



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:00 pm GMT

PDB ID : 1VQN
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (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

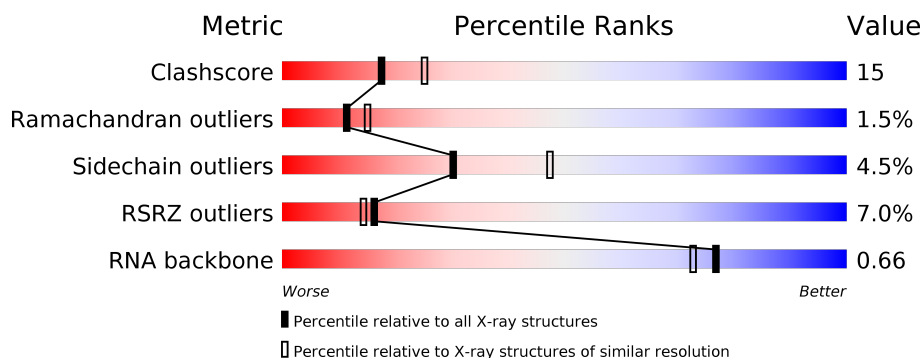
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)
RNA backbone	2636	1023 (2.80-2.00)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div>62% 27% 5% 6%</div> </div>
2	9	122	<div> <div>5%</div> <div>57% 32% 11%</div> </div>
3	4	4	<div> <div>50% 50%</div> </div>
4	5	6	<div> <div>17% 17%</div> <div>67% 17%</div> </div>
5	A	240	<div> <div>5%</div> <div>61% 33% 5%</div> </div>
6	B	338	<div> <div>3%</div> <div>57% 39%</div> </div>

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Mol	Chain	Length	Quality of chain
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	

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Mol	Chain	Length	Quality of chain
32	3	92	
33	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
34	MG	0	8047	-	-	-	X
36	NA	0	9152	-	-	-	X
36	NA	0	9184	-	-	-	X
38	SR	B	9521	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99077 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			

- 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*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	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 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	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 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

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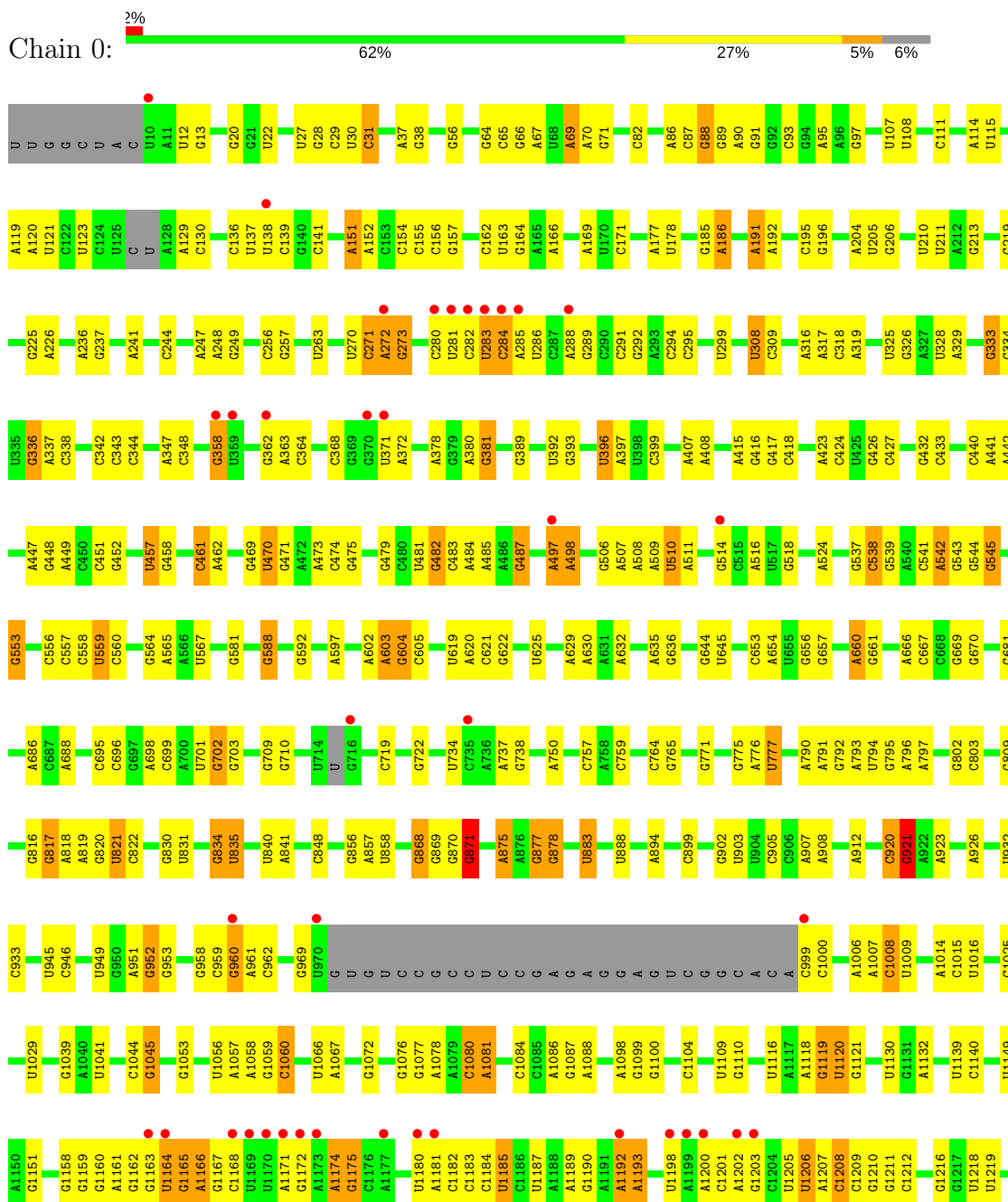
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0

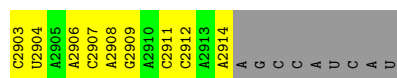
3 Residue-property plots

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

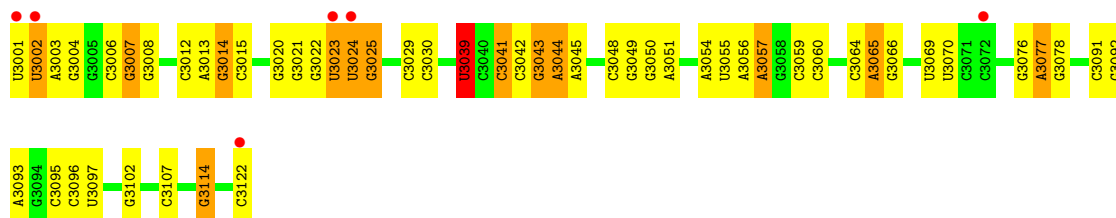
- Molecule 1: 23S ribosomal rna



U2796	U2671	G2564	A2467	C2351	C2243	U1846	U1741	C1633	A1482	C1343	A1232
A2800	C2672	C2565	A2468	A2352	C2248	A1847	G1744	G1634	A1483	U1350	A1233
U2807	U2673	A2568	A2469	A2353	G2249	G1848	G1745	U1635	G1484	U1351	U1234
U2808	C2676	A2569	C2472	A2354	G2250	C1853	U1748	G1636	G1491	A1352	A1236
G2809	A2681	G2578	C2476	A2355	G2251	C1856	U1751	A1637	U1503	C1353	U1237
G2810	C2682	U2586	C2477	A2356	A2252	G1857	G1752	A1641	U1504	C1360	U1238
A2811	A2689	U2587	A2478	G2357	G2253	C1863	C1755	A1642	A1505	G1363	U1239
A2812	A2694	G2588	A2479	A2361	G2254	G1867	A1756	U1654	U1506	A1242	A1243
G2813	G2712	U2589	G2480	A2362	A2255	G1868	G1757	G1655	U1511	C1244	A1245
A2814	G2713	U2590	G2481	A2363	G2256	G1877	U1766	A1657	U1512	C1245	A1246
G2815	U2714	C2591	G2482	A2364	G2257	U1878	U1771	A1666	U1524	C1250	C1250
A2816	U2715	G2592	A2483	G2365	A2258	U1879	C1772	A1667	G1525	C1251	A1252
U2817	G2716	C2599	C2487	A2369	U2265	U1880	G1773	U1668	A1528	U1378	A1253
A2818	A2699	A2600	A2490	A2372	A2266	A1881	U1778	A1669	C1529	C1384	C1257
G2819	C2717	G2601	A2491	U2373	G2270	U1882	A1779	G1670	C1535	A1406	A1261
A2820	A2718	G2602	U2492	A2374	G2271	C1883	U1784	A1680	C1536	A1407	A1262
C2821	G2720	C2603	U2493	A2375	G2272	U1884	U1785	A1681	C1552	U1468	U1266
C2824	U2721	U2607	C2494	A2376	A2291	A1885	G1777	A1682	U1554	G1409	C1267
G2825	U2724	C2608	C2502	C2377	A2291	A1886	A1788	A1683	U1555	A1414	C1268
A2826	G2725	G2613	A2503	U2378	C2296	G1902	U1789	A1684	A1569	U1415	A1278
G2827	U2726	U2619	A2504	U2378	U2297	U1903	G1794	A1685	U	U1418	U1279
C2828	U2727	U2620	A2505	U2378	U2297	A1904	G1795	A1686	U1561	C1289	C1289
G2829	U2735	U2621	A2506	A2401	A2301	A1919	U1796	A1687	C1562	G1290	G1290
U2837	U2736	U2622	A2507	A2402	A2302	A1921	A1797	C1692	C1574	C1422	A1294
A2840	G2737	C2626	C2508	G2412	A2302	A1922	C1798	C1700	C1575	C1426	U1298
A2841	C2738	G2627	A2511	A2413	C2309	G1929	G1799	A1701	U1702	A1427	G1299
G2842	C2747	U2630	U2512	A2414	C2313	C1940	C1816	A1710	G1589	U1435	U1306
A2851	G2748	U2631	U2513	A2415	C2313	A1941	U1817	C1714	G1592	U1440	A1307
U2853	U2749	G2632	C2515	A2416	C2317	C1943	G1818	C1715	C1594	G1441	A1308
A2856	G2750	A2633	C2516	C2417	C2317	C1944	G1819	A1716	G1595	A1442	G1311
C2857	G2751	G2634	C2517	U2418	C2320	C1945	G1820	A1717	U1596	C1451	G1312
U2866	A2761	A2637	A2521	U2419	A2321	C1946	A1821	A1718	A1597	G1452	A1313
C2867	C2762	U2637	G2524	G2420	A2331	G1947	A1822	G1718	A1598	G1453	U1314
U2868	C2767	G2642	G2525	U2421	G2334	G1948	C1826	U1722	A1603	U1454	G1315
G2862	A2768	U2643	C2526	U2422	C2335	G1951	G1827	G1723	G1604	A1458	G1325
U2866	G2770	C2644	U2531	G2426	U2336	U	G1828	U1724	G1605	C1462	A1328
G2867	A2776	U2645	A2532	C2427	G2337	A	A1829	C1725	A1606	U1473	U1333
U2876	G2777	U2648	C2533	A2434	U2338	A	C1834	G1730	A1607	C1474	C1334
G2876	A2778	A2649	C2534	C2443	G2338	A	U1835	A1732	A1615	C1477	A1341
U2877	G2779	U2652	U2535	U2444	A	A	A1836	A1733	U1625	U1478	G1342
G2878	C2780	A2653	C2536	U2445	C	A	U1837	A1736	A1626	C1477	G1342
A2879	U2781	U2654	G2537	G2446	G	C	G1838	A1739	G1627	U1478	G1342
U2883	G2782	U2661	U2541	G2453	G2337	U	A1839	A1739	A1630	U1478	G1342
G2884	A2783	G2662	C2542	A	G2338	A	C1834	G1730	A1607	U1478	G1342
A2890	G2785	U2663	C2543	A2456	A	A	U1835	A1732	A1615	C1462	A1328
C2894	G2786	A2664	C2544	U2457	C	U	A1836	A1733	U1625	U1473	U1333
A2895	C2787	A	C2545	G	G	U	U1837	A1736	A1626	C1474	C1334
G2896	U2793	U	G2344	A	A	G	G1838	A1739	A1630	U1478	G1342
C2897	G2794	G2667	A2345	C	C	A	A1839	G1730	A1626	C1477	A1341
U2898	C2795	G2670	C2346	C	C	C	A1840	U1740	A1630	U1478	G1342



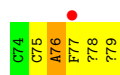
• Molecule 2: 5S ribosomal RNA



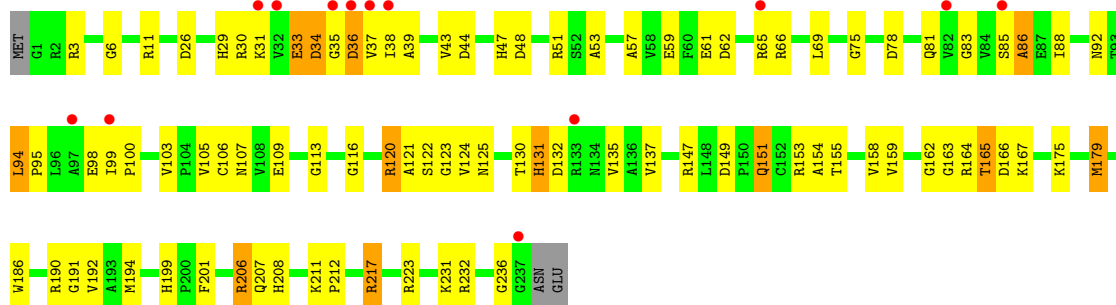
• Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'



• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

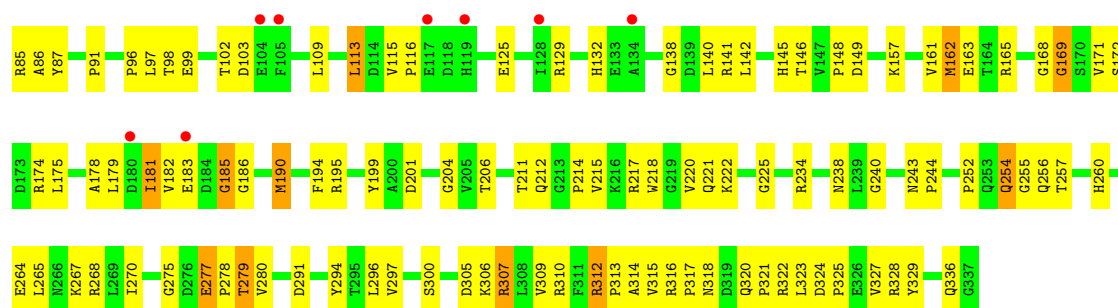


• Molecule 5: 50S ribosomal protein L2P



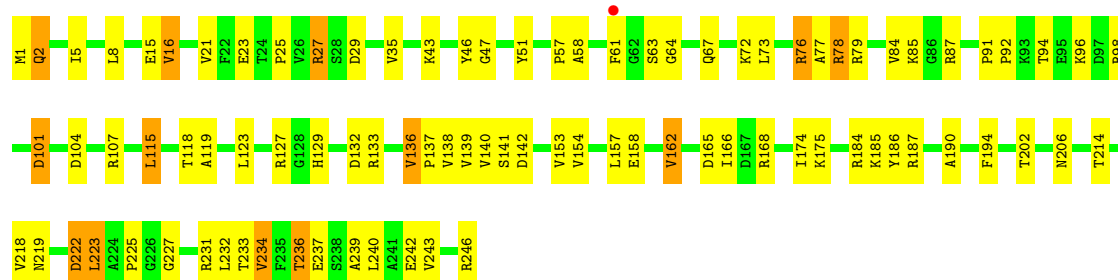
• Molecule 6: 50S ribosomal protein L3P





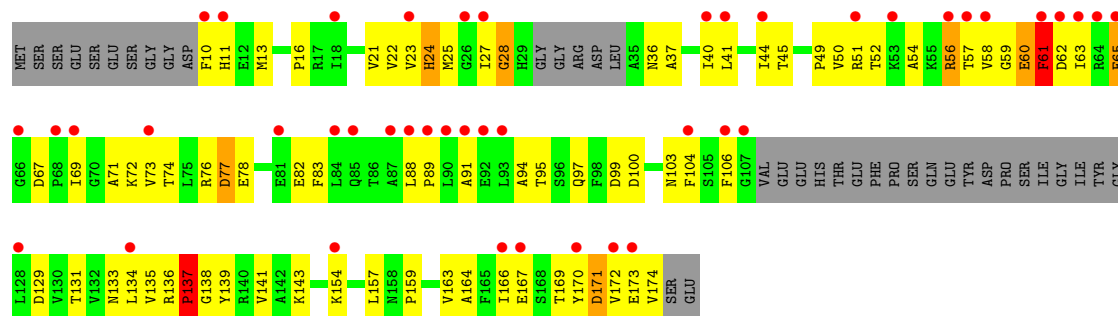
• Molecule 7: 50S ribosomal protein L4E

Chain C: 63% 31% 5%



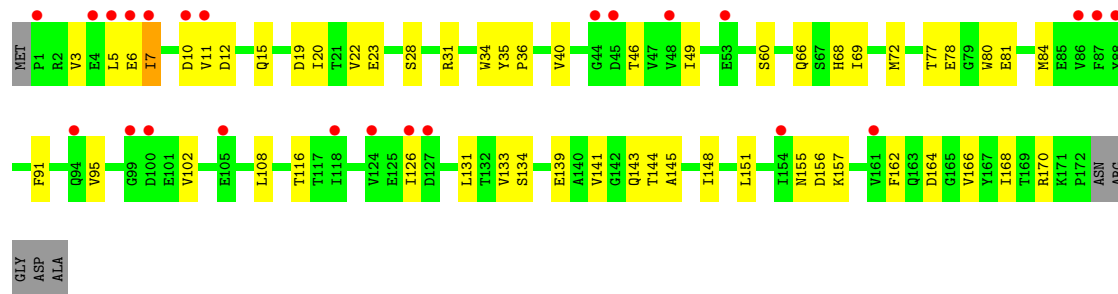
• Molecule 8: 50S ribosomal protein L5P

Chain D: 25% 36% 38% 21%

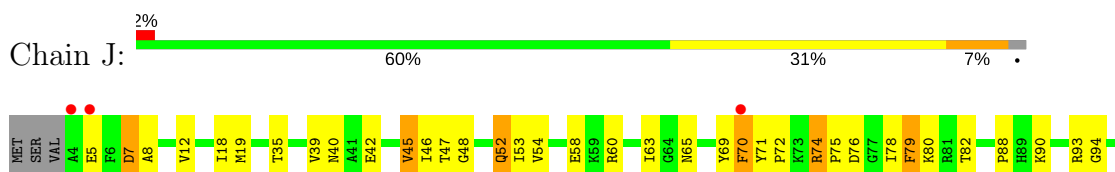


• Molecule 9: 50S ribosomal protein L6P

Chain E: 13% 66% 30%



• Molecule 10: 50S ribosomal protein L7AE





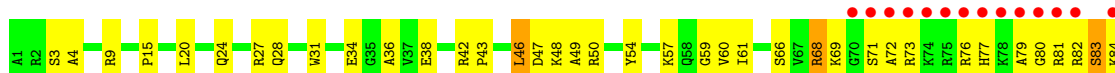
• Molecule 14: 50S ribosomal protein L14P



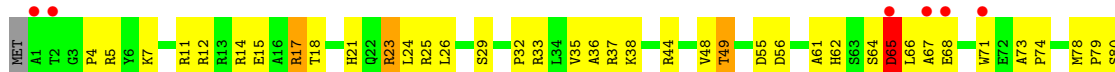
• Molecule 15: 50S ribosomal protein L15P



• Molecule 16: 50S Ribosomal Protein L15E

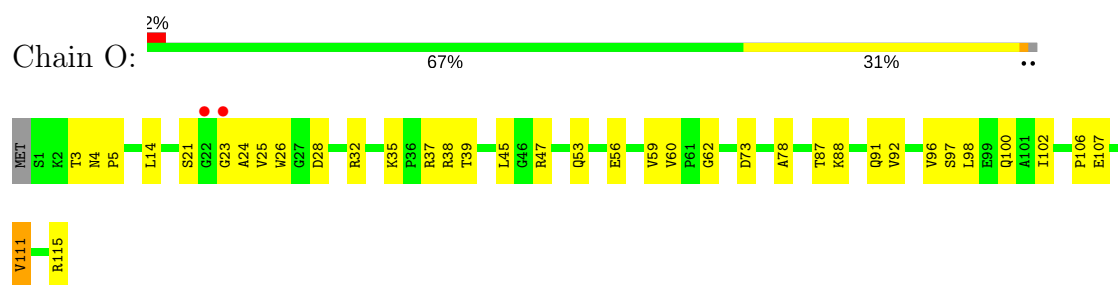


• Molecule 17: 50S ribosomal protein L18P

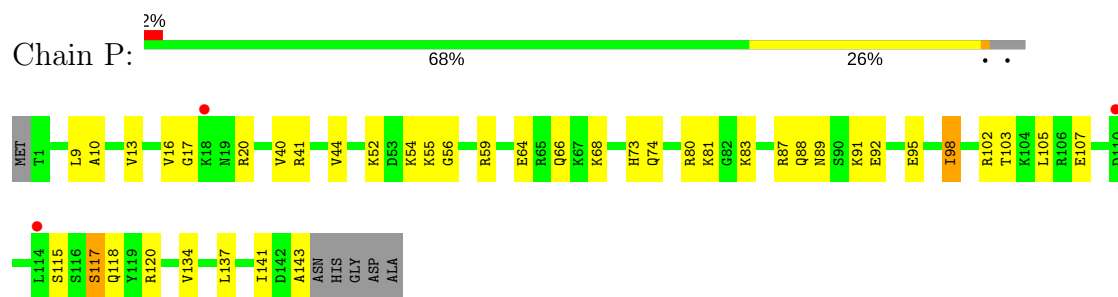


• Molecule 18: 50S ribosomal protein L18e

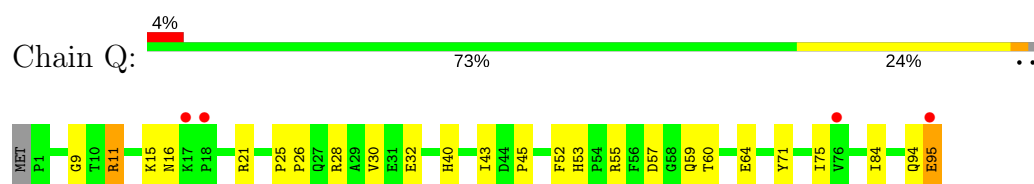




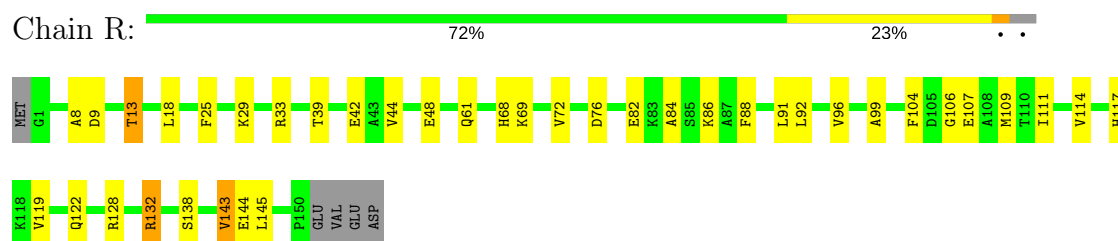
- Molecule 19: 50S ribosomal protein L19E



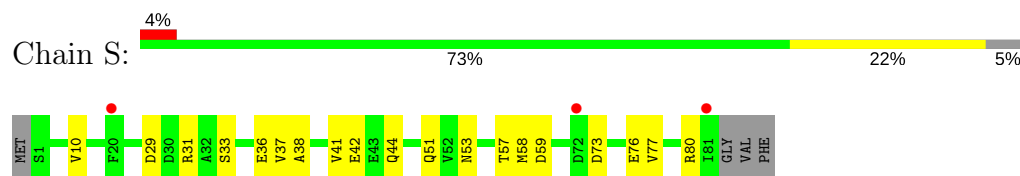
- Molecule 20: 50S ribosomal protein L21e



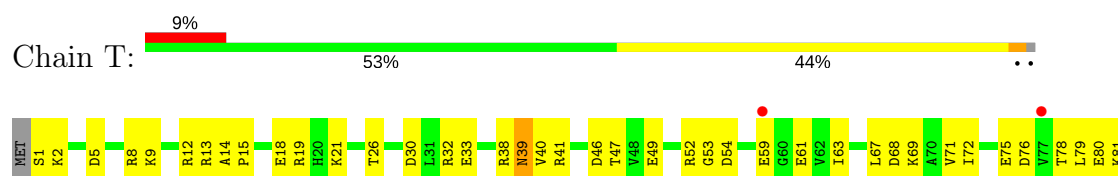
- Molecule 21: 50S ribosomal protein L22P

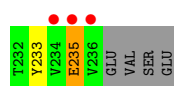


- Molecule 22: 50S ribosomal protein L23P

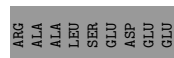
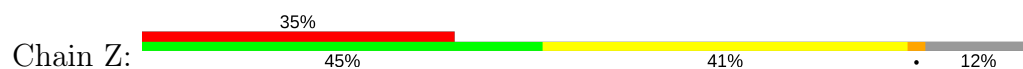


- Molecule 23: 50S ribosomal protein L24P





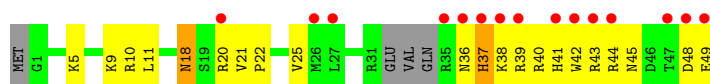
- Molecule 29: 50S ribosomal protein L37Ae



- Molecule 30: 50S ribosomal protein L37e



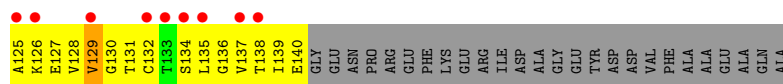
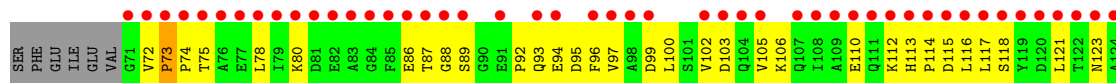
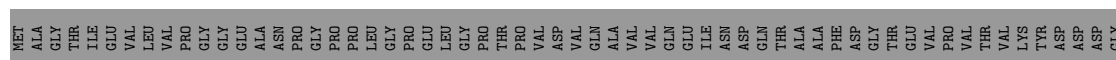
- Molecule 31: 50S ribosomal protein L39e



- Molecule 32: 50S ribosomal protein L44E



- Molecule 33: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACA, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/65959	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00
1	0	2726	U	N1-C1'-C2'	6.13	121.97	114.00
1	0	1504	A	C1'-O4'-C4'	-6.08	105.03	109.90
1	0	777	U	O4'-C1'-N1	5.98	112.98	108.20
2	9	3039	U	N1-C1'-C2'	5.95	121.73	114.00
1	0	1120	U	C5'-C4'-C3'	-5.79	106.73	116.00
1	0	2467	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	2541	U	C2'-C3'-O3'	5.76	122.91	113.70
1	0	1819	G	C1'-O4'-C4'	-5.69	105.35	109.90
1	0	1504	A	N9-C1'-C2'	5.65	121.34	114.00
1	0	1979	G	C2'-C3'-O3'	5.55	122.58	113.70
1	0	2291	A	N9-C1'-C2'	5.45	121.09	114.00
1	0	206	G	C5'-C4'-C3'	-5.26	107.58	116.00
1	0	2313	C	C5'-C4'-O4'	5.26	115.42	109.10
1	0	841	A	C1'-O4'-C4'	-5.24	105.70	109.90
1	0	1615	A	C5'-C4'-C3'	5.20	124.33	116.00
1	0	2301	A	N9-C1'-C2'	5.12	120.66	114.00
1	0	1352	A	OP1-P-O3'	5.07	116.36	105.20
1	0	921	G	N9-C1'-C2'	5.05	120.57	114.00
1	0	1261	A	N9-C1'-C2'	5.05	120.57	114.00
1	0	457	U	C1'-O4'-C4'	-5.04	105.86	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	389	G	C5'-C4'-C3'	-5.00	108.00	116.00

