:CB	2.68	0.41
38:9:1056:HOH:O	16:N:7:LYS:HE2	2.21	0.41
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.21	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
23:U:6:CYS:HA	23:U:13:ILE:HD11	2.03	0.41
25:W:13:MET:CE	25:W:18:GLN:HA	2.51	0.41
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.41
26:X:7:GLU:HA	26:X:74:ALA:O	2.19	0.41
1:O:1355:A:H2'	38:O:4429:HOH:O	2.21	0.41
1:O:1477:C:H5'	1:O:1868:G:H5''	2.03	0.41
1:O:1006:A:N1	1:O:2311:A:H1'	2.35	0.41
1:O:2564:G:OP2	1:O:2565:C:H5''	2.21	0.41
1:O:2812:A:C2	1:O:2814:A:N6	2.75	0.41
1:O:2842:G:H2'	1:O:2843:A:H5'	2.03	0.41
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.13	0.41
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.85	0.41
6:C:130:GLU:HA	6:C:130:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:16:ASP:O	8:E:17:HIS:HB2	2.19	0.41
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.41
16:N:37:ARG:NH2	38:N:9331:HOH:O	2.53	0.41
1:O:120:A:H2'	1:O:120:A:N3	2.36	0.41
1:O:1419:U:H2'	1:O:1685:A:C2	2.56	0.41
1:O:1762:C:H4'	38:O:4949:HOH:O	2.19	0.41
1:O:1815:A:H4'	1:O:2751:C:O4'	2.21	0.41
1:O:204:A:C2'	1:O:205:U:H5'	2.51	0.41
1:O:2379:G:N7	1:O:2408:A:N1	2.68	0.41
1:O:2455:A:H2'	1:O:2456:A:O4'	2.20	0.41
1:O:250:C:H2'	1:O:251:C:C6	2.55	0.41
1:O:2668:G:H2'	1:O:2669:U:C6	2.56	0.41
1:O:2735:U:H2'	1:O:2736:U:C6	2.55	0.41
1:O:825:U:H5''	1:O:826:U:OP1	2.21	0.41
1:O:907:A:H2'	1:O:908:A:H8	1.84	0.41
1:O:941:G:C5	1:O:942:U:C4	3.09	0.41
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.41
5:B:217:ARG:CG	5:B:257:THR:HG22	2.48	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.20	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
7:D:27:ILE:HG22	7:D:28:GLY:N	2.34	0.41
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.03	0.41
11:H:51:VAL:HG21	11:H:127:VAL:HG11	2.03	0.41
11:H:9:ILE:HG23	11:H:126:ARG:NE	2.36	0.41
38:O:7175:HOH:O	19:Q:16:ASN:HB2	2.21	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.44	0.41
1:O:1307:A:H2'	1:O:1308:A:C8	2.56	0.41
1:O:2255:A:C6	1:O:2256:G:C5	3.09	0.41
1:O:377:C:H5	38:O:3616:HOH:O	2.03	0.41
1:O:451:C:O2'	1:O:452:G:H5'	2.21	0.41
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.55	0.41
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.41
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.90	0.41
5:B:184:ASP:HB2	5:B:185:GLY:H	1.71	0.41
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.03	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.91	0.41
32:I:132:CYS:O	32:I:135:LEU:N	2.52	0.41
17:O:81:PHE:N	17:O:81:PHE:CD1	2.88	0.41
18:P:59:ARG:O	18:P:63:ARG:HG3	2.21	0.41
25:W:5:VAL:HG11	25:W:153:MET:CE	2.51	0.41
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1386:G:O2'	1:0:1387:G:H5'	2.21	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
1:0:482:G:H4'	1:0:508:A:N1	2.36	0.41
4:A:36:ASP:C	4:A:38:ILE:N	2.71	0.41
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.85	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.03	0.41
9:F:111:ILE:O	9:F:115:VAL:HG23	2.21	0.41
12:J:39:VAL:CG1	12:J:40:ASN:N	2.84	0.41
13:K:10:GLN:N	13:K:10:GLN:NE2	2.43	0.41
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.55	0.41
15:M:65:VAL:HG21	15:M:105:ALA:HB2	2.03	0.41
18:P:115:SER:C	18:P:117:SER:N	2.74	0.41
23:U:49:LEU:HG	38:U:3805:HOH:O	2.20	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.21	0.41
1:0:1778:A:H2'	1:0:1779:A:H5'	2.02	0.41
1:0:200:U:O2'	1:0:201:G:H5'	2.21	0.41
1:0:2079:G:H2'	1:0:2080:G:O4'	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.41
1:0:432:G:O2'	1:0:433:C:H5'	2.20	0.41
1:0:645:U:O2	1:0:761:A:H2	2.04	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.41
1:0:876:A:H2'	1:0:876:A:N3	2.35	0.41
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.85	0.41
6:C:19:PRO:HG2	6:C:22:PHE:CD1	2.56	0.41
6:C:39:GLN:O	6:C:43:LYS:HD3	2.20	0.41
1:0:894:A:C2	6:C:87:ARG:NH2	2.88	0.41
8:E:75:GLY:HA2	8:E:79:GLY:HA2	2.03	0.41
10:G:12:ILE:HG13	38:G:6833:HOH:O	2.21	0.41
12:J:131:THR:CG2	12:J:134:GLU:HG3	2.51	0.41
1:0:1119:G:P	12:J:49:ARG:HH11	2.44	0.41
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.55	0.41
1:0:1396:C:H4'	18:P:2:ASP:OD1	2.21	0.41
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.20	0.41
22:T:19:ARG:NH1	22:T:68:ASP:O	2.54	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.86	0.41
1:0:1123:A:C2	1:0:1129:C:H4'	2.56	0.41
1:0:1744:G:C2'	1:0:1745:G:H5'	2.51	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.56	0.41
2:9:3041:C:H5''	7:D:48:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.51	0.41
5:B:57:GLU:OE1	5:B:60:SER:HB2	2.21	0.41
6:C:77:ALA:O	6:C:78:ARG:HG3	2.21	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.56	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.77	0.41
11:H:99:LYS:CG	11:H:119:LYS:HD3	2.51	0.41
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.21	0.41
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.53	0.41
15:M:72:ALA:HB2	15:M:93:ARG:HG2	2.03	0.41
1:O:710:G:OP1	17:O:24:ALA:HB3	2.21	0.41
1:O:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
22:T:41:ARG:O	22:T:43:ASN:ND2	2.53	0.41
1:O:907:A:H4'	1:O:1328:A:C2	2.56	0.40
1:O:1543:G:N1	1:O:1641:A:OP2	2.41	0.40
1:O:1682:A:H5''	38:O:9769:HOH:O	2.20	0.40
1:O:1790:C:H2'	1:O:1791:U:C6	2.55	0.40
1:O:2615:U:C5	1:O:2616:G:C6	3.09	0.40
1:O:353:G:O2'	1:O:354:A:H5'	2.22	0.40
1:O:475:G:H5'	6:C:73:LEU:CD2	2.50	0.40
1:O:542:A:O2'	1:O:543:G:H5'	2.21	0.40
2:9:3033:U:H2'	38:9:3797:HOH:O	2.21	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
