



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:00 AM GMT

PDB ID : 1YI2
Title : Crystal Structure Of Erythromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-11
Resolution : 2.65 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

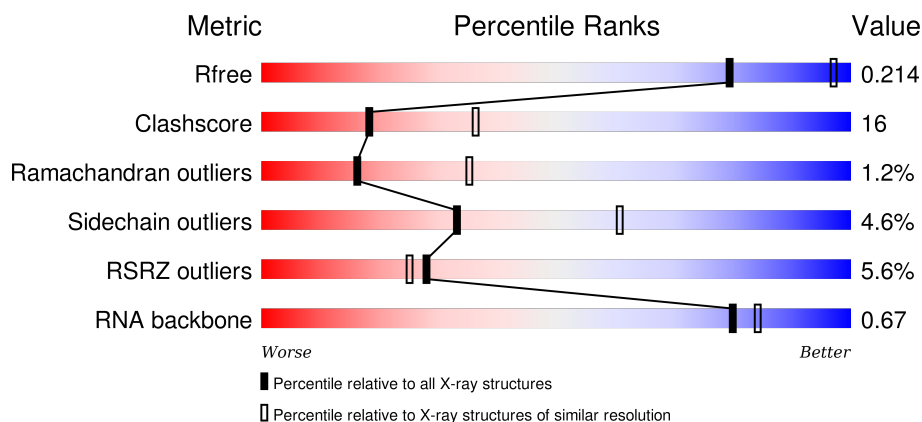
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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




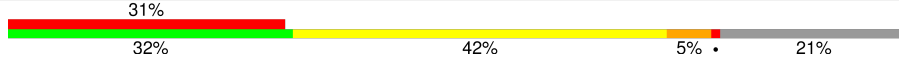


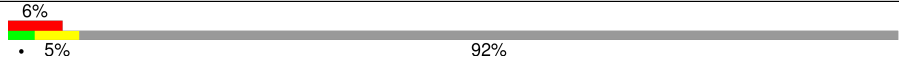
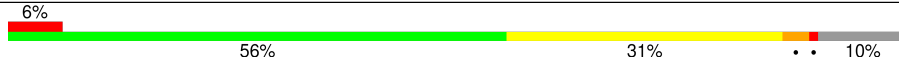

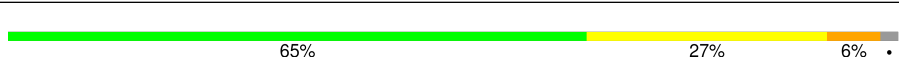
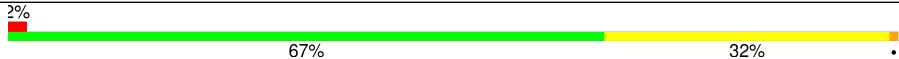
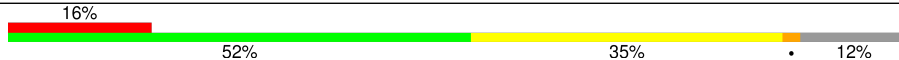
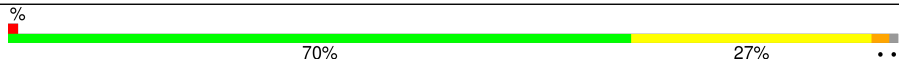
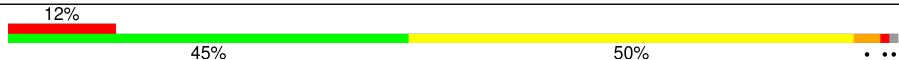


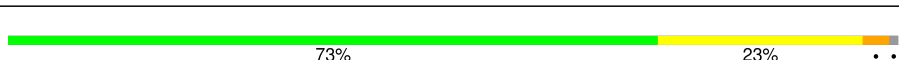
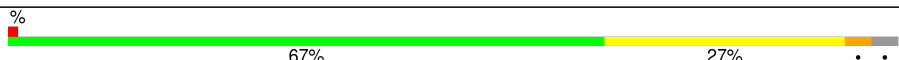
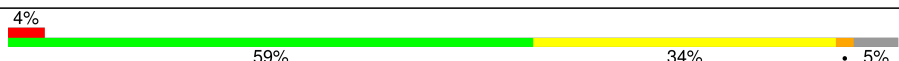
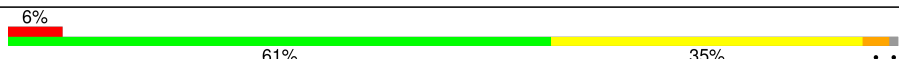

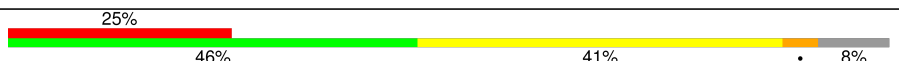
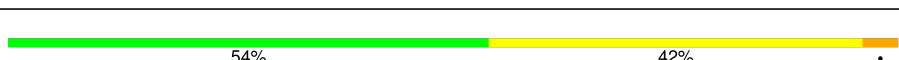
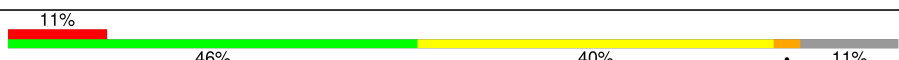
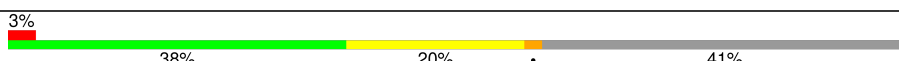

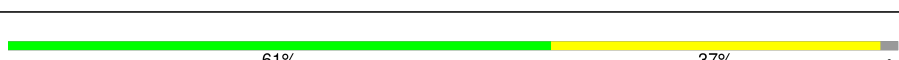
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)
RNA backbone	2183	1001 (3.08-2.24)

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> <div></div> <div>62%</div> <div>27%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>35%</div> <div>8%</div> <div></div> </div> </div>
3	A	240	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>31%</div> <div>5%</div> <div></div> </div> </div>
4	B	338	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>44%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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
32	ERY	0	9000	-	-	-	X
33	MG	0	8088	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8510	-	-	-	X
35	NA	0	8514	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8540	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8578	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	0	8815	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

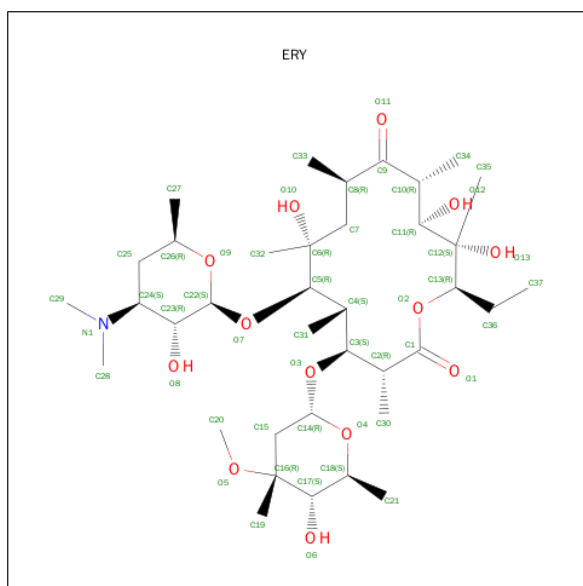
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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

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

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

- Molecule 32 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			51	37	1	13		

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	C	1	Total	Na	0	0
			1	1		
35	A	1	Total	Na	0	0
			1	1		
35	T	1	Total	Na	0	0
			1	1		
35	R	3	Total	Na	0	0
			3	3		
35	9	2	Total	Na	0	0
			2	2		
35	L	1	Total	Na	0	0
			1	1		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total	Cl	0	0
			10	10		

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5869	Total 5869	O 5869	0	0
38	9	138	Total 138	O 138	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	121	Total 121	O 121	0	0
38	B	151	Total 151	O 151	0	0
38	C	168	Total 168	O 168	0	0
38	D	50	Total 50	O 50	0	0
38	E	42	Total 42	O 42	0	0
38	F	28	Total 28	O 28	0	0
38	G	19	Total 19	O 19	0	0
38	H	71	Total 71	O 71	0	0
38	I	9	Total 9	O 9	0	0
38	J	55	Total 55	O 55	0	0
38	K	61	Total 61	O 61	0	0
38	L	81	Total 81	O 81	0	0
38	M	124	Total 124	O 124	0	0
38	N	67	Total 67	O 67	0	0
38	O	43	Total 43	O 43	0	0
38	P	66	Total 66	O 66	0	0
38	Q	49	Total 49	O 49	0	0
38	R	80	Total 80	O 80	0	0
38	S	37	Total 37	O 37	0	0
38	T	37	Total 37	O 37	0	0
38	U	27	Total 27	O 27	0	0

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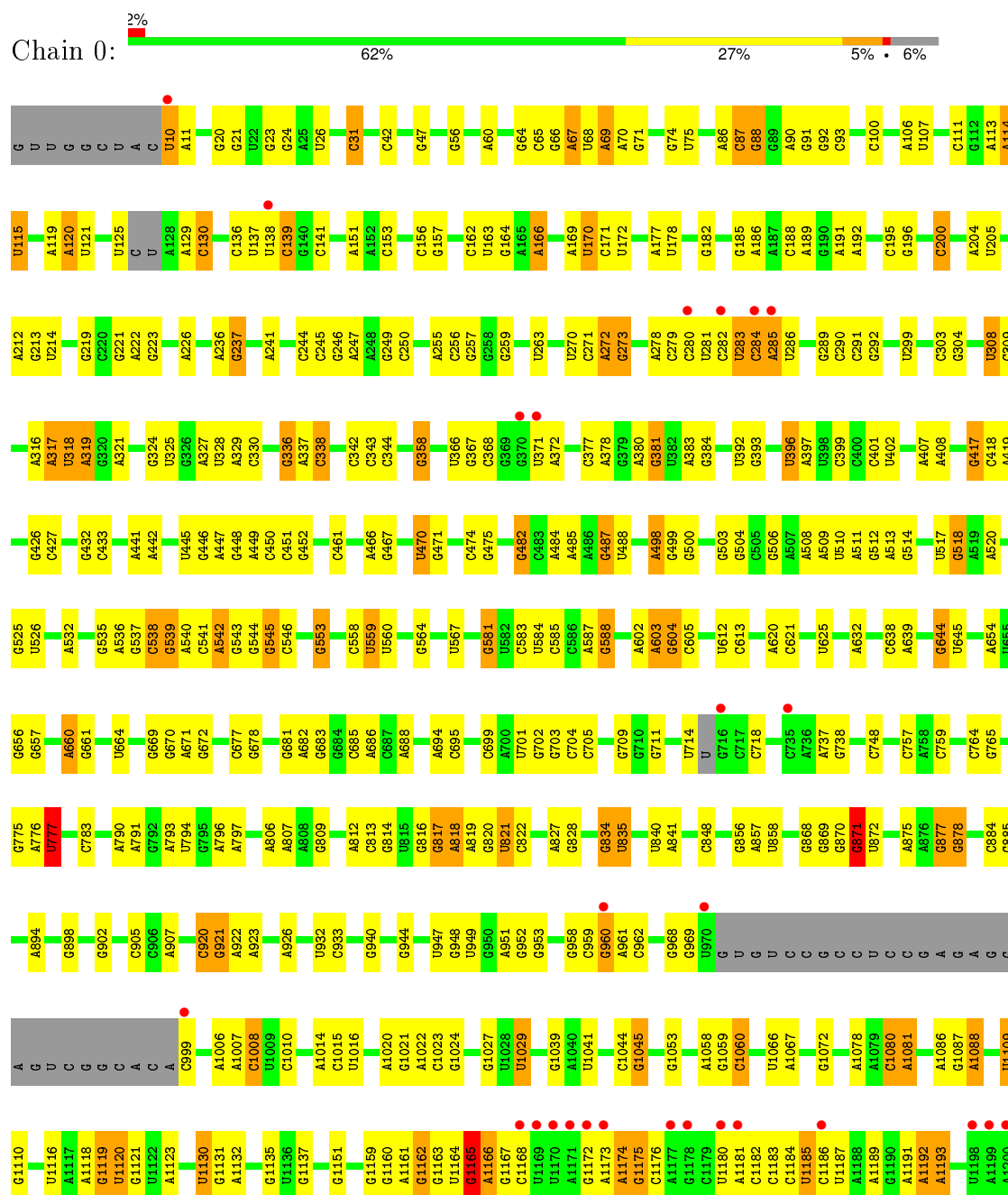
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	14	Total 14	O 14	0	0
38	W	73	Total 73	O 73	0	0
38	X	27	Total 27	O 27	0	0
38	Y	94	Total 94	O 94	0	0
38	Z	30	Total 30	O 30	0	0
38	1	54	Total 54	O 54	0	0
38	2	45	Total 45	O 45	0	0
38	3	78	Total 78	O 78	0	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

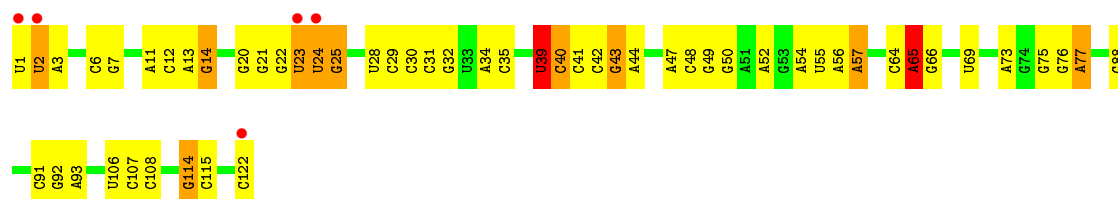
• Molecule 1: 23S Ribosomal RNA



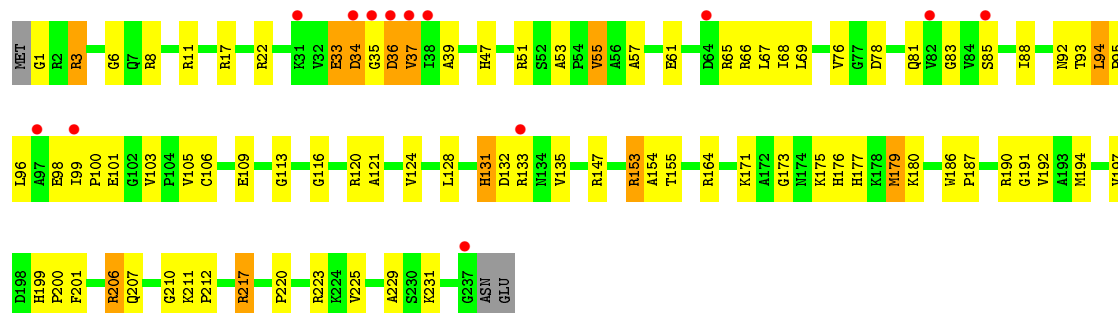
C2779	C2780	A2853	G2583	A2434	C2326	C	C	U	A2054	C1940	U1791	G1886	G1589	U1460	U1333	C1201
G2781	U2781	A2864	C2534	C2443	G2338	C	G	A	A2054	A1941	C1798	C1687	G1592	U1461	U1334	A1202
G2782	U2782	A	U2535	U2444	A	U	U	G	U2064	A1942	C1819	C1692	C1593	C1462	C1335	G1203
A2783	C2536	U	C2537	U2445	C	C	C	A	G	C1943	G1820	A1701	C1594	A1470	G1340	C1204
A2784	G2537		G	G2446	G	G	G	U	G	G1947	G1820	U1702	G1595	C1474	U1205	U1206
C2785	C2668	C2667	U2541	G2453	A	U	U	C	G	G1948	U1825	U1702	U1596	C1341	A1207	C1208
G2786	U2669	C2668	C2547	A2456	G2344	G	G	C	U	G1949	C1826	A1711	A1597	C1477	C1342	C1209
C2787	U2671	U2671	C2548	U2457	G2345	C	C	U	G	G1950	G1826	A1712	A1598	G1210	C1343	C1209
A2788	C2576		C2549	C2346	A2081	U	U	U	A	G1951	A1829	G1717	A1603	G1351	G1352	G1210
U2791	C2576		C2552	G2462	A2089	U	U	A	A	U	C1830	A1717	A1604	A1482	A1352	C1213
A2792	A2553		A2553	A2353	G2090	U	U	C	A	A	C1830	A1717	G1604	C1483	C1353	G1214
A2793	G2679		G2679	A2354	G2091	A	A	A	C	A	C1834	U1722	G1605	U1488	A1215	G1216
G2794	A2680		C2559	A2355	G2092	G	G	A	G	U	U1835	U1723	A1606	C1360	C1363	C1229
C2795	C2681		C2559	A2356	G2093	A	A	A	C	A	A1840	U1724	A1607	G1363	A1230	C1230
U2796	C2682		C2559	A2357	G2094	U	U	U	U	G	A1845	C1725	G1613	G1376	U1237	C1238
A2800	U2563		G2563	A2468	A2095	G	G	G	G	U	U1846	G1730	G1614	A1372	U1239	G1239
A2801	G2564		G2564	A2469	A2096	U	U	A	A	C	U1847	G1731	A1615	U1234	G1235	U1234
A2801	C2565		C2565	G2359	A2096	A	A	C	C	C	U1848	A1732	A1616	G1235	A1236	U1235
U2807	G2570		G2570	C2360	A2101	C	C	C	C	C	A1849	C1733	C1617	A1376	C1377	U1237
A2811	C2577		C2577	A2362	G2102	C	C	C	C	C	G1849	A1733	A1624	U1380	U1380	G1238
A2812	G2577		G2577	G2363	A2103	G	G	C	C	U	U1850	C1734	U1503	A1406	A1407	G1239
G2813	C2578		C2578	A2364	C2104	C	C	C	C	U	G1851	C1735	A1504	U1251	C1251	A1252
A2813	G2578		G2578	G2365	G2110	G	G	C	C	U	U1852	A1736	U1505	C1253	C1253	C1253
U2814	C2586		C2586	A2369	G2111	C	C	C	C	U	A1853	G1741	U1524	U1266	U1266	U1266
G2815	U2587		U2587	A2372	U2115	U	U	A	A	U	C1856	A1742	A1525	C1267	C1267	C1267
G2816	C2588		C2588	U2372	U2116	A	A	C	C	U	G1857	C1762	A1526	C1268	C1268	C1268
U2817	U2589		U2589	U2373	C2132	G	G	C	C	U	C1858	C1763	A1527	G1269	G1269	G1269
C2821	C2592		C2592	A2379	A2135	C	C	C	C	U	G1859	U1766	A1528	C1273	C1273	C1273
A2825	G2597		G2597	A2380	G2136	C	C	C	C	U	U1877	C1767	G1535	U1278	U1278	U1278
G2826	U2598		U2598	C2381	A2136	G	G	C	C	U	G1878	C1768	C1536	C1279	C1279	C1279
G2827	C2599		C2599	C2382	A2137	C	C	C	C	U	C1880	U1767	C1537	U1287	U1287	U1287
U2828	U2599		U2599	C2383	A2138	C	C	C	C	U	C1881	C1768	U1544	C1288	C1288	C1288
C2831	G2601		G2601	A2385	A2139	C	C	C	C	U	C1882	C1769	C1545	G1295	G1295	G1295
G2832	C2602		C2602	U2386	G2136	C	C	C	C	U	U1887	U1770	G1552	U1298	U1298	U1298
U2833	G2603		G2603	U2387	A2137	C	C	C	C	U	G1888	U1771	C1553	G1299	G1299	G1299
G2834	A2604		A2604	C2388	A2138	C	C	C	C	U	G1889	C1772	C1554	U1314	U1314	U1314
C2840	U2607		U2607	C2392	A2139	C	C	C	C	U	U1896	U1773	A1559	C1451	C1451	C1451
A2841	C2608		C2608	A2401	A2140	C	C	C	C	U	A1904	G1774	U1561	U1442	U1442	U1442
G2842	G2609		G2609	A2402	A2141	C	C	C	C	U	U1905	C1775	U1562	A1328	A1328	A1328
C2846	U2613		U2613	C2403	A2142	C	C	C	C	U	A1919	G1776	C1436	U1450	U1450	U1450
U2847	C2629		C2629	G2412	A2143	C	C	C	C	U	C1920	A1778	U1451	C1451	C1451	C1451
G2850	G2630		G2630	A2413	A2144	C	C	C	C	U	A1921	C1779	U1452	U1452	U1452	U1452
A2851	C2633		C2633	A2414	A2145	C	C	C	C	U	G1925	A1783	C1563	U1453	U1453	U1453
A2852	A2635		A2635	A2415	A2146	C	C	C	C	U	U1926	U1784	C1564	C1454	C1454	C1454
G2862	G2636		G2636	G2417	A2147	C	C	C	C	U	A1927	C1787	A1573	U1455	U1455	U1455
U2866	A2637		A2637	U2418	A2148	C	C	C	C	U	G1927	U1788	A1580	C1456	C1456	C1456
G2867	G2638		G2638	U2419	A2149	C	C	C	C	U	A1930	U1789	A1581	U1457	U1457	U1457
A2868	C2643		C2643	G2421	A2150	C	C	C	C	U	A1931	C1789	C1458	U1458	U1458	U1458
G2876	A2649		A2649	U2422	A2151	C	C	C	C	U	G1932	U1790	A1582	C1459	C1459	C1459
U2877	C2652		C2652	G2426	A2152	C	C	C	C	U	A1933	C1790	A1583	U1460	U1460	U1460
A2879	U2652		U2652	U2527	A2153	C	C	C	C	U	G1934	C1791	A1584	C1461	C1461	C1461



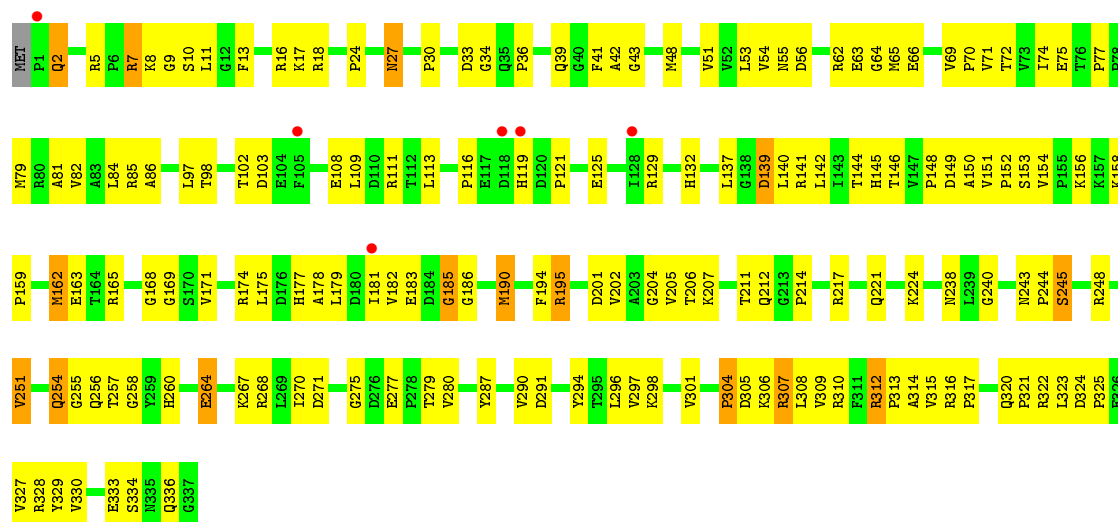
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P

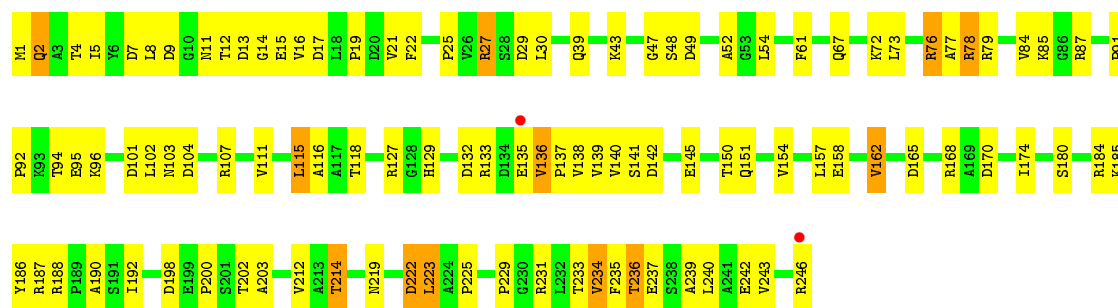


• Molecule 4: 50S ribosomal protein L3P

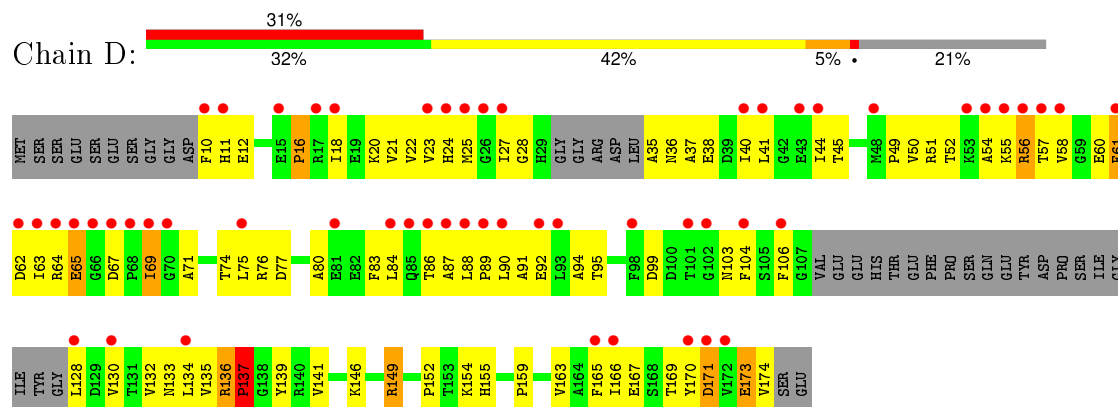


• Molecule 5: 50S ribosomal protein L4E

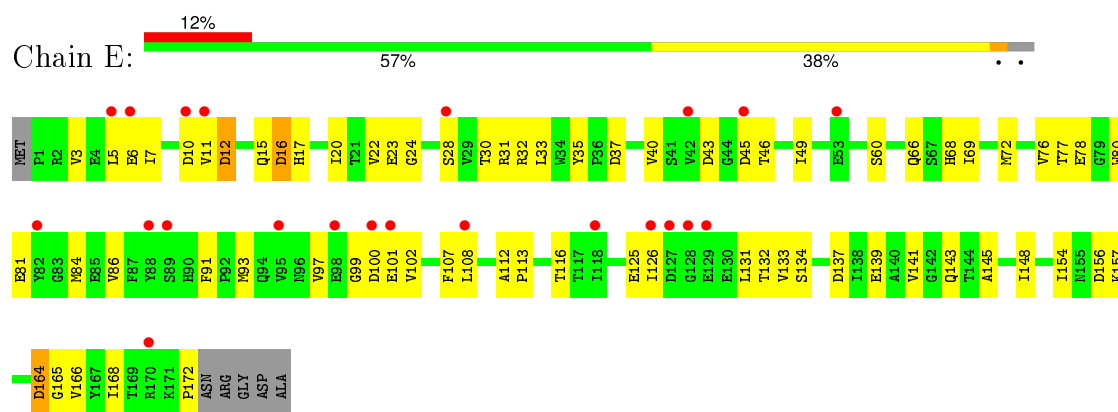




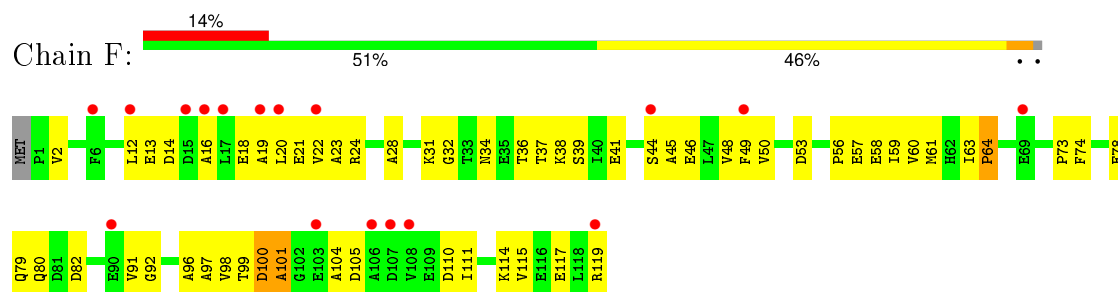
• Molecule 6: 50S ribosomal protein L5P



• Molecule 7: 50S ribosomal protein L6P



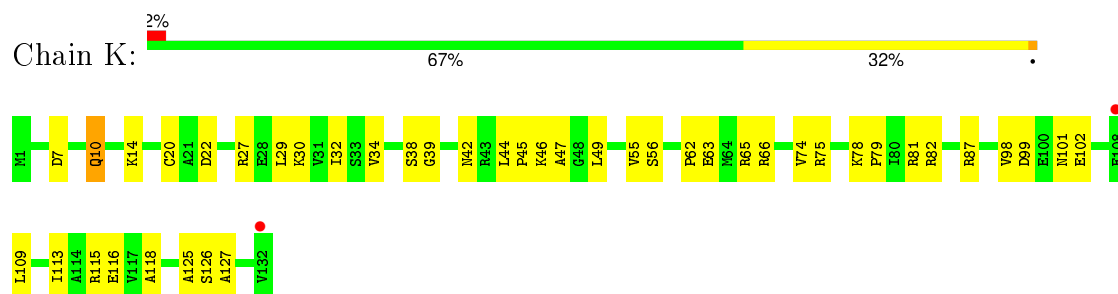
• Molecule 8: 50S ribosomal protein L7AE