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1458	A	Sidechain
1	0	1491	G	Sidechain
1	0	1592	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1885	A	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	2115	U	Sidechain
1	0	22	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2645	U	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2726	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	507	A	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	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	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	66	0	0	0	0
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	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 (2220) 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:O:1160:G:H5'	1:O:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04
23:T:9:LYS:HE3	23:T:13:ARG:NH1	1.73	1.04
13:J:93:ARG:HH11	13:J:93:ARG:HB3	1.21	1.02
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.38	1.02
8:D:25:MET:HE2	8:D:41:LEU:HG	1.41	1.00
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.44	0.99
1:O:871:G:C8	1:O:871:G:H5'	1.96	0.99
22:S:51:GLN:HE21	22:S:53:ASN:HD21	1.05	0.99
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.46	0.98
7:C:236:THR:HG22	7:C:239:ALA:H	1.24	0.98
1:O:156:C:H5''	16:M:171:ARG:HD3	1.46	0.97
5:A:211:LYS:HG2	5:A:212:PRO:HD2	1.45	0.96
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.80	0.96
10:F:91:VAL:HG12	10:F:92:GLY:H	1.26	0.96
23:T:71:VAL:HG11	23:T:90:PRO:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:78:ARG:HG3	7:C:78:ARG:HH11	1.30	0.96
1:0:1771:U:H5'	29:Z:20:ARG:HH21	1.31	0.95
1:0:871:G:H8	1:0:871:G:H5'	1.28	0.95
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.95
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
14:K:10:GLN:H	14:K:10:GLN:HE21	0.93	0.92
1:0:1242:A:H5'	13:J:82:THR:HG23	1.50	0.92
17:N:11:ARG:HG3	17:N:14:ARG:HH12	1.34	0.92
14:K:10:GLN:H	14:K:10:GLN:NE2	1.66	0.91
8:D:28:GLY:HA2	8:D:69:ILE:HG23	1.52	0.91
1:0:1372:A:H3'	40:0:7638:HOH:O	1.70	0.91
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.53	0.91
5:A:81:GLN:HB2	5:A:92:ASN:ND2	1.86	0.90
26:W:6:GLN:HB2	26:W:26:ILE:HD12	1.53	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.90
17:N:144:GLY:O	17:N:147:ILE:HG22	1.70	0.90
28:Y:235:GLU:H	28:Y:235:GLU:CD	1.75	0.90
6:B:238:ASN:HD22	6:B:240:GLY:H	1.18	0.90
31:2:18:ASN:HD21	31:2:40:ARG:H	1.17	0.89
14:K:74:VAL:HG13	14:K:113:ILE:HG23	1.54	0.89
6:B:307:ARG:HH11	6:B:307:ARG:HG3	1.36	0.89
12:H:29:ALA:HB3	12:H:66:ARG:HH12	1.37	0.89
7:C:1:MET:HG2	7:C:2:GLN:H	1.38	0.89
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.55	0.89
8:D:58:VAL:HB	8:D:62:ASP:HB3	1.54	0.89
18:O:32:ARG:HE	18:O:35:LYS:HD2	1.36	0.88
14:K:81:ARG:HB2	14:K:87:ARG:HH11	1.37	0.88
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.88
14:K:74:VAL:HG11	14:K:113:ILE:HG12	1.54	0.88
1:0:289:G:H22	1:0:363:A:H2	1.21	0.87
16:M:102:GLU:OE1	16:M:164:THR:HG21	1.73	0.87
19:P:115:SER:H	19:P:118:GLN:HE21	1.20	0.87
21:R:25:PHE:CE2	21:R:29:LYS:HE2	2.09	0.87
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
17:N:49:THR:HG22	17:N:56:ASP:HB2	1.55	0.86
29:Z:11:SER:HB3	29:Z:23:ARG:HB2	1.55	0.86
17:N:113:SER:HB2	40:N:9354:HOH:O	1.75	0.86
17:N:83:LEU:HD13	17:N:175:LEU:HD23	1.56	0.85
7:C:5:ILE:HD11	7:C:16:VAL:HG22	1.57	0.85
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.07	0.85
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85
26:W:137:GLN:HE21	26:W:141:HIS:HE1	1.25	0.85
9:E:15:GLN:HG2	9:E:19:ASP:O	1.77	0.85
8:D:172:VAL:HG12	8:D:173:GLU:H	1.40	0.85
29:Z:37:HIS:HB2	29:Z:47:VAL:HB	1.59	0.84
16:M:99:ARG:HH21	16:M:170:ASN:HD22	1.25	0.84
21:R:8:ALA:HB1	21:R:13:THR:HG21	1.58	0.84
28:Y:200:THR:HG22	28:Y:201:GLU:HG3	1.58	0.84
14:K:10:GLN:N	14:K:10:GLN:HE21	1.74	0.84
15:L:80:ASP:HB2	15:L:90:ARG:O	1.78	0.83
2:9:3006:C:H5''	17:N:37:ARG:NH1	1.94	0.83
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.83
19:P:115:SER:OG	19:P:118:GLN:HG3	1.78	0.83
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.83
5:A:192:VAL:HG22	40:A:9617:HOH:O	1.78	0.83
26:W:122:ARG:HH11	26:W:122:ARG:HG2	1.43	0.83
1:0:2717:C:C2'	1:0:2718:C:H5''	2.08	0.83
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.82
1:0:2840:A:OP1	6:B:211:THR:HG23	1.77	0.82
29:Z:36:ASP:HB3	29:Z:45:ASP:HB3	1.62	0.82
12:H:56:GLN:HE22	12:H:93:GLN:HG2	1.45	0.82
14:K:39:GLY:HA2	40:K:4183:HOH:O	1.80	0.82
6:B:162:MET:CE	6:B:310:ARG:HD3	2.10	0.82
2:9:3006:C:H5''	17:N:37:ARG:HH12	1.45	0.81
21:R:99:ALA:HB1	21:R:109:MET:HE1	1.61	0.81
1:0:871:G:H8	1:0:871:G:C5'	1.94	0.81
16:M:134:ILE:HG23	16:M:141:ILE:HD13	1.63	0.81
31:2:41:HIS:H	31:2:45:ASN:HD22	1.26	0.81
1:0:288:A:H61	1:0:364:C:H42	1.29	0.80
5:A:191:GLY:HA2	5:A:194:MET:CE	2.11	0.80
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.63	0.80
14:K:107:THR:HG22	14:K:108:GLU:HG3	1.64	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
8:D:136:ARG:HH12	8:D:157:LEU:HA	1.46	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.81	0.79
26:W:6:GLN:HB2	26:W:26:ILE:CD1	2.13	0.79
26:W:88:THR:HB	40:W:6679:HOH:O	1.82	0.79
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.79
1:0:2716:G:H5''	6:B:206:THR:HG21	1.65	0.79
14:K:4:LEU:HD22	14:K:116:GLU:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:12:ILE:N	11:G:13:PRO:HD3	1.97	0.79
27:X:72:VAL:HG22	27:X:85:VAL:HG12	1.64	0.79
1:0:1603:A:H5'	1:0:1605:G:O4'	1.83	0.79
1:0:1119:G:H2'	13:J:52:GLN:NE2	1.98	0.79
14:K:98:VAL:HG13	14:K:102:GLU:HA	1.63	0.79
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.64	0.79
17:N:11:ARG:HA	17:N:14:ARG:NH1	1.97	0.79
26:W:4:LEU:HD22	26:W:52:VAL:HG21	1.63	0.79
1:0:2534:C:H1'	40:0:4081:HOH:O	1.80	0.78
21:R:99:ALA:HB1	21:R:109:MET:CE	2.12	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.11	0.78
33:I:102:VAL:HG12	33:I:106:LYS:HE3	1.62	0.78
16:M:107:ARG:HH11	16:M:107:ARG:HG3	1.47	0.78
1:0:969:G:H1	1:0:999:C:H42	1.32	0.78
26:W:88:THR:HG23	26:W:110:GLN:NE2	1.99	0.78
1:0:2054:A:N3	21:R:128:ARG:NH2	2.31	0.78
1:0:1973:A:H5'	1:0:1973:A:H8	1.49	0.77
31:2:22:PRO:HG2	31:2:25:VAL:HG23	1.67	0.77
17:N:12:ARG:HD3	17:N:18:THR:OG1	1.85	0.77
1:0:2073:G:H5''	40:0:4400:HOH:O	1.83	0.77
12:H:27:LYS:H	12:H:59:HIS:HD2	1.30	0.77
1:0:1118:A:H3'	1:0:1118:A:H8	1.50	0.77
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.66	0.77
5:A:199:HIS:HD2	5:A:201:PHE:H	1.32	0.76
21:R:18:LEU:HD12	21:R:143:VAL:HG11	1.68	0.76
13:J:93:ARG:NH1	13:J:93:ARG:HB3	1.99	0.76
10:F:91:VAL:HG12	10:F:92:GLY:N	2.01	0.76
40:0:5371:HOH:O	13:J:47:THR:HB	1.83	0.76
26:W:122:ARG:HH11	26:W:122:ARG:CG	1.97	0.76
26:W:125:HIS:HD2	26:W:127:GLY:H	1.30	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.50	0.76
14:K:98:VAL:CG1	14:K:102:GLU:HA	2.15	0.76
1:0:560:C:H42	1:0:597:A:H61	1.33	0.76
17:N:11:ARG:HG3	17:N:14:ARG:NH1	2.01	0.76
1:0:1041:U:H5'	40:L:9491:HOH:O	1.85	0.76
8:D:57:THR:HG23	8:D:63:ILE:HA	1.67	0.76
16:M:79:ALA:HB3	16:M:81:ARG:NH1	2.00	0.76
1:0:1667:A:H8	1:0:1667:A:H5'	1.51	0.75
1:0:960:G:H4'	40:0:7866:HOH:O	1.84	0.75
2:9:3014:G:H8	2:9:3014:G:H5'	1.50	0.75
21:R:111:ILE:HG23	21:R:145:LEU:HD11	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.50	0.75
13:J:93:ARG:HH11	13:J:93:ARG:CB	2.00	0.75
1:O:1119:G:N2	1:O:1246:A:C2	2.53	0.75
1:O:2533:C:H5'	1:O:2533:C:H6	1.51	0.75
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.68	0.75
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.75
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.68	0.75
5:A:153:ARG:HH11	5:A:153:ARG:HB2	1.50	0.75
13:J:19:MET:HE1	13:J:132:LEU:HD21	1.69	0.75
25:V:39:ALA:N	25:V:40:PRO:HD2	2.02	0.75
26:W:13:MET:HE1	26:W:18:GLN:HA	1.67	0.75
1:O:1116:U:O2'	1:O:1118:A:H2	1.67	0.74
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.67	0.74
13:J:19:MET:HE3	13:J:132:LEU:HD11	1.68	0.74
14:K:14:LYS:HB2	14:K:45:PRO:HG2	1.70	0.74
32:3:70:ARG:HG2	32:3:77:ALA:HB2	1.69	0.74
5:A:206:ARG:HD3	5:A:206:ARG:H	1.51	0.74
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.69	0.74
1:O:1244:U:OP1	13:J:18:ILE:HD13	1.87	0.74
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.18	0.74
1:O:1118:A:C8	1:O:1118:A:H3'	2.22	0.74
29:Z:46:ARG:HD2	29:Z:59:TYR:HB2	1.68	0.74
1:O:281:U:H2'	1:O:282:C:O4'	1.86	0.74
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.69	0.74
5:A:35:GLY:O	5:A:36:ASP:HB3	1.88	0.74
33:I:78:LEU:HD12	33:I:112:LYS:HZ2	1.53	0.74
17:N:80:SER:HB2	40:N:9333:HOH:O	1.85	0.74
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.70	0.74
21:R:39:THR:HB	21:R:42:GLU:HG3	1.69	0.74
1:O:1377:C:H6	1:O:1377:C:H5'	1.52	0.73
28:Y:154:ARG:HH12	28:Y:155:ARG:HG3	1.53	0.73
1:O:1751:G:H2'	1:O:1752:G:H5''	1.70	0.73
9:E:36:PRO:HD3	13:J:127:ILE:HD12	1.68	0.73
13:J:74:ARG:HB3	13:J:74:ARG:HH11	1.51	0.73
15:L:143:THR:HG22	15:L:144:ASP:H	1.52	0.73
26:W:88:THR:HG22	26:W:89:ASP:N	2.03	0.73
1:O:1206:U:H6	1:O:1206:U:H5'	1.52	0.73
33:I:99:ASP:OD1	33:I:138:THR:HB	1.89	0.73
22:S:57:THR:HG22	22:S:59:ASP:H	1.54	0.73
32:3:65:THR:HG22	32:3:67:LEU:HG	1.69	0.73
7:C:236:THR:HG22	7:C:239:ALA:N	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:567:U:H5''	40:W:5817:HOH:O	1.88	0.73
1:0:111:C:O2'	30:1:20:ARG:HG2	1.88	0.73
25:V:1:THR:HG23	25:V:2:VAL:H	1.54	0.73
26:W:137:GLN:HE21	26:W:141:HIS:CE1	2.07	0.73
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.73
23:T:49:GLU:HB3	23:T:59:GLU:HG2	1.71	0.73
16:M:69:LYS:O	16:M:73:ARG:NH2	2.22	0.72
18:O:32:ARG:HD3	18:O:32:ARG:O	1.87	0.72
1:0:506:G:H22	1:0:509:A:H5''	1.53	0.72
1:0:1118:A:H62	1:0:1244:U:H3	1.35	0.72
1:0:870:G:C2'	1:0:871:G:H5''	2.18	0.72
1:0:656:G:H5'	18:O:3:THR:HB	1.71	0.72
1:0:2890:A:H1'	24:U:56:ARG:NH2	2.04	0.72
15:L:143:THR:HG22	15:L:144:ASP:N	2.05	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.72
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.05	0.72
1:0:545:G:H8	1:0:545:G:H5'	1.55	0.71
19:P:115:SER:H	19:P:118:GLN:NE2	1.88	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.90	0.71
14:K:74:VAL:CG1	14:K:113:ILE:HG12	2.19	0.71
14:K:81:ARG:HB2	14:K:87:ARG:NH1	2.04	0.71
1:0:2851:G:H2'	1:0:2852:A:H5'	1.72	0.71
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.71	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.91	0.71
8:D:58:VAL:HG12	8:D:60:GLU:HG2	1.72	0.71
33:I:110:GLU:HA	33:I:113:HIS:NE2	2.06	0.71
10:F:58:GLU:OE1	16:M:27:ARG:NH2	2.23	0.71
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.71	0.71
13:J:74:ARG:NH1	13:J:76:ASP:HB2	2.06	0.71
14:K:29:LEU:HB3	14:K:55:VAL:CG1	2.19	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.72	0.71
1:0:1299:G:O6	15:L:6:ARG:HD3	1.91	0.71
28:Y:165:GLU:HB3	40:Y:9390:HOH:O	1.90	0.71
1:0:1701:A:H4'	1:0:1702:U:H5''	1.73	0.70
40:0:7889:HOH:O	6:B:211:THR:HG21	1.91	0.70
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.26	0.70
16:M:31:TRP:HA	16:M:34:GLU:HG3	1.72	0.70
7:C:236:THR:CG2	7:C:239:ALA:H	2.04	0.70
1:0:2364:A:H5''	20:Q:15:LYS:HD3	1.73	0.70
1:0:962:C:H1'	17:N:5:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:77:VAL:HG21	10:F:83:LEU:HD13	1.74	0.70
26:W:80:ASP:O	26:W:84:VAL:HG23	1.90	0.70
10:F:96:ALA:HA	40:F:3111:HOH:O	1.91	0.70
12:H:21:THR:O	12:H:120:ILE:HD12	1.92	0.70
19:P:115:SER:N	19:P:118:GLN:HE21	1.89	0.70
27:X:74:ALA:HB2	27:X:85:VAL:HG13	1.72	0.70
16:M:79:ALA:HB3	16:M:81:ARG:HH12	1.57	0.70
7:C:132:ASP:HB3	40:C:9172:HOH:O	1.91	0.70
33:I:132:CYS:HB3	33:I:137:VAL:HB	1.74	0.70
5:A:33:GLU:CD	5:A:33:GLU:H	1.93	0.70
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.04	0.70
17:N:17:ARG:HB3	17:N:17:ARG:HH11	1.57	0.70
19:P:59:ARG:NH2	19:P:66:GLN:HE22	1.89	0.70
30:1:25:LYS:HD2	31:2:48:ASP:HA	1.72	0.70
6:B:275:GLY:O	6:B:291:ASP:HA	1.91	0.70
23:T:71:VAL:HG11	23:T:90:PRO:CB	2.21	0.70
33:I:78:LEU:HD12	33:I:112:LYS:NZ	2.07	0.69
26:W:52:VAL:HG22	26:W:53:ALA:H	1.57	0.69
1:0:1160:G:H5'	1:0:1161:A:C5'	2.18	0.69
31:2:18:ASN:HD21	31:2:40:ARG:N	1.89	0.69
30:1:28:HIS:CD2	30:1:31:LYS:HG3	2.27	0.69
10:F:37:THR:O	10:F:41:GLU:HG3	1.93	0.69
1:0:1771:U:H5'	29:Z:20:ARG:NH2	2.07	0.69
1:0:542:A:C8	1:0:542:A:H5'	2.22	0.69
1:0:481:U:H5''	40:0:6167:HOH:O	1.92	0.69
6:B:125:GLU:O	6:B:129:ARG:HG3	1.93	0.69
1:0:2491:G:H1'	40:0:7335:HOH:O	1.93	0.69
22:S:77:VAL:O	22:S:80:ARG:HG2	1.92	0.69
28:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.92	0.69
5:A:51:ARG:HB2	40:A:9591:HOH:O	1.93	0.69
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.74	0.69
12:H:56:GLN:NE2	12:H:126:ARG:HE	1.90	0.69
26:W:13:MET:HE3	26:W:17:ILE:HG22	1.74	0.69
26:W:88:THR:HG22	26:W:89:ASP:H	1.57	0.69
1:0:380:A:OP2	16:M:9:ARG:HD2	1.93	0.69
8:D:172:VAL:HG12	8:D:173:GLU:N	2.07	0.69
1:0:1474:C:C6	1:0:1474:C:H5'	2.26	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.74	0.69
18:O:32:ARG:NE	18:O:35:LYS:HD2	2.08	0.69
1:0:2749:U:H5'	40:0:8429:HOH:O	1.92	0.68
26:W:122:ARG:NH2	26:W:154:ARG:HG2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:76:ARG:HH11	27:X:76:ARG:HG3	1.57	0.68
1:O:871:G:C8	1:O:871:G:C5'	2.70	0.68
26:W:130:HIS:O	26:W:136:GLY:HA3	1.93	0.68
16:M:107:ARG:NH1	16:M:107:ARG:HG3	2.05	0.68
6:B:238:ASN:HD22	6:B:240:GLY:N	1.92	0.68
14:K:23:ASN:HD21	14:K:107:THR:HB	1.58	0.68
15:L:67:ARG:O	15:L:71:GLU:HG3	1.93	0.68
33:I:134:SER:O	33:I:135:LEU:HD23	1.93	0.68
21:R:18:LEU:HD12	21:R:143:VAL:CG1	2.23	0.68
26:W:137:GLN:NE2	26:W:141:HIS:HE1	1.90	0.68
26:W:81:ASP:OD1	26:W:92:ASP:HB2	1.94	0.68
7:C:2:GLN:HB3	40:C:9195:HOH:O	1.94	0.68
9:E:6:GLU:HA	9:E:46:THR:HG22	1.74	0.68
13:J:131:THR:HG22	13:J:134:GLU:H	1.56	0.68
1:O:1201:C:H2'	1:O:1202:A:H5'	1.74	0.68
12:H:56:GLN:NE2	12:H:93:GLN:HG2	2.08	0.68
14:K:81:ARG:HD3	14:K:87:ARG:NH1	2.08	0.68
19:P:91:LYS:O	19:P:95:GLU:HG3	1.93	0.68
1:O:1116:U:O2'	1:O:1118:A:C2	2.46	0.67
13:J:74:ARG:HH12	13:J:76:ASP:HB2	1.60	0.67
17:N:62:HIS:HB3	17:N:65:ASP:OD1	1.95	0.67
1:O:1182:C:H1'	1:O:1192:A:H8	1.58	0.67
6:B:62:ARG:HA	6:B:65:MET:CE	2.24	0.67
12:H:30:GLN:H	12:H:66:ARG:NH1	1.93	0.67
12:H:59:HIS:HA	12:H:62:LEU:HD23	1.76	0.67
21:R:18:LEU:HB2	21:R:143:VAL:CG1	2.24	0.67
18:O:96:VAL:HG13	18:O:100:GLN:HB2	1.75	0.67
1:O:2908:A:H2'	1:O:2909:G:O4'	1.95	0.67
1:O:1166:A:H1'	1:O:1192:A:C2	2.29	0.67
8:D:159:PRO:O	8:D:163:VAL:HG23	1.94	0.67
27:X:71:ARG:HD3	40:X:2171:HOH:O	1.95	0.67
1:O:1184:C:H1'	40:O:7899:HOH:O	1.93	0.67
1:O:2676:C:H4'	13:J:70:PHE:CE1	2.30	0.67
1:O:2676:C:H4'	13:J:70:PHE:CD1	2.30	0.67
23:T:115:GLU:HG3	23:T:116:ASP:N	2.09	0.67
24:U:5:GLU:HG2	24:U:10:GLY:O	1.95	0.67
1:O:2468:A:H61	32:3:48:ASN:HD21	1.43	0.67
1:O:883:U:H2'	1:O:883:U:O2	1.95	0.67
5:A:199:HIS:CD2	5:A:201:PHE:H	2.11	0.67
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.75	0.67
12:H:27:LYS:N	12:H:59:HIS:HD2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:797:A:C4'	29:Z:10:ARG:N	2.57	0.67
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
26:W:21:LEU:CD2	26:W:48:VAL:HG11	2.19	0.66
1:0:1183:C:H2'	40:0:6739:HOH:O	1.94	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
10:F:13:GLU:OE2	10:F:78:GLU:HG2	1.95	0.66
27:X:71:ARG:HB3	27:X:88:GLU:OE1	1.95	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.95	0.66
1:0:2073:G:OP2	1:0:2490:A:H5'	1.94	0.66
5:A:153:ARG:NH1	5:A:153:ARG:HB2	2.10	0.66
19:P:59:ARG:HH22	19:P:66:GLN:HE22	1.42	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.66
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.76	0.66
28:Y:189:ASN:HA	28:Y:217:ILE:HD11	1.78	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
6:B:140:LEU:HA	40:B:9575:HOH:O	1.95	0.66
28:Y:144:ARG:HH11	28:Y:144:ARG:CG	2.09	0.66
1:0:2505:G:O2'	1:0:2506:A:H5'	1.96	0.66
29:Z:22:SER:O	29:Z:26:VAL:HG23	1.94	0.66
6:B:51:VAL:HG23	6:B:329:TYR:O	1.96	0.66
26:W:68:THR:HG23	26:W:69:ARG:HG2	1.78	0.66
10:F:58:GLU:CD	16:M:27:ARG:HH22	1.97	0.66
1:0:1116:U:H3	1:0:1246:A:H62	1.44	0.65
1:0:1159:G:H21	1:0:1189:A:H8	1.44	0.65
6:B:254:GLN:HG2	6:B:255:GLY:N	2.10	0.65
22:S:10:VAL:HG11	25:V:36:ALA:HA	1.78	0.65
6:B:53:LEU:HD11	6:B:327:VAL:HG22	1.77	0.65
13:J:45:VAL:HG11	13:J:121:LEU:HD22	1.79	0.65
18:O:32:ARG:HH21	18:O:35:LYS:NZ	1.94	0.65
19:P:9:LEU:O	19:P:13:VAL:HG12	1.97	0.65
23:T:41:ARG:HG2	23:T:41:ARG:HH11	1.59	0.65
1:0:1687:C:O2	30:1:9:GLY:HA2	1.97	0.65
6:B:16:ARG:NH1	40:B:9612:HOH:O	2.28	0.65
7:C:162:VAL:HG22	7:C:232:LEU:HD21	1.77	0.65
15:L:73:VAL:HG23	15:L:74:THR:H	1.62	0.65
23:T:49:GLU:OE2	23:T:97:ARG:HD2	1.95	0.65
28:Y:144:ARG:CZ	40:Y:9409:HOH:O	2.44	0.65
18:O:32:ARG:HH21	18:O:35:LYS:HZ2	1.44	0.65
23:T:32:ARG:NH1	23:T:38:ARG:HH12	1.94	0.65
1:0:1162:G:H1'	33:I:117:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:48:ASP:HB3	40:A:9591:HOH:O	1.95	0.65
12:H:166:SER:HB3	12:H:167:PRO:HD3	1.78	0.65
1:O:2661:U:H3	1:O:2812:A:H62	1.43	0.65
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.79	0.65
1:O:2521:A:OP2	12:H:3:ALA:HB3	1.96	0.65
17:N:48:VAL:CG1	17:N:55:ASP:HB3	2.27	0.65
28:Y:144:ARG:HG3	28:Y:144:ARG:HH11	1.60	0.65
1:O:1175:G:H1'	1:O:1193:A:H2'	1.78	0.65
6:B:307:ARG:NH1	6:B:307:ARG:HG3	2.05	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.41	0.64
1:O:1730:G:H5'	1:O:1731:C:C5	2.31	0.64
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.64
16:M:134:ILE:CG2	16:M:141:ILE:HD13	2.26	0.64
1:O:2896:A:H5''	40:O:6599:HOH:O	1.96	0.64
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.78	0.64
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.97	0.64
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.96	0.64
17:N:139:TRP:HA	17:N:139:TRP:CE3	2.33	0.64
26:W:88:THR:HG23	26:W:110:GLN:HE21	1.61	0.64
26:W:48:VAL:HG12	26:W:48:VAL:O	1.97	0.64
1:O:1209:C:H2'	1:O:1210:G:H8	1.61	0.64
1:O:272:A:H5'	1:O:273:G:OP2	1.97	0.64
16:M:68:ARG:NH2	16:M:73:ARG:HD3	2.13	0.64
18:O:21:SER:OG	18:O:106:PRO:HB2	1.98	0.64
23:T:112:LEU:HD23	23:T:119:ALA:HB3	1.79	0.64
29:Z:42:CYS:SG	29:Z:43:GLY:N	2.70	0.64
1:O:544:G:C2'	1:O:545:G:H5''	2.27	0.64
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.78	0.64
6:B:41:PHE:CD2	6:B:190:MET:HE3	2.32	0.64
1:O:1878:G:H1'	40:O:6620:HOH:O	1.97	0.64
1:O:381:G:H5''	40:M:9373:HOH:O	1.97	0.64
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.80	0.64
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.78	0.64
13:J:75:PRO:HG2	13:J:105:LEU:HD21	1.79	0.64
24:U:45:GLU:HB2	24:U:48:ASN:ND2	2.12	0.64
31:2:18:ASN:ND2	31:2:40:ARG:H	1.93	0.64
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.61	0.64
14:K:49:LEU:HD12	14:K:80:ILE:HG21	1.80	0.64
16:M:187:LEU:CD2	16:M:194:ALA:HB3	2.28	0.64
20:Q:75:ILE:HD13	20:Q:84:ILE:HD11	1.78	0.64
1:O:709:G:O2'	18:O:25:VAL:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:9:LYS:HE3	23:T:13:ARG:HH12	1.58	0.64
26:W:108:ARG:HG3	26:W:114:PRO:HG3	1.80	0.64
33:I:125:ALA:O	33:I:129:VAL:HG23	1.97	0.64
1:O:2064:U:H5'	1:O:2652:U:H4'	1.80	0.64
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.26	0.64
14:K:75:ARG:HD3	14:K:112:PRO:O	1.98	0.64
21:R:111:ILE:HG23	21:R:145:LEU:CD1	2.28	0.64
7:C:157:LEU:HD13	7:C:166:ILE:HD11	1.81	0.63
12:H:166:SER:CB	12:H:167:PRO:CD	2.75	0.63
33:I:110:GLU:HA	33:I:113:HIS:CE1	2.33	0.63
2:9:3039:U:HO2'	2:9:3042:C:H5	1.44	0.63
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.63
7:C:77:ALA:O	7:C:78:ARG:HG3	1.97	0.63
28:Y:126:PRO:HG2	28:Y:128:PHE:CE1	2.33	0.63
1:O:1427:A:H61	1:O:1440:U:H1'	1.62	0.63
1:O:263:U:O4'	10:F:59:ILE:HD13	1.99	0.63
5:A:36:ASP:OD2	5:A:85:SER:HB2	1.98	0.63
17:N:164:ASP:CG	17:N:167:ASP:HA	2.18	0.63
33:I:113:HIS:N	33:I:114:PRO:HD2	2.14	0.63
16:M:80:GLY:O	16:M:81:ARG:HD2	1.99	0.63
1:O:447:A:P	23:T:1:SER:HB2	2.38	0.63
1:O:2587:OMU:H5	40:O:7918:HOH:O	1.97	0.63
1:O:88:G:H2'	1:O:89:G:C8	2.34	0.63
25:V:20:LEU:HD22	25:V:60:GLN:HE22	1.63	0.63
1:O:2541:U:H4'	1:O:2542:C:OP1	1.97	0.63
14:K:55:VAL:HG12	14:K:56:SER:N	2.13	0.63
40:O:9739:HOH:O	16:M:82:ARG:HD2	1.98	0.63
2:9:3014:G:C8	2:9:3014:G:H5'	2.33	0.63
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.80	0.63
1:O:2533:C:C6	1:O:2533:C:H5'	2.32	0.62
13:J:90:LYS:HB2	37:J:9302:CL:CL	2.35	0.62
30:1:25:LYS:HD2	31:2:49:GLU:H	1.64	0.62
32:3:38:ARG:HB3	32:3:42:ARG:HH12	1.64	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.15	0.62
30:1:45:ARG:NH2	40:1:9488:HOH:O	2.31	0.62
1:O:1206:U:H2'	1:O:1207:A:O4'	2.00	0.62
1:O:1528:A:H2'	1:O:1529:G:O4'	1.98	0.62
12:H:27:LYS:H	12:H:59:HIS:CD2	2.17	0.62
12:H:40:ALA:HB1	12:H:137:TYR:CE2	2.34	0.62
31:2:22:PRO:HG2	31:2:25:VAL:CG2	2.29	0.62
16:M:164:THR:HG22	16:M:166:ALA:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:4:LEU:HD11	26:W:45:VAL:HG12	1.81	0.62
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.64	0.62
1:0:524:A:H5''	21:R:29:LYS:HD3	1.82	0.62
30:1:10:LYS:HG3	40:1:9492:HOH:O	1.98	0.62
2:9:3029:C:O3'	8:D:138:GLY:HA2	2.00	0.62
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.80	0.62
17:N:139:TRP:HA	17:N:139:TRP:HE3	1.65	0.62
17:N:154:LEU:HG	17:N:155:GLU:H	1.63	0.62
21:R:18:LEU:HB2	21:R:143:VAL:HG13	1.82	0.62
21:R:44:VAL:O	21:R:48:GLU:HG3	2.00	0.62
23:T:71:VAL:HG12	23:T:72:ILE:N	2.15	0.62
26:W:141:HIS:HB2	26:W:146:ILE:HG12	1.80	0.62
27:X:25:ARG:HD3	27:X:64:ALA:O	1.99	0.62
1:0:1183:C:N4	1:0:1184:C:H41	1.98	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
2:9:3051:A:H5'	17:N:160:SER:HB3	1.82	0.62
40:9:4707:HOH:O	17:N:147:ILE:HD12	1.99	0.62
19:P:80:ARG:HG2	19:P:87:ARG:CZ	2.30	0.62
1:0:1118:A:H8	1:0:1119:G:H5''	1.64	0.62
1:0:1328:A:OP1	28:Y:169:ARG:HD2	2.00	0.62
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.15	0.62
12:H:20:ILE:HG23	12:H:120:ILE:HD11	1.81	0.62
16:M:164:THR:HG22	16:M:167:GLY:H	1.65	0.62
1:0:470:U:O2'	30:1:16:HIS:HD2	1.83	0.62
2:9:3029:C:H2'	2:9:3030:C:H5'	1.81	0.62
11:G:12:ILE:N	11:G:13:PRO:CD	2.63	0.62
19:P:64:GLU:HG2	40:P:165:HOH:O	2.00	0.62
29:Z:72:GLU:OE1	29:Z:77:LYS:HE2	1.99	0.62
30:1:8:GLN:HE22	30:1:11:LYS:NZ	1.97	0.61
6:B:141:ARG:HD2	6:B:163:GLU:OE2	1.99	0.61
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.81	0.61
13:J:19:MET:CE	13:J:132:LEU:HD11	2.29	0.61
14:K:109:LEU:HD13	14:K:113:ILE:HD11	1.81	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
6:B:225:GLY:HA3	40:B:9562:HOH:O	2.00	0.61
24:U:14:GLU:O	24:U:17:THR:HB	2.01	0.61
28:Y:112:GLU:OE1	28:Y:112:GLU:HA	2.00	0.61
28:Y:187:VAL:HG12	28:Y:205:ILE:HA	1.81	0.61
1:0:2807:U:P	6:B:27:ASN:HD21	2.24	0.61
1:0:485:A:N3	1:0:487:G:H5''	2.14	0.61
30:1:25:LYS:HD2	31:2:49:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:11:ARG:CG	17:N:14:ARG:HH12	2.09	0.61
24:U:52:THR:HG22	24:U:54:THR:N	2.16	0.61
1:O:289:G:N2	1:O:363:A:H2	1.94	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.15	0.61
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.00	0.61
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.61
6:B:175:LEU:O	6:B:175:LEU:HD23	2.00	0.61
8:D:59:GLY:O	8:D:61:PHE:N	2.33	0.61
25:V:56:ILE:HG22	25:V:60:GLN:HE21	1.66	0.61
6:B:217:ARG:HG3	6:B:257:THR:HG22	1.80	0.61
27:X:43:VAL:HG12	27:X:44:ASP:N	2.16	0.61
1:O:282:C:H1'	1:O:368:C:N4	2.15	0.61
8:D:136:ARG:NH1	8:D:157:LEU:HA	2.15	0.61
9:E:35:TYR:HA	13:J:127:ILE:HD12	1.82	0.61
18:O:25:VAL:HG23	18:O:26:TRP:N	2.16	0.61
1:O:553:G:P	28:Y:204:ARG:HH22	2.23	0.61
1:O:280:C:H2'	1:O:281:U:O4'	2.01	0.61
5:A:191:GLY:HA2	5:A:194:MET:HE3	1.81	0.61
17:N:164:ASP:OD1	17:N:167:ASP:HA	2.01	0.61
20:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.00	0.61
6:B:329:TYR:CE2	24:U:15:PRO:HG2	2.35	0.61
27:X:66:THR:HG23	27:X:67:PRO:HD2	1.83	0.61
5:A:69:LEU:HD23	5:A:107:ASN:HB2	1.81	0.61
1:O:263:U:O2	16:M:42:ARG:HD2	2.01	0.61
1:O:2563:U:H2'	1:O:2565:C:O5'	2.00	0.61
32:3:65:THR:HG23	32:3:88:LEU:HD22	1.83	0.61
6:B:102:THR:CG2	6:B:182:VAL:HG12	2.31	0.61
8:D:13:MET:HA	8:D:137:PRO:HG2	1.83	0.61
17:N:132:ASN:O	17:N:135:VAL:HG12	2.00	0.61
1:O:475:G:OP1	7:C:73:LEU:HD22	2.01	0.60
5:A:81:GLN:HB2	5:A:92:ASN:HD21	1.62	0.60
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.36	0.60
8:D:58:VAL:CG1	8:D:60:GLU:HG2	2.30	0.60
17:N:61:ALA:HB3	17:N:88:ALA:HB2	1.83	0.60
1:O:2769:C:C2'	1:O:2770:G:H5'	2.32	0.60
5:A:123:GLY:HA3	5:A:162:GLY:HA2	1.83	0.60
7:C:136:VAL:HG22	7:C:137:PRO:HA	1.83	0.60
9:E:68:HIS:O	9:E:72:MET:HG3	2.00	0.60
1:O:902:G:N7	15:L:18:HIS:HD2	1.99	0.60
26:W:21:LEU:HD22	26:W:26:ILE:CD1	2.31	0.60
7:C:139:VAL:HG13	40:C:9254:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:129:VAL:O	33:I:129:VAL:HG12	2.01	0.60
33:I:92:PRO:C	33:I:94:GLU:H	2.05	0.60
16:M:71:SER:HB2	16:M:92:THR:HG22	1.83	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.36	0.60
1:0:2426:G:H1'	40:0:6592:HOH:O	2.00	0.60
1:0:338:C:H4'	7:C:174:ILE:CD1	2.32	0.60
16:M:183:THR:HG22	16:M:194:ALA:HB1	1.82	0.60
25:V:39:ALA:N	25:V:40:PRO:CD	2.64	0.60
28:Y:187:VAL:HB	28:Y:203:VAL:HG22	1.83	0.60
1:0:2365:G:H5''	40:Q:6597:HOH:O	2.01	0.60
1:0:848:C:H5'	40:0:7714:HOH:O	2.02	0.60
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.83	0.60
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.02	0.60
8:D:94:ALA:HA	8:D:174:VAL:HA	1.83	0.60
1:0:1201:C:H5''	40:0:6728:HOH:O	2.01	0.60
1:0:156:C:H5''	16:M:171:ARG:CD	2.28	0.60
2:9:3013:A:O2'	2:9:3014:G:H5''	2.01	0.60
1:0:1943:C:H4'	5:A:211:LYS:O	2.02	0.60
10:F:58:GLU:HA	10:F:61:MET:HE2	1.82	0.60
1:0:2346:C:O2'	8:D:52:THR:HG21	2.00	0.60
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.60
22:S:57:THR:HG22	22:S:59:ASP:N	2.16	0.60
1:0:796:A:HO2'	29:Z:10:ARG:N	1.98	0.60