8:E:73:PHE:O	8:E:76:VAL:HG22	2.21	0.40
11:H:154:TYR:HD1	11:H:154:TYR:C	2.24	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.63	0.40
15:M:164:THR:HG22	15:M:166:ALA:N	2.36	0.40
16:N:164:ASP:CG	16:N:167:ASP:HA	2.39	0.40
1:O:1370:G:O5'	20:R:62:HIS:HB3	2.21	0.40
38:O:4650:HOH:O	25:W:14:HIS:HA	2.20	0.40
1:O:1434:A:H2'	1:O:1436:C:C5	2.56	0.40
1:O:1730:G:H2'	1:O:1730:G:N3	2.36	0.40
1:O:1739:G:O2'	1:O:1740:U:H5'	2.21	0.40
1:O:2506:A:O2'	1:O:2507:G:P	2.79	0.40
1:O:2765:C:H2'	1:O:2766:A:H8	1.87	0.40
1:O:354:A:H2'	1:O:355:C:C6	2.56	0.40
1:O:10:U:H1'	1:O:532:A:H62	1.86	0.40
1:O:702:G:O2'	1:O:703:G:H5'	2.22	0.40
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.73	0.40
1:O:474:C:O2'	6:C:73:LEU:HD21	2.21	0.40
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.40
7:D:86:THR:HG23	38:D:7477:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2690:U:H4'	8:E:111:LYS:CE	2.51	0.40
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.56	0.40
16:N:101:VAL:HG12	38:N:9327:HOH:O	2.22	0.40
16:N:157:PRO:HA	38:N:9322:HOH:O	2.21	0.40
16:N:63:SER:HB2	16:N:75:THR:HB	2.03	0.40
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.04	0.40
20:R:99:ALA:CB	20:R:109:MET:CE	2.95	0.40
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.41	0.40
23:U:35:LYS:HE2	23:U:51:TRP:CH2	2.56	0.40
27:Y:197:ASP:OD1	27:Y:197:ASP:C	2.60	0.40
1:O:1139:U:H2'	1:O:1140:C:H6	1.85	0.40
1:O:1613:C:H2'	1:O:1614:G:O4'	2.21	0.40
1:O:1985:U:C2	1:O:1996:U:O4'	2.75	0.40
1:O:2061:C:H2'	1:O:2062:A:H5'	2.04	0.40
1:O:566:A:H2'	1:O:567:U:O4'	2.21	0.40
1:O:999:C:H2'	1:O:1000:C:O4'	2.21	0.40
4:A:194:MET:CE	4:A:199:HIS:HB2	2.51	0.40
4:A:223:ARG:CZ	38:A:9317:HOH:O	2.69	0.40
5:B:53:LEU:HD12	5:B:327:VAL:HA	2.04	0.40
7:D:104:PHE:CE2	7:D:166:ILE:CD1	3.04	0.40
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.93	0.40
8:E:87:PHE:O	8:E:93:MET:HE3	2.21	0.40
12:J:130:VAL:CG1	12:J:131:THR:N	2.85	0.40
12:J:51:GLU:O	12:J:55:GLU:HG3	2.20	0.40
1:O:2453:G:H4'	14:L:50:GLY:C	2.41	0.40
16:N:67:ALA:O	16:N:69:TYR:N	2.54	0.40
18:P:135:ALA:O	18:P:139:ARG:HG3	2.22	0.40
1:O:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
20:R:76:ASP:N	20:R:76:ASP:OD1	2.53	0.40
23:U:37:GLU:O	23:U:40:ALA:HB3	2.22	0.40
25:W:85:ALA:HB2	25:W:91:ASP:O	2.21	0.40
1:O:1079:A:H4'	1:O:2078:U:H5'	2.04	0.40
1:O:1158:G:O2'	1:O:1159:G:H5'	2.21	0.40
1:O:1194:A:C2'	1:O:1195:G:H5'	2.51	0.40
1:O:1196:C:H2'	1:O:1197:G:H5'	2.04	0.40
1:O:1311:G:C2	1:O:1312:G:C8	3.09	0.40
1:O:2067:A:H2'	1:O:2068:G:O4'	2.21	0.40
1:O:2456:A:H2'	1:O:2457:U:C6	2.56	0.40
1:O:338:C:H4'	6:C:174:ILE:HD12	2.03	0.40
1:O:601:G:O2'	1:O:602:A:H5'	2.21	0.40
1:O:615:G:H2'	1:O:616:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3034:A:H2'	2:9:3035:C:O4'	2.21	0.40
5:B:175:LEU:O	5:B:175:LEU:HD23	2.21	0.40
11:H:20:ILE:CG2	11:H:120:ILE:HD11	2.52	0.40
11:H:63:GLU:OE1	11:H:66:ARG:NH1	2.54	0.40
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.40
14:L:125:PHE:CE2	14:L:140:VAL:HG22	2.56	0.40
21:S:81:ILE:HG12	38:S:9134:HOH:O	2.21	0.40
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.94	0.40
28:Z:67:GLY:N	28:Z:70:LYS:O	2.54	0.40
1:0:1335:C:H2'	1:0:1336:U:C6	2.57	0.40
1:0:2093:G:H5''	38:B:9326:HOH:O	2.21	0.40
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.40
1:0:912:A:C4	1:0:1294:A:C2	3.10	0.40
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	2.04	0.40
4:A:65:ARG:C	4:A:66:ARG:HG3	2.42	0.40
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.35	0.40
5:B:316:ARG:N	5:B:317:PRO:HD3	2.37	0.40
5:B:76:THR:N	5:B:77:PRO:HD3	2.37	0.40
7:D:173:GLU:CG	7:D:174:VAL:H	2.35	0.40
8:E:102:VAL:HG11	8:E:148:ILE:HG12	2.03	0.40
11:H:88:ARG:H	11:H:88:ARG:HG2	1.68	0.40
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.34	0.40
12:J:39:VAL:HG12	12:J:40:ASN:CG	2.42	0.40
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.22	0.40
20:R:106:GLY:HA2	20:R:109:MET:HE3	2.02	0.40
20:R:61:GLN:CD	38:R:9338:HOH:O	2.60	0.40
25:W:130:HIS:O	25:W:136:GLY:HA3	2.22	0.40
1:0:622:G:P	27:Y:148:GLY:HA3	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	10	17
5	B	335/338 (99%)	298 (89%)	31 (9%)	6 (2%)	9	16
6	C	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	36	57
7	D	134/177 (76%)	101 (75%)	23 (17%)	10 (8%)	1	1
8	E	170/178 (96%)	158 (93%)	12 (7%)	0	100	100
9	F	117/120 (98%)	108 (92%)	3 (3%)	6 (5%)	2	2
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	145 (93%)	8 (5%)	3 (2%)	9	15
12	J	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	12	22
13	K	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	7	11
14	L	141/165 (86%)	121 (86%)	16 (11%)	4 (3%)	5	8
15	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	3	4
17	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	19	34
18	P	141/149 (95%)	138 (98%)	2 (1%)	1 (1%)	24	42
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
21	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	19	34
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	4	6
25	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	24	42
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	13	23
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	9 (13%)	2 (3%)	5	8
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	6	10
31	3	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	7	11
32	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	11	20
All	All	3705/4430 (84%)	3373 (91%)	273 (7%)	59 (2%)	11	19