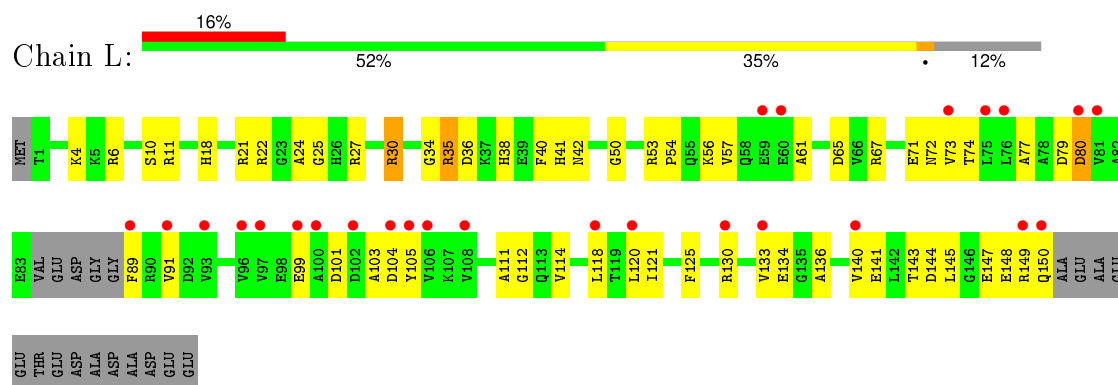
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



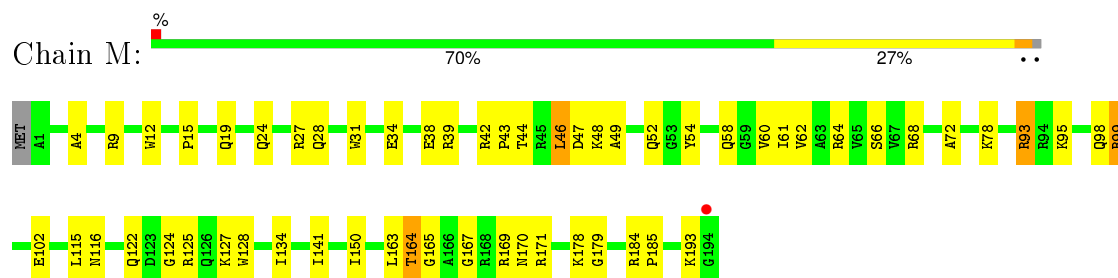
- Molecule 13: 50S ribosomal protein L14P



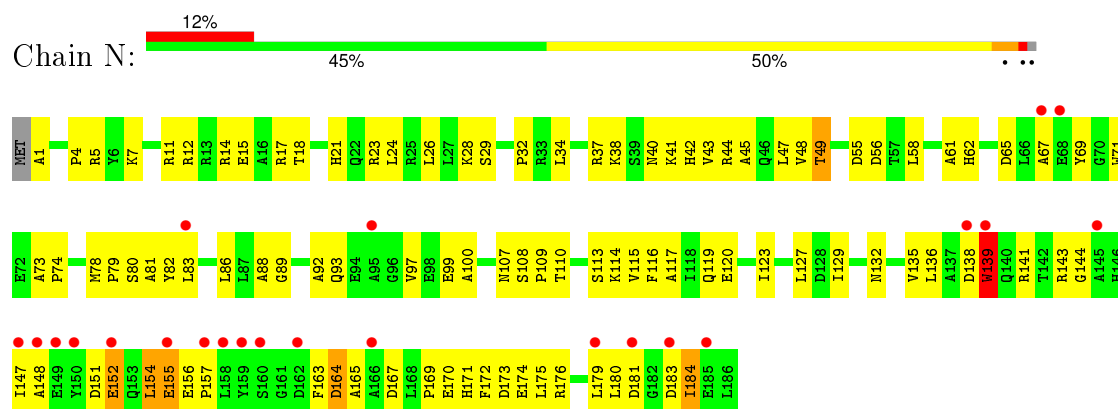
- Molecule 14: 50S ribosomal protein L15P



- Molecule 15: 50S Ribosomal Protein L15E

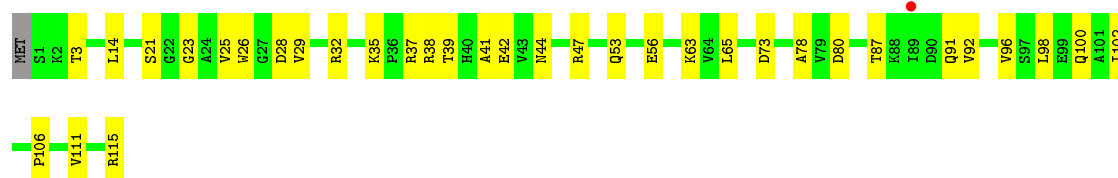


- Molecule 16: 50S ribosomal protein L18P

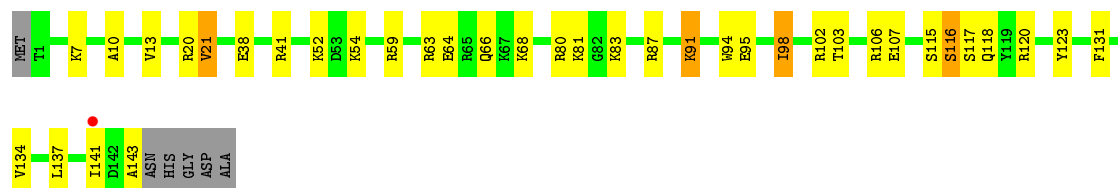


- Molecule 17: 50S ribosomal protein L18e





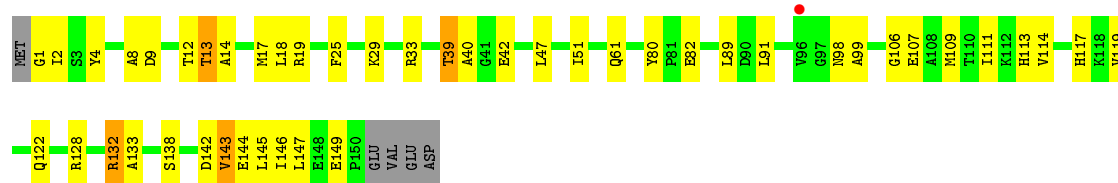
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



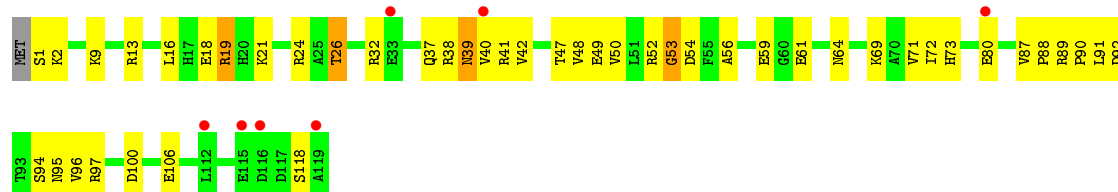
- Molecule 20: 50S ribosomal protein L22P



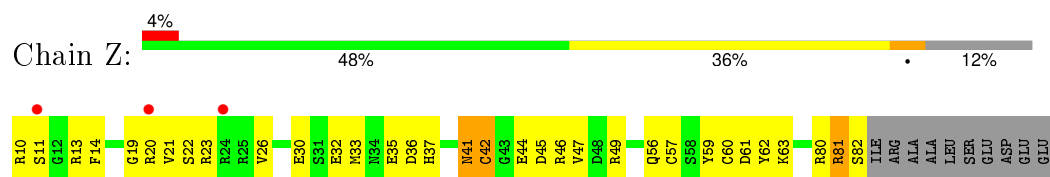
- Molecule 21: 50S ribosomal protein L23P



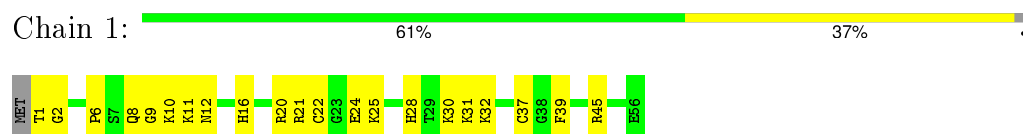
- Molecule 22: 50S ribosomal protein L24P



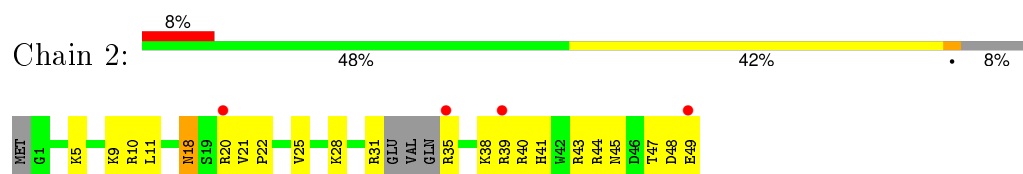
- Molecule 28: 50S ribosomal protein L37Ae



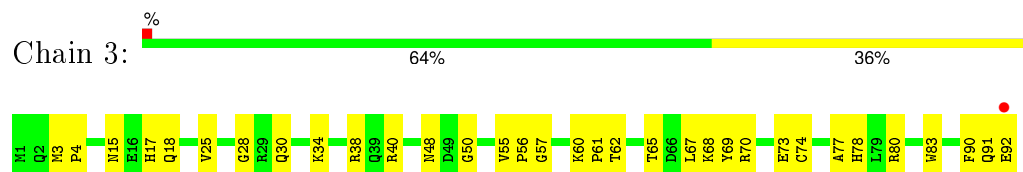
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.44Å 299.99Å 574.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 49.81 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.65) 94.5 (49.81-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.214 0.177 , 0.214	Depositor DCC
R_{free} test set	4878 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 495739 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99086	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.36	0/65957	0.69	23/102867 (0.0%)
2	9	0.33	0/2904	0.70	2/4526 (0.0%)
3	A	0.32	0/1786	0.64	0/2408
4	B	0.32	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.31	0/1111	0.55	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.31	0/901	0.55	0/1224
9	G	0.27	0/241	0.45	0/324
10	H	0.39	0/1302	0.66	1/1743 (0.1%)
11	I	0.30	0/526	0.54	0/716
12	J	0.35	0/1136	0.61	0/1530
13	K	0.33	0/1001	0.68	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.33	0/1582	0.62	0/2117
16	N	0.29	0/1474	0.61	0/1999
17	O	0.33	0/874	0.59	0/1181
18	P	0.33	0/1147	0.53	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.34	0/1172	0.63	0/1578
21	S	0.33	0/648	0.57	1/875 (0.1%)
22	T	0.30	0/958	0.62	0/1289
23	U	0.33	0/417	0.55	0/562
24	V	0.29	0/502	0.55	0/675
25	W	0.34	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.35	0/1146	0.62	0/1536
28	Z	0.33	0/589	0.65	0/787
29	1	0.38	0/438	0.63	0/578
30	2	0.33	0/401	0.54	0/529
31	3	0.37	0/771	0.58	0/1024
All	All	0.35	0/98702	0.67	27/147588 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	45
2	9	0	2
All	All	1	47

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.25	129.85	109.50
1	0	1942	A	C5'-C4'-C3'	7.55	128.08	116.00
2	9	39	U	N1-C1'-C2'	7.02	123.12	114.00
1	0	871	G	C5'-C4'-O4'	-6.90	100.82	109.10
1	0	1504	A	C1'-O4'-C4'	-6.19	104.95	109.90
1	0	2291	A	N9-C1'-C2'	6.19	122.04	114.00
1	0	2313	C	C5'-C4'-O4'	6.07	116.38	109.10
1	0	2467	A	C1'-O4'-C4'	-5.84	105.23	109.90
1	0	777	U	O4'-C1'-N1	5.83	112.86	108.20
1	0	1120	U	C5'-C4'-C3'	-5.72	106.84	116.00
1	0	1819	G	C5'-C4'-C3'	5.68	125.08	116.00
1	0	2316	G	C5'-C4'-C3'	-5.63	106.99	116.00
1	0	2526	C	N1-C1'-C2'	5.48	121.13	114.00
1	0	1971	G	N9-C1'-C2'	5.42	121.05	114.00
1	0	1979	G	N9-C1'-C2'	5.41	121.03	114.00
2	9	65	A	N9-C1'-C2'	5.32	120.91	114.00
21	S	27	ALA	N-CA-C	-5.31	96.67	111.00
10	H	115	GLY	N-CA-C	-5.27	99.91	113.10
1	0	2726	U	N1-C1'-C2'	5.26	120.84	114.00
1	0	1878	G	N9-C1'-C2'	-5.24	106.23	112.00
1	0	1592	G	N9-C1'-C2'	5.21	120.77	114.00
1	0	1504	A	N9-C1'-C2'	5.05	120.57	114.00
1	0	841	A	C1'-O4'-C4'	-5.04	105.87	109.90
1	0	1942	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	0	535	G	N9-C1'-C2'	5.04	120.55	114.00
1	0	1165	G	C1'-O4'-C4'	-5.04	105.87	109.90
1	0	2313	C	C1'-O4'-C4'	-5.03	105.88	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1653	A	Sidechain
1	0	1681	G	Sidechain
1	0	1682	A	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	221	G	Sidechain
1	0	2315	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	396	U	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
2	9	39	U	Sidechain
2	9	65	A	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59020	0	29810	809	0
2	9	2599	0	1325	63	0
3	A	1753	0	1766	111	0
4	B	2625	0	2533	172	0
5	C	1859	0	1816	122	0
6	D	1094	0	1085	92	0
7	E	1357	0	1266	74	0
8	F	890	0	843	60	0
9	G	240	0	231	19	0
10	H	1282	0	1292	70	0
11	I	519	0	500	57	0
12	J	1120	0	1098	55	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1558	0	1566	58	0
16	N	1445	0	1401	112	0
17	O	865	0	873	29	0
18	P	1136	0	1123	41	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	52	0
21	S	641	0	605	25	0
22	T	950	0	923	45	0
23	U	410	0	364	28	0
24	V	499	0	511	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	1196	0	1137	97	0
26	X	654	0	653	48	0
27	Y	1130	0	1133	62	0
28	Z	578	0	539	27	0
29	1	431	0	426	30	0
30	2	396	0	413	32	0
31	3	755	0	728	29	0
32	0	51	0	67	0	0
33	0	108	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5869	0	0	162	0
38	1	54	0	0	2	0
38	2	45	0	0	6	0
38	3	78	0	0	10	0
38	9	138	0	0	9	0
38	A	121	0	0	16	0
38	B	151	0	0	20	0
38	C	168	0	0	27	0
38	D	50	0	0	17	0
38	E	42	0	0	11	0
38	F	28	0	0	8	0
38	G	19	0	0	1	0
38	H	71	0	0	17	0
38	I	9	0	0	4	0
38	J	55	0	0	3	0
38	K	61	0	0	11	0
38	L	81	0	0	23	0
38	M	124	0	0	12	0
38	N	67	0	0	13	0
38	O	43	0	0	6	0
38	P	66	0	0	2	0
38	Q	49	0	0	6	0
38	R	80	0	0	7	0
38	S	37	0	0	5	0
38	T	37	0	0	6	0
38	U	27	0	0	4	0
38	V	14	0	0	3	0
38	W	73	0	0	11	0
38	X	27	0	0	9	0
38	Y	94	0	0	14	0
38	Z	30	0	0	1	0
All	All	99086	0	59985	2356	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 16.

