



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1KQS  
Title : The Haloarcula marismortui 50S Complexed with a Pretranslocational Intermediate in Protein Synthesis  
Authors : Schmeing, T.M.; Seila, A.C.; Hansen, J.L.; Freeborn, B.; Soukup, J.K.; Scaringe, S.A.; Strobel, S.A.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2002-01-07  
Resolution : 3.10 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

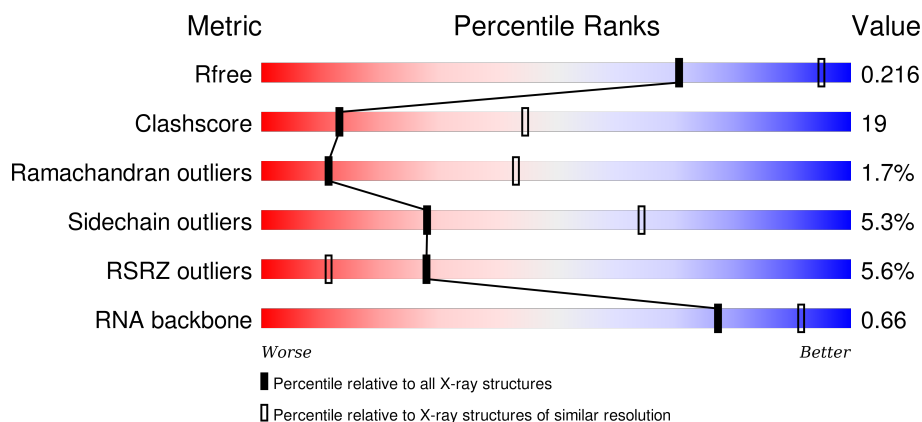
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div>57%</div> <div>32%</div> <div>5% • 6%</div> </div>
2	9	122	<div> <div>5%</div> <div>52%</div> <div>38%</div> <div>9% •</div> </div>
3	3	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
4	4	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	A	239	
6	B	337	
7	C	246	
8	D	176	
9	E	177	
10	F	119	
11	G	348	
12	H	167	
13	I	145	
14	J	132	
15	K	164	
16	L	194	
17	M	186	
18	N	115	
19	O	148	
20	P	95	
21	Q	154	
22	R	84	
23	S	119	
24	T	66	
25	U	70	
26	V	154	
27	W	91	
28	X	240	
29	Y	73	

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Mol	Chain	Length	Quality of chain
30	Z	56	
31	1	48	
32	2	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
33	MG	0	8053	-	-	-	X
33	MG	0	8064	-	-	-	X
33	MG	2	8078	-	-	-	X
33	MG	Y	8105	-	-	-	X
34	K	0	8201	-	-	-	X
34	K	0	8202	-	-	-	X
35	NA	0	8303	-	-	-	X
35	NA	0	8308	-	-	-	X
35	NA	0	8310	-	-	-	X
35	NA	0	8321	-	-	-	X
35	NA	0	8323	-	-	-	X
35	NA	0	8325	-	-	-	X
35	NA	0	8326	-	-	-	X
35	NA	0	8331	-	-	-	X
35	NA	0	8332	-	-	-	X
35	NA	0	8340	-	-	-	X
35	NA	0	8350	-	-	-	X
35	NA	0	8356	-	-	-	X
35	NA	0	8361	-	-	-	X
35	NA	0	8362	-	-	-	X
35	NA	0	8364	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8372	-	-	-	X
35	NA	0	8373	-	-	-	X
35	NA	0	8374	-	-	-	X
35	NA	0	8376	-	-	-	X
35	NA	0	8379	-	-	-	X
35	NA	0	8381	-	-	-	X
35	NA	0	8382	-	-	-	X
35	NA	9	8383	-	-	-	X
35	NA	Q	8386	-	-	-	X
36	CL	0	8505	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CL	0	8515	-	-	-	X
36	CL	2	8504	-	-	-	X
36	CL	B	8519	-	-	-	X
36	CL	N	8508	-	-	-	X
39	ACA	4	78	-	-	-	X
40	BTN	4	79	-	-	-	X
41	CD	2	8404	-	-	-	X
41	CD	T	8401	-	-	-	X
41	CD	Y	8403	-	-	-	X

## 2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 98688 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	? 3377779

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

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

- Molecule 3 is a RNA chain called CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a RNA chain called CC-Pmn-pcb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	DELETION	UNP P20279
B	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	K	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	M	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	N	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	O	143	Total	C	N	O	0	0	0
			1133	680	230	223			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	P	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	S	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	V	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Y	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	DELETION	UNP P22452

- Molecule 32 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	110	Total	Mg	0	0
			110	110		
33	J	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	X	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		
33	S	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	73	Total	Na	0	0
			73	73		
35	P	1	Total	Na	0	0
			1	1		
35	Q	3	Total	Na	0	0
			3	3		

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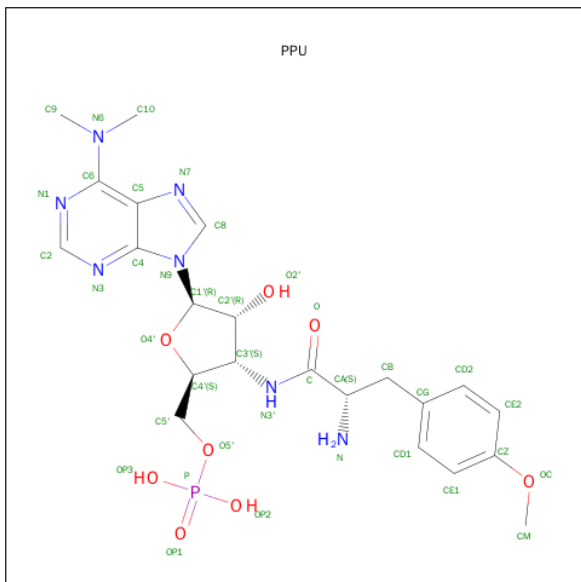
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	I	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	A	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0

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

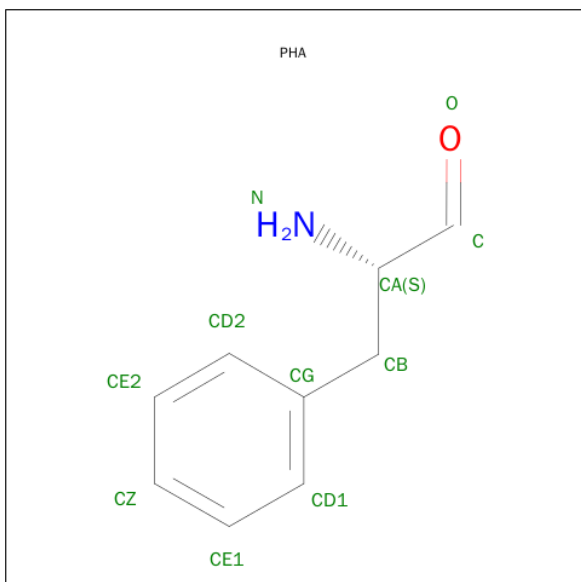
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	Q	1	Total 1	Cl 1	0	0
36	K	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	I	3	Total 3	Cl 3	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula:  $C_{22}H_{30}N_7O_8P$ ).



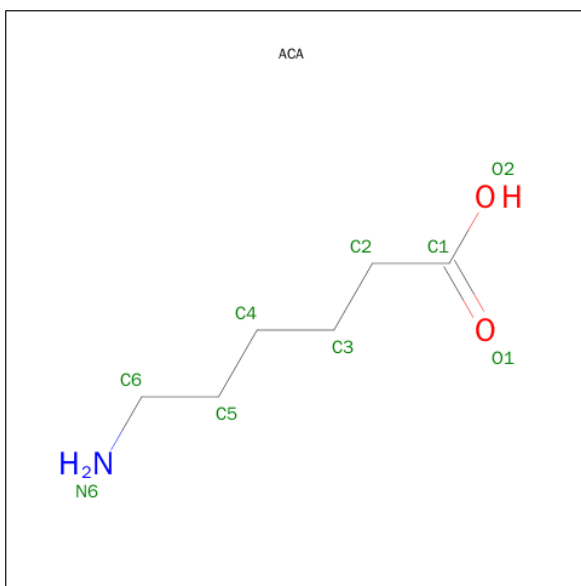
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	4	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 38 is PHENYLALANINAL (three-letter code: PHA) (formula:  $C_9H_{11}NO$ ).



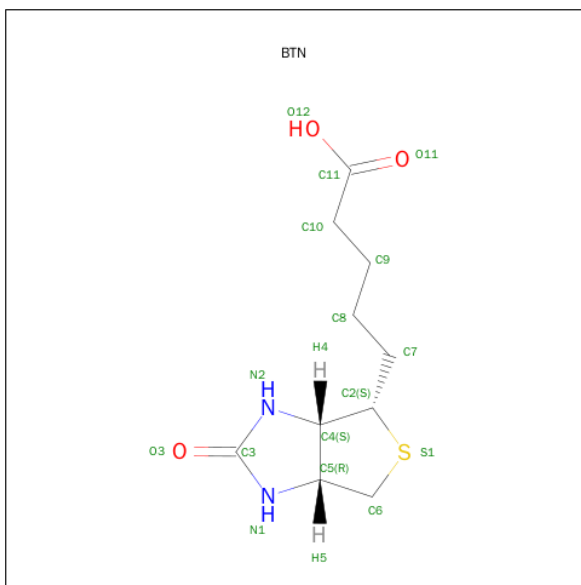
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 39 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
39	4	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 40 is BIOTIN (three-letter code: BTN) (formula:  $C_{10}H_{16}N_2O_3S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	Z	1	Total Cd 1 1	0	0
41	Y	1	Total Cd 1 1	0	0
41	T	1	Total Cd 1 1	0	0
41	2	1	Total Cd 1 1	0	0
41	N	1	Total Cd 1 1	0	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	0	5873	Total O 5873 5873	0	0
42	9	140	Total O 140 140	0	0
42	3	4	Total O 4 4	0	0
42	4	4	Total O 4 4	0	0
42	A	132	Total O 132 132	0	0
42	B	143	Total O 143 143	0	0
42	C	176	Total O 176 176	0	0
42	D	51	Total O 51 51	0	0
42	E	44	Total O 44 44	0	0
42	F	29	Total O 29 29	0	0
42	G	22	Total O 22 22	0	0
42	H	78	Total O 78 78	0	0
42	I	57	Total O 57 57	0	0
42	J	61	Total O 61 61	0	0
42	K	84	Total O 84 84	0	0

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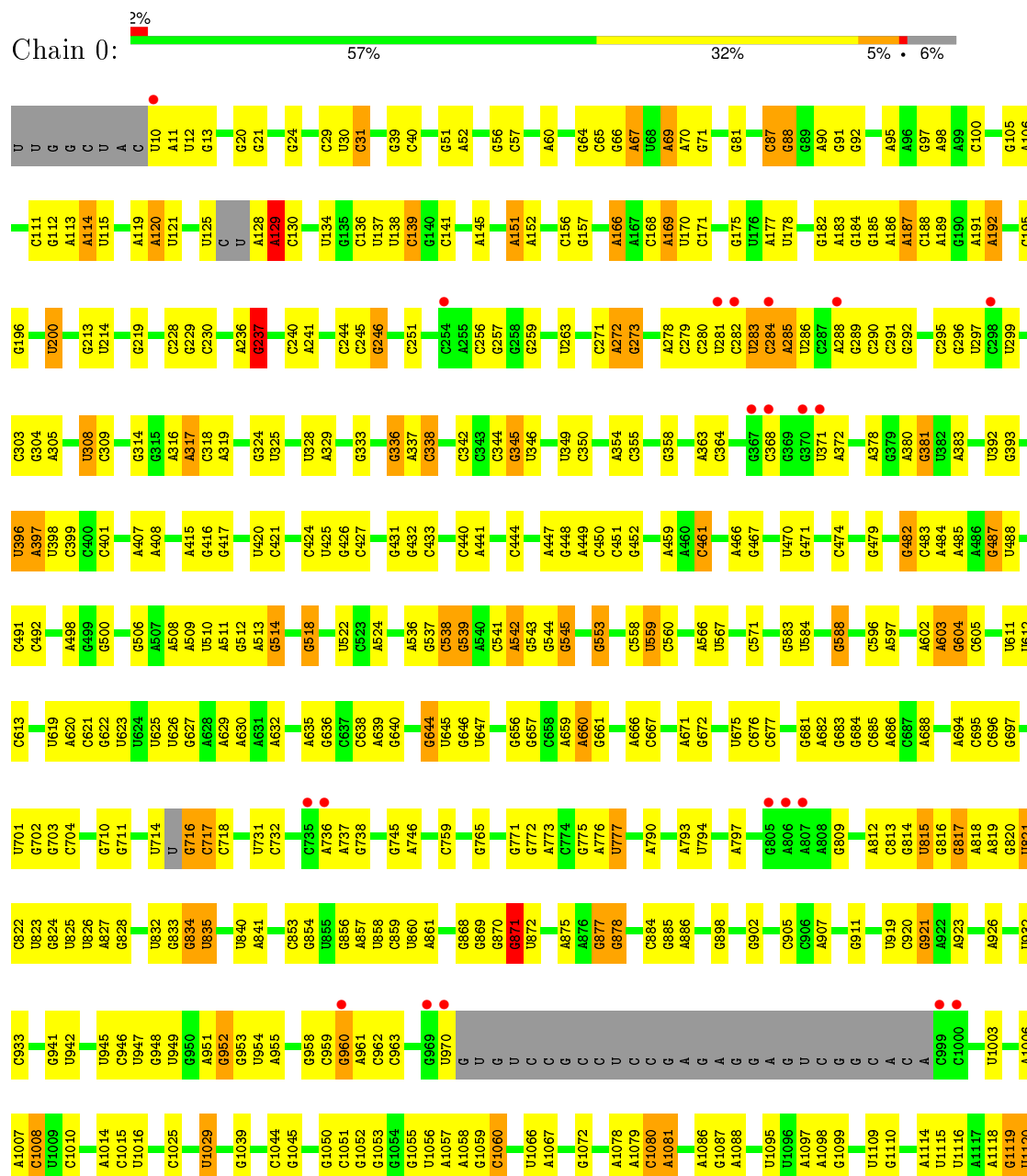
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	L	138	Total 138	O 138	0	0
42	M	70	Total 70	O 70	0	0
42	N	42	Total 42	O 42	0	0
42	O	67	Total 67	O 67	0	0
42	P	56	Total 56	O 56	0	0
42	Q	87	Total 87	O 87	0	0
42	R	36	Total 36	O 36	0	0
42	S	37	Total 37	O 37	0	0
42	T	26	Total 26	O 26	0	0
42	U	16	Total 16	O 16	0	0
42	V	66	Total 66	O 66	0	0
42	W	30	Total 30	O 30	0	0
42	X	96	Total 96	O 96	0	0
42	Y	33	Total 33	O 33	0	0
42	Z	55	Total 55	O 55	0	0
42	1	42	Total 42	O 42	0	0
42	2	76	Total 76	O 76	0	0

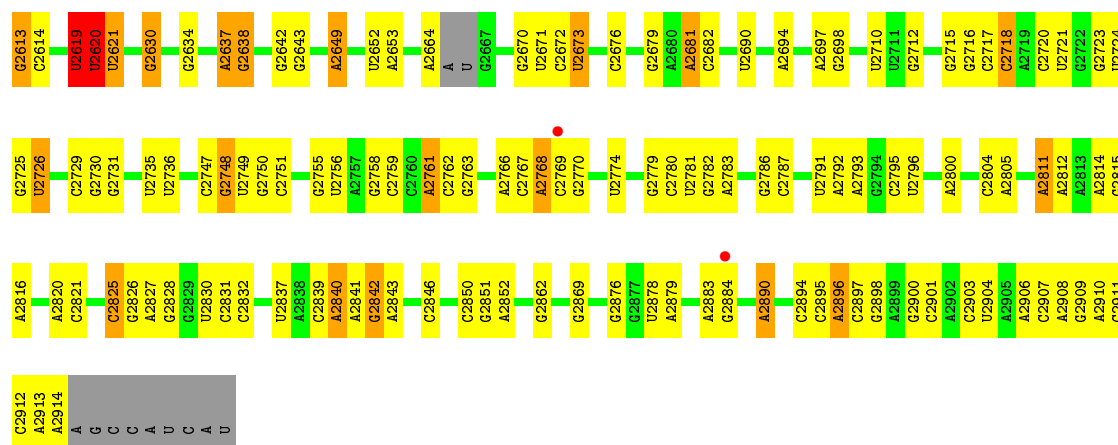
### 3 Residue-property plots

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.

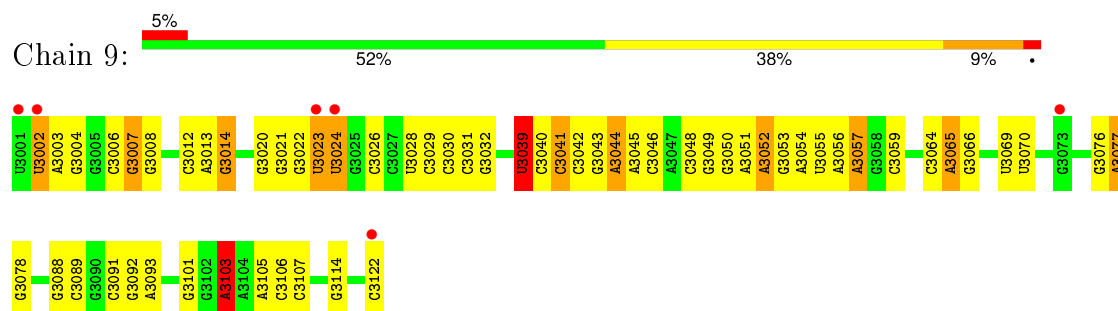
#### • Molecule 1: 23S rRNA



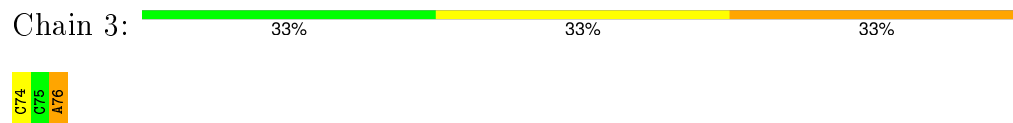
A2511	C2431	G2336	C2241	G2113	G2009	A1904	A1767	G1666	U	G1441	G1316	U1206	G1121
A2524	C2432	G2338	U2242	C2114	A2010	A1909	C1768	A1667	U1561	G1442	G1316	A1207	U1122
C2526	A2433	A	C2247	U2115	A2011	A1910	C1769	U1668	G1562	A1563	G1325	C1209	A1123
U2527	U2435	A	G2248	U2116	U2012	G1911	U1770	U1669	C1564	C1450	G1325	G1210	U1130
A2437	U2436	G	G2249	C2119	G2013	A1912	U1771	G1670	G1568	C1451	A1328	G1211	U1131
A2438	A	A	G2250	U2120	A2015	G1913	G1772	U1677	U1569	G1460	A1329	C1212	A1132
C2439	G2344	G	G2251	U2121	U2016	A1919	A1778	A1678	A1572	U1461	A1330	C1213	A1133
C2440	A2345	C	A2252	G2122	A2019	A1923	A1779	C1679	A1572	C1462	A1331	G1214	G1134
C2441	C2346	C	G2253	A2123	A2019	G1923	A1783	G1680	A1573	A1463	A1332	G1215	G1135
G2443	G2349	C	G2256	U2128	G2033	A1924	U1784	A1682	A1580	U1464	A1334	G1216	G1137
U2444	G2257	A	G2257	U2129	U2034	G1925	U1784	A1682	A1580	G1224	G1340	G1224	G1151
U2445	A2353	G	A2258	U2133	A2039	A1930	C1787	G1683	G1588	A1470	G1340	C1225	G1151
U2446	A2354	C	U2265	G2134	A1931	A1931	U1788	A1684	G1589	A1471	A1341	C1229	G1158
G2453	G2355	G	A2266	A2135	G2044	C1940	U1788	A1685	G1592	C1472	C1342	G1238	G1159
C2454	G2357	G	G2267	G2136	G2046	A1941	C1798	C1686	G1593	U1473	C1343	U1234	G1160
U2457	U2358	C	C2268	A	C2047	A1941	C1798	C1687	C1593	C1474	A1344	G1235	A1161
U2458	G2359	C	C2269	A	C2047	A1942	A1804	C1692	C1594	C1477	A1345	A1236	G1162
G2459	C2360	A	G2270	G	G2050	C1943	G1805	C1699	C1595	U1478	U1346	U1237	G1163
A2460	A2361	C	G2271	C	G2050	G1948	G1806	C1700	U1596	C1483	A1352	G1238	G1164
G2461	G2363	C	C2272	U	A2054	G1948	C1810	C1701	A1597	C1484	C1353	G1239	G1165
G2462	A2364	G	A2273	G	A2054	G1948	C1810	U1702	A1598	A1485	G1353	A1242	A1166
A2463	G2365	A	G2274	U	U2064	G1981	A1815	U1710	A1603	G1477	C1360	G1243	G1167
C2464	U2276	G	G2275	C	U2064	G1981	C1816	A1710	A1604	A1494	C1366	U1244	C1168
A2465	U2277	C	U2277	G	G2068	A	U1817	A1711	G1605	C1495	C1366	U1244	C1169
A2466	A2369	C	C2281	C	G2072	C	C1818	A1712	C1609	C1496	A1372	A1246	U1170
A2467	A2372	A	U2282	C	G2073	C	G1819	A1717	G1497	G1497	A1372	U1249	G1172
A2468	U2373	A	U2282	C	A2074	U	G1820	U1717	G1610	U1499	C1377	C1250	A1173
A2469	G2379	G	G2285	G	U2078	G	G1828	U1722	C1613	U1500	C1378	C1251	G1175
C2472	A2380	U	A2291	U	G2079	A	A1829	G1723	G1614	U1503	U1380	A1252	C1176
A2474	C2381	G	A2300	G	G2080	C	C1830	U1724	A1615	U1504	C1380	C1253	A1177
C2475	A2382	A	A2301	A	A2081	C	C1834	C1725	A1616	U1505	C1384	U1266	U1180
C2476	A2401	A	A2302	C	C2084	U1984	U1835	G1730	C1617	U1506	G1385	C1267	A1181
C2477	A2402	U	A2302	C	A2085	A1969	A1840	C1731	A1624	A1515	U1388	C1268	C1182
A2478	C2403	C	U2308	U	A2085	G1970	A1840	A1732	U1625	C1516	U1389	C1269	C1183
G2480	A2408	C	C2309	C	C2088	G1971	C1856	C1734	A1626	C1517	A1390	C1273	C1184
A2483	C2409	A	G2310	G	A2089	A1972	G1868	C1735	G1627	G1523	A1391	U1279	U1185
A2488	G2412	C	A2311	C	G2090	G1974	U1874	A1736	C1633	G1523	A1392	A1287	C1186
A2489	A2413	C	G2312	C	G2093	A1978	U1878	U1741	G1634	U1524	A1393	A1288	A1187
A2490	G2414	G	C2313	G	G2093	G1979	A1878	A1742	U1635	G1525	C1394	A1289	A1188
A2490	A2415	U	G2315	G	G2094	G1979	U1879	G1743	G1636	A1526	A1398	C1289	G1190
C2493	G2418	C	G2316	A	A2095	U1980	U1879	G1743	A1637	A1528	A1399	A1298	A1192
C2502	U2419	G	C2317	A	A2096	U1982	C1880	G1751	A1641	G1529	A1407	U1298	A1193
G2503	G2420	U	U2320	C	G2099	C1982	C1881	G1752	A1642	G1535	A1407	G1299	G1197
A2504	G2421	G	A2321	C	A2100	C1983	C1882	C1753	G1535	C1536	U1419	U1304	U1198
G2505	U2422	A	C2324	C	A2101	G1994	G1883	A1759	U1654	C1545	U1422	C1305	A1199
A2506	G2426	C	G2325	U	G2102	G1995	G1884	G1760	G1655	C1546	C1423	A1306	A1200
G2507	C2427	U	U2326	A	A2103	U1996	A1885	U1761	G1656	G1567	U1435	A1307	C1201
C2508	G2428	C	C2329	C	G2110	U2004	U1887	C1762	A1657	G1567	A1436	A1308	A1202
A2510	A2430	C	U2330	A	G2111	G2005	G1902	C1763	A1658	U1435	A1436	G1311	G1203
		G	G2237	A	A2112	U2008	U1903	U1766	C1660	A1559		G1312	U1205