All (59) Ramachandran outliers are listed below:

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

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	170 (95%)	9 (5%)	27	49
5	B	282/283 (100%)	266 (94%)	16 (6%)	23	42
6	C	193/193 (100%)	178 (92%)	15 (8%)	14	26
7	D	117/148 (79%)	111 (95%)	6 (5%)	26	48
8	E	152/156 (97%)	151 (99%)	1 (1%)	85	95
9	F	93/94 (99%)	93 (100%)	0	100	100
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	124 (94%)	8 (6%)	20	39
12	J	118/121 (98%)	109 (92%)	9 (8%)	14	28
13	K	106/106 (100%)	102 (96%)	4 (4%)	36	62
14	L	113/127 (89%)	107 (95%)	6 (5%)	25	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	M	158/158 (100%)	153 (97%)	5 (3%)	42	69
16	N	149/150 (99%)	142 (95%)	7 (5%)	29	52
17	O	93/94 (99%)	89 (96%)	4 (4%)	32	56
18	P	113/117 (97%)	110 (97%)	3 (3%)	48	75
19	Q	79/80 (99%)	76 (96%)	3 (4%)	36	62
20	R	117/122 (96%)	115 (98%)	2 (2%)	63	85
21	S	71/74 (96%)	70 (99%)	1 (1%)	69	88
22	T	105/106 (99%)	99 (94%)	6 (6%)	23	42
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	35	61
25	W	130/130 (100%)	126 (97%)	4 (3%)	43	70
26	X	66/74 (89%)	62 (94%)	4 (6%)	20	39
27	Y	120/196 (61%)	112 (93%)	8 (7%)	18	34
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	52	78
31	3	79/79 (100%)	77 (98%)	2 (2%)	50	77
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2967 (96%)	126 (4%)	33	59

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

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

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

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

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

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

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

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

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

### 5.3.3 RNA ⓘ

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

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

All (251) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G

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Mol	Chain	Res	Type
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	905	C
1	0	920	C

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Mol	Chain	Res	Type
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C

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

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

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Mol	Chain	Res	Type
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A

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

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	87	C
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1692	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	0	2587	1	14,22,23	1.03	1 (7%)	18,31,34	3.69	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.04	2 (10%)	22,38,41	2.46	4 (18%)
1	UR3	0	2619	1	13,22,23	0.84	0	15,32,35	0.68	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	5.38	4 (20%)
1	1MA	0	628	1	16,25,26	1.04	1 (6%)	12,37,40	1.25	1 (8%)
3	5AA	4	76	1,3	17,26,27	1.02	1 (5%)	16,38,41	1.07	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.10	1.47	1.52
3	4	76	5AA	C3'-N3'	-3.38	1.42	1.47
1	0	2588	OMG	C8-N7	-2.17	1.30	1.34
1	0	2621	PSU	C4-N3	2.61	1.37	1.33
1	0	2621	PSU	C2-N1	2.66	1.43	1.38
1	0	2587	OMU	C4-N3	2.72	1.37	1.33
1	0	628	1MA	C6-N6	3.03	1.34	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2588	OMG	C6-N1	3.40	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-16.97	114.77	128.41
1	0	2588	OMG	C5-C6-N1	-8.35	111.59	123.47
1	0	2621	PSU	C5-C4-N3	-8.33	114.63	125.36
1	0	628	1MA	C2-N3-C4	-3.71	110.83	116.51
1	0	2587	OMU	C5-C4-N3	-3.66	114.67	123.17
1	0	2588	OMG	C2-N3-C4	-2.75	111.94	115.16
1	0	2588	OMG	N3-C2-N1	-2.36	123.95	127.41
3	4	76	5AA	C9-N6-C6	2.01	125.59	119.51
1	0	2621	PSU	C6-N1-C2	2.65	119.60	115.36
3	4	76	5AA	C2-N1-C6	2.89	118.82	111.81
1	0	2588	OMG	C6-N1-C2	6.32	125.15	116.06
1	0	2621	PSU	C4-N3-C2	14.16	127.20	115.14
1	0	2587	OMU	C4-N3-C2	15.11	127.14	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.49	48 (1%) 70 72	24, 49, 93, 155	0
2	9	122/122 (100%)	-0.29	5 (4%) 37 40	45, 66, 91, 152	0
3	4	5/8 (62%)	-0.71	0 100 100	41, 45, 47, 49	0
4	A	237/240 (98%)	0.39	17 (7%) 15 16	30, 51, 89, 114	0
5	B	337/338 (99%)	0.30	11 (3%) 46 50	31, 61, 90, 100	0
6	C	246/246 (100%)	-0.05	4 (1%) 72 74	28, 48, 71, 82	0
7	D	140/177 (79%)	2.54	74 (52%) 0 0	59, 106, 130, 136	0
8	E	172/178 (96%)	1.10	27 (15%) 2 1	52, 76, 101, 111	0
9	F	119/120 (99%)	0.99	27 (22%) 0 0	52, 74, 100, 116	0
10	G	29/348 (8%)	2.64	19 (65%) 0 0	74, 92, 104, 108	0
11	H	160/171 (93%)	0.39	8 (5%) 29 31	42, 60, 91, 100	0
12	J	142/145 (97%)	0.13	0 100 100	40, 56, 77, 99	0
13	K	132/132 (100%)	0.20	3 (2%) 60 63	35, 58, 80, 85	0
14	L	145/165 (87%)	0.85	28 (19%) 1 1	28, 69, 114, 127	0
15	M	194/194 (100%)	0.04	2 (1%) 82 84	32, 43, 59, 66	0
16	N	186/187 (99%)	0.84	36 (19%) 1 1	40, 64, 113, 119	0
17	O	115/116 (99%)	0.15	3 (2%) 56 59	39, 58, 75, 90	0
18	P	143/149 (95%)	0.30	5 (3%) 44 47	43, 58, 70, 78	0
19	Q	95/96 (98%)	0.14	2 (2%) 63 66	38, 47, 60, 72	0
20	R	150/155 (96%)	-0.07	0 100 100	33, 48, 65, 76	0
21	S	81/85 (95%)	0.19	2 (2%) 57 60	45, 59, 78, 88	0
22	T	119/120 (99%)	0.42	3 (2%) 57 60	40, 58, 85, 96	0
23	U	53/66 (80%)	0.28	2 (3%) 40 43	46, 62, 76, 86	0
24	V	65/71 (91%)	1.62	22 (33%) 0 0	56, 76, 112, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.07	0 100 100	39, 55, 74, 86	0
26	X	82/92 (89%)	0.65	12 (14%) 2 2	46, 63, 85, 101	0
27	Y	142/241 (58%)	0.27	8 (5%) 24 26	30, 49, 70, 92	0
28	Z	73/83 (87%)	0.18	5 (6%) 17 18	46, 60, 76, 94	0
29	1	56/57 (98%)	-0.35	0 100 100	27, 34, 39, 52	0
30	2	46/50 (92%)	1.61	14 (30%) 0 0	36, 65, 120, 122	0
31	3	92/92 (100%)	0.32	5 (5%) 26 27	35, 55, 71, 87	0
32	I	70/162 (43%)	4.52	59 (84%) 0 0	108, 126, 148, 149	0
All	All	6651/7482 (88%)	0.11	451 (6%) 17 18	24, 55, 103, 155	0