All (2356) 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)
10:H:172:GLU:HB2	38:H:8591:HOH:O	1.34	1.21
1:0:1160:G:H5'	1:0:1161:A:H5'	1.24	1.17
5:C:236:THR:HG22	5:C:239:ALA:H	1.04	1.16
10:H:174:LEU:HA	38:H:8571:HOH:O	1.50	1.11
2:9:6:C:H5''	16:N:37:ARG:NH1	1.66	1.10
6:D:154:LYS:HD2	6:D:154:LYS:H	1.21	1.03
1:0:1242:A:H5'	12:J:82:THR:HG23	1.35	1.03
1:0:156:C:H5''	15:M:171:ARG:HD3	1.38	1.02
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.40	1.01
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.40	1.00
13:K:10:GLN:H	13:K:10:GLN:NE2	1.59	0.99
5:C:78:ARG:HG3	5:C:78:ARG:HH11	1.23	0.99
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.44	0.99
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.43	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.46	0.98
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.46	0.97
1:0:871:G:C8	1:0:871:G:H5'	1.98	0.97
2:9:56:A:H2'	2:9:57:A:H5''	1.44	0.97
1:0:1559:A:H1'	38:0:5823:HOH:O	1.64	0.96
1:0:871:G:H8	1:0:871:G:H5'	1.29	0.96
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.10	0.96
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.47	0.95
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.81	0.95
12:J:76:ASP:HA	38:J:5907:HOH:O	1.67	0.95
2:9:6:C:H5''	16:N:37:ARG:HH12	1.24	0.94
2:9:76:G:H3'	2:9:77:A:H5''	1.47	0.94
18:P:115:SER:H	18:P:118:GLN:HE21	0.96	0.93
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.51	0.93
15:M:164:THR:HG22	15:M:167:GLY:H	1.33	0.93
16:N:144:GLY:O	16:N:147:ILE:HG22	1.67	0.93
3:A:35:GLY:O	3:A:36:ASP:HB3	1.68	0.93
13:K:10:GLN:N	13:K:10:GLN:HE21	1.65	0.92
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.92
30:2:41:HIS:H	30:2:45:ASN:HD22	1.13	0.92
1:0:1751:G:H2'	1:0:1752:G:H5''	1.50	0.92
13:K:39:GLY:HA2	38:K:4183:HOH:O	1.70	0.92
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.50	0.91
1:0:2717:C:C2'	1:0:2718:C:H5''	2.00	0.91
1:0:381:G:H5''	38:0:4294:HOH:O	1.70	0.91
1:0:545:G:H8	1:0:545:G:H5'	1.36	0.90
5:C:236:THR:HG22	5:C:239:ALA:N	1.84	0.90
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.52	0.90
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.71	0.90
10:H:170:ARG:HD2	38:H:8540:HOH:O	1.72	0.90
1:O:21:G:H5'	20:R:2:ILE:HA	1.54	0.90
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.50	0.90
1:O:1474:C:H6	1:O:1474:C:H5'	1.37	0.89
25:W:88:THR:HB	38:W:6679:HOH:O	1.73	0.89
4:B:62:ARG:HA	4:B:65:MET:HE3	1.52	0.89
1:O:2506:A:HO2'	1:O:2507:G:H8	0.89	0.88
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.56	0.88
4:B:238:ASN:HD22	4:B:240:GLY:H	1.22	0.88
1:O:541:C:H2'	1:O:542:A:H5''	1.55	0.87
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.75	0.87
1:O:1835:U:H5	1:O:1840:A:N7	1.72	0.87
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.20	0.86
28:Z:10:ARG:HA	38:Z:8714:HOH:O	1.75	0.86
1:O:1160:G:C5'	1:O:1161:A:H5'	2.06	0.86
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.56	0.86
1:O:962:C:H1'	16:N:5:ARG:NH1	1.90	0.86
1:O:542:A:H5'	1:O:542:A:H8	1.40	0.86
7:E:100:ASP:HB2	38:E:2789:HOH:O	1.74	0.86
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.56	0.85
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.41	0.85
1:O:2812:A:H2	1:O:2814:A:H62	1.25	0.85
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.58	0.85
1:O:2890:A:H1'	23:U:56:ARG:NH2	1.92	0.85
1:O:2716:G:H5''	4:B:206:THR:HG21	1.59	0.84
5:C:236:THR:H	5:C:239:ALA:HB3	1.43	0.84
1:O:1667:A:H8	1:O:1667:A:H5'	1.39	0.84
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.76	0.84
6:D:25:MET:HE2	6:D:41:LEU:HG	1.60	0.83
1:O:214:U:H5'	38:O:6098:HOH:O	1.78	0.83
4:B:86:ALA:HA	38:B:8879:HOH:O	1.78	0.83
1:O:1116:U:HO2'	1:O:1118:A:H2	0.85	0.83
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.60	0.83
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.83
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.09	0.83
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.58	0.83
1:O:282:C:H1'	1:O:368:C:N4	1.92	0.83
1:O:1184:C:H1'	38:O:7413:HOH:O	1.77	0.83
2:9:73:A:H61	2:9:108:C:H42	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:HO2'	1:0:1189:A:H2	1.27	0.83
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.61	0.83
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.60	0.83
4:B:321:PRO:HA	38:B:8961:HOH:O	1.79	0.82
1:0:1160:G:H5'	1:0:1161:A:C5'	2.07	0.82
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.93	0.82
8:F:91:VAL:HG12	8:F:92:GLY:H	1.45	0.81
3:A:191:GLY:HA2	3:A:194:MET:CE	2.10	0.81
1:0:2586:U:H3	1:0:2592:G:H22	1.26	0.81
14:L:133:VAL:HA	38:L:8871:HOH:O	1.81	0.81
1:0:21:G:C5'	20:R:2:ILE:HA	2.10	0.81
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.61	0.81
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.79	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.46	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.80
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.95	0.80
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.12	0.80
1:0:1162:G:H1'	11:I:112:LEU:HD11	1.62	0.80
1:0:962:C:H1'	16:N:5:ARG:HH12	1.43	0.80
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.64	0.80
5:C:132:ASP:HB3	38:C:8564:HOH:O	1.82	0.80
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.63	0.80
6:D:57:THR:HG23	6:D:63:ILE:HA	1.62	0.80
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.26	0.80
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.64	0.80
2:9:14:G:H5'	2:9:14:G:H8	1.47	0.79
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.45	0.79
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.63	0.79
18:P:115:SER:N	18:P:118:GLN:HE21	1.79	0.79
4:B:179:LEU:O	4:B:183:GLU:HG2	1.83	0.79
13:K:10:GLN:H	13:K:10:GLN:HE21	0.85	0.79
1:0:2291:A:C8	1:0:2309:C:H5'	2.18	0.78
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.48	0.78
25:W:13:MET:HE1	25:W:18:GLN:HA	1.64	0.78
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.82	0.78
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.48	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.78
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.64	0.78
1:0:2756:U:H3	1:0:2896:A:H2	1.30	0.78
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.49	0.78
20:R:99:ALA:HB1	20:R:109:MET:CE	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:C2'	1:0:542:A:H5''	2.14	0.77
4:B:140:LEU:HD23	38:B:8879:HOH:O	1.82	0.77
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.77
1:0:960:G:H4'	38:0:7379:HOH:O	1.83	0.77
1:0:1701:A:H4'	1:0:1702:U:H5''	1.64	0.77
5:C:242:GLU:HG3	38:C:8583:HOH:O	1.83	0.77
10:H:30:LYS:H	10:H:62:HIS:HD2	1.31	0.77
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.65	0.77
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.77
1:0:182:G:H5'	38:0:5115:HOH:O	1.83	0.77
1:0:236:A:H4'	1:0:237:G:H5'	1.67	0.77
38:0:6824:HOH:O	15:M:178:LYS:HB2	1.84	0.77
14:L:148:GLU:HA	38:L:8870:HOH:O	1.85	0.76
38:9:8673:HOH:O	16:N:23:ARG:HD3	1.83	0.76
27:Y:174:VAL:HG13	27:Y:177:LYS:HD2	1.65	0.76
1:0:1450:C:H4'	1:0:1451:C:OP2	1.86	0.76
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.50	0.76
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.48	0.76
1:0:870:G:C2'	1:0:871:G:H5''	2.15	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.33	0.76
1:0:1118:A:H3'	1:0:1118:A:H8	1.51	0.76
1:0:200:C:H2'	38:0:3429:HOH:O	1.85	0.75
8:F:96:ALA:HA	38:F:3111:HOH:O	1.84	0.75
1:0:1183:C:H2'	38:0:6204:HOH:O	1.86	0.75
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.85	0.75
1:0:877:G:H5'	1:0:878:G:OP1	1.87	0.75
12:J:45:VAL:HG23	12:J:130:VAL:O	1.85	0.75
16:N:113:SER:HB2	38:N:8860:HOH:O	1.85	0.75
1:0:2908:A:H2'	1:0:2909:G:O4'	1.87	0.75
8:F:58:GLU:HA	8:F:61:MET:HE2	1.69	0.75
1:0:272:A:H3'	38:0:7476:HOH:O	1.87	0.75
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.83	0.75
1:0:2637:A:H5'	38:0:9265:HOH:O	1.85	0.75
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.69	0.75
2:9:56:A:C2'	2:9:57:A:H5''	2.16	0.75
25:W:65:VAL:HA	25:W:68:THR:HG22	1.69	0.75
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.69	0.75
8:F:91:VAL:HG12	8:F:92:GLY:N	2.01	0.74
1:0:1603:A:H5'	1:0:1605:G:O4'	1.87	0.74
1:0:2426:G:H1'	38:0:6048:HOH:O	1.86	0.74
38:0:5416:HOH:O	9:G:12:ILE:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1234:U:N3	4:B:244:PRO:HB3	2.02	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.15	0.74
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.84	0.74
1:0:544:G:H2'	1:0:545:G:H5''	1.69	0.74
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.69	0.74
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.69	0.74
38:0:7172:HOH:O	3:A:11:ARG:HA	1.88	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.00	0.74
1:0:2533:C:H6	1:0:2533:C:H5'	1.51	0.74
20:R:39:THR:HG22	20:R:42:GLU:H	1.52	0.74
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.18	0.74
5:C:236:THR:HA	38:C:8650:HOH:O	1.87	0.74
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.00	0.74
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.05	0.74
5:C:1:MET:HG2	5:C:2:GLN:H	1.52	0.74
1:0:657:G:OP1	5:C:27:ARG:NH2	2.20	0.74
1:0:1118:A:C8	1:0:1118:A:H3'	2.22	0.74
1:0:2508:C:H2'	38:0:6705:HOH:O	1.88	0.73
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.87	0.73
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.70	0.73
11:I:94:ASP:OD1	11:I:133:THR:HB	1.88	0.73
1:0:1474:C:C6	1:0:1474:C:H5'	2.23	0.73
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.19	0.73
1:0:396:U:H1'	38:0:7576:HOH:O	1.87	0.73
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.70	0.73
20:R:39:THR:HG23	20:R:107:GLU:O	1.89	0.73
25:W:88:THR:HG22	25:W:89:ASP:H	1.52	0.73
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.89	0.73
1:0:1206:U:H5'	1:0:1206:U:H6	1.54	0.73
1:0:450:C:OP1	5:C:184:ARG:NH2	2.21	0.73
24:V:12:THR:HG22	24:V:15:GLU:CG	2.18	0.73
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.70	0.73
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.73
24:V:42:ASN:HB3	38:V:7247:HOH:O	1.87	0.72
14:L:77:ALA:HB3	38:L:8830:HOH:O	1.89	0.72
1:0:2768:A:H5''	38:0:4399:HOH:O	1.89	0.72
1:0:559:U:H5'	1:0:559:U:H6	1.54	0.72
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.54	0.72
2:9:6:C:C5'	16:N:37:ARG:NH1	2.51	0.72
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.70	0.72
23:U:9:CYS:HA	23:U:52:THR:HG23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:12:ILE:HD12	10:H:57:THR:HG22	1.70	0.71
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.71
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.55	0.71
15:M:58:GLN:HG3	38:M:8907:HOH:O	1.88	0.71
1:0:545:G:C8	1:0:545:G:H5'	2.24	0.71
1:0:711:G:H1'	38:0:7045:HOH:O	1.88	0.71
2:9:75:G:H1	2:9:106:U:H3	1.38	0.71
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
1:0:281:U:H2'	1:0:282:C:O4'	1.91	0.71
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.71	0.71
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.72	0.71
1:0:2054:A:N3	20:R:128:ARG:NH2	2.39	0.70
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.89	0.70
18:P:64:GLU:HG2	38:P:170:HOH:O	1.90	0.70
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.72	0.70
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.52	0.70
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.71	0.70
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.74	0.70
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.71	0.70
1:0:1819:G:H2'	1:0:1820:G:H4'	1.73	0.70
1:0:2783:A:H3'	38:0:5190:HOH:O	1.91	0.70
5:C:139:VAL:HG13	38:C:8647:HOH:O	1.91	0.70
1:0:1641:A:H2'	1:0:1642:A:H5'	1.72	0.70
16:N:132:ASN:O	16:N:135:VAL:HG12	1.91	0.70
1:0:2851:G:O2'	1:0:2852:A:H5'	1.90	0.70
5:C:2:GLN:HB3	38:C:8536:HOH:O	1.91	0.70
2:9:69:U:OP1	16:N:4:PRO:HG3	1.92	0.70
5:C:236:THR:HG21	38:C:8575:HOH:O	1.92	0.70
5:C:236:THR:CG2	5:C:239:ALA:H	1.95	0.70
10:H:12:ILE:O	10:H:12:ILE:HG22	1.90	0.70
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.72	0.70
1:0:1701:A:H5'	38:0:6242:HOH:O	1.90	0.70
1:0:645:U:OP2	14:L:4:LYS:HE2	1.91	0.70
27:Y:141:THR:HG23	38:Y:8887:HOH:O	1.91	0.69
16:N:80:SER:HB2	38:N:8837:HOH:O	1.92	0.69
1:0:56:G:H5''	24:V:50:ARG:NH1	2.07	0.69
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.73	0.69
1:0:56:G:H5''	24:V:50:ARG:HH12	1.57	0.69
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.92	0.69
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.23	0.69
1:0:1666:C:H2'	1:0:1667:A:H5'	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1189:A:H1'	1:0:1209:C:C1'	2.22	0.69
1:0:2533:C:C6	1:0:2533:C:H5'	2.26	0.69
1:0:2629:C:N4	3:A:206:ARG:HH21	1.91	0.69
2:9:114:G:O6	16:N:11:ARG:HD3	1.91	0.69
14:L:143:THR:HG22	14:L:144:ASP:N	2.07	0.69
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.06	0.69
16:N:164:ASP:CG	16:N:167:ASP:HA	2.13	0.69
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.75	0.69
7:E:166:VAL:HG12	38:E:3134:HOH:O	1.92	0.69
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.56	0.68
11:I:120:ALA:O	11:I:124:VAL:HG23	1.92	0.68
14:L:79:ASP:HB3	38:L:8857:HOH:O	1.91	0.68
11:I:73:LEU:HD12	11:I:107:LYS:NZ	2.09	0.68
12:J:19:MET:CE	12:J:132:LEU:HD11	2.24	0.68
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.09	0.68
1:0:1751:G:C2'	1:0:1752:G:H5''	2.23	0.68
1:0:1119:G:N2	1:0:1246:A:C2	2.62	0.68
27:Y:144:ARG:CZ	38:Y:8910:HOH:O	2.41	0.68
2:9:39:U:H1'	2:9:44:A:H61	1.57	0.68
1:0:447:A:OP2	22:T:1:SER:HB2	1.93	0.68
1:0:2755:G:H1'	38:0:4650:HOH:O	1.94	0.68
26:X:78:GLU:HG2	26:X:79:GLU:H	1.58	0.68
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.26	0.68
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.94	0.68
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.28	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.93	0.68
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.76	0.68
14:L:143:THR:HG21	38:L:8838:HOH:O	1.92	0.68
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.94	0.68
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.75	0.68
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.67
1:0:2004:U:H4'	38:0:5268:HOH:O	1.93	0.67
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.76	0.67
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.76	0.67
1:0:1372:A:H3'	38:0:7141:HOH:O	1.94	0.67
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.10	0.67
1:0:544:G:C2'	1:0:545:G:H5''	2.24	0.67
10:H:165:ARG:HD3	38:H:8583:HOH:O	1.94	0.67
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.76	0.67
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.76	0.67
4:B:41:PHE:HB3	4:B:190:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:114:ASP:HB2	38:H:8547:HOH:O	1.94	0.67
1:O:1130:U:H5'	38:O:7620:HOH:O	1.94	0.67
38:O:6240:HOH:O	28:Z:33:MET:HE3	1.95	0.67
5:C:140:VAL:HB	38:C:8650:HOH:O	1.94	0.67
15:M:164:THR:HG22	15:M:167:GLY:N	2.07	0.67
1:O:506:G:H22	1:O:509:A:H5'	1.58	0.67
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.25	0.67
17:O:32:ARG:HD3	17:O:32:ARG:O	1.94	0.67
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.77	0.67
3:A:223:ARG:HG3	38:A:8900:HOH:O	1.94	0.67
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.25	0.67
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.77	0.67
30:2:41:HIS:HD2	30:2:44:ARG:H	1.41	0.67
1:O:1667:A:C8	1:O:1667:A:H5'	2.28	0.67
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.92	0.67
24:V:39:ALA:N	24:V:40:PRO:HD2	2.09	0.67
20:R:39:THR:HB	20:R:42:GLU:HG3	1.76	0.66
11:I:88:GLN:HA	11:I:91:PHE:CE2	2.30	0.66
24:V:4:HIS:HB3	38:V:6622:HOH:O	1.94	0.66
2:9:35:C:H5''	38:9:8653:HOH:O	1.96	0.66
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.40	0.66
1:O:2840:A:OP1	4:B:211:THR:HG23	1.95	0.66
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.77	0.66
4:B:41:PHE:HA	4:B:79:MET:HE2	1.77	0.66
12:J:99:GLU:HA	38:J:7377:HOH:O	1.95	0.66
2:9:14:G:H5'	2:9:14:G:C8	2.29	0.66
15:M:169:ARG:HD2	38:M:8892:HOH:O	1.94	0.66
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.11	0.66
7:E:11:VAL:HG12	7:E:12:ASP:N	2.10	0.66
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.96	0.66
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.09	0.66
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.78	0.66
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.14	0.66
7:E:6:GLU:HA	7:E:46:THR:HG22	1.76	0.66
38:O:3826:HOH:O	10:H:14:LYS:HE2	1.96	0.66
1:O:1835:U:C5	1:O:1840:A:N7	2.60	0.66
1:O:1189:A:H1'	1:O:1209:C:H1'	1.78	0.66
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.11	0.66
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.24	0.65
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.96	0.65
4:B:140:LEU:HA	38:B:8879:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:21:SER:OG	17:O:106:PRO:HB2	1.96	0.65
9:G:64:ASN:HD22	9:G:64:ASN:N	1.93	0.65
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.27	0.65
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.78	0.65
6:D:136:ARG:HD2	6:D:155:HIS:O	1.96	0.65
1:O:272:A:H5'	1:O:273:G:OP2	1.96	0.65
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.79	0.65
16:N:169:PRO:O	16:N:172:PHE:HB3	1.96	0.65
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.62	0.65
1:O:2850:C:H6	1:O:2850:C:H5'	1.59	0.65
1:O:2780:C:H1'	7:E:143:GLN:HE21	1.61	0.65
6:D:99:ASP:HB3	6:D:103:ASN:H	1.61	0.65
1:O:338:C:H4'	5:C:174:ILE:CD1	2.27	0.65
2:9:54:A:O2'	2:9:55:U:H5'	1.96	0.65
2:9:39:U:H1'	2:9:44:A:N6	2.10	0.65
16:N:154:LEU:O	16:N:155:GLU:HB3	1.97	0.65
1:O:814:G:H4'	38:O:3121:HOH:O	1.96	0.65
5:C:233:THR:HG22	5:C:234:VAL:H	1.62	0.65
21:S:37:VAL:O	21:S:41:VAL:HG23	1.96	0.65
1:O:871:G:C8	1:O:871:G:C5'	2.73	0.65
1:O:1741:U:H5'	1:O:1742:A:OP1	1.97	0.65
27:Y:133:HIS:HD2	38:Y:8880:HOH:O	1.79	0.65
18:P:115:SER:H	18:P:118:GLN:NE2	1.81	0.65
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.79	0.65
10:H:61:ARG:HG3	10:H:61:ARG:HH11	1.62	0.65
38:C:8559:HOH:O	17:O:3:THR:HG21	1.96	0.65
24:V:64:GLY:O	24:V:65:ASP:HB2	1.95	0.65
21:S:43:GLU:HB3	38:S:8545:HOH:O	1.97	0.65
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.77	0.65
25:W:38:THR:HG22	25:W:39:ASP:H	1.61	0.64
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.78	0.64
6:D:99:ASP:HA	38:D:5675:HOH:O	1.97	0.64
3:A:121:ALA:O	3:A:124:VAL:HG22	1.97	0.64
1:O:2488:A:H61	1:O:2534:C:H42	1.43	0.64
6:D:163:VAL:HA	38:D:6326:HOH:O	1.96	0.64
11:I:124:VAL:HG13	11:I:134:ILE:HD11	1.79	0.64
14:L:143:THR:HG22	14:L:144:ASP:H	1.62	0.64
1:O:1634:G:H3'	38:O:3873:HOH:O	1.96	0.64
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.79	0.64
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.79	0.64
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.38	0.64
11:I:108:HIS:HE1	11:I:116:LEU:HD22	1.62	0.64
24:V:44:GLY:O	24:V:48:GLU:HG2	1.97	0.64
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.13	0.64
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.80	0.64
1:0:1086:A:C6	25:W:11:VAL:HG11	2.32	0.64
8:F:46:GLU:OE1	8:F:100:ASP:HA	1.97	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
6:D:154:LYS:H	6:D:154:LYS:CD	2.00	0.64
38:0:6723:HOH:O	16:N:4:PRO:HD2	1.97	0.64
1:0:2243:C:H5''	38:0:3732:HOH:O	1.98	0.64
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.80	0.64
2:9:73:A:N6	2:9:108:C:H42	1.96	0.64
2:9:92:G:H2'	2:9:93:A:C8	2.33	0.64
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.63	0.64
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.79	0.63
38:0:9348:HOH:O	29:1:1:THR:HA	1.98	0.63
3:A:164:ARG:NE	38:A:8886:HOH:O	2.31	0.63
12:J:19:MET:HE1	12:J:132:LEU:HD11	1.80	0.63
1:0:1679:C:H5'	38:0:9314:HOH:O	1.99	0.63
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.79	0.63
4:B:56:ASP:OD1	4:B:322:ARG:HB3	1.98	0.63
2:9:49:G:H5''	38:9:8665:HOH:O	1.97	0.63
1:0:797:A:C4'	28:Z:10:ARG:N	2.61	0.63
1:0:777:U:O2'	29:1:11:LYS:HG2	1.98	0.63
18:P:91:LYS:O	18:P:95:GLU:HG3	1.98	0.63
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.80	0.63
1:0:1189:A:H1'	1:0:1209:C:O4'	1.99	0.63
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.81	0.63
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.79	0.63
5:C:142:ASP:OD1	5:C:237:GLU:HB3	1.99	0.63
11:I:70:THR:HA	11:I:107:LYS:HZ3	1.64	0.63
38:E:2512:HOH:O	12:J:127:ILE:HD11	1.98	0.63
1:0:603:A:H5''	1:0:604:G:OP1	1.99	0.63
31:3:73:GLU:HB3	38:3:8865:HOH:O	1.97	0.63
1:0:1377:C:H6	1:0:1377:C:H5'	1.64	0.63
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.79	0.63
20:R:9:ASP:O	20:R:13:THR:HB	1.98	0.63
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.13	0.63
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.80	0.63
1:0:558:C:C2'	1:0:559:U:H5''	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.62	0.63
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.98	0.63
3:A:199:HIS:HD2	3:A:201:PHE:H	1.46	0.63
10:H:12:ILE:HG23	10:H:129:ARG:CZ	2.29	0.63
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.80	0.63
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.81	0.63
14:L:22:ARG:HG2	38:L:8823:HOH:O	1.98	0.63
24:V:13:PRO:O	24:V:17:GLU:HG3	1.99	0.63
1:O:2505:G:O2'	1:O:2506:A:H5'	1.99	0.63
5:C:16:VAL:HG12	5:C:17:ASP:H	1.64	0.63
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.64	0.63
6:D:25:MET:CE	6:D:37:ALA:HB1	2.29	0.62
1:O:2630:G:O6	3:A:206:ARG:NH2	2.32	0.62
1:O:2320:U:H4'	1:O:2321:A:O4'	1.98	0.62
1:O:2491:G:H1'	38:O:6818:HOH:O	1.98	0.62
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.26	0.62
11:I:87:PRO:C	11:I:89:GLU:H	2.02	0.62
23:U:17:THR:HG22	23:U:18:GLY:N	2.14	0.62
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.81	0.62
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.81	0.62
24:V:56:ILE:O	24:V:60:GLN:HG3	2.00	0.62
1:O:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
1:O:2694:A:H4'	7:E:91:PHE:CE1	2.34	0.62
12:J:107:ASN:ND2	12:J:109:TYR:H	1.97	0.62
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.29	0.62
16:N:151:ASP:O	16:N:154:LEU:HB2	2.00	0.62
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.64	0.62
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.82	0.62
14:L:136:ALA:HB3	38:L:8871:HOH:O	1.98	0.62
30:2:35:ARG:HB2	38:2:2691:HOH:O	1.99	0.62
38:O:4202:HOH:O	30:2:38:LYS:HE3	1.99	0.62
5:C:16:VAL:HG12	5:C:17:ASP:N	2.14	0.62
1:O:2420:G:O2'	1:O:2421:G:H5'	2.00	0.62
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.15	0.62
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.35	0.62
2:9:29:C:H2'	2:9:30:C:H5'	1.82	0.62
2:9:73:A:H61	2:9:108:C:N4	1.97	0.62
1:O:21:G:H4'	20:R:2:ILE:HG22	1.81	0.62
1:O:282:C:O2'	1:O:283:U:H5'	2.00	0.62
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.35	0.62
15:M:60:VAL:C	15:M:61:ILE:HD12	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.97	0.62
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.82	0.61
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.14	0.61
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.35	0.61
10:H:31:ILE:HA	10:H:66:GLU:OE1	2.00	0.61
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.80	0.61
1:O:2502:C:C2'	1:O:2503:A:H5'	2.30	0.61
1:O:2710:U:H1'	38:O:7568:HOH:O	2.00	0.61
1:O:558:C:O2'	1:O:559:U:H5''	2.00	0.61
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.61
1:O:870:G:OP2	3:A:3:ARG:HD3	2.00	0.61
11:I:101:LYS:O	11:I:105:GLU:HG3	2.00	0.61
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.30	0.61
1:O:2578:G:H5'	1:O:2578:G:H8	1.65	0.61
3:A:33:GLU:O	3:A:34:ASP:HB2	2.01	0.61
29:1:10:LYS:HG3	38:1:8732:HOH:O	1.99	0.61
1:O:31:C:H2'	38:O:7636:HOH:O	2.00	0.61
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.30	0.61
4:B:304:PRO:HD2	4:B:307:ARG:HD2	1.82	0.61
4:B:275:GLY:O	4:B:291:ASP:HA	2.01	0.61
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.02	0.61
26:X:31:ILE:O	26:X:35:GLU:HG3	1.99	0.61
20:R:33:ARG:NH1	38:R:8840:HOH:O	2.33	0.61
1:O:709:G:O2'	17:O:25:VAL:HG12	2.01	0.61
30:2:41:HIS:N	30:2:45:ASN:HD22	1.93	0.61
1:O:1185:U:H5'	38:O:7413:HOH:O	2.01	0.61
1:O:1701:A:H4'	1:O:1702:U:C5'	2.29	0.61
1:O:1477:C:H5'	1:O:1868:G:C5'	2.31	0.61
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.83	0.61
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.31	0.61
4:B:51:VAL:HG13	4:B:53:LEU:HD13	1.82	0.61
1:O:447:A:P	22:T:1:SER:HB2	2.41	0.61
5:C:12:THR:HB	38:C:8640:HOH:O	2.00	0.61
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.82	0.61
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.82	0.61
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.83	0.61
5:C:77:ALA:O	5:C:78:ARG:HG3	2.00	0.61
8:F:61:MET:HB3	15:M:19:GLN:OE1	2.01	0.61
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.83	0.61
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.82	0.60
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.82	0.60
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.23	0.60
14:L:114:VAL:HG11	38:L:8871:HOH:O	1.99	0.60
4:B:41:PHE:CD2	4:B:190:MET:HE3	2.36	0.60
1:O:1008:C:H5''	10:H:19:ARG:HH12	1.66	0.60
11:I:108:HIS:N	11:I:109:PRO:HD2	2.17	0.60
1:O:31:C:H4'	38:O:7373:HOH:O	2.01	0.60
38:O:6657:HOH:O	27:Y:165:GLU:HB3	2.00	0.60
9:G:16:LYS:O	9:G:20:VAL:HG23	2.01	0.60
21:S:57:THR:HG22	21:S:59:ASP:H	1.65	0.60
1:O:1505:U:H6	1:O:1505:U:H5'	1.65	0.60
1:O:1080:C:H4'	1:O:1081:A:OP1	2.00	0.60
6:D:166:ILE:HB	38:D:6326:HOH:O	2.00	0.60
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.83	0.60
1:O:797:A:H4'	28:Z:10:ARG:N	2.16	0.60
1:O:558:C:H2'	1:O:559:U:C5'	2.31	0.60
3:A:53:ALA:HB3	38:A:8905:HOH:O	2.02	0.60
1:O:470:U:O2'	29:1:16:HIS:HD2	1.85	0.60
1:O:2717:C:H2'	1:O:2718:C:C5'	2.28	0.60
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.01	0.60
8:F:99:THR:HA	38:F:3461:HOH:O	2.01	0.60
3:A:164:ARG:CZ	38:A:8886:HOH:O	2.48	0.60
1:O:584:U:H3'	38:O:6051:HOH:O	2.00	0.60
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.36	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.02	0.60
5:C:145:GLU:HG3	38:C:8575:HOH:O	2.01	0.60
13:K:55:VAL:HG12	13:K:56:SER:N	2.16	0.60
14:L:133:VAL:HB	38:L:8856:HOH:O	2.00	0.60
12:J:131:THR:HB	12:J:134:GLU:HG3	1.82	0.60
1:O:136:C:H2'	1:O:137:U:O4'	2.02	0.60
17:O:73:ASP:HA	17:O:92:VAL:O	2.00	0.60
6:D:50:VAL:O	6:D:71:ALA:HA	2.02	0.60
4:B:16:ARG:NH1	38:B:8918:HOH:O	2.34	0.60
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.33	0.60
1:O:1593:C:H5'	18:P:116:SER:O	2.01	0.60
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.67	0.60
11:I:129:SER:O	11:I:130:LEU:HD23	2.01	0.60
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.15	0.60
3:A:88:ILE:HG22	3:A:88:ILE:O	2.00	0.60
1:O:396:U:O2'	1:O:418:C:H4'	2.02	0.60
4:B:162:MET:CE	4:B:308:LEU:HD21	2.24	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:9208:HOH:O	3:A:11:ARG:HD3	2.02	0.60
25:W:38:THR:HG22	38:W:3580:HOH:O	2.01	0.60
17:O:26:TRP:HB2	38:O:3062:HOH:O	2.02	0.60
38:O:6978:HOH:O	3:A:211:LYS:HG2	2.01	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.83	0.59
1:O:818:A:O2'	28:Z:13:ARG:HD3	2.02	0.59
1:O:1058:A:H2'	1:O:1060:C:H5''	1.82	0.59
3:A:109:GLU:HG2	3:A:116:GLY:N	2.17	0.59
1:O:1168:C:H4'	38:I:5128:HOH:O	2.01	0.59
12:J:131:THR:HG22	12:J:134:GLU:H	1.65	0.59
1:O:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.59
5:C:246:ARG:NH2	38:C:8627:HOH:O	2.33	0.59
1:O:2064:U:H5'	1:O:2652:U:H4'	1.84	0.59
25:W:126:ASP:HB3	25:W:135:GLY:O	2.02	0.59
12:J:103:VAL:HG12	38:J:5907:HOH:O	2.00	0.59
4:B:62:ARG:CA	4:B:65:MET:HE3	2.29	0.59
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.02	0.59
1:O:2036:C:O4'	13:K:44:LEU:HG	2.02	0.59
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.71	0.59
3:A:94:LEU:N	3:A:94:LEU:HD23	2.18	0.59
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.67	0.59
1:O:2414:A:H2'	1:O:2415:A:C8	2.36	0.59
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.49	0.59
1:O:1187:U:O2'	1:O:1189:A:H2	1.84	0.59
1:O:506:G:H22	1:O:509:A:H5''	1.68	0.59
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.32	0.59
4:B:51:VAL:HG23	4:B:330:VAL:HG22	1.83	0.59
5:C:246:ARG:NE	38:C:8627:HOH:O	2.35	0.59
1:O:1596:U:H2'	1:O:1598:A:OP2	2.02	0.59
29:1:25:LYS:O	29:1:25:LYS:HG2	2.02	0.59
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.37	0.59
25:W:13:MET:CE	25:W:17:ILE:HG22	2.32	0.59
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.33	0.59
3:A:192:VAL:HG13	38:A:8855:HOH:O	2.03	0.59
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.84	0.59
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.59
20:R:132:ARG:CZ	38:R:8878:HOH:O	2.51	0.59
1:O:542:A:H5'	1:O:542:A:C8	2.29	0.59
23:U:14:GLU:O	23:U:17:THR:HB	2.02	0.59
18:P:103:THR:O	18:P:107:GLU:HG3	2.03	0.59
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.03	0.59
1:0:188:C:H5''	15:M:163:LEU:HD21	1.84	0.59
2:9:13:A:O2'	2:9:14:G:H5''	2.03	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.67	0.59
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.59
38:9:8665:HOH:O	16:N:147:ILE:HB	2.00	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.18	0.58
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.84	0.58
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.01	0.58
38:0:3737:HOH:O	22:T:9:LYS:HD3	2.03	0.58
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.38	0.58
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.03	0.58
18:P:134:VAL:O	18:P:137:LEU:HB3	2.03	0.58
1:0:1278:A:H4'	1:0:1279:U:C4	2.37	0.58
11:I:87:PRO:O	11:I:89:GLU:HG3	2.03	0.58
1:0:285:A:H2'	1:0:286:U:O4'	2.04	0.58
26:X:30:MET:HE1	26:X:55:ASN:HA	1.84	0.58
1:0:1159:G:H21	1:0:1189:A:H8	1.52	0.58
1:0:2769:C:C2'	1:0:2770:G:H5'	2.34	0.58
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.68	0.58
1:0:2717:C:O2'	1:0:2718:C:H5''	2.03	0.58
1:0:1183:C:N4	1:0:1184:C:H41	2.01	0.58
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.69	0.58
1:0:1120:U:H5'	1:0:1121:G:OP2	2.02	0.58
4:B:185:GLY:HA2	38:B:8934:HOH:O	2.04	0.58
1:0:2769:C:H2'	1:0:2770:G:O4'	2.03	0.58
11:I:70:THR:HA	11:I:107:LYS:NZ	2.17	0.58
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.04	0.58
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.68	0.58
1:0:2748:G:H5'	38:0:7487:HOH:O	2.02	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
18:P:143:ALA:HA	38:P:192:HOH:O	2.02	0.58
5:C:162:VAL:HG13	5:C:192:ILE:HD11	1.83	0.58
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.34	0.58
1:0:1299:G:O6	14:L:6:ARG:HD3	2.04	0.58
14:L:104:ASP:HB2	38:L:8874:HOH:O	2.03	0.58
10:H:30:LYS:H	10:H:62:HIS:CD2	2.16	0.58
24:V:38:GLY:C	24:V:40:PRO:HD2	2.24	0.58
1:0:2265:U:H2'	1:0:2266:A:C8	2.39	0.58
1:0:793:A:H5''	18:P:83:LYS:HG2	1.86	0.58
3:A:211:LYS:NZ	38:A:8919:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:NH2	38:Y:8910:HOH:O	2.37	0.57
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.33	0.57
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.86	0.57
1:O:20:G:H21	20:R:117:HIS:HD2	1.52	0.57
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.86	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.33	0.57
6:D:64:ARG:HB3	6:D:67:ASP:OD2	2.04	0.57
1:O:1667:A:H2'	1:O:1668:U:C6	2.39	0.57
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.34	0.57
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.04	0.57
1:O:1741:U:O2'	1:O:2723:G:H4'	2.05	0.57
1:O:485:A:N3	1:O:487:G:H5''	2.19	0.57
1:O:2241:C:O2'	1:O:2242:U:H5'	2.04	0.57
1:O:1878:G:H1'	38:O:6077:HOH:O	2.04	0.57
31:3:62:THR:HB	38:3:8854:HOH:O	2.04	0.57
6:D:149:ARG:NH1	38:D:3066:HOH:O	2.37	0.57
1:O:1187:U:H2'	38:O:6847:HOH:O	2.04	0.57
6:D:65:GLU:HG3	38:D:6752:HOH:O	2.03	0.57
1:O:263:U:O4'	8:F:59:ILE:HD13	2.04	0.57
4:B:63:GLU:HG3	4:B:63:GLU:O	2.05	0.57
25:W:38:THR:HG22	25:W:39:ASP:N	2.20	0.57
15:M:61:ILE:HG13	38:M:8922:HOH:O	2.03	0.57
1:O:1477:C:H5'	1:O:1868:G:H5''	1.86	0.57
27:Y:155:ARG:NH1	38:Y:8856:HOH:O	2.36	0.57
38:K:1387:HOH:O	23:U:20:MET:HE3	2.03	0.57
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.87	0.57
7:E:68:HIS:O	7:E:72:MET:HG3	2.05	0.57
1:O:1163:G:H5'	11:I:110:ASP:O	2.05	0.57
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.29	0.57
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.85	0.57
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.86	0.57
7:E:31:ARG:NH1	38:E:5919:HOH:O	2.37	0.57
1:O:121:U:OP2	30:2:10:ARG:NH2	2.35	0.57
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.85	0.57
15:M:64:ARG:HD2	38:M:8887:HOH:O	2.04	0.57
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.86	0.57
1:O:1242:A:H5'	12:J:82:THR:CG2	2.23	0.57
20:R:39:THR:HB	20:R:42:GLU:CG	2.34	0.57
23:U:52:THR:HG22	23:U:54:THR:N	2.20	0.57
21:S:33:SER:O	21:S:37:VAL:HG23	2.04	0.57
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1926:G:H2'	1:0:1927:A:C8	2.40	0.57
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.39	0.57
26:X:25:ARG:HD3	26:X:64:ALA:O	2.05	0.57
5:C:214:THR:HG23	38:C:8636:HOH:O	2.04	0.57
25:W:88:THR:HG22	25:W:89:ASP:N	2.19	0.57
1:0:1834:C:H2'	1:0:1840:A:N6	2.20	0.57
3:A:105:VAL:HG12	3:A:106:CYS:N	2.20	0.57
26:X:30:MET:CE	26:X:58:ALA:HB3	2.35	0.57
1:0:2748:G:H2'	38:0:7487:HOH:O	2.04	0.57
1:0:1766:U:O2	1:0:1778:A:H5'	2.04	0.57
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.35	0.57
31:3:56:PRO:N	38:3:8853:HOH:O	2.38	0.57
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.68	0.57
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.19	0.57
1:0:558:C:H2'	1:0:559:U:H5'	1.87	0.57
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.69	0.57
1:0:2346:C:O2'	6:D:52:THR:HG21	2.04	0.57
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.04	0.57
27:Y:115:ARG:NE	38:Y:8854:HOH:O	2.37	0.57
22:T:106:GLU:HG3	38:T:4913:HOH:O	2.05	0.57
1:0:2756:U:N3	1:0:2896:A:H2	2.03	0.56
23:U:52:THR:CG2	23:U:54:THR:HB	2.35	0.56
7:E:69:ILE:HA	7:E:72:MET:CE	2.35	0.56
3:A:199:HIS:CD2	3:A:201:PHE:H	2.22	0.56
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.35	0.56
1:0:2502:C:H2'	1:0:2503:A:H5'	1.87	0.56
1:0:69:A:H5'	1:0:69:A:C8	2.40	0.56
38:0:9071:HOH:O	4:B:214:PRO:HD2	2.05	0.56
10:H:41:LYS:HE2	10:H:45:ASP:HB2	1.86	0.56
16:N:37:ARG:NE	38:N:8834:HOH:O	2.38	0.56
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.33	0.56
1:0:2323:G:H5'	38:0:6971:HOH:O	2.05	0.56
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.87	0.56
1:0:2094:G:H4'	4:B:245:SER:HB3	1.86	0.56
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.87	0.56
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.31	0.56
12:J:52:GLN:HG3	12:J:53:ILE:N	2.21	0.56
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.32	0.56
25:W:6:GLN:HG2	25:W:29:VAL:HA	1.87	0.56
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.56
14:L:144:ASP:HA	14:L:147:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.71	0.56
1:0:1060:C:H6	1:0:1060:C:H5'	1.70	0.56
1:0:244:C:OP2	8:F:38:LYS:HE3	2.04	0.56
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.40	0.56
25:W:130:HIS:O	25:W:136:GLY:HA3	2.05	0.56
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.40	0.56
38:0:7404:HOH:O	5:C:188:ARG:HD2	2.05	0.56
5:C:25:PRO:HG2	38:C:8523:HOH:O	2.05	0.56
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.87	0.56
1:0:2896:A:H5''	38:0:6055:HOH:O	2.04	0.56
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.35	0.56
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.05	0.56
24:V:39:ALA:C	24:V:41:GLU:H	2.09	0.56
6:D:135:VAL:HG22	6:D:136:ARG:N	2.20	0.56
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.40	0.56
4:B:85:ARG:NH1	38:B:8935:HOH:O	2.39	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.06	0.56
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.50	0.56
5:C:115:LEU:O	5:C:118:THR:HB	2.06	0.56
1:0:1132:A:N6	1:0:1229:C:H2'	2.21	0.56
4:B:137:LEU:HD21	4:B:140:LEU:HD21	1.88	0.56
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.56
2:9:44:A:O4'	6:D:76:ARG:NE	2.39	0.56
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.86	0.56
5:C:233:THR:HG22	5:C:234:VAL:N	2.19	0.56
4:B:297:VAL:HB	38:B:8907:HOH:O	2.06	0.56
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.36	0.56
1:0:125:U:H2'	38:0:3747:HOH:O	2.05	0.56
4:B:280:VAL:HG13	4:B:333:GLU:O	2.06	0.56
4:B:248:ARG:O	4:B:251:VAL:HG13	2.05	0.56
2:9:1:U:H5''	2:9:3:A:OP1	2.06	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
31:3:17:HIS:O	31:3:18:GLN:HG3	2.06	0.56
3:A:109:GLU:HG2	3:A:116:GLY:H	1.71	0.56
1:0:1377:C:H5'	1:0:1377:C:C6	2.41	0.56
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.88	0.56
4:B:145:HIS:HD2	4:B:146:THR:O	1.87	0.56
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.09	0.56
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.87	0.56
1:0:447:A:O2'	1:0:448:G:H5'	2.06	0.56
3:A:65:ARG:C	3:A:66:ARG:HG3	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.88	0.56
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.06	0.56
1:0:902:G:N7	14:L:18:HIS:HD2	2.03	0.56
11:I:129:SER:N	38:I:7330:HOH:O	2.37	0.56
5:C:1:MET:HG2	5:C:2:GLN:N	2.20	0.56
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.41	0.56
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.88	0.56
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.06	0.56
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.06	0.56
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.56
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.54	0.55
4:B:238:ASN:HD22	4:B:240:GLY:N	1.97	0.55
14:L:145:LEU:O	14:L:148:GLU:HG3	2.06	0.55
6:D:135:VAL:HG22	6:D:136:ARG:H	1.71	0.55
8:F:28:ALA:CB	8:F:99:THR:HG23	2.36	0.55
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.70	0.55
1:0:2559:C:H4'	38:0:7209:HOH:O	2.04	0.55
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.55
1:0:1166:A:H1'	1:0:1192:A:C2	2.41	0.55
1:0:2629:C:H41	3:A:206:ARG:HH21	1.54	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.55
1:0:2712:G:H5'	38:K:4183:HOH:O	2.06	0.55
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.40	0.55
11:I:130:LEU:HA	38:I:7210:HOH:O	2.06	0.55
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.34	0.55