1:0:2427:C:OP2	32:3:84:ARG:HD2	2.00	0.60
2:9:3004:G:H21	17:N:44:ARG:NH1	2.00	0.60
26:W:21:LEU:HB3	26:W:26:ILE:HG12	1.83	0.60
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.60
8:D:135:VAL:HG22	8:D:136:ARG:N	2.17	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.83	0.60
10:F:46:GLU:O	10:F:73:PRO:HD2	2.02	0.60
26:W:125:HIS:CD2	26:W:127:GLY:H	2.16	0.60
1:0:236:A:H8	1:0:236:A:OP1	1.84	0.60
33:I:113:HIS:CE1	33:I:121:LEU:HD22	2.36	0.60
1:0:1164:U:OP1	33:I:74:PRO:HA	2.01	0.60
14:K:113:ILE:HG22	14:K:114:ALA:N	2.16	0.60
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.82	0.59
13:J:75:PRO:HD3	13:J:136:SER:OG	2.01	0.59
19:P:16:VAL:HG12	19:P:17:GLY:N	2.17	0.59
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.84	0.59
6:B:71:VAL:HG11	6:B:296:LEU:HD22	1.83	0.59
12:H:170:ASN:N	12:H:170:ASN:HD22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:39:ALA:C	25:V:41:GLU:H	2.06	0.59
25:V:56:ILE:O	25:V:60:GLN:HG3	2.02	0.59
1:0:396:U:O2'	1:0:418:C:H4'	2.02	0.59
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.83	0.59
40:0:4936:HOH:O	16:M:83:SER:HB3	2.01	0.59
25:V:11:MET:HB3	25:V:15:GLU:HB2	1.84	0.59
28:Y:154:ARG:NH1	28:Y:155:ARG:HG3	2.16	0.59
5:A:153:ARG:CB	5:A:153:ARG:HH11	2.15	0.59
17:N:162:ASP:HA	40:N:9328:HOH:O	2.03	0.59
26:W:119:HIS:HD2	26:W:120:PRO:O	1.86	0.59
6:B:62:ARG:HA	6:B:65:MET:HE3	1.83	0.59
33:I:106:LYS:O	33:I:110:GLU:HG3	2.02	0.59
1:0:1555:G:H4'	1:0:1630:A:H2	1.68	0.59
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.59
1:0:462:A:N3	31:2:37:HIS:HB3	2.18	0.59
10:F:91:VAL:CG1	10:F:92:GLY:H	2.10	0.59
33:I:105:VAL:HG11	33:I:129:VAL:HG22	1.84	0.59
23:T:38:ARG:NH1	40:T:6217:HOH:O	2.35	0.59
31:2:36:ASN:HB3	31:2:39:ARG:NE	2.17	0.59
7:C:236:THR:H	7:C:239:ALA:HB3	1.68	0.59
1:0:1946:C:H2'	1:0:1971:G:C8	2.37	0.59
5:A:33:GLU:O	5:A:34:ASP:HB2	2.02	0.59
7:C:233:THR:HG22	7:C:234:VAL:N	2.17	0.59
17:N:23:ARG:HH11	17:N:23:ARG:HG2	1.67	0.59
1:0:1187:U:HO2'	1:0:1189:A:H2	1.51	0.58
1:0:1418:U:OP1	31:2:42:TRP:HB3	2.02	0.58
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.58
1:0:2649:A:H5'	1:0:2649:A:H8	1.67	0.58
1:0:316:A:H5'	23:T:54:ASP:OD2	2.02	0.58
5:A:36:ASP:C	5:A:38:ILE:H	2.06	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.58
1:0:797:A:H4'	29:Z:10:ARG:N	2.18	0.58
6:B:265:LEU:HD21	6:B:316:ARG:HD3	1.85	0.58
12:H:46:GLN:HE21	12:H:137:TYR:HE2	1.51	0.58
14:K:62:PRO:HG3	14:K:65:ARG:HH21	1.66	0.58
25:V:12:THR:HG22	25:V:15:GLU:CG	2.21	0.58
1:0:343:C:O2'	1:0:344:C:H5'	2.02	0.58
6:B:254:GLN:HG2	6:B:255:GLY:H	1.68	0.58
32:3:55:VAL:HG22	40:3:9444:HOH:O	2.02	0.58
16:M:24:GLN:NE2	16:M:27:ARG:HH11	2.02	0.58
29:Z:11:SER:CB	29:Z:23:ARG:HB2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1973:A:H5'	1:0:1973:A:C8	2.37	0.58
6:B:145:HIS:HD2	6:B:146:THR:O	1.85	0.58
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.85	0.58
1:0:1163:G:H5'	33:I:115:ASP:O	2.04	0.58
14:K:109:LEU:CD1	14:K:113:ILE:HD11	2.32	0.58
15:L:148:GLU:HB2	40:L:9486:HOH:O	2.03	0.58
16:M:164:THR:HG22	16:M:166:ALA:H	1.68	0.58
17:N:143:ARG:HH21	17:N:169:PRO:HB2	1.68	0.58
17:N:78:MET:HB2	17:N:79:PRO:HD3	1.85	0.58
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.58
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.58
6:B:87:TYR:O	6:B:138:GLY:N	2.27	0.58
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
14:K:32:ILE:HD11	14:K:56:SER:HB3	1.86	0.58
8:D:50:VAL:O	8:D:71:ALA:HA	2.04	0.58
1:0:2081:A:H4'	13:J:69:TYR:CE1	2.39	0.58
15:L:133:VAL:HA	40:L:9470:HOH:O	2.04	0.58
24:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
7:C:168:ARG:NH2	7:C:190:ALA:O	2.36	0.58
12:H:58:ARG:HG3	12:H:58:ARG:HH11	1.68	0.58
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
1:0:969:G:H1	1:0:999:C:N4	2.01	0.58
6:B:85:ARG:NH1	40:B:9629:HOH:O	2.37	0.58
13:J:47:THR:HG22	13:J:48:GLY:N	2.17	0.58
26:W:38:THR:HG22	26:W:39:ASP:N	2.19	0.58
7:C:242:GLU:HB2	40:C:9192:HOH:O	2.04	0.58
17:N:115:VAL:HG22	40:N:9354:HOH:O	2.04	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.19	0.57
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.86	0.57
1:0:474:C:O3'	7:C:73:LEU:HD21	2.03	0.57
8:D:25:MET:CE	8:D:37:ALA:HB1	2.33	0.57
9:E:81:GLU:HG2	9:E:134:SER:CB	2.33	0.57
10:F:60:VAL:HG12	10:F:60:VAL:O	2.04	0.57
12:H:30:GLN:H	12:H:66:ARG:HH11	1.51	0.57
1:0:2443:C:O3'	15:L:56:LYS:HE3	2.04	0.57
32:3:60:LYS:HG3	32:3:61:PRO:HD2	1.85	0.57
6:B:5:ARG:HH11	6:B:8:LYS:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:54:VAL:HG11	13:J:138:THR:HG21	1.86	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.57
17:N:110:THR:HB	17:N:113:SER:OG	2.04	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.65	0.57
11:G:24:VAL:O	11:G:28:GLU:HB2	2.04	0.57
18:O:25:VAL:HG23	18:O:26:TRP:H	1.69	0.57
25:V:64:GLY:O	25:V:65:ASP:HB2	2.03	0.57
5:A:179:MET:HG2	5:A:186:TRP:CB	2.35	0.57
5:A:88:ILE:HG22	5:A:88:ILE:O	2.03	0.57
8:D:138:GLY:N	40:D:7597:HOH:O	2.36	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1878:G:HO2'	1:0:1879:U:H6	1.49	0.57
1:0:2541:U:H3'	1:0:2541:U:H6	1.70	0.57
6:B:321:PRO:HA	40:B:9650:HOH:O	2.03	0.57
13:J:74:ARG:O	13:J:78:ILE:HG12	2.03	0.57
1:0:1666:C:O2'	1:0:1667:A:H5''	2.04	0.57
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.86	0.57
25:V:55:ARG:O	25:V:59:ILE:HG12	2.04	0.57
27:X:37:LEU:CD1	27:X:85:VAL:HG21	2.25	0.57
6:B:17:LYS:O	6:B:260:HIS:HD2	1.87	0.57
8:D:170:TYR:O	8:D:171:ASP:HB3	2.03	0.57
26:W:139:GLY:O	26:W:141:HIS:HD2	1.87	0.57
29:Z:30:GLU:HA	29:Z:33:MET:HE3	1.87	0.57
1:0:1352:A:O2'	1:0:1353:C:OP1	2.22	0.57
5:A:165:THR:HG22	40:A:9604:HOH:O	2.05	0.57
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.57
1:0:1625:U:H4'	40:0:5209:HOH:O	2.05	0.57
1:0:1919:A:H4'	40:0:5385:HOH:O	2.05	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.57
1:0:462:A:C2	31:2:37:HIS:HB3	2.39	0.57
2:9:3008:G:O6	17:N:11:ARG:NH1	2.33	0.57
16:M:77:HIS:HD2	16:M:79:ALA:O	1.88	0.57
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.35	0.56
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.56
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.86	0.56
33:I:128:VAL:C	33:I:130:GLY:H	2.08	0.56
1:0:20:G:H21	21:R:117:HIS:HD2	1.53	0.56
26:W:88:THR:CG2	26:W:89:ASP:H	2.18	0.56
1:0:1684:A:H1'	31:2:43:ARG:HH22	1.70	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.69	0.56
1:0:2824:C:H5''	1:0:2825:C:H5'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.39	0.56
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.04	0.56
1:0:2815:G:N7	13:J:80:LYS:NZ	2.53	0.56
16:M:60:VAL:C	16:M:61:ILE:HD12	2.25	0.56
24:U:17:THR:CG2	24:U:18:GLY:N	2.67	0.56
26:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.56
1:0:1189:A:H1'	1:0:1209:C:O4'	2.05	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.56
13:J:99:GLU:HA	40:J:7377:HOH:O	2.05	0.56
14:K:114:ALA:HB3	14:K:117:VAL:HG23	1.86	0.56
21:R:9:ASP:O	21:R:13:THR:HB	2.05	0.56
28:Y:235:GLU:CD	28:Y:235:GLU:N	2.52	0.56
1:0:1426:C:H2'	40:0:3203:HOH:O	2.05	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
8:D:49:PRO:HA	8:D:73:VAL:HG22	1.87	0.56
24:U:17:THR:HG22	24:U:18:GLY:N	2.19	0.56
26:W:4:LEU:O	26:W:32:CYS:HA	2.05	0.56
28:Y:187:VAL:HB	28:Y:203:VAL:CG2	2.35	0.56
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.56
1:0:757:C:OP1	15:L:27:ARG:HD2	2.05	0.56
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.87	0.56
17:N:169:PRO:O	17:N:172:PHE:HB3	2.06	0.56
19:P:10:ALA:HA	19:P:13:VAL:CG1	2.35	0.56
26:W:122:ARG:CG	26:W:122:ARG:NH1	2.64	0.56
29:Z:29:ILE:O	29:Z:33:MET:HB2	2.06	0.56
1:0:2346:C:O5'	1:0:2346:C:H6	1.87	0.56
1:0:93:C:H5''	25:V:1:THR:HB	1.88	0.56
40:0:9699:HOH:O	6:B:214:PRO:HD2	2.04	0.56
15:L:121:ILE:HG12	15:L:141:GLU:HB2	1.87	0.56
19:P:40:VAL:O	19:P:44:VAL:HG23	2.05	0.56
1:0:1118:A:C8	1:0:1119:G:H5''	2.40	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
1:0:538:C:OP2	28:Y:134:HIS:HE1	1.89	0.56
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.35	0.56
1:0:2721:U:H4'	14:K:87:ARG:HG3	1.87	0.56
40:0:3149:HOH:O	19:P:81:LYS:HG2	2.06	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.88	0.56
1:0:920:C:H4'	1:0:921:G:C2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:57:ALA:HB1	5:A:65:ARG:HE	1.69	0.56
8:D:103:ASN:ND2	8:D:134:LEU:H	2.03	0.56
1:0:244:C:OP2	10:F:38:LYS:HE3	2.05	0.56
40:0:8433:HOH:O	12:H:154:TYR:HB2	2.06	0.56
15:L:136:ALA:HB3	40:L:9470:HOH:O	2.06	0.56
1:0:2421:G:H1'	40:0:4280:HOH:O	2.06	0.56
1:0:1594:C:OP2	19:P:120:ARG:HD2	2.06	0.56
21:R:18:LEU:HG	21:R:91:LEU:HD13	1.88	0.56
26:W:149:LEU:HG	26:W:153:MET:CE	2.36	0.56
27:X:30:MET:HE1	27:X:58:ALA:HB3	1.88	0.56
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.56
1:0:949:U:H4'	20:Q:95:GLU:HA	1.86	0.56
8:D:135:VAL:HG21	8:D:139:TYR:CG	2.41	0.56
8:D:76:ARG:O	8:D:77:ASP:HB2	2.06	0.56
1:0:2032:U:H2'	1:0:2033:G:H5''	1.88	0.55
1:0:120:A:H5'	30:1:20:ARG:HH21	1.71	0.55
6:B:297:VAL:HB	40:B:9600:HOH:O	2.05	0.55
14:K:34:VAL:HG22	14:K:47:ALA:HB2	1.86	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
8:D:135:VAL:HG22	8:D:136:ARG:H	1.71	0.55
1:0:1060:C:H6	1:0:1060:C:H5'	1.72	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:621:C:H5'	28:Y:132:ASP:OD2	2.07	0.55
2:9:3024:U:H3'	2:9:3025:G:H5'	1.88	0.55
8:D:24:HIS:HB2	8:D:72:LYS:CB	2.35	0.55
1:0:1748:U:H4'	40:0:7953:HOH:O	2.04	0.55
1:0:2481:G:H5''	40:0:5094:HOH:O	2.05	0.55
5:A:125:ASN:HB3	5:A:158:VAL:HG12	1.88	0.55
6:B:305:ASP:O	6:B:306:LYS:HB2	2.07	0.55
25:V:1:THR:HG23	25:V:2:VAL:N	2.20	0.55
1:0:2416:G:O2'	17:N:25:ARG:HG2	2.05	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.37	0.55
1:0:1180:U:O2'	33:I:92:PRO:HD2	2.05	0.55
1:0:164:G:H4'	15:L:30:ARG:HD3	1.89	0.55
17:N:86:LEU:HD12	17:N:125:ALA:HB2	1.88	0.55
1:0:1205:U:H2'	1:0:1206:U:H5'	1.89	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.55
1:0:407:A:H2'	1:0:408:A:C8	2.41	0.55
12:H:166:SER:HB3	12:H:167:PRO:CD	2.35	0.55
1:0:834:G:H4'	1:0:835:U:OP2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:57:LYS:HE2	16:M:140:ALA:O	2.06	0.55
1:O:2851:G:O2'	1:O:2852:A:H5'	2.05	0.55
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.42	0.55
16:M:34:GLU:HB3	16:M:38:GLU:HG3	1.89	0.55
1:O:121:U:OP2	31:2:10:ARG:NH2	2.35	0.55
1:O:137:U:H2'	1:O:139:C:C5	2.42	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.37	0.55
1:O:1168:C:H5''	33:I:87:THR:CG2	2.37	0.55
16:M:120:VAL:HG11	16:M:130:GLU:HG3	1.88	0.55
29:Z:37:HIS:O	29:Z:45:ASP:HA	2.07	0.55
1:O:2591:C:H2'	1:O:2592:G:O4'	2.06	0.55
6:B:5:ARG:NH1	6:B:8:LYS:HE2	2.22	0.55
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.07	0.55
13:J:130:VAL:HG12	13:J:131:THR:N	2.22	0.55
13:J:76:ASP:HA	40:J:5907:HOH:O	2.06	0.55
15:L:10:SER:O	15:L:11:ARG:HB3	2.06	0.55
23:T:63:ILE:HD11	23:T:75:GLU:HB2	1.89	0.55
27:X:78:GLU:HG2	27:X:79:GLU:OE2	2.07	0.55
27:X:9:VAL:HG22	27:X:88:GLU:OE2	2.07	0.55
1:O:1595:G:O2'	1:O:1596:U:H5'	2.06	0.54
1:O:2270:G:H4'	5:A:223:ARG:HH12	1.72	0.54
6:B:40:GLY:HA3	40:B:9641:HOH:O	2.06	0.54
14:K:30:LYS:O	14:K:55:VAL:HG13	2.06	0.54
17:N:32:PRO:HD2	17:N:99:GLU:O	2.06	0.54
28:Y:108:ASP:N	28:Y:108:ASP:OD1	2.36	0.54
28:Y:154:ARG:HH12	28:Y:155:ARG:CG	2.20	0.54
6:B:221:GLN:HE22	14:K:42:ASN:HD22	1.55	0.54
29:Z:53:GLY:HA2	29:Z:67:GLY:O	2.06	0.54
1:O:2670:G:O2'	1:O:2671:U:H5'	2.07	0.54
8:D:24:HIS:HB2	8:D:72:LYS:HB3	1.89	0.54
14:K:4:LEU:CD2	14:K:116:GLU:HB3	2.36	0.54
28:Y:133:HIS:HD2	40:Y:9381:HOH:O	1.90	0.54
1:O:1202:A:H2'	1:O:1203:G:O4'	2.08	0.54
5:A:65:ARG:C	5:A:66:ARG:HG3	2.26	0.54
1:O:1451:C:H5'	1:O:1505:U:C5	2.43	0.54
1:O:2414:A:H2'	1:O:2415:A:C8	2.43	0.54
5:A:192:VAL:HB	40:A:9580:HOH:O	2.06	0.54
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.72	0.54
6:B:321:PRO:HG3	40:B:9595:HOH:O	2.06	0.54
7:C:1:MET:HG2	7:C:2:GLN:N	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:87:THR:O	18:O:91:GLN:HG3	2.07	0.54
1:O:1189:A:O2'	1:O:1208:C:H2'	2.07	0.54
2:9:3107:C:H5	40:9:3167:HOH:O	1.90	0.54
1:O:1853:C:OP1	5:A:231:LYS:HG3	2.08	0.54
9:E:144:THR:O	9:E:148:ILE:HG13	2.08	0.54
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.36	0.54
15:L:53:ARG:NH2	15:L:57:VAL:HG12	2.22	0.54
16:M:164:THR:CG2	16:M:165:GLY:N	2.70	0.54
1:O:291:C:H2'	1:O:292:G:O4'	2.08	0.54
9:E:145:ALA:HB1	9:E:168:ILE:HD11	1.88	0.54
1:O:2748:G:H2'	40:0:7972:HOH:O	2.07	0.54
1:O:95:A:H5''	1:O:97:G:O4'	2.08	0.54
40:0:7978:HOH:O	16:M:91:ILE:HG12	2.07	0.54
18:O:47:ARG:HG3	18:O:47:ARG:HH11	1.73	0.54
1:O:1773:G:C8	29:Z:16:ALA:HA	2.43	0.54
29:Z:57:CYS:SG	29:Z:59:TYR:HB3	2.48	0.54
1:O:441:A:H1'	1:O:442:A:N7	2.22	0.54
1:O:482:G:H4'	1:O:508:A:N1	2.23	0.54
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.73	0.54
18:O:97:SER:H	18:O:100:GLN:NE2	2.05	0.54
28:Y:189:ASN:HD22	28:Y:189:ASN:C	2.11	0.54
1:O:1377:C:H5'	1:O:1377:C:C6	2.38	0.54
1:O:328:U:O4'	7:C:202:THR:HG22	2.08	0.54
1:O:603:A:H5''	1:O:604:G:OP1	2.08	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.73	0.54
8:D:154:LYS:HD2	8:D:154:LYS:H	1.73	0.54
33:I:113:HIS:HE1	33:I:121:LEU:HD22	1.70	0.54
16:M:187:LEU:HD23	16:M:194:ALA:HB3	1.89	0.54
23:T:32:ARG:NH1	23:T:38:ARG:NH1	2.54	0.54
1:O:1847:A:OP1	5:A:175:LYS:HG3	2.08	0.53
1:O:2837:U:H2'	40:0:7305:HOH:O	2.09	0.53
5:A:105:VAL:HG12	5:A:106:CYS:N	2.24	0.53
16:M:61:ILE:N	16:M:61:ILE:HD12	2.23	0.53
28:Y:170:SER:OG	28:Y:175:ARG:HG3	2.08	0.53
1:O:1477:C:O2'	1:O:1478:U:H5'	2.08	0.53
1:O:1730:G:C5'	1:O:1731:C:C6	2.91	0.53
5:A:217:ARG:HH11	5:A:217:ARG:CG	2.20	0.53
16:M:182:LYS:O	16:M:194:ALA:HB2	2.07	0.53
1:O:1172:G:H1'	40:0:5505:HOH:O	2.09	0.53
1:O:1766:U:O2	1:O:1778:A:H5'	2.08	0.53
1:O:475:G:H5'	7:C:73:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1184:C:H4'	33:I:126:LYS:HB3	1.89	0.53
33:I:93:GLN:HA	33:I:96:PHE:HE2	1.73	0.53
19:P:103:THR:O	19:P:107:GLU:HG3	2.08	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.53
1:0:653:C:H2'	1:0:654:A:C8	2.43	0.53
31:2:36:ASN:HB3	31:2:39:ARG:HG3	1.90	0.53
32:3:56:PRO:HA	40:3:9486:HOH:O	2.09	0.53
6:B:102:THR:HG21	6:B:182:VAL:O	2.07	0.53
6:B:320:GLN:HE21	6:B:321:PRO:HD2	1.73	0.53
8:D:36:ASN:HA	40:D:7500:HOH:O	2.07	0.53
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.08	0.53
18:O:14:LEU:CD2	18:O:102:ILE:HD11	2.38	0.53
18:O:53:GLN:HG2	18:O:56:GLU:OE1	2.08	0.53
1:0:1066:U:H2'	1:0:1067:A:C8	2.44	0.53
1:0:1838:U:H1'	1:0:2644:C:H5'	1.91	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
30:1:25:LYS:HD2	31:2:48:ASP:CA	2.38	0.53
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.89	0.53
7:C:25:PRO:HG2	40:C:9126:HOH:O	2.09	0.53
15:L:119:THR:HG23	15:L:139:SER:OG	2.08	0.53
23:T:47:THR:HB	23:T:100:ASP:HB3	1.90	0.53
1:0:1077:G:H2'	1:0:1080:C:H42	1.73	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.53
1:0:2883:A:H2'	1:0:2884:G:O4'	2.09	0.53
9:E:3:VAL:CG2	9:E:49:ILE:HB	2.38	0.53
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.44	0.53
1:0:151:A:H2'	1:0:152:A:O4'	2.08	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.70	0.53
1:0:516:A:H5'	40:0:6167:HOH:O	2.09	0.53
1:0:775:G:OP1	30:1:16:HIS:HE1	1.91	0.53
1:0:447:A:OP2	23:T:1:SER:HB2	2.08	0.53
7:C:233:THR:HG22	7:C:234:VAL:H	1.73	0.53
26:W:88:THR:HG22	26:W:90:TYR:HD1	1.72	0.53
28:Y:112:GLU:CD	28:Y:115:ARG:NH1	2.63	0.53
1:0:1786:C:OP1	19:P:74:GLN:HG2	2.09	0.53
1:0:545:G:C8	1:0:545:G:H5'	2.42	0.53
5:A:121:ALA:O	5:A:124:VAL:HG22	2.09	0.53
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.44	0.53
14:K:49:LEU:HD12	14:K:80:ILE:HD13	1.90	0.53
18:O:97:SER:OG	18:O:100:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:N2	1:0:1634:G:H1'	2.24	0.53
1:0:1667:A:H2'	1:0:1668:U:C6	2.44	0.53
1:0:1741:U:H3'	40:0:3363:HOH:O	2.09	0.53
30:1:1:THR:HA	40:1:9468:HOH:O	2.08	0.53
40:0:4793:HOH:O	31:2:38:LYS:HE3	2.08	0.53
19:P:16:VAL:HG13	19:P:20:ARG:NH1	2.24	0.53
1:0:1252:A:H2'	1:0:1253:C:O4'	2.09	0.52
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
1:0:362:G:H2'	1:0:363:A:C8	2.44	0.52
1:0:1836:A:H1'	30:1:1:THR:O	2.09	0.52
32:3:30:GLN:HG3	40:3:9452:HOH:O	2.09	0.52
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.91	0.52
8:D:62:ASP:HA	40:D:4233:HOH:O	2.08	0.52
10:F:48:VAL:HG12	10:F:97:ALA:CB	2.39	0.52
33:I:113:HIS:N	33:I:114:PRO:CD	2.72	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
1:0:2817:G:P	40:0:8435:HOH:O	2.67	0.52
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.24	0.52
7:C:194:PHE:CD2	7:C:234:VAL:HG11	2.43	0.52
33:I:138:THR:HG22	33:I:139:ILE:N	2.24	0.52
22:S:73:ASP:OD1	22:S:76:GLU:HG3	2.09	0.52
27:X:12:ILE:HD12	27:X:36:HIS:ND1	2.24	0.52
6:B:36:PRO:HB3	6:B:174:ARG:CB	2.40	0.52
9:E:10:ASP:HA	40:E:3707:HOH:O	2.08	0.52
17:N:86:LEU:HD21	17:N:180:LEU:CD1	2.40	0.52
21:R:114:VAL:HA	21:R:144:GLU:O	2.09	0.52
26:W:88:THR:CG2	26:W:89:ASP:N	2.69	0.52
40:0:5237:HOH:O	29:Z:13:ARG:HD3	2.09	0.52
4:5:77:PHE:CE1	4:5:79:BTN:H62	2.43	0.52
7:C:236:THR:HG22	7:C:239:ALA:CB	2.40	0.52
15:L:134:GLU:HG3	40:L:9452:HOH:O	2.09	0.52
26:W:13:MET:CE	26:W:17:ILE:HG22	2.39	0.52
26:W:29:VAL:O	26:W:30:ASN:HB2	2.10	0.52
5:A:43:VAL:HG21	5:A:59:GLU:HG3	1.90	0.52
7:C:246:ARG:NH1	40:C:9180:HOH:O	2.43	0.52
12:H:63:GLU:HA	40:H:9546:HOH:O	2.08	0.52
19:P:98:ILE:HD12	19:P:102:ARG:NE	2.25	0.52
1:0:2326:U:H4'	1:0:2412:G:C4'	2.40	0.52
1:0:2644:C:O2'	1:0:2645:U:H5'	2.08	0.52
1:0:1562:C:H42	1:0:2738:G:H1	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:28:HIS:HD2	30:1:31:LYS:H	1.57	0.52
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.90	0.52
6:B:41:PHE:CG	6:B:79:MET:HE2	2.45	0.52
18:O:78:ALA:C	18:O:98:LEU:HD13	2.30	0.52
25:V:12:THR:HG23	25:V:14:ALA:H	1.73	0.52
26:W:52:VAL:HG22	26:W:53:ALA:N	2.23	0.52
1:O:2502:C:H2'	1:O:2503:A:H5'	1.91	0.52
32:3:70:ARG:HB3	40:3:9508:HOH:O	2.09	0.52
17:N:24:LEU:HD22	40:Q:2847:HOH:O	2.10	0.52
1:O:1462:C:H2'	1:O:1463:A:C8	2.45	0.52
5:A:109:GLU:HG2	5:A:116:GLY:N	2.25	0.52
23:T:40:VAL:HG22	23:T:41:ARG:N	2.25	0.52
1:O:497:A:H2'	1:O:498:A:C5'	2.40	0.52
8:D:136:ARG:HB3	8:D:137:PRO:HD2	1.91	0.52
12:H:38:LYS:HE2	12:H:42:ASP:HB2	1.92	0.52
14:K:34:VAL:CG2	14:K:47:ALA:HB2	2.39	0.52
16:M:31:TRP:CA	16:M:34:GLU:HG3	2.40	0.52
1:O:2419:U:H5''	1:O:2420:G:H5'	1.91	0.52
2:9:3069:U:OP1	17:N:4:PRO:HG3	2.10	0.52
12:H:76:GLU:O	12:H:77:LEU:HD23	2.09	0.52
16:M:107:ARG:NH1	40:M:9378:HOH:O	2.43	0.52
23:T:19:ARG:HD3	23:T:67:LEU:O	2.10	0.52
40:K:7438:HOH:O	24:U:20:MET:HE1	2.09	0.52
28:Y:184:GLU:OE1	28:Y:204:ARG:NH1	2.43	0.52
1:O:1119:G:H2'	13:J:52:GLN:HE22	1.73	0.51
6:B:41:PHE:HB3	6:B:190:MET:CE	2.40	0.51
6:B:254:GLN:HG3	40:B:9531:HOH:O	2.10	0.51
8:D:65:GLU:HA	40:D:6752:HOH:O	2.08	0.51
13:J:130:VAL:HG12	13:J:131:THR:H	1.74	0.51
15:L:36:ASP:HB2	40:L:9431:HOH:O	2.09	0.51
28:Y:187:VAL:HG23	40:Y:9369:HOH:O	2.10	0.51
1:O:2320:U:H4'	1:O:2321:A:O4'	2.10	0.51
1:O:2645:U:OP2	1:O:2645:U:C6	2.63	0.51
1:O:497:A:H2'	1:O:498:A:H5'	1.91	0.51
1:O:899:C:H5'	40:O:3792:HOH:O	2.09	0.51
6:B:58:PRO:HA	6:B:63:GLU:OE2	2.11	0.51
11:G:64:ASN:N	11:G:64:ASN:HD22	2.07	0.51
12:H:63:GLU:O	12:H:67:LEU:HB2	2.09	0.51
13:J:71:TYR:CD1	13:J:72:PRO:HD2	2.45	0.51
2:9:3051:A:H5'	17:N:160:SER:CB	2.40	0.51
23:T:49:GLU:CB	23:T:59:GLU:HG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.51
1:0:2415:A:H2'	1:0:2416:G:H5'	1.91	0.51
30:1:21:ARG:HD2	30:1:37:CYS:SG	2.51	0.51
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.10	0.51
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.40	0.51
7:C:127:ARG:CZ	7:C:225:PRO:HG2	2.40	0.51
7:C:236:THR:HA	40:C:9257:HOH:O	2.10	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.57	0.51
5:A:36:ASP:O	5:A:38:ILE:N	2.44	0.51
5:A:94:LEU:HD12	5:A:98:GLU:HB2	1.91	0.51
33:I:89:SER:HB3	33:I:97:VAL:CG2	2.40	0.51
24:U:9:CYS:O	24:U:52:THR:HG23	2.10	0.51
27:X:76:ARG:NH1	27:X:76:ARG:HG3	2.24	0.51
1:0:1234:U:N3	6:B:244:PRO:HB3	2.25	0.51
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.94	0.51
8:D:49:PRO:HB3	40:D:5828:HOH:O	2.10	0.51
9:E:34:TRP:O	13:J:127:ILE:HD11	2.11	0.51
16:M:99:ARG:NH2	16:M:170:ASN:HD22	2.00	0.51
17:N:67:ALA:HA	17:N:71:TRP:HB3	1.93	0.51
1:0:1384:C:H5'	27:X:30:MET:HG2	1.92	0.51
6:B:41:PHE:HB3	6:B:190:MET:HE3	1.93	0.51
6:B:199:TYR:CE2	6:B:268:ARG:HB2	2.46	0.51
1:0:926:A:H5'	15:L:39:GLU:OE2	2.09	0.51
1:0:1189:A:H3'	40:0:8193:HOH:O	2.10	0.51
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.51
1:0:317:A:H5''	23:T:52:ARG:HD2	1.92	0.51
40:0:5933:HOH:O	5:A:164:ARG:CZ	2.59	0.51
18:O:106:PRO:HG2	18:O:107:GLU:OE1	2.10	0.51
23:T:112:LEU:CD2	23:T:119:ALA:HB3	2.39	0.51
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.51
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.11	0.51
5:A:211:LYS:CG	5:A:212:PRO:HD2	2.30	0.51
10:F:36:THR:HG23	10:F:97:ALA:HB2	1.93	0.51
33:I:78:LEU:CD1	33:I:112:LYS:HZ2	2.24	0.51
18:O:73:ASP:HA	18:O:92:VAL:O	2.11	0.51
21:R:106:GLY:HA2	21:R:109:MET:HE3	1.92	0.51
21:R:39:THR:HG22	21:R:107:GLU:O	2.10	0.51
1:0:1484:G:H2'	40:0:9725:HOH:O	2.11	0.51
1:0:1669:A:H2'	1:0:1670:G:C8	2.46	0.51
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.51
11:G:67:LEU:O	11:G:71:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:35:ARG:HB2	15:L:35:ARG:NH1	2.25	0.51
1:0:1886:A:O2'	29:Z:20:ARG:HB2	2.11	0.51
1:0:1160:G:HO2'	1:0:1190:G:H8	1.59	0.51
1:0:475:G:C5'	7:C:73:LEU:HD23	2.40	0.51
1:0:2694:A:H4'	9:E:91:PHE:HE1	1.76	0.51
12:H:56:GLN:HE21	12:H:126:ARG:HE	1.56	0.51
40:0:7340:HOH:O	16:M:178:LYS:HB2	2.11	0.51
17:N:66:LEU:HD11	17:N:175:LEU:HD21	1.92	0.51
1:0:308:U:H5'	23:T:97:ARG:NH2	2.26	0.51
1:0:1077:G:H2'	1:0:1080:C:N4	2.25	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
1:0:1306:U:OP1	7:C:184:ARG:HD2	2.11	0.50
1:0:1717:A:H5''	19:P:54:LYS:HB2	1.92	0.50
1:0:2421:G:H2'	40:0:4646:HOH:O	2.10	0.50
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.50
2:9:3054:A:H2	40:9:3535:HOH:O	1.93	0.50
2:9:3054:A:O2'	2:9:3055:U:H5'	2.11	0.50
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.92	0.50
6:B:72:THR:HB	40:B:9600:HOH:O	2.11	0.50
13:J:45:VAL:HG11	13:J:121:LEU:CD2	2.40	0.50
14:K:115:ARG:HG3	14:K:116:GLU:N	2.27	0.50
15:L:145:LEU:O	15:L:145:LEU:HD23	2.11	0.50
22:S:29:ASP:OD1	22:S:31:ARG:NH1	2.44	0.50
29:Z:30:GLU:HG2	29:Z:33:MET:HE3	1.94	0.50
1:0:2016:U:H2'	1:0:2017:U:O4'	2.10	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
1:0:299:U:H5'	40:0:7775:HOH:O	2.11	0.50
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.50
6:B:265:LEU:CD2	6:B:316:ARG:HD3	2.41	0.50
7:C:236:THR:HG21	40:C:9184:HOH:O	2.10	0.50
8:D:104:PHE:CE2	8:D:166:ILE:HD13	2.46	0.50
33:I:87:THR:HG22	33:I:88:GLY:N	2.25	0.50
20:Q:75:ILE:HD13	20:Q:84:ILE:CD1	2.41	0.50
26:W:21:LEU:HD22	26:W:26:ILE:HD13	1.92	0.50
1:0:2296:C:H2'	1:0:2297:U:H6	1.77	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.50
31:2:20:ARG:HG3	31:2:39:ARG:HH21	1.76	0.50
40:0:7989:HOH:O	32:3:61:PRO:HG2	2.10	0.50
17:N:179:LEU:HD23	17:N:184:ILE:HD12	1.94	0.50
19:P:115:SER:HG	19:P:118:GLN:HG3	1.76	0.50
40:0:6777:HOH:O	28:Y:158:LYS:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.47	0.50
1:0:2906:A:H5'	1:0:2907:C:O4'	2.12	0.50
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.50
9:E:133:VAL:HG12	9:E:141:VAL:HG13	1.94	0.50
21:R:92:LEU:HD23	21:R:145:LEU:HD21	1.94	0.50
1:0:177:A:H2'	1:0:178:U:O4'	2.11	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.94	0.50
1:0:2816:A:H2'	40:0:8435:HOH:O	2.12	0.50
5:A:163:GLY:HA2	5:A:166:ASP:OD2	2.12	0.50
6:B:268:ARG:NH2	6:B:325:PRO:HG3	2.25	0.50
13:J:75:PRO:HG2	13:J:105:LEU:CD2	2.41	0.50
26:W:122:ARG:CZ	40:W:5817:HOH:O	2.58	0.50
2:9:3059:C:H2'	2:9:3060:C:C6	2.46	0.50
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.92	0.50
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.42	0.50
12:H:158:THR:HB	12:H:159:PRO:HD3	1.94	0.50
13:J:74:ARG:NH1	13:J:105:LEU:HD11	2.27	0.50
1:0:1992:U:OP2	14:K:66:ARG:HD2	2.11	0.50
16:M:82:ARG:O	16:M:84:LYS:N	2.44	0.50
21:R:69:LYS:HB2	21:R:72:VAL:HG23	1.92	0.50
1:0:1714:C:O2'	1:0:1715:C:H5'	2.11	0.50
1:0:2338:G:OP1	8:D:97:GLN:HG2	2.11	0.50
10:F:48:VAL:HG12	10:F:97:ALA:HB2	1.94	0.50
1:0:155:C:OP2	16:M:188:ARG:HD3	2.11	0.50
26:W:110:GLN:NE2	26:W:110:GLN:HA	2.27	0.50
26:W:5:VAL:HG22	26:W:32:CYS:HB2	1.93	0.50
28:Y:107:PRO:HD3	28:Y:182:PHE:CE1	2.46	0.50
1:0:123:U:H5'	40:0:7132:HOH:O	2.12	0.50
1:0:2769:C:H2'	1:0:2770:G:H5'	1.92	0.50
7:C:154:VAL:O	7:C:158:GLU:HG3	2.12	0.50
29:Z:10:ARG:HA	40:Z:9215:HOH:O	2.11	0.50
1:0:1751:G:C2'	1:0:1752:G:H5''	2.40	0.50
1:0:247:A:H2'	40:0:4495:HOH:O	2.11	0.50
1:0:2827:A:H2'	1:0:2828:G:O4'	2.12	0.50
2:9:3007:G:H4'	17:N:55:ASP:OD2	2.12	0.50
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.50
6:B:58:PRO:HA	6:B:63:GLU:CD	2.32	0.50
8:D:28:GLY:CA	8:D:69:ILE:HG23	2.35	0.50
1:0:962:C:H1'	17:N:5:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:126:PRO:HG2	28:Y:128:PHE:CZ	2.47	0.50
1:0:1745:G:H22	1:0:2033:G:H5'	1.77	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.49
7:C:57:PRO:HG2	7:C:73:LEU:HD13	1.93	0.49
8:D:25:MET:SD	8:D:40:ILE:HD11	2.51	0.49
10:F:13:GLU:OE1	10:F:77:VAL:HG13	2.12	0.49
18:O:96:VAL:CG1	18:O:100:GLN:HB2	2.40	0.49
19:P:13:VAL:HG11	19:P:40:VAL:CG1	2.42	0.49
1:0:204:A:H2'	1:0:205:U:H5'	1.93	0.49
1:0:2748:G:H1'	40:0:8408:HOH:O	2.11	0.49
1:0:926:A:O2'	15:L:41:HIS:HD2	1.95	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
6:B:310:ARG:HD2	40:B:9586:HOH:O	2.10	0.49
6:B:51:VAL:HG23	6:B:327:VAL:HG13	1.94	0.49
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.47	0.49