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	96	PHE	15.2
32	I	133	THR	13.6
24	V	1	THR	13.1
32	I	102	VAL	12.5
32	I	93	GLN	11.6
7	D	63	ILE	9.7
30	2	38	LYS	9.3
16	N	166	ALA	9.2
2	9	3001	U	9.0
7	D	88	LEU	8.7
32	I	116	LEU	8.7
7	D	69	ILE	8.4
32	I	71	GLY	8.3
10	G	23	ILE	8.2
32	I	79	ILE	8.0
10	G	27	ILE	7.5
32	I	117	LEU	7.4
7	D	57	THR	7.4
32	I	109	ALA	7.4
7	D	26	GLY	7.3
24	V	39	ALA	7.3
30	2	41	HIS	7.2
7	D	44	ILE	7.2
7	D	64	ARG	7.0
4	A	37	VAL	6.9
32	I	113	HIS	6.9

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Mol	Chain	Res	Type	RSRZ
24	V	40	PRO	6.8
32	I	137	VAL	6.7
7	D	84	LEU	6.6
32	I	118	SER	6.6
24	V	38	GLY	6.5
32	I	75	THR	6.5
7	D	85	GLN	6.4
30	2	44	ARG	6.4
7	D	58	VAL	6.2
32	I	105	VAL	6.2
7	D	172	VAL	6.2
7	D	170	TYR	6.1
7	D	61	PHE	6.0
32	I	88	GLY	5.9
7	D	66	GLY	5.8
32	I	85	PHE	5.8
32	I	103	ASP	5.6
30	2	42	TRP	5.5
10	G	24	VAL	5.5
32	I	111	GLN	5.5
7	D	75	LEU	5.5
32	I	77	GLU	5.5
30	2	45	ASN	5.3
30	2	48	ASP	5.3
1	0	2237	G	5.3
30	2	49	GLU	5.3
7	D	10	PHE	5.3
30	2	37	HIS	5.3
24	V	43	PRO	5.2
26	X	88	GLU	5.2
2	9	3024	U	5.2
32	I	129	VAL	5.1
1	0	1173	A	5.1
7	D	23	VAL	5.1
8	E	42	VAL	5.1
7	D	41	LEU	5.1
8	E	44	GLY	5.0
7	D	40	ILE	4.9
2	9	3023	U	4.8
32	I	119	TYR	4.8
7	D	87	ALA	4.8
32	I	115	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
32	I	81	ASP	4.7
32	I	114	PRO	4.7
32	I	94	GLU	4.6
7	D	165	PHE	4.6
32	I	126	LYS	4.6
32	I	92	PRO	4.5
7	D	56	ARG	4.5
32	I	74	PRO	4.5
16	N	159	TYR	4.4
32	I	78	LEU	4.4
1	0	1177	A	4.4
1	0	960	G	4.4
32	I	97	VAL	4.4
16	N	160	SER	4.4
1	0	282	C	4.3
32	I	72	VAL	4.3
4	A	31	LYS	4.3
21	S	81	ILE	4.3
7	D	98	PHE	4.3
7	D	68	PRO	4.3
11	H	73	LEU	4.3
7	D	90	LEU	4.2
1	0	1172	G	4.2
32	I	106	LYS	4.2
1	0	2238	A	4.2
7	D	18	ILE	4.2
9	F	17	LEU	4.2
10	G	71	LEU	4.2
14	L	97	VAL	4.1
32	I	89	SER	4.1
9	F	119	ARG	4.1
32	I	121	LEU	4.1
24	V	37	GLY	4.1
7	D	89	PRO	4.1
7	D	51	ARG	4.1
30	2	39	ARG	4.1
30	2	36	ASN	4.0
7	D	65	GLU	4.0
14	L	106	VAL	4.0
16	N	67	ALA	4.0
14	L	60	GLU	4.0
24	V	41	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
7	D	166	ILE	4.0
8	E	11	VAL	4.0
8	E	87	PHE	4.0
16	N	152	GLU	4.0
7	D	86	THR	4.0
32	I	136	GLY	4.0
1	0	970	U	3.9
32	I	73	PRO	3.9
30	2	47	THR	3.9
10	G	26	MET	3.9
32	I	76	ALA	3.9
7	D	59	GLY	3.9
7	D	62	ASP	3.9
32	I	107	GLN	3.9
1	0	1951	G	3.8
32	I	91	GLU	3.8
7	D	128	LEU	3.8
9	F	16	ALA	3.8
7	D	49	PRO	3.8
7	D	106	PHE	3.8
7	D	92	GLU	3.8
7	D	93	LEU	3.8
16	N	158	LEU	3.8
7	D	104	PHE	3.8
7	D	27	ILE	3.7
32	I	139	ILE	3.7
7	D	134	LEU	3.7
32	I	135	LEU	3.7
1	0	1199	A	3.7
14	L	80	ASP	3.7
32	I	95	ASP	3.7
32	I	125	ALA	3.7
8	E	76	VAL	3.6
9	F	106	ALA	3.6
14	L	105	TYR	3.6
1	0	1171	A	3.6
27	Y	236	VAL	3.6
1	0	1525	G	3.6
8	E	100	ASP	3.6
7	D	81	GLU	3.6
27	Y	235	GLU	3.6
32	I	104	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
7	D	73	VAL	3.6
4	A	35	GLY	3.6
7	D	135	VAL	3.6
8	E	8	PRO	3.5
7	D	25	MET	3.5
9	F	45	ALA	3.5
32	I	98	ALA	3.5
8	E	88	TYR	3.5
7	D	70	GLY	3.5
1	0	10	U	3.5
32	I	132	CYS	3.5
8	E	45	ASP	3.5
9	F	117	GLU	3.4
30	2	43	ARG	3.4
9	F	44	SER	3.4
32	I	128	VAL	3.4
5	B	119	HIS	3.4
26	X	41	PHE	3.4
17	O	22	GLY	3.4
7	D	71	ALA	3.4
14	L	142	LEU	3.3
16	N	175	LEU	3.3
32	I	86	GLU	3.3
32	I	138	THR	3.3
1	0	735	C	3.3
7	D	167	GLU	3.3