1:0:1819:G:H5'	38:0:4679:HOH:O	2.06	0.55
7:E:137:ASP:O	7:E:141:VAL:HG23	2.05	0.55
38:0:7093:HOH:O	29:1:1:THR:HB	2.05	0.55
1:0:2064:U:H5'	1:0:2652:U:O3'	2.07	0.55
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.55
1:0:926:A:O2'	14:L:41:HIS:HD2	1.89	0.55
4:B:305:ASP:O	4:B:306:LYS:HB2	2.07	0.55
22:T:26:THR:HA	22:T:39:ASN:HB3	1.88	0.55
6:D:92:GLU:HB2	38:D:3862:HOH:O	2.07	0.55
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.87	0.55
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.71	0.55
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.37	0.55
7:E:107:PHE:CE2	7:E:108:LEU:HD13	2.42	0.55
16:N:37:ARG:NH2	38:N:8834:HOH:O	2.39	0.55
25:W:139:GLY:O	25:W:141:HIS:CD2	2.60	0.55
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.36	0.55
26:X:25:ARG:NH1	38:X:3861:HOH:O	2.40	0.55
11:I:71:ALA:O	11:I:75:LYS:HG3	2.07	0.55
1:0:417:G:P	38:0:7367:HOH:O	2.64	0.55
9:G:23:ILE:O	9:G:27:ILE:HG13	2.06	0.55
2:9:6:C:OP1	16:N:37:ARG:NH1	2.40	0.55
12:J:19:MET:HE2	12:J:79:PHE:HA	1.88	0.55
1:0:318:U:O2'	1:0:338:C:H2'	2.06	0.55
1:0:656:G:H5'	17:O:3:THR:HB	1.88	0.55
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.36	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.70	0.55
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.42	0.55
8:F:37:THR:O	8:F:41:GLU:HG3	2.05	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.89	0.55
1:0:282:C:H1'	1:0:368:C:H42	1.71	0.55
11:I:118:ASN:HA	11:I:121:LYS:HD2	1.88	0.55
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.06	0.55
1:0:2365:G:H4'	19:Q:45:PRO:O	2.07	0.55
22:T:47:THR:HB	22:T:100:ASP:HB3	1.88	0.55
1:0:796:A:HO2'	28:Z:10:ARG:N	2.04	0.55
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.55
1:0:119:A:H2'	1:0:120:A:H5''	1.88	0.55
1:0:536:A:H3'	38:0:5012:HOH:O	2.06	0.55
5:C:78:ARG:CG	5:C:78:ARG:HH11	2.06	0.55
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.55
1:0:1926:G:H2'	1:0:1927:A:H8	1.72	0.55
4:B:119:HIS:O	4:B:121:PRO:HD3	2.07	0.55
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.88	0.55
1:0:2878:U:H2'	1:0:2879:A:O4'	2.07	0.55
1:0:1130:U:H2'	1:0:1131:G:O4'	2.07	0.54
8:F:46:GLU:O	8:F:73:PRO:HD2	2.07	0.54
2:9:48:C:H4'	16:N:141:ARG:HH21	1.72	0.54
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.37	0.54
38:0:9689:HOH:O	4:B:254:GLN:HG3	2.06	0.54
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.54
2:9:30:C:OP1	6:D:137:PRO:O	2.25	0.54
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.72	0.54
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.42	0.54
1:0:1044:C:H5''	38:0:9020:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:21:GLU:O	8:F:24:ARG:HG3	2.07	0.54
3:A:217:ARG:CG	3:A:217:ARG:HH11	2.19	0.54
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.89	0.54
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.05	0.54
1:0:1701:A:H5''	1:0:1702:U:H3'	1.89	0.54
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.90	0.54
21:S:57:THR:HG22	21:S:59:ASP:N	2.22	0.54
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.54
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.90	0.54
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.89	0.54
1:0:1342:C:O2'	1:0:1343:C:H5'	2.08	0.54
11:I:124:VAL:O	11:I:124:VAL:HG12	2.07	0.54
1:0:204:A:H2'	1:0:205:U:H5'	1.88	0.54
38:0:4042:HOH:O	4:B:27:ASN:HB2	2.07	0.54
2:9:55:U:H4'	2:9:56:A:H8	1.71	0.54
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.55	0.54
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.54
23:U:9:CYS:CA	23:U:52:THR:HG23	2.38	0.54
27:Y:144:ARG:NH1	38:Y:8874:HOH:O	2.39	0.54
1:0:299:U:H5'	38:0:7287:HOH:O	2.07	0.54
31:3:70:ARG:HB3	38:3:8877:HOH:O	2.07	0.54
10:H:48:VAL:HA	10:H:170:ARG:O	2.07	0.54
20:R:132:ARG:HG2	20:R:133:ALA:N	2.21	0.54
1:0:553:G:P	27:Y:204:ARG:HH22	2.30	0.54
1:0:2301:A:H5''	1:0:2302:A:H5'	1.90	0.54
1:0:1119:G:H8	12:J:52:GLN:HE22	1.54	0.54
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.68	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
1:0:69:A:H5'	1:0:69:A:H8	1.73	0.54
6:D:36:ASN:HA	38:D:7500:HOH:O	2.07	0.54
38:0:6243:HOH:O	27:Y:158:LYS:HD3	2.07	0.54
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.31	0.54
1:0:500:G:H21	20:R:98:ASN:HD21	1.54	0.54
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.89	0.54
13:K:87:ARG:NE	38:K:4854:HOH:O	2.41	0.54
1:0:485:A:HO2'	1:0:487:G:H8	1.56	0.54
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.73	0.54
2:9:31:C:H1'	38:9:8593:HOH:O	2.08	0.54
5:C:219:ASN:O	5:C:222:ASP:OD1	2.25	0.54
1:0:138:U:H5''	1:0:139:C:OP2	2.08	0.54
1:0:517:U:H1'	38:0:7523:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.89	0.54
1:0:1506:U:H6	1:0:1506:U:H5'	1.72	0.54
18:P:115:SER:C	18:P:117:SER:H	2.12	0.54
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.88	0.54
1:0:1641:A:C2'	1:0:1642:A:H5'	2.38	0.54
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.72	0.54
21:S:33:SER:OG	21:S:36:GLU:HG3	2.08	0.54
2:9:91:C:H2'	2:9:92:G:O4'	2.08	0.54
1:0:67:A:H5''	1:0:69:A:C8	2.43	0.54
8:F:101:ALA:HA	38:F:5413:HOH:O	2.08	0.54
27:Y:216:ARG:HD3	38:Y:8868:HOH:O	2.08	0.54
1:0:88:G:H5'	1:0:88:G:H8	1.72	0.54
25:W:80:ASP:O	25:W:84:VAL:HG23	2.07	0.53
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.90	0.53
9:G:64:ASN:N	9:G:64:ASN:ND2	2.55	0.53
8:F:28:ALA:HB3	8:F:99:THR:O	2.08	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.41	0.53
1:0:2604:A:H5'	38:0:5748:HOH:O	2.08	0.53
1:0:2256:G:H2'	1:0:2257:G:C5'	2.38	0.53
31:3:48:ASN:ND2	31:3:50:GLY:H	2.05	0.53
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.90	0.53
18:P:115:SER:O	18:P:117:SER:N	2.41	0.53
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.73	0.53
8:F:91:VAL:CG1	8:F:92:GLY:H	2.17	0.53
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.53
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.91	0.53
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.89	0.53
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.89	0.53
16:N:37:ARG:CZ	38:N:8834:HOH:O	2.56	0.53
1:0:1116:U:O2'	1:0:1118:A:C2	2.48	0.53
16:N:110:THR:HB	16:N:113:SER:OG	2.08	0.53
1:0:1086:A:N6	25:W:11:VAL:HG11	2.23	0.53
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.37	0.53
1:0:2256:G:H2'	1:0:2257:G:H5'	1.91	0.53
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.07	0.53
1:0:407:A:H5'	38:0:5983:HOH:O	2.07	0.53
1:0:1525:G:H5'	1:0:1526:A:OP2	2.08	0.53
1:0:775:G:OP1	29:1:16:HIS:HE1	1.92	0.53
1:0:2346:C:O5'	1:0:2346:C:H6	1.92	0.53
19:Q:53:HIS:ND1	19:Q:55:ARG:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:328:U:O4'	5:C:202:THR:HG22	2.08	0.53
1:0:602:A:O2'	1:0:605:C:H4'	2.07	0.53
2:9:64:C:H2'	2:9:65:A:H5'	1.90	0.53
1:0:1527:A:H1'	1:0:1528:A:C8	2.43	0.53
21:S:52:VAL:C	21:S:53:ASN:HD22	2.11	0.53
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.91	0.53
14:L:21:ARG:N	38:L:8831:HOH:O	2.41	0.53
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.44	0.53
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.90	0.53
26:X:76:ARG:O	26:X:77:PHE:HB3	2.08	0.53
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.91	0.53
1:0:2256:G:C2'	1:0:2257:G:H5'	2.39	0.53
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.08	0.53
17:O:87:THR:O	17:O:91:GLN:HG3	2.08	0.53
1:0:285:A:C2	1:0:368:C:H4'	2.43	0.53
1:0:1185:U:H2'	1:0:1186:C:C6	2.43	0.53
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.44	0.53
1:0:1266:U:H4'	27:Y:115:ARG:HH21	1.73	0.53
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
1:0:399:C:H5'	15:M:179:GLY:O	2.09	0.53
1:0:1333:U:H2'	1:0:1334:C:C6	2.44	0.53
1:0:1289:C:O2'	1:0:1290:G:H5'	2.09	0.53
5:C:39:GLN:O	5:C:43:LYS:HD3	2.09	0.53
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.33	0.53
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.37	0.53
23:U:52:THR:HG22	23:U:54:THR:H	1.74	0.53
9:G:20:VAL:O	9:G:24:VAL:HG23	2.09	0.53
21:S:77:VAL:O	21:S:80:ARG:HG2	2.08	0.53
1:0:2526:C:O2'	1:0:2527:U:H5'	2.09	0.53
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.44	0.53
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.24	0.53
1:0:316:A:H5'	22:T:54:ASP:OD2	2.08	0.53
1:0:2649:A:H5'	1:0:2649:A:H8	1.73	0.53
1:0:1205:U:H2'	1:0:1206:U:H5''	1.90	0.53
16:N:152:GLU:C	16:N:154:LEU:H	2.10	0.53
1:0:2300:A:H4'	1:0:2301:A:O5'	2.09	0.53
5:C:61:PHE:HB3	38:C:8643:HOH:O	2.09	0.53
21:S:81:ILE:HG12	38:S:8538:HOH:O	2.08	0.53
12:J:130:VAL:HG12	12:J:131:THR:N	2.24	0.52
14:L:61:ALA:HA	38:L:8862:HOH:O	2.08	0.52
21:S:11:THR:H	21:S:14:ALA:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:18:GLU:O	22:T:21:LYS:HG2	2.09	0.52
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.09	0.52
8:F:117:GLU:C	8:F:119:ARG:H	2.11	0.52
12:J:74:ARG:O	12:J:78:ILE:HG12	2.09	0.52
12:J:107:ASN:C	12:J:107:ASN:HD22	2.12	0.52
1:O:2064:U:H4'	1:O:2653:A:OP1	2.09	0.52
18:P:103:THR:HA	18:P:106:ARG:NH1	2.24	0.52
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.08	0.52
22:T:80:GLU:HA	38:T:6653:HOH:O	2.08	0.52
38:O:9529:HOH:O	18:P:81:LYS:HG2	2.09	0.52
10:H:50:ILE:HG12	10:H:168:VAL:HG22	1.92	0.52
1:O:2401:A:H5'	38:O:9483:HOH:O	2.10	0.52
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.38	0.52
3:A:192:VAL:HB	38:A:8892:HOH:O	2.10	0.52
2:9:34:A:H2'	2:9:35:C:O4'	2.08	0.52
1:O:654:A:OP2	17:O:38:ARG:HD3	2.09	0.52
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.52
10:H:146:ALA:O	10:H:149:VAL:HG12	2.09	0.52
4:B:125:GLU:O	4:B:129:ARG:HG3	2.09	0.52
1:O:1135:G:H5'	38:O:5887:HOH:O	2.08	0.52
1:O:1236:A:H2'	1:O:1237:U:O4'	2.09	0.52
1:O:794:U:H3	1:O:819:A:H61	1.57	0.52
1:O:1636:G:O2'	1:O:1637:A:H5'	2.09	0.52
1:O:1942:A:O2'	1:O:1943:C:H5'	2.10	0.52
7:E:80:TRP:O	7:E:134:SER:HA	2.09	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.90	0.52
7:E:77:THR:OG1	7:E:78:GLU:N	2.43	0.52
1:O:1544:U:H2'	1:O:1545:C:H6	1.75	0.52
5:C:127:ARG:HD2	5:C:229:PRO:O	2.09	0.52
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.39	0.52
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.23	0.52
24:V:5:VAL:HG23	38:V:2271:HOH:O	2.09	0.52
1:O:1535:G:H2'	1:O:1536:C:C6	2.44	0.52
1:O:1173:A:H2	38:O:6239:HOH:O	1.92	0.52
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.24	0.52
2:9:55:U:H4'	2:9:56:A:C8	2.45	0.52
4:B:254:GLN:HG2	4:B:255:GLY:N	2.24	0.52
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.55	0.52
1:O:447:A:OP1	22:T:2:LYS:HG2	2.09	0.52
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2237:G:H1'	38:0:4818:HOH:O	2.10	0.52
24:V:55:ARG:O	24:V:59:ILE:HG12	2.10	0.52
1:0:474:C:O3'	5:C:73:LEU:HD21	2.09	0.52
1:0:2862:G:H4'	4:B:336:GLN:O	2.09	0.52
38:0:9545:HOH:O	25:W:119:HIS:HE1	1.92	0.52
8:F:19:ALA:O	8:F:22:VAL:HG22	2.10	0.52
31:3:65:THR:HG23	31:3:67:LEU:HG	1.90	0.52
2:9:49:G:O2'	2:9:50:G:H5'	2.09	0.52
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.92	0.52
23:U:52:THR:HG22	23:U:54:THR:HB	1.92	0.52
1:0:343:C:O2'	1:0:344:C:H5'	2.09	0.52
1:0:2668:G:H2'	1:0:2669:U:C6	2.45	0.52
1:0:588:G:O6	25:W:154:ARG:NH1	2.42	0.52
4:B:294:TYR:HE2	38:B:8954:HOH:O	1.93	0.52
1:0:2715:G:N2	4:B:264:GLU:OE1	2.41	0.52
1:0:926:A:O2'	14:L:41:HIS:CD2	2.63	0.52
1:0:638:C:H2'	1:0:639:A:C8	2.45	0.52
1:0:2506:A:H1'	38:0:3728:HOH:O	2.09	0.52
27:Y:187:VAL:HB	38:Y:8869:HOH:O	2.10	0.52
4:B:41:PHE:CB	4:B:190:MET:HE3	2.40	0.52
13:K:34:VAL:HB	38:K:7169:HOH:O	2.10	0.52
1:0:407:A:H2'	1:0:408:A:C8	2.45	0.52
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.52
3:A:179:MET:HG2	3:A:186:TRP:CG	2.45	0.52
7:E:145:ALA:HB1	7:E:168:ILE:HD11	1.92	0.52
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.09	0.52
4:B:43:GLY:O	4:B:308:LEU:HD12	2.10	0.52
1:0:960:G:H2'	1:0:960:G:N3	2.25	0.52
3:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.91	0.52
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.91	0.52
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.40	0.52
10:H:39:LYS:HD3	38:H:8578:HOH:O	2.09	0.52
1:0:2718:C:H6	1:0:2718:C:H5'	1.76	0.51
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.45	0.51
1:0:1681:G:H5''	1:0:1682:A:H5'	1.91	0.51
4:B:103:ASP:HB2	38:B:8894:HOH:O	2.10	0.51
22:T:41:ARG:HH11	22:T:41:ARG:HG2	1.75	0.51
3:A:211:LYS:HB2	38:A:8918:HOH:O	2.09	0.51
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.51
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.39	0.51
25:W:125:HIS:CD2	25:W:127:GLY:H	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:111:VAL:HB	38:C:8522:HOH:O	2.10	0.51
5:C:168:ARG:NH2	5:C:190:ALA:O	2.43	0.51
1:0:1730:G:H5''	1:0:1731:C:H6	1.76	0.51
2:9:76:G:C3'	2:9:77:A:H5''	2.31	0.51
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.90	0.51
27:Y:117:LEU:CD1	27:Y:174:VAL:HG11	2.40	0.51
1:0:2815:G:N7	12:J:80:LYS:NZ	2.58	0.51
5:C:133:ARG:NE	5:C:135:GLU:O	2.43	0.51
21:S:57:THR:CG2	21:S:58:MET:N	2.73	0.51
4:B:195:ARG:CG	4:B:323:LEU:HD22	2.40	0.51
1:0:1044:C:H5	38:0:6557:HOH:O	1.92	0.51
1:0:474:C:O3'	5:C:73:LEU:CD2	2.58	0.51
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.51
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.91	0.51
7:E:11:VAL:HG12	7:E:12:ASP:H	1.72	0.51
1:0:2468:A:H61	31:3:48:ASN:HD21	1.57	0.51
5:C:13:ASP:OD1	5:C:13:ASP:O	2.27	0.51
4:B:202:VAL:HG11	4:B:301:VAL:HG13	1.93	0.51
10:H:172:GLU:CD	38:H:8591:HOH:O	2.48	0.51
38:0:6815:HOH:O	3:A:211:LYS:HD3	2.11	0.51
38:0:7373:HOH:O	22:T:9:LYS:HB2	2.10	0.51
25:W:65:VAL:HA	25:W:68:THR:CG2	2.40	0.51
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.92	0.51
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.10	0.51
9:G:67:LEU:O	9:G:71:LEU:HG	2.10	0.51
13:K:115:ARG:HG3	13:K:116:GLU:N	2.25	0.51
1:0:558:C:H5'	38:0:5218:HOH:O	2.11	0.51
29:1:45:ARG:NH2	38:1:8728:HOH:O	2.32	0.51
1:0:1979:G:H2'	38:0:3283:HOH:O	2.10	0.51
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.42	0.51
6:D:23:VAL:O	6:D:23:VAL:HG23	2.11	0.51
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.41	0.51
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.93	0.51
26:X:45:GLU:HG3	38:X:6178:HOH:O	2.09	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
8:F:78:GLU:HG3	38:F:5966:HOH:O	2.10	0.51
4:B:82:VAL:HG12	4:B:82:VAL:O	2.09	0.51
1:0:1189:A:H3'	38:0:7628:HOH:O	2.10	0.51
1:0:1682:A:H5''	38:0:9445:HOH:O	2.11	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:51:GLN:HB3	21:S:67:ARG:NH1	2.24	0.51
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.92	0.51
8:F:91:VAL:CG1	8:F:92:GLY:N	2.71	0.51
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.93	0.51
1:0:2533:C:H6	1:0:2533:C:C5'	2.22	0.51
26:X:78:GLU:HG2	26:X:79:GLU:N	2.26	0.51
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.51	0.51
21:S:23:LYS:HE2	38:S:8532:HOH:O	2.10	0.51
7:E:99:GLY:N	38:E:4191:HOH:O	2.44	0.51
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.41	0.51
9:G:12:ILE:N	9:G:13:PRO:HD3	2.26	0.51
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.10	0.51
1:0:2781:U:H2'	1:0:2782:G:H5'	1.92	0.51
38:0:6240:HOH:O	28:Z:49:ARG:HD2	2.11	0.51
3:A:51:ARG:NH1	3:A:120:ARG:O	2.44	0.51
1:0:2256:G:O2'	1:0:2257:G:H5'	2.11	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.51
1:0:958:G:H2'	1:0:959:C:C6	2.46	0.51
38:0:7309:HOH:O	3:A:177:HIS:HE1	1.94	0.51
1:0:559:U:H2'	1:0:560:U:O4'	2.11	0.50
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.50
1:0:944:G:H21	25:W:44:MET:CE	2.24	0.50
1:0:1625:U:H4'	38:0:4635:HOH:O	2.11	0.50
1:0:1176:C:H1'	38:0:3909:HOH:O	2.10	0.50
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.93	0.50
38:0:6167:HOH:O	4:B:2:GLN:HA	2.10	0.50
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.23	0.50
1:0:644:G:H5'	1:0:644:G:N3	2.25	0.50
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.50
28:Z:81:ARG:O	28:Z:82:SER:C	2.50	0.50
26:X:75:ALA:O	26:X:83:ALA:HA	2.10	0.50
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.94	0.50
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.76	0.50
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.37	0.50
20:R:29:LYS:NZ	38:R:8837:HOH:O	2.43	0.50
15:M:61:ILE:HA	38:M:8922:HOH:O	2.11	0.50
5:C:79:ARG:O	5:C:87:ARG:HG2	2.11	0.50
5:C:95:GLU:HG3	38:C:8671:HOH:O	2.11	0.50
12:J:133:GLY:O	12:J:137:GLU:HG3	2.10	0.50
8:F:58:GLU:HA	8:F:61:MET:CE	2.40	0.50
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:259:G:H21	15:M:58:GLN:NE2	2.09	0.50
4:B:48:MET:HG2	4:B:72:THR:HA	1.93	0.50
4:B:139:ASP:CB	4:B:165:ARG:HE	2.23	0.50
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.42	0.50
5:C:165:ASP:O	5:C:168:ARG:HB3	2.11	0.50
1:0:2679:G:H2'	1:0:2681:A:OP2	2.12	0.50
7:E:32:ARG:O	7:E:33:LEU:HD23	2.12	0.50
1:0:1687:C:O2	29:1:9:GLY:HA2	2.11	0.50
1:0:1825:U:O2'	1:0:1826:C:H5'	2.11	0.50
5:C:180:SER:HB2	38:C:8644:HOH:O	2.12	0.50
1:0:42:C:H1'	38:0:4644:HOH:O	2.10	0.50
1:0:1603:A:H5''	1:0:1605:G:H5'	1.93	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.89	0.50
1:0:1201:C:H2'	1:0:1202:A:H5'	1.93	0.50
8:F:46:GLU:N	38:F:3461:HOH:O	2.43	0.50
4:B:329:TYR:HE2	23:U:15:PRO:HG2	1.77	0.50
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.41	0.50
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.93	0.50
1:0:1790:C:H2'	1:0:1791:U:H6	1.75	0.50
1:0:1434:A:H2'	1:0:1436:C:C5	2.46	0.50
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.10	0.50
5:C:236:THR:O	5:C:237:GLU:C	2.49	0.50
1:0:2506:A:O2'	1:0:2507:G:O5'	2.29	0.50
11:I:133:THR:HG22	11:I:134:ILE:N	2.26	0.50
11:I:134:ILE:HG22	11:I:135:GLU:N	2.26	0.50
1:0:2781:U:C2'	1:0:2782:G:H5'	2.42	0.50
1:0:660:A:H4'	1:0:661:G:O5'	2.12	0.50
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.50
25:W:38:THR:HB	38:W:5390:HOH:O	2.12	0.50
4:B:7:ARG:HD3	4:B:9:GLY:O	2.11	0.50
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.40	0.50
14:L:104:ASP:HB3	38:L:8862:HOH:O	2.10	0.50
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.92	0.50
1:0:2601:A:N1	13:K:38:SER:HB2	2.27	0.50
1:0:2563:U:H2'	1:0:2565:C:O5'	2.11	0.50
6:D:154:LYS:HD2	6:D:154:LYS:N	2.06	0.50
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.76	0.50
6:D:35:ALA:N	38:D:5576:HOH:O	2.45	0.50
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.92	0.50
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.40	0.50
1:0:1862:C:H1'	38:0:7172:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:134:ILE:C	11:I:135:GLU:HG3	2.32	0.50
5:C:133:ARG:NH2	38:C:8629:HOH:O	2.44	0.50
31:3:3:MET:O	31:3:90:PHE:HA	2.12	0.50
1:0:1537:C:H1'	38:0:6542:HOH:O	2.11	0.50
1:0:1180:U:H4'	11:I:86:GLU:HG2	1.94	0.50
15:M:164:THR:HG23	15:M:165:GLY:N	2.26	0.50
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.42	0.50
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.93	0.50
17:O:25:VAL:HG23	17:O:26:TRP:N	2.27	0.50
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.76	0.50
6:D:94:ALA:HA	6:D:174:VAL:O	2.11	0.50
27:Y:235:GLU:H	27:Y:235:GLU:CD	2.13	0.50
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.46	0.50
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.93	0.50
5:C:140:VAL:HG12	5:C:141:SER:N	2.25	0.49
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.59	0.49
16:N:11:ARG:NH2	38:N:8819:HOH:O	2.45	0.49
20:R:132:ARG:NH2	38:R:8878:HOH:O	2.45	0.49
2:9:2:U:OP2	2:9:3:A:H5'	2.12	0.49
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.49
6:D:51:ARG:HD3	38:D:7636:HOH:O	2.10	0.49
14:L:42:ASN:HB2	38:L:8873:HOH:O	2.12	0.49
3:A:210:GLY:HA3	38:A:8883:HOH:O	2.12	0.49
1:0:2570:G:H5''	38:0:4876:HOH:O	2.12	0.49
1:0:21:G:H5''	20:R:1:GLY:O	2.13	0.49
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.27	0.49
8:F:48:VAL:HG12	8:F:97:ALA:HB2	1.94	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
1:0:694:A:H2'	1:0:695:C:H5'	1.94	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.46	0.49
1:0:2507:G:H2'	1:0:2510:C:H42	1.77	0.49
6:D:28:GLY:CA	6:D:69:ILE:HG23	2.36	0.49
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.44	0.49
5:C:246:ARG:NH1	38:C:8571:HOH:O	2.45	0.49
1:0:1528:A:H2'	1:0:1529:G:O4'	2.12	0.49
1:0:316:A:N3	1:0:336:G:O2'	2.44	0.49
16:N:176:ARG:O	16:N:180:LEU:HD13	2.13	0.49
1:0:2445:U:H2'	1:0:2446:G:C8	2.47	0.49
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.94	0.49
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.94	0.49
4:B:258:GLY:H	4:B:260:HIS:CE1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:279:THR:OG1	4:B:290:VAL:HB	2.12	0.49
21:S:57:THR:HG22	21:S:58:MET:N	2.27	0.49
1:0:894:A:C2	5:C:87:ARG:NH2	2.81	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
7:E:101:GLU:HB2	7:E:116:THR:O	2.12	0.49
6:D:128:LEU:N	38:D:6007:HOH:O	2.46	0.49
1:0:1615:A:H5'	38:0:4158:HOH:O	2.11	0.49
4:B:217:ARG:CG	4:B:257:THR:HG22	2.42	0.49
1:0:284:C:H4'	1:0:285:A:O5'	2.12	0.49
11:I:108:HIS:N	11:I:109:PRO:CD	2.76	0.49
1:0:64:G:H2'	1:0:65:C:O4'	2.13	0.49
38:0:4337:HOH:O	3:A:212:PRO:HB2	2.12	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.42	0.49
1:0:281:U:H3'	38:0:7159:HOH:O	2.11	0.49
25:W:26:ILE:O	25:W:26:ILE:HG13	2.12	0.49
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.48	0.49
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.93	0.49
29:1:25:LYS:HD2	30:2:49:GLU:H	1.77	0.49
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.49
4:B:280:VAL:CG1	4:B:334:SER:HA	2.43	0.49
1:0:2649:A:C8	1:0:2649:A:H5'	2.48	0.49
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.92	0.49
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.95	0.49
10:H:151:GLU:OE1	10:H:151:GLU:HA	2.13	0.49
22:T:69:LYS:O	22:T:71:VAL:HG23	2.13	0.49
10:H:41:LYS:HE2	10:H:45:ASP:CB	2.43	0.49
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.27	0.49
1:0:1175:G:H1'	1:0:1193:A:H2'	1.94	0.49
1:0:1733:A:H4'	4:B:212:GLN:HA	1.93	0.49
6:D:25:MET:CE	6:D:41:LEU:HG	2.37	0.49
25:W:149:LEU:HG	25:W:153:MET:CE	2.42	0.49
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.95	0.49
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.94	0.49
16:N:171:HIS:CE1	38:N:8868:HOH:O	2.66	0.49
10:H:61:ARG:HG3	10:H:61:ARG:NH1	2.28	0.49
7:E:69:ILE:HA	7:E:72:MET:HE2	1.94	0.49
16:N:151:ASP:OD1	16:N:154:LEU:HD13	2.13	0.49
16:N:154:LEU:O	16:N:155:GLU:CB	2.61	0.49
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.53	0.49
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.94	0.49
16:N:65:ASP:HB3	38:N:8824:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:30:ARG:NH2	38:L:8820:HOH:O	2.42	0.49
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.47	0.49
1:0:1544:U:H2'	1:0:1545:C:C6	2.48	0.49
28:Z:80:ARG:O	28:Z:81:ARG:O	2.30	0.49
1:0:2825:C:H4'	1:0:2826:G:O5'	2.13	0.49
1:0:2403:C:H3'	38:0:5171:HOH:O	2.11	0.49
14:L:67:ARG:O	14:L:71:GLU:HG3	2.12	0.49
1:0:380:A:OP2	15:M:9:ARG:HD2	2.12	0.49
7:E:132:THR:HB	38:E:2227:HOH:O	2.13	0.49
25:W:5:VAL:O	25:W:52:VAL:HG22	2.13	0.49
1:0:1450:C:O2'	1:0:1494:A:H5'	2.12	0.49
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.13	0.49
1:0:1191:A:H2'	1:0:1193:A:H5'	1.95	0.49
1:0:757:C:OP1	14:L:27:ARG:HD2	2.12	0.49
20:R:119:VAL:HG12	20:R:119:VAL:O	2.12	0.49
1:0:714:U:H3'	38:0:6893:HOH:O	2.13	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.48
1:0:558:C:H2'	1:0:559:U:H5''	1.94	0.48
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.27	0.48
6:D:56:ARG:N	38:D:6752:HOH:O	2.45	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.27	0.48
25:W:41:TYR:HA	25:W:44:MET:HE3	1.95	0.48
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.95	0.48
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.33	0.48
1:0:2894:C:O2'	1:0:2895:C:H5'	2.12	0.48
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.28	0.48
11:I:108:HIS:CE1	11:I:116:LEU:HD22	2.44	0.48
4:B:17:LYS:O	4:B:260:HIS:HD2	1.96	0.48
1:0:820:G:O2'	1:0:856:G:H4'	2.13	0.48
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.48	0.48
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.27	0.48
15:M:61:ILE:CG2	15:M:62:VAL:N	2.75	0.48
1:0:475:G:H5'	5:C:73:LEU:HD23	1.95	0.48
1:0:2251:G:H2'	1:0:2252:A:C8	2.47	0.48
15:M:46:LEU:HG	38:M:8921:HOH:O	2.13	0.48
22:T:61:GLU:HG3	38:T:3851:HOH:O	2.13	0.48
3:A:55:VAL:HG22	3:A:68:ILE:O	2.13	0.48
1:0:1589:G:N2	1:0:1605:G:H1'	2.28	0.48
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.41	0.48
1:0:2004:U:H2'	1:0:2004:U:O2	2.12	0.48
38:0:5903:HOH:O	18:P:87:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:43:VAL:HG12	26:X:44:ASP:H	1.78	0.48
5:C:157:LEU:HD22	5:C:162:VAL:CG1	2.43	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.13	0.48
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.96	0.48
4:B:102:THR:HG21	4:B:182:VAL:O	2.13	0.48
1:O:2670:G:O2'	1:O:2671:U:H5'	2.14	0.48
5:C:78:ARG:CG	5:C:78:ARG:NH1	2.70	0.48
13:K:30:LYS:O	13:K:55:VAL:HG13	2.13	0.48
1:O:1183:C:H42	1:O:1184:C:H41	1.62	0.48
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.28	0.48
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.43	0.48
27:Y:144:ARG:NE	38:Y:8910:HOH:O	2.46	0.48
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.13	0.48
5:C:246:ARG:CZ	38:C:8627:HOH:O	2.62	0.48
1:O:1972:U:H2'	1:O:1973:A:H5'	1.96	0.48
22:T:87:VAL:HB	38:T:5545:HOH:O	2.13	0.48
1:O:1675:C:H5''	30:2:5:LYS:HD2	1.95	0.48
1:O:790:A:H2'	1:O:791:A:O4'	2.13	0.48
10:H:23:ILE:HG23	10:H:123:ILE:HD11	1.95	0.48
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.12	0.48
38:9:8638:HOH:O	16:N:41:LYS:HD3	2.13	0.48
1:O:1118:A:C8	1:O:1119:G:H5''	2.48	0.48
4:B:315:VAL:HG23	4:B:316:ARG:HG2	1.96	0.48
11:I:100:VAL:HG11	11:I:124:VAL:CG2	2.43	0.48
23:U:44:ARG:HB3	38:U:3805:HOH:O	2.13	0.48
30:2:48:ASP:O	30:2:49:GLU:HB2	2.14	0.48
1:O:1787:C:H4'	1:O:2883:A:O4'	2.13	0.48
1:O:120:A:H2'	1:O:120:A:N3	2.29	0.48
1:O:2800:A:H5'	1:O:2801:A:OP2	2.13	0.48
14:L:149:ARG:O	14:L:150:GLN:HB2	2.14	0.48
1:O:2314:G:C2'	1:O:2315:C:H5'	2.44	0.48
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.95	0.48
38:0:6088:HOH:O	30:2:20:ARG:HB3	2.13	0.48
5:C:2:GLN:HB3	38:C:8586:HOH:O	2.12	0.48
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.14	0.48
25:W:151:GLU:O	25:W:154:ARG:HB3	2.13	0.48
6:D:21:VAL:HG23	6:D:80:ALA:HB1	1.95	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.48
4:B:171:VAL:O	4:B:175:LEU:HB2	2.14	0.48
22:T:37:GLN:OE1	22:T:118:SER:HA	2.12	0.48
1:O:821:U:H2'	1:O:822:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
1:0:484:A:N1	1:0:506:G:H4'	2.29	0.48
7:E:81:GLU:HG2	7:E:134:SER:CB	2.43	0.48
6:D:86:THR:C	6:D:89:PRO:HD2	2.34	0.48
1:0:952:G:N3	1:0:2302:A:H2'	2.28	0.48
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.44	0.48
1:0:377:C:H5	38:0:3296:HOH:O	1.97	0.48
10:H:157:TYR:CD1	10:H:157:TYR:C	2.86	0.48
10:H:12:ILE:HD12	10:H:57:THR:CG2	2.41	0.48
4:B:62:ARG:HA	4:B:65:MET:CE	2.35	0.48
1:0:1641:A:H2'	1:0:1642:A:C5'	2.42	0.48
1:0:1972:U:H2'	1:0:1973:A:C5'	2.44	0.48
1:0:1120:U:H5''	1:0:1120:U:C6	2.49	0.48
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.67	0.48
1:0:564:G:H1'	38:0:6268:HOH:O	2.12	0.48
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.48	0.48
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.95	0.48
1:0:2050:G:H5''	20:R:80:TYR:O	2.13	0.48
23:U:47:ARG:HG3	38:U:4381:HOH:O	2.13	0.48
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.76	0.48
10:H:30:LYS:N	10:H:62:HIS:HD2	2.07	0.48
8:F:50:VAL:CG2	8:F:63:ILE:HG21	2.44	0.48
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.14	0.48
8:F:28:ALA:HB3	8:F:99:THR:HG23	1.94	0.48
1:0:1020:A:H1'	38:Q:6976:HOH:O	2.12	0.48
1:0:2362:A:H2'	1:0:2363:G:C8	2.49	0.48
1:0:170:U:H2'	1:0:171:C:H5'	1.94	0.48
1:0:2787:C:H2'	1:0:2788:A:O4'	2.13	0.48
28:Z:46:ARG:CD	28:Z:59:TYR:HB2	2.29	0.47
38:0:7373:HOH:O	22:T:9:LYS:HD2	2.13	0.47
1:0:2909:G:H2'	1:0:2910:A:H8	1.79	0.47
7:E:7:ILE:HD11	7:E:11:VAL:C	2.34	0.47
7:E:7:ILE:HG22	7:E:45:ASP:O	2.14	0.47
1:0:1881:A:OP1	3:A:199:HIS:HE1	1.97	0.47
2:9:20:G:O2'	2:9:21:G:H5'	2.14	0.47
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.28	0.47
1:0:2597:U:H2'	1:0:2598:U:H5'	1.96	0.47
1:0:245:C:H2'	38:0:5530:HOH:O	2.14	0.47
3:A:8:ARG:HG2	38:A:8850:HOH:O	2.13	0.47
1:0:281:U:O2'	1:0:282:C:H5'	2.14	0.47
24:V:1:THR:O	24:V:4:HIS:CE1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.93	0.47
1:0:2768:A:H3'	38:0:4399:HOH:O	2.14	0.47
1:0:2421:G:H3'	1:0:2422:U:H5''	1.95	0.47
2:9:29:C:C2'	2:9:30:C:H5'	2.44	0.47
5:C:246:ARG:NH1	5:C:246:ARG:HB3	2.29	0.47
26:X:41:PHE:O	26:X:43:VAL:HG23	2.14	0.47
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.96	0.47
1:0:2897:C:H2'	1:0:2898:G:H8	1.78	0.47
38:0:6278:HOH:O	6:D:55:LYS:HB2	2.13	0.47
16:N:67:ALA:C	16:N:69:TYR:H	2.16	0.47
20:R:47:LEU:O	20:R:51:ILE:HG13	2.14	0.47
1:0:1353:C:P	38:0:4647:HOH:O	2.72	0.47
1:0:2779:G:H21	7:E:143:GLN:NE2	2.11	0.47
1:0:338:C:H4'	5:C:174:ILE:HD11	1.94	0.47
3:A:33:GLU:OE1	3:A:33:GLU:N	2.43	0.47
16:N:181:ASP:O	16:N:184:ILE:HG22	2.15	0.47
24:V:7:GLU:O	24:V:11:MET:HG3	2.13	0.47
16:N:170:GLU:O	16:N:174:GLU:HG3	2.14	0.47
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.28	0.47
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	0.47
1:0:2135:A:O2'	1:0:2136:G:H5'	2.14	0.47
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.42	0.47
15:M:9:ARG:HG3	38:M:8846:HOH:O	2.14	0.47
1:0:820:G:C6	3:A:171:LYS:HB2	2.48	0.47
6:D:10:PHE:N	38:D:7345:HOH:O	2.46	0.47
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.14	0.47
11:I:87:PRO:C	11:I:89:GLU:N	2.66	0.47
38:0:3224:HOH:O	11:I:87:PRO:HD2	2.15	0.47
25:W:69:ARG:NH2	38:W:4276:HOH:O	2.24	0.47
1:0:907:A:H4'	1:0:1328:A:C2	2.49	0.47
1:0:1299:G:H5'	38:0:4049:HOH:O	2.13	0.47
10:H:157:TYR:HD1	10:H:157:TYR:C	2.18	0.47
8:F:31:LYS:HE3	38:F:2623:HOH:O	2.14	0.47
25:W:129:LYS:HG2	38:W:1990:HOH:O	2.14	0.47
1:0:1252:A:H2'	1:0:1253:C:O4'	2.15	0.47
1:0:2001:G:O2'	1:0:2002:C:H5'	2.14	0.47
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.50	0.47
13:K:99:ASP:OD1	13:K:101:ASN:N	2.46	0.47
8:F:57:GLU:O	8:F:61:MET:HG3	2.14	0.47
1:0:1205:U:H2'	1:0:1206:U:H5'	1.97	0.47
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:4165:HOH:O	27:Y:186:ARG:HD2	2.14	0.47
4:B:24:PRO:HG2	4:B:204:GLY:HA2	1.95	0.47
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.32	0.47
5:C:22:PHE:HA	5:C:116:ALA:HA	1.96	0.47
27:Y:95:THR:N	27:Y:236:VAL:O	2.46	0.47
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.14	0.47
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.97	0.47
3:A:37:VAL:HG13	38:A:8909:HOH:O	2.13	0.47
1:0:371:U:H2'	1:0:372:A:H8	1.79	0.47
25:W:149:LEU:HG	25:W:153:MET:HE2	1.97	0.47
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.21	0.47
10:H:65:LEU:H	10:H:65:LEU:HD22	1.79	0.47
13:K:65:ARG:HD3	38:K:5358:HOH:O	2.14	0.47
16:N:115:VAL:HG23	38:N:8860:HOH:O	2.15	0.47
11:I:133:THR:HG22	11:I:134:ILE:H	1.78	0.47
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.96	0.47
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.30	0.47
13:K:34:VAL:HG21	13:K:46:LYS:O	2.15	0.47
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.27	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.47	0.47
8:F:111:ILE:O	8:F:115:VAL:HG23	2.15	0.47
1:0:1163:G:N2	38:0:4693:HOH:O	2.45	0.47
38:0:7404:HOH:O	5:C:188:ARG:CD	2.61	0.47
1:0:1044:C:H3'	1:0:1045:G:H5"	1.97	0.47
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.47	0.47
4:B:270:ILE:O	4:B:271:ASP:HB2	2.15	0.47
26:X:8:ARG:NH1	38:X:2479:HOH:O	2.41	0.47
22:T:41:ARG:NH1	22:T:42:VAL:O	2.48	0.47
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.97	0.47
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.30	0.47
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.15	0.47
13:K:55:VAL:CG1	13:K:56:SER:N	2.77	0.47
7:E:69:ILE:HA	7:E:72:MET:HE3	1.97	0.47
1:0:449:A:N7	5:C:43:LYS:HG2	2.30	0.47
1:0:475:G:OP1	5:C:73:LEU:HD22	2.15	0.47
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.13	0.47
1:0:1497:G:H4'	1:0:1627:G:O2'	2.14	0.47
1:0:783:C:OP1	3:A:180:LYS:HE3	2.14	0.47
14:L:89:PHE:N	38:L:8869:HOH:O	2.48	0.47
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.49	0.47
1:0:920:C:H5'	1:0:921:G:C4	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:58:THR:O	24:V:62:GLU:HG3	2.15	0.47
1:0:290:C:O2'	1:0:291:C:H5'	2.14	0.47
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.97	0.47
25:W:76:ASP:O	25:W:77:ALA:C	2.53	0.47
10:H:66:GLU:HA	38:H:8580:HOH:O	2.15	0.47
14:L:121:ILE:HA	14:L:141:GLU:O	2.14	0.47
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.15	0.47
1:0:2252:A:C5	1:0:2253:G:H1'	2.50	0.47
10:H:91:ARG:NH1	10:H:138:THR:OG1	2.43	0.47
1:0:2456:A:H5'	38:0:5653:HOH:O	2.15	0.47
1:0:2392:C:H4'	38:0:4243:HOH:O	2.14	0.47
1:0:157:G:H4'	15:M:95:LYS:HE3	1.97	0.46
25:W:4:LEU:O	25:W:32:CYS:HA	2.15	0.46
8:F:60:VAL:HG12	8:F:60:VAL:O	2.15	0.46
16:N:163:PHE:O	16:N:164:ASP:O	2.32	0.46
3:A:131:HIS:O	3:A:132:ASP:HB2	2.14	0.46
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.97	0.46
1:0:612:U:H2'	1:0:613:C:C6	2.50	0.46
22:T:71:VAL:HG12	22:T:72:ILE:N	2.30	0.46
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.44	0.46
2:9:28:U:H5''	16:N:40:ASN:ND2	2.30	0.46
1:0:292:G:H2'	1:0:358:G:N2	2.29	0.46
6:D:167:GLU:C	6:D:169:THR:H	2.19	0.46
7:E:154:ILE:HD11	7:E:157:LYS:HE2	1.97	0.46
3:A:105:VAL:HG13	3:A:155:THR:O	2.15	0.46
10:H:69:ARG:HB3	38:H:8580:HOH:O	2.15	0.46
38:0:4936:HOH:O	10:H:61:ARG:HG3	2.15	0.46
1:0:1477:C:C5'	1:0:1868:G:H5''	2.45	0.46
5:C:4:THR:HG21	5:C:12:THR:HG22	1.96	0.46
3:A:66:ARG:HH11	3:A:66:ARG:CB	2.28	0.46
1:0:951:A:C2'	1:0:952:G:H5'	2.45	0.46
7:E:43:ASP:HA	38:E:5864:HOH:O	2.15	0.46
4:B:84:LEU:HD23	4:B:142:LEU:HD23	1.97	0.46
26:X:70:ILE:HG23	26:X:70:ILE:O	2.15	0.46
4:B:42:ALA:HB1	4:B:308:LEU:HD11	1.97	0.46
2:9:49:G:H2'	2:9:50:G:O4'	2.16	0.46
1:0:542:A:H2'	1:0:543:G:O4'	2.15	0.46
1:0:1189:A:O2'	1:0:1208:C:H2'	2.15	0.46
11:I:95:LEU:O	11:I:134:ILE:HG23	2.15	0.46
2:9:31:C:H2'	2:9:32:G:O4'	2.16	0.46
1:0:303:C:H2'	1:0:304:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:110:ASP:O	8:F:114:LYS:HG3	2.15	0.46
11:I:126:THR:O	11:I:126:THR:HG22	2.14	0.46
5:C:237:GLU:HB2	38:C:8633:HOH:O	2.15	0.46
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.96	0.46
6:D:57:THR:HG23	6:D:63:ILE:CA	2.41	0.46
1:0:1234:U:C4	4:B:244:PRO:HB3	2.51	0.46
1:0:2768:A:O2'	1:0:2769:C:H5'	2.15	0.46
2:9:107:C:H5	38:9:8634:HOH:O	1.99	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
3:A:153:ARG:HD3	38:A:8828:HOH:O	2.14	0.46
14:L:104:ASP:O	14:L:105:TYR:HB3	2.15	0.46
6:D:62:ASP:HA	38:D:4233:HOH:O	2.16	0.46
1:0:1175:G:H8	1:0:1193:A:HO2'	1.63	0.46
1:0:392:U:C5'	15:M:193:LYS:HB3	2.46	0.46
1:0:2638:G:H5'	38:0:4893:HOH:O	2.16	0.46
4:B:238:ASN:ND2	4:B:240:GLY:H	2.02	0.46
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.44	0.46
1:0:1209:C:H2'	1:0:1210:G:H8	1.81	0.46
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.81	0.46
3:A:132:ASP:OD1	3:A:133:ARG:N	2.45	0.46
31:3:18:GLN:HG2	38:3:8816:HOH:O	2.14	0.46
38:0:9615:HOH:O	8:F:38:LYS:HE2	2.15	0.46
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.98	0.46
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.15	0.46
1:0:1503:U:H2'	1:0:1504:A:O4'	2.16	0.46
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.16	0.46
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.96	0.46
14:L:72:ASN:HB2	38:L:8880:HOH:O	2.16	0.46
20:R:114:VAL:HG13	20:R:114:VAL:O	2.15	0.46
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.50	0.46
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.98	0.46
1:0:1819:G:H2'	1:0:1820:G:C4'	2.41	0.46
15:M:169:ARG:NH1	38:M:8872:HOH:O	2.48	0.46
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.98	0.46
10:H:88:MET:HA	10:H:139:ALA:HA	1.98	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.46
1:0:256:C:H2'	1:0:257:G:O4'	2.16	0.46
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.48	0.46
3:A:93:THR:HG23	3:A:154:ALA:O	2.16	0.46
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:99:THR:HG23	8:F:99:THR:O	2.15	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.46	0.46
1:0:2837:U:H2'	38:0:6789:HOH:O	2.16	0.46
1:0:816:G:H5'	1:0:1598:A:H4'	1.97	0.46
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.97	0.46
21:S:53:ASN:N	21:S:53:ASN:HD22	2.14	0.46
5:C:54:LEU:HD23	5:C:79:ARG:HG3	1.98	0.46
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.16	0.46
31:3:15:ASN:ND2	38:3:8851:HOH:O	2.48	0.46
24:V:49:LEU:O	24:V:53:ILE:HG13	2.16	0.46
1:0:2385:G:H2'	1:0:2386:U:C6	2.51	0.46
1:0:1555:G:H4'	1:0:1630:A:H2	1.79	0.46
1:0:2005:G:OP2	1:0:2005:G:H3'	2.16	0.46
4:B:162:MET:CE	4:B:310:ARG:HD3	2.46	0.46
12:J:131:THR:HG22	12:J:133:GLY:N	2.31	0.46
38:0:9889:HOH:O	12:J:46:ILE:HA	2.16	0.46
20:R:39:THR:HB	20:R:42:GLU:CD	2.36	0.46
4:B:16:ARG:NE	38:B:8853:HOH:O	2.30	0.46
1:0:1595:G:O2'	1:0:1596:U:H5'	2.16	0.46
27:Y:216:ARG:CD	38:Y:8868:HOH:O	2.64	0.46
1:0:1427:A:H61	1:0:1440:U:C1'	2.29	0.46
14:L:10:SER:O	14:L:11:ARG:HB3	2.15	0.46
1:0:1123:A:C6	1:0:1238:C:H5'	2.51	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.16	0.46
15:M:78:LYS:NZ	38:M:8876:HOH:O	2.49	0.46
1:0:1119:G:H8	12:J:52:GLN:NE2	2.14	0.46
11:I:94:ASP:HA	11:I:133:THR:O	2.15	0.46
1:0:1206:U:H2'	1:0:1207:A:O4'	2.16	0.46
16:N:163:PHE:O	16:N:164:ASP:OD1	2.34	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.16	0.46
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.45	0.46
2:9:64:C:C2'	2:9:65:A:H5'	2.46	0.46
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.16	0.46
1:0:1398:G:O2'	1:0:1399:A:H5'	2.16	0.46
31:3:30:GLN:NE2	38:3:8857:HOH:O	2.47	0.46
15:M:12:TRP:O	15:M:15:PRO:HD3	2.16	0.46
25:W:122:ARG:HH11	25:W:122:ARG:HG3	1.81	0.46
1:0:166:A:N7	14:L:25:GLY:HA2	2.31	0.46
4:B:54:VAL:HB	38:B:8914:HOH:O	2.15	0.46
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.99	0.45
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:11:VAL:CG1	7:E:12:ASP:N	2.77	0.45
2:9:88:G:OP1	25:W:130:HIS:NE2	2.46	0.45
20:R:47:LEU:HB2	20:R:89:LEU:HD21	1.98	0.45
17:O:44:ASN:OD1	17:O:65:LEU:HB2	2.16	0.45
19:Q:11:ARG:NH1	38:Q:5620:HOH:O	2.49	0.45
20:R:4:TYR:N	38:R:8844:HOH:O	2.49	0.45
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.51	0.45
1:0:445:U:H2'	1:0:446:G:H8	1.81	0.45