33:I:131:THR:O	33:I:135:LEU:HG	2.12	0.49
13:J:19:MET:HE2	13:J:79:PHE:HA	1.92	0.49
25:V:59:ILE:O	25:V:63:GLU:HG2	2.11	0.49
1:0:820:G:H5'	1:0:821:U:H5'	1.94	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
7:C:127:ARG:HD3	7:C:129:HIS:HE1	1.76	0.49
13:J:88:PRO:O	13:J:94:GLY:HA3	2.12	0.49
15:L:143:THR:CG2	15:L:144:ASP:N	2.75	0.49
17:N:119:GLN:O	17:N:123:ILE:HG13	2.12	0.49
17:N:89:GLY:O	17:N:92:ALA:HB3	2.12	0.49
28:Y:177:LYS:HD3	28:Y:181:GLY:O	2.12	0.49
1:0:1506:U:H5'	1:0:1506:U:H6	1.78	0.49
30:1:21:ARG:HD2	30:1:39:PHE:HB2	1.95	0.49
32:3:3:MET:O	32:3:90:PHE:HA	2.12	0.49
2:9:3095:C:O2'	2:9:3096:C:H5'	2.12	0.49
11:G:20:VAL:O	11:G:24:VAL:HG23	2.13	0.49
13:J:12:VAL:HG21	13:J:116:LEU:HD11	1.94	0.49
14:K:22:ASP:O	14:K:110:LYS:HE3	2.12	0.49
14:K:55:VAL:CG1	14:K:56:SER:N	2.74	0.49
23:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.49
23:T:38:ARG:HG3	23:T:38:ARG:HH11	1.77	0.49
27:X:61:ARG:HH11	27:X:61:ARG:HG3	1.77	0.49
1:0:1056:U:H2'	1:0:1057:A:O4'	2.11	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
1:0:734:U:H1'	1:0:737:A:N6	2.27	0.49
32:3:25:VAL:HG22	32:3:68:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:84:LEU:HD13	6:B:84:LEU:O	2.13	0.49
8:D:10:PHE:CE1	8:D:11:HIS:HB3	2.47	0.49
1:O:2333:G:P	8:D:56:ARG:HH22	2.36	0.49
8:D:56:ARG:N	40:D:6752:HOH:O	2.46	0.49
9:E:81:GLU:HA	9:E:133:VAL:O	2.12	0.49
14:K:125:ALA:C	14:K:127:ALA:H	2.14	0.49
10:F:38:LYS:NZ	16:M:3:SER:HA	2.27	0.49
1:O:1755:A:H2'	1:O:1756:G:O4'	2.12	0.49
1:O:288:A:H2'	1:O:289:G:C8	2.47	0.49
1:O:333:G:O2'	1:O:334:G:H5'	2.13	0.49
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.42	0.49
24:U:39:ASN:ND2	24:U:44:ARG:HH11	2.10	0.49
25:V:1:THR:CG2	25:V:2:VAL:H	2.19	0.49
1:O:1119:G:H8	13:J:52:GLN:NE2	2.10	0.49
1:O:1878:G:O2'	1:O:1879:U:OP2	2.30	0.49
1:O:2453:G:H5''	40:L:9438:HOH:O	2.12	0.49
1:O:2531:U:O2'	1:O:2532:A:H5'	2.12	0.49
1:O:2735:U:H2'	1:O:2736:U:C6	2.47	0.49
1:O:830:G:O2'	1:O:831:U:H5'	2.13	0.49
1:O:960:G:H2'	1:O:960:G:N3	2.28	0.49
3:4:75:C:N4	3:4:76:PPU:H102	2.28	0.49
2:9:3078:G:N2	2:9:3102:G:H2'	2.28	0.49
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.43	0.49
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.43	0.49
10:F:34:ASN:HA	16:M:4:ALA:HB2	1.93	0.49
17:N:152:GLU:C	17:N:154:LEU:H	2.16	0.49
19:P:16:VAL:HG13	19:P:20:ARG:CZ	2.43	0.49
1:O:793:A:H5''	19:P:83:LYS:HG2	1.95	0.49
21:R:18:LEU:HB2	21:R:143:VAL:HG12	1.94	0.49
25:V:12:THR:HG23	25:V:14:ALA:N	2.27	0.49
25:V:1:THR:HG22	25:V:48:GLU:OE1	2.13	0.49
1:O:1666:C:H2'	1:O:1667:A:C5'	2.42	0.49
1:O:2032:U:C2'	1:O:2033:G:H5''	2.42	0.49
1:O:2781:U:H1'	9:E:139:GLU:OE2	2.12	0.49
1:O:669:G:O2'	1:O:670:G:H5'	2.12	0.49
5:A:94:LEU:N	5:A:94:LEU:HD23	2.28	0.49
12:H:148:GLU:HA	12:H:148:GLU:OE1	2.11	0.49
21:R:99:ALA:HB1	21:R:109:MET:HE3	1.92	0.49
23:T:41:ARG:NH1	23:T:41:ARG:HG2	2.27	0.49
23:T:69:LYS:O	23:T:71:VAL:HG23	2.13	0.49
1:O:2252:A:H2'	1:O:2253:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.46	0.49
6:B:41:PHE:CG	6:B:190:MET:HE3	2.47	0.49
8:D:172:VAL:CG1	8:D:173:GLU:H	2.18	0.49
8:D:37:ALA:O	8:D:40:ILE:HG12	2.12	0.49
9:E:11:VAL:HG12	9:E:12:ASP:N	2.26	0.49
9:E:80:TRP:O	9:E:134:SER:HA	2.13	0.49
20:Q:32:GLU:HA	20:Q:71:TYR:OH	2.13	0.49
21:R:84:ALA:O	21:R:88:PHE:HD1	1.96	0.49
26:W:122:ARG:HG3	26:W:152:ALA:O	2.13	0.49
1:O:2445:U:H2'	1:O:2446:G:C8	2.47	0.49
1:O:65:C:O2'	1:O:66:G:H5'	2.12	0.49
6:B:62:ARG:HA	6:B:65:MET:HE2	1.93	0.49
8:D:51:ARG:HD3	40:D:7636:HOH:O	2.13	0.49
12:H:69:ALA:HB2	12:H:153:ALA:HB2	1.94	0.49
17:N:155:GLU:O	17:N:156:GLU:HG3	2.12	0.49
17:N:164:ASP:OD2	17:N:167:ASP:HA	2.12	0.49
18:O:97:SER:H	18:O:100:GLN:HE21	1.59	0.49
28:Y:186:ARG:HH11	28:Y:186:ARG:HG2	1.76	0.49
1:O:1730:G:H5'	1:O:1731:C:H5	1.77	0.48
1:O:2265:U:H2'	1:O:2266:A:C8	2.48	0.48
30:1:25:LYS:HG3	31:2:49:GLU:H	1.77	0.48
12:H:170:ASN:N	12:H:170:ASN:ND2	2.61	0.48
1:O:2784:A:H1'	9:E:60:SER:OG	2.13	0.48
1:O:750:A:O3'	7:C:101:ASP:HB2	2.12	0.48
31:2:41:HIS:HD2	31:2:44:ARG:H	1.61	0.48
33:I:138:THR:HG22	33:I:139:ILE:H	1.78	0.48
14:K:28:GLU:HB3	14:K:59:LYS:HB2	1.94	0.48
16:M:99:ARG:HH21	16:M:170:ASN:ND2	2.02	0.48
5:A:167:LYS:HB2	29:Z:29:ILE:HD13	1.95	0.48
1:O:2809:G:H2'	1:O:2810:G:O4'	2.13	0.48
2:9:3024:U:H3'	2:9:3025:G:C5'	2.43	0.48
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.14	0.48
8:D:99:ASP:HB3	8:D:103:ASN:H	1.77	0.48
15:L:97:VAL:HG12	15:L:98:GLU:O	2.13	0.48
1:O:2064:U:H5'	1:O:2652:U:O3'	2.13	0.48
1:O:399:C:H5'	16:M:179:GLY:O	2.13	0.48
1:O:426:G:H2'	1:O:427:C:O4'	2.13	0.48
1:O:1654:U:H2'	5:A:47:HIS:HD2	1.77	0.48
8:D:103:ASN:HD21	8:D:134:LEU:H	1.60	0.48
1:O:1242:A:C5'	13:J:82:THR:HG23	2.34	0.48
40:O:6232:HOH:O	14:K:87:ARG:CZ	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:36:ALA:HB1	40:M:9352:HOH:O	2.13	0.48
40:O:5270:HOH:O	17:N:21:HIS:HD2	1.94	0.48
20:Q:40:HIS:CD2	20:Q:60:THR:HG23	2.49	0.48
20:Q:75:ILE:CD1	20:Q:84:ILE:HD11	2.42	0.48
22:S:44:GLN:HE21	25:V:28:LEU:CD2	2.27	0.48
26:W:65:VAL:HA	26:W:68:THR:HG22	1.95	0.48
28:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.46	0.48
1:O:2541:U:H3'	1:O:2541:U:C6	2.47	0.48
6:B:146:THR:C	6:B:148:PRO:HD3	2.34	0.48
8:D:134:LEU:CD1	8:D:166:ILE:HD11	2.41	0.48
10:F:117:GLU:C	10:F:119:ARG:H	2.17	0.48
21:R:96:VAL:HG13	21:R:106:GLY:HA3	1.96	0.48
1:O:1171:A:H2'	1:O:1172:G:H5'	1.94	0.48
1:O:2456:A:H2'	1:O:2457:U:C6	2.48	0.48
1:O:2779:G:H21	9:E:143:GLN:NE2	2.12	0.48
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.96	0.48
12:H:3:ALA:HA	12:H:58:ARG:NH1	2.28	0.48
25:V:7:GLU:O	25:V:11:MET:HG3	2.13	0.48
27:X:61:ARG:HB2	27:X:65:ASN:O	2.14	0.48
1:O:1736:A:H1'	40:O:8069:HOH:O	2.13	0.48
30:1:28:HIS:CE1	30:1:31:LYS:HE2	2.49	0.48
32:3:42:ARG:HH11	32:3:42:ARG:HG3	1.79	0.48
13:J:39:VAL:HG11	13:J:107:ASN:CG	2.34	0.48
17:N:154:LEU:O	17:N:155:GLU:HB3	2.14	0.48
1:O:31:C:OP2	23:T:8:ARG:NH1	2.44	0.48
27:X:61:ARG:HD2	27:X:65:ASN:O	2.14	0.48
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.48
12:H:116:ALA:O	12:H:117:PHE:C	2.52	0.48
12:H:58:ARG:O	12:H:62:LEU:HD22	2.14	0.48
23:T:61:GLU:HG3	40:T:3851:HOH:O	2.14	0.48
25:V:39:ALA:O	25:V:41:GLU:N	2.47	0.48
1:O:1044:C:H3'	1:O:1045:G:H5''	1.96	0.48
1:O:1730:G:C5'	1:O:1731:C:H6	2.26	0.48
1:O:2480:G:H3'	40:O:4750:HOH:O	2.14	0.48
1:O:241:A:C2	1:O:378:A:H4'	2.49	0.48
1:O:602:A:O2'	1:O:605:C:H4'	2.12	0.48
1:O:656:G:OP2	18:O:37:ARG:HD2	2.13	0.48
1:O:776:A:OP1	30:1:28:HIS:HE1	1.97	0.48
6:B:277:GLU:N	6:B:278:PRO:HD2	2.29	0.48
9:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:47:THR:CG2	13:J:48:GLY:N	2.77	0.48
16:M:134:ILE:O	16:M:136:PRO:HD3	2.13	0.48
40:O:7242:HOH:O	17:N:4:PRO:HD2	2.12	0.48
26:W:88:THR:HG22	26:W:90:TYR:CD1	2.49	0.48
1:O:1236:A:C8	13:J:63:ILE:HD11	2.49	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.14	0.48
4:5:75:C:H2'	4:5:76:A:O4'	2.14	0.48
16:M:59:GLY:HA3	16:M:141:ILE:HD12	1.96	0.48
21:R:29:LYS:NZ	40:R:9449:HOH:O	2.47	0.48
22:S:57:THR:HG22	22:S:58:MET:N	2.28	0.48
27:X:9:VAL:HG13	27:X:88:GLU:OE1	2.14	0.48
1:O:1098:A:H2'	1:O:1099:G:O4'	2.14	0.47
1:O:1189:A:H1'	1:O:1209:C:C1'	2.44	0.47
1:O:2862:G:H4'	6:B:336:GLN:O	2.14	0.47
1:O:558:C:C2'	1:O:559:U:C5'	2.92	0.47
10:F:49:PHE:HE1	10:F:98:VAL:HG23	1.79	0.47
1:O:2504:A:H4'	12:H:71:ARG:HH11	1.80	0.47
6:B:91:PRO:O	13:J:144:THR:HG21	2.14	0.47
14:K:10:GLN:N	14:K:10:GLN:NE2	2.48	0.47
15:L:145:LEU:O	15:L:148:GLU:HG3	2.13	0.47
24:U:4:ARG:HH11	24:U:4:ARG:HG2	1.79	0.47
1:O:2253:G:O2'	1:O:2254:G:H5'	2.15	0.47
1:O:2719:A:C2	6:B:70:PRO:HG3	2.49	0.47
12:H:46:GLN:NE2	12:H:137:TYR:HE2	2.11	0.47
23:T:26:THR:HA	23:T:39:ASN:HB3	1.96	0.47
23:T:96:VAL:CG1	23:T:97:ARG:N	2.78	0.47
1:O:308:U:C4	1:O:342:C:H1'	2.49	0.47
30:1:25:LYS:CD	31:2:49:GLU:H	2.27	0.47
7:C:133:ARG:NH1	40:C:9220:HOH:O	2.47	0.47
12:H:38:LYS:HE2	12:H:42:ASP:CB	2.45	0.47
33:I:139:ILE:C	33:I:140:GLU:HG3	2.34	0.47
13:J:54:VAL:O	13:J:58:GLU:HG3	2.14	0.47
1:O:392:U:C5'	16:M:193:LYS:HB3	2.45	0.47
21:R:82:GLU:O	21:R:86:LYS:HG3	2.14	0.47
25:V:5:VAL:CG1	25:V:9:ARG:NH1	2.77	0.47
1:O:1058:A:H2'	1:O:1060:C:H5''	1.96	0.47
1:O:1149:U:H5''	1:O:1151:G:O4'	2.14	0.47
1:O:210:U:H2'	1:O:211:U:C6	2.49	0.47
1:O:2626:C:H2'	1:O:2627:G:C8	2.50	0.47
1:O:347:A:H2'	1:O:348:C:O4'	2.14	0.47
32:3:11:CYS:HB2	32:3:20:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3076:G:H3'	2:9:3077:A:C5'	2.26	0.47
6:B:254:GLN:NE2	40:B:9587:HOH:O	2.44	0.47
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.31	0.47
9:E:49:ILE:HD11	9:E:69:ILE:HD12	1.96	0.47
12:H:77:LEU:HD12	12:H:83:TYR:CD2	2.49	0.47
18:O:39:THR:O	18:O:115:ARG:NH2	2.47	0.47
21:R:119:VAL:HG12	21:R:119:VAL:O	2.13	0.47
22:S:57:THR:CG2	22:S:58:MET:N	2.77	0.47
1:0:912:A:C4	1:0:1294:A:C2	3.02	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
32:3:17:HIS:O	32:3:18:GLN:HG3	2.15	0.47
5:A:123:GLY:HA3	5:A:162:GLY:CA	2.44	0.47
6:B:178:ALA:O	6:B:182:VAL:HG23	2.15	0.47
7:C:157:LEU:CD1	7:C:166:ILE:HD11	2.44	0.47
17:N:15:GLU:HB3	17:N:17:ARG:HD2	1.97	0.47
26:W:64:THR:O	26:W:68:THR:HG22	2.15	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47
1:0:329:A:OP2	7:C:206:ASN:HB2	2.15	0.47
2:9:3003:A:H2'	40:9:2430:HOH:O	2.15	0.47
6:B:87:TYR:OH	6:B:163:GLU:OE2	2.30	0.47
1:0:1167:G:H4'	33:I:135:LEU:HD22	1.96	0.47
17:N:154:LEU:O	17:N:155:GLU:CB	2.63	0.47
19:P:141:ILE:C	19:P:143:ALA:H	2.17	0.47
29:Z:32:GLU:CD	29:Z:70:LYS:HZ2	2.18	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
1:0:2434:A:O3'	32:3:28:GLY:HA3	2.15	0.47
32:3:20:HIS:HA	32:3:70:ARG:O	2.15	0.47
7:C:140:VAL:HB	40:C:9257:HOH:O	2.14	0.47
8:D:173:GLU:HG3	8:D:174:VAL:N	2.30	0.47
16:M:165:GLY:O	16:M:169:ARG:HG3	2.15	0.47
17:N:7:LYS:HE3	20:Q:21:ARG:O	2.13	0.47
1:0:1667:A:C8	1:0:1667:A:H5'	2.40	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.30	0.47
1:0:635:A:H2'	1:0:636:G:H5''	1.96	0.47
1:0:999:C:H2'	1:0:1000:C:O4'	2.15	0.47
32:3:91:GLN:O	32:3:92:GLU:HB2	2.15	0.47
2:9:3048:C:H4'	17:N:141:ARG:HH21	1.79	0.47
6:B:75:GLU:C	6:B:77:PRO:HD3	2.35	0.47
10:F:14:ASP:O	10:F:18:GLU:HG3	2.14	0.47
10:F:60:VAL:O	10:F:60:VAL:CG1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:142:ASN:O	13:J:144:THR:N	2.48	0.47
14:K:113:ILE:CG2	14:K:114:ALA:N	2.77	0.47
15:L:53:ARG:HH22	15:L:57:VAL:HG12	1.80	0.47
16:M:86:GLN:O	16:M:88:VAL:HG23	2.15	0.47
21:R:132:ARG:NH2	40:R:9489:HOH:O	2.46	0.47
22:S:38:ALA:O	22:S:42:GLU:HG3	2.15	0.47
24:U:49:LEU:HG	40:U:3805:HOH:O	2.14	0.47
25:V:64:GLY:O	25:V:65:ASP:CB	2.62	0.47
27:X:7:GLU:HA	27:X:74:ALA:O	2.15	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.47
1:0:1787:C:OP1	19:P:68:LYS:HE2	2.14	0.47
1:0:1921:A:O2'	1:0:1922:A:H5'	2.15	0.47
1:0:764:C:H2'	1:0:765:G:O4'	2.15	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
6:B:215:VAL:HA	6:B:220:VAL:HG22	1.97	0.47
6:B:294:TYR:HE2	40:B:9643:HOH:O	1.97	0.47
33:I:102:VAL:O	33:I:106:LYS:HG3	2.14	0.47
33:I:75:THR:HA	33:I:112:LYS:NZ	2.29	0.47
13:J:19:MET:CE	13:J:132:LEU:HD21	2.44	0.47
1:0:171:C:OP2	16:M:84:LYS:HG3	2.14	0.47
17:N:167:ASP:C	17:N:168:LEU:HG	2.35	0.47
17:N:17:ARG:HB3	17:N:17:ARG:NH1	2.27	0.47
17:N:64:SER:C	17:N:66:LEU:H	2.18	0.47
26:W:149:LEU:HG	26:W:153:MET:HE2	1.96	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.97	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
5:A:69:LEU:HD23	5:A:107:ASN:CB	2.45	0.47
40:0:5212:HOH:O	6:B:300:SER:HB3	2.15	0.47
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.95	0.47
9:E:77:THR:OG1	9:E:78:GLU:N	2.47	0.47
14:K:7:ASP:OD2	14:K:81:ARG:NH2	2.48	0.47
15:L:97:VAL:HB	15:L:100:ALA:HB2	1.97	0.47
15:L:21:ARG:N	40:L:9425:HOH:O	2.47	0.47
24:U:52:THR:HG22	24:U:54:THR:H	1.79	0.47
27:X:80:GLU:HG2	27:X:80:GLU:O	2.15	0.47
1:0:1299:G:N7	15:L:6:ARG:NH1	2.63	0.47
1:0:1634:G:H3'	40:0:4467:HOH:O	2.14	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.47
1:0:1783:A:O2'	1:0:1784:U:H5'	2.15	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.33	0.47
9:E:157:LYS:HD2	9:E:162:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:58:GLU:HA	10:F:61:MET:HG3	1.97	0.47
33:I:72:VAL:CG1	33:I:73:PRO:HD2	2.45	0.47
13:J:52:GLN:HG3	13:J:53:ILE:N	2.30	0.47
22:S:53:ASN:ND2	40:S:9479:HOH:O	2.49	0.47
1:0:1268:C:O2'	28:Y:169:ARG:HB2	2.15	0.47
1:0:1192:A:H3'	1:0:1193:A:H5'	1.96	0.46
1:0:1794:G:N2	1:0:1796:A:H3'	2.30	0.46
1:0:2374:A:H2'	1:0:2375:G:C8	2.51	0.46
1:0:451:C:O2'	1:0:452:G:H5'	2.15	0.46
1:0:657:G:OP1	7:C:27:ARG:NH2	2.30	0.46
7:C:153:VAL:O	7:C:157:LEU:HG	2.15	0.46
1:0:894:A:N1	7:C:87:ARG:NH2	2.63	0.46
8:D:154:LYS:HD2	8:D:154:LYS:N	2.30	0.46
8:D:65:GLU:HG3	40:D:6752:HOH:O	2.14	0.46
33:I:100:LEU:O	33:I:139:ILE:HG23	2.15	0.46
17:N:38:LYS:HD3	17:N:107:ASN:ND2	2.29	0.46
28:Y:155:ARG:NH1	40:Y:9355:HOH:O	2.49	0.46
1:0:1180:U:H1'	40:I:1549:HOH:O	2.14	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.46
1:0:1406:A:H5'	1:0:1407:A:C8	2.51	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
1:0:2270:G:H4'	5:A:223:ARG:NH1	2.30	0.46
1:0:449:A:N7	7:C:43:LYS:HG2	2.31	0.46
1:0:603:A:H1'	1:0:605:C:C2	2.50	0.46
32:3:65:THR:HG22	32:3:67:LEU:CG	2.42	0.46
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.96	0.46
8:D:166:ILE:HB	40:D:6326:HOH:O	2.14	0.46
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.97	0.46
10:F:102:GLY:O	10:F:103:GLU:HB2	2.15	0.46
33:I:112:LYS:C	33:I:114:PRO:HD2	2.35	0.46
14:K:81:ARG:HD3	14:K:87:ARG:CZ	2.44	0.46
23:T:75:GLU:O	23:T:76:ASP:HB2	2.16	0.46
1:0:56:G:H5''	25:V:50:ARG:NH1	2.31	0.46
40:0:5814:HOH:O	26:W:122:ARG:NH2	2.47	0.46
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.46
1:0:1679:C:H5'	40:0:9938:HOH:O	2.16	0.46
5:A:65:ARG:HH11	5:A:65:ARG:HG2	1.80	0.46
8:D:60:GLU:O	8:D:60:GLU:HG3	2.15	0.46
10:F:105:ASP:O	10:F:109:GLU:HB2	2.16	0.46
10:F:56:PRO:HB2	10:F:58:GLU:OE1	2.16	0.46
15:L:57:VAL:HG12	15:L:57:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:88:THR:HG23	26:W:110:GLN:HB3	1.97	0.46
1:O:1799:G:H21	19:P:88:GLN:NE2	2.14	0.46
1:O:2453:G:H5'	40:O:5233:HOH:O	2.16	0.46
40:O:3854:HOH:O	6:B:222:LYS:HE2	2.16	0.46
6:B:62:ARG:HG2	6:B:65:MET:HE3	1.97	0.46
7:C:218:VAL:HG12	40:C:9232:HOH:O	2.16	0.46
8:D:172:VAL:CG1	8:D:173:GLU:N	2.78	0.46
13:J:131:THR:HG22	13:J:133:GLY:N	2.30	0.46
25:V:29:ASN:O	25:V:33:VAL:HG23	2.16	0.46
25:V:4:HIS:O	25:V:8:ILE:HG13	2.15	0.46
1:O:1435:U:H5'	40:O:3203:HOH:O	2.15	0.46
1:O:2072:G:H3'	1:O:2073:G:C5'	2.45	0.46
4:5:78:ACA:H61	4:5:79:BTN:H101	1.60	0.46
6:B:41:PHE:HA	6:B:79:MET:CE	2.45	0.46
8:D:58:VAL:N	8:D:62:ASP:O	2.45	0.46
10:F:57:GLU:O	10:F:61:MET:HG3	2.15	0.46
24:U:45:GLU:HB2	24:U:48:ASN:HD22	1.78	0.46
27:X:72:VAL:CG2	27:X:85:VAL:HG12	2.42	0.46
28:Y:102:LEU:HD11	28:Y:225:GLY:HA2	1.97	0.46
1:O:1014:A:H2'	1:O:1015:C:H5'	1.97	0.46
1:O:2587:OMU:H6	1:O:2587:OMU:O5'	2.16	0.46
1:O:702:G:O2'	1:O:703:G:H5'	2.16	0.46
30:1:56:GLU:HG2	30:1:56:GLU:OXT	2.16	0.46
6:B:14:GLY:HA2	6:B:15:PRO:C	2.36	0.46
18:O:26:TRP:N	40:O:3062:HOH:O	2.49	0.46
26:W:4:LEU:CD2	26:W:52:VAL:HG21	2.39	0.46
1:O:1636:G:O2'	1:O:1637:A:H5'	2.15	0.46
1:O:1789:G:O6	19:P:73:HIS:HE1	1.99	0.46
1:O:2511:A:H2'	1:O:2512:U:O4'	2.15	0.46
1:O:319:A:H4'	1:O:338:C:C5	2.49	0.46
6:B:215:VAL:HB	6:B:234:ARG:HH12	1.81	0.46
7:C:236:THR:O	7:C:237:GLU:C	2.53	0.46
8:D:10:PHE:CG	8:D:11:HIS:N	2.84	0.46
12:H:45:VAL:HA	12:H:167:PRO:O	2.15	0.46
12:H:58:ARG:HG3	12:H:58:ARG:NH1	2.30	0.46
33:I:103:ASP:HA	33:I:106:LYS:HD2	1.97	0.46
21:R:39:THR:CG2	21:R:107:GLU:O	2.63	0.46
23:T:71:VAL:HG13	23:T:91:LEU:O	2.16	0.46
28:Y:99:ALA:HB2	28:Y:233:TYR:CZ	2.51	0.46
29:Z:17:ARG:HD3	40:Z:9220:HOH:O	2.15	0.46
29:Z:39:CYS:SG	29:Z:41:ASN:HB3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1778:A:H2'	1:0:1779:A:H5'	1.97	0.46
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.46
2:9:3057:A:H8	8:D:141:VAL:HG21	1.80	0.46
6:B:87:TYR:HD1	40:B:9575:HOH:O	1.99	0.46
7:C:236:THR:O	7:C:239:ALA:N	2.49	0.46
1:0:894:A:C2	7:C:87:ARG:NH2	2.83	0.46
33:I:99:ASP:O	33:I:100:LEU:HD23	2.16	0.46
13:J:71:TYR:CG	13:J:72:PRO:HD2	2.51	0.46
15:L:79:ASP:HB3	40:L:9453:HOH:O	2.15	0.46
17:N:183:ASP:O	17:N:184:ILE:O	2.34	0.46
21:R:114:VAL:HG13	21:R:114:VAL:O	2.15	0.46
26:W:142:ASP:HB2	40:W:6373:HOH:O	2.15	0.46
27:X:34:ARG:NH1	27:X:48:VAL:O	2.48	0.46
27:X:43:VAL:CG1	27:X:44:ASP:N	2.79	0.46
1:0:1015:C:H2'	1:0:1016:U:C6	2.51	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.16	0.46
1:0:2487:C:H5	40:0:5422:HOH:O	1.98	0.46
6:B:51:VAL:HG21	6:B:327:VAL:HG13	1.94	0.46
12:H:9:ILE:HD12	12:H:54:THR:HG22	1.97	0.46
14:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.46
15:L:91:VAL:CG1	15:L:120:LEU:HD23	2.46	0.46
27:X:20:GLU:HG3	27:X:21:PRO:HD2	1.98	0.46
1:0:1200:A:H3'	40:0:6272:HOH:O	2.15	0.46
1:0:1298:U:H2'	1:0:1299:G:C8	2.50	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.46
1:0:1799:G:H21	19:P:88:GLN:HE22	1.64	0.46
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.46
1:0:802:G:H2'	1:0:803:C:C6	2.50	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
2:9:3064:C:H2'	2:9:3065:A:H5'	1.97	0.46
2:9:3092:G:H2'	2:9:3093:A:C8	2.51	0.46
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.51	0.46
6:B:217:ARG:HG3	6:B:257:THR:CG2	2.46	0.46
7:C:107:ARG:NE	40:C:9266:HOH:O	2.32	0.46
10:F:107:ASP:O	10:F:111:ILE:HG13	2.16	0.46
25:V:45:ARG:HA	25:V:48:GLU:HB2	1.98	0.46
1:0:2904:U:H4'	27:X:8:ARG:NH1	2.31	0.46
28:Y:152:LYS:HB3	28:Y:160:LYS:HG3	1.98	0.46
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.45
1:0:1878:G:O2'	1:0:1879:U:C5	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:6:ARG:HA	32:3:20:HIS:O	2.16	0.45
5:A:217:ARG:NH1	5:A:217:ARG:CG	2.78	0.45
5:A:232:ARG:NH2	5:A:236:GLY:O	2.45	0.45
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.16	0.45
1:0:2346:C:H4'	8:D:52:THR:CG2	2.47	0.45
12:H:54:THR:O	12:H:55:VAL:HG13	2.16	0.45
14:K:101:ASN:O	14:K:102:GLU:HB2	2.17	0.45
26:W:21:LEU:HD13	26:W:26:ILE:HD11	1.99	0.45
26:W:3:ALA:O	26:W:54:PHE:HA	2.16	0.45
1:0:1067:A:H5'	40:0:4906:HOH:O	2.15	0.45
1:0:2338:G:H2'	8:D:129:ASP:OD1	2.16	0.45
6:B:42:ALA:H	6:B:79:MET:HE2	1.81	0.45
6:B:86:ALA:HA	40:B:9575:HOH:O	2.15	0.45
7:C:5:ILE:HG13	7:C:15:GLU:HA	1.99	0.45
7:C:78:ARG:CG	7:C:78:ARG:NH1	2.76	0.45
13:J:8:ALA:HA	13:J:35:THR:HG22	1.98	0.45
26:W:11:VAL:O	26:W:12:ASN:HB2	2.15	0.45
26:W:59:GLN:NE2	26:W:97:ALA:HB3	2.32	0.45
28:Y:117:LEU:HA	28:Y:174:VAL:HG11	1.98	0.45
1:0:1942:A:H3'	40:0:7785:HOH:O	2.16	0.45
1:0:1980:U:H5'	1:0:2626:C:H1'	1.98	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
5:A:130:THR:HB	5:A:137:VAL:HB	1.97	0.45
12:H:43:TYR:HA	12:H:44:PRO:HD3	1.77	0.45
17:N:110:THR:HB	17:N:113:SER:HG	1.80	0.45
19:P:10:ALA:HA	19:P:13:VAL:HG12	1.98	0.45
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.45
1:0:1205:U:H2'	1:0:1206:U:H5''	1.99	0.45
1:0:1441:G:H1'	40:0:8275:HOH:O	2.16	0.45
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.45
1:0:2003:U:H4'	1:0:2004:U:H5	1.80	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
1:0:558:C:H2'	1:0:559:U:H5''	1.97	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
6:B:168:GLY:O	6:B:169:GLY:O	2.35	0.45
8:D:167:GLU:C	8:D:169:THR:H	2.20	0.45
33:I:116:LEU:HD22	33:I:127:GLU:OE1	2.17	0.45
16:M:66:SER:HB3	16:M:128:TRP:CD1	2.51	0.45
28:Y:107:PRO:HB3	28:Y:182:PHE:CE2	2.51	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.16	0.45
1:0:2747:C:H4'	40:0:8429:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:27:U:H2'	1:0:28:G:O4'	2.17	0.45
1:0:447:A:OP1	23:T:2:LYS:HG2	2.16	0.45
6:B:97:LEU:HD21	40:B:9637:HOH:O	2.17	0.45
1:0:2101:A:H2'	7:C:63:SER:OG	2.16	0.45
15:L:90:ARG:NH2	15:L:121:ILE:HD11	2.32	0.45
16:M:68:ARG:O	16:M:68:ARG:HD3	2.17	0.45
17:N:154:LEU:CG	17:N:155:GLU:H	2.25	0.45
17:N:73:ALA:HB1	17:N:74:PRO:CD	2.46	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.45
2:9:3045:A:H4'	8:D:143:LYS:O	2.16	0.45
9:E:95:VAL:HG11	9:E:131:LEU:HD11	1.97	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.35	0.45
9:E:69:ILE:HA	9:E:72:MET:CE	2.47	0.45
12:H:136:ALA:HB3	12:H:146:VAL:HG21	1.97	0.45
33:I:89:SER:HB2	33:I:95:ASP:HB2	1.99	0.45
13:J:131:THR:HB	13:J:134:GLU:OE1	2.16	0.45
15:L:143:THR:CG2	15:L:144:ASP:H	2.23	0.45
15:L:77:ALA:C	15:L:79:ASP:H	2.20	0.45
23:T:78:THR:HB	23:T:87:VAL:O	2.17	0.45
22:S:10:VAL:HG11	25:V:36:ALA:CA	2.45	0.45
25:V:8:ILE:HG21	25:V:59:ILE:HG13	1.98	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
5:A:223:ARG:CZ	40:A:9562:HOH:O	2.64	0.45
33:I:75:THR:OG1	33:I:112:LYS:HE2	2.17	0.45
15:L:101:ASP:C	15:L:103:ALA:H	2.20	0.45
20:Q:30:VAL:HG12	20:Q:30:VAL:O	2.17	0.45
40:0:6180:HOH:O	23:T:68:ASP:HB2	2.16	0.45
23:T:85:GLU:CG	23:T:86:GLU:N	2.79	0.45
24:U:14:GLU:OE1	24:U:15:PRO:HD2	2.17	0.45
26:W:108:ARG:CG	26:W:114:PRO:HG3	2.44	0.45
26:W:85:ALA:HB2	26:W:91:ASP:O	2.17	0.45
26:W:88:THR:CG2	26:W:90:TYR:HD1	2.29	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.45
1:0:1201:C:C2'	1:0:1202:A:H5'	2.43	0.45
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.45
1:0:2256:G:H2'	1:0:2257:G:H5'	1.99	0.45
1:0:962:C:H5'	40:0:7430:HOH:O	2.16	0.45
5:A:131:HIS:O	5:A:132:ASP:HB2	2.17	0.45
7:C:133:ARG:NE	7:C:138:VAL:HG22	2.30	0.45
7:C:119:ALA:HA	7:C:137:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.99	0.45
20:Q:53:HIS:CE1	20:Q:55:ARG:HB2	2.52	0.45
23:T:71:VAL:HG12	23:T:72:ILE:H	1.82	0.45
1:O:1477:C:H5'	1:O:1868:G:C5'	2.47	0.45
1:O:790:A:H1'	1:O:1710:A:H2'	1.99	0.45
1:O:2250:G:OP1	5:A:31:LYS:HD3	2.17	0.45
1:O:1168:C:H5''	33:I:87:THR:HG23	1.99	0.45
14:K:80:ILE:O	14:K:87:ARG:HA	2.16	0.45
15:L:149:ARG:O	15:L:150:GLN:HB2	2.16	0.45
16:M:46:LEU:HD22	16:M:50:ARG:HG3	1.98	0.45
20:Q:40:HIS:HD2	20:Q:60:THR:HG23	1.82	0.45
21:R:119:VAL:CG1	21:R:119:VAL:O	2.64	0.45
28:Y:187:VAL:HG23	28:Y:192:ASP:HB3	1.98	0.45
1:O:1015:C:H2'	1:O:1016:U:H6	1.81	0.45
1:O:1180:U:H2'	1:O:1181:A:O4'	2.17	0.45
1:O:2256:G:C2'	1:O:2257:G:H5'	2.47	0.45
1:O:2541:U:C6	1:O:2541:U:C3'	3.00	0.45
1:O:622:G:P	28:Y:148:GLY:HA3	2.57	0.45
1:O:816:G:H5'	1:O:1598:A:H4'	1.97	0.45
1:O:907:A:H2'	1:O:908:A:C8	2.51	0.45
5:A:206:ARG:N	5:A:206:ARG:HD3	2.27	0.45
12:H:146:VAL:HG22	40:H:9543:HOH:O	2.17	0.45
16:M:120:VAL:CG1	16:M:130:GLU:HG3	2.46	0.45
16:M:158:ARG:HB2	16:M:163:LEU:HB2	1.97	0.45
18:O:47:ARG:HG3	18:O:47:ARG:NH1	2.32	0.45
19:P:16:VAL:HG12	19:P:17:GLY:H	1.80	0.45
24:U:4:ARG:NH1	24:U:4:ARG:HG2	2.32	0.45
28:Y:144:ARG:CG	28:Y:144:ARG:NH1	2.71	0.45
5:A:167:LYS:HE3	29:Z:26:VAL:HG13	1.99	0.45
1:O:1350:U:H2'	1:O:1351:G:O4'	2.17	0.44
1:O:2724:U:H2'	1:O:2725:G:O4'	2.17	0.44
1:O:2769:C:H2'	1:O:2770:G:O4'	2.17	0.44
4:5:76:A:OP1	4:5:76:A:H4'	2.17	0.44
5:A:105:VAL:HG12	5:A:106:CYS:H	1.82	0.44
6:B:175:LEU:C	6:B:175:LEU:HD23	2.37	0.44
6:B:41:PHE:CB	6:B:190:MET:HE3	2.47	0.44
9:E:170:ARG:HE	9:E:170:ARG:HB2	1.67	0.44
10:F:33:THR:HG21	10:F:59:ILE:O	2.17	0.44
15:L:89:PHE:CD1	15:L:89:PHE:N	2.85	0.44
17:N:49:THR:HG22	17:N:56:ASP:CB	2.39	0.44
18:O:24:ALA:O	18:O:28:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2365:G:H4'	20:Q:45:PRO:O	2.17	0.44
27:X:21:PRO:HG2	27:X:24:LYS:HD3	1.98	0.44
28:Y:163:THR:HB	40:Y:9397:HOH:O	2.16	0.44
1:0:1163:G:H1	1:0:1184:C:N4	2.15	0.44
1:0:2443:C:H5'	15:L:57:VAL:HG21	1.99	0.44
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.44
2:9:3001:U:H5''	2:9:3003:A:OP1	2.17	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.44
2:9:3056:A:C3'	2:9:3057:A:H5''	2.47	0.44
9:E:31:ARG:NH1	40:E:5919:HOH:O	2.49	0.44
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.44
12:H:58:ARG:HG3	40:H:9520:HOH:O	2.18	0.44
14:K:115:ARG:O	14:K:118:ALA:HB3	2.16	0.44
15:L:145:LEU:C	15:L:145:LEU:HD23	2.38	0.44
1:0:1593:C:OP1	19:P:117:SER:HB3	2.17	0.44
25:V:42:ASN:O	25:V:44:GLY:N	2.50	0.44
1:0:2726:U:O2	1:0:2749:U:O5'	2.34	0.44
1:0:656:G:H1'	40:C:9267:HOH:O	2.17	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44
6:B:113:LEU:HD21	6:B:161:VAL:HG21	1.98	0.44
6:B:185:GLY:HA2	40:B:9628:HOH:O	2.16	0.44
6:B:41:PHE:HA	6:B:79:MET:HE1	1.99	0.44
6:B:8:LYS:HG3	6:B:220:VAL:HG12	1.99	0.44
7:C:107:ARG:NH1	40:C:9238:HOH:O	2.50	0.44
7:C:115:LEU:O	7:C:118:THR:HB	2.17	0.44
9:E:22:VAL:O	9:E:28:SER:HA	2.17	0.44
33:I:97:VAL:N	33:I:136:GLY:O	2.51	0.44
13:J:39:VAL:CG1	13:J:40:ASN:N	2.81	0.44
27:X:41:PHE:O	27:X:43:VAL:HG23	2.16	0.44
27:X:73:ARG:HB2	27:X:88:GLU:OE2	2.17	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
5:A:179:MET:HG2	5:A:186:TRP:CG	2.52	0.44
8:D:78:GLU:O	8:D:82:GLU:HG3	2.18	0.44
10:F:5:ASP:O	10:F:119:ARG:NH1	2.50	0.44
13:J:42:GLU:O	13:J:131:THR:HG23	2.18	0.44
15:L:35:ARG:HB2	15:L:35:ARG:HH11	1.82	0.44
1:0:154:C:P	16:M:188:ARG:HH12	2.40	0.44
19:P:143:ALA:HA	40:P:164:HOH:O	2.17	0.44
1:0:2100:A:H4'	7:C:64:GLY:O	2.16	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H5'	40:0:6529:HOH:O	2.18	0.44
1:0:82:C:OP1	23:T:67:LEU:HB2	2.18	0.44
2:9:3114:G:O6	17:N:11:ARG:HD3	2.17	0.44
12:H:29:ALA:C	12:H:30:GLN:HG3	2.38	0.44
1:0:1104:C:H4'	13:J:88:PRO:HD3	1.99	0.44
1:0:1185:U:H5'	40:0:7899:HOH:O	2.18	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.52	0.44
1:0:1552:G:H2'	1:0:1553:C:C6	2.52	0.44
1:0:2019:A:H5'	40:0:5087:HOH:O	2.17	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.44
6:B:53:LEU:CD1	6:B:327:VAL:HG22	2.46	0.44
6:B:85:ARG:HB2	6:B:99:GLU:HG2	1.99	0.44
33:I:92:PRO:O	33:I:94:GLU:N	2.50	0.44
18:O:60:VAL:HG12	18:O:62:GLY:H	1.81	0.44
23:T:71:VAL:CG1	23:T:72:ILE:N	2.80	0.44
25:V:56:ILE:HG22	25:V:60:GLN:NE2	2.32	0.44
40:0:3165:HOH:O	26:W:119:HIS:HE1	2.01	0.44
1:0:1266:U:H4'	28:Y:115:ARG:HH21	1.82	0.44