### • Molecule 2: 5S RRNA



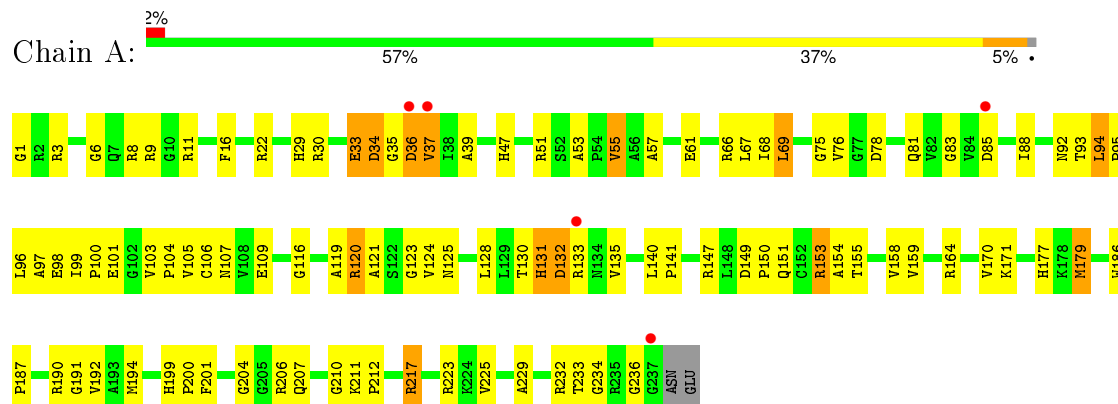
### • Molecule 3: CCA



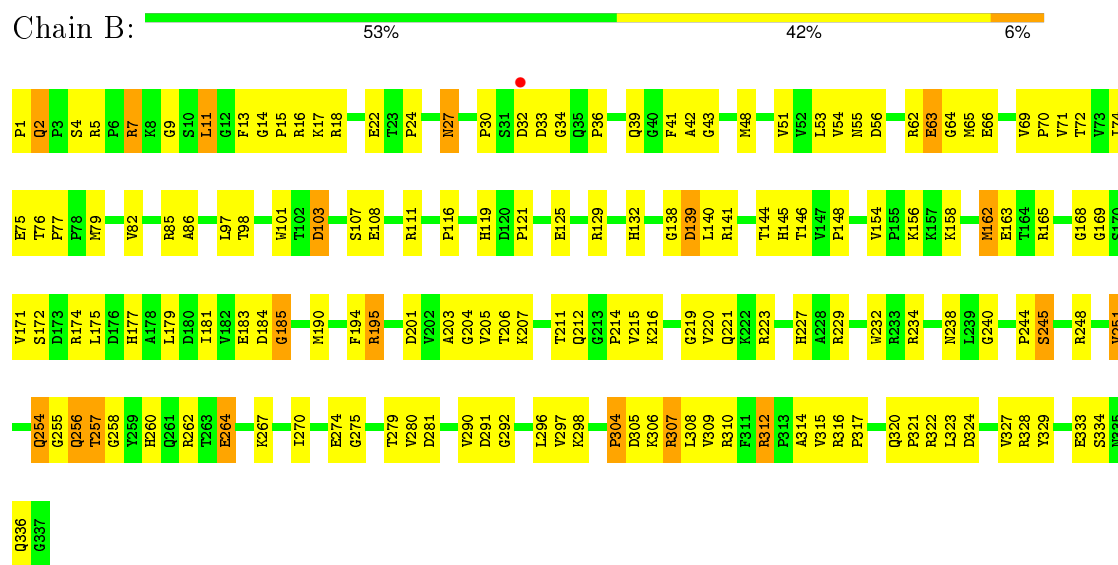
### • Molecule 4: CC-Pmn-pcb



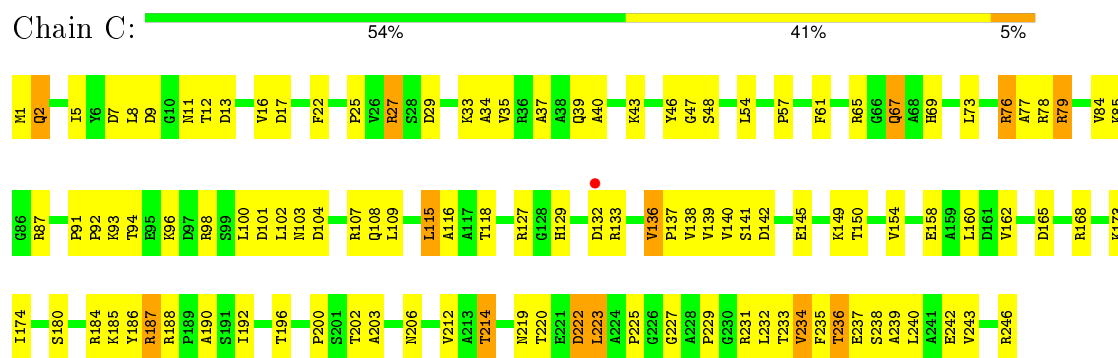
### • Molecule 5: RIBOSOMAL PROTEIN L2



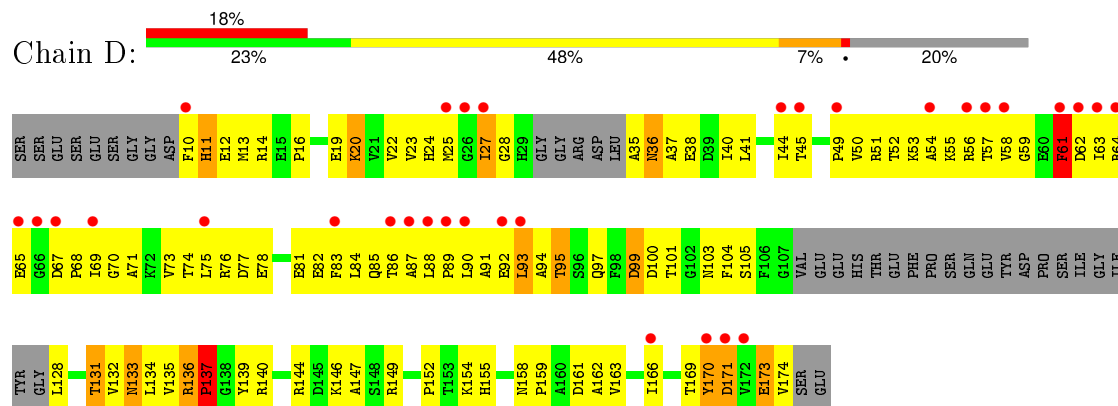
- Molecule 6: RIBOSOMAL PROTEIN L3



- Molecule 7: RIBOSOMAL PROTEIN L4

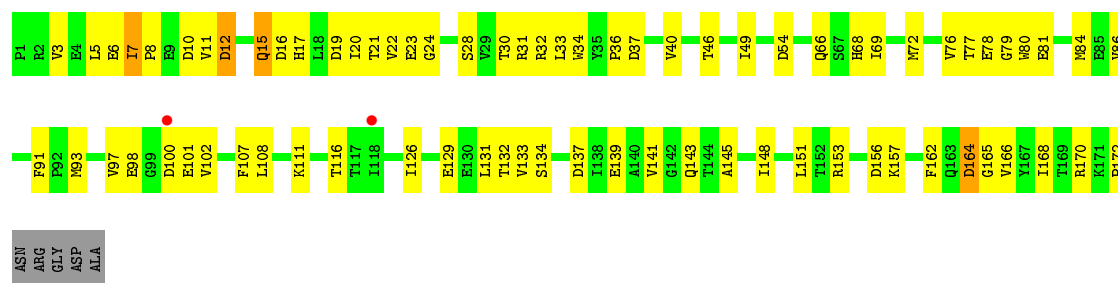


- Molecule 8: RIBOSOMAL PROTEIN L5

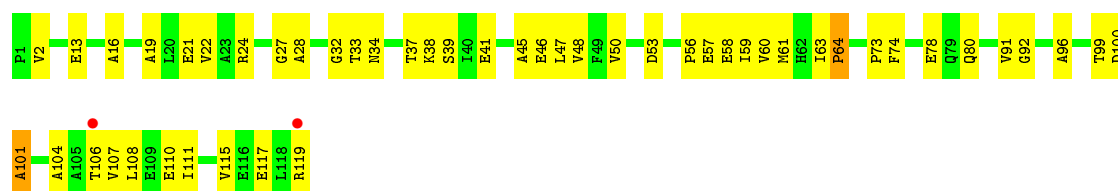


- Molecule 9: RIBOSOMAL PROTEIN L6

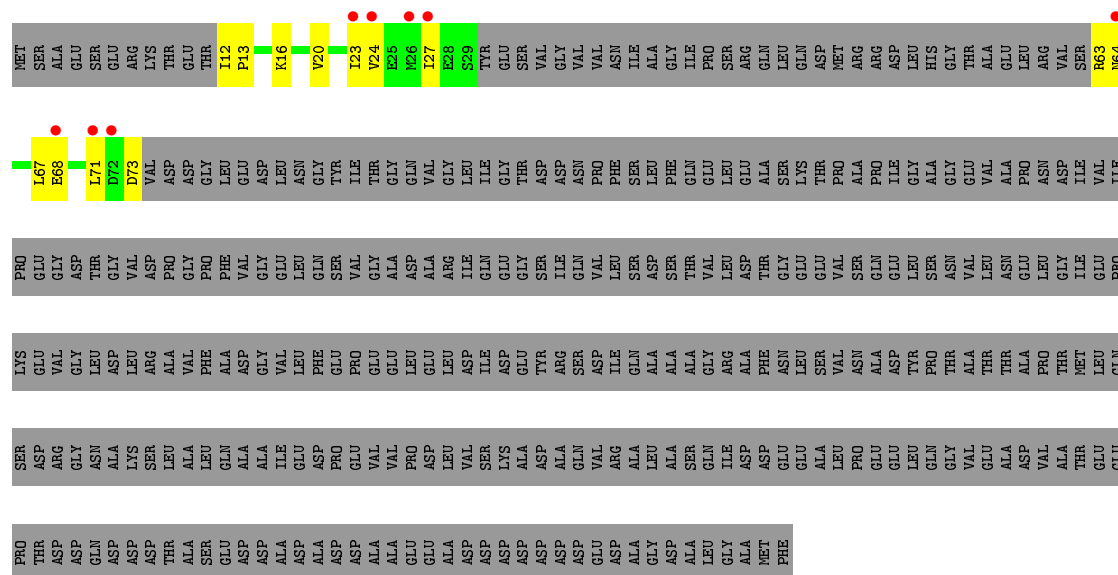




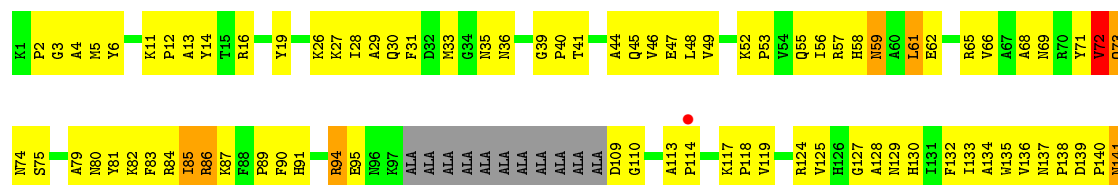
• Molecule 10: RIBOSOMAL PROTEIN L7AE

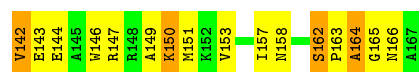


• Molecule 11: RIBOSOMAL PROTEIN L10



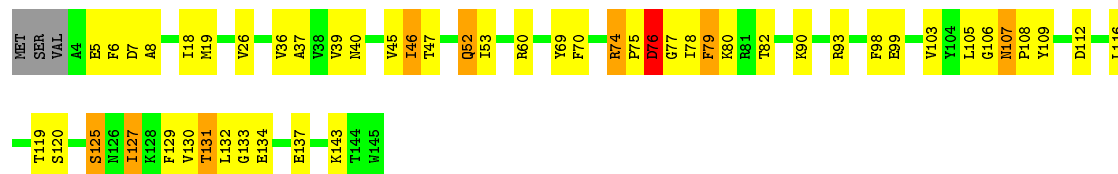
• Molecule 12: RIBOSOMAL PROTEIN L10E





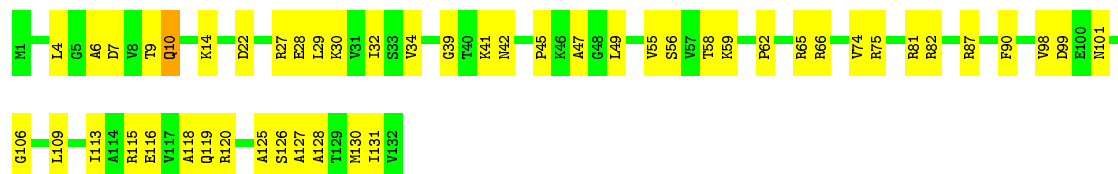
• Molecule 13: RIBOSOMAL PROTEIN L13

Chain I: 63% 29% 6% ••



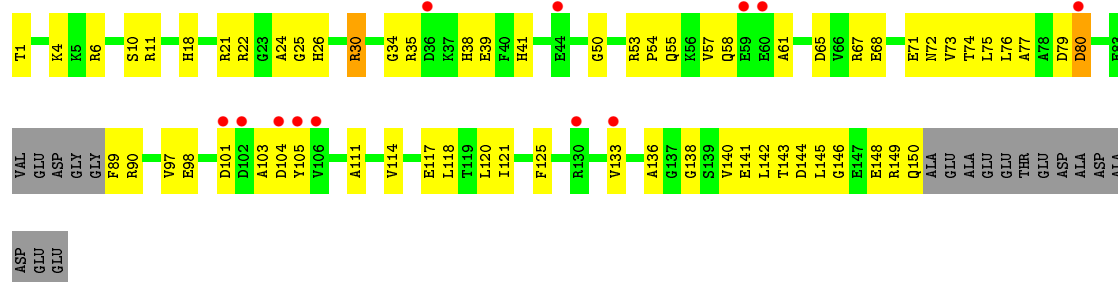
• Molecule 14: RIBOSOMAL PROTEIN L14

Chain J: 63% 36% •



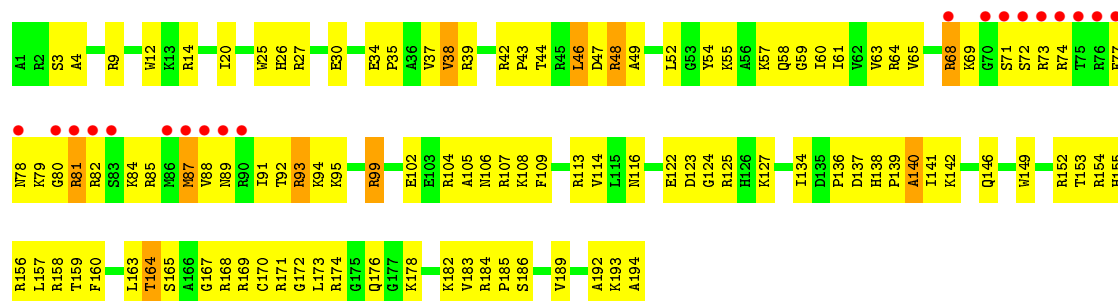
• Molecule 15: RIBOSOMAL PROTEIN L15

Chain K: 7% 49% 38% 12% •

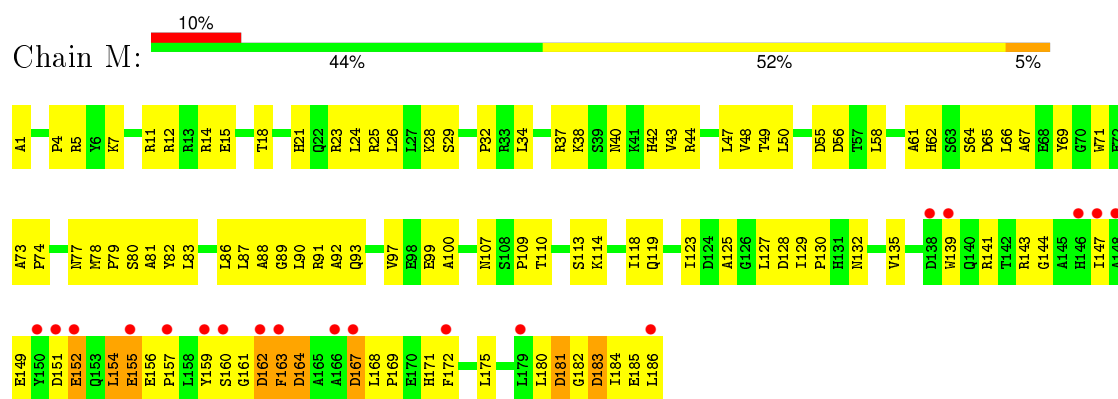


• Molecule 16: RIBOSOMAL PROTEIN L15E

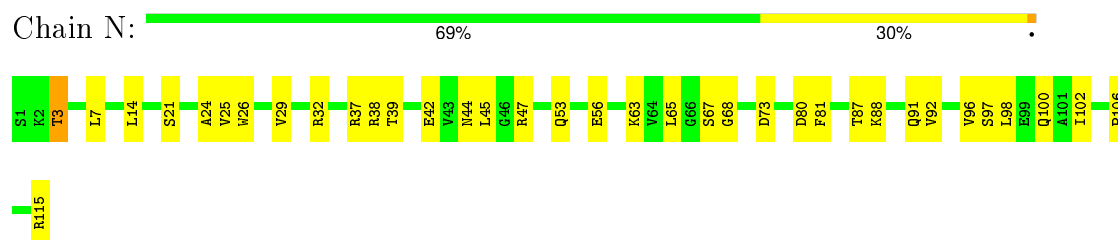
Chain L: 10% 42% 53% 5% •



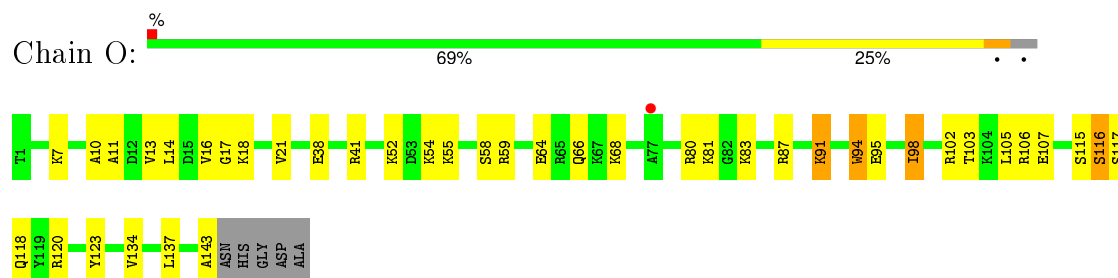
• Molecule 17: RIBOSOMAL PROTEIN L18



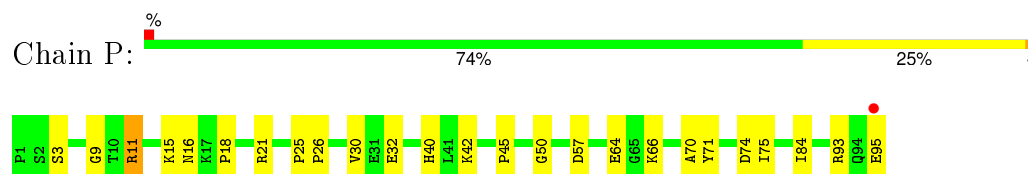
• Molecule 18: RIBOSOMAL PROTEIN L18E



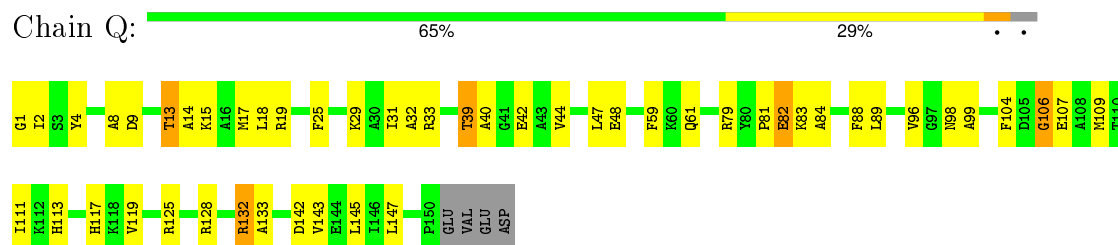
• Molecule 19: RIBOSOMAL PROTEIN L19E



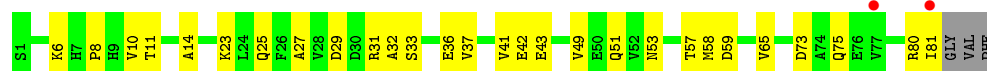
• Molecule 20: RIBOSOMAL PROTEIN L21E



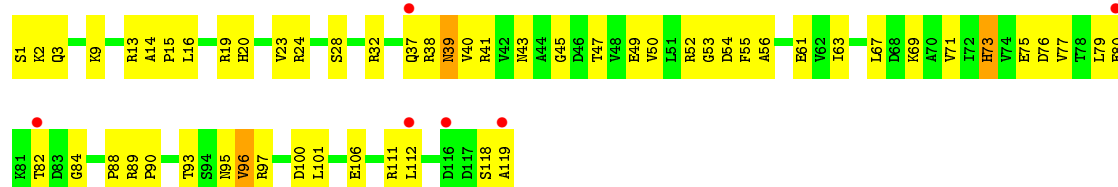
• Molecule 21: RIBOSOMAL PROTEIN L22



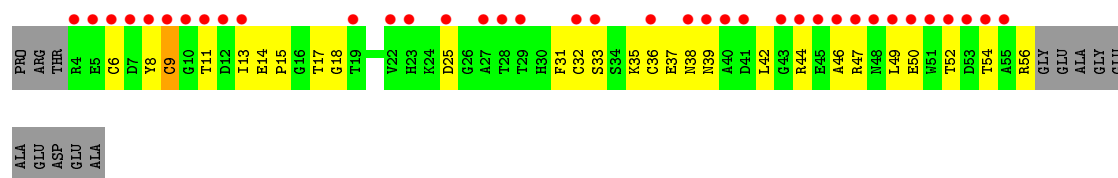
• Molecule 22: RIBOSOMAL PROTEIN L23



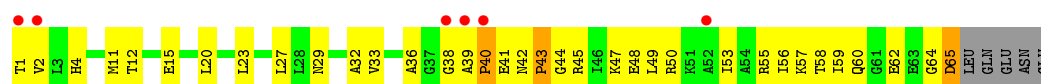
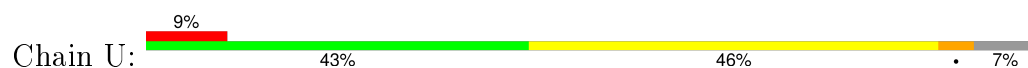
• Molecule 23: RIBOSOMAL PROTEIN L24



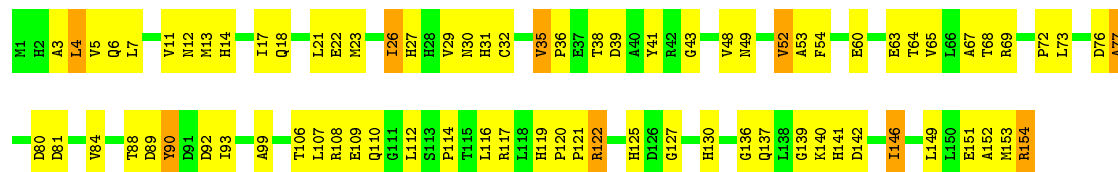
• Molecule 24: RIBOSOMAL PROTEIN L24E



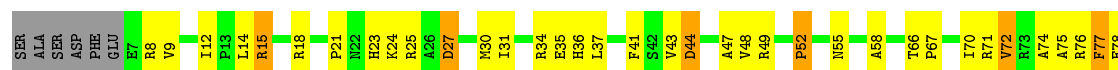
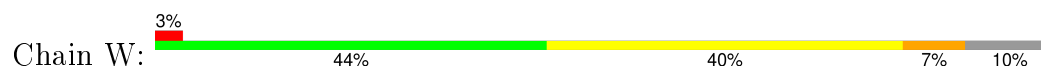
• Molecule 25: RIBOSOMAL PROTEIN L29



• Molecule 26: RIBOSOMAL PROTEIN L30

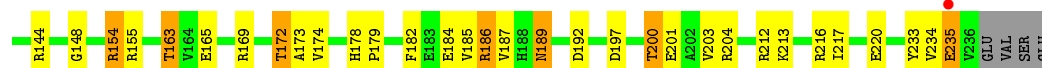
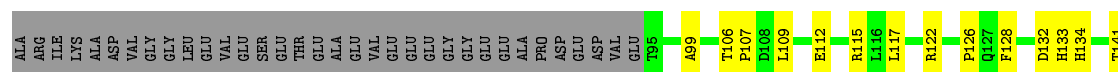


• Molecule 27: RIBOSOMAL PROTEIN L31E

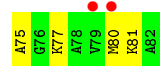
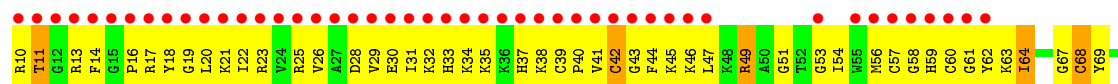




• Molecule 28: RIBOSOMAL PROTEIN L32E



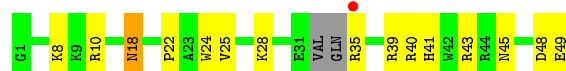
• Molecule 29: RIBOSOMAL PROTEIN L37Ae



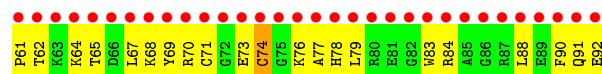
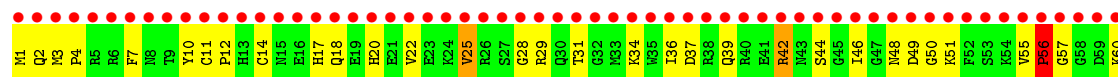
• Molecule 30: RIBOSOMAL PROTEIN L37E



• Molecule 31: RIBOSOMAL PROTEIN L39E



• Molecule 32: RIBOSOMAL PROTEIN L44E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.78 Å   300.35 Å   574.96 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.10 44.78 – 3.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 95.4 (44.78-3.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 3.06 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.173   ,   0.220 0.172   ,   0.216	Depositor DCC
$R_{free}$ test set	3206 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 340532 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	98688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, CL, NA, K, ACA, CD, PPU, BTN, PHA

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	0.41	2/66076 (0.0%)	0.70	27/103052 (0.0%)
2	9	0.39	0/2905	0.75	2/4528 (0.0%)
3	3	0.82	0/65	0.87	0/99
4	4	0.49	0/40	0.62	0/60
5	A	0.34	0/1787	0.66	0/2409
6	B	0.35	0/2689	0.64	0/3652
7	C	0.39	0/1883	0.64	0/2551
8	D	0.32	0/1111	0.59	0/1498
9	E	0.34	0/1382	0.58	0/1880
10	F	0.33	0/896	0.56	0/1219
11	G	0.29	0/241	0.48	0/324
12	H	0.39	0/1246	0.76	2/1686 (0.1%)
13	I	0.38	0/1135	0.62	0/1530
14	J	0.35	0/1003	0.66	0/1351
15	K	0.34	0/1126	0.65	0/1504
16	L	0.41	0/1633	0.71	0/2180
17	M	0.29	0/1473	0.63	0/1999
18	N	0.35	0/873	0.62	0/1181
19	O	0.35	0/1143	0.54	0/1521
20	P	0.36	0/748	0.66	0/1005
21	Q	0.37	0/1172	0.66	0/1578
22	R	0.34	0/648	0.58	0/875
23	S	0.34	0/957	0.64	0/1289
24	T	0.34	0/417	0.56	0/562
25	U	0.30	0/502	0.57	0/675
26	V	0.37	0/1218	0.64	0/1655
27	W	0.35	0/664	0.61	0/895
28	X	0.38	0/1146	0.65	0/1536
29	Y	0.34	0/575	0.66	0/763
30	Z	0.41	0/437	0.64	0/578
31	1	0.32	0/398	0.54	0/527
32	2	0.39	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.40	2/98360 (0.0%)	0.69	31/147186 (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	37
2	9	0	1
26	V	0	1
All	All	1	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	U	O5'-C5'	-7.09	1.31	1.42
1	0	2620	U	C2'-O2'	6.66	1.50	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1164	U	OP1-P-O3'	-12.07	78.64	105.20
1	0	1164	U	OP2-P-O3'	-10.75	81.56	105.20
1	0	1165	G	O5'-P-OP2	9.72	122.36	110.70
1	0	1563	G	C2'-C3'-O3'	9.36	130.09	109.50
1	0	2619	U	C5'-C4'-C3'	-9.23	101.24	116.00
1	0	1979	G	C2'-C3'-O3'	8.86	128.98	109.50
1	0	2620	U	O5'-P-OP2	-8.34	98.20	105.70
1	0	1942	A	C5'-C4'-C3'	8.11	128.97	116.00
2	9	3103	A	C5'-C4'-O4'	7.78	118.43	109.10
2	9	3039	U	N1-C1'-C2'	6.68	122.69	114.00
1	0	1504	A	C1'-O4'-C4'	-6.47	104.72	109.90
1	0	871	G	C5'-C4'-O4'	-6.38	101.44	109.10
1	0	1120	U	C5'-C4'-C3'	-6.36	105.82	116.00
1	0	2620	U	C4'-C3'-O3'	-6.12	96.56	109.40
1	0	2313	C	C5'-C4'-O4'	6.09	116.41	109.10
1	0	2620	U	O4'-C4'-C3'	6.00	110.90	106.10
12	H	74	ASN	N-CA-C	-5.87	95.15	111.00
1	0	1819	G	C5'-C4'-C3'	5.79	125.26	116.00
1	0	2726	U	N1-C1'-C2'	5.73	121.45	114.00
1	0	2620	U	C5'-C4'-C3'	-5.72	106.84	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2619	U	C5'-C4'-O4'	5.49	115.69	109.10
1	0	1504	A	N9-C1'-C2'	5.30	120.89	114.00
12	H	141	ASN	N-CA-C	-5.22	96.91	111.00
1	0	1592	G	N9-C1'-C2'	5.20	120.77	114.00
1	0	129	A	C2'-C3'-O3'	5.19	122.01	113.70
1	0	1829	A	N9-C1'-C2'	-5.14	106.35	112.00
1	0	2313	C	C5'-C4'-C3'	5.13	124.21	116.00
1	0	237	G	N9-C1'-C2'	-5.10	106.39	112.00
1	0	841	A	C1'-O4'-C4'	-5.05	105.86	109.90
1	0	2313	C	C1'-O4'-C4'	-5.04	105.87	109.90
1	0	1819	G	C4'-C3'-C2'	-5.00	97.59	102.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1342	C	Sidechain
1	0	1524	U	Sidechain
1	0	1614	G	Sidechain
1	0	1653	A	Sidechain
1	0	171	C	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	2308	U	Sidechain
1	0	246	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	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2619	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2673	U	Sidechain
1	0	2774	U	Sidechain
1	0	2793	A	Sidechain
1	0	2811	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	393	G	Sidechain
1	0	396	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
26	V	90	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29805	983	0
2	9	2600	0	1326	68	0
3	3	59	0	35	4	0
4	4	37	0	23	5	0
5	A	1754	0	1763	130	0
6	B	2624	0	2533	167	0
7	C	1858	0	1816	130	0
8	D	1094	0	1085	133	0
9	E	1357	0	1266	78	0
10	F	885	0	854	63	0
11	G	240	0	231	20	0
12	H	1215	0	1215	162	0
13	I	1119	0	1098	64	0
14	J	993	0	1027	58	0
15	K	1114	0	1072	64	0
16	L	1605	0	1676	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	1444	0	1401	139	0
18	N	864	0	873	33	0
19	O	1133	0	1127	43	0
20	P	734	0	729	23	0
21	Q	1149	0	1122	57	0
22	R	641	0	605	26	0
23	S	949	0	923	53	0
24	T	410	0	366	35	0
25	U	499	0	511	34	0
26	V	1195	0	1137	104	0
27	W	654	0	653	51	0
28	X	1130	0	1133	57	0
29	Y	563	0	601	72	0
30	Z	430	0	426	24	0
31	1	393	0	406	18	0
32	2	755	0	731	63	0
33	0	110	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	3	0	0	0	0
35	R	1	0	0	0	0
36	0	10	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	4	37	0	26	2	0
38	4	11	0	8	1	0
39	4	8	0	10	0	0
40	4	15	0	15	2	0
41	2	1	0	0	0	0
41	N	1	0	0	0	0
41	T	1	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	0	0
42	0	5873	0	0	207	0
42	1	42	0	0	3	0
42	2	76	0	0	7	0
42	3	4	0	0	3	0
42	4	4	0	0	0	0
42	9	140	0	0	11	0
42	A	132	0	0	16	0
42	B	143	0	0	23	0
42	C	176	0	0	35	0
42	D	51	0	0	19	0
42	E	44	0	0	10	0
42	F	29	0	0	12	0
42	G	22	0	0	5	0
42	H	78	0	0	22	0
42	I	57	0	0	4	0
42	J	61	0	0	9	0
42	K	84	0	0	19	0
42	L	138	0	0	22	0
42	M	70	0	0	15	0
42	N	42	0	0	7	0
42	O	67	0	0	6	0
42	P	56	0	0	3	0
42	Q	87	0	0	9	0
42	R	36	0	0	6	0
42	S	37	0	0	9	0
42	T	26	0	0	4	0
42	U	16	0	0	3	0
42	V	66	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	W	30	0	0	5	0
42	X	96	0	0	17	0
42	Y	33	0	0	12	0
42	Z	55	0	0	3	0
All	All	98688	0	59628	2828	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 19.