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.45
4:B:62:ARG:NH2	4:B:66:GLU:O	2.48	0.45
6:D:40:ILE:HG23	38:D:5583:HOH:O	2.16	0.45
25:W:4:LEU:HD21	25:W:52:VAL:HG11	1.99	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.76	0.45
2:9:34:A:H8	2:9:34:A:O5'	1.99	0.45
10:H:41:LYS:HD3	10:H:46:TYR:OH	2.16	0.45
10:H:149:VAL:HG13	38:H:8577:HOH:O	2.16	0.45
1:0:2793:A:H2'	1:0:2794:G:H5'	1.98	0.45
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.45
1:0:1768:C:H2'	1:0:1769:C:O4'	2.16	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.16	0.45
1:0:1996:U:O2'	1:0:1997:A:H5'	2.16	0.45
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.97	0.45
16:N:147:ILE:HG23	16:N:148:ALA:N	2.31	0.45
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.44	0.45
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.23	0.45
1:0:2769:C:H2'	1:0:2770:G:H5'	1.99	0.45
1:0:2769:C:H2'	1:0:2770:G:C5'	2.45	0.45
7:E:139:GLU:CD	38:E:5919:HOH:O	2.54	0.45
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.52	0.45
16:N:154:LEU:C	16:N:156:GLU:H	2.19	0.45
1:0:2419:U:H5''	1:0:2420:G:H5'	1.99	0.45
1:0:1333:U:H2'	1:0:1334:C:H6	1.82	0.45
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.31	0.45
1:0:1790:C:H2'	1:0:1791:U:C6	2.50	0.45
1:0:65:C:O2'	1:0:66:G:H5'	2.16	0.45
1:0:2361:A:H5''	38:0:9001:HOH:O	2.17	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.45
1:0:2900:G:H2'	1:0:2901:C:O4'	2.16	0.45
7:E:37:ASP:OD1	12:J:125:SER:HB3	2.16	0.45
1:0:1617:C:C4	1:0:1643:C:H4'	2.51	0.45
1:0:1559:A:OP2	1:0:1559:A:H8	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.49	0.45
2:9:20:G:H3'	38:9:8633:HOH:O	2.16	0.45
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.16	0.45
16:N:183:ASP:O	16:N:184:ILE:O	2.34	0.45
11:I:84:SER:HB3	11:I:92:VAL:CG2	2.47	0.45
1:0:24:G:N2	1:0:518:G:H1'	2.32	0.45
5:C:150:THR:HA	5:C:203:ALA:O	2.15	0.45
1:0:249:G:O2'	1:0:250:C:H5'	2.17	0.45
1:0:1352:A:N1	5:C:48:SER:HB3	2.31	0.45
7:E:22:VAL:O	7:E:28:SER:HA	2.17	0.45
1:0:709:G:O2'	17:O:25:VAL:CG1	2.64	0.45
6:D:18:ILE:HD13	6:D:84:LEU:CD1	2.47	0.45
4:B:248:ARG:NH2	38:B:8824:HOH:O	2.49	0.45
23:U:13:ILE:HG12	23:U:32:CYS:CB	2.46	0.45
25:W:108:ARG:NH2	38:W:2359:HOH:O	2.50	0.45
1:0:289:G:O2'	1:0:290:C:H5'	2.16	0.45
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.16	0.45
16:N:43:VAL:HG11	16:N:81:ALA:HA	1.97	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.16	0.45
17:O:39:THR:O	17:O:115:ARG:NH2	2.49	0.45
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.31	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.46	0.45
15:M:61:ILE:N	15:M:61:ILE:HD12	2.32	0.45
1:0:100:C:H4'	22:T:16:LEU:HB2	1.98	0.45
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.45
17:O:41:ALA:HA	38:O:5104:HOH:O	2.17	0.45
16:N:100:ALA:O	16:N:129:ILE:HG23	2.16	0.45
4:B:75:GLU:C	4:B:77:PRO:HD3	2.36	0.45
4:B:148:PRO:HD2	38:B:8880:HOH:O	2.16	0.45
9:G:19:GLU:HG2	9:G:66:LEU:HD13	1.99	0.45
1:0:2714:U:H4'	4:B:10:SER:HB2	1.98	0.45
1:0:2498:C:O2'	1:0:2499:U:H5'	2.15	0.45
10:H:172:GLU:CB	38:H:8591:HOH:O	2.20	0.45
14:L:143:THR:CG2	14:L:144:ASP:H	2.28	0.45
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.97	0.45
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.99	0.45
7:E:31:ARG:HH12	7:E:68:HIS:CE1	2.35	0.45
15:M:61:ILE:HG22	15:M:62:VAL:N	2.31	0.45
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.16	0.45
29:1:28:HIS:HD2	29:1:30:LYS:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:106:A:H2'	1:0:107:U:O4'	2.17	0.45
5:C:7:ASP:OD1	5:C:11:ASN:O	2.34	0.45
3:A:135:VAL:HG21	3:A:147:ARG:HG2	1.98	0.45
1:0:426:G:H2'	1:0:427:C:O4'	2.17	0.45
4:B:268:ARG:NE	38:B:8909:HOH:O	2.50	0.45
27:Y:185:VAL:HG12	38:Y:8869:HOH:O	2.17	0.45
13:K:98:VAL:CG1	13:K:99:ASP:N	2.80	0.45
12:J:42:GLU:O	12:J:131:THR:HG23	2.17	0.45
11:I:94:ASP:HB3	11:I:135:GLU:OE1	2.17	0.45
24:V:39:ALA:O	24:V:41:GLU:N	2.50	0.45
6:D:99:ASP:CB	6:D:103:ASN:H	2.30	0.45
25:W:38:THR:O	25:W:42:ARG:HB2	2.16	0.45
1:0:86:A:C2	30:2:25:VAL:HG13	2.52	0.45
26:X:30:MET:CE	26:X:55:ASN:HA	2.46	0.45
1:0:1023:C:H2'	1:0:1024:G:O4'	2.16	0.45
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.83	0.45
1:0:2115:U:H2'	1:0:2116:U:C6	2.52	0.45
1:0:932:U:H2'	1:0:933:C:C6	2.52	0.45
25:W:90:TYR:CE2	25:W:99:ALA:HB2	2.51	0.45
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.99	0.45
24:V:1:THR:HG23	24:V:2:VAL:N	2.24	0.45
1:0:1450:C:C4'	1:0:1451:C:OP2	2.60	0.45
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.82	0.45
20:R:17:MET:CE	20:R:19:ARG:NH2	2.78	0.45
25:W:39:ASP:HB2	38:W:3580:HOH:O	2.17	0.45
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.45	0.45
14:L:6:ARG:NH2	38:L:8849:HOH:O	2.50	0.45
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.98	0.45
1:0:407:A:H8	38:0:4433:HOH:O	2.00	0.45
3:A:179:MET:HA	3:A:179:MET:CE	2.45	0.45
16:N:67:ALA:C	16:N:69:TYR:N	2.70	0.45
1:0:1482:A:O2'	1:0:1483:C:H5'	2.17	0.45
1:0:512:G:O3'	1:0:513:A:H8	2.00	0.45
1:0:1422:U:H2'	1:0:1423:C:C6	2.52	0.45
16:N:37:ARG:HD3	36:N:8807:CL:CL	2.54	0.45
25:W:90:TYR:N	25:W:90:TYR:CD1	2.85	0.45
20:R:29:LYS:HD3	38:R:8830:HOH:O	2.16	0.45
1:0:1279:U:O2	1:0:1279:U:H2'	2.16	0.45
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.98	0.45
1:0:68:U:O2'	1:0:69:A:H5"	2.17	0.45
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1730:G:C5'	1:0:1731:C:C6	3.00	0.45
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.80	0.45
10:H:72:ALA:HB2	10:H:156:ALA:HB2	1.99	0.45
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.16	0.45
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.47	0.45
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.16	0.45
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.17	0.45
8:F:32:GLY:N	38:F:311:HOH:O	2.50	0.44
14:L:91:VAL:HB	38:L:885:HOH:O	2.17	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.51	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.44
1:0:2036:C:C1'	13:K:44:LEU:HG	2.47	0.44
1:0:2002:C:H2'	1:0:2003:U:H5'	1.99	0.44
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.32	0.44
8:F:20:LEU:HD13	8:F:49:PHE:CE1	2.52	0.44
8:F:34:ASN:HA	15:M:4:ALA:HB2	2.00	0.44
14:L:101:ASP:C	14:L:103:ALA:H	2.19	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.17	0.44
1:0:1940:C:H4'	38:0:729:HOH:O	2.15	0.44
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.44
13:K:20:CYS:HB2	13:K:29:LEU:HG	2.00	0.44
10:H:6:ALA:CA	10:H:61:ARG:HH12	2.29	0.44
1:0:2846:C:OP1	4:B:158:LYS:HD3	2.17	0.44
1:0:816:G:C6	1:0:817:G:N1	2.85	0.44
25:W:122:ARG:HG3	25:W:152:ALA:O	2.18	0.44
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.16	0.44
2:9:23:U:O2'	2:9:24:U:H4'	2.17	0.44
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.18	0.44
31:3:74:CYS:N	38:3:8865:HOH:O	2.50	0.44
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.33	0.44
2:9:47:A:C2	2:9:48:C:C2	3.05	0.44
6:D:170:TYR:O	6:D:171:ASP:HB3	2.17	0.44
1:0:671:A:O2'	1:0:672:G:H2'	2.17	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.51	0.44
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.48	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.80	0.44
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.45	0.44
1:0:656:G:OP2	17:O:37:ARG:HD2	2.18	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.17	0.44
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:175:LEU:HD23	4:B:175:LEU:O	2.18	0.44
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.33	0.44
30:2:31:ARG:NH1	38:2:7177:HOH:O	2.50	0.44
1:0:1771:U:O2'	1:0:1773:G:N7	2.49	0.44
19:Q:4:ASN:ND2	38:Q:7115:HOH:O	2.51	0.44
25:W:107:LEU:O	25:W:112:LEU:HB2	2.17	0.44
16:N:15:GLU:HB3	16:N:17:ARG:HG3	2.00	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.32	0.44
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.99	0.44
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.46	0.44
6:D:35:ALA:C	6:D:37:ALA:H	2.21	0.44
2:9:14:G:O2'	16:N:1:ALA:HB2	2.17	0.44
1:0:2754:G:C2'	1:0:2755:G:H5'	2.48	0.44
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.20	0.44
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.99	0.44
14:L:57:VAL:O	14:L:57:VAL:HG12	2.17	0.44
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.82	0.44
1:0:587:A:H5''	38:0:7237:HOH:O	2.17	0.44
1:0:1783:A:O2'	1:0:1784:U:H5'	2.17	0.44
3:A:173:GLY:O	3:A:176:HIS:HB3	2.17	0.44
1:0:2667:G:H1'	1:0:2914:A:N3	2.32	0.44
20:R:122:GLN:HB3	20:R:138:SER:HB2	2.00	0.44
23:U:37:GLU:HB3	38:U:408:HOH:O	2.17	0.44
1:0:1942:A:H3'	38:0:7297:HOH:O	2.18	0.44
1:0:1562:C:N4	38:0:5823:HOH:O	2.49	0.44
10:H:12:ILE:HG23	10:H:129:ARG:NE	2.32	0.44
16:N:147:ILE:CG2	16:N:148:ALA:N	2.81	0.44
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.17	0.44
15:M:78:LYS:HD3	38:M:8940:HOH:O	2.17	0.44
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.33	0.44
6:D:38:GLU:HB3	6:D:49:PRO:HG3	1.99	0.44
1:0:2515:C:H2'	1:0:2516:G:O4'	2.17	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44
1:0:2453:G:H4'	14:L:50:GLY:C	2.38	0.44
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.44
1:0:1613:C:H2'	1:0:1614:G:O4'	2.17	0.44
1:0:1593:C:OP1	18:P:117:SER:HB3	2.18	0.44
11:I:127:CYS:C	11:I:129:SER:H	2.21	0.44
1:0:1268:C:O2'	1:0:1269:G:H5'	2.17	0.44
7:E:22:VAL:HG12	7:E:76:VAL:HG11	2.00	0.44
7:E:23:GLU:HG2	7:E:28:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:74:ILE:HG13	38:B:8907:HOH:O	2.17	0.44
4:B:307:ARG:HH11	4:B:307:ARG:HB2	1.83	0.44
1:0:1441:G:H1'	38:0:7711:HOH:O	2.18	0.44
21:S:81:ILE:HG23	38:S:8538:HOH:O	2.17	0.44
3:A:186:TRP:CG	3:A:187:PRO:HA	2.53	0.44
1:0:1393:A:H2'	1:0:1394:C:C6	2.53	0.44
16:N:119:GLN:O	16:N:123:ILE:HG13	2.18	0.44
4:B:81:ALA:O	4:B:186:GLY:HA3	2.17	0.44
1:0:1213:C:O2'	1:0:1214:G:H5'	2.17	0.44
17:O:63:LYS:HG3	17:O:80:ASP:O	2.18	0.44
1:0:2359:G:H3'	38:0:5649:HOH:O	2.17	0.44
8:F:79:GLN:HG3	8:F:82:ASP:OD2	2.18	0.44
1:0:1552:G:H2'	1:0:1553:C:C6	2.53	0.44
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.48	0.44
1:0:1184:C:O2'	1:0:1185:U:OP2	2.32	0.44
4:B:312:ARG:HG2	4:B:313:PRO:N	2.32	0.44
7:E:133:VAL:HG12	7:E:141:VAL:HG13	2.00	0.44
5:C:214:THR:HB	38:C:8525:HOH:O	2.17	0.44
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.48	0.44
31:3:70:ARG:HD3	38:3:8877:HOH:O	2.17	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.17	0.44
5:C:222:ASP:N	5:C:222:ASP:OD1	2.48	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.44
4:B:84:LEU:HD23	4:B:178:ALA:HB1	2.00	0.44
1:0:1754:A:H2'	1:0:1755:A:O4'	2.18	0.44
38:0:9106:HOH:O	5:C:103:ASN:HB3	2.17	0.44
1:0:834:G:H3'	1:0:835:U:H4'	1.99	0.44
5:C:84:VAL:O	5:C:85:LYS:HB2	2.18	0.44
1:0:738:G:H3'	38:0:6999:HOH:O	2.18	0.44
18:P:115:SER:C	18:P:117:SER:N	2.71	0.44
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.33	0.44
4:B:7:ARG:CG	4:B:7:ARG:HH11	2.26	0.44
1:0:2846:C:H4'	4:B:156:LYS:HB3	2.00	0.44
1:0:583:C:H2'	1:0:584:U:H6	1.83	0.44
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.99	0.44
3:A:217:ARG:NH1	3:A:217:ARG:CG	2.77	0.44
1:0:1015:C:H2'	1:0:1016:U:C6	2.52	0.44
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.44
1:0:1391:G:H2'	1:0:1392:A:H5'	1.99	0.44
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.18	0.44
13:K:63:GLU:CG	38:K:6344:HOH:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:90:LYS:HB2	36:J:8802:CL:CL	2.55	0.44
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.16	0.44
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.78	0.43
11:I:87:PRO:HD3	38:I:6825:HOH:O	2.18	0.43
19:Q:18:PRO:O	19:Q:21:ARG:HB2	2.18	0.43
2:9:114:G:H2'	2:9:115:C:C6	2.53	0.43
1:0:2781:U:H2'	1:0:2782:G:C5'	2.48	0.43
1:0:2720:C:O2	13:K:87:ARG:NH2	2.50	0.43
12:J:107:ASN:HD22	12:J:109:TYR:H	1.63	0.43
17:O:25:VAL:O	17:O:29:VAL:HG23	2.18	0.43
1:0:585:C:H6	38:0:6051:HOH:O	2.00	0.43
30:2:49:GLU:HB2	38:2:719:HOH:O	2.17	0.43
5:C:157:LEU:HD22	5:C:162:VAL:HG12	2.00	0.43
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.99	0.43
2:9:3:A:H2	2:9:21:G:N3	2.16	0.43
8:F:36:THR:HG23	8:F:97:ALA:HB2	2.00	0.43
7:E:125:GLU:HB2	7:E:132:THR:CG2	2.48	0.43
3:A:57:ALA:HA	3:A:67:LEU:HD23	2.00	0.43
31:3:91:GLN:O	31:3:92:GLU:HB2	2.18	0.43
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.48	0.43
1:0:93:C:H5''	24:V:1:THR:HG21	1.99	0.43
8:F:60:VAL:HG13	8:F:63:ILE:HG13	2.00	0.43
3:A:192:VAL:CG1	3:A:192:VAL:O	2.65	0.43
7:E:11:VAL:HG11	7:E:22:VAL:HG13	2.00	0.43
1:0:2850:C:C6	1:0:2850:C:H5'	2.47	0.43
6:D:99:ASP:HB2	6:D:103:ASN:O	2.18	0.43
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.48	0.43
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	2.00	0.43
7:E:154:ILE:HG23	7:E:154:ILE:O	2.18	0.43
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.43
1:0:321:A:H1'	38:0:6985:HOH:O	2.18	0.43
16:N:114:LYS:O	16:N:117:ALA:HB3	2.18	0.43
1:0:441:A:H1'	1:0:442:A:N7	2.33	0.43
1:0:23:G:H1'	1:0:520:A:N6	2.33	0.43
26:X:74:ALA:HB2	26:X:85:VAL:CG1	2.48	0.43
28:Z:46:ARG:O	28:Z:57:CYS:HA	2.17	0.43
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.34	0.43
1:0:1209:C:H4'	38:0:5241:HOH:O	2.19	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
25:W:48:VAL:HG12	25:W:52:VAL:HB	1.99	0.43
10:H:70:LEU:O	10:H:74:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.18	0.43
29:1:2:GLY:O	29:1:6:PRO:HG2	2.18	0.43
1:O:162:C:H2'	1:O:163:U:H5'	2.00	0.43
4:B:177:HIS:O	4:B:181:ILE:HG13	2.18	0.43
1:O:812:A:H2'	1:O:813:C:O4'	2.17	0.43
1:O:1363:G:OP1	5:C:76:ARG:NH2	2.45	0.43
3:A:211:LYS:CB	38:A:8918:HOH:O	2.67	0.43
2:9:57:A:C8	6:D:141:VAL:HG21	2.53	0.43
6:D:35:ALA:HB3	38:D:3279:HOH:O	2.18	0.43
25:W:5:VAL:HG11	25:W:153:MET:CE	2.48	0.43
6:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.64	0.43
9:G:71:LEU:C	9:G:73:ASP:H	2.21	0.43
1:O:661:G:C5	1:O:686:A:C2	3.06	0.43
7:E:132:THR:O	7:E:132:THR:HG23	2.18	0.43
30:2:20:ARG:CG	30:2:21:VAL:N	2.82	0.43
5:C:7:ASP:C	5:C:9:ASP:H	2.21	0.43
16:N:38:LYS:HD2	16:N:114:LYS:HE3	2.01	0.43
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.87	0.43
1:O:2326:C:H4'	1:O:2412:G:H4'	2.01	0.43
38:O:4697:HOH:O	16:N:21:HIS:HD2	2.01	0.43
1:O:2379:G:H5'	1:O:2381:C:O4'	2.18	0.43
1:O:1242:A:OP2	12:J:60:ARG:NH2	2.45	0.43
3:A:211:LYS:CB	3:A:212:PRO:HD2	2.33	0.43
15:M:95:LYS:HG2	15:M:99:ARG:HB3	1.99	0.43
11:I:130:LEU:HB2	11:I:132:VAL:HG23	1.99	0.43
14:L:134:GLU:HG3	38:L:8856:HOH:O	2.18	0.43
25:W:6:GLN:HA	25:W:52:VAL:HG23	2.00	0.43
16:N:73:ALA:N	38:N:8868:HOH:O	2.51	0.43
4:B:16:ARG:NH2	38:B:8853:HOH:O	2.40	0.43
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.86	0.43
1:O:1878:G:O2'	1:O:1879:U:OP2	2.37	0.43
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.19	0.43
10:H:149:VAL:HG22	38:H:8577:HOH:O	2.19	0.43
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.54	0.43
30:2:5:LYS:O	30:2:9:LYS:HG3	2.18	0.43
3:A:37:VAL:HG22	38:A:8895:HOH:O	2.18	0.43
1:O:581:G:H5'	38:O:7630:HOH:O	2.18	0.43
1:O:503:G:H2'	1:O:504:G:H8	1.84	0.43
1:O:47:G:N3	1:O:114:A:C2	2.87	0.43
25:W:48:VAL:HG12	25:W:48:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.43
6:D:76:ARG:O	6:D:77:ASP:HB2	2.19	0.43
3:A:113:GLY:HA2	3:A:153:ARG:NH2	2.34	0.43
2:9:28:U:H2'	2:9:29:C:C6	2.54	0.43
1:0:949:U:H4'	19:Q:95:GLU:HA	1.99	0.43
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.43
26:X:18:ARG:NH1	38:X:4132:HOH:O	2.48	0.43
21:S:50:GLU:OE2	21:S:69:SER:HB3	2.19	0.43
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.58	0.43
15:M:115:LEU:HD23	15:M:150:ILE:HD12	2.00	0.43
1:0:1589:G:H4'	38:0:6807:HOH:O	2.18	0.43
23:U:9:CYS:HA	23:U:52:THR:CG2	2.45	0.43
4:B:41:PHE:HA	4:B:79:MET:CE	2.47	0.43
1:0:2265:U:H2'	1:0:2266:A:H8	1.81	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	2.01	0.43
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.87	0.43
8:F:14:ASP:O	8:F:18:GLU:HG3	2.18	0.43
2:9:42:C:H5'	2:9:43:G:OP2	2.18	0.43
1:0:1087:G:H4'	1:0:1088:A:OP1	2.19	0.43
1:0:2132:C:H1'	15:M:124:GLY:HA3	2.01	0.43
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.18	0.43
6:D:67:ASP:O	6:D:69:ILE:HG13	2.18	0.43
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.00	0.43
1:0:1299:G:N7	14:L:6:ARG:NH1	2.67	0.43
19:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.18	0.43
15:M:47:ASP:CG	15:M:48:LYS:N	2.72	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.53	0.43
1:0:226:A:H1'	1:0:393:G:C5	2.54	0.43
1:0:1380:U:H5'	38:0:9209:HOH:O	2.19	0.43
29:1:22:CYS:SG	29:1:24:GLU:HB2	2.58	0.43
38:0:5479:HOH:O	4:B:298:LYS:HD3	2.18	0.43
38:9:8665:HOH:O	16:N:147:ILE:HD12	2.18	0.43
1:0:1167:G:O2'	1:0:1168:C:H5'	2.18	0.43
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.51	0.43
10:H:66:GLU:O	10:H:70:LEU:HB2	2.19	0.43
1:0:1131:G:C6	1:0:1230:A:C4	3.07	0.43
20:R:61:GLN:CD	38:R:8837:HOH:O	2.56	0.43
1:0:1925:G:O2'	1:0:1926:G:H5'	2.19	0.43
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.49	0.43
1:0:87:C:H2'	30:2:28:LYS:O	2.19	0.43
1:0:1172:G:H5''	38:0:7212:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:10:ASP:HA	38:E:3707:HOH:O	2.19	0.43
1:0:451:C:O2'	1:0:452:G:H5'	2.19	0.43
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.43
10:H:87:LYS:NZ	10:H:87:LYS:HB2	2.33	0.43
31:3:34:LYS:HD2	31:3:34:LYS:N	2.33	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.19	0.43
25:W:65:VAL:CA	25:W:68:THR:HG22	2.42	0.43
8:F:60:VAL:O	8:F:60:VAL:CG1	2.67	0.43
2:9:92:G:C6	2:9:93:A:C6	3.07	0.43
16:N:49:THR:HB	16:N:58:LEU:CD1	2.49	0.43
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.48	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.53	0.43
23:U:34:SER:HA	23:U:37:GLU:OE1	2.19	0.43
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.43
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.43
1:0:2387:U:H2'	1:0:2388:C:C6	2.54	0.43
27:Y:105:LYS:HE2	27:Y:198:GLY:O	2.19	0.43
4:B:217:ARG:CD	4:B:257:THR:HG22	2.49	0.42
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.00	0.42
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.34	0.42
1:0:1163:G:N2	38:0:6005:HOH:O	2.51	0.42
16:N:120:GLU:HG3	16:N:136:LEU:HD13	2.01	0.42
1:0:703:G:O2'	1:0:704:C:H5'	2.19	0.42
1:0:1109:U:O4	12:J:21:ARG:HA	2.19	0.42
1:0:2831:C:H2'	1:0:2832:C:H5'	2.01	0.42
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.42
15:M:98:GLN:O	15:M:102:GLU:HG3	2.19	0.42
38:0:6207:HOH:O	23:U:56:ARG:HD3	2.19	0.42
38:0:3737:HOH:O	22:T:9:LYS:CD	2.65	0.42
1:0:1684:A:O2'	1:0:1685:A:H5''	2.18	0.42
20:R:106:GLY:HA2	20:R:109:MET:CE	2.49	0.42
1:0:1702:U:H5'	38:0:3411:HOH:O	2.19	0.42
5:C:27:ARG:HG2	5:C:30:LEU:HD12	2.01	0.42
1:0:2504:A:H4'	10:H:74:ARG:HH11	1.84	0.42
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.18	0.42
6:D:86:THR:O	6:D:90:LEU:HG	2.19	0.42
3:A:51:ARG:HB2	38:A:8905:HOH:O	2.18	0.42
1:0:2415:A:O2'	16:N:29:SER:HB3	2.19	0.42
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.67	0.42
14:L:73:VAL:HG23	14:L:74:THR:N	2.34	0.42
18:P:94:TRP:CH2	18:P:98:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:612:U:H2'	1:0:613:C:H6	1.84	0.42
1:0:488:U:H2'	38:0:3984:HOH:O	2.18	0.42
1:0:324:G:O2'	1:0:325:U:H5'	2.20	0.42
1:0:969:G:H1	1:0:999:C:H42	1.67	0.42
2:9:56:A:C3'	2:9:57:A:H5''	2.48	0.42
2:9:57:A:O2'	6:D:152:PRO:HD2	2.19	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
1:0:2784:A:H1'	7:E:60:SER:OG	2.19	0.42
7:E:15:GLN:HG3	7:E:20:ILE:HG12	2.00	0.42
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.42
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.85	0.42
5:C:133:ARG:HD2	38:C:8613:HOH:O	2.19	0.42
1:0:2883:A:H2'	1:0:2884:G:O4'	2.20	0.42
25:W:125:HIS:HD2	25:W:127:GLY:H	1.67	0.42
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.50	0.42
6:D:20:LYS:HA	6:D:75:LEU:O	2.20	0.42
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.52	0.42
16:N:44:ARG:HG3	16:N:45:ALA:N	2.34	0.42
27:Y:122:ARG:NH2	38:Y:8834:HOH:O	2.51	0.42
4:B:72:THR:HB	38:B:8907:HOH:O	2.19	0.42
10:H:50:ILE:HG21	38:H:8577:HOH:O	2.19	0.42
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.84	0.42
1:0:682:A:H2'	1:0:683:G:O4'	2.19	0.42
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.42
1:0:2092:G:H2'	1:0:2613:G:OP1	2.20	0.42
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.55	0.42
7:E:93:MET:HE1	7:E:165:GLY:N	2.35	0.42
3:A:17:ARG:HD2	38:A:8838:HOH:O	2.20	0.42
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.19	0.42
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.37	0.42
1:0:1761:U:H5'	18:P:81:LYS:O	2.20	0.42
1:0:1730:G:H5''	1:0:1731:C:C6	2.52	0.42
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.01	0.42
8:F:20:LEU:O	8:F:23:ALA:HB3	2.19	0.42
1:0:2719:A:C2	4:B:70:PRO:HG3	2.54	0.42
1:0:1495:C:H1'	1:0:1573:A:H1'	2.02	0.42
1:0:419:A:H1'	1:0:1921:A:C2	2.54	0.42
8:F:56:PRO:CG	15:M:44:THR:HA	2.50	0.42
1:0:1624:A:H5'	1:0:1626:A:O4'	2.19	0.42
1:0:10:U:O4	1:0:532:A:OP2	2.38	0.42
17:O:35:LYS:HD3	38:O:3360:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1201:C:H5''	38:0:6193:HOH:O	2.19	0.42
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.65	0.42
4:B:55:ASN:HB3	4:B:64:GLY:H	1.85	0.42
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.45	0.42
1:0:255:A:H2'	1:0:256:C:O4'	2.19	0.42
1:0:1423:C:O2'	1:0:1424:A:H5'	2.19	0.42
1:0:2453:G:H5''	38:L:8842:HOH:O	2.19	0.42
16:N:38:LYS:HB2	16:N:38:LYS:HE3	1.77	0.42
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:1762:C:H2'	1:0:1763:C:H6	1.84	0.42
17:O:78:ALA:C	17:O:98:LEU:HD13	2.40	0.42
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.42
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.85	0.42
1:0:1167:G:H4'	11:I:130:LEU:HD22	2.02	0.42
6:D:35:ALA:C	6:D:37:ALA:N	2.73	0.42
1:0:212:A:O4'	1:0:214:U:C6	2.73	0.42
12:J:45:VAL:HG22	12:J:46:ILE:N	2.34	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
1:0:2694:A:C4'	7:E:91:PHE:HE1	2.26	0.42
38:0:7503:HOH:O	31:3:60:LYS:HG3	2.18	0.42
7:E:11:VAL:CG1	7:E:12:ASP:H	2.33	0.42
15:M:28:GLN:HA	15:M:31:TRP:HB2	2.01	0.42
1:0:1377:C:H1'	38:0:9033:HOH:O	2.19	0.42
31:3:70:ARG:CB	38:3:8877:HOH:O	2.67	0.42
1:0:1334:C:H2'	1:0:1335:C:H6	1.85	0.42
16:N:24:LEU:O	16:N:28:LYS:HG3	2.20	0.42
1:0:1730:G:H5'	1:0:1731:C:C5	2.54	0.42
16:N:62:HIS:O	16:N:65:ASP:OD1	2.37	0.42
9:G:63:ARG:N	38:G:2569:HOH:O	2.53	0.42
6:D:170:TYR:CD1	6:D:170:TYR:N	2.88	0.42
1:0:812:A:H1'	38:0:3936:HOH:O	2.18	0.42
1:0:2821:C:H4'	4:B:116:PRO:HB3	2.01	0.42
10:H:80:LEU:HD12	10:H:86:TYR:CD2	2.55	0.42
10:H:83:GLU:HA	38:H:8584:HOH:O	2.20	0.42
1:0:2866:U:H4'	1:0:2867:G:H5'	2.01	0.42
5:C:154:VAL:O	5:C:158:GLU:HG3	2.20	0.42
38:0:4592:HOH:O	3:A:6:GLY:HA3	2.20	0.42
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.42
1:0:1461:U:H2'	1:0:1462:C:C6	2.54	0.42
30:2:18:ASN:O	30:2:18:ASN:ND2	2.53	0.42
16:N:82:TYR:C	16:N:82:TYR:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2716:G:C5'	4:B:206:THR:HG21	2.42	0.42
1:0:1119:G:H22	1:0:1246:A:H2	1.58	0.42
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.53	0.42
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	0.42
1:0:470:U:O2'	29:1:16:HIS:CD2	2.68	0.42
26:X:43:VAL:HG11	26:X:82:GLU:HA	2.02	0.42
26:X:25:ARG:HD2	38:X:3861:HOH:O	2.19	0.42
5:C:129:HIS:HD2	5:C:165:ASP:OD2	2.01	0.42
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.50	0.42
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.54	0.42
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.42
1:0:222:A:H2'	1:0:223:G:O4'	2.19	0.42
14:L:36:ASP:HB2	38:L:8836:HOH:O	2.19	0.42
1:0:327:A:H4'	1:0:329:A:C8	2.55	0.42
1:0:189:A:OP1	15:M:171:ARG:NH2	2.52	0.42
1:0:544:G:H2'	1:0:545:G:C5'	2.46	0.42
27:Y:189:ASN:CA	27:Y:217:ILE:HD11	2.47	0.42
25:W:48:VAL:CG1	25:W:48:VAL:O	2.67	0.42
25:W:4:LEU:HD23	25:W:4:LEU:HA	1.85	0.42
1:0:1702:U:H1'	38:0:5732:HOH:O	2.20	0.42
9:G:64:ASN:O	9:G:68:GLU:HG3	2.20	0.42
21:S:57:THR:HG23	38:S:8530:HOH:O	2.19	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.54	0.42
1:0:485:A:O2'	1:0:487:G:H5'	2.20	0.42
10:H:46:TYR:HA	10:H:47:PRO:HD3	1.78	0.42
9:G:71:LEU:C	9:G:73:ASP:N	2.73	0.42
23:U:33:SER:O	23:U:37:GLU:HG3	2.20	0.42
15:M:72:ALA:HB2	15:M:93:ARG:HG2	2.00	0.42
1:0:130:C:H5'	38:0:5173:HOH:O	2.19	0.42
11:I:96:SER:H	11:I:99:GLN:NE2	2.18	0.42
1:0:2472:C:O2'	1:0:2634:G:H4'	2.20	0.42
1:0:366:U:H2'	1:0:367:G:O4'	2.19	0.42
1:0:1375:A:C2'	1:0:1376:G:H5'	2.50	0.42
4:B:320:GLN:NE2	4:B:321:PRO:CD	2.80	0.42
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.42	0.42
26:X:76:ARG:NH1	26:X:76:ARG:CG	2.81	0.42
3:A:192:VAL:HG12	3:A:192:VAL:O	2.19	0.42
7:E:24:GLY:CA	7:E:76:VAL:HB	2.50	0.42
12:J:107:ASN:C	12:J:107:ASN:ND2	2.73	0.42
17:O:23:GLY:C	38:O:3062:HOH:O	2.59	0.42
16:N:58:LEU:N	16:N:58:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3:A:OP2	2:9:25:G:N2	2.53	0.42
7:E:108:LEU:HD11	7:E:164:ASP:HB2	2.02	0.42
4:B:271:ASP:HB3	4:B:296:LEU:HD12	2.01	0.42
10:H:139:ALA:HB3	10:H:149:VAL:HG21	2.02	0.42
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.55	0.42
23:U:47:ARG:CG	38:U:4381:HOH:O	2.67	0.42
16:N:21:HIS:HB2	38:N:8833:HOH:O	2.19	0.42
10:H:141:CYS:HB2	38:H:8545:HOH:O	2.20	0.42
1:0:567:U:H5'	38:W:5817:HOH:O	2.19	0.42
1:0:247:A:H2'	38:0:3902:HOH:O	2.19	0.42
1:0:922:A:N7	1:0:2281:C:H5'	2.35	0.42
1:0:1415:G:H5'	29:1:12:ASN:O	2.19	0.42
1:0:1829:A:H2'	1:0:1830:C:H5'	2.02	0.42
5:C:185:LYS:HD3	5:C:186:TYR:CE1	2.55	0.42
27:Y:220:GLU:HG2	38:Y:8847:HOH:O	2.19	0.42
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.64	0.41
4:B:55:ASN:CB	4:B:63:GLU:HA	2.46	0.41
4:B:146:THR:O	4:B:159:PRO:HB3	2.19	0.41
1:0:1181:A:H2'	1:0:1182:C:O4'	2.20	0.41
1:0:317:A:OP1	22:T:52:ARG:O	2.38	0.41
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.49	0.41
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.35	0.41
16:N:86:LEU:HD21	16:N:180:LEU:HD11	2.02	0.41
1:0:2681:A:H4'	1:0:2682:C:H5'	2.02	0.41
1:0:2324:G:H4'	1:0:2418:G:O2'	2.20	0.41
1:0:2880:A:H2'	1:0:2881:C:H5'	2.02	0.41
1:0:1887:U:OP1	28:Z:21:VAL:HG23	2.20	0.41
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.02	0.41
5:C:49:ASP:HB3	5:C:52:ALA:HB2	2.02	0.41
1:0:172:U:H5'	38:0:4135:HOH:O	2.18	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.19	0.41
30:2:11:LEU:HD23	30:2:11:LEU:HA	1.85	0.41
38:0:3224:HOH:O	11:I:87:PRO:CD	2.68	0.41
11:I:88:GLN:NE2	11:I:128:THR:HG21	2.35	0.41
5:C:188:ARG:NH2	38:C:8524:HOH:O	2.53	0.41
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.41
1:0:1460:G:OP1	3:A:17:ARG:NH1	2.52	0.41
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.52	0.41
5:C:102:LEU:HD12	38:C:8515:HOH:O	2.20	0.41
1:0:74:G:H2'	1:0:75:U:C6	2.54	0.41
14:L:35:ARG:O	14:L:40:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.19	0.41
4:B:153:SER:HB2	4:B:287:TYR:CZ	2.54	0.41
25:W:26:ILE:O	25:W:26:ILE:CG1	2.67	0.41
25:W:69:ARG:NE	38:W:4276:HOH:O	2.48	0.41
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.83	0.41
1:0:1819:G:H2'	1:0:1820:G:C5'	2.50	0.41
16:N:151:ASP:OD2	16:N:165:ALA:O	2.38	0.41
1:0:2036:C:C4'	13:K:44:LEU:HG	2.51	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.54	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.52	0.41
4:B:30:PRO:HB2	4:B:39:GLN:HE21	1.85	0.41
1:0:1625:U:H3'	1:0:1625:U:H6	1.85	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.41
4:B:149:ASP:HB2	38:B:8880:HOH:O	2.21	0.41
1:0:130:C:H2'	38:0:3149:HOH:O	2.19	0.41
2:9:11:A:O2'	2:9:12:C:H3'	2.19	0.41
1:0:677:C:O2'	1:0:678:G:H5'	2.20	0.41
1:0:2353:A:H4'	1:0:2354:A:O5'	2.19	0.41
1:0:1515:A:H2'	1:0:1516:U:C6	2.55	0.41
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.67	0.41
24:V:12:THR:H	24:V:15:GLU:HB2	1.85	0.41
6:D:57:THR:HG23	6:D:63:ILE:HG22	2.03	0.41
1:0:137:U:OP1	1:0:259:G:O2'	2.38	0.41
4:B:41:PHE:CG	4:B:190:MET:HE3	2.55	0.41
15:M:39:ARG:NH2	38:M:8922:HOH:O	2.53	0.41
1:0:1973:A:H2'	1:0:1974:G:O4'	2.21	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.20	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
1:0:1850:U:H2'	1:0:1851:G:C8	2.55	0.41
4:B:109:LEU:HG	4:B:113:LEU:HD12	2.02	0.41
1:0:113:A:H2'	1:0:115:U:O4	2.20	0.41
1:0:1711:A:O2'	1:0:1712:A:H5'	2.20	0.41
10:H:115:GLY:N	38:H:8589:HOH:O	2.54	0.41
4:B:224:LYS:HA	4:B:224:LYS:HD3	1.95	0.41
4:B:255:GLY:O	4:B:257:THR:HG23	2.20	0.41
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.35	0.41
1:0:645:U:OP2	14:L:4:LYS:CE	2.63	0.41
4:B:41:PHE:HB3	4:B:190:MET:CE	2.46	0.41
24:V:60:GLN:O	24:V:65:ASP:N	2.52	0.41
1:0:1973:A:H5'	1:0:1973:A:C8	2.52	0.41
20:R:145:LEU:HD12	20:R:146:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.21	0.41
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.55	0.41
1:0:2588:OMG:H3'	1:0:2589:U:H5''	2.02	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
18:P:98:ILE:HD13	18:P:98:ILE:O	2.20	0.41
1:0:1398:G:H2'	1:0:1399:A:C8	2.55	0.41
5:C:7:ASP:O	5:C:9:ASP:N	2.53	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.85	0.41
16:N:93:GLN:HG2	38:N:8858:HOH:O	2.20	0.41
1:0:1314:U:H2'	38:0:5832:HOH:O	2.20	0.41
25:W:59:GLN:NE2	25:W:97:ALA:HB3	2.35	0.41
1:0:1904:A:H2'	1:0:1905:U:O4'	2.20	0.41
16:N:108:SER:HA	16:N:109:PRO:HD3	1.85	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.43	0.41
6:D:23:VAL:HG11	6:D:83:PHE:CZ	2.55	0.41
1:0:1500:U:P	18:P:41:ARG:HH22	2.43	0.41
16:N:157:PRO:HA	38:N:8826:HOH:O	2.21	0.41
12:J:6:PHE:O	12:J:8:ALA:N	2.53	0.41
5:C:107:ARG:CZ	5:C:107:ARG:HB3	2.50	0.41
1:0:2000:G:O2'	1:0:2001:G:H5'	2.20	0.41
1:0:2832:C:H5	38:0:7166:HOH:O	2.04	0.41
27:Y:219:GLU:HG3	27:Y:220:GLU:N	2.35	0.41
1:0:947:U:O2'	1:0:948:G:H5'	2.20	0.41
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.21	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.91	0.41
6:D:16:PRO:HB2	6:D:165:PHE:CG	2.56	0.41
5:C:140:VAL:CG1	5:C:141:SER:N	2.84	0.41
4:B:190:MET:CE	4:B:194:PHE:CD1	3.04	0.41
5:C:136:VAL:HA	5:C:137:PRO:C	2.41	0.41
29:1:25:LYS:HE2	38:2:7213:HOH:O	2.20	0.41
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.24	0.41
6:D:65:GLU:HA	38:D:6752:HOH:O	2.20	0.41
26:X:25:ARG:HG2	38:X:5356:HOH:O	2.20	0.41
1:0:245:C:H2'	1:0:246:G:H5'	2.03	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:737:A:H2'	1:0:738:G:O4'	2.20	0.41
15:M:125:ARG:HD3	38:M:8897:HOH:O	2.20	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
12:J:54:VAL:HG11	12:J:138:THR:HG21	2.02	0.41
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.40	0.41
1:0:2764:C:O2'	1:0:2765:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:705:C:H2'	1:0:705:C:O2	2.21	0.41
2:9:57:A:H8	6:D:141:VAL:HG21	1.86	0.41
4:B:313:PRO:O	4:B:314:ALA:C	2.58	0.41
10:H:69:ARG:CZ	38:H:8580:HOH:O	2.69	0.41
1:0:2840:A:H3'	38:0:7595:HOH:O	2.20	0.41
38:0:7401:HOH:O	4:B:211:THR:HG21	2.20	0.41
8:F:100:ASP:HB3	38:F:5691:HOH:O	2.19	0.41
1:0:1594:C:O2'	1:0:1607:A:H4'	2.21	0.41
1:0:317:A:H5'	38:0:3753:HOH:O	2.19	0.41
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.03	0.41
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.21	0.41
1:0:1015:C:H2'	1:0:1016:U:H6	1.85	0.41
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.56	0.41
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.51	0.41
1:0:164:G:O3'	14:L:30:ARG:HB2	2.21	0.41
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.03	0.41
4:B:102:THR:HG23	4:B:182:VAL:HG12	2.03	0.41
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.20	0.41
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.20	0.41
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.56	0.41
1:0:153:C:P	38:0:6803:HOH:O	2.79	0.41
26:X:27:ASP:OD2	26:X:27:ASP:N	2.52	0.41
1:0:1167:G:H2'	1:0:1168:C:O4'	2.21	0.41
1:0:2270:G:C4'	3:A:223:ARG:HH12	2.25	0.41
20:R:39:THR:O	20:R:40:ALA:C	2.59	0.41
1:0:711:G:C2	1:0:718:C:C2	3.09	0.41
2:9:106:U:O2'	2:9:107:C:H5'	2.21	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.56	0.41
26:X:78:GLU:CG	26:X:79:GLU:H	2.31	0.41
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.84	0.41
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.21	0.41
1:0:958:G:H2'	1:0:959:C:H6	1.86	0.41
1:0:820:G:C5	3:A:171:LYS:HB2	2.55	0.41
5:C:21:VAL:HG23	5:C:22:PHE:CD1	2.56	0.41
11:I:92:VAL:HG12	11:I:92:VAL:O	2.20	0.41
5:C:151:GLN:O	5:C:154:VAL:HB	2.21	0.41
1:0:940:G:C5	1:0:1027:G:C2	3.09	0.41
38:0:6229:HOH:O	18:P:63:ARG:NH2	2.51	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.21	0.41
16:N:32:PRO:HD2	16:N:99:GLU:O	2.21	0.41
1:0:498:A:H2'	1:0:499:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:401:C:H2'	1:0:402:U:C6	2.56	0.41
4:B:144:THR:HG21	38:B:8926:HOH:O	2.21	0.41
1:0:383:A:H2'	1:0:384:G:O4'	2.21	0.41
1:0:2372:A:H2'	1:0:2373:U:C6	2.56	0.41
25:W:63:GLU:HG2	25:W:93:ILE:HG22	2.02	0.41
4:B:13:PHE:N	4:B:13:PHE:CD1	2.89	0.41
1:0:1592:G:O2'	1:0:1593:C:O4'	2.37	0.41
1:0:2505:G:C2'	1:0:2506:A:H5'	2.50	0.41
11:I:87:PRO:HB3	11:I:130:LEU:N	2.37	0.41
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.66	0.41
5:C:16:VAL:CG1	5:C:17:ASP:N	2.82	0.41
11:I:105:GLU:HA	11:I:108:HIS:CE1	2.56	0.41
1:0:1684:A:H1'	30:2:43:ARG:NH2	2.25	0.41
7:E:20:ILE:O	7:E:30:THR:HA	2.21	0.41
3:A:99:ILE:O	3:A:131:HIS:CE1	2.74	0.41
1:0:92:G:H4'	24:V:44:GLY:HA3	2.02	0.41
18:P:141:ILE:O	18:P:143:ALA:N	2.47	0.41
9:G:27:ILE:HD12	9:G:70:ALA:HB1	2.02	0.41
1:0:1675:C:O2'	1:0:1676:G:H5'	2.21	0.41
4:B:84:LEU:HD23	4:B:142:LEU:CD2	2.51	0.41
10:H:86:TYR:C	10:H:86:TYR:CD1	2.94	0.41
1:0:2791:U:H1'	1:0:2792:A:H5''	2.02	0.41
4:B:150:ALA:O	4:B:152:PRO:HD3	2.21	0.41
1:0:2443:C:H1'	14:L:56:LYS:HE3	2.03	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.92	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.42	0.41
1:0:545:G:H2'	1:0:546:C:O4'	2.21	0.40
1:0:396:U:P	31:3:38:ARG:HH11	2.43	0.40
11:I:70:THR:OG1	11:I:107:LYS:HE2	2.22	0.40
1:0:338:C:H5''	38:0:3781:HOH:O	2.21	0.40
20:R:18:LEU:HB2	20:R:143:VAL:HG12	2.01	0.40
30:2:35:ARG:HG2	38:2:6391:HOH:O	2.21	0.40
4:B:307:ARG:HH11	4:B:307:ARG:CG	2.34	0.40
1:0:1505:U:C6	1:0:1505:U:H5'	2.50	0.40
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.56	0.40
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.21	0.40
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.55	0.40
1:0:539:G:H2'	1:0:540:A:C8	2.55	0.40
1:0:2361:A:H2'	1:0:2362:A:C8	2.55	0.40
9:G:19:GLU:HG2	9:G:66:LEU:CD1	2.51	0.40
7:E:156:ASP:N	7:E:156:ASP:OD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:685:C:O2	1:0:748:C:H4'	2.20	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.56	0.40
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	2.01	0.40
1:0:213:G:O2'	1:0:214:U:OP2	2.39	0.40
14:L:130:ARG:HA	38:L:8856:HOH:O	2.21	0.40
1:0:2316:G:H4'	38:0:6048:HOH:O	2.21	0.40
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.21	0.40
1:0:2415:A:H2'	1:0:2416:G:H5'	2.02	0.40
20:R:113:HIS:O	20:R:145:LEU:HD12	2.21	0.40
5:C:219:ASN:OD1	5:C:222:ASP:OD1	2.40	0.40
26:X:80:GLU:N	38:X:5564:HOH:O	2.54	0.40
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	2.03	0.40
1:0:330:C:H5	5:C:170:ASP:OD2	2.04	0.40
1:0:2766:A:O2'	1:0:2767:C:H5'	2.20	0.40
14:L:120:LEU:HD12	14:L:133:VAL:HG21	2.03	0.40
25:W:21:LEU:CD2	25:W:26:ILE:HD11	2.44	0.40
1:0:2269:C:H2'	1:0:2270:G:H5'	2.03	0.40
18:P:59:ARG:NH2	18:P:66:GLN:NE2	2.60	0.40
1:0:1234:U:C2	4:B:244:PRO:HB3	2.56	0.40
20:R:25:PHE:CE2	20:R:29:LYS:CE	3.05	0.40
4:B:207:LYS:HG2	4:B:304:PRO:HB3	2.02	0.40
1:0:2807:U:P	4:B:27:ASN:HD21	2.45	0.40
31:3:65:THR:HB	31:3:83:TRP:H	1.87	0.40
1:0:1755:A:H2'	1:0:1756:G:O4'	2.21	0.40
4:B:174:ARG:HA	4:B:177:HIS:HB3	2.02	0.40
1:0:848:C:H5'	38:0:7224:HOH:O	2.22	0.40
1:0:1947:G:N2	1:0:1966:U:C2	2.89	0.40
1:0:525:G:H2'	1:0:526:U:O4'	2.20	0.40
1:0:1930:A:H2'	1:0:1931:A:C8	2.56	0.40
1:0:466:A:H2'	1:0:467:G:O4'	2.21	0.40
5:C:145:GLU:OE1	5:C:198:ASP:HB2	2.21	0.40
30:2:41:HIS:H	30:2:45:ASN:ND2	1.97	0.40
30:2:41:HIS:CD2	30:2:44:ARG:H	2.29	0.40
27:Y:189:ASN:ND2	27:Y:192:ASP:N	2.70	0.40
6:D:37:ALA:O	6:D:40:ILE:HG12	2.22	0.40
13:K:65:ARG:O	13:K:66:ARG:HB2	2.21	0.40
4:B:305:ASP:O	4:B:306:LYS:CB	2.68	0.40
16:N:183:ASP:O	16:N:184:ILE:C	2.60	0.40
4:B:77:PRO:HG2	4:B:151:VAL:CG2	2.51	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.22	0.40
5:C:14:GLY:O	5:C:15:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2577:A:H5'	38:0:7697:HOH:O	2.21	0.40
1:0:1735:C:O2'	1:0:1736:A:H5'	2.20	0.40
6:D:11:HIS:CG	6:D:12:GLU:N	2.90	0.40
1:0:2812:A:N7	38:0:7464:HOH:O	2.37	0.40
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.29	0.40
8:F:63:ILE:HB	8:F:64:PRO:CD	2.47	0.40
1:0:1205:U:C2'	1:0:1206:U:H5''	2.51	0.40
2:9:39:U:H3'	2:9:40:C:H5''	2.04	0.40
7:E:35:TYR:HA	12:J:127:ILE:HD12	2.02	0.40
2:9:28:U:H5''	16:N:40:ASN:HD21	1.85	0.40
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.51	0.40
6:D:173:GLU:O	6:D:174:VAL:C	2.60	0.40
1:0:2564:G:OP2	1:0:2565:C:H5''	2.22	0.40
1:0:968:G:O2'	1:0:969:G:H5'	2.21	0.40
14:L:35:ARG:HD3	14:L:35:ARG:C	2.41	0.40
1:0:2708:G:H2'	1:0:2709:G:O4'	2.22	0.40
38:0:7370:HOH:O	3:A:22:ARG:HD2	2.21	0.40
1:0:1041:U:H4'	1:0:1295:G:H5'	2.04	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	
3	A	235/240 (98%)	213 (91%)	20 (8%)	2 (1%)	21	44
4	B	335/338 (99%)	300 (90%)	30 (9%)	5 (2%)	13	28
5	C	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	39	65
6	D	134/177 (76%)	98 (73%)	27 (20%)	9 (7%)	1	1
7	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
8	F	117/120 (98%)	101 (86%)	12 (10%)	4 (3%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	15	33
11	I	68/162 (42%)	53 (78%)	15 (22%)	0	100	100
12	J	140/145 (97%)	130 (93%)	5 (4%)	5 (4%)	4	8
13	K	130/132 (98%)	119 (92%)	10 (8%)	1 (1%)	24	47
14	L	141/165 (86%)	121 (86%)	19 (14%)	1 (1%)	26	51
15	M	192/195 (98%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	6	13
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	133 (94%)	7 (5%)	1 (1%)	26	51
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	44
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	56 (89%)	5 (8%)	2 (3%)	5	10
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	15	33
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	2	3
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	17	38
All	All	3705/4437 (84%)	3374 (91%)	285 (8%)	46 (1%)	16	35