1:0:1162:G:H1'	33:I:117:LEU:CD1	2.47	0.44
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.44
1:0:2296:C:H2'	1:0:2297:U:C6	2.52	0.44
1:0:2533:C:H6	1:0:2533:C:C5'	2.25	0.44
1:0:2748:G:H4'	1:0:2749:U:C5'	2.47	0.44
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.44
31:2:5:LYS:O	31:2:9:LYS:HG3	2.17	0.44
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.44
6:B:217:ARG:HD3	6:B:218:TRP:NE1	2.33	0.44
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.18	0.44
6:B:96:PRO:HG3	40:B:9629:HOH:O	2.17	0.44
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.33	0.44
8:D:60:GLU:O	8:D:61:PHE:C	2.55	0.44
33:I:139:ILE:HG22	33:I:140:GLU:N	2.32	0.44
1:0:645:U:OP2	15:L:4:LYS:HE2	2.18	0.44
16:M:98:GLN:O	16:M:102:GLU:HG3	2.17	0.44
16:M:82:ARG:O	16:M:83:SER:C	2.56	0.44
25:V:5:VAL:HG23	40:V:2271:HOH:O	2.18	0.44
26:W:122:ARG:NE	40:W:5817:HOH:O	2.50	0.44
27:X:18:ARG:NH1	40:X:4132:HOH:O	2.50	0.44
27:X:9:VAL:HG13	27:X:88:GLU:OE2	2.17	0.44
28:Y:203:VAL:CG1	28:Y:228:VAL:HG22	2.48	0.44
1:0:1044:C:H5''	40:0:9648:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1350:U:H1'	40:0:3273:HOH:O	2.17	0.44
1:0:2335:C:H2'	1:0:2336:G:H8	1.83	0.44
1:0:2712:G:H5'	40:K:4183:HOH:O	2.17	0.44
1:0:2895:C:H4'	40:X:4132:HOH:O	2.18	0.44
1:0:29:C:O2'	1:0:30:U:H5'	2.18	0.44
1:0:656:G:H4'	40:C:9167:HOH:O	2.18	0.44
5:A:103:VAL:O	5:A:105:VAL:HG23	2.18	0.44
1:0:1119:G:H8	13:J:52:GLN:HE22	1.66	0.44
1:0:1771:U:C4'	29:Z:20:ARG:HE	2.30	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.53	0.44
1:0:1244:U:H2'	13:J:47:THR:HG21	1.99	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.18	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.81	0.44
6:B:71:VAL:CG1	6:B:296:LEU:HD22	2.48	0.44
12:H:55:VAL:HG12	40:H:9540:HOH:O	2.18	0.44
18:O:4:ASN:HA	18:O:5:PRO:HD3	1.90	0.44
40:0:4557:HOH:O	23:T:82:THR:HA	2.17	0.44
27:X:31:ILE:O	27:X:35:GLU:HG3	2.16	0.44
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.18	0.43
1:0:2044:G:OP1	27:X:23:HIS:HE1	2.01	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.33	0.43
1:0:556:C:H2'	1:0:557:C:C6	2.53	0.43
5:A:132:ASP:HB3	5:A:135:VAL:H	1.83	0.43
7:C:219:ASN:N	7:C:222:ASP:OD1	2.44	0.43
13:J:75:PRO:HB3	13:J:132:LEU:HB3	2.00	0.43
15:L:144:ASP:O	15:L:147:GLU:HB2	2.18	0.43
21:R:61:GLN:NE2	40:R:9449:HOH:O	2.50	0.43
23:T:38:ARG:HG3	23:T:38:ARG:NH1	2.32	0.43
1:0:1086:A:C6	26:W:11:VAL:HG11	2.52	0.43
27:X:61:ARG:HG3	27:X:61:ARG:NH1	2.33	0.43
29:Z:30:GLU:HA	29:Z:33:MET:HB3	1.99	0.43
1:0:157:G:H4'	16:M:95:LYS:HE2	1.99	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.53	0.43
1:0:2503:A:OP1	12:H:151:ARG:NH2	2.42	0.43
1:0:338:C:H5''	40:C:9230:HOH:O	2.16	0.43
5:A:29:HIS:CD2	5:A:153:ARG:NH1	2.86	0.43
5:A:105:VAL:HG13	5:A:155:THR:O	2.18	0.43
6:B:279:THR:CG2	6:B:280:VAL:N	2.80	0.43
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.51	0.43
19:P:55:LYS:CG	19:P:56:GLY:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:25:PRO:HA	20:Q:26:PRO:HD3	1.85	0.43
23:T:30:ASP:O	23:T:33:GLU:HB3	2.18	0.43
23:T:96:VAL:HG13	23:T:97:ARG:N	2.32	0.43
28:Y:106:THR:HG23	28:Y:107:PRO:HD2	1.98	0.43
28:Y:151:SER:HB3	28:Y:154:ARG:HB3	2.00	0.43
31:2:41:HIS:CD2	31:2:44:ARG:H	2.35	0.43
2:9:3057:A:C8	8:D:141:VAL:HG21	2.52	0.43
6:B:181:ILE:HG22	6:B:186:GLY:HA2	1.98	0.43
6:B:243:ASN:HA	6:B:244:PRO:C	2.37	0.43
8:D:88:LEU:N	8:D:89:PRO:CD	2.81	0.43
12:H:169:GLY:C	12:H:170:ASN:HD22	2.20	0.43
28:Y:216:ARG:HD2	40:Y:9368:HOH:O	2.16	0.43
29:Z:60:CYS:O	29:Z:61:ASP:HB2	2.18	0.43
1:0:1174:A:H62	1:0:1200:A:H2'	1.83	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
1:0:2787:C:H5	40:0:5178:HOH:O	2.01	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
5:A:123:GLY:HA2	5:A:159:VAL:O	2.18	0.43
40:0:5154:HOH:O	5:A:206:ARG:HD3	2.18	0.43
15:L:130:ARG:O	15:L:131:GLU:C	2.57	0.43
16:M:49:ALA:C	16:M:54:TYR:HB3	2.39	0.43
16:M:72:ALA:HB2	16:M:93:ARG:HG2	2.01	0.43
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:1928:C:C2'	1:0:1929:G:H5'	2.47	0.43
2:9:3042:C:H5'	2:9:3043:G:OP2	2.17	0.43
2:9:3044:A:O4'	8:D:76:ARG:NE	2.51	0.43
1:0:1884:G:O6	5:A:190:ARG:HD2	2.16	0.43
6:B:36:PRO:HB3	6:B:174:ARG:HB2	1.99	0.43
7:C:123:LEU:HA	7:C:123:LEU:HD23	1.86	0.43
7:C:142:ASP:CG	7:C:237:GLU:HB3	2.39	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.18	0.43
9:E:84:MET:CE	9:E:148:ILE:HD12	2.45	0.43
17:N:11:ARG:CG	17:N:14:ARG:NH1	2.73	0.43
17:N:71:TRP:CE3	17:N:175:LEU:HD22	2.53	0.43
20:Q:59:GLN:HB3	40:Q:6286:HOH:O	2.17	0.43
20:Q:64:GLU:OE1	20:Q:64:GLU:HA	2.18	0.43
26:W:106:THR:OG1	26:W:109:GLU:HG3	2.18	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.51	0.43
1:0:1511:U:O2'	1:0:1512:G:H5'	2.18	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2363:G:O3'	20:Q:11:ARG:NH1	2.51	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.43
1:0:2776:A:H2'	1:0:2777:G:O4'	2.18	0.43
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.43
1:0:588:G:O6	26:W:154:ARG:NH1	2.52	0.43
7:C:51:TYR:CD1	30:1:56:GLU:HB2	2.54	0.43
9:E:35:TYR:HB2	40:E:5715:HOH:O	2.18	0.43
10:F:11:ASP:O	10:F:14:ASP:HB2	2.17	0.43
12:H:47:ILE:HG21	40:H:9543:HOH:O	2.18	0.43
1:0:903:U:O4	15:L:18:HIS:HB2	2.17	0.43
21:R:104:PHE:HB3	21:R:109:MET:CE	2.49	0.43
26:W:110:GLN:HE21	26:W:110:GLN:HA	1.84	0.43
40:O:6985:HOH:O	28:Y:141:THR:HG23	2.19	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.83	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	1.98	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.43
30:1:53:LYS:HA	30:1:53:LYS:HD3	1.84	0.43
7:C:194:PHE:HA	7:C:234:VAL:HG13	2.01	0.43
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.01	0.43
12:H:56:GLN:HG2	12:H:126:ARG:HG2	2.00	0.43
12:H:83:TYR:C	12:H:83:TYR:CD1	2.92	0.43
33:I:132:CYS:C	33:I:134:SER:H	2.21	0.43
15:L:12:THR:HG21	15:L:16:GLY:O	2.18	0.43
16:M:107:ARG:CG	16:M:107:ARG:NH1	2.77	0.43
16:M:24:GLN:O	16:M:28:GLN:HG3	2.19	0.43
7:C:27:ARG:HD2	18:O:5:PRO:HD2	2.01	0.43
19:P:13:VAL:HG21	19:P:41:ARG:HG2	2.01	0.43
23:T:79:LEU:HG	23:T:89:ARG:HB2	2.01	0.43
26:W:146:ILE:HA	26:W:146:ILE:HD13	1.92	0.43
1:0:2856:A:P	27:X:15:ARG:HH22	2.42	0.43
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.43
1:0:2001:G:O2'	1:0:2002:C:H5'	2.19	0.43
1:0:2015:A:O2'	1:0:2016:U:H5'	2.19	0.43
1:0:830:G:H2'	1:0:831:U:C6	2.54	0.43
6:B:109:LEU:HD11	6:B:113:LEU:HD11	2.00	0.43
10:F:49:PHE:CB	10:F:83:LEU:HD11	2.49	0.43
10:F:52:GLU:HG3	10:F:77:VAL:O	2.19	0.43
33:I:132:CYS:C	33:I:134:SER:N	2.71	0.43
40:C:9167:HOH:O	18:O:3:THR:HG21	2.18	0.43
28:Y:112:GLU:OE2	28:Y:115:ARG:NH1	2.52	0.43
1:0:1979:G:HO2'	1:0:1980:U:P	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	13:J:70:PHE:HD1	1.83	0.43
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.43
1:0:710:G:N2	1:0:719:C:C2	2.87	0.43
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.43
40:0:4966:HOH:O	5:A:11:ARG:CZ	2.67	0.43
5:A:217:ARG:HH11	5:A:217:ARG:HG3	1.84	0.43
12:H:166:SER:HB2	12:H:167:PRO:CD	2.48	0.43
1:0:1185:U:H4'	33:I:123:ASN:HB3	2.00	0.43
17:N:48:VAL:HG11	17:N:55:ASP:HB3	1.99	0.43
17:N:74:PRO:HG2	17:N:159:TYR:CE1	2.54	0.43
24:U:52:THR:CG2	24:U:54:THR:HB	2.49	0.43
26:W:108:ARG:HE	26:W:114:PRO:CG	2.32	0.43
1:0:2515:C:H2'	1:0:2516:G:O4'	2.19	0.43
1:0:821:U:H2'	1:0:822:C:H6	1.84	0.43
1:0:883:U:C2'	1:0:883:U:O2	2.65	0.43
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.87	0.43
10:F:101:ALA:HA	40:F:5413:HOH:O	2.19	0.43
12:H:2:PRO:HD2	12:H:5:MET:SD	2.58	0.43
13:J:39:VAL:HG21	13:J:107:ASN:ND2	2.34	0.43
14:K:13:GLU:OE1	14:K:44:LEU:HD12	2.19	0.43
19:P:105:LEU:CD2	19:P:137:LEU:HD21	2.49	0.43
19:P:55:LYS:HG2	19:P:56:GLY:N	2.33	0.43
25:V:5:VAL:HG11	25:V:9:ARG:NH1	2.33	0.43
28:Y:107:PRO:HB3	28:Y:182:PHE:CD2	2.54	0.43
1:0:818:A:O2'	29:Z:13:ARG:HD2	2.19	0.43
1:0:1008:C:H2'	1:0:1009:U:C6	2.54	0.42
1:0:185:G:H4'	1:0:186:A:H4'	2.00	0.42
1:0:2072:G:N2	40:0:7335:HOH:O	2.50	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.42
1:0:2851:G:H4'	6:B:157:LYS:NZ	2.34	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.33	0.42
5:A:207:GLN:O	5:A:208:HIS:HB3	2.19	0.42
6:B:102:THR:HG23	6:B:182:VAL:HG12	1.99	0.42
6:B:190:MET:CE	6:B:194:PHE:CD1	3.01	0.42
7:C:246:ARG:HB3	7:C:246:ARG:NH1	2.33	0.42
22:S:37:VAL:O	22:S:41:VAL:HG23	2.18	0.42
25:V:12:THR:OG1	25:V:13:PRO:HD2	2.19	0.42
1:0:797:A:O4'	29:Z:10:ARG:N	2.51	0.42
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.52	0.42
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.42
1:0:2748:G:H5'	40:0:7972:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:461:C:N3	1:0:479:G:H5'	2.34	0.42
1:0:920:C:H5'	1:0:921:G:C4	2.54	0.42
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.42
31:2:44:ARG:HA	31:2:44:ARG:HD3	1.78	0.42
33:I:102:VAL:HG23	33:I:140:GLU:O	2.18	0.42
15:L:91:VAL:HG12	15:L:120:LEU:HD23	2.01	0.42
16:M:42:ARG:HA	16:M:43:PRO:HD3	1.87	0.42
40:9:5851:HOH:O	17:N:115:VAL:HG13	2.19	0.42
1:0:2866:U:C4	24:U:50:GLU:HB3	2.55	0.42
26:W:142:ASP:HB3	26:W:145:GLY:H	1.84	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.30	0.42
1:0:1315:G:C4	28:Y:212:ARG:HB2	2.55	0.42
1:0:1363:G:OP1	7:C:76:ARG:NH2	2.48	0.42
1:0:1947:G:H2'	1:0:1948:G:H8	1.84	0.42
1:0:2134:G:C6	1:0:2258:A:C8	3.08	0.42
1:0:2663:U:O2	40:0:8435:HOH:O	2.22	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.54	0.42
1:0:709:G:O2'	18:O:25:VAL:CG1	2.67	0.42
1:0:816:G:C6	1:0:817:G:N1	2.87	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
31:2:48:ASP:O	31:2:49:GLU:HB2	2.19	0.42
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.42
12:H:154:TYR:C	12:H:154:TYR:CD1	2.92	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.42
1:0:2415:A:O2'	17:N:29:SER:HB3	2.19	0.42
1:0:483:C:C4	1:0:484:A:C6	3.07	0.42
1:0:945:U:H2'	1:0:946:C:C6	2.55	0.42
32:3:18:GLN:OE1	32:3:73:GLU:HB3	2.19	0.42
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.84	0.42
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.85	0.42
11:G:64:ASN:N	11:G:64:ASN:ND2	2.67	0.42
17:N:181:ASP:O	17:N:184:ILE:HG22	2.19	0.42
18:O:98:LEU:O	18:O:102:ILE:HG13	2.19	0.42
1:0:1257:C:H2'	1:0:1258:G:O4'	2.19	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.19	0.42
40:0:7289:HOH:O	7:C:175:LYS:HE3	2.19	0.42
13:J:132:LEU:HA	13:J:132:LEU:HD23	1.82	0.42
16:M:167:GLY:O	16:M:171:ARG:HG3	2.20	0.42
18:O:59:VAL:HG21	18:O:111:VAL:HG21	2.02	0.42
19:P:13:VAL:HG11	19:P:40:VAL:HG12	2.01	0.42
21:R:122:GLN:HB3	21:R:138:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:33:SER:OG	22:S:36:GLU:HG3	2.19	0.42
22:S:51:GLN:HE21	22:S:53:ASN:ND2	1.90	0.42
23:T:14:ALA:HA	23:T:15:PRO:HD3	1.95	0.42
27:X:20:GLU:CG	27:X:21:PRO:HD2	2.49	0.42
29:Z:32:GLU:HA	29:Z:35:GLU:HG3	2.01	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.20	0.42
1:0:1574:C:H6	1:0:1574:C:O5'	2.02	0.42
1:0:2248:C:H3'	40:0:5967:HOH:O	2.18	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.42
1:0:2713:G:O2'	1:0:2714:U:H5'	2.20	0.42
1:0:2793:A:H2'	1:0:2794:G:H5'	2.00	0.42
1:0:325:U:H2'	1:0:326:G:H8	1.84	0.42
5:A:109:GLU:HG2	5:A:116:GLY:H	1.85	0.42
5:A:113:GLY:HA2	5:A:153:ARG:NH2	2.34	0.42
14:K:49:LEU:CD1	14:K:80:ILE:HD13	2.49	0.42
16:M:15:PRO:HA	16:M:20:LEU:HD23	2.02	0.42
2:9:3004:G:O2'	17:N:44:ARG:NH2	2.53	0.42
1:0:710:G:H5'	18:O:25:VAL:CG1	2.49	0.42
1:0:107:U:H2'	1:0:108:U:H5'	2.02	0.42
1:0:1298:U:H2'	1:0:1299:G:H8	1.85	0.42
1:0:1422:U:H2'	1:0:1423:C:C6	2.55	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.20	0.42
1:0:470:U:O2'	30:1:16:HIS:CD2	2.70	0.42
1:0:564:G:H1'	40:0:6803:HOH:O	2.18	0.42
2:9:3023:U:O2'	2:9:3024:U:H4'	2.19	0.42
7:C:133:ARG:HE	7:C:138:VAL:HG22	1.85	0.42
13:J:74:ARG:HH12	13:J:76:ASP:CB	2.30	0.42
17:N:36:ALA:HB1	17:N:118:ILE:HD12	2.02	0.42
18:O:38:ARG:NH1	40:O:7674:HOH:O	2.53	0.42
23:T:12:ARG:NH1	40:T:3035:HOH:O	2.47	0.42
25:V:1:THR:CG2	25:V:2:VAL:N	2.82	0.42
26:W:73:LEU:HA	26:W:73:LEU:HD12	1.83	0.42
1:0:1205:U:C2'	1:0:1206:U:H5''	2.50	0.42
1:0:271:C:C2	1:0:273:G:O4'	2.73	0.42
1:0:2821:C:H4'	6:B:116:PRO:HG3	2.01	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.20	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
5:A:51:ARG:NH1	5:A:120:ARG:O	2.53	0.42
6:B:17:LYS:O	6:B:260:HIS:CD2	2.70	0.42
7:C:218:VAL:N	40:C:9232:HOH:O	2.52	0.42
10:F:67:ALA:HB1	10:F:72:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:14:TYR:CD2	12:H:94:VAL:HB	2.54	0.42
33:I:118:SER:HB2	33:I:123:ASN:HB2	2.02	0.42
15:L:6:ARG:NH2	40:L:9444:HOH:O	2.53	0.42
20:Q:94:GLN:O	20:Q:95:GLU:HB2	2.20	0.42
27:X:7:GLU:HA	27:X:75:ALA:HA	2.00	0.42
1:O:1733:A:H4'	6:B:212:GLN:HA	2.02	0.42
1:O:2716:G:H5''	6:B:206:THR:CG2	2.45	0.42
1:O:380:A:H2'	40:O:7673:HOH:O	2.19	0.42
1:O:695:C:H2'	1:O:696:C:C6	2.54	0.42
5:A:33:GLU:OE1	5:A:33:GLU:N	2.36	0.42
6:B:277:GLU:N	6:B:278:PRO:CD	2.82	0.42
10:F:99:THR:HG23	10:F:99:THR:O	2.19	0.42
11:G:23:ILE:O	11:G:27:ILE:HG13	2.20	0.42
12:H:51:VAL:CG1	12:H:53:GLU:O	2.67	0.42
14:K:20:CYS:HB2	14:K:29:LEU:HG	2.01	0.42
15:L:133:VAL:HB	40:L:9452:HOH:O	2.19	0.42
16:M:47:ASP:CG	16:M:48:LYS:N	2.73	0.42
17:N:173:ASP:O	17:N:177:GLU:HB2	2.20	0.42
2:9:3006:C:H4'	17:N:35:VAL:HG11	2.02	0.42
17:N:61:ALA:CB	17:N:88:ALA:HB2	2.48	0.42
22:S:51:GLN:NE2	22:S:53:ASN:HD21	1.90	0.42
29:Z:46:ARG:O	29:Z:57:CYS:HA	2.19	0.42
1:O:1314:U:H2'	40:O:6383:HOH:O	2.20	0.42
1:O:1367:A:H2'	1:O:1368:U:O4'	2.19	0.42
1:O:1940:C:H4'	40:O:7785:HOH:O	2.19	0.42
1:O:2089:A:O2'	1:O:2090:G:H5'	2.20	0.42
1:O:2456:A:H2'	1:O:2457:U:H6	1.85	0.42
1:O:2642:G:H2'	1:O:2643:G:O4'	2.20	0.42
1:O:1739:G:H1'	1:O:2726:U:O4	2.20	0.42
32:3:48:ASN:ND2	32:3:50:GLY:H	2.18	0.42
1:O:1363:G:P	7:C:76:ARG:HH22	2.43	0.42
8:D:10:PHE:CD1	8:D:11:HIS:N	2.88	0.42
11:G:63:ARG:HB2	11:G:66:LEU:HG	2.02	0.42
33:I:92:PRO:HD3	40:I:1549:HOH:O	2.19	0.42
15:L:104:ASP:HB2	40:L:9460:HOH:O	2.19	0.42
27:X:80:GLU:HB3	40:X:5564:HOH:O	2.19	0.42
1:O:1311:G:O2'	1:O:1312:G:H5'	2.20	0.41
1:O:1473:U:O2'	1:O:1474:C:H5''	2.20	0.41
1:O:226:A:H1'	1:O:393:G:C5	2.54	0.41
1:O:629:A:H2'	1:O:630:A:O4'	2.20	0.41
32:3:55:VAL:HB	32:3:56:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:69:TYR:O	32:3:77:ALA:HA	2.19	0.41
5:A:122:SER:O	5:A:124:VAL:HG13	2.20	0.41
6:B:62:ARG:CA	6:B:65:MET:HE3	2.49	0.41
7:C:21:VAL:C	7:C:23:GLU:H	2.23	0.41
8:D:167:GLU:OE2	8:D:173:GLU:HB3	2.20	0.41
33:I:74:PRO:C	33:I:112:LYS:HZ1	2.23	0.41
1:0:1242:A:OP2	13:J:60:ARG:NH2	2.46	0.41
1:0:1380:U:O4	1:0:2748:G:O2'	2.28	0.41
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.41
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.41
1:0:2256:G:O2'	1:0:2257:G:H5'	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.85	0.41
1:0:396:U:OP2	32:3:38:ARG:HD2	2.19	0.41
32:3:62:THR:HB	40:3:9487:HOH:O	2.20	0.41
5:A:36:ASP:O	5:A:36:ASP:CG	2.59	0.41
6:B:115:VAL:HA	6:B:116:PRO:HD3	1.93	0.41
40:0:7470:HOH:O	6:B:264:GLU:HG3	2.19	0.41
10:F:70:LYS:C	10:F:72:VAL:H	2.22	0.41
40:0:7460:HOH:O	20:Q:9:GLY:HA2	2.20	0.41
25:V:45:ARG:O	25:V:48:GLU:N	2.53	0.41
5:A:75:GLY:HA2	29:Z:64:PHE:HA	2.02	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.20	0.41
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.35	0.41
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.21	0.41
8:D:163:VAL:HA	40:D:6326:HOH:O	2.20	0.41
8:D:170:TYR:CD1	8:D:170:TYR:N	2.89	0.41
8:D:173:GLU:O	8:D:174:VAL:C	2.59	0.41
12:H:169:GLY:HA3	40:H:9557:HOH:O	2.20	0.41
33:I:80:LYS:HD3	33:I:86:GLU:O	2.20	0.41
19:P:16:VAL:CG1	19:P:17:GLY:N	2.83	0.41
26:W:38:THR:HG22	26:W:39:ASP:H	1.85	0.41
1:0:1086:A:N6	26:W:11:VAL:HG11	2.35	0.41
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.41
1:0:1174:A:C6	1:0:1201:C:H4'	2.55	0.41
1:0:1451:C:H5'	1:0:1505:U:C4	2.56	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
16:M:81:ARG:HG2	16:M:85:ARG:O	2.19	0.41
18:O:14:LEU:HG	18:O:102:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:89:ASN:HB3	19:P:92:GLU:HB2	2.01	0.41
20:Q:28:ARG:HG2	40:Q:4350:HOH:O	2.20	0.41
24:U:47:ARG:HG2	24:U:54:THR:HG21	2.03	0.41
28:Y:154:ARG:HH11	28:Y:154:ARG:CG	2.34	0.41
1:0:1181:A:H2'	1:0:1182:C:H5'	2.03	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.04	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:790:A:H1'	1:0:1710:A:O2'	2.21	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.55	0.41
1:0:20:G:H5''	1:0:510:U:O4	2.21	0.41
5:A:29:HIS:CD2	5:A:153:ARG:HH12	2.37	0.41
5:A:53:ALA:HB3	40:A:9591:HOH:O	2.20	0.41
15:L:145:LEU:C	15:L:147:GLU:H	2.23	0.41
15:L:73:VAL:HG23	15:L:74:THR:N	2.32	0.41
21:R:96:VAL:O	21:R:99:ALA:HB3	2.20	0.41
26:W:5:VAL:O	26:W:52:VAL:CG2	2.68	0.41
1:0:1524:U:HO2'	1:0:1525:G:P	2.44	0.41
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.41
1:0:2324:G:N2	1:0:2377:U:H1'	2.36	0.41
1:0:407:A:H8	40:0:5010:HOH:O	2.03	0.41
5:A:6:GLY:HA3	40:A:9557:HOH:O	2.20	0.41
5:A:36:ASP:HA	5:A:83:GLY:HA3	2.02	0.41
6:B:294:TYR:C	6:B:294:TYR:CD1	2.93	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.67	0.41
6:B:81:ALA:HB1	6:B:142:LEU:HD13	2.03	0.41
33:I:110:GLU:HA	33:I:113:HIS:CD2	2.55	0.41
14:K:2:GLU:O	14:K:3:ALA:C	2.58	0.41
14:K:41:LYS:O	14:K:42:ASN:HB2	2.20	0.41
17:N:170:GLU:O	17:N:174:GLU:HG3	2.21	0.41
26:W:21:LEU:HD22	26:W:26:ILE:HD11	2.02	0.41
1:0:1535:G:H2'	1:0:1536:C:C6	2.56	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.21	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.41
1:0:447:A:OP1	23:T:1:SER:HB2	2.21	0.41
30:1:8:GLN:HE22	30:1:11:LYS:HZ2	1.65	0.41
2:9:3039:U:O2'	2:9:3042:C:H5	2.03	0.41
5:A:30:ARG:HB3	5:A:30:ARG:HE	1.64	0.41
5:A:95:PRO:HA	5:A:153:ARG:HA	2.03	0.41
15:L:35:ARG:HD3	15:L:35:ARG:C	2.41	0.41
15:L:66:VAL:HG23	15:L:67:ARG:N	2.35	0.41
16:M:164:THR:CG2	16:M:166:ALA:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:108:SER:HA	17:N:109:PRO:HD3	1.80	0.41
18:O:45:LEU:CD1	18:O:88:LYS:HD2	2.51	0.41
29:Z:30:GLU:HG2	29:Z:33:MET:CE	2.51	0.41
1:O:1076:G:C2	1:O:1084:C:C2	3.09	0.41
1:O:1427:A:N6	1:O:1440:U:H1'	2.33	0.41
1:O:1594:C:O2'	1:O:1607:A:H4'	2.21	0.41
1:O:1849:G:H1'	1:O:2011:A:N1	2.35	0.41
1:O:2335:C:H2'	1:O:2336:G:C8	2.56	0.41
31:2:11:LEU:HA	31:2:11:LEU:HD23	1.91	0.41
31:2:39:ARG:HG2	40:2:3143:HOH:O	2.21	0.41
6:B:18:ARG:HE	6:B:256:GLN:NE2	2.19	0.41
7:C:61:PHE:HB3	40:C:9251:HOH:O	2.20	0.41
9:E:69:ILE:HA	9:E:72:MET:HE3	2.01	0.41
10:F:12:LEU:HD23	10:F:12:LEU:O	2.21	0.41
13:J:143:LYS:HA	13:J:145:TRP:CZ3	2.55	0.41
15:L:124:ASP:OD1	15:L:149:ARG:NH2	2.54	0.41
15:L:94:ARG:NH1	15:L:143:THR:HG21	2.36	0.41
16:M:76:ARG:HG3	16:M:88:VAL:HG21	2.03	0.41
40:O:3646:HOH:O	19:P:91:LYS:HA	2.21	0.41
21:R:33:ARG:NH1	40:R:9452:HOH:O	2.51	0.41
40:O:4333:HOH:O	23:T:9:LYS:HD2	2.20	0.41
25:V:43:PRO:O	25:V:46:ILE:HG22	2.19	0.41
1:O:1025:C:H5'	26:W:23:MET:O	2.21	0.41
26:W:5:VAL:O	26:W:52:VAL:HG23	2.20	0.41
29:Z:39:CYS:HA	29:Z:40:PRO:HD3	1.97	0.41
1:O:1821:A:O2'	1:O:1822:A:H5'	2.21	0.41
1:O:271:C:H41	1:O:378:A:H2	1.68	0.41
1:O:2748:G:H4'	1:O:2749:U:H5'	2.02	0.41
1:O:2819:C:O4'	6:B:96:PRO:HB2	2.21	0.41
1:O:2820:A:H2'	1:O:2821:C:C6	2.56	0.41
40:O:3421:HOH:O	6:B:252:PRO:HD3	2.21	0.41
6:B:27:ASN:H	6:B:27:ASN:HD22	1.69	0.41
6:B:41:PHE:CD1	6:B:79:MET:CE	3.04	0.41
8:D:23:VAL:O	8:D:23:VAL:HG23	2.21	0.41
10:F:79:GLN:HB2	10:F:82:ASP:OD2	2.21	0.41
33:I:92:PRO:C	33:I:94:GLU:N	2.72	0.41
33:I:93:GLN:HA	33:I:96:PHE:CE2	2.54	0.41
14:K:98:VAL:HG11	14:K:102:GLU:HA	1.99	0.41
1:O:392:U:H5''	16:M:193:LYS:HB3	2.01	0.41
19:P:134:VAL:O	19:P:137:LEU:HB3	2.21	0.41
23:T:81:LYS:HD2	23:T:87:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:45:GLU:HG3	40:X:6178:HOH:O	2.21	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:2336:G:H1'	40:D:5675:HOH:O	2.20	0.41
1:0:284:C:H4'	1:0:285:A:H8	1.86	0.41
1:0:737:A:H3'	1:0:737:A:C8	2.56	0.41
1:0:1882:C:OP1	5:A:192:VAL:HG23	2.21	0.41
1:0:875:A:C2	5:A:194:MET:SD	3.14	0.41
5:A:65:ARG:NH1	5:A:65:ARG:HG2	2.36	0.41
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.33	0.41
6:B:312:ARG:HG2	6:B:313:PRO:N	2.34	0.41
9:E:84:MET:HB2	9:E:131:LEU:HB2	2.03	0.41
1:0:1181:A:H4'	33:I:92:PRO:HG2	2.03	0.41
14:K:107:THR:HG22	14:K:108:GLU:CG	2.44	0.41
14:K:118:ALA:O	14:K:119:GLN:C	2.59	0.41
17:N:33:ARG:NH1	17:N:103:ASP:OD2	2.47	0.41
17:N:24:LEU:HD13	20:Q:26:PRO:HB3	2.02	0.41
26:W:54:PHE:CZ	26:W:140:LYS:HB2	2.55	0.41
27:X:30:MET:CE	27:X:58:ALA:HB3	2.50	0.41
29:Z:36:ASP:HB3	29:Z:45:ASP:O	2.21	0.41
1:0:1453:G:H2'	1:0:1454:U:O4'	2.21	0.41
1:0:1834:C:H2'	1:0:1840:A:N6	2.36	0.41
1:0:2767:C:OP1	6:B:318:ASN:ND2	2.54	0.41
1:0:2828:G:H2'	1:0:2829:G:O4'	2.21	0.41
1:0:791:A:H2'	1:0:792:G:O4'	2.21	0.41
30:1:28:HIS:O	30:1:32:LYS:N	2.49	0.41
31:2:20:ARG:HG3	31:2:21:VAL:H	1.86	0.41
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.41
15:L:120:LEU:HD12	15:L:133:VAL:HG21	2.02	0.41
18:O:14:LEU:HD23	18:O:102:ILE:HD11	2.02	0.41
18:O:60:VAL:C	18:O:62:GLY:H	2.24	0.41
21:R:68:HIS:CD2	21:R:76:ASP:HB2	2.56	0.41
24:U:17:THR:HG21	40:U:3194:HOH:O	2.21	0.41
26:W:4:LEU:HD23	26:W:54:PHE:HB3	2.03	0.41
28:Y:178:HIS:CG	28:Y:179:PRO:HD2	2.56	0.41
1:0:1724:U:H5''	40:0:4311:HOH:O	2.19	0.40
1:0:1816:C:H2'	1:0:1817:U:O4'	2.21	0.40
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.40
1:0:2720:C:O2	14:K:87:ARG:NH2	2.54	0.40
1:0:556:C:H2'	1:0:557:C:H6	1.86	0.40
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.40
5:A:135:VAL:HG13	5:A:135:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:140:VAL:HG12	7:C:141:SER:N	2.36	0.40
7:C:72:LYS:HG2	7:C:77:ALA:HA	2.02	0.40
9:E:7:ILE:HD11	9:E:11:VAL:C	2.41	0.40
12:H:114:ARG:O	12:H:115:ALA:C	2.60	0.40
40:O:9644:HOH:O	15:L:30:ARG:HD2	2.20	0.40
25:V:1:THR:OG1	25:V:2:VAL:N	2.53	0.40
28:Y:186:ARG:HG2	28:Y:186:ARG:NH1	2.36	0.40
1:O:1119:G:C6	1:O:1244:U:C5	3.09	0.40
1:O:2329:C:O2'	1:O:2330:U:H5'	2.21	0.40
1:O:2361:A:H2'	1:O:2362:A:O4'	2.21	0.40
1:O:2748:G:C5'	40:O:7972:HOH:O	2.69	0.40
5:A:38:ILE:HD13	5:A:38:ILE:HA	1.92	0.40
6:B:278:PRO:HD3	6:B:294:TYR:CE2	2.56	0.40
8:D:21:VAL:HA	8:D:131:THR:O	2.21	0.40
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.51	0.40
10:F:72:VAL:HA	10:F:73:PRO:HD3	1.92	0.40
17:N:37:ARG:HA	17:N:37:ARG:HD3	1.69	0.40
20:Q:43:ILE:HG13	20:Q:52:PHE:CZ	2.56	0.40
25:V:1:THR:O	25:V:2:VAL:C	2.59	0.40
26:W:4:LEU:CD1	26:W:24:LEU:HD13	2.51	0.40
1:O:120:A:H2'	1:O:120:A:N3	2.37	0.40
1:O:1589:G:N2	1:O:1605:G:H1'	2.35	0.40
1:O:1829:A:C8	1:O:1885:A:C8	3.09	0.40
1:O:2824:C:C5'	1:O:2825:C:H5'	2.51	0.40
5:A:43:VAL:O	5:A:44:ASP:HB2	2.21	0.40
5:A:81:GLN:H	5:A:92:ASN:CG	2.24	0.40
5:A:85:SER:O	5:A:86:ALA:C	2.60	0.40
6:B:81:ALA:O	6:B:186:GLY:HA3	2.22	0.40
6:B:279:THR:HG23	6:B:280:VAL:N	2.35	0.40
6:B:60:SER:HA	6:B:61:PRO:HD3	1.92	0.40
1:O:2101:A:H5'	7:C:63:SER:HB3	2.04	0.40
7:C:84:VAL:HG12	7:C:85:LYS:HG2	2.04	0.40
8:D:91:ALA:HB2	8:D:106:PHE:CD2	2.56	0.40
8:D:67:ASP:O	8:D:69:ILE:HG13	2.21	0.40
12:H:78:GLY:C	12:H:80:GLU:H	2.25	0.40
17:N:103:ASP:OD1	17:N:103:ASP:C	2.60	0.40
23:T:18:GLU:O	23:T:21:LYS:HG2	2.22	0.40
25:V:42:ASN:HB3	40:V:7247:HOH:O	2.21	0.40
25:V:8:ILE:CG2	25:V:59:ILE:HG13	2.51	0.40
28:Y:115:ARG:NE	40:Y:9353:HOH:O	2.55	0.40
28:Y:187:VAL:CG1	28:Y:205:ILE:HG12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:96:GLU:O	28:Y:235:GLU:HA	2.21	0.40
1:0:1235:G:C1'	13:J:63:ILE:HG23	2.51	0.40
1:0:1299:G:N2	40:0:5226:HOH:O	2.53	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.21	0.40
1:0:294:C:H2'	1:0:295:C:O4'	2.21	0.40
40:0:7989:HOH:O	32:3:60:LYS:HG3	2.21	0.40
15:L:65:ASP:CG	15:L:111:ALA:HB3	2.42	0.40
18:O:59:VAL:HG23	18:O:111:VAL:HG23	2.02	0.40
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.56	0.40
1:0:1081:A:H5''	40:0:3742:HOH:O	2.21	0.40
1:0:1626:A:H2'	1:0:1627:G:C5'	2.52	0.40
1:0:2819:C:H2'	1:0:2820:A:C8	2.56	0.40
1:0:423:A:O2'	1:0:424:C:H5'	2.21	0.40
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.40
30:1:25:LYS:CG	31:2:49:GLU:H	2.35	0.40
32:3:30:GLN:HE21	32:3:30:GLN:HB3	1.61	0.40
2:9:3002:U:OP2	2:9:3003:A:H5'	2.22	0.40
2:9:3008:G:OP1	17:N:23:ARG:NH1	2.51	0.40
2:9:3091:C:H2'	2:9:3092:G:O4'	2.22	0.40
1:0:1881:A:OP1	5:A:199:HIS:HE1	2.04	0.40
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.52	0.40
7:C:57:PRO:HG2	7:C:73:LEU:CD1	2.51	0.40
11:G:16:LYS:O	11:G:20:VAL:HG23	2.22	0.40
13:J:103:VAL:HG12	40:J:5907:HOH:O	2.21	0.40
13:J:80:LYS:HE2	13:J:98:PHE:CZ	2.56	0.40
15:L:67:ARG:HB2	15:L:112:GLY:HA3	2.03	0.40
18:O:23:GLY:C	40:O:3062:HOH:O	2.59	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	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	13	18
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	11	15
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	21	31
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	6	6
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	6	6
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	5	4
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	21	31
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	12	17
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	31	44
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	2	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	10	13
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	2	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	2
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	6	7
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	16	22
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	5	4
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	11	15