All (2828) 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)
12:H:86:ARG:NH1	12:H:133:ILE:HG13	1.61	1.16
25:U:12:THR:HG22	25:U:15:GLU:HG3	1.34	1.09
7:C:236:THR:HG22	7:C:239:ALA:H	0.97	1.07
1:O:156:C:H5''	16:L:171:ARG:HD3	1.38	1.05
12:H:45:GLN:HB3	12:H:163:PRO:HD2	1.40	1.04
17:M:47:LEU:HD11	17:M:127:LEU:HD21	1.40	1.02
16:L:87:MET:HG2	32:2:46:ILE:HG21	1.40	1.02
1:O:871:G:H8	1:O:871:G:H5'	1.21	1.02
1:O:871:G:C8	1:O:871:G:H5'	1.95	1.01
1:O:1134:G:H4'	12:H:151:MET:HE1	1.42	1.01
12:H:86:ARG:HH11	12:H:133:ILE:CG1	1.74	1.00
14:J:10:GLN:NE2	14:J:10:GLN:H	1.60	1.00
29:Y:46:LYS:HD3	29:Y:59:HIS:HB2	1.41	1.00
7:C:5:ILE:HD11	7:C:16:VAL:HG23	1.43	0.99
23:S:71:VAL:HG11	23:S:90:PRO:HB3	1.39	0.99
12:H:165:GLY:HA3	42:H:8399:HOH:O	1.61	0.99
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	0.99
8:D:25:MET:HE2	8:D:41:LEU:HG	1.44	0.98
1:O:870:G:H2'	1:O:871:G:H5''	1.42	0.98
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.44	0.98
2:9:3056:A:H2'	2:9:3057:A:H5''	1.45	0.98
16:L:52:LEU:HD11	42:L:8618:HOH:O	1.61	0.98
5:A:211:LYS:HB3	5:A:212:PRO:HD2	1.44	0.98
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.45	0.97
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.45	0.97
7:C:2:GLN:HB3	42:C:8337:HOH:O	1.62	0.96
27:W:37:LEU:HD13	27:W:85:VAL:HG21	1.47	0.96
1:O:1751:G:H2'	1:O:1752:G:H5''	1.47	0.95
1:O:1242:A:H5'	13:I:82:THR:HG23	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:10:GLN:H	14:J:10:GLN:HE21	0.99	0.95
1:0:856:G:H2'	42:0:4905:HOH:O	1.67	0.95
1:0:960:G:H4'	42:0:6897:HOH:O	1.66	0.95
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.81	0.95
28:X:200:THR:HG22	28:X:201:GLU:HG3	1.47	0.94
7:C:236:THR:HG22	7:C:239:ALA:N	1.82	0.94
1:0:2717:C:H2'	1:0:2718:C:H5''	1.49	0.94
6:B:238:ASN:HD22	6:B:240:GLY:H	1.09	0.94
2:9:3006:C:H5''	17:M:37:ARG:NH1	1.81	0.94
31:1:41:HIS:H	31:1:45:ASN:HD22	1.14	0.94
6:B:86:ALA:HA	42:B:8579:HOH:O	1.68	0.94
12:H:27:LYS:H	12:H:58:HIS:HD2	1.13	0.93
32:2:70:ARG:HG2	32:2:77:ALA:HB2	1.51	0.93
12:H:29:ALA:HB3	12:H:65:ARG:HH12	1.33	0.93
1:0:21:G:H5'	21:Q:2:ILE:HA	1.50	0.93
19:O:115:SER:H	19:O:118:GLN:HE21	1.00	0.93
8:D:105:SER:HB2	8:D:131:THR:HG23	1.50	0.93
21:Q:99:ALA:HB1	21:Q:109:MET:HE1	1.50	0.93
1:0:1166:A:H1'	1:0:1192:A:C2	2.03	0.93
1:0:2533:C:H6	1:0:2533:C:H5'	1.34	0.93
17:M:87:LEU:HD12	17:M:186:LEU:HD21	1.49	0.93
26:V:88:THR:HB	42:V:6679:HOH:O	1.69	0.92
42:0:4697:HOH:O	14:J:39:GLY:HA2	1.67	0.92
1:0:1835:U:H5	1:0:1840:A:N7	1.66	0.92
10:F:91:VAL:HG12	10:F:92:GLY:H	1.35	0.92
42:0:3938:HOH:O	16:L:146:GLN:HG2	1.69	0.91
12:H:55:GLN:HE21	12:H:124:ARG:HE	1.16	0.91
16:L:102:GLU:OE1	16:L:164:THR:HG21	1.69	0.91
14:J:81:ARG:HB2	14:J:87:ARG:HH11	1.35	0.90
2:9:3076:G:H3'	2:9:3077:A:H5''	1.54	0.90
1:0:545:G:H8	1:0:545:G:H5'	1.37	0.90
12:H:150:LYS:HB2	12:H:157:ILE:HD12	1.54	0.89
13:I:76:ASP:HA	42:I:5907:HOH:O	1.70	0.89
6:B:162:MET:HE3	6:B:308:LEU:HD21	1.54	0.89
16:L:106:ASN:ND2	36:L:8518:CL:CL	2.42	0.89
12:H:162:SER:HB2	12:H:163:PRO:HD3	1.52	0.89
12:H:139:ASP:HA	42:H:8370:HOH:O	1.70	0.89
1:0:962:C:H1'	17:M:5:ARG:NH1	1.88	0.89
6:B:140:LEU:HA	42:B:8579:HOH:O	1.73	0.89
12:H:86:ARG:HH11	12:H:133:ILE:HG13	0.79	0.88
12:H:26:LYS:HD2	12:H:28:ILE:HD12	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:6:GLN:HB2	26:V:26:ILE:HD12	1.55	0.88
14:J:10:GLN:N	14:J:10:GLN:HE21	1.72	0.88
26:V:88:THR:HG22	26:V:89:ASP:H	1.38	0.87
10:F:96:ALA:HA	42:F:3111:HOH:O	1.74	0.87
2:9:3023:U:H5''	2:9:3024:U:OP2	1.73	0.87
29:Y:40:PRO:HD3	29:Y:47:LEU:HD11	1.54	0.87
16:L:35:PRO:CG	16:L:38:VAL:HG23	2.04	0.87
1:0:381:G:H5''	42:0:3798:HOH:O	1.74	0.87
1:0:1701:A:H5'	42:0:5760:HOH:O	1.75	0.86
19:O:115:SER:H	19:O:118:GLN:NE2	1.73	0.86
20:P:25:PRO:HB2	42:P:4350:HOH:O	1.75	0.86
8:D:154:LYS:HD2	8:D:154:LYS:H	1.37	0.86
8:D:27:ILE:HG22	8:D:28:GLY:H	1.40	0.86
1:0:1771:U:H4'	29:Y:20:LEU:HD21	1.57	0.86
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.56	0.86
1:0:1116:U:O2'	1:0:1118:A:H2	1.59	0.86
1:0:1164:U:C4'	1:0:1165:G:OP1	2.22	0.85
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.58	0.85
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.57	0.85
7:C:242:GLU:HG3	42:C:8388:HOH:O	1.74	0.85
15:K:79:ASP:HB3	42:K:8565:HOH:O	1.77	0.85
14:J:29:LEU:HB3	14:J:55:VAL:HG11	1.58	0.85
5:A:192:VAL:HB	42:A:8602:HOH:O	1.76	0.85
13:I:131:THR:HG22	13:I:134:GLU:H	1.41	0.85
16:L:89:ASN:HA	42:L:8556:HOH:O	1.75	0.85
14:J:14:LYS:HB2	14:J:45:PRO:HG2	1.57	0.85
1:0:1603:A:H5'	1:0:1605:G:O4'	1.77	0.85
23:S:9:LYS:HE3	23:S:13:ARG:NH1	1.91	0.85
1:0:2717:C:C2'	1:0:2718:C:H5''	2.07	0.84
16:L:35:PRO:HG2	16:L:38:VAL:HG23	1.57	0.84
1:0:506:G:H22	1:0:509:A:H5'	1.40	0.84
5:A:35:GLY:O	5:A:36:ASP:HB3	1.78	0.84
1:0:870:G:C2'	1:0:871:G:H5''	2.06	0.84
17:M:144:GLY:O	17:M:147:ILE:HG22	1.76	0.84
42:0:4333:HOH:O	16:L:14:ARG:HG2	1.78	0.83
18:N:42:GLU:HB2	42:N:2176:HOH:O	1.77	0.83
1:0:542:A:H5'	1:0:542:A:H8	1.43	0.83
1:0:289:G:H22	1:0:363:A:H2	1.27	0.83
9:E:97:VAL:HG12	42:E:4191:HOH:O	1.77	0.83
1:0:1165:G:H4'	1:0:1174:A:O2'	1.78	0.83
1:0:2506:A:O2'	1:0:2507:G:H8	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:187:VAL:HG23	28:X:192:ASP:HB2	1.60	0.83
42:9:5071:HOH:O	17:M:23:ARG:HD3	1.78	0.83
22:R:51:GLN:HE21	22:R:53:ASN:HD21	1.27	0.83
1:0:2586:U:H3	1:0:2592:G:H22	1.23	0.83
13:I:74:ARG:HB3	13:I:74:ARG:HH11	1.43	0.82
21:Q:9:ASP:O	21:Q:13:THR:HB	1.79	0.82
12:H:26:LYS:HG2	12:H:28:ILE:H	1.44	0.82
12:H:59:ASN:HD22	12:H:59:ASN:N	1.78	0.82
12:H:59:ASN:HD22	12:H:59:ASN:H	1.26	0.82
16:L:164:THR:HG22	16:L:167:GLY:H	1.42	0.82
16:L:164:THR:HG23	16:L:165:SER:N	1.94	0.82
29:Y:39:CYS:HA	29:Y:47:LEU:HD11	1.61	0.82
19:O:115:SER:OG	19:O:118:GLN:HG3	1.79	0.82
17:M:7:LYS:HE3	20:P:21:ARG:O	1.78	0.82
7:C:132:ASP:HB3	42:C:8368:HOH:O	1.78	0.82
42:0:5772:HOH:O	8:D:99:ASP:HA	1.80	0.81
1:0:2435:U:OP1	32:2:28:GLY:HA3	1.80	0.81
42:0:4423:HOH:O	2:9:3103:A:H4'	1.80	0.81
12:H:162:SER:HB2	12:H:163:PRO:CD	2.10	0.81
1:0:2716:G:H5''	6:B:206:THR:HG21	1.61	0.81
5:A:223:ARG:HG3	42:A:8609:HOH:O	1.77	0.81
27:W:78:GLU:HG2	27:W:79:GLU:H	1.46	0.81
26:V:137:GLN:HE21	26:V:141:HIS:HE1	1.24	0.81
1:0:21:G:C5'	21:Q:2:ILE:HA	2.10	0.81
12:H:139:ASP:N	12:H:140:PRO:HD3	1.95	0.81
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.61	0.81
6:B:321:PRO:HA	42:B:8654:HOH:O	1.81	0.81
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.44	0.81
17:M:83:LEU:HD13	17:M:175:LEU:HD23	1.64	0.80
1:0:1165:G:OP1	1:0:1165:G:H3'	1.81	0.80
1:0:2578:G:H5'	1:0:2578:G:H8	1.45	0.80
14:J:81:ARG:HB2	14:J:87:ARG:NH1	1.97	0.80
29:Y:38:LYS:HG2	29:Y:45:LYS:HG2	1.63	0.80
21:Q:8:ALA:HB1	21:Q:13:THR:HG21	1.64	0.80
8:D:20:LYS:HA	8:D:75:LEU:O	1.82	0.80
26:V:4:LEU:HD22	26:V:52:VAL:HG21	1.64	0.79
9:E:37:ASP:OD1	13:I:125:SER:HB3	1.82	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.83	0.79
42:0:5268:HOH:O	16:L:170:CYS:SG	2.39	0.79
26:V:72:PRO:HG2	26:V:77:ALA:HB3	1.63	0.79
1:0:1372:A:H3'	42:0:6659:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:H3	1:0:1246:A:H62	1.30	0.79
28:X:187:VAL:HG23	28:X:192:ASP:CB	2.13	0.79
10:F:91:VAL:HG12	10:F:92:GLY:N	1.96	0.79
12:H:14:TYR:H	12:H:91:HIS:CE1	2.01	0.79
32:2:25:VAL:HG22	32:2:68:LYS:HG3	1.65	0.79
42:0:3217:HOH:O	16:L:157:LEU:HD11	1.83	0.79
42:0:4017:HOH:O	12:H:151:MET:HE2	1.83	0.79
1:0:506:G:H22	1:0:509:A:C5'	1.94	0.79
15:K:68:GLU:HA	42:K:8549:HOH:O	1.82	0.79
1:0:2506:A:HO2'	1:0:2507:G:H8	0.81	0.78
1:0:338:C:H5''	42:C:8427:HOH:O	1.82	0.78
1:0:1667:A:H8	1:0:1667:A:H5'	1.47	0.78
12:H:142:VAL:HG13	42:H:8381:HOH:O	1.81	0.78
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.83	0.78
7:C:78:ARG:HH11	7:C:78:ARG:HG3	1.48	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.83	0.78
42:0:6246:HOH:O	17:M:4:PRO:HD2	1.83	0.78
16:L:169:ARG:HD2	42:L:8591:HOH:O	1.83	0.78
12:H:4:ALA:HB3	42:H:8365:HOH:O	1.83	0.77
1:0:2748:G:H2'	42:0:7009:HOH:O	1.84	0.77
2:9:3056:A:C2'	2:9:3057:A:H5''	2.14	0.77
1:0:1118:A:H3'	1:0:1118:A:H8	1.49	0.77
1:0:1184:C:H1'	42:0:6934:HOH:O	1.83	0.77
2:9:3048:C:H4'	17:M:141:ARG:HH21	1.50	0.77
1:0:558:C:H5'	42:0:4735:HOH:O	1.84	0.77
16:L:172:GLY:O	16:L:183:VAL:HG11	1.85	0.77
12:H:41:THR:HA	42:H:8396:HOH:O	1.85	0.77
1:0:2502:C:H2'	1:0:2503:A:H5'	1.67	0.77
12:H:137:ASN:O	12:H:139:ASP:N	2.18	0.77
27:W:71:ARG:HB3	27:W:88:GLU:OE1	1.84	0.77
26:V:122:ARG:HG2	26:V:122:ARG:HH11	1.48	0.77
7:C:236:THR:HG21	42:C:8380:HOH:O	1.83	0.77
16:L:87:MET:CG	32:2:46:ILE:HG21	2.14	0.77
17:M:113:SER:HB2	42:M:8561:HOH:O	1.84	0.77
29:Y:39:CYS:SG	29:Y:47:LEU:HD21	2.24	0.77
1:0:541:C:H2'	1:0:542:A:H5''	1.65	0.77
15:K:133:VAL:HA	42:K:8578:HOH:O	1.83	0.77
16:L:69:LYS:O	16:L:73:ARG:NH2	2.18	0.77
25:U:12:THR:HG22	25:U:15:GLU:CG	2.12	0.77
12:H:55:GLN:NE2	12:H:124:ARG:HE	1.83	0.77
1:0:2099:G:H1	40:4:79:BTN:H92	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H4'	1:0:1702:U:H5''	1.66	0.76
29:Y:38:LYS:HE2	29:Y:45:LYS:HE2	1.68	0.76
5:A:69:LEU:HD21	5:A:120:ARG:HB3	1.67	0.76
1:0:1684:A:H1'	31:1:43:ARG:HH22	1.50	0.76
21:Q:39:THR:HB	21:Q:42:GLU:HG3	1.67	0.76
1:0:2526:C:O2'	1:0:2527:U:H5'	1.86	0.76
9:E:100:ASP:HB2	42:E:2789:HOH:O	1.86	0.76
1:0:272:A:H3'	42:0:6997:HOH:O	1.84	0.76
4:4:74:C:H2'	4:4:75:C:H5'	1.66	0.76
12:H:47:GLU:HB3	12:H:133:ILE:HD13	1.67	0.76
1:0:1118:A:H3'	1:0:1118:A:C8	2.20	0.76
1:0:1164:U:H3	1:0:1192:A:H2	1.31	0.76
12:H:5:MET:HG3	42:H:8365:HOH:O	1.85	0.76
6:B:41:PHE:HB3	6:B:190:MET:HE1	1.68	0.76
2:9:3006:C:H5''	17:M:37:ARG:HH12	1.48	0.76
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.76
14:J:74:VAL:HG13	14:J:113:ILE:HG23	1.68	0.76
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.86	0.76
1:0:2421:G:H3'	1:0:2422:U:H5''	1.67	0.76
17:M:49:THR:HG22	17:M:56:ASP:HB2	1.68	0.76
18:N:14:LEU:HD23	18:N:102:ILE:HD11	1.67	0.75
28:X:220:GLU:HG2	42:X:8551:HOH:O	1.86	0.75
1:0:1164:U:H4'	1:0:1165:G:OP1	1.86	0.75
1:0:2420:G:O2'	1:0:2421:G:H5'	1.87	0.75
1:0:282:C:H1'	1:0:368:C:N4	2.01	0.75
1:0:1160:G:C5'	1:0:1161:A:H5'	2.16	0.75
7:C:139:VAL:HG13	42:C:8452:HOH:O	1.84	0.75
1:0:2812:A:H2	1:0:2814:A:H62	1.34	0.75
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.69	0.75
29:Y:30:GLU:HA	29:Y:33:HIS:HB3	1.68	0.75
1:0:541:C:C2'	1:0:542:A:H5''	2.17	0.75
1:0:2533:C:C6	1:0:2533:C:H5'	2.22	0.74
13:I:107:ASN:ND2	13:I:109:TYR:H	1.84	0.74
1:0:346:U:H4'	42:0:6317:HOH:O	1.87	0.74
26:V:88:THR:HG23	26:V:110:GLN:NE2	2.02	0.74
13:I:74:ARG:CB	13:I:74:ARG:HH11	2.00	0.74
13:I:99:GLU:HA	42:I:7377:HOH:O	1.85	0.74
1:0:2502:C:C2'	1:0:2503:A:H5'	2.18	0.74
27:W:72:VAL:HG22	27:W:85:VAL:HG12	1.69	0.74
12:H:75:SER:O	12:H:79:ALA:HB2	1.87	0.74
23:S:61:GLU:HG3	42:S:3851:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3069:U:OP1	17:M:4:PRO:HG3	1.88	0.74
1:0:2094:G:H4'	6:B:245:SER:HB3	1.70	0.74
1:0:553:G:P	28:X:204:ARG:HH22	2.11	0.74
7:C:5:ILE:HD11	7:C:16:VAL:CG2	2.16	0.74
5:A:153:ARG:HH11	5:A:153:ARG:HB2	1.52	0.74
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.74
6:B:162:MET:CE	6:B:308:LEU:HD21	2.18	0.74
6:B:258:GLY:H	6:B:260:HIS:CE1	2.05	0.74
1:0:2421:G:H3'	1:0:2422:U:C5'	2.18	0.74
18:N:32:ARG:O	18:N:32:ARG:HD3	1.86	0.74
1:0:288:A:H61	1:0:364:C:H42	1.34	0.74
17:M:48:VAL:CG1	17:M:55:ASP:HB3	2.17	0.74
26:V:13:MET:HE3	26:V:17:ILE:HG22	1.69	0.74
20:P:64:GLU:HG3	20:P:74:ASP:OD2	1.88	0.73
12:H:47:GLU:HB3	12:H:133:ILE:CD1	2.18	0.73
7:C:140:VAL:HB	42:C:8455:HOH:O	1.88	0.73
19:O:59:ARG:NH2	19:O:66:GLN:HE22	1.85	0.73
18:N:47:ARG:HG3	18:N:47:ARG:HH11	1.52	0.73
19:O:115:SER:N	19:O:118:GLN:HE21	1.82	0.73
42:O:3277:HOH:O	16:L:189:VAL:HG21	1.87	0.73
5:A:121:ALA:O	5:A:124:VAL:HG22	1.88	0.73
23:S:9:LYS:HB2	42:S:7242:HOH:O	1.88	0.73
1:0:560:C:H42	1:0:597:A:H61	1.36	0.73
16:L:186:SER:O	16:L:189:VAL:HG12	1.88	0.73
1:0:1878:G:H1'	42:O:5597:HOH:O	1.88	0.73
9:E:11:VAL:HG12	9:E:12:ASP:N	2.03	0.73
29:Y:37:HIS:HB2	29:Y:47:LEU:HB2	1.70	0.73
1:0:711:G:H1'	42:O:6565:HOH:O	1.88	0.73
6:B:62:ARG:HA	6:B:65:MET:HE2	1.69	0.73
12:H:2:PRO:HB2	42:H:8365:HOH:O	1.89	0.73
22:R:57:THR:HG22	22:R:59:ASP:H	1.53	0.73
21:Q:106:GLY:HA2	21:Q:109:MET:HE3	1.71	0.73
1:0:1835:U:C5	1:0:1840:A:N7	2.55	0.73
8:D:64:ARG:HG2	8:D:67:ASP:HB3	1.71	0.73
1:0:1919:A:H4'	42:O:4320:HOH:O	1.87	0.73
31:1:41:HIS:N	31:1:45:ASN:HD22	1.84	0.72
25:U:39:ALA:N	25:U:40:PRO:HD2	2.04	0.72
25:U:1:THR:HG23	25:U:2:VAL:H	1.54	0.72
21:Q:39:THR:HG23	21:Q:107:GLU:O	1.89	0.72
26:V:22:GLU:HG2	26:V:27:HIS:CD2	2.23	0.72
1:0:111:C:O2'	30:Z:20:ARG:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.72	0.72
1:0:1474:C:H6	1:0:1474:C:H5'	1.53	0.72
1:0:1909:A:N1	1:0:2128:G:H1'	2.04	0.72
28:X:200:THR:HG22	28:X:201:GLU:CG	2.19	0.72
31:1:41:HIS:H	31:1:45:ASN:ND2	1.88	0.72
12:H:140:PRO:HB3	42:H:8381:HOH:O	1.90	0.72
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.24	0.72
42:9:4707:HOH:O	17:M:147:ILE:HD12	1.88	0.72
8:D:19:GLU:O	8:D:20:LYS:HG2	1.89	0.72
16:L:139:PRO:O	16:L:140:ALA:HB3	1.89	0.72
1:0:450:C:OP1	7:C:184:ARG:NH2	2.19	0.72
6:B:71:VAL:HG11	6:B:296:LEU:HB3	1.71	0.72
11:G:12:ILE:HA	42:G:4499:HOH:O	1.88	0.72
1:0:2004:U:H4'	42:0:4785:HOH:O	1.88	0.72
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.55	0.71
1:0:2637:A:H4'	1:0:2638:G:O5'	1.89	0.71
27:W:76:ARG:HH11	27:W:76:ARG:HG3	1.54	0.71
42:0:6403:HOH:O	28:X:212:ARG:HD2	1.89	0.71
14:J:22:ASP:HB2	42:J:5264:HOH:O	1.89	0.71
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
17:M:61:ALA:HB3	17:M:88:ALA:HB2	1.70	0.71
24:T:9:CYS:SG	24:T:11:THR:HG23	2.31	0.71
1:0:1191:A:H3'	1:0:1192:A:H5''	1.72	0.71
27:W:25:ARG:HD2	42:W:3861:HOH:O	1.90	0.71
1:0:1187:U:H2'	42:0:6368:HOH:O	1.91	0.71
2:9:3014:G:H8	2:9:3014:G:H5'	1.54	0.71
1:0:236:A:H4'	1:0:237:G:H5'	1.73	0.71
5:A:36:ASP:OD2	5:A:85:ASP:HB2	1.90	0.71
21:Q:99:ALA:HB1	21:Q:109:MET:CE	2.19	0.71
26:V:6:GLN:HB2	26:V:26:ILE:CD1	2.20	0.71
1:0:1666:C:H2'	1:0:1667:A:H5'	1.72	0.71
6:B:145:HIS:HD2	6:B:146:THR:O	1.73	0.71
15:K:143:THR:HG22	15:K:144:ASP:N	2.06	0.71
1:0:2466:G:OP1	42:0:3138:HOH:O	2.08	0.71
1:0:1209:C:H4'	42:0:4758:HOH:O	1.90	0.71
42:0:3048:HOH:O	16:L:152:ARG:HG3	1.91	0.71
5:A:33:GLU:O	5:A:34:ASP:HB2	1.90	0.71
23:S:69:LYS:O	23:S:71:VAL:HG23	1.91	0.70
26:V:21:LEU:HD22	26:V:26:ILE:CD1	2.21	0.70
1:0:182:G:H5'	42:0:4630:HOH:O	1.90	0.70
1:0:1209:C:H2'	1:0:1210:G:H8	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:6:GLU:HA	9:E:46:THR:HG22	1.72	0.70
1:0:2508:C:H2'	42:0:6228:HOH:O	1.91	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.20	0.70
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.72	0.70
25:U:12:THR:CG2	25:U:15:GLU:HG3	2.19	0.70
26:V:21:LEU:HD22	26:V:26:ILE:HD11	1.72	0.70
26:V:122:ARG:HH21	26:V:154:ARG:HD2	1.56	0.70
31:1:35:ARG:HB2	42:1:2691:HOH:O	1.92	0.70
1:0:545:G:C8	1:0:545:G:H5'	2.25	0.70
1:0:284:C:H4'	1:0:285:A:O5'	1.89	0.70
1:0:2604:A:H5'	42:0:5266:HOH:O	1.90	0.70
16:L:139:PRO:O	16:L:140:ALA:CB	2.40	0.70
2:9:3029:C:H2'	2:9:3030:C:H5'	1.73	0.70
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.07	0.70
1:0:2748:G:H5'	42:0:7009:HOH:O	1.92	0.70
1:0:396:U:H1'	42:0:7100:HOH:O	1.89	0.70
1:0:1206:U:H6	1:0:1206:U:H5'	1.56	0.70
1:0:544:G:H2'	1:0:545:G:H5''	1.73	0.70
9:E:107:PHE:CE2	9:E:108:LEU:HD13	2.26	0.70
24:T:9:CYS:HA	24:T:52:THR:HG23	1.73	0.69
19:O:103:THR:HA	19:O:106:ARG:NH1	2.06	0.69
12:H:162:SER:CB	12:H:163:PRO:HD3	2.21	0.69
12:H:27:LYS:H	12:H:58:HIS:CD2	2.04	0.69
1:0:2419:U:H5''	1:0:2420:G:H5'	1.72	0.69
13:I:75:PRO:HG2	13:I:105:LEU:HD21	1.72	0.69
15:K:67:ARG:O	15:K:71:GLU:HG3	1.91	0.69
12:H:27:LYS:N	12:H:58:HIS:HD2	1.88	0.69
1:0:657:G:OP1	7:C:27:ARG:NH2	2.25	0.69
1:0:962:C:H1'	17:M:5:ARG:HH12	1.57	0.69
13:I:45:VAL:HG23	13:I:130:VAL:O	1.92	0.69
1:0:281:U:H2'	1:0:282:C:O4'	1.92	0.69
27:W:15:ARG:HH11	27:W:15:ARG:HB3	1.57	0.69
17:M:164:ASP:CG	17:M:167:ASP:HA	2.13	0.69
8:D:146:LYS:NZ	17:M:107:ASN:HD21	1.90	0.69
42:0:9657:HOH:O	16:L:87:MET:HE3	1.93	0.69
12:H:49:VAL:O	12:H:157:ILE:HG23	1.93	0.69
42:0:6348:HOH:O	16:L:178:LYS:HB2	1.92	0.69
1:0:2291:A:C8	1:0:2309:C:H5'	2.28	0.69
12:H:45:GLN:HE21	12:H:135:TRP:HE1	1.38	0.69
13:I:19:MET:CE	13:I:132:LEU:HD11	2.23	0.69
1:0:559:U:H5'	1:0:559:U:H6	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2426:G:H1'	42:O:5568:HOH:O	1.91	0.69
26:V:88:THR:HG22	26:V:89:ASP:N	2.08	0.69
1:O:1185:U:H2'	1:O:1186:C:C6	2.28	0.69
10:F:99:THR:HA	42:F:3461:HOH:O	1.93	0.69
14:J:82:ARG:NH2	14:J:115:ARG:HG2	2.08	0.69
1:O:56:G:H5''	25:U:50:ARG:HH12	1.57	0.69
16:L:122:GLU:OE2	16:L:127:LYS:HE2	1.93	0.69
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.75	0.69
7:C:162:VAL:HG12	7:C:192:ILE:HD11	1.74	0.69
1:O:2890:A:H1'	24:T:56:ARG:NH2	2.07	0.69
1:O:1625:U:H4'	42:O:4142:HOH:O	1.91	0.68
24:T:13:ILE:HG12	24:T:32:CYS:HB3	1.72	0.68
29:Y:42:CYS:SG	29:Y:44:PHE:HB2	2.33	0.68
6:B:238:ASN:ND2	6:B:240:GLY:H	1.88	0.68
16:L:106:ASN:HD22	16:L:114:VAL:HG23	1.57	0.68
14:J:74:VAL:HG11	14:J:113:ILE:HG12	1.74	0.68
25:U:42:ASN:HB3	42:U:7247:HOH:O	1.92	0.68
1:O:1160:G:H5'	1:O:1161:A:C5'	2.19	0.68
1:O:1741:U:H5'	1:O:1742:A:OP1	1.93	0.68
26:V:68:THR:HG23	26:V:69:ARG:HG2	1.76	0.68
14:J:28:GLU:OE2	14:J:58:THR:HG21	1.94	0.68
8:D:55:LYS:HA	42:D:6752:HOH:O	1.94	0.68
1:O:2768:A:H2'	1:O:2769:C:O4'	1.92	0.68
7:C:236:THR:H	7:C:239:ALA:HB3	1.58	0.68
17:M:159:TYR:HB3	17:M:162:ASP:HB2	1.76	0.68
1:O:214:U:H5'	42:O:5617:HOH:O	1.92	0.68
26:V:4:LEU:HD22	26:V:52:VAL:CG2	2.24	0.68
1:O:2241:C:O2'	1:O:2242:U:H5'	1.93	0.68
1:O:1751:G:C2'	1:O:1752:G:H5''	2.22	0.68
31:I:39:ARG:HG2	42:I:3143:HOH:O	1.93	0.68
1:O:1679:C:H5'	42:O:8828:HOH:O	1.94	0.68
8:D:57:THR:HG23	8:D:63:ILE:HG22	1.76	0.68
1:O:738:G:H3'	42:O:6518:HOH:O	1.93	0.68
2:9:3092:G:H2'	2:9:3093:A:C8	2.29	0.67
1:O:2346:C:O2'	8:D:52:THR:HG21	1.93	0.67
1:O:1130:U:H2'	1:O:1131:G:O4'	1.94	0.67
12:H:130:HIS:CD2	12:H:133:ILE:HD11	2.29	0.67
26:V:4:LEU:HD23	26:V:54:PHE:HB3	1.76	0.67
1:O:1119:G:H2'	13:I:52:GLN:NE2	2.09	0.67
11:G:12:ILE:N	11:G:13:PRO:HD3	2.10	0.67
24:T:46:ALA:HB1	24:T:52:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1:MET:HG2	7:C:2:GLN:H	1.58	0.67
28:X:186:ARG:HG2	28:X:186:ARG:HH11	1.57	0.67
13:I:103:VAL:HG12	42:I:5907:HOH:O	1.94	0.67
21:Q:39:THR:HG22	21:Q:42:GLU:H	1.60	0.67
29:Y:49:ARG:HD2	42:Y:8424:HOH:O	1.94	0.67
26:V:122:ARG:NH2	26:V:154:ARG:HD2	2.09	0.67
7:C:12:THR:HB	42:C:8445:HOH:O	1.95	0.67
12:H:46:VAL:HG12	12:H:146:TRP:HZ3	1.60	0.67
16:L:104:ARG:O	16:L:108:LYS:HE2	1.94	0.67
1:O:1244:U:OP1	13:I:18:ILE:HD13	1.95	0.67
1:O:56:G:H5''	25:U:50:ARG:NH1	2.08	0.67
1:O:1328:A:OP1	28:X:169:ARG:HD2	1.95	0.67
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.77	0.67
1:O:156:C:H5''	16:L:171:ARG:CD	2.22	0.67
1:O:1377:C:H6	1:O:1377:C:H5'	1.61	0.67
16:L:12:TRP:CE2	16:L:20:ILE:HD11	2.30	0.67
21:Q:18:LEU:HD12	21:Q:143:VAL:HG11	1.76	0.67
16:L:37:VAL:HG21	16:L:108:LYS:HG3	1.77	0.66
16:L:173:LEU:HD23	16:L:183:VAL:HG12	1.76	0.66
16:L:34:GLU:HB3	16:L:35:PRO:HD2	1.77	0.66
17:M:164:ASP:OD2	17:M:167:ASP:HA	1.95	0.66
25:U:56:ILE:O	25:U:60:GLN:HG3	1.95	0.66
42:O:4444:HOH:O	12:H:57:ARG:HG3	1.95	0.66
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.10	0.66
19:O:103:THR:O	19:O:107:GLU:HG3	1.94	0.66
5:A:53:ALA:HB3	42:A:8614:HOH:O	1.95	0.66
12:H:56:ILE:HG22	12:H:61:LEU:HD22	1.76	0.66
13:I:75:PRO:HG2	13:I:105:LEU:CD2	2.25	0.66
6:B:7:ARG:HG2	6:B:7:ARG:HH11	1.61	0.66
17:M:12:ARG:HD3	17:M:18:THR:OG1	1.96	0.66
1:O:1058:A:H2'	1:O:1060:C:H5''	1.77	0.66
1:O:1299:G:O6	15:K:6:ARG:HD3	1.96	0.66
1:O:1080:C:H4'	1:O:1081:A:OP1	1.94	0.66
25:U:4:HIS:HB3	42:U:6622:HOH:O	1.94	0.66
8:D:35:ALA:N	42:D:5576:HOH:O	2.27	0.66
26:V:88:THR:HG23	26:V:110:GLN:HE21	1.59	0.66
1:O:31:C:H4'	42:S:7242:HOH:O	1.94	0.66
19:O:38:GLU:HA	19:O:41:ARG:NH1	2.11	0.66
13:I:107:ASN:HD21	13:I:109:TYR:HB2	1.61	0.66
21:Q:18:LEU:HB2	21:Q:143:VAL:CG1	2.26	0.66
12:H:118:PRO:HD2	42:H:8339:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:183:ASP:OD2	17:M:186:LEU:HD12	1.96	0.66
1:O:1886:A:N3	42:O:4293:HOH:O	2.28	0.66