23	U	47	ARG	3.3
4	A	36	ASP	3.3
11	H	45	VAL	3.3
14	L	149	ARG	3.3
14	L	104	ASP	3.2
16	N	164	ASP	3.2
24	V	8	ILE	3.2
4	A	85	SER	3.2
1	0	1279	U	3.2
26	X	85	VAL	3.2
16	N	149	GLU	3.2
27	Y	98	GLN	3.2
26	X	71	ARG	3.2
7	D	130	VAL	3.2
32	I	110	GLU	3.1
7	D	29	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
16	N	148	ALA	3.1
26	X	10	VAL	3.1
9	F	49	PHE	3.1
32	I	122	THR	3.1
14	L	96	VAL	3.1
7	D	17	ARG	3.1
9	F	22	VAL	3.1
1	O	280	C	3.0
32	I	124	ALA	3.0
11	H	37	GLN	3.0
18	P	114	LEU	3.0
14	L	130	ARG	3.0
4	A	38	ILE	3.0
16	N	143	ARG	3.0
7	D	157	LEU	3.0
16	N	157	PRO	3.0
7	D	171	ASP	3.0
7	D	45	THR	3.0
9	F	103	GLU	3.0
9	F	26	THR	3.0
30	2	20	ARG	2.9
10	G	73	ASP	2.9
10	G	20	VAL	2.9
1	O	2004	U	2.9
30	2	35	ARG	2.9
14	L	145	LEU	2.9
6	C	61	PHE	2.9
26	X	72	VAL	2.9
26	X	80	GLU	2.9
7	D	24	HIS	2.9
22	T	35	TYR	2.9
4	A	33	GLU	2.8
9	F	18	GLU	2.8
14	L	102	ASP	2.8
8	E	48	VAL	2.8
7	D	53	LYS	2.8
14	L	150	GLN	2.8
26	X	77	PHE	2.8
32	I	108	ILE	2.8
22	T	119	ALA	2.8
8	E	5	LEU	2.8
8	E	108	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
9	F	12	LEU	2.8
14	L	76	LEU	2.8
16	N	154	LEU	2.8
14	L	133	VAL	2.8
10	G	67	LEU	2.8
14	L	120	LEU	2.8
1	0	2254	G	2.8
10	G	28	GLU	2.8
5	B	181	ILE	2.8
14	L	121	ILE	2.8
1	0	2769	C	2.8
8	E	10	ASP	2.8
26	X	73	ARG	2.8
1	0	272	A	2.8
1	0	2508	C	2.8
16	N	180	LEU	2.8
4	A	34	ASP	2.8
1	0	370	G	2.8
22	T	112	LEU	2.8
16	N	140	GLN	2.7
8	E	118	ILE	2.7
32	I	87	THR	2.7
1	0	2250	G	2.7
7	D	55	LYS	2.7
1	0	497	A	2.7
2	9	3122	C	2.7
16	N	182	GLY	2.7
1	0	283	U	2.7
14	L	81	VAL	2.7
24	V	33	VAL	2.7
16	N	139	TRP	2.7
11	H	146	VAL	2.7
5	B	106	HIS	2.7
9	F	107	ASP	2.7
31	3	92	GLU	2.6
24	V	59	ILE	2.6
16	N	138	ASP	2.6
4	A	32	VAL	2.6
16	N	95	ALA	2.6
4	A	237	GLY	2.6
24	V	3	LEU	2.6
7	D	94	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
9	F	108	VAL	2.6
27	Y	95	THR	2.6
5	B	105	PHE	2.6
18	P	141	ILE	2.6
1	0	999	C	2.6
16	N	183	ASP	2.6
8	E	7	ILE	2.6
6	C	135	GLU	2.6
7	D	48	MET	2.6
7	D	129	ASP	2.6
9	F	19	ALA	2.6
14	L	108	VAL	2.6
27	Y	108	ASP	2.6
4	A	97	ALA	2.6
9	F	98	VAL	2.6
1	0	1169	U	2.6
2	9	3002	U	2.6
1	0	1163	G	2.6
4	A	133	ARG	2.6
1	0	2251	G	2.5
1	0	284	C	2.5
7	D	173	GLU	2.5
7	D	164	ALA	2.5
1	0	2850	C	2.5
10	G	66	LEU	2.5
16	N	68	GLU	2.5
1	0	281	U	2.5
1	0	1198	U	2.5
28	Z	11	SER	2.5
18	P	71	TYR	2.5
7	D	11	HIS	2.5
11	H	47	ILE	2.5
7	D	47	GLN	2.5
23	U	54	THR	2.5
32	I	100	LEU	2.5
1	0	285	A	2.5
24	V	36	ALA	2.5
8	E	95	VAL	2.5
8	E	161	VAL	2.5
9	F	118	LEU	2.5
1	0	1179	C	2.5
10	G	69	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
28	Z	59	TYR	2.4
32	I	112	LYS	2.4
5	B	117	GLU	2.4
10	G	25	GLU	2.4
24	V	9	ARG	2.4
11	H	50	ILE	2.4
16	N	155	GLU	2.4
8	E	170	ARG	2.4
1	0	2239	C	2.4
8	E	128	GLY	2.4
9	F	20	LEU	2.4
14	L	118	LEU	2.4
7	D	67	ASP	2.4
28	Z	21	VAL	2.4
16	N	150	TYR	2.4
7	D	83	PHE	2.4
28	Z	20	ARG	2.4
31	3	22	VAL	2.4
1	0	1625	U	2.4
8	E	126	ILE	2.4
24	V	46	ILE	2.4
14	L	125	PHE	2.4
1	0	1162	G	2.4
10	G	65	THR	2.4
24	V	45	ARG	2.4
7	D	43	GLU	2.4
16	N	147	ILE	2.4
16	N	145	ALA	2.4
4	A	94	LEU	2.4
5	B	1	PRO	2.3
31	3	1	MET	2.3
16	N	165	ALA	2.3
16	N	162	ASP	2.3
16	N	184	ILE	2.3
7	D	80	ALA	2.3
15	M	194	ALA	2.3
19	Q	95	GLU	2.3
7	D	105	SER	2.3
1	0	1000	C	2.3
14	L	100	ALA	2.3
10	G	21	ASP	2.3
1	0	1948	G	2.3