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER
13	J	143	LYS
15	L	80	ASP
17	N	154	LEU
17	N	184	ILE
29	Z	81	ARG
5	A	37	VAL
6	B	34	GLY
8	D	27	ILE
8	D	61	PHE
8	D	65	GLU
12	H	168	ALA
15	L	143	THR
16	M	83	SER
23	T	53	GLY
25	V	43	PRO
29	Z	20	ARG
31	2	37	HIS
33	I	129	VAL
5	A	86	ALA
6	B	185	GLY
8	D	28	GLY
8	D	56	ARG
8	D	164	ALA
10	F	71	GLY
17	N	183	ASP
23	T	46	ASP
5	A	34	ASP
7	C	8	LEU
7	C	58	ALA
8	D	171	ASP
12	H	16	ARG
12	H	81	GLY
13	J	5	GLU
13	J	7	ASP
17	N	65	ASP
17	N	155	GLU
17	N	162	ASP
8	D	77	ASP

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Mol	Chain	Res	Type
10	F	100	ASP
14	K	126	SER
17	N	164	ASP
17	N	167	ASP
29	Z	42	CYS
32	3	56	PRO
6	B	2	GLN
8	D	16	PRO
13	J	65	ASN
17	N	68	GLU
25	V	40	PRO
25	V	2	VAL
6	B	181	ILE
33	I	73	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	
5	A	179/182 (98%)	165 (92%)	14 (8%)	14	21
6	B	282/283 (100%)	267 (95%)	15 (5%)	25	40
7	C	193/193 (100%)	173 (90%)	20 (10%)	8	11
8	D	117/148 (79%)	112 (96%)	5 (4%)	32	49
9	E	152/156 (97%)	146 (96%)	6 (4%)	35	54
10	F	93/94 (99%)	91 (98%)	2 (2%)	55	74
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	36	55
13	J	118/121 (98%)	108 (92%)	10 (8%)	12	18
14	K	106/106 (100%)	101 (95%)	5 (5%)	29	45
15	L	113/127 (89%)	110 (97%)	3 (3%)	48	68
16	M	158/158 (100%)	153 (97%)	5 (3%)	42	62
17	N	149/150 (99%)	142 (95%)	7 (5%)	29	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	O	93/94 (99%)	92 (99%)	1 (1%)	76	88
19	P	113/117 (97%)	110 (97%)	3 (3%)	48	68
20	Q	79/80 (99%)	75 (95%)	4 (5%)	26	42
21	R	117/122 (96%)	114 (97%)	3 (3%)	49	70
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	36	55
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	58	77
26	W	130/130 (100%)	124 (95%)	6 (5%)	29	46
27	X	66/74 (89%)	63 (96%)	3 (4%)	30	47
28	Y	120/196 (61%)	109 (91%)	11 (9%)	10	15
29	Z	60/68 (88%)	59 (98%)	1 (2%)	63	80
30	1	46/47 (98%)	45 (98%)	1 (2%)	55	74
31	2	42/46 (91%)	41 (98%)	1 (2%)	52	72
32	3	79/79 (100%)	77 (98%)	2 (2%)	50	71
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	30	47