17:M:119:GLN:O	17:M:123:ILE:HG13	1.95	0.66
1:O:282:C:H1'	1:O:368:C:H42	1.60	0.66
24:T:14:GLU:O	24:T:17:THR:HB	1.96	0.66
17:M:71:TRP:CE3	17:M:175:LEU:HD22	2.32	0.65
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.65
11:G:12:ILE:HD12	42:G:692:HOH:O	1.96	0.65
5:A:131:HIS:O	5:A:132:ASP:HB2	1.94	0.65
7:C:214:THR:HG21	42:C:8409:HOH:O	1.95	0.65
1:O:603:A:H5''	1:O:604:G:OP1	1.96	0.65
1:O:902:G:N7	15:K:18:HIS:HD2	1.93	0.65
16:L:74:ARG:HG3	16:L:74:ARG:HH11	1.61	0.65
12:H:150:LYS:HE2	42:H:8383:HOH:O	1.96	0.65
2:9:3006:C:OP1	17:M:37:ARG:NH1	2.29	0.65
5:A:76:VAL:HG23	29:Y:63:LYS:HB3	1.79	0.65
23:S:9:LYS:HE3	23:S:13:ARG:HH11	1.60	0.65
13:I:93:ARG:HB3	13:I:93:ARG:HH11	1.62	0.65
1:O:1923:G:H4'	32:2:31:THR:O	1.97	0.65
7:C:236:THR:HA	42:C:8455:HOH:O	1.97	0.65
17:M:86:LEU:HD12	17:M:125:ALA:HB2	1.79	0.65
22:R:57:THR:HG22	22:R:59:ASP:N	2.11	0.65
14:J:62:PRO:HG3	14:J:65:ARG:HH21	1.61	0.65
6:B:62:ARG:HA	6:B:65:MET:CE	2.25	0.65
1:O:1329:A:H2	42:O:4159:HOH:O	1.78	0.65
14:J:62:PRO:HG3	14:J:65:ARG:NH2	2.12	0.65
14:J:27:ARG:HD2	42:J:4747:HOH:O	1.96	0.65
6:B:238:ASN:HD22	6:B:240:GLY:N	1.89	0.65
14:J:55:VAL:HG12	14:J:56:SER:N	2.12	0.65
1:O:2637:A:H3'	3:3:74:C:O5'	1.96	0.65
5:A:191:GLY:HA2	5:A:194:MET:CE	2.26	0.65
8:D:23:VAL:O	8:D:23:VAL:HG23	1.96	0.65
14:J:115:ARG:HG3	14:J:116:GLU:N	2.12	0.65
12:H:141:ASN:HA	42:H:8366:HOH:O	1.97	0.65
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.77	0.64
32:2:55:VAL:HG22	42:2:8511:HOH:O	1.97	0.64
1:O:1172:G:H1'	42:O:4446:HOH:O	1.96	0.64
9:E:166:VAL:HG12	42:E:3134:HOH:O	1.96	0.64
1:O:1641:A:H2'	1:O:1642:A:H5'	1.79	0.64
1:O:645:U:OP2	15:K:4:LYS:HE2	1.96	0.64
1:O:182:G:H4'	16:L:157:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2421:G:H4'	42:0:4252:HOH:O	1.97	0.64
8:D:64:ARG:CG	8:D:67:ASP:HB3	2.27	0.64
32:2:65:THR:HG23	32:2:67:LEU:HG	1.79	0.64
8:D:25:MET:CE	8:D:41:LEU:HG	2.23	0.64
6:B:264:GLU:HG2	6:B:267:LYS:CE	2.23	0.64
19:O:58:SER:HB3	42:O:183:HOH:O	1.96	0.64
29:Y:54:ILE:HD12	42:Y:8415:HOH:O	1.96	0.64
1:0:447:A:OP1	23:S:2:LYS:HG2	1.97	0.64
22:R:51:GLN:HE21	22:R:53:ASN:ND2	1.95	0.64
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.79	0.64
5:A:191:GLY:HA2	5:A:194:MET:HE3	1.79	0.64
1:0:2310:G:OP2	12:H:114:PRO:HD2	1.97	0.64
1:0:470:U:O2'	30:Z:16:HIS:HD2	1.79	0.64
42:0:7025:HOH:O	32:2:60:LYS:HG3	1.97	0.64
23:S:32:ARG:NH1	23:S:38:ARG:HH12	1.96	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.96	0.64
5:A:36:ASP:HA	5:A:83:GLY:HA3	1.80	0.64
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.79	0.64
8:D:69:ILE:O	8:D:69:ILE:HG22	1.96	0.64
8:D:97:GLN:HG2	8:D:97:GLN:O	1.96	0.64
13:I:19:MET:HE3	13:I:132:LEU:HD11	1.79	0.64
17:M:154:LEU:O	17:M:155:GLU:HB3	1.98	0.64
1:0:1234:U:N3	6:B:244:PRO:HB3	2.13	0.64
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.80	0.64
11:G:64:ASN:N	11:G:64:ASN:HD22	1.94	0.64
17:M:37:ARG:NE	42:M:8535:HOH:O	2.29	0.64
1:0:69:A:H5'	1:0:69:A:C8	2.33	0.64
6:B:221:GLN:HE22	14:J:42:ASN:HD22	1.44	0.64
42:0:4307:HOH:O	13:I:47:THR:HB	1.97	0.64
12:H:59:ASN:H	12:H:59:ASN:ND2	1.95	0.64
1:0:383:A:H4'	42:0:4807:HOH:O	1.96	0.64
12:H:58:HIS:HA	12:H:61:LEU:HD23	1.80	0.64
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.79	0.64
26:V:130:HIS:O	26:V:136:GLY:HA3	1.97	0.64
12:H:163:PRO:HG2	42:H:8338:HOH:O	1.97	0.64
12:H:28:ILE:HA	12:H:62:GLU:OE1	1.98	0.64
12:H:55:GLN:HE22	12:H:91:HIS:CD2	2.16	0.64
31:1:22:PRO:HG2	31:1:25:VAL:HG23	1.79	0.64
13:I:133:GLY:O	13:I:137:GLU:HG3	1.98	0.64
42:0:5006:HOH:O	16:L:58:GLN:HG3	1.97	0.64
1:0:125:U:H2'	42:0:3260:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:6612:HOH:O	30:Z:1:THR:HB	1.97	0.63
16:L:84:LYS:HE2	42:L:8579:HOH:O	1.98	0.63
28:X:187:VAL:CG2	28:X:192:ASP:HB2	2.27	0.63
18:N:14:LEU:CD2	18:N:102:ILE:HD11	2.27	0.63
6:B:36:PRO:HA	6:B:168:GLY:CA	2.28	0.63
1:O:1119:G:H22	1:O:1246:A:H2	1.45	0.63
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.80	0.63
6:B:125:GLU:O	6:B:129:ARG:HG3	1.99	0.63
1:O:2459:G:OP1	32:2:64:LYS:N	2.18	0.63
16:L:87:MET:HG2	32:2:46:ILE:CG2	2.23	0.63
12:H:26:LYS:HD2	12:H:28:ILE:CD1	2.26	0.63
15:K:148:GLU:HA	42:K:8577:HOH:O	1.97	0.63
12:H:83:PHE:HZ	12:H:146:TRP:HE1	1.46	0.63
1:O:289:G:N2	1:O:363:A:H2	1.94	0.63
15:K:120:LEU:HD12	15:K:133:VAL:HG21	1.80	0.63
29:Y:30:GLU:HA	29:Y:33:HIS:CB	2.28	0.63
8:D:65:GLU:HG3	42:D:6752:HOH:O	1.99	0.63
12:H:69:ASN:O	12:H:72:VAL:HG12	1.97	0.63
12:H:136:VAL:HG22	12:H:137:ASN:O	1.97	0.63
1:O:285:A:H2'	1:O:286:U:O4'	1.98	0.63
27:W:41:PHE:O	27:W:43:VAL:HG23	1.98	0.63
15:K:1:THR:HA	42:K:8529:HOH:O	1.99	0.63
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.81	0.63
1:O:338:C:H4'	7:C:174:ILE:CD1	2.28	0.63
6:B:41:PHE:HA	6:B:79:MET:HE2	1.81	0.63
17:M:61:ALA:CB	17:M:88:ALA:HB2	2.29	0.63
1:O:2769:C:H2'	1:O:2770:G:O4'	1.99	0.63
6:B:175:LEU:C	6:B:175:LEU:HD23	2.19	0.63
12:H:33:MET:HB2	12:H:83:PHE:HB3	1.81	0.63
1:O:1118:A:H62	1:O:1244:U:H3	1.46	0.63
1:O:371:U:H2'	1:O:372:A:H8	1.63	0.63
12:H:53:PRO:HG3	12:H:127:GLY:H	1.64	0.63
10:F:110:GLU:HG2	42:F:6926:HOH:O	1.98	0.63
1:O:871:G:C8	1:O:871:G:C5'	2.75	0.63
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.81	0.63
8:D:105:SER:CB	8:D:131:THR:HG23	2.27	0.63
26:V:110:GLN:NE2	26:V:110:GLN:HA	2.14	0.63
16:L:138:HIS:ND1	16:L:139:PRO:O	2.24	0.62
1:O:2432:C:O2'	1:O:2433:A:H5'	1.98	0.62
18:N:38:ARG:NH1	42:N:7674:HOH:O	2.30	0.62
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:84:ARG:NH2	12:H:135:TRP:HH2	1.96	0.62
1:0:272:A:H5'	1:0:273:G:OP2	1.98	0.62
8:D:95:THR:O	8:D:97:GLN:N	2.28	0.62
16:L:164:THR:CG2	16:L:165:SER:N	2.62	0.62
7:C:115:LEU:HD21	7:C:243:VAL:HG13	1.81	0.62
6:B:307:ARG:HB2	6:B:307:ARG:HH11	1.64	0.62
1:0:2054:A:N3	21:Q:128:ARG:NH2	2.47	0.62
30:Z:8:GLN:HE22	30:Z:11:LYS:NZ	1.97	0.62
26:V:90:TYR:N	26:V:90:TYR:CD1	2.66	0.62
21:Q:132:ARG:HG2	21:Q:133:ALA:N	2.14	0.62
1:0:2851:G:O2'	1:0:2852:A:H5'	1.98	0.62
22:R:33:SER:O	22:R:37:VAL:HG23	2.00	0.62
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.82	0.62
21:Q:18:LEU:HB2	21:Q:143:VAL:HG12	1.81	0.62
5:A:194:MET:HE1	5:A:199:HIS:HB2	1.81	0.62
12:H:71:TYR:C	12:H:73:GLN:H	2.03	0.62
18:N:87:THR:O	18:N:91:GLN:HG3	1.98	0.62
17:M:32:PRO:HD2	17:M:99:GLU:O	2.00	0.62
42:O:3551:HOH:O	6:B:27:ASN:HB2	1.99	0.62
29:Y:10:ARG:HA	42:Y:8414:HOH:O	1.98	0.62
17:M:151:ASP:O	17:M:154:LEU:HB2	2.00	0.62
16:L:68:ARG:HD3	16:L:68:ARG:O	1.99	0.62
1:0:2361:A:H5''	42:O:8523:HOH:O	1.99	0.62
28:X:133:HIS:HD2	42:X:8583:HOH:O	1.82	0.62
12:H:48:LEU:HG	12:H:157:ILE:HG21	1.82	0.62
7:C:115:LEU:O	7:C:118:THR:HB	1.99	0.62
6:B:140:LEU:HD23	42:B:8579:HOH:O	1.99	0.62
1:0:69:A:H5'	1:0:69:A:H8	1.65	0.62
5:A:211:LYS:HB3	5:A:212:PRO:CD	2.24	0.62
1:0:544:G:C2'	1:0:545:G:H5''	2.30	0.62
1:0:1886:A:H4'	42:Y:8405:HOH:O	1.98	0.62
1:0:1116:U:HO2'	1:0:1118:A:H2	0.76	0.62
1:0:1972:U:H2'	1:0:1973:A:H5'	1.82	0.62
5:A:94:LEU:N	5:A:94:LEU:HD23	2.15	0.61
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.81	0.61
16:L:164:THR:HG22	16:L:167:GLY:N	2.13	0.61
27:W:78:GLU:CG	27:W:79:GLU:H	2.11	0.61
5:A:200:PRO:HG2	5:A:225:VAL:HG21	1.82	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.34	0.61
28:X:216:ARG:HD3	42:X:8570:HOH:O	2.01	0.61
1:0:2505:G:O2'	1:0:2506:A:H5'	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:73:ALA:N	42:M:8568:HOH:O	2.33	0.61
1:0:1170:U:O2'	1:0:1172:G:N7	2.27	0.61
1:0:2276:U:H2'	1:0:2277:U:C6	2.35	0.61
1:0:188:C:H5''	16:L:163:LEU:HD21	1.82	0.61
12:H:44:ALA:HA	12:H:163:PRO:O	2.00	0.61
2:9:3006:C:C5'	17:M:37:ARG:NH1	2.59	0.61
22:R:51:GLN:NE2	22:R:53:ASN:HD21	1.96	0.61
15:K:136:ALA:HB3	42:K:8578:HOH:O	2.00	0.61
1:0:1829:A:N6	29:Y:18:TYR:HA	2.15	0.61
26:V:13:MET:HE1	26:V:18:GLN:HA	1.80	0.61
23:S:63:ILE:HD11	23:S:75:GLU:HB2	1.82	0.61
10:F:91:VAL:CG1	10:F:92:GLY:H	2.11	0.61
26:V:137:GLN:HE21	26:V:141:HIS:CE1	2.13	0.61
1:0:558:C:O2'	1:0:559:U:H5''	2.00	0.61
6:B:148:PRO:HD2	42:B:8580:HOH:O	2.00	0.61
19:O:98:ILE:HD12	19:O:102:ARG:NE	2.16	0.61
29:Y:28:ASP:O	29:Y:31:ILE:HG22	2.01	0.61
32:2:62:THR:HB	42:2:8557:HOH:O	2.00	0.61
16:L:74:ARG:O	16:L:88:VAL:HG13	2.00	0.61
1:0:1116:U:O2'	1:0:1118:A:C2	2.42	0.61
1:0:2896:A:H5''	42:0:5575:HOH:O	2.00	0.61
29:Y:51:GLY:HA3	42:Y:8415:HOH:O	2.01	0.61
1:0:2427:C:OP2	32:2:84:ARG:HD2	2.00	0.61
26:V:81:ASP:OD1	26:V:92:ASP:HB2	1.99	0.61
17:M:184:ILE:HG22	17:M:185:GLU:HG3	1.82	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.81	0.61
42:C:8360:HOH:O	18:N:3:THR:HG21	1.99	0.61
7:C:118:THR:O	7:C:136:VAL:HG13	2.00	0.61
6:B:141:ARG:HD2	6:B:163:GLU:OE2	2.01	0.61
12:H:144:GLU:OE1	12:H:144:GLU:HA	2.00	0.61
32:2:10:TYR:HB2	32:2:17:HIS:CE1	2.36	0.61
1:0:2710:U:H1'	42:0:7092:HOH:O	2.00	0.61
1:0:1559:A:H1'	42:0:5338:HOH:O	2.01	0.61
1:0:1474:C:C6	1:0:1474:C:H5'	2.34	0.61
1:0:1766:U:O2	1:0:1778:A:H5'	2.01	0.61
2:9:3039:U:H1'	2:9:3044:A:H61	1.64	0.61
1:0:1003:U:HO2'	12:H:90:PHE:HE1	1.48	0.61
32:2:70:ARG:HB3	42:2:8576:HOH:O	2.00	0.61
9:E:79:GLY:HA3	42:E:7046:HOH:O	2.00	0.61
17:M:91:ARG:HG3	17:M:186:LEU:HD23	1.82	0.60
21:Q:33:ARG:NH1	42:Q:8544:HOH:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:25:PRO:HG2	42:C:8324:HOH:O	1.99	0.60
1:O:431:G:P	16:L:48:ARG:HH12	2.25	0.60
21:Q:44:VAL:O	21:Q:48:GLU:HG3	2.02	0.60
1:O:775:G:OP1	30:Z:16:HIS:HE1	1.84	0.60
28:X:144:ARG:CZ	42:X:8612:HOH:O	2.48	0.60
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.84	0.60
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.60
8:D:36:ASN:HA	42:D:7500:HOH:O	2.00	0.60
1:O:1120:U:H5'	1:O:1121:G:OP2	2.00	0.60
16:L:52:LEU:HD21	42:L:8618:HOH:O	2.00	0.60
26:V:13:MET:CE	26:V:17:ILE:HG22	2.30	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.36	0.60
1:O:2783:A:H3'	42:O:4708:HOH:O	1.99	0.60
1:O:1114:A:H2'	1:O:1115:U:H6	1.66	0.60
1:O:2437:A:H2'	1:O:2438:G:C8	2.37	0.60
17:M:80:SER:HB2	42:M:8537:HOH:O	1.99	0.60
1:O:299:U:H5'	42:O:6806:HOH:O	2.01	0.60
1:O:2587:U:H2'	1:O:2589:U:H5''	1.82	0.60
16:L:104:ARG:O	16:L:108:LYS:HG2	2.01	0.60
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.14	0.60
21:Q:39:THR:HB	21:Q:42:GLU:CG	2.30	0.60
1:O:2676:C:H4'	13:I:70:PHE:CE1	2.35	0.60
1:O:1594:C:OP2	19:O:120:ARG:HD2	2.01	0.60
1:O:263:U:O4'	10:F:59:ILE:HD13	2.01	0.60
12:H:46:VAL:O	12:H:146:TRP:HH2	1.84	0.60
12:H:166:ASN:HD22	12:H:166:ASN:N	1.98	0.60
1:O:1119:G:N2	1:O:1246:A:C2	2.63	0.60
29:Y:30:GLU:HB3	29:Y:34:LYS:HE3	1.84	0.60
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.82	0.60
1:O:20:G:H21	21:Q:117:HIS:HD2	1.49	0.60
16:L:61:ILE:HA	42:L:8627:HOH:O	2.01	0.60
10:F:107:VAL:O	10:F:111:ILE:HG13	2.01	0.60
22:R:81:ILE:HG23	42:R:8336:HOH:O	2.02	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.84	0.60
9:E:7:ILE:HD11	9:E:11:VAL:C	2.22	0.60
19:O:38:GLU:HA	19:O:41:ARG:HH11	1.67	0.60
6:B:207:LYS:HG2	6:B:304:PRO:HB3	1.83	0.60
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.82	0.60
19:O:87:ARG:HG2	42:O:186:HOH:O	2.01	0.60
1:O:2908:A:H2'	1:O:2909:G:O4'	2.01	0.60
19:O:16:VAL:HG12	19:O:17:GLY:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:74:ARG:O	13:I:78:ILE:HG12	2.01	0.60
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.31	0.60
1:O:2690:U:O2'	9:E:111:LYS:HE3	2.02	0.60
1:O:1741:U:O2'	1:O:2723:G:H4'	2.01	0.60
17:M:169:PRO:O	17:M:172:PHE:HB3	2.02	0.60
30:Z:21:ARG:HD2	30:Z:37:CYS:SG	2.41	0.60
13:I:39:VAL:HG12	13:I:40:ASN:ND2	2.17	0.59
19:O:59:ARG:HH22	19:O:66:GLN:HE22	1.51	0.59
1:O:1197:G:N2	42:O:5710:HOH:O	2.34	0.59
1:O:31:C:H2'	42:O:7158:HOH:O	2.01	0.59
12:H:59:ASN:ND2	12:H:59:ASN:N	2.50	0.59
29:Y:29:VAL:O	29:Y:33:HIS:HB2	2.02	0.59
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.84	0.59
16:L:60:ILE:C	16:L:61:ILE:HD12	2.23	0.59
17:M:86:LEU:O	17:M:90:LEU:HG	2.02	0.59
1:O:2578:G:C8	1:O:2578:G:H5'	2.34	0.59
12:H:127:GLY:O	12:H:128:ALA:HB3	2.03	0.59
29:Y:61:GLY:HA3	42:Y:8422:HOH:O	2.02	0.59
7:C:16:VAL:HG12	7:C:17:ASP:N	2.16	0.59
8:D:99:ASP:HB2	8:D:103:ASN:HB2	1.84	0.59
10:F:58:GLU:OE1	16:L:27:ARG:NH2	2.34	0.59
1:O:797:A:C4'	29:Y:10:ARG:N	2.65	0.59
12:H:35:ASN:ND2	12:H:80:ASN:HA	2.18	0.59
1:O:1187:U:O2'	1:O:1189:A:H2	1.86	0.59
1:O:2756:U:H3	1:O:2896:A:H2	1.49	0.59
1:O:1130:U:H5'	42:O:7141:HOH:O	2.02	0.59
30:Z:25:LYS:O	30:Z:25:LYS:HG2	2.02	0.59
29:Y:47:LEU:HD23	29:Y:57:CYS:HB2	1.85	0.59
42:O:6498:HOH:O	5:A:211:LYS:HG2	2.02	0.59
7:C:118:THR:HG23	42:C:8305:HOH:O	2.02	0.59
1:O:2718:C:H6	1:O:2718:C:H5'	1.68	0.59
1:O:1667:A:C8	1:O:1667:A:H5'	2.35	0.59
5:A:88:ILE:HD13	5:A:100:PRO:CD	2.31	0.59
5:A:81:GLN:HB2	5:A:92:ASN:ND2	2.17	0.59
1:O:2755:G:H1'	42:O:4158:HOH:O	2.03	0.59
16:L:87:MET:CB	32:2:46:ILE:HG21	2.33	0.59
16:L:74:ARG:NH1	16:L:74:ARG:HG3	2.18	0.59
8:D:25:MET:CE	8:D:37:ALA:HB1	2.32	0.59
16:L:38:VAL:C	16:L:63:VAL:HG13	2.23	0.59
14:J:106:GLY:HA3	42:J:5264:HOH:O	2.02	0.59
29:Y:31:ILE:O	29:Y:35:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:34:VAL:HG22	14:J:47:ALA:HB2	1.85	0.59
42:O:5501:HOH:O	20:P:50:GLY:HA2	2.02	0.59
23:S:101:LEU:HD13	23:S:112:LEU:HD11	1.85	0.59
1:O:189:A:OP1	16:L:171:ARG:NH2	2.36	0.59
2:9:3048:C:H4'	17:M:141:ARG:NH2	2.17	0.59
12:H:75:SER:C	12:H:79:ALA:HB2	2.23	0.59
26:V:65:VAL:HA	26:V:68:THR:HG22	1.84	0.59
7:C:180:SER:HB2	42:C:8449:HOH:O	2.01	0.59
25:U:64:GLY:O	25:U:65:ASP:HB2	2.03	0.59
1:O:1053:G:OP1	12:H:12:PRO:HG3	2.02	0.59
13:I:107:ASN:HD22	13:I:107:ASN:C	2.06	0.59
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.84	0.59
22:R:43:GLU:HB3	42:R:8344:HOH:O	2.03	0.59
8:D:91:ALA:HB1	42:D:5198:HOH:O	2.03	0.59
26:V:21:LEU:HD21	26:V:48:VAL:HG11	1.84	0.59
17:M:48:VAL:HG11	17:M:55:ASP:HB3	1.82	0.59
9:E:23:GLU:HG2	9:E:28:SER:CB	2.33	0.59
8:D:95:THR:C	8:D:97:GLN:H	2.06	0.59
1:O:88:G:H5'	1:O:88:G:H8	1.68	0.59
16:L:65:VAL:HG21	16:L:105:ALA:HB2	1.85	0.59
5:A:88:ILE:HG22	5:A:88:ILE:O	2.02	0.59
1:O:2408:A:HO2'	32:2:10:TYR:HD1	1.48	0.59
21:Q:104:PHE:HB2	21:Q:109:MET:HE1	1.84	0.58
15:K:145:LEU:O	15:K:148:GLU:HG3	2.03	0.58
20:P:11:ARG:HD3	42:P:5620:HOH:O	2.03	0.58
26:V:108:ARG:HE	26:V:114:PRO:HG3	1.66	0.58
32:2:48:ASN:ND2	32:2:50:GLY:H	2.00	0.58
1:O:240:C:H4'	16:L:146:GLN:NE2	2.18	0.58
1:O:2676:C:H4'	13:I:70:PHE:HE1	1.68	0.58
42:O:7149:HOH:O	16:L:154:ARG:HB2	2.03	0.58
12:H:109:ASP:HB2	42:H:8345:HOH:O	2.03	0.58
8:D:37:ALA:O	8:D:40:ILE:HG12	2.03	0.58
11:G:12:ILE:N	11:G:13:PRO:CD	2.66	0.58
24:T:13:ILE:HG12	24:T:32:CYS:CB	2.32	0.58
9:E:101:GLU:HB2	9:E:116:THR:O	2.03	0.58
42:O:9200:HOH:O	6:B:254:GLN:HG3	2.02	0.58
23:S:71:VAL:HG11	23:S:90:PRO:CB	2.26	0.58
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.85	0.58
8:D:64:ARG:CD	8:D:67:ASP:HB3	2.33	0.58
14:J:34:VAL:HB	42:J:7169:HOH:O	2.02	0.58
32:2:3:MET:O	32:2:90:PHE:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:111:ILE:HG23	21:Q:145:LEU:HD11	1.85	0.58
7:C:145:GLU:HG3	42:C:8380:HOH:O	2.02	0.58
16:L:87:MET:CB	32:2:46:ILE:HD13	2.33	0.58
17:M:141:ARG:N	42:M:8571:HOH:O	2.34	0.58
1:0:558:C:H2'	1:0:559:U:H5'	1.86	0.58
16:L:172:GLY:C	16:L:183:VAL:HG11	2.24	0.58
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
2:9:3013:A:O2'	2:9:3014:G:H5''	2.03	0.58
27:W:43:VAL:HG12	27:W:44:ASP:N	2.18	0.58
42:0:6923:HOH:O	6:B:211:THR:HG21	2.04	0.58
5:A:109:GLU:HG2	5:A:116:GLY:N	2.18	0.58
1:0:2047:C:H5'	42:0:9316:HOH:O	2.04	0.58
16:L:64:ARG:HD2	42:L:8586:HOH:O	2.03	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
9:E:69:ILE:HA	9:E:72:MET:CE	2.33	0.58
26:V:11:VAL:O	26:V:12:ASN:HB2	2.04	0.58
26:V:90:TYR:CE2	26:V:99:ALA:HB2	2.38	0.58
9:E:132:THR:HB	42:E:2227:HOH:O	2.03	0.58
26:V:84:VAL:HG12	42:V:6679:HOH:O	2.04	0.58
25:U:39:ALA:N	25:U:40:PRO:CD	2.66	0.58
6:B:7:ARG:HD3	6:B:9:GLY:O	2.03	0.58
7:C:246:ARG:NE	42:C:8430:HOH:O	2.36	0.58
1:0:2547:C:OP2	6:B:5:ARG:NH1	2.36	0.58
21:Q:119:VAL:HG21	21:Q:142:ASP:CG	2.24	0.58
1:0:1008:C:H5''	12:H:16:ARG:HH12	1.68	0.58
13:I:45:VAL:HG21	13:I:129:PHE:CD1	2.39	0.58
28:X:189:ASN:C	28:X:189:ASN:HD22	2.06	0.58
11:G:12:ILE:HB	42:G:4714:HOH:O	2.03	0.58
1:0:1209:C:H2'	1:0:1210:G:C8	2.38	0.58
1:0:1168:C:H2'	1:0:1169:U:O4'	2.03	0.58
25:U:58:THR:O	25:U:62:GLU:HG3	2.04	0.58
8:D:38:GLU:HB3	8:D:49:PRO:HG2	1.86	0.58
1:0:821:U:H5''	42:0:9545:HOH:O	2.02	0.58
12:H:136:VAL:HG23	42:H:8343:HOH:O	2.02	0.58
26:V:21:LEU:HD21	26:V:48:VAL:CG1	2.33	0.58
6:B:145:HIS:CD2	6:B:146:THR:O	2.56	0.58
6:B:275:GLY:O	6:B:291:ASP:HA	2.04	0.58
6:B:30:PRO:HB2	6:B:39:GLN:NE2	2.19	0.58
5:A:164:ARG:NE	42:A:8596:HOH:O	2.36	0.58
8:D:27:ILE:HG22	8:D:28:GLY:N	2.13	0.57
1:0:1205:U:C2'	1:0:1206:U:H5''	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:39:ALA:C	25:U:41:GLU:H	2.08	0.57
1:0:1477:C:O2'	1:0:1478:U:H5'	2.04	0.57
15:K:77:ALA:HB3	42:K:8537:HOH:O	2.02	0.57
2:9:3020:G:O2'	2:9:3021:G:H5'	2.04	0.57
29:Y:58:GLY:HA3	42:Y:8434:HOH:O	2.05	0.57
7:C:76:ARG:HD3	42:C:8372:HOH:O	2.03	0.57
29:Y:11:THR:CG2	29:Y:23:ARG:HB2	2.35	0.57
1:0:371:U:H2'	1:0:372:A:C8	2.39	0.57
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.38	0.57
42:0:9038:HOH:O	19:O:81:LYS:HG2	2.04	0.57
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.57
1:0:2637:A:H5''	3:3:74:C:H5'	1.86	0.57
26:V:38:THR:HG22	42:V:3580:HOH:O	2.03	0.57
29:Y:62:TYR:CE2	29:Y:64:ILE:HG23	2.39	0.57
27:W:78:GLU:HG2	27:W:79:GLU:N	2.17	0.57
14:J:74:VAL:CG1	14:J:113:ILE:HG12	2.35	0.57
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.87	0.57
30:Z:25:LYS:HE2	42:1:7213:HOH:O	2.02	0.57
1:0:65:C:O2'	1:0:66:G:H5'	2.03	0.57
1:0:818:A:O2'	29:Y:13:ARG:HD3	2.04	0.57
12:H:26:LYS:HD3	12:H:89:PRO:HG3	1.86	0.57
1:0:2781:U:C2'	1:0:2782:G:H5'	2.35	0.57
1:0:121:U:OP2	31:1:10:ARG:NH2	2.36	0.57
15:K:54:PRO:HG2	15:K:57:VAL:CG2	2.34	0.57
1:0:1528:A:H2'	1:0:1529:G:O4'	2.04	0.57
6:B:63:GLU:HG3	6:B:63:GLU:O	2.04	0.57
1:0:183:A:H5'	16:L:157:LEU:HD12	1.87	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.35	0.57
13:I:39:VAL:HG11	13:I:107:ASN:HB2	1.86	0.57
1:0:2409:C:H4'	32:2:17:HIS:HB2	1.87	0.57
8:D:50:VAL:O	8:D:71:ALA:HA	2.05	0.57
1:0:157:G:H4'	16:L:95:LYS:HE3	1.85	0.57
12:H:157:ILE:HG22	12:H:158:ASN:N	2.19	0.57
1:0:380:A:OP2	16:L:9:ARG:HD2	2.04	0.57
8:D:19:GLU:HG3	42:D:6165:HOH:O	2.04	0.57
1:0:567:U:H5''	42:V:5817:HOH:O	2.05	0.57
6:B:168:GLY:N	6:B:174:ARG:HD3	2.20	0.57
1:0:681:G:N3	1:0:681:G:H5'	2.20	0.57
11:G:63:ARG:N	42:G:2569:HOH:O	2.37	0.57
42:0:3996:HOH:O	16:L:94:LYS:HE3	2.05	0.57
1:0:485:A:N3	1:0:487:G:H5''	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2365:G:H4'	20:P:45:PRO:O	2.04	0.57
17:M:38:LYS:HD2	17:M:114:LYS:HE3	1.87	0.57
15:K:138:GLY:HA3	42:K:8559:HOH:O	2.04	0.57
12:H:47:GLU:CB	12:H:133:ILE:HD13	2.35	0.57
10:F:58:GLU:HA	10:F:61:MET:HE2	1.85	0.57
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.57
1:0:714:U:H3'	42:0:6416:HOH:O	2.04	0.57
1:0:1176:C:H1'	42:0:3420:HOH:O	2.04	0.57
1:0:1942:A:H3'	42:0:6815:HOH:O	2.05	0.57
1:0:1834:C:H2'	1:0:1840:A:N6	2.19	0.57
16:L:30:GLU:O	16:L:34:GLU:HG3	2.04	0.57
29:Y:11:THR:OG1	29:Y:23:ARG:HB2	2.05	0.57
1:0:2781:U:H2'	1:0:2782:G:H5'	1.86	0.57
15:K:143:THR:HG22	15:K:144:ASP:H	1.70	0.57
22:R:37:VAL:O	22:R:41:VAL:HG23	2.05	0.57
1:0:2840:A:OP1	6:B:211:THR:HG23	2.04	0.57
16:L:113:ARG:NH2	16:L:156:ARG:HG2	2.19	0.57
21:Q:106:GLY:HA2	21:Q:109:MET:CE	2.34	0.56
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.87	0.56
1:0:1086:A:C6	26:V:11:VAL:HG11	2.40	0.56
1:0:136:C:H2'	1:0:137:U:O4'	2.05	0.56
1:0:1887:U:OP1	29:Y:21:LYS:HE3	2.05	0.56
1:0:1634:G:H3'	42:0:3383:HOH:O	2.04	0.56
17:M:34:LEU:HA	17:M:47:LEU:HD23	1.86	0.56
17:M:89:GLY:O	17:M:92:ALA:HB3	2.05	0.56
2:9:3049:G:H5''	42:9:4707:HOH:O	2.04	0.56
26:V:122:ARG:NH2	42:V:4276:HOH:O	2.37	0.56
16:L:185:PRO:HG2	16:L:189:VAL:HG11	1.87	0.56
7:C:162:VAL:HG13	7:C:232:LEU:HD21	1.87	0.56
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.04	0.56
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.56
8:D:38:GLU:OE2	8:D:51:ARG:CZ	2.54	0.56
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.88	0.56
16:L:52:LEU:HD13	16:L:116:ASN:HB3	1.88	0.56