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
6	D	173	GLU
8	F	101	ALA
14	L	80	ASP
16	N	154	LEU
16	N	164	ASP

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Mol	Chain	Res	Type
16	N	184	ILE
28	Z	81	ARG
4	B	34	GLY
4	B	139	ASP
4	B	169	GLY
5	C	8	LEU
8	F	44	SER
10	H	172	GLU
12	J	5	GLU
18	P	116	SER
31	3	57	GLY
4	B	185	GLY
6	D	56	ARG
6	D	171	ASP
22	T	53	GLY
24	V	43	PRO
25	W	49	ASN
25	W	77	ALA
6	D	27	ILE
6	D	65	GLU
6	D	137	PRO
12	J	89	HIS
16	N	139	TRP
28	Z	20	ARG
28	Z	41	ASN
28	Z	42	CYS
6	D	61	PHE
8	F	100	ASP
12	J	7	ASP
12	J	65	ASN
12	J	143	LYS
13	K	126	SER
16	N	155	GLU
4	B	2	GLN
6	D	16	PRO
10	H	143	VAL
6	D	69	ILE
8	F	64	PRO
24	V	40	PRO
3	A	37	VAL

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	
3	A	179/182 (98%)	167 (93%)	12 (7%)	20	41
4	B	282/283 (100%)	265 (94%)	17 (6%)	24	47
5	C	193/193 (100%)	175 (91%)	18 (9%)	11	23
6	D	117/148 (79%)	111 (95%)	6 (5%)	29	55
7	E	152/156 (97%)	147 (97%)	5 (3%)	45	73
8	F	93/94 (99%)	91 (98%)	2 (2%)	60	84
9	G	27/283 (10%)	26 (96%)	1 (4%)	41	69
10	H	134/145 (92%)	128 (96%)	6 (4%)	34	61
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	106 (90%)	12 (10%)	9	19
13	K	106/106 (100%)	103 (97%)	3 (3%)	51	79
14	L	113/127 (89%)	109 (96%)	4 (4%)	43	71
15	M	158/159 (99%)	152 (96%)	6 (4%)	40	68
16	N	149/150 (99%)	144 (97%)	5 (3%)	44	72
17	O	93/94 (99%)	91 (98%)	2 (2%)	60	84
18	P	113/117 (97%)	109 (96%)	4 (4%)	43	71
19	Q	79/80 (99%)	74 (94%)	5 (6%)	22	44
20	R	117/122 (96%)	112 (96%)	5 (4%)	35	63
21	S	71/74 (96%)	68 (96%)	3 (4%)	36	64
22	T	105/106 (99%)	99 (94%)	6 (6%)	25	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	39	67
25	W	130/130 (100%)	125 (96%)	5 (4%)	40	68
26	X	66/74 (89%)	63 (96%)	3 (4%)	34	61
27	Y	120/196 (61%)	113 (94%)	7 (6%)	25	48
28	Z	60/68 (88%)	59 (98%)	1 (2%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	82
31	3	79/79 (100%)	78 (99%)	1 (1%)	76	91
All	All	3095/3619 (86%)	2953 (95%)	142 (5%)	33	61