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	26	ASP
5	A	33	GLU
5	A	36	ASP
5	A	62	ASP
5	A	78	ASP
5	A	94	LEU
5	A	120	ARG
5	A	131	HIS
5	A	151	GLN
5	A	165	THR
5	A	179	MET
5	A	206	ARG
5	A	217	ARG
6	B	11	LEU

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Mol	Chain	Res	Type
6	B	27	ASN
6	B	82	VAL
6	B	84	LEU
6	B	98	THR
6	B	103	ASP
6	B	113	LEU
6	B	149	ASP
6	B	162	MET
6	B	190	MET
6	B	254	GLN
6	B	277	GLU
6	B	279	THR
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	16	VAL
7	C	27	ARG
7	C	67	GLN
7	C	76	ARG
7	C	78	ARG
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	162	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	243	VAL
8	D	24	HIS
8	D	61	PHE
8	D	100	ASP
8	D	133	ASN
8	D	137	PRO
9	E	7	ILE
9	E	102	VAL
9	E	108	LEU

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Mol	Chain	Res	Type
9	E	155	ASN
9	E	156	ASP
9	E	164	ASP
10	F	12	LEU
10	F	46	GLU
12	H	18	GLU
12	H	84	LYS
12	H	88	ARG
12	H	154	TYR
12	H	159	PRO
13	J	7	ASP
13	J	45	VAL
13	J	46	ILE
13	J	52	GLN
13	J	70	PHE
13	J	74	ARG
13	J	79	PHE
13	J	107	ASN
13	J	127	ILE
13	J	131	THR
14	K	4	LEU
14	K	10	GLN
14	K	56	SER
14	K	84	ASP
14	K	100	GLU
15	L	35	ARG
15	L	43	HIS
15	L	140	VAL
16	M	46	LEU
16	M	68	ARG
16	M	93	ARG
16	M	99	ARG
16	M	116	ASN
17	N	17	ARG
17	N	23	ARG
17	N	26	LEU
17	N	49	THR
17	N	65	ASP
17	N	139	TRP
17	N	152	GLU
18	O	111	VAL
19	P	52	LYS

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Mol	Chain	Res	Type
19	P	98	ILE
19	P	117	SER
20	Q	11	ARG
20	Q	16	ASN
20	Q	57	ASP
20	Q	95	GLU
21	R	13	THR
21	R	132	ARG
21	R	143	VAL
23	T	5	ASP
23	T	39	ASN
23	T	80	GLU
23	T	89	ARG
25	V	65	ASP
26	W	26	ILE
26	W	35	VAL
26	W	78	ASP
26	W	122	ARG
26	W	142	ASP
26	W	146	ILE
27	X	72	VAL
27	X	79	GLU
27	X	82	GLU
28	Y	103	THR
28	Y	141	THR
28	Y	144	ARG
28	Y	154	ARG
28	Y	163	THR
28	Y	174	VAL
28	Y	187	VAL
28	Y	189	ASN
28	Y	200	THR
28	Y	231	PRO
28	Y	235	GLU
29	Z	44	GLU
30	1	47	ASP
31	2	18	ASN
32	3	11	CYS
32	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	29	HIS
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	221	GLN
6	B	238	ASN
6	B	256	GLN
6	B	260	HIS
6	B	320	GLN
6	B	332	ASN
7	C	2	GLN
7	C	39	GLN
7	C	129	HIS
8	D	47	GLN
8	D	103	ASN
8	D	133	ASN
9	E	106	ASN
9	E	143	GLN
11	G	64	ASN
12	H	56	GLN
12	H	59	HIS
12	H	70	ASN
12	H	170	ASN
13	J	52	GLN
13	J	107	ASN
14	K	10	GLN
15	L	18	HIS
15	L	41	HIS
15	L	42	ASN
16	M	24	GLN
16	M	77	HIS
16	M	170	ASN
17	N	93	GLN
17	N	107	ASN
17	N	153	GLN
18	O	100	GLN
19	P	50	GLN
19	P	66	GLN
19	P	73	HIS
19	P	88	GLN
19	P	89	ASN
19	P	118	GLN
20	Q	16	ASN

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Mol	Chain	Res	Type
20	Q	40	HIS
21	R	61	GLN
21	R	94	ASN
21	R	98	ASN
21	R	113	HIS
21	R	117	HIS
22	S	44	GLN
22	S	53	ASN
22	S	55	GLN
23	T	37	GLN
23	T	39	ASN
24	U	39	ASN
24	U	48	ASN
25	V	60	GLN
26	W	2	HIS
26	W	28	HIS
26	W	110	GLN
26	W	119	HIS
26	W	125	HIS
26	W	141	HIS
27	X	22	ASN
27	X	23	HIS
28	Y	119	GLN
28	Y	134	HIS
28	Y	149	GLN
28	Y	189	ASN
29	Z	41	ASN
30	1	8	GLN
30	1	16	HIS
30	1	28	HIS
31	2	16	ASN
31	2	18	ASN
31	2	41	HIS
31	2	45	ASN
32	3	30	GLN
32	3	48	ASN
33	I	113	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	33 (1%)

All (249) 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	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A

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Mol	Chain	Res	Type
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G

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Mol	Chain	Res	Type
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
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	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1528	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	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	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U

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Mol	Chain	Res	Type
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U

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Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G

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Mol	Chain	Res	Type
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
4	5	76	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A

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Mol	Chain	Res	Type
1	0	2852	A
2	9	3065	A

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

8 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	1.00	2 (14%)	18,31,34	3.61	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.08	2 (10%)	22,38,41	2.47	4 (18%)
1	UR3	0	2619	1,38	13,22,23	0.96	0	15,32,35	0.67	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	5.42	4 (20%)
1	1MA	0	628	1,36	16,25,26	1.03	1 (6%)	12,37,40	1.25	1 (8%)
3	PPU	4	76	1,3	17,26,41	0.71	0	16,38,60	1.03	1 (6%)
3	HFA	4	77	3	11,11,12	0.88	1 (9%)	13,13,15	0.73	1 (7%)
4	ACA	5	78	4	7,7,8	2.14	1 (14%)	5,6,8	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,38	-	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	1,36	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1
4	ACA	5	78	4	-	0/4/5/6	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	78	ACA	C3-C2	-5.05	1.32	1.52
1	0	2621	PSU	C5-C1'	-4.71	1.48	1.52
1	0	2588	OMG	C8-N7	-2.16	1.30	1.34
1	0	2587	OMU	C6-C5	-2.09	1.33	1.38
3	4	77	HFA	OA-CA	2.13	1.48	1.43
1	0	2621	PSU	C2-N1	2.58	1.43	1.38
1	0	2587	OMU	C4-N3	2.65	1.37	1.33
1	0	628	1MA	C6-N6	2.98	1.34	1.27
1	0	2621	PSU	C4-N3	3.17	1.38	1.33
1	0	2588	OMG	C6-N1	3.31	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	-17.23	114.56	128.41
1	0	2621	PSU	C5-C4-N3	-8.31	114.65	125.36
1	0	2588	OMG	C5-C6-N1	-8.29	111.69	123.47
1	0	628	1MA	C2-N3-C4	-3.72	110.83	116.51
1	0	2587	OMU	C5-C4-N3	-3.60	114.82	123.17
1	0	2588	OMG	C2-N3-C4	-2.79	111.91	115.16
1	0	2588	OMG	N3-C2-N1	-2.39	123.91	127.41
3	4	77	HFA	CB-CA-C	-2.03	107.83	111.64
1	0	2621	PSU	C6-N1-C2	2.78	119.80	115.36
3	4	76	PPU	C2-N1-C6	2.91	118.88	111.81
1	0	2588	OMG	C6-N1-C2	6.31	125.14	116.06
1	0	2621	PSU	C4-N3-C2	14.22	127.24	115.14
1	0	2587	OMU	C4-N3-C2	14.73	126.81	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	3	0
1	0	2619	UR3	1	0
3	4	76	PPU	1	0
4	5	78	ACA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.63	62 (2%) 60 57	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.24	6 (4%) 29 28	41, 69, 93, 152	0
3	4	2/4 (50%)	-1.10	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	-0.08	1 (25%) 0 0	55, 57, 58, 66	0
5	A	237/240 (98%)	0.33	13 (5%) 25 24	31, 54, 86, 106	0
6	B	337/338 (99%)	0.14	11 (3%) 46 44	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.06	1 (0%) 92 91	27, 49, 70, 87	0
8	D	140/177 (79%)	1.71	44 (31%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.74	24 (13%) 2 2	44, 66, 86, 92	0
10	F	119/120 (99%)	1.00	27 (22%) 0 0	49, 74, 100, 112	0
11	G	29/348 (8%)	2.39	18 (62%) 0 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.60	16 (10%) 7 6	47, 65, 96, 103	0
13	J	142/145 (97%)	-0.01	3 (2%) 63 60	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.15	2 (1%) 73 71	37, 48, 71, 84	0
15	L	145/165 (87%)	0.60	15 (10%) 6 6	29, 69, 112, 121	0
16	M	194/194 (100%)	0.52	19 (9%) 7 7	37, 48, 85, 93	0
17	N	186/187 (99%)	0.90	33 (17%) 1 1	49, 68, 112, 119	0
18	O	115/116 (99%)	0.16	2 (1%) 70 67	40, 59, 73, 81	0
19	P	143/149 (95%)	0.24	3 (2%) 63 60	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.05	4 (4%) 36 34	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.14	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.30	3 (3%) 41 40	43, 61, 84, 97	0
23	T	119/120 (99%)	0.67	11 (9%) 9 8	41, 59, 85, 110	0
24	U	53/66 (80%)	0.26	2 (3%) 40 39	42, 56, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.61	16 (24%) 0 0	56, 78, 115, 120	0
26	W	154/154 (100%)	0.02	2 (1%) 77 75	40, 53, 74, 82	0
27	X	82/92 (89%)	0.67	13 (15%) 2 1	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.10	8 (5%) 24 23	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.74	29 (39%) 0 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.43	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.44	15 (32%) 0 0	41, 68, 96, 102	0
32	3	92/92 (100%)	0.33	6 (6%) 19 17	41, 61, 73, 86	0
33	I	70/162 (43%)	5.01	57 (81%) 0 0	111, 125, 142, 144	0
All	All	6652/7484 (88%)	0.03	466 (7%) 16 14	24, 54, 100, 153	0

All (466) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	71	GLY	15.4
25	V	1	THR	14.2
33	I	79	ILE	12.3
33	I	76	ALA	12.1
33	I	133	THR	11.9
8	D	63	ILE	11.6
29	Z	11	SER	11.4
23	T	119	ALA	10.9
2	9	3001	U	10.2
33	I	85	PHE	10.0
17	N	166	ALA	9.5
8	D	57	THR	9.2
16	M	70	GLY	9.0
29	Z	22	SER	8.9
31	2	49	GLU	8.8
33	I	88	GLY	8.5
25	V	40	PRO	8.5
25	V	39	ALA	8.2
33	I	121	LEU	8.2
33	I	81	ASP	8.1
33	I	75	THR	8.1
33	I	77	GLU	7.9
33	I	137	VAL	7.9
33	I	116	LEU	7.8
33	I	91	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
33	I	105	VAL	7.7
16	M	79	ALA	7.7
33	I	118	SER	7.4
33	I	129	VAL	7.4
33	I	109	ALA	7.4
33	I	87	THR	7.2
33	I	96	PHE	7.1
8	D	90	LEU	7.1
33	I	78	LEU	7.0
5	A	37	VAL	6.8
33	I	126	LYS	6.8
31	2	48	ASP	6.6
2	9	3024	U	6.4
33	I	113	HIS	6.4
33	I	132	CYS	6.3
5	A	237	GLY	6.3
33	I	89	SER	6.3
1	0	282	C	6.1
29	Z	20	ARG	6.0
33	I	93	GLN	5.9
33	I	108	ILE	5.9
23	T	118	SER	5.8
31	2	39	ARG	5.8
29	Z	45	ASP	5.7
33	I	74	PRO	5.5
33	I	111	GLN	5.5
8	D	69	ILE	5.5
25	V	38	GLY	5.5
33	I	107	GLN	5.4
16	M	74	LYS	5.4
27	X	88	GLU	5.4
8	D	64	ARG	5.3
2	9	3023	U	5.2
33	I	83	ALA	5.2
29	Z	18	TYR	5.2
33	I	104	GLN	5.1
31	2	41	HIS	5.1
33	I	80	LYS	5.1
16	M	75	ARG	5.0
27	X	80	GLU	5.0
29	Z	25	ARG	5.0
14	K	132	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
17	N	155	GLU	5.0
29	Z	12	GLY	5.0
33	I	98	ALA	5.0
11	G	26	MET	4.9
11	G	69	ARG	4.9
16	M	86	GLN	4.9
25	V	41	GLU	4.8
29	Z	32	GLU	4.8
1	0	1951	G	4.8
1	0	1199	A	4.8
8	D	61	PHE	4.8
29	Z	21	VAL	4.8
17	N	68	GLU	4.7
33	I	125	ALA	4.7
16	M	71	SER	4.6
29	Z	14	PHE	4.6
16	M	87	GLY	4.6
33	I	138	THR	4.6
15	L	81	VAL	4.6
29	Z	23	ARG	4.6
11	G	23	ILE	4.6
11	G	71	LEU	4.5
31	2	44	ARG	4.5
31	2	47	THR	4.5
33	I	86	GLU	4.5
33	I	102	VAL	4.5
17	N	163	PHE	4.4
8	D	66	GLY	4.4
8	D	170	TYR	4.4
17	N	175	LEU	4.4
2	9	3002	U	4.3
23	T	117	ASP	4.3
1	0	1177	A	4.3
1	0	1172	G	4.3
1	0	2237	G	4.3
1	0	497	A	4.3
1	0	1169	U	4.3
11	G	27	ILE	4.2
17	N	147	ILE	4.2
23	T	116	ASP	4.2
11	G	66	LEU	4.2
9	E	10	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
33	I	114	PRO	4.2
27	X	77	PHE	4.2
12	H	138	CYS	4.2
8	D	44	ILE	4.1
9	E	45	ASP	4.1
1	0	2004	U	4.1
29	Z	37	HIS	4.0
1	0	2508	C	4.0
29	Z	34	ASN	4.0
12	H	73	LEU	4.0
15	L	80	ASP	4.0
12	H	74	ILE	4.0
8	D	26	GLY	4.0
1	0	280	C	4.0
28	Y	216	ARG	4.0
12	H	78	GLY	3.9
33	I	112	LYS	3.9
15	L	93	VAL	3.9
31	2	38	LYS	3.9
28	Y	235	GLU	3.9
8	D	134	LEU	3.9
33	I	122	THR	3.8
10	F	107	ASP	3.8
27	X	41	PHE	3.8
29	Z	24	ARG	3.8
10	F	28	ALA	3.8
8	D	92	GLU	3.7
5	A	31	LYS	3.7
8	D	56	ARG	3.7
15	L	76	LEU	3.7
5	A	133	ARG	3.7
1	0	285	A	3.7
29	Z	33	MET	3.7
1	0	2511	A	3.6
16	M	78	LYS	3.6
25	V	59	ILE	3.6
8	D	154	LYS	3.6
33	I	119	TYR	3.6
12	H	146	VAL	3.6
8	D	10	PHE	3.5
29	Z	19	GLY	3.5
8	D	73	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
9	E	100	ASP	3.5
25	V	37	GLY	3.5
16	M	77	HIS	3.5
1	0	970	U	3.5
9	E	87	PHE	3.5
33	I	134	SER	3.5
1	0	1173	A	3.5
31	2	42	TRP	3.5
29	Z	31	SER	3.5
25	V	36	ALA	3.4
9	E	86	VAL	3.4
10	F	117	GLU	3.4
8	D	40	ILE	3.4
8	D	128	LEU	3.4
31	2	35	ARG	3.4
33	I	99	ASP	3.4
8	D	166	ILE	3.4
17	N	185	GLU	3.4
15	L	97	VAL	3.4
27	X	7	GLU	3.4
17	N	178	THR	3.4
1	0	960	G	3.4
1	0	1198	U	3.4
15	L	100	ALA	3.4
15	L	91	VAL	3.4
33	I	84	GLY	3.3
8	D	88	LEU	3.3
32	3	92	GLU	3.3
1	0	1202	A	3.3
25	V	63	GLU	3.3
22	S	81	ILE	3.3
25	V	8	ILE	3.3
23	T	82	THR	3.3
5	A	36	ASP	3.3
1	0	1948	G	3.3
1	0	2645	U	3.3
1	0	514	G	3.3
16	M	81	ARG	3.3
8	D	18	ILE	3.3
10	F	16	ALA	3.3
8	D	27	ILE	3.3
17	N	95	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
5	A	35	GLY	3.3
16	M	80	GLY	3.2
16	M	72	ALA	3.2
22	S	20	PHE	3.2
33	I	117	LEU	3.2
29	Z	29	ILE	3.2
1	0	1163	G	3.2
8	D	68	PRO	3.2
1	0	2238	A	3.2
8	D	62	ASP	3.2
1	0	1965	C	3.2
27	X	85	VAL	3.2
1	0	272	A	3.2
8	D	41	LEU	3.2
1	0	1966	U	3.2
17	N	184	ILE	3.2
17	N	134	ASP	3.2
15	L	60	GLU	3.2
29	Z	30	GLU	3.2
15	L	145	LEU	3.2
33	I	120	ASP	3.1
8	D	172	VAL	3.1
9	E	124	VAL	3.1
10	F	100	ASP	3.1
15	L	120	LEU	3.1
31	2	27	LEU	3.1
31	2	26	MET	3.1
12	H	171	ALA	3.1
33	I	123	ASN	3.1
8	D	53	LYS	3.1
6	B	104	GLU	3.1
10	F	17	LEU	3.1
33	I	73	PRO	3.1
16	M	76	ARG	3.1
17	N	2	THR	3.1
5	A	32	VAL	3.1
8	D	11	HIS	3.1
13	J	70	PHE	3.1
29	Z	10	ARG	3.1
9	E	127	ASP	3.0
1	0	1950	G	3.0
5	A	65	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
17	N	139	TRP	3.0
17	N	180	LEU	3.0
20	Q	95	GLU	3.0
1	0	735	C	3.0
9	E	88	TYR	3.0
1	0	716	G	3.0
6	B	2	GLN	3.0
10	F	49	PHE	3.0
8	D	107	GLY	3.0
15	L	102	ASP	2.9
33	I	82	GLU	2.9
31	2	37	HIS	2.9
11	G	22	ALA	2.9
28	Y	95	THR	2.9
33	I	72	VAL	2.9
1	0	1180	U	2.9
1	0	284	C	2.9
8	D	173	GLU	2.9
10	F	44	SER	2.9
1	0	1168	C	2.9
17	N	179	LEU	2.9
1	0	358	G	2.9
9	E	6	GLU	2.9
12	H	47	ILE	2.9
29	Z	59	TYR	2.9
8	D	85	GLN	2.9
11	G	73	ASP	2.9
10	F	106	ALA	2.9
12	H	149	ALA	2.9
10	F	22	VAL	2.9
33	I	94	GLU	2.9
1	0	1981	A	2.8
25	V	3	LEU	2.8
10	F	119	ARG	2.8
24	U	47	ARG	2.8
10	F	99	THR	2.8
29	Z	16	ALA	2.8
11	G	72	ASP	2.8
29	Z	26	VAL	2.8
29	Z	36	ASP	2.8
33	I	115	ASP	2.8
1	0	281	U	2.8