1:0:1180:U:H2'	1:0:1181:A:O4'	2.05	0.56
16:L:37:VAL:HG21	16:L:108:LYS:CG	2.35	0.56
23:S:9:LYS:CE	23:S:13:ARG:NH1	2.64	0.56
1:0:281:U:O2'	1:0:282:C:H5'	2.06	0.56
29:Y:25:ARG:O	29:Y:29:VAL:HG23	2.05	0.56
9:E:11:VAL:HG12	9:E:12:ASP:H	1.69	0.56
8:D:86:THR:O	8:D:90:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2285:G:H1	3:3:74:C:H42	1.51	0.56
21:Q:18:LEU:HD12	21:Q:143:VAL:CG1	2.35	0.56
1:0:2459:G:P	32:2:64:LYS:HB2	2.46	0.56
1:0:660:A:H4'	1:0:661:G:O5'	2.06	0.56
6:B:103:ASP:HB2	42:B:8589:HOH:O	2.04	0.56
6:B:85:ARG:NH1	42:B:8632:HOH:O	2.38	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.05	0.56
1:0:625:U:H5''	1:0:1044:C:N4	2.20	0.56
15:K:149:ARG:O	15:K:150:GLN:HB2	2.06	0.56
1:0:960:G:H2'	1:0:960:G:N3	2.21	0.56
31:1:18:ASN:HD21	31:1:40:ARG:H	1.53	0.56
2:9:3029:C:C2'	2:9:3030:C:H5'	2.35	0.56
7:C:246:ARG:NH2	42:C:8430:HOH:O	2.37	0.56
19:O:105:LEU:HD21	19:O:137:LEU:HD21	1.86	0.56
1:0:2089:A:O2'	1:0:2090:G:H5'	2.06	0.56
1:0:2679:G:H2'	1:0:2681:A:OP2	2.05	0.56
1:0:1730:G:H5'	1:0:1731:C:C5	2.41	0.56
1:0:1119:G:H8	13:I:52:GLN:HE22	1.54	0.56
28:X:185:VAL:HG12	42:X:8571:HOH:O	2.04	0.56
8:D:99:ASP:CB	8:D:103:ASN:H	2.19	0.56
26:V:122:ARG:HH22	26:V:154:ARG:C	2.09	0.56
11:G:12:ILE:HG22	11:G:12:ILE:O	2.05	0.56
24:T:9:CYS:CA	24:T:52:THR:HG23	2.35	0.56
10:F:46:GLU:N	42:F:3461:HOH:O	2.39	0.56
10:F:47:LEU:HB2	10:F:108:LEU:HD11	1.88	0.56
2:9:3044:A:O4'	8:D:76:ARG:NE	2.39	0.56
16:L:55:LYS:HB2	16:L:60:ILE:CD1	2.35	0.56
28:X:235:GLU:H	28:X:235:GLU:CD	2.07	0.56
25:U:44:GLY:O	25:U:48:GLU:HG2	2.05	0.56
1:0:1123:A:C6	1:0:1238:C:H5'	2.41	0.56
1:0:2329:C:O2'	1:0:2330:U:H5'	2.06	0.56
1:0:1132:A:N6	1:0:1229:C:H2'	2.21	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.06	0.56
17:M:71:TRP:HE3	17:M:175:LEU:HD22	1.69	0.56
42:J:408:HOH:O	24:T:37:GLU:HB3	2.04	0.56
5:A:199:HIS:CD2	5:A:201:PHE:H	2.24	0.56
17:M:154:LEU:HG	17:M:155:GLU:H	1.71	0.56
7:C:133:ARG:HD2	42:C:8417:HOH:O	2.06	0.56
1:0:2469:A:H1'	42:O:9736:HOH:O	2.06	0.56
23:S:9:LYS:HD2	42:S:7242:HOH:O	2.06	0.56
1:0:558:C:C2'	1:0:559:U:H5''	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:7:ILE:HD11	9:E:11:VAL:O	2.06	0.56
1:O:2781:U:H1'	9:E:139:GLU:OE2	2.06	0.56
16:L:149:TRP:O	16:L:152:ARG:HG2	2.04	0.56
31:1:48:ASP:O	31:1:49:GLU:HB2	2.06	0.56
2:9:3051:A:H5'	17:M:160:SER:HB3	1.88	0.56
1:O:659:A:H5''	42:O:6568:HOH:O	2.06	0.56
27:W:74:ALA:CB	27:W:85:VAL:HG22	2.36	0.56
1:O:797:A:H4'	29:Y:10:ARG:N	2.21	0.56
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.88	0.56
8:D:174:VAL:HG13	42:D:6555:HOH:O	2.06	0.56
2:9:3039:U:H1'	2:9:3044:A:N6	2.21	0.56
1:O:1669:A:H2'	1:O:1670:G:C8	2.41	0.56
1:O:157:G:H4'	16:L:95:LYS:CE	2.37	0.55
1:O:2502:C:H4'	12:H:151:MET:HG2	1.88	0.55
17:M:37:ARG:NH2	42:M:8535:HOH:O	2.38	0.55
10:F:91:VAL:CG1	10:F:92:GLY:N	2.67	0.55
1:O:1118:A:C8	1:O:1118:A:C3'	2.85	0.55
26:V:141:HIS:HB2	26:V:146:ILE:HG12	1.87	0.55
21:Q:39:THR:CB	21:Q:42:GLU:HG3	2.36	0.55
10:F:101:ALA:HA	42:F:5413:HOH:O	2.06	0.55
27:W:43:VAL:CG1	27:W:47:ALA:HB3	2.36	0.55
1:O:2081:A:H4'	13:I:69:TYR:CE1	2.41	0.55
1:O:1687:C:O2	30:Z:9:GLY:HA2	2.06	0.55
28:X:106:THR:HG23	28:X:107:PRO:HD2	1.87	0.55
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.36	0.55
2:9:3054:A:O2'	2:9:3055:U:H5'	2.06	0.55
7:C:77:ALA:O	7:C:78:ARG:HG3	2.06	0.55
5:A:153:ARG:CB	5:A:153:ARG:HH11	2.19	0.55
1:O:2694:A:H4'	9:E:91:PHE:CE1	2.40	0.55
28:X:163:THR:HG23	42:X:8529:HOH:O	2.06	0.55
1:O:138:U:H5''	1:O:139:C:OP2	2.06	0.55
1:O:2563:U:H2'	1:O:2565:C:O5'	2.06	0.55
7:C:142:ASP:OD1	7:C:237:GLU:HB3	2.06	0.55
1:O:1733:A:H4'	6:B:212:GLN:HA	1.87	0.55
1:O:2769:C:O2'	1:O:2770:G:H5'	2.06	0.55
1:O:2694:A:H4'	9:E:91:PHE:HE1	1.70	0.55
6:B:75:GLU:C	6:B:77:PRO:HD3	2.26	0.55
21:Q:17:MET:HE1	21:Q:19:ARG:NH2	2.22	0.55
27:W:72:VAL:HG22	27:W:85:VAL:CG1	2.35	0.55
13:I:39:VAL:CG1	13:I:107:ASN:HB2	2.36	0.55
6:B:51:VAL:HG23	6:B:329:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2672:C:H1'	42:B:8632:HOH:O	2.06	0.55
1:O:1717:A:H5''	19:O:54:LYS:HB2	1.89	0.55
32:2:11:CYS:HB2	32:2:20:HIS:CE1	2.41	0.55
1:O:2115:U:H2'	1:O:2116:U:C6	2.41	0.55
12:H:85:ILE:HB	12:H:132:PHE:CE2	2.41	0.55
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.72	0.55
17:M:37:ARG:CZ	42:M:8535:HOH:O	2.54	0.55
14:J:87:ARG:CZ	42:J:4854:HOH:O	2.54	0.55
16:L:57:LYS:HE2	16:L:140:ALA:O	2.06	0.55
19:O:10:ALA:HA	19:O:13:VAL:HG12	1.88	0.55
6:B:138:GLY:O	6:B:139:ASP:O	2.24	0.55
42:O:4996:HOH:O	6:B:298:LYS:HD3	2.06	0.55
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.22	0.55
1:O:2359:G:H3'	42:O:5166:HOH:O	2.05	0.55
21:Q:14:ALA:HB3	21:Q:147:LEU:HB2	1.87	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
30:Z:28:HIS:HD2	30:Z:30:LYS:H	1.54	0.55
29:Y:39:CYS:HA	29:Y:47:LEU:CD1	2.35	0.55
17:M:87:LEU:CD1	17:M:186:LEU:HD21	2.31	0.55
1:O:542:A:H5'	1:O:542:A:C8	2.33	0.55
1:O:2316:G:H8	42:O:5129:HOH:O	1.88	0.55
32:2:69:TYR:HB2	32:2:78:HIS:CE1	2.42	0.55
23:S:37:GLN:OE1	23:S:118:SER:HA	2.06	0.55
16:L:71:SER:HB2	16:L:92:THR:HG22	1.88	0.55
1:O:1182:C:H1'	1:O:1192:A:H8	1.72	0.55
22:R:57:THR:HG22	22:R:58:MET:N	2.20	0.55
1:O:2769:C:C2'	1:O:2770:G:H5'	2.37	0.55
5:A:199:HIS:HD2	5:A:201:PHE:H	1.55	0.55
6:B:304:PRO:HD2	6:B:307:ARG:HD2	1.87	0.55
27:W:21:PRO:HG2	27:W:24:LYS:HD3	1.87	0.55
1:O:184:G:H5''	16:L:153:THR:HG22	1.88	0.55
1:O:1773:G:C8	29:Y:16:PRO:HA	2.41	0.55
42:O:3173:HOH:O	16:L:79:LYS:HD3	2.06	0.55
17:M:67:ALA:HA	17:M:71:TRP:H	1.71	0.55
1:O:2094:G:C4'	6:B:245:SER:HB3	2.36	0.55
7:C:93:LYS:O	7:C:98:ARG:NH2	2.40	0.55
1:O:2638:G:H1'	42:O:7230:HOH:O	2.05	0.55
7:C:246:ARG:HB3	7:C:246:ARG:NH1	2.22	0.55
18:N:96:VAL:HA	42:N:4258:HOH:O	2.05	0.55
16:L:59:GLY:HA3	16:L:141:ILE:HD12	1.89	0.55
10:F:48:VAL:CG2	10:F:74:PHE:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:74:C:C2'	4:4:75:C:H5'	2.35	0.55
27:W:76:ARG:O	27:W:77:PHE:HB3	2.06	0.55
31:1:22:PRO:HG2	31:1:25:VAL:CG2	2.36	0.55
16:L:61:ILE:N	16:L:61:ILE:HD12	2.22	0.55
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.55
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.71	0.55
28:X:185:VAL:HA	42:X:8565:HOH:O	2.06	0.55
27:W:9:VAL:HG13	27:W:88:GLU:OE2	2.07	0.55
21:Q:40:ALA:O	21:Q:44:VAL:HG23	2.07	0.55
9:E:137:ASP:O	9:E:141:VAL:HG23	2.07	0.55
17:M:139:TRP:HA	17:M:139:TRP:CE3	2.41	0.55
17:M:58:LEU:HD12	17:M:58:LEU:N	2.22	0.55
1:0:1759:A:N3	1:0:1818:C:H2'	2.21	0.55
8:D:10:PHE:CG	8:D:11:HIS:N	2.75	0.55
12:H:150:LYS:CB	12:H:157:ILE:HD12	2.33	0.54
29:Y:57:CYS:SG	29:Y:59:HIS:HB3	2.47	0.54
27:W:37:LEU:CD1	27:W:85:VAL:HG21	2.30	0.54
17:M:90:LEU:HB2	17:M:186:LEU:HD22	1.87	0.54
6:B:315:VAL:HG23	6:B:316:ARG:HG2	1.89	0.54
1:0:1500:U:P	19:O:41:ARG:HH22	2.30	0.54
2:9:3042:C:H2'	42:9:6700:HOH:O	2.07	0.54
1:0:2594:C:O2'	1:0:2595:U:H5'	2.07	0.54
17:M:11:ARG:HG3	17:M:14:ARG:NH1	2.21	0.54
15:K:104:ASP:O	15:K:105:TYR:HB3	2.06	0.54
28:X:126:PRO:HG2	28:X:128:PHE:CE1	2.42	0.54
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.89	0.54
1:0:1134:G:C4'	12:H:151:MET:HE1	2.26	0.54
7:C:233:THR:HG22	7:C:234:VAL:N	2.22	0.54
6:B:254:GLN:HG2	6:B:255:GLY:N	2.21	0.54
6:B:55:ASN:HB3	6:B:63:GLU:HA	1.89	0.54
15:K:30:ARG:NH2	42:K:8527:HOH:O	2.40	0.54
1:0:1189:A:H1'	1:0:1209:C:C1'	2.37	0.54
10:F:48:VAL:HG23	10:F:74:PHE:CB	2.37	0.54
1:0:1525:G:H5'	1:0:1526:A:OP2	2.07	0.54
28:X:112:GLU:OE1	28:X:112:GLU:HA	2.08	0.54
18:N:39:THR:O	18:N:115:ARG:NH2	2.40	0.54
12:H:3:GLY:HA2	12:H:57:ARG:NH1	2.22	0.54
28:X:141:THR:HG23	42:X:8589:HOH:O	2.08	0.54
1:0:1735:C:O2'	1:0:1736:A:H5'	2.07	0.54
1:0:1192:A:H3'	1:0:1193:A:H5'	1.90	0.54
13:I:19:MET:HE2	13:I:79:PHE:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:ASP:O	7:C:108:GLN:HG3	2.07	0.54
1:O:2346:C:O5'	1:O:2346:C:H6	1.90	0.54
32:2:11:CYS:SG	32:2:71:CYS:HB2	2.48	0.54
1:O:1595:G:O2'	1:O:1596:U:H5'	2.08	0.54
1:O:1699:C:H4'	42:O:5916:HOH:O	2.06	0.54
16:L:87:MET:HB3	32:2:46:ILE:HD13	1.90	0.54
13:I:130:VAL:HG12	13:I:131:THR:N	2.21	0.54
9:E:11:VAL:CG1	9:E:12:ASP:N	2.70	0.54
1:O:2316:G:H4'	42:O:5568:HOH:O	2.07	0.54
5:A:101:GLU:OE2	5:A:131:HIS:HB2	2.08	0.54
23:S:24:ARG:HH21	23:S:39:ASN:HD22	1.54	0.54
1:O:2559:C:H4'	42:O:6727:HOH:O	2.07	0.54
1:O:2830:U:H3'	42:O:4704:HOH:O	2.07	0.54
1:O:1535:G:H2'	1:O:1536:C:C6	2.43	0.54
1:O:2073:G:OP2	1:O:2490:A:H5'	2.07	0.54
29:Y:18:TYR:HB3	29:Y:22:ILE:HG21	1.90	0.54
30:Z:1:THR:HA	42:Z:8411:HOH:O	2.07	0.54
6:B:139:ASP:HB2	6:B:165:ARG:HE	1.73	0.54
1:O:2122:C:H3'	42:O:4767:HOH:O	2.08	0.54
42:O:6473:HOH:O	20:P:9:GLY:HA2	2.07	0.54
1:O:12:U:H2'	1:O:13:G:H5'	1.89	0.54
16:L:72:SER:OG	16:L:74:ARG:HB2	2.07	0.54
16:L:74:ARG:NH2	42:L:8634:HOH:O	2.41	0.54
29:Y:47:LEU:CD2	29:Y:57:CYS:HB2	2.37	0.54
13:I:74:ARG:NH1	13:I:76:ASP:HB2	2.23	0.54
1:O:2506:A:O2'	1:O:2507:G:O5'	2.26	0.54
11:G:64:ASN:O	11:G:68:GLU:HG3	2.08	0.54
9:E:69:ILE:HA	9:E:72:MET:HE2	1.89	0.54
15:K:54:PRO:HG2	15:K:57:VAL:HG21	1.88	0.54
9:E:31:ARG:NH1	42:E:5919:HOH:O	2.40	0.54
7:C:61:PHE:HB3	42:C:8448:HOH:O	2.07	0.54
28:X:172:THR:HG22	28:X:173:ALA:N	2.21	0.54
26:V:119:HIS:HD2	26:V:120:PRO:O	1.91	0.54
7:C:219:ASN:O	7:C:222:ASP:OD1	2.25	0.54
10:F:19:ALA:O	10:F:22:VAL:HG22	2.08	0.54
23:S:73:HIS:CD2	23:S:88:PRO:HG3	2.43	0.54
8:D:51:ARG:HD3	42:D:7636:HOH:O	2.08	0.54
12:H:139:ASP:N	12:H:140:PRO:CD	2.70	0.54
1:O:289:G:O2'	1:O:290:C:H5'	2.08	0.54
5:A:132:ASP:OD1	5:A:133:ARG:N	2.40	0.54
19:O:80:ARG:HG2	19:O:87:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:8591:HOH:O	6:B:214:PRO:HD2	2.06	0.54
1:O:328:U:O4'	7:C:202:THR:HG22	2.07	0.54
9:E:137:ASP:OD1	9:E:139:GLU:HB2	2.08	0.54
27:W:25:ARG:NH1	42:W:3861:HOH:O	2.41	0.54
27:W:15:ARG:NH1	27:W:15:ARG:HB3	2.22	0.54
6:B:175:LEU:O	6:B:175:LEU:HD23	2.08	0.54
1:O:1527:A:H1'	1:O:1528:A:C8	2.43	0.54
42:O:4554:HOH:O	6:B:216:LYS:HA	2.08	0.54
26:V:125:HIS:HE1	42:V:3071:HOH:O	1.90	0.54
6:B:248:ARG:NH1	42:B:8612:HOH:O	2.40	0.54
1:O:820:G:OP2	5:A:171:LYS:NZ	2.35	0.53
26:V:6:GLN:CB	26:V:26:ILE:HD12	2.33	0.53
7:C:214:THR:HG23	42:C:8441:HOH:O	2.07	0.53
8:D:140:ARG:O	8:D:144:ARG:HG2	2.08	0.53
25:U:49:LEU:O	25:U:53:ILE:HG13	2.08	0.53
1:O:2779:G:H21	9:E:143:GLN:NE2	2.05	0.53
19:O:13:VAL:HG21	19:O:41:ARG:HG2	1.90	0.53
17:M:154:LEU:HG	17:M:155:GLU:N	2.23	0.53
2:9:3041:C:O4'	8:D:50:VAL:HG23	2.08	0.53
8:D:166:ILE:HD12	42:D:6326:HOH:O	2.07	0.53
26:V:21:LEU:HB3	26:V:26:ILE:HG12	1.90	0.53
15:K:114:VAL:HG11	42:K:8578:HOH:O	2.08	0.53
12:H:3:GLY:HA2	12:H:57:ARG:HH12	1.72	0.53
5:A:109:GLU:HG2	5:A:116:GLY:H	1.72	0.53
29:Y:53:GLY:HA2	29:Y:67:GLY:O	2.07	0.53
1:O:2312:G:H2'	1:O:2313:C:H5'	1.90	0.53
13:I:26:VAL:HG13	13:I:36:VAL:HG11	1.90	0.53
8:D:23:VAL:HG21	8:D:45:THR:CG2	2.37	0.53
26:V:4:LEU:O	26:V:32:CYS:HA	2.08	0.53
1:O:1829:A:H61	29:Y:18:TYR:HA	1.71	0.53
13:I:107:ASN:HD22	13:I:109:TYR:H	1.56	0.53
22:R:57:THR:CG2	22:R:58:MET:N	2.70	0.53
1:O:2768:A:O2'	1:O:2769:C:H5'	2.09	0.53
7:C:65:ARG:HG3	7:C:67:GLN:HB2	1.90	0.53
12:H:166:ASN:ND2	12:H:166:ASN:N	2.57	0.53
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.44	0.53
14:J:109:LEU:HD13	14:J:113:ILE:HD11	1.89	0.53
15:K:143:THR:CG2	15:K:144:ASP:N	2.70	0.53
5:A:194:MET:CE	5:A:199:HIS:HB2	2.39	0.53
12:H:53:PRO:HA	12:H:125:VAL:O	2.07	0.53
1:O:120:A:N3	1:O:120:A:H2'	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:OP2	18:N:37:ARG:HD2	2.09	0.53
6:B:32:ASP:HA	42:B:8571:HOH:O	2.08	0.53
1:0:2502:C:C4'	12:H:151:MET:HG2	2.39	0.53
1:0:821:U:H2'	1:0:822:C:H6	1.72	0.53
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.41	0.53
1:0:542:A:H2'	1:0:543:G:O4'	2.08	0.53
1:0:1930:A:H1'	1:0:2128:G:H5'	1.89	0.53
24:T:9:CYS:HA	24:T:52:THR:CG2	2.39	0.53
14:J:58:THR:HG22	14:J:59:LYS:HG3	1.91	0.53
42:0:3675:HOH:O	28:X:186:ARG:HD2	2.08	0.53
17:M:152:GLU:C	17:M:154:LEU:H	2.10	0.53
1:0:2363:G:O3'	20:P:11:ARG:NH1	2.41	0.53
26:V:38:THR:HB	42:V:5390:HOH:O	2.08	0.53
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.41	0.53
6:B:82:VAL:O	6:B:82:VAL:HG12	2.08	0.53
1:0:1422:U:H2'	1:0:1423:C:C6	2.44	0.53
32:2:73:GLU:HB3	42:2:8567:HOH:O	2.07	0.53
1:0:1353:C:P	42:0:4154:HOH:O	2.66	0.53
42:0:8630:HOH:O	16:L:82:ARG:HD2	2.09	0.53
12:H:62:GLU:HA	42:H:8385:HOH:O	2.07	0.53
42:3:7215:HOH:O	37:4:76:PPU:HD2	2.09	0.53
14:J:75:ARG:CZ	42:J:4172:HOH:O	2.57	0.53
1:0:283:U:H5''	1:0:284:C:P	2.48	0.53
8:D:94:ALA:HB3	8:D:174:VAL:HA	1.91	0.53
25:U:64:GLY:O	25:U:65:ASP:CB	2.56	0.53
1:0:119:A:H2'	1:0:120:A:H5''	1.91	0.53
1:0:514:G:O5'	1:0:514:G:H8	1.91	0.53
15:K:21:ARG:N	42:K:8538:HOH:O	2.42	0.53
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.44	0.53
23:S:47:THR:HB	23:S:100:ASP:HB3	1.91	0.53
21:Q:82:GLU:HG3	21:Q:83:LYS:N	2.23	0.53
1:0:349:U:O2'	1:0:350:C:H5'	2.09	0.53
1:0:1242:A:OP2	13:I:60:ARG:NH2	2.41	0.53
1:0:1060:C:H6	1:0:1060:C:H5'	1.74	0.53
16:L:47:ASP:CG	16:L:48:ARG:N	2.62	0.53
14:J:30:LYS:O	14:J:55:VAL:HG13	2.09	0.53
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.77	0.53
1:0:1189:A:H1'	1:0:1209:C:O4'	2.09	0.53
27:W:15:ARG:HH11	27:W:15:ARG:CB	2.21	0.53
17:M:157:PRO:HA	42:M:8526:HOH:O	2.08	0.53
17:M:11:ARG:O	17:M:15:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:671:A:O2'	1:0:672:G:H2'	2.09	0.53
1:0:2379:G:H4'	1:0:2380:A:H5''	1.90	0.53
17:M:110:THR:HB	17:M:113:SER:OG	2.09	0.53
19:O:105:LEU:CD2	19:O:137:LEU:HD21	2.39	0.53
9:E:80:TRP:O	9:E:134:SER:HA	2.08	0.53
17:M:29:SER:HA	42:M:8558:HOH:O	2.08	0.53
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.53
12:H:86:ARG:HD3	12:H:130:HIS:HD2	1.73	0.52
16:L:87:MET:HB3	32:2:46:ILE:HG21	1.91	0.52
6:B:333:GLU:HB2	24:T:14:GLU:OE2	2.09	0.52
5:A:199:HIS:HD2	5:A:201:PHE:HB2	1.74	0.52
32:2:11:CYS:HB2	32:2:20:HIS:HE1	1.74	0.52
1:0:316:A:H5'	23:S:54:ASP:OD2	2.10	0.52
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.91	0.52
1:0:2019:A:H5'	42:0:4012:HOH:O	2.09	0.52
9:E:10:ASP:HA	42:E:3707:HOH:O	2.09	0.52
1:0:338:C:H4'	7:C:174:ILE:HD12	1.91	0.52
1:0:553:G:O4'	1:0:1325:G:H5'	2.08	0.52
18:N:47:ARG:NH1	18:N:47:ARG:HG3	2.22	0.52
6:B:27:ASN:HB3	42:B:8625:HOH:O	2.09	0.52
1:0:2301:A:H5''	1:0:2302:A:H5'	1.90	0.52
1:0:951:A:C2'	1:0:952:G:H5'	2.39	0.52
1:0:1213:C:O2'	1:0:1214:G:H5'	2.09	0.52
1:0:2382:A:H5'	42:2:8538:HOH:O	2.09	0.52
23:S:1:SER:N	42:S:5837:HOH:O	2.42	0.52
1:0:1279:U:H5''	42:0:9091:HOH:O	2.09	0.52
1:0:2717:C:O2'	1:0:2718:C:H5''	2.09	0.52
5:A:69:LEU:CD2	5:A:120:ARG:HB3	2.39	0.52
17:M:159:TYR:HE2	17:M:163:PHE:HE2	1.58	0.52
1:0:1377:C:H5'	1:0:1377:C:C6	2.42	0.52
9:E:15:GLN:NE2	9:E:40:VAL:O	2.42	0.52
1:0:1044:C:H5''	42:0:8544:HOH:O	2.08	0.52
1:0:297:U:H1'	42:0:3425:HOH:O	2.09	0.52
16:L:87:MET:CG	32:2:46:ILE:HD13	2.40	0.52
15:K:143:THR:HG22	15:K:145:LEU:H	1.73	0.52
1:0:661:G:C5	1:0:686:A:C2	2.97	0.52
7:C:57:PRO:HD2	7:C:73:LEU:HD22	1.91	0.52
1:0:500:G:H21	21:Q:98:ASN:HD21	1.56	0.52
14:J:32:ILE:HD11	14:J:56:SER:HB3	1.91	0.52
1:0:1874:U:H2'	5:A:120:ARG:HG3	1.92	0.52
1:0:1159:G:H21	1:0:1189:A:H8	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:470:U:O2'	30:Z:16:HIS:CD2	2.62	0.52
15:K:57:VAL:HG12	15:K:57:VAL:O	2.10	0.52
42:0:9445:HOH:O	27:W:23:HIS:HD2	1.92	0.52
27:W:18:ARG:NH1	42:W:4132:HOH:O	2.37	0.52
1:0:2445:U:H2'	1:0:2446:G:C8	2.45	0.52
12:H:157:ILE:CG2	12:H:158:ASN:N	2.73	0.52
1:0:820:G:O2'	1:0:856:G:H4'	2.10	0.52
8:D:86:THR:HG23	42:D:7477:HOH:O	2.09	0.52
10:F:99:THR:HG23	10:F:99:THR:O	2.09	0.52
6:B:305:ASP:O	6:B:306:LYS:HB2	2.10	0.52
1:0:920:C:H5'	1:0:921:G:C4	2.44	0.52
5:A:8:ARG:HG2	42:A:8556:HOH:O	2.10	0.52
14:J:87:ARG:NE	42:J:4854:HOH:O	2.42	0.52
26:V:5:VAL:HG22	26:V:32:CYS:HB2	1.91	0.52
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.91	0.52
8:D:135:VAL:HG22	8:D:136:ARG:H	1.73	0.52
1:0:920:C:H5''	1:0:921:G:O5'	2.09	0.52
30:Z:10:LYS:HG3	42:Z:8434:HOH:O	2.10	0.52
5:A:179:MET:HG2	5:A:186:TRP:CG	2.45	0.52
2:9:3023:U:C5'	2:9:3024:U:OP2	2.54	0.52
13:I:46:ILE:HG12	13:I:53:ILE:HD13	1.92	0.52
28:X:187:VAL:HB	42:X:8571:HOH:O	2.09	0.52
28:X:187:VAL:HG23	28:X:192:ASP:HB3	1.88	0.52
1:0:2748:G:H1'	42:0:7371:HOH:O	2.10	0.52
1:0:2815:G:N7	13:I:80:LYS:NZ	2.57	0.52
6:B:280:VAL:HG13	6:B:333:GLU:O	2.10	0.52
24:T:17:THR:HG22	24:T:18:GLY:N	2.25	0.52
8:D:94:ALA:O	8:D:95:THR:O	2.28	0.52
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.28	0.52
1:0:1505:U:H5'	1:0:1505:U:H6	1.74	0.52
7:C:40:ALA:HB3	7:C:100:LEU:HD12	1.92	0.52
29:Y:46:LYS:O	29:Y:57:CYS:HA	2.09	0.52
12:H:14:TYR:N	12:H:91:HIS:CE1	2.75	0.52
8:D:86:THR:C	8:D:89:PRO:HD2	2.30	0.52
26:V:64:THR:O	26:V:68:THR:HG22	2.10	0.52
1:0:2438:G:H2'	1:0:2439:C:O4'	2.10	0.52
10:F:107:VAL:HG23	42:F:6617:HOH:O	2.09	0.52
2:9:3020:G:H3'	42:9:2984:HOH:O	2.10	0.52
42:0:5686:HOH:O	6:B:2:GLN:HA	2.10	0.52
1:0:970:U:H2'	42:0:5804:HOH:O	2.10	0.52
1:0:2281:C:C2'	1:0:2282:U:H5'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:8:TYR:CD2	24:T:36:CYS:HB3	2.44	0.52
26:V:122:ARG:NE	42:V:5817:HOH:O	2.42	0.52
29:Y:19:GLY:O	29:Y:23:ARG:HG2	2.09	0.52
27:W:76:ARG:HG3	27:W:76:ARG:NH1	2.24	0.52
17:M:171:HIS:CE1	42:M:8568:HOH:O	2.62	0.52
10:F:46:GLU:O	10:F:73:PRO:HD2	2.10	0.52
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.10	0.52
1:O:1887:U:OP1	29:Y:21:LYS:HG3	2.10	0.52
16:L:134:ILE:HG23	16:L:141:ILE:HD13	1.91	0.52
7:C:33:LYS:HE2	42:C:8364:HOH:O	2.10	0.52
28:X:99:ALA:HB2	28:X:233:TYR:CZ	2.45	0.52
1:O:1398:G:H2'	1:O:1399:A:C8	2.45	0.52
1:O:834:G:H4'	1:O:835:U:OP2	2.10	0.52
1:O:407:A:H5'	42:O:5500:HOH:O	2.10	0.52
1:O:2015:A:H2'	1:O:2016:U:O4'	2.09	0.52
23:S:71:VAL:CG1	23:S:90:PRO:HB3	2.27	0.51
16:L:37:VAL:CG1	16:L:63:VAL:HG11	2.40	0.51
1:O:1010:C:H4'	17:M:4:PRO:HB2	1.92	0.51
21:Q:39:THR:HB	21:Q:42:GLU:CD	2.30	0.51
1:O:2524:G:H21	1:O:2526:C:N4	2.08	0.51
1:O:1189:A:O2'	1:O:1208:C:H2'	2.10	0.51
28:X:144:ARG:NE	42:X:8612:HOH:O	2.43	0.51
26:V:106:THR:OG1	26:V:109:GLU:HG3	2.10	0.51
1:O:1592:G:O2'	1:O:1593:C:O4'	2.28	0.51
1:O:29:C:O2'	1:O:30:U:H5'	2.11	0.51
1:O:1942:A:O2'	1:O:1943:C:H5'	2.10	0.51
1:O:1191:A:C3'	1:O:1192:A:H5''	2.41	0.51
1:O:2123:A:OP1	16:L:89:ASN:ND2	2.43	0.51
28:X:189:ASN:ND2	28:X:192:ASP:H	2.08	0.51
28:X:186:ARG:NH1	28:X:186:ARG:HG2	2.24	0.51
5:A:99:ILE:O	5:A:131:HIS:CE1	2.62	0.51
1:O:1477:C:H5'	1:O:1868:G:C5'	2.40	0.51
30:Z:28:HIS:O	30:Z:32:LYS:N	2.40	0.51
1:O:449:A:N7	7:C:43:LYS:HG2	2.24	0.51
16:L:155:HIS:CE1	16:L:158:ARG:HE	2.29	0.51
26:V:149:LEU:HG	26:V:153:MET:CE	2.39	0.51
29:Y:42:CYS:SG	29:Y:43:GLY:N	2.83	0.51
26:V:88:THR:HG23	26:V:110:GLN:HB3	1.91	0.51
1:O:1884:G:O6	5:A:190:ARG:HD2	2.10	0.51
1:O:1829:A:H5''	42:O:9576:HOH:O	2.09	0.51
17:M:154:LEU:O	17:M:155:GLU:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.39	0.51
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.43	0.51
6:B:248:ARG:O	6:B:251:VAL:CG1	2.58	0.51
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.73	0.51
25:U:11:MET:HB3	25:U:15:GLU:HB2	1.91	0.51
26:V:21:LEU:HD13	26:V:26:ILE:HD11	1.92	0.51
1:0:1667:A:H2'	1:0:1668:U:C6	2.45	0.51
32:2:74:CYS:SG	32:2:76:LYS:HB2	2.50	0.51
12:H:162:SER:CB	12:H:163:PRO:CD	2.83	0.51
2:9:3076:G:C3'	2:9:3077:A:H5''	2.33	0.51
7:C:107:ARG:NE	42:C:8462:HOH:O	2.29	0.51
5:A:105:VAL:HG13	5:A:155:THR:O	2.11	0.51
21:Q:132:ARG:CZ	42:Q:8585:HOH:O	2.58	0.51
8:D:11:HIS:O	8:D:12:GLU:HB3	2.10	0.51
7:C:200:PRO:HB3	7:C:212:VAL:HG23	1.92	0.51
1:0:2251:G:H2'	1:0:2252:A:C8	2.45	0.51
28:X:155:ARG:NH1	42:X:8559:HOH:O	2.44	0.51
1:0:2670:G:O2'	1:0:2671:U:H5'	2.10	0.51
12:H:83:PHE:CD1	12:H:134:ALA:HB2	2.46	0.51
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.51
1:0:1181:A:H2'	1:0:1182:C:O4'	2.11	0.51
8:D:64:ARG:O	8:D:67:ASP:OD2	2.28	0.51
2:9:3003:A:H2'	42:9:2430:HOH:O	2.10	0.51
15:K:104:ASP:HB3	42:K:8570:HOH:O	2.10	0.51
16:L:155:HIS:ND1	16:L:158:ARG:NE	2.54	0.51
18:N:21:SER:OG	18:N:106:PRO:HB2	2.11	0.51
1:0:1753:C:O2	6:B:229:ARG:NH2	2.43	0.51
1:0:2114:C:OP1	5:A:1:GLY:HA2	2.11	0.51
12:H:13:ALA:HA	12:H:91:HIS:CE1	2.46	0.51
29:Y:26:VAL:O	29:Y:30:GLU:HG3	2.11	0.51
1:0:1189:A:H1'	1:0:1209:C:H1'	1.93	0.51