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	69	LEU
3	A	78	ASP
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	206	ARG
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	97	LEU
4	B	98	THR
4	B	162	MET
4	B	190	MET
4	B	195	ARG
4	B	245	SER
4	B	251	VAL
4	B	254	GLN
4	B	264	GLU
4	B	277	GLU
4	B	304	PRO
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG

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Mol	Chain	Res	Type
5	C	78	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	115	LEU
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
6	D	24	HIS
6	D	61	PHE
6	D	133	ASN
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
7	E	12	ASP
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
7	E	164	ASP
8	F	12	LEU
8	F	105	ASP
9	G	64	ASN
10	H	33	GLN
10	H	87	LYS
10	H	91	ARG
10	H	114	ASP
10	H	157	TYR
10	H	172	GLU
12	J	46	ILE
12	J	47	THR
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP

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Mol	Chain	Res	Type
12	J	120	SER
12	J	127	ILE
12	J	131	THR
12	J	132	LEU
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP
14	L	99	GLU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	26	LEU
16	N	49	THR
16	N	138	ASP
16	N	139	TRP
16	N	152	GLU
17	O	28	ASP
17	O	111	VAL
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	55	ARG
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	82	GLU
20	R	132	ARG
20	R	143	VAL
21	S	53	ASN
21	S	71	ASP
21	S	80	ARG
22	T	19	ARG

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Mol	Chain	Res	Type
22	T	26	THR
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	43	PRO
24	V	65	ASP
25	W	4	LEU
25	W	52	VAL
25	W	73	LEU
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	72	VAL
27	Y	115	ARG
27	Y	163	THR
27	Y	172	THR
27	Y	189	ASN
27	Y	203	VAL
27	Y	204	ARG
27	Y	220	GLU
28	Z	41	ASN
30	2	18	ASN
31	3	40	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	92	ASN
3	A	199	HIS
4	B	27	ASN
4	B	106	HIS
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN

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Mol	Chain	Res	Type
5	C	39	GLN
5	C	129	HIS
5	C	151	GLN
5	C	163	HIS
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	71	ASN
7	E	90	HIS
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	73	ASN
10	H	148	HIS
11	I	88	GLN
11	I	108	HIS
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	137	ASN
15	M	170	ASN
16	N	40	ASN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	22	GLN

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Mol	Chain	Res	Type
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
20	R	123	GLN
21	S	53	ASN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
24	V	4	HIS
24	V	60	GLN
25	W	27	HIS
25	W	28	HIS
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	37	HIS
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	240 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2867/3044 (94%)	256 (8%)	36 (1%)

All (256) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	317	A
1	0	319	A
1	0	336	G

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Mol	Chain	Res	Type
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	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	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G

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Mol	Chain	Res	Type
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	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

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

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Mol	Chain	Res	Type
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	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

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Mol	Chain	Res	Type
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
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	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	7	G
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U

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Mol	Chain	Res	Type
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	52	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	169	A
1	0	318	U
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1563	G
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A

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Mol	Chain	Res	Type
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
2	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMU	0	2587	1	12,22,23	0.97	1 (8%)	19,31,34	3.15	2 (10%)
1	OMG	0	2588	1	17,26,27	1.04	1 (5%)	21,38,41	2.51	3 (14%)
1	UR3	0	2619	1	12,22,23	0.92	0	16,32,35	0.79	0
1	PSU	0	2621	1	13,21,22	1.55	2 (15%)	18,30,33	6.12	3 (16%)
1	1MA	0	628	1	14,25,26	0.94	1 (7%)	15,37,40	1.22	1 (6%)

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	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.62	1.48	1.52
1	0	2587	OMU	C4-N3	2.29	1.37	1.33
1	0	628	1MA	C6-N6	2.54	1.33	1.29
1	0	2621	PSU	C4-N3	2.72	1.38	1.33
1	0	2588	OMG	C6-N1	3.22	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.50	114.62	128.33
1	0	2588	OMG	C5-C6-N1	-8.70	111.70	123.59
1	0	628	1MA	C2-N3-C4	-3.67	110.72	116.40
1	0	2587	OMU	C5-C4-N3	-3.24	114.81	123.12
1	0	2588	OMG	N3-C2-N1	-2.22	124.06	127.44
1	0	2621	PSU	C6-N1-C2	2.83	120.02	115.47
1	0	2588	OMG	C6-N1-C2	6.58	125.08	115.94
1	0	2587	OMU	C4-N3-C2	13.14	127.15	114.14
1	0	2621	PSU	C4-N3-C2	13.91	127.27	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2588	OMG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	ERY	0	9000	-	53,53,53	1.15	3 (5%)	82,82,82	0.97	3 (3%)

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
32	ERY	0	9000	-	-	0/72/107/107	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	ERY	C2-C3	2.07	1.60	1.55
32	0	9000	ERY	C7-C6	2.29	1.58	1.54
32	0	9000	ERY	C6-C5	2.78	1.61	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	ERY	C3-C2-C1	-2.63	104.71	109.86
32	0	9000	ERY	C25-C24-C23	-2.42	106.50	110.03
32	0	9000	ERY	C6-C5-C4	-2.26	110.94	114.11

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%)	-0.43	46 (1%) 73 72	26, 49, 94, 152	0
2	9	122/122 (100%)	-0.38	5 (4%) 41 39	40, 65, 90, 154	0
3	A	237/240 (98%)	0.24	13 (5%) 29 26	31, 54, 88, 109	0
4	B	337/338 (99%)	0.06	6 (1%) 71 70	30, 58, 83, 92	0
5	C	246/246 (100%)	-0.06	2 (0%) 87 87	26, 48, 73, 82	0
6	D	140/177 (79%)	1.90	55 (39%) 0 0	56, 101, 125, 132	0
7	E	172/178 (96%)	0.81	22 (12%) 5 3	49, 71, 90, 94	0
8	F	119/120 (99%)	0.82	17 (14%) 4 2	51, 76, 95, 111	0
9	G	29/348 (8%)	2.72	22 (75%) 0 0	77, 93, 102, 105	0
10	H	160/177 (90%)	0.26	11 (6%) 20 17	39, 59, 92, 99	0
11	I	70/162 (43%)	4.29	63 (90%) 0 0	109, 122, 139, 141	0
12	J	142/145 (97%)	0.01	0 100 100	38, 53, 75, 95	0
13	K	132/132 (100%)	-0.07	2 (1%) 76 75	34, 55, 75, 86	0
14	L	145/165 (87%)	0.68	26 (17%) 2 1	27, 68, 109, 122	0
15	M	194/195 (99%)	-0.15	1 (0%) 91 92	35, 46, 61, 70	0
16	N	186/187 (99%)	0.64	23 (12%) 5 4	41, 64, 108, 119	0
17	O	115/116 (99%)	0.05	1 (0%) 85 86	39, 57, 74, 78	0
18	P	143/149 (95%)	0.15	1 (0%) 89 89	41, 58, 71, 80	0
19	Q	95/96 (98%)	-0.07	0 100 100	38, 46, 62, 76	0
20	R	150/155 (96%)	-0.11	1 (0%) 89 89	35, 48, 67, 77	0
21	S	81/85 (95%)	0.20	3 (3%) 45 44	47, 63, 83, 88	0
22	T	119/120 (99%)	0.45	7 (5%) 26 23	40, 61, 85, 97	0
23	U	53/66 (80%)	0.24	1 (1%) 70 69	46, 59, 76, 86	0
24	V	65/71 (91%)	1.65	18 (27%) 1 0	58, 77, 114, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.17	0 100 100	35, 50, 67, 78	0
26	X	82/92 (89%)	0.52	10 (12%) 5 4	48, 61, 85, 101	0
27	Y	142/241 (58%)	0.10	7 (4%) 33 31	28, 47, 71, 89	0
28	Z	73/83 (87%)	0.18	3 (4%) 41 39	52, 64, 80, 95	0
29	1	56/57 (98%)	-0.46	0 100 100	29, 36, 42, 52	0
30	2	46/50 (92%)	0.39	4 (8%) 13 9	37, 61, 87, 102	0
31	3	92/92 (100%)	0.25	1 (1%) 82 82	37, 56, 70, 83	0
All	All	6646/7481 (88%)	0.03	371 (5%) 28 25	26, 55, 99, 154	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	128	THR	13.3
24	V	1	THR	11.1
11	I	91	PHE	9.4
24	V	39	ALA	8.9
11	I	88	GLN	8.5
11	I	108	HIS	8.4
11	I	66	GLY	7.8
6	D	63	ILE	7.8
11	I	104	ALA	7.5
2	9	1	U	7.5
11	I	132	VAL	7.4
11	I	74	ILE	7.4
24	V	40	PRO	7.2
6	D	10	PHE	6.9
11	I	112	LEU	6.8
9	G	27	ILE	6.7
6	D	69	ILE	6.6
11	I	80	PHE	6.5
11	I	92	VAL	6.3
11	I	70	THR	6.3
11	I	72	GLU	6.2
11	I	97	VAL	6.2
6	D	18	ILE	6.2
11	I	71	ALA	6.1
26	X	88	GLU	5.9
11	I	113	SER	5.8
6	D	64	ARG	5.7
14	L	105	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
11	I	106	GLN	5.5
24	V	43	PRO	5.5
16	N	166	ALA	5.3
3	A	37	VAL	5.3
11	I	100	VAL	5.3
11	I	98	ASP	5.3
9	G	23	ILE	5.2
11	I	86	GLU	5.1
11	I	83	GLY	5.1
1	0	1198	U	5.0
9	G	24	VAL	5.0
11	I	111	LEU	5.0
1	0	1173	A	4.9
14	L	106	VAL	4.9
6	D	57	THR	4.9
11	I	116	LEU	4.8
24	V	38	GLY	4.8
3	A	35	GLY	4.8
1	0	1177	A	4.8
6	D	85	GLN	4.7
6	D	170	TYR	4.7
2	9	23	U	4.6
11	I	134	ILE	4.6
6	D	88	LEU	4.6
6	D	89	PRO	4.6
22	T	119	ALA	4.6
6	D	17	ARG	4.5
1	0	2237	G	4.5
8	F	119	ARG	4.5
11	I	109	PRO	4.5
11	I	84	SER	4.5
2	9	24	U	4.4
1	0	1199	A	4.4
14	L	60	GLU	4.4
27	Y	235	GLU	4.4
6	D	106	PHE	4.4
6	D	26	GLY	4.3
11	I	79	GLY	4.3
11	I	127	CYS	4.3
1	0	282	C	4.3
7	E	45	ASP	4.3
11	I	118	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
6	D	165	PHE	4.2
6	D	58	VAL	4.2
11	I	130	LEU	4.2
6	D	61	PHE	4.1
11	I	102	GLN	4.1
6	D	171	ASP	4.1
6	D	66	GLY	4.1
30	2	35	ARG	4.0
6	D	62	ASP	4.0
11	I	99	GLN	4.0
1	0	1169	U	4.0
6	D	93	LEU	4.0
8	F	16	ALA	4.0
11	I	76	ASP	4.0
1	0	1172	G	3.9
6	D	27	ILE	3.9
8	F	17	LEU	3.9
1	0	1171	A	3.9
1	0	1951	G	3.9
1	0	970	U	3.9
6	D	166	ILE	3.9
16	N	152	GLU	3.8
10	H	174	LEU	3.8
6	D	65	GLU	3.8
21	S	81	ILE	3.8
6	D	25	MET	3.8
11	I	117	THR	3.8
9	G	20	VAL	3.8
6	D	68	PRO	3.7
16	N	149	GLU	3.7
11	I	131	GLY	3.7
15	M	194	GLY	3.7
11	I	78	ALA	3.7
1	0	2004	U	3.7
11	I	135	GLU	3.7
6	D	90	LEU	3.6
11	I	87	PRO	3.6
24	V	37	GLY	3.6
7	E	108	LEU	3.5
16	N	183	ASP	3.5
1	0	1525	G	3.5
1	0	735	C	3.5