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Mol	Chain	Res	Type	RSRZ
24	V	2	VAL	2.3
9	F	99	THR	2.3
4	A	96	LEU	2.3
5	B	104	GLU	2.3
19	Q	76	VAL	2.2
32	I	84	GLY	2.2
14	L	99	GLU	2.2
8	E	93	MET	2.2
14	L	73	VAL	2.2
27	Y	96	GLU	2.2
5	B	123	ALA	2.2
17	O	24	ALA	2.2
9	F	47	LEU	2.2
10	G	15	TRP	2.2
4	A	82	VAL	2.2
7	D	72	LYS	2.2
31	3	13	HIS	2.2
27	Y	97	LEU	2.2
16	N	181	ASP	2.2
26	X	9	VAL	2.2
5	B	35	GLN	2.2
21	S	20	PHE	2.2
1	0	1190	G	2.2
9	F	109	GLU	2.2
18	P	77	ALA	2.2
24	V	52	ALA	2.2
26	X	74	ALA	2.2
6	C	132	ASP	2.2
1	0	2249	G	2.2
7	D	50	VAL	2.2
10	G	12	ILE	2.2
11	H	74	ILE	2.2
10	G	63	ARG	2.2
1	0	372	A	2.2
31	3	2	GLN	2.1
9	F	15	ASP	2.1
9	F	100	ASP	2.1
10	G	72	ASP	2.1
32	I	120	ASP	2.1
18	P	67	LYS	2.1
24	V	11	MET	2.1
10	G	70	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
13	K	132	VAL	2.1
14	L	91	VAL	2.1
14	L	93	VAL	2.1
28	Z	24	ARG	2.1
8	E	6	GLU	2.1
15	M	164	THR	2.1
1	O	1950	G	2.1
16	N	172	PHE	2.1
16	N	186	LEU	2.1
14	L	144	ASP	2.1
1	O	1130	U	2.1
24	V	49	LEU	2.1
4	A	65	ARG	2.1
8	E	2	ARG	2.1
13	K	101	ASN	2.1
24	V	44	GLY	2.1
1	O	1180	U	2.1
14	L	61	ALA	2.1
17	O	111	VAL	2.1
7	D	74	THR	2.1
8	E	46	THR	2.1
16	N	178	THR	2.1
6	C	237	GLU	2.1
16	N	179	LEU	2.1
8	E	72	MET	2.1
1	O	138	U	2.1
8	E	86	VAL	2.1
11	H	171	ALA	2.1
32	I	83	ALA	2.1
24	V	62	GLU	2.1
4	A	99	ILE	2.1
26	X	82	GLU	2.1
27	Y	216	ARG	2.1
5	B	121	PRO	2.1
9	F	29	VAL	2.1
9	F	110	ASP	2.1
7	D	38	GLU	2.1
16	N	177	GLU	2.0
1	O	279	C	2.0
13	K	108	GLU	2.0
9	F	27	GLY	2.0
7	D	52	THR	2.0