1:0:1299:G:N2	42:0:4159:HOH:O	2.43	0.51
1:0:710:G:OP1	18:N:24:ALA:HB3	2.10	0.51
1:0:2111:G:H1'	42:0:8565:HOH:O	2.08	0.51
29:Y:22:ILE:O	29:Y:26:VAL:HG23	2.11	0.51
8:D:57:THR:HG23	8:D:63:ILE:CB	2.41	0.51
6:B:280:VAL:CG1	6:B:334:SER:HA	2.40	0.51
11:G:64:ASN:N	11:G:64:ASN:ND2	2.57	0.51
1:0:2408:A:H1'	32:2:10:TYR:CD1	2.46	0.51
1:0:1114:A:H2'	1:0:1115:U:C6	2.46	0.51
21:Q:17:MET:CE	21:Q:19:ARG:NH2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:694:A:H2'	1:0:695:C:H5'	1.92	0.51
6:B:204:GLY:HA3	42:B:8650:HOH:O	2.11	0.51
42:0:9295:HOH:O	14:J:39:GLY:HA3	2.10	0.51
5:A:37:VAL:HG22	42:A:8604:HOH:O	2.10	0.51
26:V:122:ARG:CG	26:V:122:ARG:HH11	2.19	0.51
1:0:1878:G:C1'	42:0:5597:HOH:O	2.54	0.51
1:0:2460:A:OP1	32:2:60:LYS:HB3	2.10	0.51
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.41	0.51
7:C:236:THR:O	7:C:237:GLU:C	2.48	0.51
1:0:820:G:C6	5:A:171:LYS:HB2	2.46	0.51
1:0:1174:A:C5	1:0:1201:C:H4'	2.45	0.51
5:A:36:ASP:HB2	5:A:85:ASP:H	1.76	0.51
13:I:80:LYS:HE2	13:I:98:PHE:CZ	2.45	0.51
14:J:28:GLU:HG2	14:J:58:THR:HB	1.93	0.51
17:M:132:ASN:O	17:M:135:VAL:HG12	2.11	0.51
1:0:1015:C:H2'	1:0:1016:U:C6	2.45	0.51
1:0:1393:A:H2'	1:0:1394:C:C6	2.46	0.51
30:Z:12:ASN:HB3	42:Z:8452:HOH:O	2.10	0.51
15:K:125:PHE:CZ	15:K:140:VAL:HG13	2.46	0.51
42:0:3499:HOH:O	6:B:48:MET:N	2.44	0.51
1:0:2502:C:H2'	1:0:2503:A:C5'	2.40	0.50
16:L:157:LEU:HB3	16:L:160:PHE:HD1	1.76	0.50
1:0:559:U:H2'	1:0:560:C:O4'	2.12	0.50
6:B:258:GLY:N	6:B:260:HIS:CE1	2.78	0.50
8:D:170:TYR:O	8:D:171:ASP:HB3	2.10	0.50
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.50
7:C:1:MET:HG2	7:C:2:GLN:N	2.24	0.50
17:M:49:THR:CG2	17:M:56:ASP:HB2	2.39	0.50
1:0:553:G:P	28:X:204:ARG:NH2	2.82	0.50
1:0:251:C:H1'	16:L:58:GLN:HE22	1.76	0.50
9:E:156:ASP:OD2	9:E:157:LYS:NZ	2.35	0.50
1:0:1787:C:OP1	19:O:68:LYS:HE2	2.11	0.50
1:0:2910:A:H5''	42:0:3616:HOH:O	2.11	0.50
1:0:2064:U:H4'	1:0:2653:A:OP1	2.11	0.50
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.93	0.50
13:I:19:MET:HE1	13:I:132:LEU:HD11	1.91	0.50
26:V:3:ALA:O	26:V:54:PHE:HA	2.10	0.50
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.40	0.50
6:B:320:GLN:HG3	6:B:321:PRO:HD2	1.93	0.50
6:B:297:VAL:HB	42:B:8602:HOH:O	2.11	0.50
6:B:7:ARG:CD	6:B:9:GLY:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2460:A:OP1	32:2:60:LYS:CB	2.60	0.50
1:0:1120:U:H5''	1:0:1120:U:C6	2.46	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.50
1:0:638:C:H2'	1:0:639:A:C8	2.46	0.50
7:C:237:GLU:HB2	42:C:8436:HOH:O	2.10	0.50
19:O:115:SER:C	19:O:117:SER:H	2.14	0.50
30:Z:25:LYS:HD2	31:1:49:GLU:H	1.76	0.50
2:9:3002:U:OP2	2:9:3003:A:H5'	2.11	0.50
1:0:771:G:OP2	16:L:79:LYS:HD2	2.11	0.50
42:0:6181:HOH:O	28:X:165:GLU:HB3	2.11	0.50
28:X:117:LEU:HD12	28:X:174:VAL:HG11	1.93	0.50
22:R:23:LYS:HE2	42:R:8330:HOH:O	2.12	0.50
5:A:125:ASN:ND2	42:A:8539:HOH:O	2.38	0.50
8:D:62:ASP:HA	42:D:4233:HOH:O	2.11	0.50
15:K:97:VAL:HG12	15:K:98:GLU:O	2.11	0.50
1:0:538:C:OP2	28:X:134:HIS:HE1	1.95	0.50
12:H:130:HIS:CG	12:H:133:ILE:HD11	2.45	0.50
12:H:147:ARG:HA	12:H:150:LYS:HZ2	1.76	0.50
19:O:115:SER:O	19:O:117:SER:N	2.45	0.50
26:V:26:ILE:HG13	26:V:26:ILE:O	2.10	0.50
27:W:9:VAL:HG13	27:W:88:GLU:OE1	2.12	0.50
10:F:58:GLU:HA	10:F:61:MET:HG3	1.93	0.50
6:B:144:THR:HG22	6:B:145:HIS:N	2.25	0.50
2:9:3028:U:H5''	17:M:40:ASN:ND2	2.27	0.50
14:J:34:VAL:CG2	14:J:47:ALA:HB2	2.42	0.50
8:D:11:HIS:C	8:D:13:MET:H	2.14	0.50
8:D:135:VAL:HG22	8:D:136:ARG:N	2.27	0.50
1:0:911:G:H5'	1:0:932:U:OP1	2.12	0.50
1:0:2614:C:HO2'	6:B:227:HIS:HD1	1.58	0.50
1:0:168:C:O2'	1:0:169:A:H5'	2.12	0.50
26:V:110:GLN:HE21	26:V:110:GLN:HA	1.75	0.50
5:A:192:VAL:HG12	5:A:192:VAL:O	2.11	0.50
7:C:162:VAL:HG12	7:C:162:VAL:O	2.11	0.50
8:D:57:THR:HG23	8:D:63:ILE:CG2	2.40	0.50
6:B:329:TYR:CE2	24:T:15:PRO:HG2	2.46	0.50
1:0:1434:A:H2'	1:0:1436:C:C5	2.45	0.50
6:B:185:GLY:HA2	42:B:8631:HOH:O	2.12	0.50
1:0:2533:C:H6	1:0:2533:C:C5'	2.17	0.50
1:0:797:A:O4'	29:Y:10:ARG:N	2.44	0.50
12:H:75:SER:HB3	12:H:79:ALA:HB1	1.93	0.50
1:0:1930:A:H2'	1:0:1931:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:172:PRO:HB3	42:E:6931:HOH:O	2.11	0.50
1:0:2842:G:H2'	1:0:2843:A:H5'	1.93	0.50
1:0:2766:A:O2'	1:0:2767:C:H5'	2.12	0.50
1:0:1119:G:H8	13:I:52:GLN:NE2	2.09	0.50
13:I:39:VAL:HG13	13:I:106:GLY:O	2.11	0.50
28:X:184:GLU:OE1	28:X:204:ARG:NH1	2.44	0.50
8:D:136:ARG:HD2	8:D:155:HIS:O	2.11	0.50
1:0:2064:U:H5'	1:0:2652:U:H4'	1.94	0.50
17:M:130:PRO:HA	42:M:8541:HOH:O	2.12	0.50
32:2:51:LYS:NZ	42:2:8533:HOH:O	2.42	0.50
17:M:24:LEU:O	17:M:28:LYS:HG2	2.12	0.50
1:0:1902:G:H2'	1:0:1903:U:O4'	2.11	0.50
13:I:45:VAL:HG22	13:I:46:ILE:N	2.26	0.50
1:0:797:A:H5'	29:Y:10:ARG:HG2	1.94	0.50
42:0:7049:HOH:O	29:Y:31:ILE:HG13	2.11	0.50
1:0:392:U:C5'	16:L:193:LYS:HB3	2.42	0.50
7:C:103:ASN:HB3	42:C:8309:HOH:O	2.10	0.50
7:C:54:LEU:HD21	7:C:87:ARG:HD2	1.94	0.50
23:S:53:GLY:HA3	42:S:6384:HOH:O	2.11	0.50
1:0:731:U:H2'	1:0:732:C:C6	2.47	0.50
8:D:49:PRO:HG3	42:D:5828:HOH:O	2.12	0.49
12:H:26:LYS:HD3	12:H:89:PRO:CG	2.42	0.49
12:H:14:TYR:HB2	42:H:8352:HOH:O	2.12	0.49
16:L:38:VAL:O	16:L:63:VAL:HG13	2.11	0.49
8:D:154:LYS:H	8:D:154:LYS:CD	2.11	0.49
1:0:1119:G:H2'	13:I:52:GLN:HE22	1.75	0.49
1:0:182:G:O3'	16:L:157:LEU:CD1	2.60	0.49
12:H:35:ASN:ND2	12:H:79:ALA:O	2.45	0.49
42:0:5726:HOH:O	24:T:56:ARG:HB3	2.12	0.49
9:E:20:ILE:CD1	9:E:33:LEU:HD12	2.42	0.49
2:9:3064:C:H2'	2:9:3065:A:H5'	1.94	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
5:A:217:ARG:HG2	5:A:229:ALA:HB2	1.94	0.49
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.49
1:0:2621:U:H5	42:0:9480:HOH:O	1.95	0.49
1:0:1810:C:OP1	24:T:44:ARG:NE	2.32	0.49
17:M:64:SER:C	17:M:66:LEU:H	2.16	0.49
17:M:100:ALA:O	17:M:129:ILE:HG23	2.12	0.49
42:0:6910:HOH:O	5:A:211:LYS:NZ	2.45	0.49
7:C:107:ARG:HH11	7:C:107:ARG:HB3	1.77	0.49
42:0:6874:HOH:O	23:S:2:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:114:LYS:O	17:M:118:ILE:HG13	2.12	0.49
9:E:31:ARG:HH12	9:E:68:HIS:CD2	2.30	0.49
1:O:1503:U:H2'	1:O:1504:A:O4'	2.12	0.49
1:O:1205:U:H2'	1:O:1206:U:H5''	1.93	0.49
4:4:74:C:H2'	4:4:75:C:C5'	2.41	0.49
9:E:11:VAL:HG13	9:E:23:GLU:O	2.11	0.49
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.49
1:O:1014:A:H2'	1:O:1015:C:H5'	1.93	0.49
2:9:3059:C:H5'	42:9:5233:HOH:O	2.11	0.49
1:O:1162:G:H2'	42:0:6056:HOH:O	2.12	0.49
1:O:1134:G:H4'	12:H:151:MET:CE	2.27	0.49
1:O:820:G:OP1	29:Y:17:ARG:NH2	2.44	0.49
1:O:1702:U:H5'	42:0:9921:HOH:O	2.12	0.49
42:0:6018:HOH:O	29:Y:22:ILE:HG13	2.12	0.49
10:F:101:ALA:HB2	10:F:108:LEU:HD22	1.95	0.49
13:I:93:ARG:HB3	13:I:93:ARG:NH1	2.27	0.49
1:O:777:U:O2'	30:Z:11:LYS:HG2	2.11	0.49
1:O:932:U:H2'	1:O:933:C:C6	2.47	0.49
7:C:7:ASP:OD1	7:C:11:ASN:O	2.30	0.49
42:0:7015:HOH:O	16:L:91:ILE:HG23	2.12	0.49
16:L:37:VAL:HG13	16:L:63:VAL:HG11	1.95	0.49
1:O:1666:C:C2'	1:O:1667:A:C5'	2.91	0.49
1:O:2748:G:C5'	42:0:7009:HOH:O	2.55	0.49
21:Q:39:THR:CG2	21:Q:42:GLU:HG3	2.42	0.49
24:T:31:PHE:CG	24:T:37:GLU:HG2	2.48	0.49
42:0:6159:HOH:O	23:S:38:ARG:NH1	2.45	0.49
7:C:150:THR:HA	7:C:203:ALA:O	2.12	0.49
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.46	0.49
9:E:86:VAL:CG1	9:E:129:GLU:HA	2.42	0.49
12:H:45:GLN:HG3	12:H:135:TRP:NE1	2.27	0.49
12:H:26:LYS:HG2	12:H:28:ILE:N	2.20	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
10:F:63:ILE:HB	10:F:64:PRO:CD	2.38	0.49
2:9:3088:G:OP1	26:V:130:HIS:NE2	2.42	0.49
1:O:2432:C:H4'	32:2:36:ILE:HG12	1.94	0.49
1:O:2256:G:H2'	1:O:2257:G:H5'	1.95	0.49
1:O:2266:A:H2'	1:O:2267:G:C8	2.47	0.49
5:A:211:LYS:HB2	42:A:8628:HOH:O	2.11	0.49
1:O:21:G:H4'	21:Q:2:ILE:HG22	1.95	0.49
1:O:907:A:H4'	1:O:1328:A:C2	2.48	0.49
17:M:184:ILE:HG22	17:M:185:GLU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:22:VAL:HG21	10:F:104:ALA:HB2	1.95	0.49
12:H:147:ARG:HA	12:H:150:LYS:NZ	2.28	0.49
2:9:3055:U:H4'	2:9:3056:A:C8	2.47	0.49
17:M:182:GLY:O	17:M:183:ASP:O	2.31	0.49
16:L:114:VAL:HB	16:L:159:THR:HG23	1.94	0.49
29:Y:23:ARG:NH1	42:Y:8404:HOH:O	2.46	0.49
1:0:2637:A:C4'	1:0:2638:G:O5'	2.60	0.49
1:0:2837:U:H1'	6:B:307:ARG:HH12	1.77	0.49
1:0:2361:A:H2'	1:0:2362:A:C8	2.48	0.49
6:B:55:ASN:HB3	6:B:64:GLY:H	1.77	0.49
1:0:2724:U:H2'	1:0:2725:G:O4'	2.12	0.49
27:W:75:ALA:O	27:W:83:ALA:HA	2.13	0.49
1:0:175:G:H2'	16:L:192:ALA:HB3	1.93	0.49
5:A:9:ARG:HG2	5:A:16:PHE:CD2	2.48	0.49
1:0:1886:A:O2'	29:Y:20:LEU:HB2	2.13	0.49
1:0:588:G:O6	26:V:154:ARG:NH1	2.46	0.49
1:0:902:G:N7	15:K:18:HIS:CD2	2.78	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
24:T:44:ARG:HB3	42:T:3805:HOH:O	2.11	0.49
1:0:1384:C:H5'	27:W:30:MET:HG2	1.95	0.49
1:0:2911:C:H2'	1:0:2912:C:C6	2.48	0.49
10:F:56:PRO:CG	16:L:44:THR:HA	2.43	0.49
16:L:74:ARG:HD3	16:L:91:ILE:HD12	1.94	0.49
12:H:29:ALA:HB3	12:H:65:ARG:NH1	2.15	0.49
5:A:97:ALA:HB2	5:A:150:PRO:HB2	1.95	0.49
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.95	0.49
1:0:919:U:H5'	1:0:2465:A:O2'	2.12	0.49
42:9:4707:HOH:O	17:M:147:ILE:HB	2.12	0.48
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.48
26:V:139:GLY:O	26:V:141:HIS:HD2	1.95	0.48
15:K:133:VAL:HB	42:K:8564:HOH:O	2.13	0.48
6:B:205:VAL:O	6:B:307:ARG:NE	2.46	0.48
6:B:119:HIS:O	6:B:121:PRO:HD3	2.12	0.48
1:0:1783:A:O2'	1:0:1784:U:H5'	2.12	0.48
1:0:621:C:H5'	28:X:132:ASP:OD2	2.12	0.48
12:H:86:ARG:NH1	12:H:130:HIS:CD2	2.81	0.48
42:0:9954:HOH:O	13:I:46:ILE:HD12	2.13	0.48
27:W:8:ARG:NH1	42:W:2479:HOH:O	2.38	0.48
1:0:244:C:OP2	10:F:38:LYS:HE3	2.13	0.48
15:K:72:ASN:O	15:K:76:LEU:HG	2.13	0.48
15:K:73:VAL:HG23	15:K:74:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1183:C:N4	42:0:3874:HOH:O	2.46	0.48
8:D:35:ALA:HB1	42:D:3279:HOH:O	2.12	0.48
14:J:29:LEU:HB3	14:J:55:VAL:CG1	2.39	0.48
16:L:139:PRO:HA	16:L:142:LYS:HB2	1.94	0.48
6:B:36:PRO:HA	6:B:168:GLY:HA2	1.94	0.48
1:0:2672:C:O2'	1:0:2673:U:H5'	2.13	0.48
6:B:248:ARG:NH2	42:B:8523:HOH:O	2.46	0.48
1:0:696:C:HO2'	1:0:697:G:H5'	1.77	0.48
6:B:24:PRO:HG2	6:B:204:GLY:HA2	1.94	0.48
1:0:1787:C:H4'	1:0:2883:A:O4'	2.13	0.48
27:W:70:ILE:O	27:W:70:ILE:HG23	2.13	0.48
14:J:99:ASP:OD1	14:J:101:ASN:N	2.45	0.48
16:L:182:LYS:HB2	16:L:194:ALA:HB2	1.95	0.48
14:J:125:ALA:C	14:J:127:ALA:H	2.16	0.48
15:K:55:GLN:HA	15:K:58:GLN:NE2	2.27	0.48
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.49	0.48
1:0:1268:C:O2'	1:0:1269:G:H5'	2.13	0.48
18:N:44:ASN:OD1	18:N:65:LEU:HB2	2.12	0.48
12:H:150:LYS:NZ	42:H:8379:HOH:O	2.44	0.48
8:D:163:VAL:HA	42:D:6326:HOH:O	2.13	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:2896:A:OP1	27:W:15:ARG:NH1	2.46	0.48
6:B:7:ARG:NH1	6:B:11:LEU:HD22	2.28	0.48
10:F:106:THR:HB	42:F:6617:HOH:O	2.13	0.48
30:Z:28:HIS:CD2	30:Z:31:LYS:HG3	2.48	0.48
6:B:1:PRO:O	6:B:2:GLN:HB2	2.14	0.48
19:O:55:LYS:HA	42:O:182:HOH:O	2.13	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.95	0.48
23:S:50:VAL:HG12	23:S:56:ALA:HA	1.95	0.48
32:2:91:GLN:O	32:2:92:GLU:HB2	2.12	0.48
1:0:2758:G:H2'	1:0:2759:C:C6	2.49	0.48
1:0:827:A:H2'	1:0:828:G:O4'	2.13	0.48
1:0:1166:A:H1'	1:0:1192:A:N1	2.25	0.48
9:E:11:VAL:CG1	9:E:12:ASP:H	2.27	0.48
6:B:62:ARG:HG2	6:B:65:MET:HE3	1.94	0.48
1:0:2004:U:H2'	1:0:2004:U:O2	2.13	0.48
24:T:52:THR:HG22	24:T:54:THR:N	2.27	0.48
24:T:6:CYS:HB2	24:T:32:CYS:HB3	1.94	0.48
9:E:32:ARG:O	9:E:33:LEU:HD23	2.12	0.48
12:H:71:TYR:C	12:H:73:GLN:N	2.65	0.48
21:Q:113:HIS:O	21:Q:145:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1730:G:H5'	1:O:1731:C:C6	2.49	0.48
9:E:31:ARG:CZ	42:E:5919:HOH:O	2.60	0.48
1:O:398:U:H2'	1:O:399:C:C6	2.48	0.48
1:O:200:U:H2'	42:O:9938:HOH:O	2.12	0.48
1:O:128:A:H3'	1:O:128:A:C8	2.47	0.48
19:O:143:ALA:HA	42:O:193:HOH:O	2.12	0.48
1:O:1342:C:O2'	1:O:1343:C:H5'	2.14	0.48
8:D:35:ALA:O	8:D:37:ALA:N	2.46	0.48
21:Q:96:VAL:HG13	21:Q:106:GLY:HA3	1.95	0.48
1:O:506:G:H22	1:O:509:A:H5''	1.75	0.48
1:O:182:G:O3'	16:L:157:LEU:HD13	2.14	0.48
6:B:41:PHE:CZ	6:B:79:MET:HG3	2.48	0.48
6:B:72:THR:HB	42:B:8602:HOH:O	2.13	0.48
1:O:1778:A:H2'	1:O:1779:A:H5'	1.95	0.48
1:O:2403:C:H5'	42:O:5501:HOH:O	2.14	0.48
5:A:164:ARG:CZ	42:A:8596:HOH:O	2.61	0.48
17:M:139:TRP:HA	17:M:139:TRP:HE3	1.79	0.48
26:V:29:VAL:O	26:V:30:ASN:HB2	2.13	0.48
1:O:1236:A:H2'	1:O:1237:U:O4'	2.14	0.48
21:Q:15:LYS:HE3	42:Q:8579:HOH:O	2.12	0.48
12:H:132:PHE:O	12:H:133:ILE:HD13	2.14	0.48
12:H:45:GLN:NE2	12:H:135:TRP:HE1	2.07	0.48
12:H:150:LYS:HA	12:H:153:VAL:HG22	1.94	0.48
1:O:1943:C:O4'	5:A:212:PRO:HA	2.13	0.48
1:O:820:G:C5	5:A:171:LYS:HB2	2.49	0.48
17:M:67:ALA:HA	17:M:71:TRP:HB3	1.95	0.48
1:O:558:C:C2'	1:O:559:U:C5'	2.91	0.48
1:O:1878:G:O2'	1:O:1879:U:C6	2.64	0.48
11:G:12:ILE:O	11:G:13:PRO:C	2.50	0.48
1:O:2466:G:H5''	42:O:3138:HOH:O	2.13	0.48
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.13	0.48
5:A:51:ARG:HB2	42:A:8614:HOH:O	2.12	0.48
1:O:1298:U:H2'	1:O:1299:G:C8	2.48	0.48
18:N:96:VAL:HG12	18:N:97:SER:O	2.14	0.48
13:I:36:VAL:HG12	13:I:37:ALA:N	2.29	0.48
16:L:47:ASP:CG	16:L:48:ARG:H	2.17	0.48
12:H:26:LYS:HD2	12:H:28:ILE:CG1	2.43	0.48
42:O:3246:HOH:O	16:L:108:LYS:HD2	2.14	0.48
1:O:1185:U:H5'	42:O:6934:HOH:O	2.14	0.48
6:B:17:LYS:O	6:B:260:HIS:HD2	1.96	0.48
1:O:2781:U:H2'	1:O:2782:G:C5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2637:A:N3	1:0:2637:A:H2'	2.28	0.48
1:0:128:A:O2'	1:0:129:A:H5'	2.14	0.48
1:0:2787:C:H5	42:0:4107:HOH:O	1.95	0.48
26:V:35:VAL:HG23	26:V:41:TYR:CD2	2.48	0.48
8:D:58:VAL:HG12	8:D:59:GLY:N	2.29	0.48
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.48
1:0:426:G:H2'	1:0:427:C:O4'	2.14	0.48
1:0:1805:G:H2'	1:0:1806:G:H8	1.78	0.48
1:0:2413:A:N7	17:M:109:PRO:HB3	2.28	0.48
7:C:127:ARG:HG2	7:C:127:ARG:NH1	2.27	0.48
15:K:143:THR:CG2	15:K:144:ASP:H	2.26	0.48
1:0:1299:G:N7	15:K:6:ARG:NH1	2.62	0.48
6:B:27:ASN:H	6:B:27:ASN:HD22	1.60	0.48
1:0:1669:A:H2'	1:0:1670:G:H8	1.79	0.48
1:0:816:G:C6	1:0:817:G:N1	2.81	0.48
9:E:36:PRO:HD3	13:I:127:ILE:HD12	1.96	0.48
14:J:130:MET:SD	24:T:25:ASP:O	2.72	0.48
8:D:23:VAL:CG2	8:D:23:VAL:O	2.62	0.48
7:C:235:PHE:HE2	7:C:243:VAL:HG21	1.79	0.48
6:B:310:ARG:HD2	42:B:8645:HOH:O	2.13	0.48
12:H:139:ASP:H	12:H:140:PRO:HD3	1.76	0.48
1:0:541:C:C2'	1:0:542:A:C5'	2.88	0.48
26:V:122:ARG:CZ	42:V:5817:HOH:O	2.62	0.48
25:U:20:LEU:HD22	25:U:60:GLN:HE22	1.79	0.48
24:T:14:GLU:OE1	24:T:15:PRO:HD2	2.14	0.48
5:A:99:ILE:O	5:A:131:HIS:HE1	1.96	0.48
1:0:2276:U:H2'	1:0:2277:U:H6	1.76	0.48
1:0:2379:G:H4'	1:0:2380:A:C5'	2.44	0.48
1:0:2119:C:O2'	1:0:2120:U:H5'	2.14	0.48
1:0:858:U:H2'	1:0:859:C:H6	1.79	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.13	0.48
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.43	0.47
11:G:16:LYS:O	11:G:20:VAL:HG23	2.14	0.47
1:0:2630:G:O6	5:A:206:ARG:NH2	2.46	0.47
6:B:177:HIS:O	6:B:181:ILE:HG13	2.14	0.47
17:M:62:HIS:HB3	17:M:65:ASP:OD1	2.13	0.47
7:C:16:VAL:HG12	7:C:17:ASP:H	1.78	0.47
6:B:162:MET:CE	6:B:310:ARG:HD3	2.44	0.47
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.47
1:0:2506:A:C1'	42:0:5531:HOH:O	2.62	0.47
1:0:2353:A:O2'	17:M:7:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:76:ARG:HD2	42:C:8439:HOH:O	2.14	0.47
1:O:2837:U:H2'	42:O:6313:HOH:O	2.14	0.47
21:Q:119:VAL:HG12	21:Q:119:VAL:O	2.14	0.47
15:K:24:ALA:HB2	15:K:30:ARG:HD2	1.96	0.47
26:V:121:PRO:CA	26:V:153:MET:HG2	2.44	0.47
1:O:2401:A:H5'	42:O:8995:HOH:O	2.14	0.47
16:L:63:VAL:HG21	16:L:109:PHE:CE1	2.49	0.47
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.96	0.47
5:A:88:ILE:CD1	5:A:100:PRO:HD3	2.42	0.47
6:B:74:ILE:HG13	42:B:8602:HOH:O	2.14	0.47
11:G:23:ILE:O	11:G:27:ILE:HG13	2.14	0.47
6:B:307:ARG:CB	6:B:307:ARG:HH11	2.27	0.47
28:X:216:ARG:CD	42:X:8570:HOH:O	2.60	0.47
16:L:61:ILE:HG13	42:L:8627:HOH:O	2.15	0.47
1:O:682:A:H2'	1:O:683:G:O4'	2.14	0.47
19:O:91:LYS:O	19:O:95:GLU:HG3	2.13	0.47
17:M:180:LEU:O	17:M:181:ASP:HB3	2.13	0.47
12:H:31:PHE:CD2	12:H:85:ILE:HG23	2.50	0.47
1:O:380:A:H5''	16:L:48:ARG:NH2	2.28	0.47
16:L:48:ARG:NH2	42:L:8564:HOH:O	2.47	0.47
1:O:1191:A:N1	1:O:1206:U:O4	2.47	0.47
7:C:107:ARG:CB	7:C:107:ARG:HH11	2.26	0.47
26:V:65:VAL:HG12	26:V:116:LEU:HD13	1.96	0.47
12:H:113:ALA:N	12:H:114:PRO:HD3	2.30	0.47
1:O:2256:G:C2'	1:O:2257:G:H5'	2.44	0.47
15:K:73:VAL:HG23	15:K:74:THR:H	1.78	0.47
1:O:1609:C:H2'	1:O:1610:G:H8	1.79	0.47
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.97	0.47
16:L:81:ARG:HG3	16:L:85:ARG:HB2	1.96	0.47
1:O:1206:U:C6	1:O:1206:U:H5'	2.42	0.47
26:V:154:ARG:HB3	26:V:154:ARG:HE	1.57	0.47
10:F:100:ASP:HB3	42:F:5691:HOH:O	2.15	0.47
13:I:93:ARG:CB	13:I:93:ARG:HH11	2.26	0.47
17:M:143:ARG:HA	17:M:172:PHE:CD2	2.49	0.47
7:C:246:ARG:CZ	42:C:8430:HOH:O	2.61	0.47
28:X:112:GLU:OE1	28:X:115:ARG:NH1	2.48	0.47
1:O:2252:A:C5	1:O:2253:G:H1'	2.50	0.47
23:S:52:ARG:HB2	23:S:95:ASN:HB3	1.97	0.47
1:O:1497:G:H4'	1:O:1627:G:O2'	2.15	0.47
1:O:2730:G:O2'	1:O:2731:G:H5'	2.15	0.47
5:A:96:LEU:HD22	5:A:128:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:29:ASN:O	25:U:33:VAL:HG23	2.13	0.47
42:A:8621:HOH:O	29:Y:75:ALA:HB3	2.14	0.47
13:I:46:ILE:HA	42:I:1123:HOH:O	2.14	0.47
1:0:541:C:H2'	1:0:542:A:H5'	1.96	0.47
1:0:281:U:H3'	42:0:6676:HOH:O	2.15	0.47
1:0:2781:U:O2'	1:0:2782:G:H5'	2.14	0.47
1:0:1342:C:C2'	1:0:1343:C:H5'	2.45	0.47
1:0:858:U:H2'	1:0:859:C:C6	2.50	0.47
8:D:128:LEU:HD23	8:D:128:LEU:C	2.35	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.15	0.47
10:F:117:GLU:C	10:F:119:ARG:H	2.18	0.47
8:D:158:ASN:HB2	8:D:161:ASP:OD2	2.15	0.47
29:Y:59:HIS:HA	42:Y:8436:HOH:O	2.14	0.47
8:D:99:ASP:HB2	8:D:103:ASN:H	1.80	0.47
1:0:2715:G:N2	6:B:264:GLU:OE1	2.47	0.47
17:M:71:TRP:N	42:M:8540:HOH:O	2.47	0.47
40:4:79:BTN:H82	40:4:79:BTN:N2	2.30	0.47
25:U:39:ALA:O	25:U:41:GLU:N	2.47	0.47
24:T:52:THR:CG2	24:T:54:THR:HB	2.45	0.47
11:G:71:LEU:C	11:G:73:ASP:H	2.18	0.47
8:D:94:ALA:HB3	8:D:174:VAL:CA	2.45	0.47
6:B:211:THR:HA	6:B:255:GLY:O	2.15	0.47
1:0:92:G:H4'	25:U:44:GLY:HA3	1.96	0.47
1:0:2274:A:H4'	16:L:77:PHE:HE1	1.80	0.47
2:9:3008:G:O6	17:M:11:ARG:NH1	2.48	0.47
18:N:39:THR:HB	42:N:3360:HOH:O	2.13	0.47
1:0:2312:G:C2'	1:0:2313:C:H5'	2.45	0.47
1:0:1398:G:O2'	1:0:1399:A:H5'	2.14	0.47
14:J:118:ALA:O	14:J:120:ARG:N	2.48	0.47
7:C:165:ASP:O	7:C:168:ARG:HB3	2.15	0.47
22:R:10:VAL:HG11	25:U:36:ALA:HA	1.96	0.47
1:0:24:G:N2	1:0:518:G:H1'	2.29	0.47
1:0:2697:A:H2'	1:0:2698:G:O4'	2.14	0.47
26:V:107:LEU:O	26:V:112:LEU:HB2	2.14	0.47
15:K:101:ASP:C	15:K:103:ALA:H	2.16	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
1:0:2100:A:H5'	42:C:8467:HOH:O	2.13	0.47
8:D:103:ASN:ND2	8:D:134:LEU:H	2.12	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.59	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.14	0.47
10:F:27:GLY:HA3	42:F:5413:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:200:PRO:HD3	42:A:8520:HOH:O	2.14	0.47
1:O:2320:U:H3'	32:2:2:GLN:HB2	1.97	0.47
5:A:217:ARG:CG	5:A:217:ARG:HH11	2.27	0.47
12:H:117:LYS:O	12:H:119:VAL:HG13	2.15	0.47
19:O:64:GLU:HG2	42:O:169:HOH:O	2.15	0.47
6:B:108:GLU:HB3	6:B:111:ARG:HD2	1.97	0.47
1:O:2467:A:H3'	42:O:4934:HOH:O	2.14	0.47
1:O:820:G:H5'	1:O:821:U:H5'	1.96	0.47
17:M:37:ARG:HA	17:M:37:ARG:HD3	1.81	0.47
16:L:39:ARG:HA	16:L:63:VAL:HG22	1.97	0.47
42:O:3250:HOH:O	23:S:9:LYS:CD	2.62	0.47
1:O:1450:C:O2'	1:O:1494:A:H5'	2.15	0.47
26:V:154:ARG:C	42:V:4276:HOH:O	2.53	0.47
7:C:168:ARG:NH2	7:C:190:ALA:O	2.48	0.47
1:O:329:A:OP2	7:C:206:ASN:HB2	2.14	0.47
42:O:5672:HOH:O	16:L:174:ARG:HD3	2.14	0.47
15:K:90:ARG:NH2	15:K:121:ILE:HD11	2.29	0.47
23:S:111:ARG:HB3	23:S:119:ALA:HB2	1.97	0.47
2:9:3006:C:C5'	17:M:37:ARG:HH12	2.23	0.47
12:H:56:ILE:HG22	12:H:61:LEU:CD2	2.43	0.47
27:W:78:GLU:CG	27:W:79:GLU:N	2.76	0.47
26:V:151:GLU:O	26:V:154:ARG:HB3	2.14	0.47
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.14	0.47
8:D:93:LEU:HG	42:D:3862:HOH:O	2.13	0.47
26:V:38:THR:HG22	26:V:39:ASP:N	2.30	0.47
30:Z:28:HIS:CE1	30:Z:31:LYS:HE2	2.50	0.47
1:O:2044:G:OP1	27:W:23:HIS:HE1	1.98	0.47
10:F:34:ASN:O	10:F:38:LYS:HG3	2.15	0.47
19:O:143:ALA:HA	42:O:168:HOH:O	2.15	0.47
42:O:9484:HOH:O	15:K:22:ARG:HG2	2.15	0.47