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Mol	Chain	Res	Type	RSRZ
10	F	110	ASP	2.8
17	N	67	ALA	2.8
24	U	43	GLY	2.8
11	G	63	ARG	2.8
23	T	112	LEU	2.8
19	P	18	LYS	2.8
8	D	51	ARG	2.8
16	M	82	ARG	2.8
1	0	1200	A	2.8
17	N	138	ASP	2.8
32	3	41	GLU	2.8
8	D	93	LEU	2.8
8	D	89	PRO	2.8
9	E	4	GLU	2.7
1	0	138	U	2.7
1	0	1171	A	2.7
8	D	91	ALA	2.7
8	D	106	PHE	2.7
10	F	12	LEU	2.7
11	G	12	ILE	2.7
17	N	156	GLU	2.7
1	0	1170	U	2.7
13	J	5	GLU	2.7
17	N	71	TRP	2.7
1	0	999	C	2.7
6	B	117	GLU	2.7
25	V	2	VAL	2.7
17	N	165	ALA	2.7
11	G	67	LEU	2.7
12	H	130	GLY	2.7
1	0	1625	U	2.7
11	G	24	VAL	2.7
1	0	10	U	2.7
8	D	167	GLU	2.7
25	V	14	ALA	2.7
27	X	71	ARG	2.7
9	E	11	VAL	2.6
10	F	108	VAL	2.6
12	H	143	ALA	2.6
1	0	1164	U	2.6
12	H	37	GLN	2.6
6	B	180	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
17	N	160	SER	2.6
1	O	1192	A	2.6
16	M	89	THR	2.6
9	E	99	GLY	2.6
27	X	10	VAL	2.6
1	O	1967	U	2.6
28	Y	102	LEU	2.6
10	F	25	ASP	2.6
10	F	98	VAL	2.6
16	M	73	ARG	2.6
17	N	1	ALA	2.6
33	I	97	VAL	2.6
25	V	43	PRO	2.6
10	F	21	GLU	2.6
17	N	159	TYR	2.6
20	Q	18	PRO	2.6
7	C	61	PHE	2.6
8	D	65	GLU	2.6
5	A	85	SER	2.5
11	G	25	GLU	2.5
16	M	84	LYS	2.5
9	E	118	ILE	2.5
17	N	172	PHE	2.5
28	Y	234	VAL	2.5
10	F	70	LYS	2.5
6	B	1	PRO	2.5
17	N	137	ALA	2.5
1	O	2769	C	2.5
10	F	75	ILE	2.5
9	E	44	GLY	2.5
19	P	114	LEU	2.5
6	B	183	GLU	2.5
13	J	4	ALA	2.5
8	D	104	PHE	2.5
20	Q	76	VAL	2.4
1	O	1525	G	2.4
33	I	135	LEU	2.4
27	X	43	VAL	2.4
23	T	77	VAL	2.4
1	O	283	U	2.4
11	G	70	ALA	2.4
5	A	99	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	0	370	G	2.4
11	G	15	TRP	2.4
28	Y	96	GLU	2.4
15	L	79	ASP	2.4
17	N	65	ASP	2.4
12	H	66	ARG	2.4
6	B	128	ILE	2.4
5	A	97	ALA	2.4
23	T	109	GLU	2.4
9	E	126	ILE	2.4
9	E	154	ILE	2.4
32	3	62	THR	2.4
8	D	84	LEU	2.4
9	E	5	LEU	2.4
9	E	48	VAL	2.3
10	F	29	VAL	2.3
1	0	288	A	2.3
2	9	3072	C	2.3
1	0	2748	G	2.3
33	I	103	ASP	2.3
33	I	124	ALA	2.3
8	D	81	GLU	2.3
29	Z	28	GLU	2.3
20	Q	17	LYS	2.3
16	M	85	ARG	2.3
31	2	36	ASN	2.3
1	0	1929	G	2.3
1	0	1947	G	2.3
10	F	15	ASP	2.3
17	N	158	LEU	2.3
31	2	20	ARG	2.3
31	2	43	ARG	2.3
6	B	105	PHE	2.3
1	0	1203	G	2.3
29	Z	35	GLU	2.3
12	H	35	ARG	2.3
27	X	72	VAL	2.3
12	H	111	ASP	2.3
22	S	72	ASP	2.3
11	G	68	GLU	2.3
23	T	115	GLU	2.3
1	0	362	G	2.2

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Mol	Chain	Res	Type	RSRZ
9	E	94	GLN	2.2
17	N	167	ASP	2.2
6	B	134	ALA	2.2
16	M	132	ILE	2.2
27	X	76	ARG	2.2
27	X	65	ASN	2.2
6	B	57	GLU	2.2
28	Y	236	VAL	2.2
8	D	87	ALA	2.2
10	F	24	ARG	2.2
9	E	1	PRO	2.2
14	K	119	GLN	2.2
17	N	106	LEU	2.2
17	N	183	ASP	2.2
28	Y	108	ASP	2.2
12	H	83	TYR	2.2
9	E	161	VAL	2.2
26	W	86	GLU	2.2
15	L	75	LEU	2.2
10	F	19	ALA	2.2
4	5	77	PHE	2.2
17	N	161	GLY	2.2
29	Z	15	GLY	2.2
6	B	119	HIS	2.2
5	A	82	VAL	2.2
8	D	58	VAL	2.2
23	T	110	ALA	2.2
29	Z	27	ALA	2.2
32	3	6	ARG	2.2
15	L	105	TYR	2.1
1	0	359	U	2.1
1	0	371	U	2.1
10	F	11	ASP	2.1
25	V	5	VAL	2.1
27	X	44	ASP	2.1
18	O	23	GLY	2.1
2	9	3122	C	2.1
15	L	148	GLU	2.1
17	N	152	GLU	2.1
18	O	22	GLY	2.1
1	0	2344	G	2.1
10	F	23	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
9	E	105	GLU	2.1
10	F	118	LEU	2.1
25	V	60	GLN	2.1
1	0	1181	A	2.1
1	0	2345	A	2.1
17	N	177	GLU	2.1
9	E	7	ILE	2.1
23	T	59	GLU	2.1
32	3	20	HIS	2.1
29	Z	44	GLU	2.1
1	0	2239	C	2.0
1	0	2747	C	2.0
19	P	110	ASP	2.0
26	W	78	ASP	2.0
5	A	38	ILE	2.0
33	I	110	GLU	2.0
8	D	23	VAL	2.0
9	E	53	GLU	2.0
12	H	137	TYR	2.0
32	3	56	PRO	2.0
11	G	20	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACA	5	78	8/9	0.88	0.30	66,72,83,86	0
3	HFA	4	77	11/12	0.95	0.20	42,44,47,48	0
1	UR3	0	2619	21/22	0.97	0.15	39,42,45,48	0
1	OMG	0	2588	24/25	0.98	0.13	31,34,39,41	0
1	OMU	0	2587	21/22	0.98	0.13	32,37,40,40	0
3	PPU	4	76	24/38	0.98	0.13	41,44,45,49	0
1	1MA	0	628	23/24	0.98	0.12	32,35,37,38	0
1	PSU	0	2621	20/21	0.98	0.14	36,38,43,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9529	1/1	-0.08	0.27	131,131,131,131	0
38	SR	0	9484	1/1	0.32	0.14	149,149,149,149	0
36	NA	0	9184	1/1	0.40	0.41	87,87,87,87	0
38	SR	0	9537	1/1	0.50	0.23	157,157,157,157	0
38	SR	0	9547	1/1	0.52	0.39	194,194,194,194	0
34	MG	0	8047	1/1	0.56	0.54	107,107,107,107	0
36	NA	0	9122	1/1	0.57	0.40	90,90,90,90	0
38	SR	9	9588	1/1	0.59	0.14	143,143,143,143	0
38	SR	B	9521	1/1	0.59	0.63	200,200,200,200	0
34	MG	0	8101	1/1	0.61	0.29	80,80,80,80	0
36	NA	0	9182	1/1	0.63	0.39	90,90,90,90	0
38	SR	0	9501	1/1	0.65	0.20	159,159,159,159	0
34	MG	0	8108	1/1	0.68	0.14	103,103,103,103	0
36	NA	D	9151	1/1	0.70	0.23	68,68,68,68	0
36	NA	0	9181	1/1	0.72	0.16	54,54,54,54	0
36	NA	0	9135	1/1	0.72	0.30	55,55,55,55	0
36	NA	0	9141	1/1	0.74	0.13	73,73,73,73	0
36	NA	9	9183	1/1	0.75	0.38	75,75,75,75	0
35	K	0	9002	1/1	0.75	0.18	88,88,88,88	0
39	CD	Z	9203	1/1	0.75	0.13	84,84,84,84	0
36	NA	0	9114	1/1	0.76	0.20	65,65,65,65	0
36	NA	0	9116	1/1	0.77	0.35	52,52,52,52	0
36	NA	0	9152	1/1	0.77	1.03	83,83,83,83	0
36	NA	0	9126	1/1	0.78	0.11	63,63,63,63	0
34	MG	0	8093	1/1	0.79	0.13	49,49,49,49	0
36	NA	J	9146	1/1	0.79	0.11	55,55,55,55	0
36	NA	0	9129	1/1	0.80	0.13	72,72,72,72	0
34	MG	0	8090	1/1	0.80	0.35	68,68,68,68	0
34	MG	0	8092	1/1	0.82	0.34	77,77,77,77	0
34	MG	0	8065	1/1	0.82	0.34	107,107,107,107	0
34	MG	0	8059	1/1	0.83	0.42	84,84,84,84	0
34	MG	0	8052	1/1	0.83	0.25	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9172	1/1	0.83	0.35	76,76,76,76	0
34	MG	0	8037	1/1	0.84	0.10	46,46,46,46	0
34	MG	0	8104	1/1	0.84	0.13	57,57,57,57	0
36	NA	R	9186	1/1	0.84	0.38	80,80,80,80	0
34	MG	0	8107	1/1	0.84	0.17	65,65,65,65	0
34	MG	0	8013	1/1	0.84	0.34	25,25,25,25	0
34	MG	0	8102	1/1	0.85	0.12	68,68,68,68	0
36	NA	0	9158	1/1	0.85	0.44	66,66,66,66	0
36	NA	0	9185	1/1	0.85	0.61	54,54,54,54	0
34	MG	0	8022	1/1	0.85	0.94	112,112,112,112	0
36	NA	0	9132	1/1	0.86	0.22	68,68,68,68	0
36	NA	0	9161	1/1	0.86	0.72	68,68,68,68	0
34	MG	0	8061	1/1	0.86	0.19	87,87,87,87	0
36	NA	0	9169	1/1	0.86	0.39	116,116,116,116	0
36	NA	0	9164	1/1	0.87	0.57	61,61,61,61	0
34	MG	0	8113	1/1	0.87	0.12	52,52,52,52	0
36	NA	0	9102	1/1	0.87	0.22	63,63,63,63	0
36	NA	S	9112	1/1	0.87	0.23	80,80,80,80	0
35	K	0	9001	1/1	0.87	0.31	74,74,74,74	0
34	MG	0	8030	1/1	0.87	0.08	37,37,37,37	0
38	SR	0	9581	1/1	0.87	0.08	130,130,130,130	0
38	SR	0	9500	1/1	0.88	1.54	200,200,200,200	0
34	MG	0	8089	1/1	0.88	0.17	61,61,61,61	0
34	MG	0	8024	1/1	0.88	0.41	86,86,86,86	0
34	MG	5	8118	1/1	0.88	0.34	45,45,45,45	0
34	MG	0	8050	1/1	0.88	0.22	89,89,89,89	0
34	MG	0	8106	1/1	0.88	0.09	51,51,51,51	0
38	SR	0	9539	1/1	0.88	0.38	157,157,157,157	0
34	MG	0	8091	1/1	0.89	0.15	64,64,64,64	0
38	SR	0	9532	1/1	0.89	0.05	120,120,120,120	0
34	MG	0	8072	1/1	0.89	0.65	89,89,89,89	0
36	NA	0	9143	1/1	0.89	0.14	40,40,40,40	0
36	NA	0	9165	1/1	0.89	0.30	45,45,45,45	0
36	NA	0	9140	1/1	0.89	0.15	57,57,57,57	0
34	MG	0	8103	1/1	0.89	0.17	67,67,67,67	0
36	NA	0	9170	1/1	0.89	0.28	77,77,77,77	0
36	NA	0	9166	1/1	0.89	0.09	74,74,74,74	0
38	SR	0	9590	1/1	0.89	0.12	131,131,131,131	0
34	MG	0	8040	1/1	0.90	0.21	92,92,92,92	0
34	MG	0	8058	1/1	0.90	0.21	41,41,41,41	0
34	MG	0	8025	1/1	0.90	0.42	27,27,27,27	0
36	NA	0	9131	1/1	0.90	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9482	1/1	0.90	0.35	135,135,135,135	0
36	NA	0	9128	1/1	0.90	0.15	49,49,49,49	0
34	MG	0	8014	1/1	0.90	0.38	73,73,73,73	0
34	MG	0	8051	1/1	0.90	0.21	36,36,36,36	0
38	SR	9	9503	1/1	0.90	0.05	122,122,122,122	0
36	NA	0	9168	1/1	0.90	0.17	69,69,69,69	0
38	SR	0	9626	1/1	0.91	0.25	154,154,154,154	0
34	MG	0	8055	1/1	0.91	0.31	97,97,97,97	0
36	NA	0	9111	1/1	0.91	0.31	63,63,63,63	0
36	NA	0	9167	1/1	0.91	0.10	65,65,65,65	0
38	SR	0	9504	1/1	0.91	0.11	108,108,108,108	0
36	NA	0	9177	1/1	0.91	0.35	77,77,77,77	0
34	MG	0	8099	1/1	0.91	0.14	75,75,75,75	0
38	SR	0	9459	1/1	0.91	0.10	103,103,103,103	0
38	SR	0	9468	1/1	0.91	0.05	128,128,128,128	0
34	MG	0	8043	1/1	0.91	0.06	52,52,52,52	0
36	NA	0	9174	1/1	0.91	0.38	65,65,65,65	0
36	NA	0	9179	1/1	0.91	0.60	121,121,121,121	0
37	CL	L	9310	1/1	0.92	0.12	58,58,58,58	0
34	MG	0	8094	1/1	0.92	0.50	72,72,72,72	0
36	NA	0	9101	1/1	0.92	0.13	46,46,46,46	0
34	MG	0	8019	1/1	0.92	0.06	51,51,51,51	0
34	MG	0	8063	1/1	0.92	0.10	65,65,65,65	0
38	SR	0	9465	1/1	0.92	0.10	107,107,107,107	0
38	SR	0	9509	1/1	0.92	0.15	95,95,95,95	0
37	CL	A	9309	1/1	0.92	0.19	66,66,66,66	0
34	MG	0	8032	1/1	0.92	0.10	48,48,48,48	0
34	MG	9	8095	1/1	0.92	0.35	55,55,55,55	0
37	CL	J	9301	1/1	0.93	0.18	60,60,60,60	0
36	NA	0	9113	1/1	0.93	0.11	60,60,60,60	0
36	NA	M	9147	1/1	0.93	0.18	42,42,42,42	0
36	NA	0	9159	1/1	0.93	0.35	58,58,58,58	0
36	NA	0	9173	1/1	0.93	0.34	69,69,69,69	0
36	NA	0	9117	1/1	0.93	0.07	51,51,51,51	0
34	MG	0	8085	1/1	0.93	0.21	63,63,63,63	0
36	NA	0	9106	1/1	0.93	0.44	44,44,44,44	0
34	MG	0	8115	1/1	0.93	0.09	59,59,59,59	0
36	NA	0	9171	1/1	0.93	0.31	61,61,61,61	0
36	NA	0	9124	1/1	0.93	0.19	50,50,50,50	0
34	MG	0	8054	1/1	0.93	0.16	63,63,63,63	0
36	NA	0	9175	1/1	0.93	0.33	55,55,55,55	0
36	NA	0	9120	1/1	0.93	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8036	1/1	0.94	0.11	65,65,65,65	0
34	MG	0	8097	1/1	0.94	0.13	57,57,57,57	0
38	SR	0	9452	1/1	0.94	0.16	106,106,106,106	0
38	SR	0	9508	1/1	0.94	0.08	97,97,97,97	0
34	MG	T	8073	1/1	0.94	0.11	43,43,43,43	0
36	NA	0	9157	1/1	0.94	0.18	47,47,47,47	0
36	NA	0	9150	1/1	0.94	0.21	47,47,47,47	0
36	NA	0	9163	1/1	0.94	0.17	73,73,73,73	0
34	MG	2	8076	1/1	0.94	0.17	64,64,64,64	0
36	NA	0	9110	1/1	0.94	0.33	46,46,46,46	0
39	CD	O	9205	1/1	0.94	0.05	132,132,132,132	0
38	SR	0	9570	1/1	0.94	0.07	111,111,111,111	0
36	NA	0	9149	1/1	0.94	0.29	49,49,49,49	0
34	MG	0	8057	1/1	0.94	0.20	77,77,77,77	0
38	SR	0	9522	1/1	0.95	0.04	114,114,114,114	0
36	NA	0	9155	1/1	0.95	0.18	60,60,60,60	0
34	MG	0	8003	1/1	0.95	0.13	35,35,35,35	0
37	CL	0	9317	1/1	0.95	0.06	52,52,52,52	0
34	MG	0	8068	1/1	0.95	0.14	48,48,48,48	0
34	MG	0	8004	1/1	0.95	0.10	35,35,35,35	0
37	CL	0	9322	1/1	0.95	0.38	61,61,61,61	0
36	NA	0	9125	1/1	0.95	0.81	92,92,92,92	0
38	SR	H	9486	1/1	0.95	0.15	125,125,125,125	0
38	SR	0	9517	1/1	0.95	0.06	110,110,110,110	0
34	MG	0	8082	1/1	0.95	0.20	82,82,82,82	0
38	SR	0	9505	1/1	0.95	0.07	106,106,106,106	0
38	SR	0	9483	1/1	0.95	0.06	77,77,77,77	0
37	CL	J	9321	1/1	0.95	0.11	66,66,66,66	0
34	MG	0	8045	1/1	0.95	0.26	72,72,72,72	0
38	SR	0	9560	1/1	0.95	0.08	101,101,101,101	0
34	MG	0	8116	1/1	0.95	0.10	64,64,64,64	0
34	MG	0	8083	1/1	0.95	0.11	53,53,53,53	0
36	NA	C	9104	1/1	0.95	0.16	33,33,33,33	0
38	SR	0	9495	1/1	0.95	0.14	111,111,111,111	0
37	CL	M	9318	1/1	0.95	0.17	41,41,41,41	0
34	MG	0	8098	1/1	0.95	0.07	45,45,45,45	0
34	MG	0	8079	1/1	0.95	0.13	33,33,33,33	0
36	NA	0	9139	1/1	0.95	0.10	43,43,43,43	0
34	MG	0	8029	1/1	0.95	0.22	35,35,35,35	0
34	MG	0	8067	1/1	0.95	0.11	40,40,40,40	0
34	MG	0	8021	1/1	0.95	0.16	56,56,56,56	0
34	MG	0	8070	1/1	0.96	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9162	1/1	0.96	0.15	52,52,52,52	0
37	CL	J	9302	1/1	0.96	0.07	53,53,53,53	0
36	NA	R	9137	1/1	0.96	0.08	36,36,36,36	0
38	SR	F	9595	1/1	0.96	0.16	109,109,109,109	0
36	NA	0	9156	1/1	0.96	0.16	57,57,57,57	0
38	SR	0	9490	1/1	0.96	0.13	116,116,116,116	0
38	SR	0	9530	1/1	0.96	0.11	72,72,72,72	0
34	MG	0	8060	1/1	0.96	0.07	82,82,82,82	0
38	SR	0	9440	1/1	0.96	0.05	72,72,72,72	0
37	CL	Y	9320	1/1	0.96	0.08	47,47,47,47	0
36	NA	0	9178	1/1	0.96	0.45	54,54,54,54	0
38	SR	0	9585	1/1	0.96	0.08	94,94,94,94	0
37	CL	3	9304	1/1	0.96	0.07	61,61,61,61	0
36	NA	0	9107	1/1	0.96	0.40	71,71,71,71	0
38	SR	0	9433	1/1	0.96	0.12	75,75,75,75	0
36	NA	0	9115	1/1	0.96	0.18	41,41,41,41	0
34	MG	0	8042	1/1	0.96	0.11	48,48,48,48	0
34	MG	Y	8109	1/1	0.96	0.12	45,45,45,45	0
34	MG	0	8112	1/1	0.96	0.06	46,46,46,46	0
36	NA	0	9105	1/1	0.96	0.09	44,44,44,44	0
37	CL	N	9307	1/1	0.96	0.16	65,65,65,65	0
38	SR	0	9447	1/1	0.97	0.07	73,73,73,73	0
34	MG	0	8027	1/1	0.97	0.24	36,36,36,36	0
37	CL	0	9316	1/1	0.97	0.26	78,78,78,78	0
34	MG	0	8002	1/1	0.97	0.09	34,34,34,34	0
34	MG	A	8066	1/1	0.97	0.10	57,57,57,57	0
37	CL	0	9311	1/1	0.97	0.15	71,71,71,71	0
38	SR	0	9426	1/1	0.97	0.08	71,71,71,71	0
34	MG	0	8009	1/1	0.97	0.10	21,21,21,21	0
34	MG	0	8114	1/1	0.97	0.47	83,83,83,83	0
38	SR	0	9466	1/1	0.97	0.06	96,96,96,96	0
38	SR	0	9545	1/1	0.97	0.06	85,85,85,85	0
38	SR	A	9437	1/1	0.97	0.10	70,70,70,70	0
37	CL	0	9315	1/1	0.97	0.09	52,52,52,52	0
34	MG	0	8012	1/1	0.97	0.22	39,39,39,39	0
38	SR	0	9601	1/1	0.97	0.06	119,119,119,119	0
38	SR	0	9438	1/1	0.97	0.09	70,70,70,70	0
34	MG	0	8117	1/1	0.97	0.12	46,46,46,46	0
38	SR	0	9446	1/1	0.97	0.07	88,88,88,88	0
34	MG	0	8044	1/1	0.97	0.06	35,35,35,35	0
38	SR	0	9534	1/1	0.97	0.14	111,111,111,111	0
36	NA	0	9127	1/1	0.97	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9442	1/1	0.97	0.10	66,66,66,66	0
38	SR	A	9436	1/1	0.97	0.06	60,60,60,60	0
34	MG	0	8088	1/1	0.97	0.11	28,28,28,28	0
34	MG	0	8046	1/1	0.97	0.05	39,39,39,39	0
36	NA	0	9108	1/1	0.97	0.10	34,34,34,34	0
36	NA	0	9160	1/1	0.97	0.17	46,46,46,46	0
36	NA	0	9138	1/1	0.97	0.07	62,62,62,62	0
38	SR	0	9568	1/1	0.97	0.07	80,80,80,80	0
34	MG	K	8069	1/1	0.97	0.17	25,25,25,25	0
38	SR	0	9405	1/1	0.97	0.16	59,59,59,59	0
38	SR	0	9432	1/1	0.97	0.14	68,68,68,68	0
34	MG	0	8041	1/1	0.97	0.09	55,55,55,55	0
36	NA	0	9134	1/1	0.97	0.10	47,47,47,47	0
34	MG	0	8084	1/1	0.97	0.40	89,89,89,89	0
37	CL	R	9306	1/1	0.97	0.10	45,45,45,45	0
34	MG	0	8110	1/1	0.97	0.11	45,45,45,45	0
38	SR	0	9489	1/1	0.98	0.11	94,94,94,94	0
34	MG	0	8075	1/1	0.98	0.07	47,47,47,47	0
38	SR	0	9464	1/1	0.98	0.05	81,81,81,81	0
38	SR	0	9477	1/1	0.98	0.10	86,86,86,86	0
38	SR	0	9421	1/1	0.98	0.10	78,78,78,78	0
34	MG	0	8001	1/1	0.98	0.19	22,22,22,22	0
38	SR	0	9629	1/1	0.98	0.08	75,75,75,75	0
38	SR	0	9566	1/1	0.98	0.04	80,80,80,80	0
38	SR	9	9481	1/1	0.98	0.08	89,89,89,89	0
34	MG	0	8020	1/1	0.98	0.16	36,36,36,36	0
34	MG	0	8056	1/1	0.98	0.23	44,44,44,44	0
38	SR	0	9454	1/1	0.98	0.10	82,82,82,82	0
38	SR	0	9435	1/1	0.98	0.08	76,76,76,76	0
37	CL	0	9305	1/1	0.98	0.07	61,61,61,61	0
38	SR	0	9427	1/1	0.98	0.12	56,56,56,56	0
38	SR	0	9443	1/1	0.98	0.10	63,63,63,63	0
34	MG	0	8031	1/1	0.98	0.12	49,49,49,49	0
38	SR	0	9475	1/1	0.98	0.13	83,83,83,83	0
38	SR	0	9445	1/1	0.98	0.09	57,57,57,57	0
36	NA	0	9118	1/1	0.98	0.21	66,66,66,66	0
38	SR	0	9506	1/1	0.98	0.04	68,68,68,68	0
36	NA	0	9154	1/1	0.98	0.15	54,54,54,54	0
36	NA	0	9130	1/1	0.98	0.15	50,50,50,50	0
38	SR	0	9461	1/1	0.98	0.06	82,82,82,82	0
34	MG	0	8039	1/1	0.98	0.17	49,49,49,49	0
34	MG	0	8096	1/1	0.98	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9456	1/1	0.98	0.10	67,67,67,67	0
38	SR	0	9469	1/1	0.98	0.05	85,85,85,85	0
38	SR	0	9455	1/1	0.98	0.10	88,88,88,88	0
36	NA	0	9136	1/1	0.98	0.12	34,34,34,34	0
34	MG	0	8005	1/1	0.98	0.06	29,29,29,29	0
38	SR	0	9457	1/1	0.98	0.08	51,51,51,51	0
38	SR	0	9414	1/1	0.98	0.12	57,57,57,57	0
38	SR	0	9441	1/1	0.98	0.07	68,68,68,68	0
34	MG	0	8017	1/1	0.98	0.14	31,31,31,31	0
36	NA	Q	9148	1/1	0.98	0.09	49,49,49,49	0
38	SR	0	9462	1/1	0.98	0.10	74,74,74,74	0
34	MG	0	8080	1/1	0.98	0.17	57,57,57,57	0
38	SR	A	9497	1/1	0.98	0.09	96,96,96,96	0
37	CL	0	9312	1/1	0.99	0.10	57,57,57,57	0
38	SR	0	9478	1/1	0.99	0.06	77,77,77,77	0
34	MG	0	8026	1/1	0.99	0.15	30,30,30,30	0
34	MG	0	8028	1/1	0.99	0.13	37,37,37,37	0
38	SR	0	9428	1/1	0.99	0.07	55,55,55,55	0
37	CL	0	9314	1/1	0.99	0.06	51,51,51,51	0
38	SR	0	9449	1/1	0.99	0.09	67,67,67,67	0
38	SR	0	9473	1/1	0.99	0.03	82,82,82,82	0
38	SR	0	9467	1/1	0.99	0.10	86,86,86,86	0
34	MG	0	8008	1/1	0.99	0.19	16,16,16,16	0
38	SR	0	9410	1/1	0.99	0.14	41,41,41,41	0
38	SR	0	9431	1/1	0.99	0.13	65,65,65,65	0
38	SR	0	9430	1/1	0.99	0.10	49,49,49,49	0
38	SR	0	9515	1/1	0.99	0.14	100,100,100,100	0
37	CL	B	9319	1/1	0.99	0.17	54,54,54,54	0
38	SR	0	9488	1/1	0.99	0.11	86,86,86,86	0
39	CD	1	9202	1/1	0.99	0.05	54,54,54,54	0
38	SR	0	9451	1/1	0.99	0.12	60,60,60,60	0
38	SR	0	9413	1/1	0.99	0.12	49,49,49,49	0
38	SR	0	9408	1/1	0.99	0.12	36,36,36,36	0
36	NA	0	9123	1/1	0.99	0.09	52,52,52,52	0
38	SR	L	9409	1/1	0.99	0.07	37,37,37,37	0
38	SR	0	9425	1/1	0.99	0.15	56,56,56,56	0
38	SR	0	9434	1/1	0.99	0.14	64,64,64,64	0
39	CD	3	9204	1/1	0.99	0.03	64,64,64,64	0
38	SR	1	9419	1/1	0.99	0.09	40,40,40,40	0
38	SR	0	9480	1/1	0.99	0.05	93,93,93,93	0
38	SR	3	9439	1/1	0.99	0.05	72,72,72,72	0
34	MG	0	8015	1/1	0.99	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9417	1/1	0.99	0.08	63,63,63,63	0
38	SR	0	9474	1/1	0.99	0.08	73,73,73,73	0
37	CL	0	9313	1/1	0.99	0.10	59,59,59,59	0
38	SR	1	9460	1/1	0.99	0.10	52,52,52,52	0
37	CL	O	9308	1/1	0.99	0.09	67,67,67,67	0
34	MG	0	8074	1/1	0.99	0.18	27,27,27,27	0
34	MG	0	8038	1/1	0.99	0.25	25,25,25,25	0
37	CL	0	9303	1/1	0.99	0.13	53,53,53,53	0
38	SR	S	9470	1/1	0.99	0.16	101,101,101,101	0
38	SR	0	9411	1/1	0.99	0.14	43,43,43,43	0
38	SR	0	9450	1/1	0.99	0.07	72,72,72,72	0
38	SR	0	9429	1/1	0.99	0.10	72,72,72,72	0
38	SR	0	9453	1/1	0.99	0.06	72,72,72,72	0
38	SR	R	9418	1/1	0.99	0.15	57,57,57,57	0
38	SR	0	9444	1/1	0.99	0.05	55,55,55,55	0
38	SR	0	9422	1/1	0.99	0.10	58,58,58,58	0
38	SR	0	9412	1/1	0.99	0.13	45,45,45,45	0
38	SR	0	9498	1/1	0.99	0.05	63,63,63,63	0
38	SR	B	9458	1/1	0.99	0.05	82,82,82,82	0
38	SR	0	9407	1/1	1.00	0.13	47,47,47,47	0
38	SR	0	9424	1/1	1.00	0.16	49,49,49,49	0
38	SR	0	9448	1/1	1.00	0.07	63,63,63,63	0
38	SR	0	9423	1/1	1.00	0.05	64,64,64,64	0
38	SR	0	9406	1/1	1.00	0.13	35,35,35,35	0
38	SR	0	9415	1/1	1.00	0.10	56,56,56,56	0
38	SR	0	9416	1/1	1.00	0.08	43,43,43,43	0
39	CD	U	9201	1/1	1.00	0.09	53,53,53,53	0
38	SR	0	9420	1/1	1.00	0.17	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.