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Mol	Chain	Res	Type	RSRZ
8	E	94	GLN	2.0
16	N	92	ALA	2.0
16	N	126	GLY	2.0
5	B	118	ASP	2.0
24	V	10	ASP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PSU	0	2621	20/21	0.98	0.13	28,31,39,40	0
1	OMU	0	2587	21/22	0.98	0.13	31,34,37,38	0
1	OMG	0	2588	24/25	0.98	0.13	30,34,37,38	0
1	UR3	0	2619	21/22	0.99	0.15	33,38,40,43	0
1	1MA	0	628	23/24	0.99	0.16	31,35,37,38	0
3	5AA	4	76	24/25	0.99	0.14	39,44,45,46	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
35	NA	9	9151	1/1	0.51	0.14	76,76,76,76	0
34	K	0	9003	1/1	0.62	0.31	82,82,82,82	0
33	MG	9	8095	1/1	0.63	0.11	72,72,72,72	0
35	NA	0	9182	1/1	0.65	0.28	74,74,74,74	0
33	MG	0	8092	1/1	0.76	0.48	95,95,95,95	0
35	NA	S	9112	1/1	0.78	0.49	76,76,76,76	0
33	MG	0	8085	1/1	0.79	0.25	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8114	1/1	0.80	0.13	64,64,64,64	0
33	MG	0	8045	1/1	0.80	0.23	65,65,65,65	0
35	NA	H	9122	1/1	0.81	0.25	77,77,77,77	0
35	NA	0	9172	1/1	0.82	0.31	59,59,59,59	0
35	NA	0	9171	1/1	0.82	0.26	60,60,60,60	0
35	NA	0	9184	1/1	0.82	0.10	75,75,75,75	0
35	NA	0	9163	1/1	0.83	0.35	71,71,71,71	0
33	MG	0	8090	1/1	0.83	0.39	80,80,80,80	0
35	NA	0	9116	1/1	0.84	0.13	36,36,36,36	0
33	MG	0	8082	1/1	0.84	0.14	66,66,66,66	0
35	NA	0	9186	1/1	0.84	0.32	75,75,75,75	0
35	NA	0	9174	1/1	0.84	0.25	59,59,59,59	0
35	NA	0	9141	1/1	0.85	0.12	46,46,46,46	0
35	NA	0	9124	1/1	0.85	0.09	59,59,59,59	0
33	MG	0	8049	1/1	0.85	0.39	90,90,90,90	0
35	NA	0	9117	1/1	0.86	0.21	72,72,72,72	0
35	NA	0	9185	1/1	0.86	0.36	60,60,60,60	0
33	MG	0	8047	1/1	0.86	0.18	102,102,102,102	0
33	MG	0	8071	1/1	0.87	0.08	53,53,53,53	0
33	MG	0	8104	1/1	0.87	0.17	53,53,53,53	0
35	NA	R	9137	1/1	0.87	0.08	42,42,42,42	0
33	MG	0	8107	1/1	0.88	0.06	45,45,45,45	0
33	MG	0	8030	1/1	0.88	0.11	35,35,35,35	0
35	NA	0	9165	1/1	0.88	0.18	39,39,39,39	0
35	NA	0	9150	1/1	0.88	0.21	44,44,44,44	0
35	NA	0	9113	1/1	0.88	0.14	59,59,59,59	0
35	NA	0	9142	1/1	0.89	0.22	52,52,52,52	0
33	MG	0	8076	1/1	0.89	0.11	57,57,57,57	0
33	MG	0	8050	1/1	0.89	0.07	63,63,63,63	0
33	MG	3	8078	1/1	0.89	0.07	46,46,46,46	0
35	NA	0	9126	1/1	0.89	0.14	40,40,40,40	0
33	MG	0	8053	1/1	0.89	0.09	51,51,51,51	0
36	CL	J	9302	1/1	0.90	0.13	70,70,70,70	0
33	MG	0	8043	1/1	0.90	0.09	42,42,42,42	0
35	NA	0	9129	1/1	0.90	0.14	53,53,53,53	0
35	NA	0	9166	1/1	0.90	0.12	77,77,77,77	0
37	CD	O	9205	1/1	0.90	0.07	137,137,137,137	0
36	CL	0	9322	1/1	0.91	0.31	76,76,76,76	0
35	NA	0	9107	1/1	0.91	0.13	43,43,43,43	0
35	NA	0	9176	1/1	0.91	0.23	43,43,43,43	0
33	MG	0	8057	1/1	0.91	0.13	39,39,39,39	0
35	NA	B	9158	1/1	0.91	1.05	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8101	1/1	0.91	0.17	69,69,69,69	0
33	MG	0	8048	1/1	0.91	0.13	60,60,60,60	0
36	CL	0	9315	1/1	0.91	0.21	69,69,69,69	0
37	CD	3	9204	1/1	0.91	0.10	62,62,62,62	0
35	NA	0	9119	1/1	0.91	0.13	42,42,42,42	0
33	MG	0	8051	1/1	0.91	0.12	56,56,56,56	0
33	MG	0	8059	1/1	0.92	0.09	51,51,51,51	0
35	NA	J	9146	1/1	0.92	0.14	37,37,37,37	0
35	NA	0	9167	1/1	0.92	0.09	40,40,40,40	0
34	K	0	9001	1/1	0.92	0.09	66,66,66,66	0
33	MG	0	8014	1/1	0.92	0.10	42,42,42,42	0
36	CL	0	9314	1/1	0.93	0.09	50,50,50,50	0
35	NA	0	9155	1/1	0.93	0.25	60,60,60,60	0
33	MG	0	8118	1/1	0.93	0.10	63,63,63,63	0
35	NA	0	9138	1/1	0.93	0.12	51,51,51,51	0
33	MG	0	8072	1/1	0.93	0.20	51,51,51,51	0
35	NA	0	9105	1/1	0.93	0.13	35,35,35,35	0
36	CL	O	9308	1/1	0.93	0.11	68,68,68,68	0
35	NA	L	9180	1/1	0.93	0.38	50,50,50,50	0
33	MG	0	8042	1/1	0.93	0.07	45,45,45,45	0
33	MG	0	8113	1/1	0.93	0.10	45,45,45,45	0
35	NA	0	9181	1/1	0.93	0.14	51,51,51,51	0
33	MG	0	8116	1/1	0.93	0.07	50,50,50,50	0
36	CL	J	9301	1/1	0.93	0.12	72,72,72,72	0
36	CL	L	9310	1/1	0.93	0.09	58,58,58,58	0
35	NA	0	9111	1/1	0.93	0.24	65,65,65,65	0
35	NA	0	9108	1/1	0.94	0.12	48,48,48,48	0
35	NA	0	9175	1/1	0.94	0.23	42,42,42,42	0
33	MG	0	8080	1/1	0.94	0.06	37,37,37,37	0
36	CL	3	9304	1/1	0.94	0.06	47,47,47,47	0
35	NA	0	9177	1/1	0.94	0.22	55,55,55,55	0
33	MG	0	8040	1/1	0.94	0.09	45,45,45,45	0
33	MG	0	8001	1/1	0.94	0.07	36,36,36,36	0
35	NA	9	9183	1/1	0.94	0.11	55,55,55,55	0
35	NA	0	9159	1/1	0.94	0.19	50,50,50,50	0
35	NA	0	9114	1/1	0.94	0.16	66,66,66,66	0
35	NA	0	9156	1/1	0.94	0.21	50,50,50,50	0
33	MG	0	8106	1/1	0.94	0.10	51,51,51,51	0
33	MG	0	8075	1/1	0.94	0.05	39,39,39,39	0
35	NA	0	9173	1/1	0.94	0.14	42,42,42,42	0
35	NA	0	9170	1/1	0.95	0.41	61,61,61,61	0
35	NA	0	9169	1/1	0.95	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8115	1/1	0.95	0.14	52,52,52,52	0
35	NA	0	9157	1/1	0.95	0.07	60,60,60,60	0
35	NA	0	9125	1/1	0.95	0.18	64,64,64,64	0
35	NA	0	9161	1/1	0.95	0.25	49,49,49,49	0
35	NA	0	9121	1/1	0.95	0.26	50,50,50,50	0
35	NA	0	9115	1/1	0.95	0.14	37,37,37,37	0
33	MG	0	8062	1/1	0.95	0.10	53,53,53,53	0
35	NA	0	9164	1/1	0.95	0.16	52,52,52,52	0
33	MG	0	8013	1/1	0.95	0.23	33,33,33,33	0
33	MG	0	8008	1/1	0.95	0.08	35,35,35,35	0
35	NA	0	9140	1/1	0.95	0.33	49,49,49,49	0
33	MG	0	8063	1/1	0.95	0.09	53,53,53,53	0
35	NA	0	9135	1/1	0.95	0.20	43,43,43,43	0
35	NA	0	9102	1/1	0.95	0.13	42,42,42,42	0
33	MG	0	8046	1/1	0.95	0.04	52,52,52,52	0
33	MG	0	8041	1/1	0.95	0.23	59,59,59,59	0
35	NA	A	9145	1/1	0.96	0.18	39,39,39,39	0
36	CL	0	9313	1/1	0.96	0.14	62,62,62,62	0
36	CL	B	9319	1/1	0.96	0.14	47,47,47,47	0
36	CL	0	9303	1/1	0.96	0.15	54,54,54,54	0