5:A:210:GLY:HA3	42:A:8594:HOH:O	2.14	0.47
1:O:278:A:H2'	1:O:279:C:O4'	2.15	0.47
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.15	0.47
42:O:9063:HOH:O	6:B:267:LYS:HD3	2.13	0.46
16:L:37:VAL:CG2	16:L:108:LYS:HG3	2.44	0.46
14:J:75:ARG:HG2	14:J:90:PHE:CD2	2.50	0.46
5:A:95:PRO:HA	5:A:153:ARG:HA	1.98	0.46
17:M:73:ALA:HB1	17:M:74:PRO:CD	2.45	0.46
1:O:474:C:O3'	7:C:73:LEU:HD21	2.16	0.46
10:F:34:ASN:HA	16:L:4:ALA:HB2	1.97	0.46
32:2:44:SER:HA	32:2:49:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:25:TRP:HE3	16:L:26:HIS:HD2	1.63	0.46
42:O:3883:HOH:O	5:A:11:ARG:CZ	2.63	0.46
1:O:2862:G:H4'	6:B:336:GLN:O	2.16	0.46
6:B:16:ARG:NH1	42:B:8613:HOH:O	2.48	0.46
17:M:47:LEU:HD13	17:M:97:VAL:HG11	1.96	0.46
2:9:3055:U:H4'	2:9:3056:A:H8	1.80	0.46
12:H:26:LYS:HD2	12:H:28:ILE:HB	1.97	0.46
1:O:1883:U:O2'	1:O:1884:G:H5'	2.14	0.46
1:O:2353:A:H4'	1:O:2354:A:O5'	2.15	0.46
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.45	0.46
1:O:1878:G:O2'	1:O:1879:U:OP2	2.33	0.46
1:O:1909:A:H2'	1:O:1910:A:C8	2.50	0.46
7:C:162:VAL:CG1	7:C:192:ILE:HD11	2.44	0.46
5:A:93:THR:C	5:A:94:LEU:HD23	2.35	0.46
23:S:28:SER:O	23:S:32:ARG:HG3	2.14	0.46
8:D:92:GLU:O	8:D:93:LEU:O	2.33	0.46
23:S:75:GLU:O	23:S:76:ASP:HB2	2.14	0.46
30:Z:25:LYS:HD2	31:1:49:GLU:N	2.30	0.46
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.46
16:L:134:ILE:CG2	16:L:141:ILE:HD13	2.46	0.46
25:U:27:LEU:HA	25:U:49:LEU:HD13	1.96	0.46
1:O:1211:G:O2'	1:O:1212:C:H5'	2.15	0.46
26:V:31:HIS:HB3	42:V:5420:HOH:O	2.14	0.46
21:Q:61:GLN:NE2	42:Q:8541:HOH:O	2.48	0.46
14:J:14:LYS:CB	14:J:45:PRO:HG2	2.36	0.46
1:O:1666:C:C2'	1:O:1667:A:H5'	2.43	0.46
29:Y:30:GLU:HB2	42:Y:8414:HOH:O	2.15	0.46
2:9:3014:G:O2'	17:M:1:ALA:HB2	2.15	0.46
10:F:99:THR:O	10:F:100:ASP:HB2	2.15	0.46
6:B:125:GLU:OE2	6:B:129:ARG:NH1	2.49	0.46
8:D:140:ARG:HH11	8:D:140:ARG:HG3	1.79	0.46
32:2:18:GLN:OE1	32:2:73:GLU:HB3	2.16	0.46
6:B:54:VAL:HB	42:B:8609:HOH:O	2.16	0.46
1:O:1304:U:H2'	1:O:1305:C:C6	2.51	0.46
24:T:39:ASN:HD22	24:T:49:LEU:HD11	1.81	0.46
1:O:622:G:O2'	1:O:623:U:H5'	2.15	0.46
12:H:47:GLU:HG2	12:H:133:ILE:HD12	1.95	0.46
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.97	0.46
5:A:35:GLY:O	5:A:36:ASP:CB	2.57	0.46
8:D:146:LYS:HZ3	17:M:107:ASN:HD21	1.61	0.46
17:M:43:VAL:HG13	17:M:118:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2883:A:H2'	1:0:2884:G:O4'	2.16	0.46
6:B:101:TRP:HB2	6:B:119:HIS:CD2	2.50	0.46
6:B:13:PHE:O	6:B:16:ARG:HD2	2.15	0.46
22:R:29:ASP:OD1	22:R:31:ARG:NH1	2.48	0.46
10:F:37:THR:O	10:F:41:GLU:HG3	2.15	0.46
42:0:6889:HOH:O	5:A:22:ARG:HD2	2.14	0.46
1:0:716:G:C2'	1:0:717:C:O5'	2.64	0.46
9:E:93:MET:HE1	9:E:165:GLY:N	2.29	0.46
1:0:461:C:H2'	42:0:3486:HOH:O	2.15	0.46
1:0:1940:C:H4'	42:0:6815:HOH:O	2.15	0.46
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.97	0.46
13:I:6:PHE:O	13:I:8:ALA:N	2.48	0.46
24:T:52:THR:HG22	24:T:54:THR:H	1.81	0.46
17:M:163:PHE:HA	42:M:8519:HOH:O	2.15	0.46
42:0:4307:HOH:O	13:I:47:THR:CB	2.59	0.46
22:R:81:ILE:HG12	42:R:8336:HOH:O	2.15	0.46
1:0:2090:G:H2'	1:0:2091:G:C8	2.50	0.46
15:K:125:PHE:CE1	15:K:140:VAL:HG13	2.51	0.46
14:J:118:ALA:C	14:J:120:ARG:H	2.19	0.46
42:0:6926:HOH:O	7:C:188:ARG:CD	2.63	0.46
2:9:3012:C:H5'	2:9:3070:U:O4'	2.16	0.46
1:0:745:G:H5''	1:0:746:A:OP1	2.16	0.46
22:R:6:LYS:HB2	22:R:27:ALA:O	2.15	0.46
1:0:57:C:H5''	42:0:6233:HOH:O	2.13	0.46
16:L:48:ARG:HH11	16:L:52:LEU:HD21	1.81	0.46
31:1:18:ASN:ND2	31:1:40:ARG:H	2.14	0.46
12:H:62:GLU:O	12:H:66:VAL:HG23	2.16	0.46
1:0:1166:A:H61	1:0:1180:U:H3	1.64	0.46
26:V:26:ILE:CG1	26:V:26:ILE:O	2.63	0.46
16:L:108:LYS:HE3	42:L:8616:HOH:O	2.15	0.46
22:R:53:ASN:ND2	42:R:8321:HOH:O	2.49	0.46
1:0:2591:C:H2'	1:0:2592:G:O4'	2.16	0.46
8:D:84:LEU:C	8:D:86:THR:H	2.18	0.46
6:B:16:ARG:NE	42:B:8551:HOH:O	2.32	0.46
23:S:20:HIS:ND1	23:S:41:ARG:NE	2.60	0.46
27:W:66:THR:HG23	27:W:67:PRO:HD2	1.96	0.46
1:0:308:U:C4	1:0:342:C:HI'	2.50	0.46
16:L:84:LYS:HD3	42:L:8532:HOH:O	2.15	0.46
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.45	0.46
17:M:5:ARG:HG3	20:P:18:PRO:CB	2.45	0.46
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:154:LEU:CG	17:M:155:GLU:H	2.27	0.46
1:O:2247:C:H5''	42:O:6813:HOH:O	2.16	0.46
6:B:223:ARG:HG3	6:B:232:TRP:O	2.15	0.46
1:O:2356:A:H2'	1:O:2357:G:O4'	2.16	0.46
1:O:2821:C:H4'	6:B:116:PRO:HB3	1.97	0.46
1:O:432:G:O2'	1:O:433:C:H5'	2.16	0.46
29:Y:39:CYS:O	29:Y:42:CYS:O	2.34	0.46
1:O:962:C:C1'	17:M:5:ARG:NH1	2.72	0.46
14:J:55:VAL:CG1	14:J:56:SER:N	2.78	0.46
1:O:2270:G:H4'	5:A:223:ARG:HH12	1.80	0.46
26:V:139:GLY:O	26:V:141:HIS:CD2	2.69	0.46
6:B:41:PHE:CE1	6:B:79:MET:HG3	2.50	0.46
1:O:2121:G:C2'	1:O:2122:C:H5'	2.46	0.46
1:O:1097:A:H5''	26:V:125:HIS:NE2	2.31	0.46
1:O:952:G:N3	1:O:2302:A:H2'	2.31	0.46
23:S:55:PHE:CD2	23:S:77:VAL:HG13	2.50	0.46
1:O:1289:C:H3'	42:O:5886:HOH:O	2.15	0.46
1:O:1056:U:H2'	1:O:1057:A:O4'	2.16	0.46
1:O:2010:A:H2'	42:O:5433:HOH:O	2.15	0.46
1:O:1003:U:O2'	12:H:90:PHE:HE1	1.99	0.46
1:O:21:G:H5''	21:Q:1:GLY:O	2.16	0.46
16:L:69:LYS:HD3	16:L:125:ARG:HA	1.98	0.46
27:W:25:ARG:HG2	42:W:5356:HOH:O	2.15	0.46
6:B:7:ARG:NH1	6:B:7:ARG:HG2	2.31	0.46
1:O:447:A:O2'	1:O:448:G:H5'	2.16	0.46
9:E:20:ILE:HD12	9:E:33:LEU:HD12	1.98	0.46
5:A:105:VAL:HG12	5:A:106:CYS:N	2.31	0.46
1:O:1120:U:H6	1:O:1120:U:H5''	1.81	0.46
42:O:4422:HOH:O	16:L:82:ARG:HD3	2.16	0.46
1:O:2904:U:H4'	27:W:8:ARG:NH1	2.30	0.46
5:A:128:LEU:HG	42:A:8583:HOH:O	2.16	0.46
1:O:1391:G:H2'	1:O:1392:A:H5'	1.98	0.46
1:O:860:U:H2'	1:O:861:A:C8	2.51	0.46
8:D:101:THR:HG22	42:D:7400:HOH:O	2.16	0.46
3:3:76:A:N6	42:3:7072:HOH:O	2.42	0.46
25:U:55:ARG:O	25:U:59:ILE:HG12	2.15	0.46
1:O:814:G:H4'	42:O:9626:HOH:O	2.16	0.46
16:L:87:MET:SD	32:2:46:ILE:HD13	2.55	0.46
5:A:192:VAL:O	5:A:207:GLN:HG2	2.16	0.46
5:A:36:ASP:CB	5:A:85:ASP:H	2.28	0.46
24:T:33:SER:O	24:T:37:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2459:G:OP2	32:2:64:LYS:HD2	2.16	0.46
1:0:1819:G:H2'	1:0:1820:G:C4'	2.46	0.46
5:A:179:MET:HG2	5:A:186:TRP:CB	2.45	0.46
1:0:716:G:H2'	1:0:717:C:O5'	2.16	0.46
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.15	0.46
23:S:19:ARG:HD3	23:S:67:LEU:O	2.14	0.46
31:1:40:ARG:HA	31:1:45:ASN:ND2	2.30	0.45
2:9:3007:G:H4'	17:M:55:ASP:OD2	2.15	0.45
7:C:160:LEU:O	7:C:162:VAL:HG23	2.16	0.45
19:O:94:TRP:CZ2	19:O:98:ILE:HG13	2.51	0.45
19:O:120:ARG:NH2	19:O:123:TYR:CD2	2.84	0.45
2:9:3002:U:OP2	2:9:3002:U:H4'	2.16	0.45
1:0:2320:U:OP2	32:2:1:MET:HA	2.16	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.33	0.45
7:C:39:GLN:O	7:C:43:LYS:HD3	2.15	0.45
1:0:113:A:OP2	1:0:114:A:H2'	2.16	0.45
1:0:2619:U:H5''	1:0:2620:U:OP2	2.15	0.45
1:0:228:C:H2'	1:0:229:G:H5'	1.98	0.45
1:0:512:G:O3'	1:0:513:A:H8	1.99	0.45
1:0:2088:C:H1'	1:0:2841:A:N1	2.31	0.45
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.44	0.45
8:D:99:ASP:HB3	8:D:103:ASN:H	1.81	0.45
8:D:99:ASP:O	8:D:159:PRO:HG3	2.15	0.45
14:J:81:ARG:HD3	14:J:87:ARG:NH1	2.30	0.45
1:0:2269:C:H2'	1:0:2270:G:O4'	2.17	0.45
8:D:67:ASP:O	8:D:69:ILE:HG13	2.16	0.45
12:H:72:VAL:HG11	12:H:81:TYR:CZ	2.51	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.52	0.45
22:R:42:GLU:HG2	22:R:49:VAL:HG23	1.98	0.45
1:0:611:U:H2'	1:0:612:U:C6	2.52	0.45
1:0:1173:A:H2'	42:0:3826:HOH:O	2.16	0.45
27:W:85:VAL:HG12	27:W:86:GLU:N	2.31	0.45
1:0:1164:U:O4'	1:0:1165:G:OP1	2.35	0.45
1:0:1205:U:H2'	1:0:1206:U:C5'	2.47	0.45
1:0:282:C:H2'	1:0:283:U:O4'	2.15	0.45
5:A:100:PRO:O	5:A:103:VAL:HG23	2.16	0.45
13:I:6:PHE:HB3	13:I:109:TYR:OH	2.16	0.45
17:M:73:ALA:HB2	17:M:163:PHE:CZ	2.51	0.45
1:0:2432:C:C1'	42:0:3566:HOH:O	2.64	0.45
1:0:170:U:H1'	32:2:50:GLY:HA3	1.98	0.45
26:V:149:LEU:HG	26:V:153:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2464:C:H5''	1:0:2465:A:OP1	2.16	0.45
1:0:1385:G:O3'	27:W:49:ARG:NH1	2.50	0.45
1:0:1066:U:H2'	1:0:1067:A:C8	2.51	0.45
1:0:703:G:O2'	1:0:704:C:H5'	2.17	0.45
21:Q:125:ARG:HG2	42:Q:8543:HOH:O	2.16	0.45
14:J:14:LYS:HG3	14:J:32:ILE:O	2.16	0.45
1:0:2637:A:H5'	1:0:2638:G:C5'	2.46	0.45
32:2:65:THR:HB	32:2:83:TRP:H	1.81	0.45
12:H:81:TYR:C	12:H:81:TYR:CD1	2.89	0.45
1:0:316:A:N3	1:0:336:G:O2'	2.43	0.45
8:D:59:GLY:O	8:D:61:PHE:N	2.41	0.45
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.47	0.45
17:M:93:GLN:HG2	42:M:8559:HOH:O	2.15	0.45
1:0:1471:A:H2'	1:0:1472:C:C6	2.51	0.45
17:M:67:ALA:C	17:M:69:TYR:N	2.70	0.45
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.45
1:0:2346:C:O3'	8:D:52:THR:HG23	2.16	0.45
30:Z:8:GLN:HE22	30:Z:11:LYS:HZ2	1.62	0.45
42:0:9054:HOH:O	26:V:119:HIS:HE1	1.98	0.45
27:W:12:ILE:HD12	27:W:36:HIS:ND1	2.32	0.45
1:0:491:C:O2'	1:0:492:C:H5'	2.17	0.45
1:0:100:C:H4'	23:S:16:LEU:HB2	1.99	0.45
17:M:78:MET:HB2	17:M:79:PRO:HD3	1.98	0.45
13:I:79:PHE:HB3	13:I:103:VAL:HG11	1.98	0.45
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.45
1:0:283:U:H5	1:0:284:C:N4	2.15	0.45
8:D:95:THR:C	8:D:97:GLN:N	2.69	0.45
17:M:77:ASN:OD1	17:M:80:SER:HB2	2.17	0.45
1:0:952:G:OP1	20:P:42:LYS:HE2	2.16	0.45
9:E:16:ASP:O	9:E:17:HIS:HB2	2.16	0.45
13:I:77:GLY:O	13:I:78:ILE:C	2.55	0.45
1:0:319:A:H4'	1:0:338:C:C4	2.52	0.45
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.45
1:0:2896:A:N3	1:0:2896:A:H2'	2.32	0.45
1:0:2768:A:H3'	42:0:3898:HOH:O	2.17	0.45
1:0:2346:C:O3'	8:D:52:THR:CG2	2.65	0.45
5:A:186:TRP:CG	5:A:187:PRO:HA	2.52	0.45
1:0:538:C:H5''	1:0:539:G:C8	2.51	0.45
1:0:926:A:O2'	15:K:41:HIS:HD2	1.99	0.45
1:0:1768:C:H2'	1:0:1769:C:O4'	2.17	0.45
15:K:38:HIS:CD2	15:K:39:GLU:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:75:ILE:CD1	20:P:84:ILE:HD11	2.47	0.45
26:V:88:THR:CG2	26:V:110:GLN:NE2	2.75	0.45
13:I:52:GLN:HG3	13:I:53:ILE:N	2.32	0.45
8:D:173:GLU:HG3	8:D:174:VAL:N	2.31	0.45
6:B:175:LEU:C	6:B:175:LEU:CD2	2.85	0.45
5:A:164:ARG:HA	29:Y:69:TYR:CE1	2.52	0.45
12:H:95:GLU:HB3	12:H:119:VAL:HG11	1.98	0.45
9:E:170:ARG:HB2	9:E:170:ARG:HE	1.56	0.45
32:2:7:PHE:HE2	32:2:22:VAL:HG21	1.82	0.45
1:O:1659:A:H2'	1:O:1660:G:O4'	2.17	0.45
9:E:24:GLY:HA3	9:E:76:VAL:HB	1.98	0.45
21:Q:4:TYR:N	42:Q:8548:HOH:O	2.50	0.45
17:M:34:LEU:HD13	17:M:47:LEU:HD21	1.98	0.45
27:W:74:ALA:HB2	27:W:85:VAL:HG13	1.98	0.45
26:V:80:ASP:O	26:V:84:VAL:HG23	2.16	0.45
1:O:1829:A:C8	1:O:1885:A:C8	3.05	0.45
9:E:23:GLU:HG2	9:E:28:SER:HB2	1.98	0.45
9:E:69:ILE:HA	9:E:72:MET:HE3	1.99	0.45
1:O:1523:G:H2'	1:O:1524:U:C6	2.52	0.45
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.52	0.45
1:O:1925:G:OP1	32:2:29:ARG:NH2	2.50	0.45
42:O:4203:HOH:O	17:M:21:HIS:HD2	2.00	0.45
1:O:2735:U:H2'	1:O:2736:U:C6	2.52	0.45
10:F:13:GLU:OE2	10:F:78:GLU:HG2	2.17	0.45
1:O:451:C:O2'	1:O:452:G:H5'	2.17	0.45
6:B:42:ALA:HB1	6:B:308:LEU:HD11	1.99	0.45
1:O:1910:A:H2	1:O:2129:U:O4'	2.00	0.45
1:O:1500:U:OP2	19:O:41:ARG:NH2	2.50	0.45
6:B:307:ARG:CG	6:B:307:ARG:HH11	2.29	0.45
10:F:24:ARG:NH2	42:F:6800:HOH:O	2.51	0.45
28:X:112:GLU:CD	28:X:115:ARG:NH1	2.70	0.45
26:V:35:VAL:HA	26:V:36:PRO:HD3	1.78	0.45
1:O:317:A:H5"	23:S:52:ARG:HD2	1.98	0.45
27:W:12:ILE:HG23	27:W:36:HIS:CG	2.51	0.45
20:P:66:LYS:HB2	20:P:70:ALA:O	2.17	0.45
1:O:1994:A:P	14:J:66:ARG:HH22	2.40	0.45
6:B:279:THR:OG1	6:B:290:VAL:HB	2.17	0.45
1:O:1165:G:C3'	1:O:1165:G:OP1	2.61	0.44
1:O:2506:A:H1'	42:O:5531:HOH:O	2.17	0.44
8:D:146:LYS:HE2	17:M:107:ASN:ND2	2.32	0.44
8:D:55:LYS:O	8:D:56:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.96	0.44
23:S:38:ARG:HG3	23:S:38:ARG:HH11	1.81	0.44
21:Q:132:ARG:NH2	42:Q:8585:HOH:O	2.50	0.44
7:C:25:PRO:HD2	42:C:8434:HOH:O	2.15	0.44
1:O:2468:A:H61	32:2:48:ASN:HD21	1.64	0.44
1:O:1654:U:H2'	5:A:47:HIS:HD2	1.81	0.44
1:O:2478:U:H2'	1:O:2479:A:C8	2.52	0.44
20:P:32:GLU:HA	20:P:71:TYR:OH	2.17	0.44
12:H:165:GLY:C	12:H:166:ASN:HD22	2.20	0.44
1:O:2505:G:H8	42:O:5114:HOH:O	2.00	0.44
27:W:9:VAL:HG13	27:W:88:GLU:CD	2.37	0.44
26:V:122:ARG:NH1	26:V:122:ARG:HG2	2.26	0.44
1:O:1159:G:H1	1:O:1208:C:H42	1.65	0.44
11:G:67:LEU:O	11:G:71:LEU:HG	2.17	0.44
1:O:776:A:OP1	30:Z:28:HIS:HE1	1.99	0.44
1:O:1266:U:H4'	28:X:115:ARG:HH21	1.81	0.44
1:O:1656:A:H2'	1:O:1657:A:O4'	2.17	0.44
27:W:34:ARG:NH1	27:W:48:VAL:O	2.49	0.44
1:O:1135:G:H5'	42:O:5403:HOH:O	2.17	0.44
1:O:2900:G:H2'	1:O:2901:C:O4'	2.17	0.44
15:K:65:ASP:CG	15:K:111:ALA:HB3	2.38	0.44
1:O:2825:C:H4'	1:O:2826:G:O5'	2.17	0.44
1:O:1029:U:O2'	1:O:1273:C:OP1	2.31	0.44
1:O:1557:G:O2'	1:O:1558:C:H5'	2.17	0.44
14:J:55:VAL:HG12	14:J:56:SER:H	1.82	0.44
1:O:1588:G:C6	1:O:1589:G:N1	2.86	0.44
1:O:541:C:O2'	1:O:542:A:H5''	2.18	0.44
26:V:122:ARG:HG2	26:V:152:ALA:O	2.17	0.44
29:Y:11:THR:HG21	29:Y:23:ARG:HB2	1.98	0.44
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.98	0.44
1:O:2839:C:H2'	1:O:2840:A:H5''	1.99	0.44
5:A:164:ARG:HB2	29:Y:68:CYS:SG	2.57	0.44
1:O:1634:G:H2'	1:O:1635:U:C6	2.52	0.44
7:C:40:ALA:CB	7:C:100:LEU:HD12	2.47	0.44
1:O:2281:C:H2'	1:O:2282:U:H5'	1.99	0.44
1:O:853:C:H2'	1:O:854:G:O4'	2.17	0.44
30:Z:2:GLY:O	30:Z:6:PRO:HG2	2.17	0.44
12:H:84:ARG:CZ	12:H:135:TRP:CH2	3.00	0.44
12:H:84:ARG:CZ	12:H:135:TRP:HH2	2.30	0.44
1:O:1942:A:H5'	5:A:233:THR:HB	1.98	0.44
12:H:26:LYS:CD	12:H:28:ILE:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:19:MET:HE1	13:I:132:LEU:HD21	1.98	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.33	0.44
1:0:2419:U:H5''	1:0:2420:G:C5'	2.43	0.44
24:T:9:CYS:O	24:T:52:THR:HG23	2.18	0.44
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.46	0.44
27:W:43:VAL:CG1	27:W:44:ASP:N	2.79	0.44
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.46	0.44
1:0:1819:G:H5'	42:0:4186:HOH:O	2.18	0.44
1:0:170:U:H5'	32:2:48:ASN:HB3	1.98	0.44
15:K:53:ARG:NH2	15:K:57:VAL:HG12	2.33	0.44
32:2:1:MET:HG3	32:2:88:LEU:HD12	1.99	0.44
28:X:107:PRO:HB3	28:X:182:PHE:CE2	2.53	0.44
27:W:30:MET:HE1	27:W:55:ASN:HA	1.98	0.44
9:E:34:TRP:O	13:I:127:ILE:HD11	2.17	0.44
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.44
27:W:31:ILE:O	27:W:35:GLU:HG3	2.16	0.44
16:L:46:LEU:HG	42:L:8625:HOH:O	2.17	0.44
28:X:109:LEU:HA	42:X:8572:HOH:O	2.18	0.44
1:0:1252:A:H2'	1:0:1253:C:O4'	2.18	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.47	0.44
1:0:2720:C:O2	14:J:87:ARG:NH2	2.50	0.44
1:0:2526:C:C2'	1:0:2527:U:H5'	2.47	0.44
10:F:57:GLU:O	10:F:61:MET:HG3	2.18	0.44
13:I:107:ASN:ND2	13:I:107:ASN:C	2.68	0.44
6:B:22:GLU:HA	6:B:205:VAL:HG21	2.00	0.44
1:0:1593:C:H5'	19:O:116:SER:O	2.17	0.44
1:0:424:C:H2'	1:0:425:U:C6	2.53	0.44
5:A:211:LYS:CB	5:A:212:PRO:HD2	2.31	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.44
25:U:1:THR:CG2	25:U:2:VAL:H	2.25	0.44
11:G:12:ILE:HG13	42:G:6833:HOH:O	2.18	0.44
15:K:146:GLY:C	15:K:148:GLU:H	2.21	0.44
9:E:116:THR:CG2	9:E:151:LEU:HD22	2.47	0.44
1:0:1015:C:H2'	1:0:1016:U:H6	1.79	0.44
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.44
25:U:55:ARG:NH2	42:U:4428:HOH:O	2.45	0.44
1:0:1615:A:H4'	42:0:5359:HOH:O	2.17	0.44
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.44
19:O:115:SER:C	19:O:117:SER:N	2.70	0.44
26:V:4:LEU:HA	26:V:4:LEU:HD23	1.75	0.44
5:A:192:VAL:CG1	5:A:192:VAL:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1589:G:N2	1:0:1605:G:H1'	2.33	0.44
26:V:122:ARG:CG	26:V:152:ALA:O	2.66	0.44
1:0:2420:G:H4'	42:0:3581:HOH:O	2.18	0.44
26:V:65:VAL:HA	26:V:68:THR:CG2	2.47	0.44
32:2:60:LYS:HG3	32:2:61:PRO:HD2	2.00	0.44
17:M:155:GLU:O	17:M:156:GLU:HG3	2.18	0.44
19:O:16:VAL:CG1	19:O:17:GLY:N	2.81	0.44
1:0:1735:C:H2'	1:0:1736:A:C8	2.51	0.44
1:0:1592:G:H2'	1:0:1593:C:C6	2.53	0.44
1:0:2064:U:H5'	1:0:2652:U:O3'	2.18	0.44
1:0:2326:U:H4'	1:0:2412:G:C4'	2.47	0.44
23:S:49:GLU:OE2	23:S:97:ARG:HD2	2.18	0.44
22:R:32:ALA:HA	22:R:36:GLU:OE1	2.17	0.44
1:0:2443:C:H3'	42:0:9967:HOH:O	2.17	0.44
13:I:90:LYS:HB2	36:I:8502:CL:CL	2.55	0.44
1:0:344:C:H2'	1:0:345:G:O4'	2.17	0.44
1:0:635:A:H2'	1:0:636:G:H5''	1.98	0.44
8:D:99:ASP:CB	8:D:103:ASN:HB2	2.47	0.44
2:9:3057:A:O2'	8:D:152:PRO:HD2	2.18	0.44
5:A:211:LYS:HD3	42:A:8618:HOH:O	2.17	0.44
16:L:173:LEU:HA	16:L:183:VAL:HG11	2.00	0.44
1:0:450:C:H4'	7:C:46:TYR:CE1	2.53	0.44
24:T:52:THR:HG22	24:T:54:THR:HB	2.00	0.44
2:9:3030:C:OP1	8:D:137:PRO:O	2.35	0.44
1:0:1329:A:C2	42:0:4159:HOH:O	2.56	0.44
12:H:141:ASN:CA	42:H:8366:HOH:O	2.61	0.44
31:1:22:PRO:HB2	31:1:24:TRP:CD1	2.53	0.44
28:X:115:ARG:NE	42:X:8557:HOH:O	2.51	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.18	0.44
1:0:2256:G:H2'	1:0:2257:G:C5'	2.48	0.44
21:Q:29:LYS:HD3	42:Q:8533:HOH:O	2.18	0.44
7:C:196:THR:HG23	42:C:8406:HOH:O	2.16	0.44
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.53	0.44
1:0:536:A:H3'	42:0:4522:HOH:O	2.17	0.44
19:O:7:LYS:CD	19:O:21:VAL:CG2	2.96	0.44
24:T:38:ASN:O	24:T:42:LEU:HG	2.18	0.44
16:L:74:ARG:CD	16:L:91:ILE:HD12	2.48	0.44
26:V:52:VAL:HG13	26:V:53:ALA:N	2.32	0.44
5:A:36:ASP:CA	5:A:83:GLY:HA3	2.46	0.44
1:0:596:C:H2'	1:0:597:A:C8	2.53	0.44
27:W:9:VAL:HG22	27:W:88:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.18	0.44
10:F:58:GLU:HG3	10:F:61:MET:HE1	1.99	0.44
2:9:3028:U:H2'	2:9:3029:C:C6	2.53	0.44
27:W:43:VAL:HG12	27:W:47:ALA:HB3	1.99	0.44
1:0:1819:G:H2'	1:0:1820:G:C5'	2.48	0.44
21:Q:25:PHE:CE2	21:Q:29:LYS:HE2	2.52	0.44
7:C:34:ALA:HB3	7:C:220:THR:HG21	1.99	0.44
7:C:13:ASP:OD1	7:C:13:ASP:O	2.36	0.44
6:B:154:VAL:HG12	6:B:156:LYS:HG2	1.98	0.44
18:N:25:VAL:HG23	18:N:26:TRP:N	2.33	0.44
1:0:166:A:N7	15:K:25:GLY:HA2	2.33	0.44
19:O:11:ALA:HB2	19:O:18:LYS:HA	2.00	0.44
12:H:86:ARG:CZ	12:H:130:HIS:CD2	3.01	0.43
17:M:47:LEU:HD12	17:M:92:ALA:HB1	2.00	0.43
1:0:506:G:N2	1:0:509:A:H5'	2.21	0.43
1:0:711:G:C2	1:0:718:C:C2	3.06	0.43
1:0:111:C:H2'	1:0:112:G:O4'	2.18	0.43
10:F:28:ALA:CB	10:F:99:THR:HG23	2.48	0.43
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.43
1:0:737:A:H2'	1:0:738:G:O4'	2.18	0.43
17:M:80:SER:CB	42:M:8537:HOH:O	2.61	0.43
10:F:16:ALA:HA	10:F:111:ILE:HD13	1.99	0.43
17:M:58:LEU:CD1	17:M:58:LEU:N	2.80	0.43
1:0:1596:U:H2'	1:0:1598:A:OP2	2.17	0.43
8:D:169:THR:O	8:D:170:TYR:HB2	2.18	0.43
11:G:20:VAL:O	11:G:24:VAL:HG23	2.18	0.43
6:B:215:VAL:O	6:B:219:GLY:HA2	2.17	0.43
20:P:3:SER:HB3	42:P:5998:HOH:O	2.17	0.43
1:0:1681:G:H5"	1:0:1682:A:H5'	2.00	0.43
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.99	0.43
1:0:2453:G:H4'	15:K:50:GLY:C	2.39	0.43
42:O:3523:HOH:O	7:C:149:LYS:HE3	2.18	0.43
16:L:107:ARG:NH1	42:L:8581:HOH:O	2.51	0.43
6:B:274:GLU:HA	6:B:292:GLY:O	2.18	0.43
1:0:886:A:OP2	1:0:2113:G:H5'	2.18	0.43
42:L:8532:HOH:O	32:2:46:ILE:HB	2.18	0.43
12:H:65:ARG:NH1	42:H:8385:HOH:O	2.51	0.43
2:9:3078:G:N2	2:9:3103:A:OP2	2.48	0.43
4:4:75:C:H2'	37:4:76:PPU:O4'	2.18	0.43
5:A:51:ARG:NH2	42:A:8551:HOH:O	2.51	0.43
6:B:139:ASP:CB	6:B:165:ARG:HE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:234:VAL:HG12	28:X:235:GLU:N	2.33	0.43
1:0:2355:G:H5''	1:0:2356:A:OP2	2.19	0.43
15:K:34:GLY:HA3	15:K:38:HIS:CE1	2.53	0.43
1:0:2314:G:O2'	1:0:2315:C:H5'	2.18	0.43
1:0:2597:U:H2'	1:0:2598:U:H5'	1.99	0.43
12:H:31:PHE:HE2	12:H:87:LYS:O	2.01	0.43
12:H:14:TYR:N	12:H:91:HIS:HE1	2.16	0.43
1:0:1771:U:C4'	29:Y:20:LEU:HD21	2.37	0.43
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.49	0.43
1:0:1189:A:N3	42:0:7150:HOH:O	2.48	0.43
24:T:6:CYS:SG	24:T:31:PHE:HA	2.58	0.43
14:J:65:ARG:CD	42:J:5358:HOH:O	2.66	0.43
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.18	0.43
18:N:98:LEU:HA	18:N:98:LEU:HD12	1.85	0.43
1:0:644:G:N3	1:0:644:G:H5'	2.33	0.43
1:0:949:U:O2'	20:P:40:HIS:HE1	2.01	0.43
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.43
1:0:95:A:H5''	1:0:97:G:O4'	2.18	0.43
42:0:6827:HOH:O	5:A:177:HIS:HE1	2.01	0.43
5:A:55:VAL:HG11	5:A:67:LEU:HD13	2.00	0.43
17:M:175:LEU:HD12	17:M:175:LEU:HA	1.85	0.43
8:D:19:GLU:O	8:D:133:ASN:HB3	2.19	0.43
24:T:17:THR:CG2	24:T:18:GLY:N	2.82	0.43
23:S:38:ARG:HG3	23:S:38:ARG:NH1	2.33	0.43
12:H:127:GLY:O	12:H:128:ALA:CB	2.65	0.43
1:0:695:C:H2'	1:0:696:C:C6	2.53	0.43
8:D:128:LEU:HB2	42:D:6007:HOH:O	2.18	0.43
42:0:8727:HOH:O	5:A:11:ARG:HD3	2.18	0.43
1:0:702:G:O2'	1:0:703:G:H5'	2.19	0.43
1:0:524:A:H5'	21:Q:29:LYS:HE2	2.00	0.43