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Mol	Chain	Res	Type	RSRZ
11	I	121	LYS	3.5
6	D	23	VAL	3.5
11	I	67	VAL	3.5
1	0	2238	A	3.5
9	G	26	MET	3.5
9	G	71	LEU	3.5
7	E	170	ARG	3.4
6	D	128	LEU	3.4
6	D	130	VAL	3.4
14	L	80	ASP	3.4
30	2	49	GLU	3.4
24	V	8	ILE	3.4
3	A	133	ARG	3.4
14	L	100	ALA	3.4
11	I	119	ALA	3.4
1	0	138	U	3.4
11	I	133	THR	3.4
16	N	147	ILE	3.4
11	I	124	VAL	3.4
24	V	41	GLU	3.4
4	B	1	PRO	3.3
11	I	93	ALA	3.3
6	D	172	VAL	3.3
28	Z	20	ARG	3.3
8	F	49	PHE	3.3
11	I	103	ILE	3.3
10	H	40	GLN	3.3
9	G	69	ARG	3.2
10	H	170	ARG	3.2
11	I	81	GLU	3.2
28	Z	11	SER	3.2
6	D	56	ARG	3.2
1	0	284	C	3.2
1	0	960	G	3.2
3	A	36	ASP	3.1
4	B	181	ILE	3.1
6	D	75	LEU	3.1
7	E	100	ASP	3.1
16	N	150	TYR	3.1
1	0	1279	U	3.1
6	D	44	ILE	3.1
6	D	98	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
9	G	28	GLU	3.1
11	I	105	GLU	3.1
14	L	81	VAL	3.1
11	I	89	GLU	3.1
6	D	104	PHE	3.1
11	I	114	TYR	3.1
16	N	159	TYR	3.1
3	A	85	SER	3.1
16	N	138	ASP	3.1
3	A	237	GLY	3.1
14	L	120	LEU	3.1
26	X	85	VAL	3.0
11	I	82	THR	3.0
6	D	134	LEU	3.0
11	I	68	PRO	3.0
11	I	101	LYS	3.0
1	0	285	A	3.0
1	0	1170	U	3.0
31	3	92	GLU	3.0
24	V	3	LEU	3.0
5	C	135	GLU	2.9
9	G	21	ASP	2.9
14	L	133	VAL	2.9
22	T	112	LEU	2.9
14	L	89	PHE	2.9
16	N	179	LEU	2.9
11	I	90	ASP	2.9
27	Y	108	ASP	2.9
4	B	119	HIS	2.9
23	U	47	ARG	2.9
6	D	87	ALA	2.9
11	I	120	ALA	2.9
14	L	149	ARG	2.9
8	F	20	LEU	2.8
24	V	6	GLN	2.8
9	G	66	LEU	2.8
11	I	110	ASP	2.8
22	T	115	GLU	2.8
16	N	160	SER	2.8
24	V	59	ILE	2.8
9	G	22	ALA	2.8
16	N	148	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
6	D	67	ASP	2.8
9	G	72	ASP	2.8
9	G	73	ASP	2.8
14	L	118	LEU	2.8
16	N	145	ALA	2.8
30	2	20	ARG	2.8
6	D	43	GLU	2.8
1	0	2239	C	2.8
27	Y	95	THR	2.8
1	0	10	U	2.8
1	0	1180	U	2.8
1	0	1202	A	2.8
7	E	10	ASP	2.8
6	D	70	GLY	2.8
7	E	88	TYR	2.8
6	D	48	MET	2.7
10	H	85	ASP	2.7
3	A	38	ILE	2.7
11	I	75	LYS	2.7
14	L	96	VAL	2.7
6	D	102	GLY	2.7
7	E	5	LEU	2.7
1	0	1950	G	2.7
1	0	1200	A	2.7
13	K	108	GLU	2.7
1	0	1948	G	2.7
26	X	10	VAL	2.7
6	D	84	LEU	2.6
6	D	86	THR	2.6
9	G	67	LEU	2.6
11	I	95	LEU	2.6
14	L	130	ARG	2.6
11	I	115	ASP	2.6
14	L	104	ASP	2.6
8	F	90	GLU	2.6
6	D	11	HIS	2.6
2	9	2	U	2.6
21	S	76	GLU	2.6
16	N	158	LEU	2.6
1	0	999	C	2.6
14	L	97	VAL	2.6
9	G	12	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	92	GLU	2.6
16	N	162	ASP	2.6
8	F	6	PHE	2.6
16	N	83	LEU	2.6
30	2	39	ARG	2.5
6	D	40	ILE	2.5
24	V	5	VAL	2.5
1	0	371	U	2.5
3	A	34	ASP	2.5
11	I	73	LEU	2.5
14	L	76	LEU	2.5
7	E	42	VAL	2.5
7	E	128	GLY	2.5
1	0	2769	C	2.5
14	L	102	ASP	2.5
6	D	55	LYS	2.5
11	I	69	PRO	2.5
16	N	157	PRO	2.5
26	X	74	ALA	2.5
9	G	25	GLU	2.5
4	B	128	ILE	2.5
6	D	81	GLU	2.5
27	Y	216	ARG	2.4
7	E	127	ASP	2.4
1	0	1626	A	2.4
9	G	15	TRP	2.4
14	L	59	GLU	2.4
3	A	31	LYS	2.4
7	E	11	VAL	2.4
10	H	48	VAL	2.4
6	D	24	HIS	2.4
11	I	123	VAL	2.4
13	K	132	VAL	2.4
3	A	64	ASP	2.4
26	X	80	GLU	2.4
1	0	1947	G	2.3
16	N	67	ALA	2.3
24	V	36	ALA	2.3
3	A	97	ALA	2.3
9	G	70	ALA	2.3
8	F	107	ASP	2.3
24	V	10	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	0	1181	A	2.3
26	X	76	ARG	2.3
16	N	181	ASP	2.3
27	Y	98	GLN	2.3
1	0	1186	C	2.3
9	G	65	THR	2.3
16	N	185	GLU	2.3
22	T	80	GLU	2.3
4	B	105	PHE	2.3
3	A	82	VAL	2.3
9	G	18	GLU	2.3
2	9	122	C	2.3
28	Z	24	ARG	2.3
7	E	101	GLU	2.3
8	F	19	ALA	2.3
17	O	89	ILE	2.3
6	D	41	LEU	2.3
8	F	106	ALA	2.3
16	N	68	GLU	2.2
26	X	7	GLU	2.2
8	F	44	SER	2.2
22	T	116	ASP	2.2
20	R	96	VAL	2.2
21	S	2	TRP	2.2
7	E	82	TYR	2.2
10	H	172	GLU	2.2
8	F	12	LEU	2.2
7	E	53	GLU	2.2
16	N	155	GLU	2.2
14	L	75	LEU	2.2
6	D	54	ALA	2.2
1	0	370	G	2.2
1	0	716	G	2.2
8	F	22	VAL	2.2
14	L	73	VAL	2.2
5	C	246	ARG	2.2
1	0	1168	C	2.2
1	0	1204	C	2.2
10	H	82	GLU	2.2
4	B	118	ASP	2.2
1	0	1178	G	2.2
7	E	28	SER	2.2

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Mol	Chain	Res	Type	RSRZ
7	E	98	GLU	2.2
8	F	103	GLU	2.2
14	L	150	GLN	2.2
26	X	77	PHE	2.2
9	G	63	ARG	2.2
14	L	99	GLU	2.2
10	H	86	TYR	2.2
1	0	280	C	2.2
10	H	169	GLU	2.2
26	X	72	VAL	2.2
16	N	139	TRP	2.1
1	0	1625	U	2.1
7	E	129	GLU	2.1
22	T	33	GLU	2.1
6	D	53	LYS	2.1
14	L	93	VAL	2.1
14	L	108	VAL	2.1
22	T	40	VAL	2.1
18	P	141	ILE	2.1
1	0	2344	G	2.1
26	X	41	PHE	2.1
7	E	6	GLU	2.1
24	V	7	GLU	2.1
24	V	63	GLU	2.1
10	H	35	LYS	2.1
24	V	2	VAL	2.1
7	E	118	ILE	2.1
10	H	76	LEU	2.1
7	E	126	ILE	2.1
27	Y	96	GLU	2.1
24	V	52	ALA	2.1
7	E	95	VAL	2.1
3	A	99	ILE	2.1
8	F	69	GLU	2.1
1	0	2345	A	2.1
11	I	129	SER	2.1
1	0	2241	C	2.0
8	F	15	ASP	2.0
27	Y	97	LEU	2.0
6	D	101	THR	2.0
8	F	108	VAL	2.0
11	I	94	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
7	E	89	SER	2.0
16	N	95	ALA	2.0
1	0	1526	A	2.0
14	L	140	VAL	2.0
9	G	64	ASN	2.0
6	D	15	GLU	2.0
14	L	91	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PSU	0	2621	20/21	0.99	0.14	-	28,31,35,36	0
1	OMU	0	2587	21/22	0.99	0.12	-	35,37,40,43	0
1	UR3	0	2619	21/22	0.99	0.12	-	35,37,41,45	0
1	1MA	0	628	23/24	0.99	0.15	-	30,33,34,36	0
1	OMG	0	2588	24/25	0.98	0.14	-	34,36,38,40	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	L	8580	1/1	0.92	0.69	40.89	60,60,60,60	0
35	NA	0	8574	1/1	0.98	0.53	36.87	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8556	1/1	0.95	0.37	23.19	44,44,44,44	0
35	NA	R	8586	1/1	0.61	0.74	21.44	87,87,87,87	0
35	NA	0	8561	1/1	0.91	0.28	20.39	58,58,58,58	0
35	NA	0	8571	1/1	0.83	0.28	19.60	58,58,58,58	0
35	NA	0	8578	1/1	0.97	0.37	19.47	52,52,52,52	0
35	NA	0	8572	1/1	0.91	0.34	14.89	64,64,64,64	0
35	NA	0	8535	1/1	0.91	0.25	13.55	49,49,49,49	0
35	NA	0	8564	1/1	0.85	0.25	13.51	49,49,49,49	0
36	CL	0	8815	1/1	0.94	0.24	13.31	81,81,81,81	0
35	NA	0	8562	1/1	0.88	0.27	13.16	63,63,63,63	0
35	NA	0	8573	1/1	0.95	0.39	12.94	58,58,58,58	0
35	NA	9	8583	1/1	0.86	0.28	11.85	58,58,58,58	0
35	NA	0	8510	1/1	0.88	0.29	11.11	45,45,45,45	0
35	NA	0	8540	1/1	0.88	0.37	11.08	52,52,52,52	0
35	NA	0	8521	1/1	0.97	0.28	8.86	57,57,57,57	0
35	NA	0	8532	1/1	0.91	0.23	8.68	40,40,40,40	0
35	NA	0	8502	1/1	0.95	0.20	6.89	56,56,56,56	0
34	K	0	8401	1/1	0.94	0.19	6.42	75,75,75,75	0
35	NA	0	8525	1/1	0.98	0.21	6.28	59,59,59,59	0
33	MG	0	8088	1/1	0.90	0.19	6.23	38,38,38,38	0
32	ERY	0	9000	51/51	0.90	0.24	5.50	69,75,79,80	0
35	NA	0	8550	1/1	0.96	0.20	5.19	47,47,47,47	0
35	NA	0	8568	1/1	0.87	0.17	5.07	76,76,76,76	0
35	NA	0	8526	1/1	0.84	0.27	4.39	55,55,55,55	0
35	NA	0	8577	1/1	0.95	0.18	3.27	62,62,62,62	0
35	NA	0	8566	1/1	0.86	0.23	2.97	59,59,59,59	0
35	NA	0	8576	1/1	0.96	0.18	2.92	52,52,52,52	0
35	NA	0	8565	1/1	0.93	0.44	2.49	46,46,46,46	0
35	NA	0	8582	1/1	0.86	0.18	2.06	80,80,80,80	0
35	NA	0	8514	1/1	0.92	0.17	2.06	40,40,40,40	0
35	NA	0	8527	1/1	0.93	0.14	0.26	45,45,45,45	0
33	MG	0	8060	1/1	0.98	0.15	0.23	42,42,42,42	0
35	NA	C	8504	1/1	0.84	0.18	0.21	46,46,46,46	0
35	NA	0	8523	1/1	0.96	0.17	0.08	38,38,38,38	0
35	NA	0	8524	1/1	0.95	0.15	-0.01	62,62,62,62	0
35	NA	0	8503	1/1	0.99	0.15	-0.07	39,39,39,39	0
35	NA	M	8547	1/1	0.96	0.14	-0.11	33,33,33,33	0
35	NA	0	8539	1/1	0.93	0.14	-0.13	28,28,28,28	0
33	MG	3	8078	1/1	0.98	0.12	-0.49	47,47,47,47	0
33	MG	0	8086	1/1	0.98	0.12	-0.68	48,48,48,48	0
36	CL	M	8818	1/1	0.99	0.14	-0.69	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8531	1/1	0.95	0.13	-0.81	40,40,40,40	0
37	CD	U	8701	1/1	0.99	0.11	-0.82	67,67,67,67	0
35	NA	Q	8548	1/1	0.91	0.16	-0.94	47,47,47,47	0
36	CL	O	8808	1/1	0.98	0.14	-0.97	72,72,72,72	0
35	NA	J	8546	1/1	0.95	0.14	-1.04	55,55,55,55	0
33	MG	0	8015	1/1	0.99	0.12	-1.29	35,35,35,35	0
35	NA	R	8537	1/1	0.94	0.12	-1.34	42,42,42,42	0
36	CL	J	8821	1/1	0.97	0.13	-1.45	55,55,55,55	0
37	CD	Z	8703	1/1	0.99	0.09	-1.51	63,63,63,63	0
33	MG	0	8044	1/1	0.97	0.10	-1.53	49,49,49,49	0
33	MG	0	8013	1/1	0.98	0.15	-1.63	45,45,45,45	0
36	CL	0	8816	1/1	0.97	0.10	-1.66	60,60,60,60	0
37	CD	1	8702	1/1	0.99	0.08	-1.77	63,63,63,63	0
37	CD	3	8704	1/1	0.99	0.07	-1.87	62,62,62,62	0
35	NA	0	8517	1/1	0.91	0.09	-2.03	46,46,46,46	0
36	CL	B	8819	1/1	0.99	0.12	-2.13	54,54,54,54	0
35	NA	0	8533	1/1	0.92	0.09	-2.21	38,38,38,38	0
33	MG	0	8064	1/1	0.96	0.10	-2.26	34,34,34,34	0
33	MG	0	8033	1/1	0.96	0.12	-2.37	32,32,32,32	0
35	NA	0	8505	1/1	0.96	0.12	-2.42	33,33,33,33	0
33	MG	T	8073	1/1	0.95	0.12	-2.44	61,61,61,61	0
36	CL	L	8810	1/1	0.96	0.09	-2.45	60,60,60,60	0
33	MG	0	8018	1/1	0.99	0.11	-2.47	45,45,45,45	0
33	MG	A	8065	1/1	0.99	0.10	-2.52	42,42,42,42	0
36	CL	3	8804	1/1	0.89	0.09	-2.54	63,63,63,63	0
33	MG	0	8070	1/1	0.93	0.08	-2.55	50,50,50,50	0
35	NA	A	8545	1/1	0.98	0.09	-2.64	50,50,50,50	0
35	NA	0	8553	1/1	0.97	0.10	-2.67	30,30,30,30	0
33	MG	0	8056	1/1	0.98	0.10	-2.72	53,53,53,53	0
33	MG	B	8055	1/1	0.98	0.07	-2.74	52,52,52,52	0
33	MG	0	8057	1/1	0.96	0.12	-2.83	49,49,49,49	0
33	MG	0	8106	1/1	0.98	0.06	-2.93	42,42,42,42	0
36	CL	0	8805	1/1	0.94	0.11	-2.95	63,63,63,63	0
33	MG	0	8074	1/1	0.99	0.05	-3.01	38,38,38,38	0
36	CL	0	8812	1/1	0.99	0.09	-3.13	54,54,54,54	0
33	MG	0	8080	1/1	0.98	0.10	-3.23	46,46,46,46	0
35	NA	H	8509	1/1	0.97	0.06	-3.67	34,34,34,34	0
35	NA	R	8538	1/1	0.95	0.07	-3.71	57,57,57,57	0
33	MG	0	8096	1/1	0.93	0.07	-3.74	45,45,45,45	0
34	K	0	8402	1/1	0.99	0.11	-3.85	59,59,59,59	0
33	MG	0	8058	1/1	0.99	0.09	-3.85	44,44,44,44	0
33	MG	0	8111	1/1	0.96	0.10	-4.19	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8017	1/1	0.99	0.04	-4.20	25,25,25,25	0
33	MG	0	8054	1/1	0.99	0.11	-4.31	32,32,32,32	0
33	MG	0	8021	1/1	0.99	0.10	-4.33	35,35,35,35	0
33	MG	0	8003	1/1	0.99	0.15	-4.39	32,32,32,32	0
33	MG	0	8020	1/1	0.99	0.09	-4.40	36,36,36,36	0
33	MG	0	8084	1/1	0.98	0.07	-4.52	48,48,48,48	0
33	MG	0	8038	1/1	0.99	0.10	-4.67	32,32,32,32	0
33	MG	0	8004	1/1	0.99	0.05	-4.74	27,27,27,27	0
35	NA	0	8544	1/1	0.98	0.05	-4.77	32,32,32,32	0
33	MG	0	8008	1/1	0.99	0.07	-4.89	33,33,33,33	0
33	MG	0	8012	1/1	0.99	0.09	-5.12	34,34,34,34	0
33	MG	0	8032	1/1	0.99	0.05	-5.37	39,39,39,39	0
33	MG	0	8010	1/1	0.98	0.09	-5.38	37,37,37,37	0
33	MG	0	8101	1/1	0.95	0.09	-5.77	58,58,58,58	0
33	MG	0	8019	1/1	0.99	0.06	-6.01	37,37,37,37	0
33	MG	0	8053	1/1	0.96	0.07	-6.05	45,45,45,45	0
35	NA	0	8520	1/1	0.98	0.10	-6.35	37,37,37,37	0
35	NA	T	8543	1/1	0.97	0.08	-6.38	39,39,39,39	0
33	MG	0	8067	1/1	0.98	0.10	-6.39	49,49,49,49	0
33	MG	0	8107	1/1	0.93	0.06	-6.44	68,68,68,68	0
33	MG	0	8001	1/1	0.99	0.08	-6.71	33,33,33,33	0
33	MG	0	8077	1/1	0.98	0.09	-7.35	30,30,30,30	0
35	NA	0	8567	1/1	0.90	0.09	-7.93	50,50,50,50	0
33	MG	0	8007	1/1	0.98	0.07	-8.42	27,27,27,27	0
33	MG	0	8006	1/1	0.96	0.06	-8.74	38,38,38,38	0
33	MG	0	8014	1/1	0.97	0.06	-9.41	34,34,34,34	0
33	MG	0	8052	1/1	0.98	0.07	-10.30	58,58,58,58	0
33	MG	0	8071	1/1	0.97	0.06	-10.40	72,72,72,72	0
33	MG	0	8091	1/1	0.98	0.06	-10.57	59,59,59,59	0
33	MG	0	8109	1/1	0.99	0.09	-11.42	23,23,23,23	0
33	MG	0	8022	1/1	0.99	0.08	-12.36	41,41,41,41	0
33	MG	0	8035	1/1	0.97	0.03	-12.48	49,49,49,49	0
33	MG	Y	8108	1/1	0.97	0.07	-12.87	40,40,40,40	0
33	MG	0	8002	1/1	0.98	0.05	-13.79	33,33,33,33	0
33	MG	0	8079	1/1	0.99	0.11	-	30,30,30,30	0
33	MG	0	8089	1/1	0.98	0.13	-	56,56,56,56	0
33	MG	0	8072	1/1	0.98	0.08	-	56,56,56,56	0
36	CL	J	8802	1/1	0.96	0.09	-	63,63,63,63	0
33	MG	0	8039	1/1	0.99	0.05	-	50,50,50,50	0
33	MG	0	8048	1/1	0.96	0.10	-	71,71,71,71	0
35	NA	S	8512	1/1	0.95	0.22	-	22,22,22,22	0
33	MG	0	8066	1/1	0.92	0.16	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8026	1/1	0.99	0.10	-	29,29,29,29	0
35	NA	0	8536	1/1	0.99	0.08	-	47,47,47,47	0
33	MG	0	8050	1/1	0.89	0.09	-	71,71,71,71	0
35	NA	0	8530	1/1	0.98	0.18	-	49,49,49,49	0
36	CL	N	8807	1/1	0.94	0.15	-	63,63,63,63	0
33	MG	0	8061	1/1	0.97	0.10	-	40,40,40,40	0
35	NA	0	8534	1/1	0.96	0.06	-	44,44,44,44	0
35	NA	0	8575	1/1	0.99	0.23	-	50,50,50,50	0
33	MG	0	8082	1/1	0.90	0.16	-	64,64,64,64	0
35	NA	0	8560	1/1	0.95	0.50	-	50,50,50,50	0
33	MG	0	8009	1/1	1.00	0.07	-	33,33,33,33	0
33	MG	0	8047	1/1	0.93	0.19	-	77,77,77,77	0
35	NA	0	8508	1/1	0.93	0.21	-	68,68,68,68	0
35	NA	H	8522	1/1	0.95	0.16	-	56,56,56,56	0
33	MG	0	8036	1/1	0.99	0.07	-	35,35,35,35	0
35	NA	0	8528	1/1	0.98	0.44	-	49,49,49,49	0
33	MG	0	8112	1/1	0.84	0.18	-	47,47,47,47	0
33	MG	0	8113	1/1	0.94	0.08	-	51,51,51,51	0
33	MG	0	8093	1/1	0.94	0.08	-	48,48,48,48	0
33	MG	0	8043	1/1	0.90	0.06	-	49,49,49,49	0
33	MG	0	8024	1/1	0.97	0.08	-	23,23,23,23	0
33	MG	0	8100	1/1	0.95	0.09	-	69,69,69,69	0
33	MG	0	8040	1/1	0.97	0.12	-	61,61,61,61	0
36	CL	A	8809	1/1	0.99	0.18	-	66,66,66,66	0
33	MG	0	8110	1/1	0.97	0.07	-	41,41,41,41	0
33	MG	0	8085	1/1	0.87	0.10	-	50,50,50,50	0
33	MG	0	8037	1/1	1.00	0.04	-	45,45,45,45	0
35	NA	0	8558	1/1	0.86	0.74	-	102,102,102,102	0
33	MG	0	8099	1/1	0.90	0.18	-	55,55,55,55	0
33	MG	0	8115	1/1	0.94	0.09	-	55,55,55,55	0
33	MG	0	8051	1/1	0.95	0.08	-	71,71,71,71	0
33	MG	0	8116	1/1	0.99	0.07	-	37,37,37,37	0
33	MG	0	8049	1/1	0.84	0.20	-	74,74,74,74	0
37	CD	O	8705	1/1	0.98	0.09	-	74,74,74,74	0
33	MG	0	8092	1/1	0.85	0.46	-	83,83,83,83	0
33	MG	0	8097	1/1	0.97	0.10	-	36,36,36,36	0
33	MG	0	8104	1/1	0.91	0.12	-	53,53,53,53	0
35	NA	0	8563	1/1	0.85	0.31	-	63,63,63,63	0
35	NA	0	8554	1/1	0.99	0.17	-	41,41,41,41	0
35	NA	0	8542	1/1	0.85	0.25	-	52,52,52,52	0
33	MG	0	8063	1/1	0.96	0.10	-	68,68,68,68	0
33	MG	0	8025	1/1	0.96	0.08	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8516	1/1	0.94	0.31	-	51,51,51,51	0
33	MG	0	8090	1/1	0.94	0.24	-	60,60,60,60	0
35	NA	0	8581	1/1	0.85	0.19	-	51,51,51,51	0
33	MG	0	8083	1/1	0.97	0.06	-	41,41,41,41	0
35	NA	0	8541	1/1	0.90	0.14	-	53,53,53,53	0
33	MG	0	8005	1/1	0.99	0.10	-	30,30,30,30	0
33	MG	0	8030	1/1	0.99	0.12	-	29,29,29,29	0
33	MG	0	8114	1/1	0.91	0.13	-	55,55,55,55	0
33	MG	0	8045	1/1	0.94	0.13	-	60,60,60,60	0
35	NA	0	8585	1/1	0.90	0.39	-	53,53,53,53	0
33	MG	0	8075	1/1	0.96	0.06	-	44,44,44,44	0
33	MG	0	8029	1/1	0.99	0.12	-	49,49,49,49	0
36	CL	0	8822	1/1	0.94	0.48	-	83,83,83,83	0
36	CL	0	8803	1/1	0.95	0.14	-	59,59,59,59	0
33	MG	0	8062	1/1	0.95	0.09	-	66,66,66,66	0
35	NA	0	8555	1/1	0.95	0.40	-	72,72,72,72	0
35	NA	0	8513	1/1	0.93	0.12	-	54,54,54,54	0
33	MG	0	8023	1/1	0.99	0.08	-	39,39,39,39	0
35	NA	0	8559	1/1	0.91	0.28	-	64,64,64,64	0
35	NA	0	8584	1/1	0.82	0.17	-	54,54,54,54	0
35	NA	9	8551	1/1	0.79	0.27	-	39,39,39,39	0
33	MG	0	8081	1/1	0.96	0.10	-	53,53,53,53	0
35	NA	0	8552	1/1	0.89	0.39	-	57,57,57,57	0
35	NA	0	8570	1/1	0.89	0.36	-	63,63,63,63	0
33	MG	0	8102	1/1	0.95	0.11	-	55,55,55,55	0
35	NA	0	8579	1/1	0.94	0.17	-	58,58,58,58	0
35	NA	0	8519	1/1	0.99	0.10	-	36,36,36,36	0
33	MG	0	8016	1/1	0.96	0.13	-	35,35,35,35	0
36	CL	0	8813	1/1	0.98	0.16	-	57,57,57,57	0
35	NA	0	8549	1/1	0.95	0.13	-	46,46,46,46	0
33	MG	K	8069	1/1	0.94	0.11	-	57,57,57,57	0
33	MG	0	8031	1/1	0.99	0.06	-	34,34,34,34	0
33	MG	0	8041	1/1	0.97	0.16	-	69,69,69,69	0
33	MG	0	8094	1/1	0.98	0.10	-	72,72,72,72	0
33	MG	0	8087	1/1	0.76	0.21	-	63,63,63,63	0
33	MG	2	8076	1/1	0.88	0.12	-	53,53,53,53	0
33	MG	0	8098	1/1	0.97	0.07	-	34,34,34,34	0
33	MG	0	8028	1/1	0.96	0.08	-	37,37,37,37	0
35	NA	0	8529	1/1	0.21	0.30	-	76,76,76,76	0
36	CL	0	8817	1/1	0.97	0.15	-	63,63,63,63	0
35	NA	0	8506	1/1	0.96	0.45	-	42,42,42,42	0
33	MG	0	8105	1/1	0.96	0.19	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8518	1/1	0.97	0.17	-	39,39,39,39	0
36	CL	J	8801	1/1	0.98	0.17	-	65,65,65,65	0
33	MG	0	8046	1/1	0.91	0.07	-	43,43,43,43	0
35	NA	0	8511	1/1	0.84	0.09	-	58,58,58,58	0
35	NA	0	8507	1/1	0.93	0.31	-	54,54,54,54	0
33	MG	0	8034	1/1	0.98	0.08	-	34,34,34,34	0
33	MG	0	8103	1/1	0.92	0.15	-	67,67,67,67	0
33	MG	0	8011	1/1	0.99	0.12	-	25,25,25,25	0
33	MG	0	8059	1/1	0.99	0.05	-	33,33,33,33	0
35	NA	0	8515	1/1	0.96	0.14	-	48,48,48,48	0
35	NA	0	8569	1/1	0.81	0.30	-	57,57,57,57	0
36	CL	0	8811	1/1	0.98	0.10	-	54,54,54,54	0
33	MG	9	8095	1/1	0.96	0.09	-	72,72,72,72	0
33	MG	0	8027	1/1	0.97	0.10	-	49,49,49,49	0
36	CL	Y	8820	1/1	0.96	0.09	-	46,46,46,46	0
35	NA	0	8557	1/1	0.91	0.08	-	60,60,60,60	0
33	MG	0	8042	1/1	0.96	0.13	-	40,40,40,40	0
33	MG	0	8068	1/1	0.95	0.09	-	68,68,68,68	0
36	CL	0	8814	1/1	0.98	0.08	-	48,48,48,48	0
35	NA	0	8501	1/1	0.98	0.20	-	35,35,35,35	0
36	CL	R	8806	1/1	0.96	0.09	-	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.