33	MG	0	8093	1/1	0.96	0.13	56,56,56,56	0
33	MG	0	8006	1/1	0.96	0.09	32,32,32,32	0
33	MG	0	8088	1/1	0.96	0.06	39,39,39,39	0
33	MG	0	8100	1/1	0.96	0.10	68,68,68,68	0
35	NA	0	9106	1/1	0.96	0.17	34,34,34,34	0
35	NA	0	9136	1/1	0.96	0.08	53,53,53,53	0
35	NA	C	9104	1/1	0.96	0.09	32,32,32,32	0
33	MG	0	8094	1/1	0.96	0.16	62,62,62,62	0
33	MG	0	8111	1/1	0.96	0.08	57,57,57,57	0
33	MG	0	8023	1/1	0.96	0.20	53,53,53,53	0
35	NA	0	9127	1/1	0.96	0.18	39,39,39,39	0
33	MG	0	8027	1/1	0.96	0.12	44,44,44,44	0
33	MG	0	8112	1/1	0.96	0.05	37,37,37,37	0
36	CL	0	9316	1/1	0.96	0.09	56,56,56,56	0
33	MG	9	8052	1/1	0.96	0.07	50,50,50,50	0
33	MG	0	8037	1/1	0.96	0.10	46,46,46,46	0
34	K	0	9002	1/1	0.96	0.06	43,43,43,43	0
33	MG	0	8103	1/1	0.96	0.20	66,66,66,66	0
35	NA	0	9160	1/1	0.96	0.24	41,41,41,41	0
33	MG	0	8091	1/1	0.97	0.07	74,74,74,74	0
33	MG	0	8032	1/1	0.97	0.16	39,39,39,39	0
35	NA	0	9130	1/1	0.97	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8024	1/1	0.97	0.15	49,49,49,49	0
33	MG	0	8039	1/1	0.97	0.08	49,49,49,49	0
33	MG	0	8070	1/1	0.97	0.12	53,53,53,53	0
35	NA	0	9152	1/1	0.97	0.30	60,60,60,60	0
33	MG	0	8021	1/1	0.97	0.14	25,25,25,25	0
35	NA	0	9168	1/1	0.97	0.13	52,52,52,52	0
35	NA	0	9110	1/1	0.97	0.14	37,37,37,37	0
33	MG	0	8108	1/1	0.97	0.09	56,56,56,56	0
33	MG	0	8054	1/1	0.97	0.11	24,24,24,24	0
33	MG	0	8087	1/1	0.97	0.21	57,57,57,57	0
35	NA	0	9178	1/1	0.97	0.31	53,53,53,53	0
33	MG	B	8055	1/1	0.97	0.20	60,60,60,60	0
33	MG	0	8036	1/1	0.97	0.14	39,39,39,39	0
35	NA	0	9133	1/1	0.97	0.16	27,27,27,27	0
35	NA	0	9101	1/1	0.97	0.22	46,46,46,46	0
33	MG	0	8084	1/1	0.97	0.11	40,40,40,40	0
35	NA	0	9149	1/1	0.97	0.09	36,36,36,36	0
33	MG	0	8098	1/1	0.97	0.11	45,45,45,45	0
36	CL	N	9307	1/1	0.97	0.16	61,61,61,61	0
33	MG	0	8019	1/1	0.97	0.10	33,33,33,33	0
33	MG	A	8065	1/1	0.97	0.14	42,42,42,42	0
33	MG	4	8119	1/1	0.97	0.08	41,41,41,41	0
33	MG	0	8003	1/1	0.97	0.13	26,26,26,26	0
33	MG	0	8022	1/1	0.97	0.06	35,35,35,35	0
35	NA	0	9131	1/1	0.97	0.13	35,35,35,35	0
33	MG	0	8007	1/1	0.97	0.08	23,23,23,23	0
33	MG	0	8020	1/1	0.97	0.14	32,32,32,32	0
33	MG	0	8086	1/1	0.97	0.07	50,50,50,50	0
35	NA	0	9179	1/1	0.97	0.20	57,57,57,57	0
33	MG	Y	8109	1/1	0.97	0.08	40,40,40,40	0
33	MG	0	8035	1/1	0.97	0.08	50,50,50,50	0
33	MG	0	8067	1/1	0.97	0.12	52,52,52,52	0
33	MG	0	8018	1/1	0.97	0.13	40,40,40,40	0
33	MG	0	8066	1/1	0.97	0.17	114,114,114,114	0
33	MG	0	8002	1/1	0.97	0.03	28,28,28,28	0
33	MG	0	8102	1/1	0.97	0.08	51,51,51,51	0
36	CL	J	9321	1/1	0.97	0.15	54,54,54,54	0
35	NA	0	9134	1/1	0.97	0.14	34,34,34,34	0
35	NA	0	9118	1/1	0.97	0.12	54,54,54,54	0
35	NA	0	9162	1/1	0.97	0.26	58,58,58,58	0
33	MG	0	8060	1/1	0.97	0.20	39,39,39,39	0
33	MG	0	8044	1/1	0.97	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	A	9309	1/1	0.98	0.21	58,58,58,58	0
33	MG	0	8028	1/1	0.98	0.15	43,43,43,43	0
33	MG	0	8017	1/1	0.98	0.10	31,31,31,31	0
33	MG	0	8026	1/1	0.98	0.12	24,24,24,24	0
33	MG	0	8015	1/1	0.98	0.10	30,30,30,30	0
33	MG	0	8034	1/1	0.98	0.12	39,39,39,39	0
33	MG	B	8056	1/1	0.98	0.15	49,49,49,49	0
33	MG	0	8099	1/1	0.98	0.14	59,59,59,59	0
33	MG	0	8038	1/1	0.98	0.17	28,28,28,28	0
33	MG	0	8110	1/1	0.98	0.06	34,34,34,34	0
33	MG	0	8058	1/1	0.98	0.16	45,45,45,45	0
33	MG	0	8079	1/1	0.98	0.12	28,28,28,28	0
33	MG	0	8096	1/1	0.98	0.09	38,38,38,38	0
33	MG	0	8016	1/1	0.98	0.19	35,35,35,35	0
36	CL	0	9305	1/1	0.98	0.10	52,52,52,52	0
35	NA	Q	9148	1/1	0.98	0.20	36,36,36,36	0
33	MG	0	8089	1/1	0.98	0.06	60,60,60,60	0
33	MG	0	8033	1/1	0.98	0.08	39,39,39,39	0
33	MG	0	8012	1/1	0.98	0.15	35,35,35,35	0
35	NA	0	9132	1/1	0.98	0.09	29,29,29,29	0
36	CL	0	9320	1/1	0.98	0.11	48,48,48,48	0
35	NA	H	9109	1/1	0.98	0.13	31,31,31,31	0
33	MG	0	8077	1/1	0.98	0.10	29,29,29,29	0
35	NA	0	9128	1/1	0.98	0.08	40,40,40,40	0
33	MG	0	8117	1/1	0.98	0.07	32,32,32,32	0
35	NA	0	9153	1/1	0.98	0.05	17,17,17,17	0
33	MG	0	8074	1/1	0.98	0.07	34,34,34,34	0
36	CL	R	9306	1/1	0.98	0.12	53,53,53,53	0
33	MG	K	8069	1/1	0.98	0.11	41,41,41,41	0
36	CL	0	9311	1/1	0.98	0.14	51,51,51,51	0
35	NA	M	9147	1/1	0.98	0.13	18,18,18,18	0
35	NA	0	9154	1/1	0.98	0.09	26,26,26,26	0
35	NA	0	9139	1/1	0.98	0.09	22,22,22,22	0
35	NA	0	9103	1/1	0.98	0.15	44,44,44,44	0
35	NA	0	9144	1/1	0.98	0.06	35,35,35,35	0
33	MG	0	8068	1/1	0.98	0.06	58,58,58,58	0
35	NA	0	9120	1/1	0.98	0.14	56,56,56,56	0
33	MG	0	8061	1/1	0.99	0.09	34,34,34,34	0
33	MG	0	8097	1/1	0.99	0.10	45,45,45,45	0
33	MG	0	8031	1/1	0.99	0.08	30,30,30,30	0
33	MG	0	8083	1/1	0.99	0.08	35,35,35,35	0
37	CD	1	9202	1/1	0.99	0.02	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8004	1/1	0.99	0.08	33,33,33,33	0
33	MG	0	8064	1/1	0.99	0.12	25,25,25,25	0
37	CD	Z	9203	1/1	0.99	0.08	61,61,61,61	0
36	CL	M	9318	1/1	0.99	0.13	36,36,36,36	0
33	MG	0	8005	1/1	0.99	0.09	24,24,24,24	0
33	MG	0	8009	1/1	0.99	0.10	31,31,31,31	0
33	MG	0	8011	1/1	0.99	0.11	23,23,23,23	0
37	CD	U	9201	1/1	0.99	0.06	73,73,73,73	0
33	MG	0	8029	1/1	0.99	0.19	32,32,32,32	0
33	MG	0	8010	1/1	0.99	0.07	30,30,30,30	0
35	NA	0	9123	1/1	0.99	0.13	52,52,52,52	0
33	MG	0	8081	1/1	0.99	0.14	43,43,43,43	0
33	MG	0	8025	1/1	0.99	0.13	48,48,48,48	0
36	CL	0	9312	1/1	0.99	0.07	52,52,52,52	0
33	MG	T	8073	1/1	0.99	0.05	49,49,49,49	0
36	CL	0	9317	1/1	0.99	0.05	61,61,61,61	0
35	NA	T	9143	1/1	0.99	0.06	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.