28:X:197:ASP:OD1	28:X:197:ASP:C	2.56	0.43
1:0:1470:A:OP1	16:L:93:ARG:HD2	2.18	0.43
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.43
1:0:629:A:H2'	1:0:630:A:O4'	2.19	0.43
16:L:95:LYS:HG2	16:L:99:ARG:HB3	2.00	0.43
12:H:46:VAL:O	12:H:146:TRP:CH2	2.68	0.43
8:D:35:ALA:C	8:D:37:ALA:N	2.72	0.43
26:V:5:VAL:O	26:V:52:VAL:HG22	2.18	0.43
1:0:288:A:H2'	1:0:289:G:C8	2.54	0.43
1:0:2349:G:OP1	8:D:20:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:125:ARG:HD3	42:L:8597:HOH:O	2.18	0.43
1:0:2542:C:H4'	4:4:75:C:O2'	2.19	0.43
1:0:2815:G:OP2	13:I:99:GLU:HG2	2.19	0.43
17:M:73:ALA:HB1	17:M:74:PRO:HD2	1.99	0.43
14:J:6:ALA:HB3	14:J:116:GLU:HG2	2.00	0.43
19:O:13:VAL:HG13	19:O:14:LEU:N	2.33	0.43
32:2:55:VAL:HB	32:2:56:PRO:HD2	2.01	0.43
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.43
8:D:10:PHE:CD1	8:D:11:HIS:N	2.86	0.43
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.43
16:L:155:HIS:CE1	16:L:158:ARG:HH21	2.36	0.43
28:X:117:LEU:HD12	28:X:174:VAL:CG1	2.49	0.43
1:0:2010:A:C2'	42:0:5433:HOH:O	2.67	0.43
9:E:162:PHE:CD1	9:E:162:PHE:N	2.86	0.43
5:A:30:ARG:HB3	5:A:30:ARG:HE	1.60	0.43
1:0:2092:G:H2'	1:0:2613:G:OP1	2.19	0.43
9:E:77:THR:OG1	9:E:78:GLU:N	2.50	0.43
15:K:10:SER:O	15:K:11:ARG:HB3	2.19	0.43
23:S:106:GLU:HG3	42:S:4913:HOH:O	2.17	0.43
7:C:142:ASP:OD2	7:C:238:SER:OG	2.33	0.43
16:L:167:GLY:O	16:L:171:ARG:HG3	2.19	0.43
17:M:5:ARG:HG3	20:P:18:PRO:HB3	1.99	0.43
29:Y:38:LYS:HE2	29:Y:45:LYS:CE	2.45	0.43
1:0:401:C:C5'	42:0:5268:HOH:O	2.65	0.43
16:L:125:ARG:NH1	42:L:8597:HOH:O	2.51	0.43
1:0:283:U:H5''	1:0:284:C:OP2	2.19	0.43
9:E:108:LEU:HD11	9:E:164:ASP:HB2	2.01	0.43
17:M:161:GLY:O	17:M:162:ASP:C	2.56	0.43
1:0:2432:C:H2'	1:0:2433:A:H8	1.84	0.43
1:0:1761:U:H5'	19:O:81:LYS:O	2.18	0.43
25:U:27:LEU:CA	25:U:49:LEU:HD13	2.49	0.43
21:Q:83:LYS:HB3	42:Q:8517:HOH:O	2.18	0.43
1:0:244:C:H6	1:0:244:C:O5'	2.00	0.43
1:0:1052:G:H2'	1:0:1052:G:N3	2.33	0.43
15:K:26:HIS:HB2	42:K:8512:HOH:O	2.18	0.43
32:2:39:GLN:HA	32:2:42:ARG:NH2	2.33	0.43
1:0:1677:U:OP2	31:1:8:LYS:NZ	2.48	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.07	0.43
1:0:2271:G:N3	1:0:2271:G:H2'	2.33	0.43
1:0:440:C:H2'	1:0:441:A:C8	2.53	0.43
1:0:2569:A:H2'	1:0:2570:G:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:127:LEU:HA	17:M:127:LEU:HD12	1.84	0.43
16:L:87:MET:HB2	16:L:91:ILE:HD11	2.00	0.43
1:0:870:G:C3'	1:0:871:G:H5''	2.49	0.43
16:L:114:VAL:HG21	16:L:159:THR:HG21	2.00	0.43
28:X:189:ASN:HA	28:X:217:ILE:HD11	2.00	0.43
1:0:338:C:H4'	7:C:174:ILE:HD11	2.00	0.43
8:D:84:LEU:HA	8:D:87:ALA:HB3	2.01	0.43
6:B:53:LEU:HD11	6:B:327:VAL:HG22	2.01	0.43
5:A:199:HIS:CD2	5:A:201:PHE:HB2	2.54	0.43
1:0:1559:A:C1'	42:0:5338:HOH:O	2.63	0.43
7:C:246:ARG:HH11	7:C:246:ARG:HB3	1.81	0.43
32:2:11:CYS:HA	32:2:12:PRO:HD2	1.83	0.43
28:X:126:PRO:HG2	28:X:128:PHE:CZ	2.54	0.43
9:E:81:GLU:HG2	9:E:134:SER:CB	2.48	0.43
1:0:1095:U:O2	26:V:120:PRO:HG2	2.18	0.43
10:F:38:LYS:NZ	16:L:3:SER:HA	2.33	0.43
22:R:29:ASP:OD1	22:R:31:ARG:HG3	2.18	0.43
1:0:466:A:H2'	1:0:467:G:O4'	2.17	0.43
12:H:36:ASN:ND2	42:H:8382:HOH:O	2.50	0.43
16:L:87:MET:H	16:L:87:MET:HG3	1.34	0.43
6:B:162:MET:HE3	6:B:308:LEU:CD2	2.36	0.43
25:U:57:LYS:HA	25:U:60:GLN:HE21	1.83	0.43
28:X:144:ARG:NH2	42:X:8612:HOH:O	2.52	0.43
15:K:104:ASP:HB2	42:K:8581:HOH:O	2.19	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.19	0.43
1:0:1200:A:H4'	42:0:6810:HOH:O	2.19	0.43
26:V:60:GLU:O	26:V:63:GLU:HB2	2.19	0.43
18:N:63:LYS:HG3	18:N:80:ASP:O	2.19	0.43
1:0:2078:U:O2'	1:0:2079:G:H5'	2.18	0.43
1:0:1419:U:H2'	1:0:1685:A:C2	2.54	0.43
12:H:151:MET:HE3	12:H:151:MET:HA	2.00	0.43
8:D:49:PRO:HA	8:D:73:VAL:HG22	2.00	0.43
1:0:1940:C:H5''	5:A:234:GLY:HA3	2.01	0.43
17:M:37:ARG:HD3	36:M:8507:CL:CL	2.56	0.43
17:M:67:ALA:C	17:M:69:TYR:H	2.22	0.43
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.43
5:A:153:ARG:NH1	5:A:153:ARG:HB2	2.28	0.43
10:F:47:LEU:HD22	10:F:108:LEU:CD1	2.49	0.43
2:9:3091:C:H2'	2:9:3092:G:O4'	2.18	0.43
1:0:677:C:H4'	7:C:246:ARG:NH2	2.34	0.43
29:Y:56:MET:HA	29:Y:62:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:24:ARG:HH21	23:S:39:ASN:ND2	2.17	0.43
16:L:82:ARG:NH2	42:L:8624:HOH:O	2.51	0.43
1:0:639:A:H2'	1:0:640:G:C8	2.53	0.43
1:0:513:A:N3	42:0:3152:HOH:O	2.37	0.43
7:C:109:LEU:O	7:C:109:LEU:HD12	2.18	0.43
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.43
1:0:583:G:H2'	1:0:584:U:H6	1.83	0.43
1:0:1345:A:H2'	1:0:1346:U:C6	2.54	0.43
1:0:2869:G:H5'	42:0:4971:HOH:O	2.17	0.43
12:H:163:PRO:O	12:H:164:ALA:HB2	2.19	0.43
2:9:3056:A:C3'	2:9:3057:A:H5''	2.49	0.43
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.99	0.43
7:C:234:VAL:HG22	7:C:234:VAL:O	2.18	0.43
1:0:2769:C:H2'	1:0:2770:G:C5'	2.49	0.43
9:E:20:ILE:HD12	9:E:33:LEU:CD1	2.49	0.43
23:S:75:GLU:HB3	42:S:4772:HOH:O	2.18	0.43
28:X:144:ARG:NH1	42:X:8577:HOH:O	2.49	0.43
16:L:154:ARG:HD3	42:L:8648:HOH:O	2.17	0.43
1:0:2547:C:H2'	1:0:2548:C:H6	1.83	0.43
21:Q:17:MET:HE3	21:Q:19:ARG:CZ	2.49	0.43
6:B:248:ARG:O	6:B:251:VAL:HG13	2.19	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.19	0.43
23:S:96:VAL:HG13	23:S:97:ARG:N	2.34	0.43
25:U:45:ARG:C	25:U:47:LYS:N	2.72	0.43
1:0:1743:G:H1'	42:0:4362:HOH:O	2.18	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
1:0:1380:U:H5'	42:0:8728:HOH:O	2.18	0.43
1:0:2457:U:H1'	32:2:79:LEU:HD13	2.01	0.43
7:C:22:PHE:HA	7:C:116:ALA:HA	2.00	0.43
7:C:127:ARG:HD2	7:C:229:PRO:O	2.19	0.42
26:V:54:PHE:CZ	26:V:140:LYS:HB2	2.53	0.42
1:0:2346:C:O5'	1:0:2346:C:C6	2.72	0.42
42:0:9457:HOH:O	32:2:84:ARG:HB2	2.19	0.42
1:0:2089:A:C2'	1:0:2090:G:H5'	2.49	0.42
1:0:2634:G:OP2	5:A:204:GLY:N	2.35	0.42
1:0:1682:A:H5''	42:0:8957:HOH:O	2.19	0.42
18:N:80:ASP:OD1	18:N:81:PHE:N	2.52	0.42
18:N:7:LEU:HD22	42:N:5650:HOH:O	2.19	0.42
1:0:1734:C:OP1	6:B:234:ARG:HD3	2.19	0.42
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.42
1:0:666:A:H2'	1:0:667:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.42
16:L:123:ASP:OD1	16:L:124:GLY:N	2.52	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
16:L:184:ARG:HG3	16:L:185:PRO:HA	2.01	0.42
1:0:1878:G:H5''	42:0:9293:HOH:O	2.19	0.42
6:B:71:VAL:CG1	6:B:296:LEU:HB3	2.47	0.42
10:F:28:ALA:HB3	10:F:99:THR:HG23	2.00	0.42
7:C:233:THR:HG22	7:C:234:VAL:H	1.84	0.42
1:0:2409:C:H4'	32:2:17:HIS:CB	2.48	0.42
6:B:4:SER:O	6:B:5:ARG:HB2	2.19	0.42
1:0:1788:U:C2	1:0:1805:G:N2	2.87	0.42
42:0:6926:HOH:O	7:C:188:ARG:HD2	2.19	0.42
1:0:2429:A:H2'	1:0:2430:A:C8	2.54	0.42
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.42
1:0:2084:C:H2'	1:0:2085:A:C8	2.54	0.42
1:0:1388:U:H2'	1:0:1389:G:O4'	2.19	0.42
1:0:420:U:H2'	1:0:421:C:C6	2.54	0.42
1:0:51:G:O2'	1:0:52:A:H5'	2.20	0.42
24:T:35:LYS:NZ	42:T:6621:HOH:O	2.44	0.42
12:H:47:GLU:CB	12:H:133:ILE:CD1	2.91	0.42
7:C:140:VAL:HG12	7:C:141:SER:N	2.34	0.42
12:H:48:LEU:HD13	12:H:146:TRP:HB3	2.00	0.42
1:0:2712:G:H5'	42:0:4697:HOH:O	2.19	0.42
6:B:162:MET:HG3	6:B:310:ARG:HD3	2.01	0.42
12:H:39:GLY:O	12:H:41:THR:N	2.52	0.42
42:9:7568:HOH:O	17:M:107:ASN:HB3	2.19	0.42
9:E:15:GLN:HG2	9:E:19:ASP:O	2.19	0.42
16:L:65:VAL:CG2	16:L:105:ALA:HB2	2.47	0.42
23:S:23:VAL:C	23:S:93:THR:HG21	2.40	0.42
28:X:178:HIS:CG	28:X:179:PRO:HD2	2.54	0.42
1:0:2894:C:O2'	1:0:2895:C:H5'	2.19	0.42
1:0:1224:G:H2'	1:0:1225:C:C6	2.54	0.42
16:L:49:ALA:C	16:L:54:TYR:HB3	2.39	0.42
42:3:6229:HOH:O	38:4:77:PHA:HA	2.20	0.42
1:0:1462:C:H2'	1:0:1463:A:C8	2.54	0.42
8:D:159:PRO:O	8:D:162:ALA:HB3	2.19	0.42
7:C:115:LEU:HA	7:C:115:LEU:HD12	1.88	0.42
7:C:76:ARG:HG2	7:C:78:ARG:NH1	2.34	0.42
14:J:74:VAL:HG12	14:J:75:ARG:HG3	2.00	0.42
13:I:107:ASN:HD22	13:I:108:PRO:N	2.17	0.42
1:0:736:A:H2'	1:0:737:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2320:U:OP2	32:2:2:GLN:N	2.53	0.42
15:K:105:TYR:C	15:K:105:TYR:CD1	2.93	0.42
5:A:179:MET:HA	5:A:179:MET:CE	2.50	0.42
18:N:25:VAL:O	18:N:29:VAL:HG23	2.19	0.42
1:0:1463:A:H2'	1:0:1464:U:C6	2.55	0.42
1:0:2649:A:H5'	1:0:2649:A:H8	1.84	0.42
1:0:684:G:H2'	1:0:685:C:C6	2.54	0.42
42:0:4097:HOH:O	5:A:6:GLY:HA3	2.17	0.42
1:0:2503:A:OP1	12:H:147:ARG:NH2	2.41	0.42
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.02	0.42
25:U:1:THR:HG23	25:U:2:VAL:N	2.29	0.42
7:C:184:ARG:HB3	42:C:8369:HOH:O	2.19	0.42
1:0:396:U:HO2'	1:0:397:A:P	2.43	0.42
5:A:75:GLY:HA2	29:Y:63:LYS:O	2.20	0.42
16:L:134:ILE:O	16:L:136:PRO:HD3	2.19	0.42
9:E:81:GLU:HA	9:E:133:VAL:O	2.19	0.42
7:C:219:ASN:N	7:C:222:ASP:OD1	2.53	0.42
23:S:41:ARG:HH11	23:S:41:ARG:HG2	1.85	0.42
16:L:123:ASP:C	16:L:123:ASP:OD1	2.58	0.42
23:S:79:LEU:HG	23:S:89:ARG:HB2	2.02	0.42
1:0:1562:C:H2'	1:0:1562:C:O2	2.19	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.20	0.42
1:0:1316:G:H1'	1:0:1340:G:N2	2.34	0.42
21:Q:84:ALA:O	21:Q:88:PHE:HD1	2.03	0.42
12:H:31:PHE:HA	12:H:85:ILE:CG2	2.50	0.42
12:H:48:LEU:CG	12:H:157:ILE:HG21	2.48	0.42
12:H:46:VAL:HG12	12:H:146:TRP:CZ3	2.46	0.42
30:Z:21:ARG:HD2	30:Z:39:PHE:HB2	2.02	0.42
32:2:3:MET:HG3	32:2:4:PRO:HD2	2.01	0.42
42:0:8898:HOH:O	16:L:94:LYS:HE2	2.20	0.42
1:0:168:C:O5'	1:0:168:C:H6	2.02	0.42
6:B:215:VAL:HA	6:B:220:VAL:HG22	2.01	0.42
5:A:57:ALA:HA	5:A:67:LEU:HD23	2.01	0.42
6:B:203:ALA:HA	6:B:262:ARG:O	2.19	0.42
2:9:3004:G:O2'	17:M:44:ARG:NH2	2.52	0.42
1:0:1352:A:N1	7:C:48:SER:HB3	2.35	0.42
8:D:41:LEU:CA	8:D:44:ILE:HG22	2.48	0.42
16:L:38:VAL:HG12	16:L:38:VAL:O	2.17	0.42
21:Q:39:THR:O	21:Q:40:ALA:C	2.57	0.42
18:N:47:ARG:NH1	42:N:4564:HOH:O	2.52	0.42
17:M:167:ASP:O	17:M:168:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2291:A:N9	1:0:2309:C:H5'	2.34	0.42
14:J:4:LEU:HD22	14:J:116:GLU:HB3	2.01	0.42
17:M:152:GLU:OE1	17:M:152:GLU:HA	2.20	0.42
21:Q:111:ILE:HG23	21:Q:145:LEU:CD1	2.49	0.42
17:M:43:VAL:HG11	17:M:81:ALA:HA	2.02	0.42
6:B:76:THR:N	6:B:77:PRO:HD3	2.34	0.42
10:F:48:VAL:HG23	10:F:74:PHE:HB3	1.96	0.42
1:0:514:G:OP1	1:0:514:G:H2'	2.20	0.42
9:E:24:GLY:N	9:E:76:VAL:HB	2.34	0.42
18:N:26:TRP:CE3	18:N:26:TRP:HA	2.55	0.42
1:0:583:G:H2'	1:0:584:U:C6	2.54	0.42
1:0:2084:C:H2'	1:0:2085:A:H8	1.84	0.42
17:M:50:LEU:HA	17:M:50:LEU:HD12	1.85	0.42
1:0:87:C:H2'	31:1:28:LYS:O	2.19	0.42
1:0:2804:C:H2'	1:0:2805:A:O4'	2.20	0.42
1:0:2561:C:OP1	9:E:153:ARG:NH2	2.52	0.42
42:0:4827:HOH:O	23:S:3:GLN:HG2	2.19	0.42
1:0:1882:C:O2'	1:0:2012:U:OP2	2.34	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.20	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.02	0.42
7:C:141:SER:HB3	42:C:8424:HOH:O	2.20	0.42
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.20	0.42
16:L:164:THR:HB	42:L:8520:HOH:O	2.18	0.42
42:0:3250:HOH:O	23:S:9:LYS:HD2	2.19	0.42
1:0:482:G:H4'	1:0:508:A:N1	2.35	0.42
5:A:103:VAL:HA	5:A:104:PRO:HD3	1.86	0.42
1:0:2815:G:H4'	1:0:2816:A:OP2	2.19	0.42
6:B:280:VAL:CG1	6:B:281:ASP:N	2.82	0.42
29:Y:13:ARG:NH1	42:Y:8418:HOH:O	2.51	0.42
1:0:1014:A:H5''	2:9:3101:G:O2'	2.20	0.42
16:L:80:GLY:O	16:L:81:ARG:HD3	2.19	0.42
1:0:1461:U:H2'	1:0:1462:C:C6	2.55	0.42
28:X:148:GLY:O	28:X:154:ARG:HD3	2.20	0.42
20:P:93:ARG:HG3	20:P:93:ARG:NH1	2.35	0.42
21:Q:31:ILE:O	21:Q:32:ALA:C	2.57	0.42
1:0:2906:A:H5'	1:0:2907:C:O4'	2.19	0.42
14:J:128:ALA:HB3	14:J:131:ILE:HD11	2.02	0.42
1:0:2050:G:OP1	21:Q:79:ARG:HB3	2.19	0.42
1:0:812:A:H2'	1:0:813:C:C6	2.55	0.42
1:0:1702:U:H5''	42:0:6687:HOH:O	2.20	0.42
15:K:142:LEU:HG	15:K:146:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:221:GLN:HE22	14:J:42:ASN:ND2	2.14	0.42
1:0:920:C:H5'	1:0:921:G:N3	2.35	0.42
1:0:694:A:C2'	1:0:695:C:H5'	2.50	0.42
1:0:814:G:N2	1:0:815:U:H1'	2.35	0.42
1:0:2453:G:H2'	1:0:2454:C:C6	2.55	0.42
12:H:110:GLY:N	42:H:8397:HOH:O	2.52	0.42
1:0:945:U:O2'	26:V:43:GLY:HA3	2.20	0.42
1:0:1496:G:H5'	1:0:1572:A:H1'	2.02	0.42
1:0:2846:C:OP1	6:B:158:LYS:HD3	2.20	0.42
7:C:173:LYS:HB3	7:C:187:ARG:HG3	2.00	0.42
1:0:1003:U:O2	12:H:90:PHE:CZ	2.73	0.42
12:H:83:PHE:HE1	12:H:146:TRP:CZ2	2.38	0.42
1:0:2533:C:O2'	1:0:2534:C:H5'	2.20	0.42
6:B:162:MET:HG3	6:B:310:ARG:NH1	2.35	0.42
6:B:43:GLY:O	6:B:308:LEU:HD12	2.19	0.42
1:0:1603:A:H5''	1:0:1605:G:H5'	2.01	0.42
28:X:189:ASN:HD22	28:X:192:ASP:H	1.68	0.42
6:B:320:GLN:HG3	6:B:321:PRO:CD	2.49	0.42
29:Y:38:LYS:HA	29:Y:45:LYS:HA	2.02	0.42
1:0:1828:G:H2'	1:0:1829:A:H5'	2.00	0.42
9:E:11:VAL:HG11	9:E:22:VAL:HG13	2.01	0.42
1:0:259:G:H21	16:L:58:GLN:NE2	2.17	0.42
12:H:71:TYR:O	12:H:73:GLN:N	2.53	0.42
17:M:38:LYS:HE3	17:M:38:LYS:HB2	1.82	0.42
1:0:314:G:N2	1:0:316:A:H3'	2.34	0.42
14:J:118:ALA:HA	14:J:125:ALA:HB2	2.02	0.42
6:B:16:ARG:NH2	42:B:8551:HOH:O	2.40	0.42
20:P:93:ARG:HG3	20:P:93:ARG:HH11	1.85	0.42
1:0:812:A:H1'	42:0:3447:HOH:O	2.20	0.42
12:H:6:TYR:HE2	12:H:94:ARG:O	2.03	0.42
32:2:34:LYS:HB2	32:2:37:ASP:OD2	2.20	0.42
1:0:2440:C:H5''	42:0:3309:HOH:O	2.19	0.42
42:0:9844:HOH:O	20:P:16:ASN:HB2	2.19	0.42
14:J:9:THR:O	14:J:10:GLN:C	2.59	0.41
1:0:2780:C:H2'	1:0:2781:U:C6	2.55	0.41
7:C:162:VAL:CG1	7:C:162:VAL:O	2.68	0.41
2:9:3092:G:H22	12:H:52:LYS:NZ	2.18	0.41
12:H:113:ALA:N	12:H:114:PRO:CD	2.83	0.41
1:0:1730:G:H4'	1:0:1731:C:O5'	2.20	0.41
9:E:126:ILE:HB	9:E:131:LEU:HD21	2.02	0.41
16:L:78:ASN:O	16:L:79:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:22:VAL:CG2	10:F:104:ALA:HB2	2.50	0.41
7:C:200:PRO:HB3	7:C:212:VAL:CG2	2.50	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.34	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.55	0.41
1:0:2271:G:P	42:0:8936:HOH:O	2.77	0.41
1:0:772:G:H2'	1:0:773:A:O4'	2.20	0.41
1:0:324:G:O2'	1:0:325:U:H5'	2.20	0.41
15:K:89:PHE:N	42:K:8576:HOH:O	2.53	0.41
1:0:2761:A:C4	1:0:2763:G:C8	3.08	0.41
1:0:240:C:C5'	16:L:146:GLN:NE2	2.83	0.41
5:A:36:ASP:O	5:A:37:VAL:C	2.58	0.41
1:0:2004:U:H1'	42:0:9687:HOH:O	2.20	0.41
32:2:84:ARG:HB3	42:2:8557:HOH:O	2.20	0.41
16:L:77:PHE:HD1	16:L:79:LYS:O	2.03	0.41
10:F:21:GLU:O	10:F:24:ARG:CG	2.67	0.41
15:K:73:VAL:HG11	15:K:118:LEU:HD21	2.02	0.41
1:0:926:A:O2'	15:K:41:HIS:CD2	2.73	0.41
18:N:53:GLN:HG2	18:N:56:GLU:OE1	2.20	0.41
27:W:27:ASP:OD2	27:W:27:ASP:N	2.52	0.41
1:0:675:U:H2'	1:0:676:C:H5'	2.01	0.41
1:0:488:U:O2'	23:S:82:THR:HG21	2.20	0.41
23:S:80:GLU:OE2	23:S:84:GLY:HA2	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.19	0.41
1:0:354:A:H2'	1:0:355:C:C6	2.55	0.41
1:0:290:C:O2'	1:0:291:C:H5'	2.19	0.41
1:0:2004:U:H2'	1:0:2005:G:OP1	2.20	0.41
26:V:125:HIS:CD2	26:V:127:GLY:H	2.38	0.41
6:B:248:ARG:O	6:B:251:VAL:HG12	2.20	0.41
1:0:710:G:P	18:N:24:ALA:HB3	2.61	0.41
23:S:55:PHE:HB2	42:S:6384:HOH:O	2.19	0.41
2:9:3064:C:C2'	2:9:3065:A:H5'	2.50	0.41
7:C:187:ARG:NH2	42:C:8370:HOH:O	2.42	0.41
20:P:16:ASN:HA	20:P:16:ASN:HD22	1.64	0.41
7:C:37:ALA:HB2	42:C:8387:HOH:O	2.20	0.41
1:0:1137:G:H1'	42:0:3367:HOH:O	2.19	0.41
1:0:134:U:C2	1:0:145:A:C2	3.09	0.41
8:D:81:GLU:O	8:D:85:GLN:HG3	2.20	0.41
1:0:1616:A:H5''	1:0:1617:C:OP1	2.20	0.41
28:X:122:ARG:NH2	42:X:8536:HOH:O	2.53	0.41
1:0:2488:A:H2	42:0:6747:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:99:ARG:HD2	16:L:167:GLY:HA2	2.02	0.41
14:J:10:GLN:NE2	14:J:10:GLN:N	2.43	0.41
17:M:69:TYR:HE2	17:M:183:ASP:OD2	2.03	0.41
1:O:2435:U:P	32:2:28:GLY:HA3	2.60	0.41
5:A:170:VAL:HG22	29:Y:22:ILE:HG23	2.01	0.41
8:D:53:LYS:HA	8:D:67:ASP:O	2.21	0.41
16:L:137:ASP:HA	16:L:142:LYS:HE3	2.03	0.41
26:V:149:LEU:HG	26:V:153:MET:HE2	2.03	0.41
7:C:7:ASP:C	7:C:9:ASP:H	2.24	0.41
1:O:1609:C:H2'	1:O:1610:G:C8	2.56	0.41
1:O:461:C:N3	1:O:479:G:H5'	2.36	0.41
1:O:229:G:O2'	1:O:230:C:H5'	2.20	0.41
1:O:945:U:H2'	1:O:946:C:C6	2.56	0.41
1:O:192:A:C4'	16:L:176:GLN:HE22	2.34	0.41
15:K:75:LEU:N	15:K:75:LEU:HD23	2.35	0.41
1:O:2237:G:H1'	42:O:4324:HOH:O	2.19	0.41
1:O:81:G:N3	1:O:98:A:C2	2.88	0.41
2:9:3026:C:P	42:9:3472:HOH:O	2.77	0.41
1:O:1545:C:H2'	1:O:1546:G:O4'	2.20	0.41
8:D:35:ALA:HB2	42:D:5858:HOH:O	2.21	0.41
1:O:1192:A:O2'	1:O:1193:A:OP1	2.29	0.41
1:O:401:C:H5'	42:O:5268:HOH:O	2.20	0.41
5:A:69:LEU:HD12	5:A:69:LEU:C	2.40	0.41
29:Y:33:HIS:HE1	29:Y:49:ARG:NE	2.19	0.41
1:O:213:G:O2'	1:O:214:U:OP2	2.39	0.41
8:D:76:ARG:O	8:D:77:ASP:HB2	2.21	0.41
1:O:1634:G:H2'	1:O:1635:U:H6	1.85	0.41
1:O:1524:U:O2'	1:O:1525:G:P	2.78	0.41
26:V:121:PRO:HA	26:V:153:MET:HG2	2.02	0.41
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.50	0.41
1:O:2911:C:H2'	1:O:2912:C:H6	1.84	0.41
17:M:42:HIS:CG	17:M:62:HIS:HE1	2.37	0.41
1:O:2729:C:O2'	1:O:2730:G:H5'	2.21	0.41
1:O:305:A:C5	1:O:329:A:C2	3.09	0.41
22:R:29:ASP:OD2	22:R:31:ARG:NH1	2.54	0.41
42:O:5719:HOH:O	5:A:22:ARG:HG2	2.19	0.41
2:9:3107:C:H5	42:9:3167:HOH:O	2.03	0.41
18:N:73:ASP:HA	18:N:92:VAL:O	2.20	0.41
1:O:2324:G:H4'	1:O:2418:G:O2'	2.20	0.41
1:O:1287:A:O4'	26:V:117:ARG:HD3	2.20	0.41
8:D:104:PHE:CE2	8:D:132:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:123:GLY:HA2	5:A:159:VAL:O	2.21	0.41
24:T:47:ARG:HG3	42:T:4381:HOH:O	2.19	0.41
1:0:459:A:H4'	42:0:8954:HOH:O	2.19	0.41
12:H:149:ALA:C	12:H:151:MET:H	2.23	0.41
12:H:68:ALA:HB2	12:H:149:ALA:HB2	2.03	0.41
1:0:2721:U:H4'	14:J:87:ARG:HG3	2.03	0.41
26:V:21:LEU:HD22	26:V:26:ILE:HD13	2.01	0.41
13:I:131:THR:HG22	13:I:134:GLU:N	2.21	0.41
1:0:508:A:H2'	1:0:509:A:H5''	2.01	0.41
26:V:122:ARG:CG	26:V:122:ARG:NH1	2.80	0.41
1:0:2812:A:N7	42:0:6984:HOH:O	2.37	0.41
10:F:33:THR:HG21	10:F:59:ILE:O	2.21	0.41
19:O:134:VAL:O	19:O:137:LEU:HB3	2.20	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.56	0.41
17:M:82:TYR:C	17:M:82:TYR:CD2	2.94	0.41
1:0:765:G:O3'	7:C:69:HIS:HB3	2.20	0.41
5:A:232:ARG:NH2	5:A:236:GLY:O	2.48	0.41
2:9:3045:A:H2'	2:9:3046:C:H6	1.86	0.41
16:L:42:ARG:HA	16:L:43:PRO:HD3	1.86	0.41
1:0:245:C:H2'	1:0:246:G:H5'	2.02	0.41
1:0:151:A:H2'	1:0:152:A:O4'	2.21	0.41
1:0:2642:G:H2'	1:0:2643:G:O4'	2.19	0.41
12:H:157:ILE:CG2	12:H:158:ASN:H	2.34	0.41
17:M:67:ALA:HA	17:M:71:TRP:CB	2.51	0.41
17:M:71:TRP:CE3	17:M:175:LEU:CD2	3.03	0.41
12:H:143:GLU:N	42:H:8381:HOH:O	2.53	0.41
26:V:21:LEU:HB3	26:V:26:ILE:CG1	2.51	0.41
1:0:1603:A:H5'	1:0:1605:G:C4'	2.50	0.41
1:0:483:C:C4	1:0:484:A:C6	3.09	0.41
1:0:319:A:H4'	1:0:338:C:C5	2.55	0.41
16:L:169:ARG:NH1	42:L:8574:HOH:O	2.54	0.41
1:0:711:G:N2	1:0:718:C:C2	2.88	0.41
1:0:1159:G:P	42:0:3774:HOH:O	2.78	0.41
8:D:93:LEU:HB3	8:D:97:GLN:OE1	2.20	0.41
2:9:3003:A:H2	2:9:3021:G:N3	2.18	0.41
15:K:72:ASN:HB2	42:K:8586:HOH:O	2.20	0.41
27:W:14:LEU:HD12	27:W:67:PRO:O	2.20	0.41
20:P:26:PRO:O	20:P:30:VAL:HG23	2.21	0.41
1:0:571:C:H6	1:0:571:C:O5'	2.03	0.41
1:0:1485:A:H4'	42:0:9780:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1568:G:O2'	1:0:1569:U:H5'	2.20	0.41
21:Q:59:PHE:HZ	21:Q:81:PRO:HG3	1.84	0.41
18:N:45:LEU:HD12	18:N:88:LYS:HD2	2.01	0.41
1:0:823:U:H2'	1:0:824:G:O4'	2.20	0.41
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.36	0.41
17:M:79:PRO:O	17:M:83:LEU:HG	2.21	0.41
1:0:1119:G:N2	1:0:1246:A:H2	2.14	0.41
17:M:162:ASP:HB3	17:M:163:PHE:H	1.63	0.41
8:D:52:THR:HB	8:D:70:GLY:O	2.21	0.41
17:M:154:LEU:HD11	17:M:157:PRO:HA	2.03	0.41
22:R:80:ARG:HG2	42:R:8336:HOH:O	2.20	0.41
1:0:2842:G:H2'	1:0:2843:A:C5'	2.51	0.41
1:0:2729:C:H2'	1:0:2730:G:H8	1.86	0.41
1:0:2011:A:P	42:0:5433:HOH:O	2.78	0.41
18:N:26:TRP:HE3	18:N:26:TRP:HA	1.85	0.41
1:0:1224:G:H2'	1:0:1225:C:H6	1.84	0.41
1:0:1055:G:OP2	12:H:94:ARG:NH1	2.54	0.41
15:K:89:PHE:N	15:K:89:PHE:CD1	2.88	0.41
1:0:2045:G:H2'	1:0:2046:G:O4'	2.21	0.41
1:0:1483:C:O2'	1:0:1484:G:H5'	2.21	0.41
22:R:11:THR:H	22:R:14:ALA:HB3	1.84	0.41
1:0:1498:G:O2'	1:0:1499:U:H5'	2.20	0.41
9:E:21:THR:HG23	9:E:30:THR:OG1	2.21	0.41
1:0:1969:A:N7	1:0:1970:G:C6	2.89	0.41
42:0:3336:HOH:O	12:H:11:LYS:HE2	2.20	0.41
22:R:8:PRO:HD2	25:U:32:ALA:HA	2.03	0.41
29:Y:41:VAL:HG12	29:Y:42:CYS:N	2.35	0.41
29:Y:46:LYS:HE2	42:Y:8434:HOH:O	2.20	0.41
8:D:27:ILE:HD11	8:D:37:ALA:CB	2.51	0.41
2:9:3056:A:H1'	8:D:14:ARG:HG2	2.03	0.41
1:0:240:C:O2	1:0:240:C:H2'	2.21	0.41
12:H:136:VAL:HG22	12:H:137:ASN:N	2.36	0.41
26:V:76:ASP:O	26:V:77:ALA:C	2.59	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
9:E:7:ILE:HA	9:E:8:PRO:HD3	1.94	0.41
25:U:38:GLY:C	25:U:40:PRO:HD2	2.41	0.41
1:0:396:U:C3'	42:0:3823:HOH:O	2.68	0.41
8:D:173:GLU:O	8:D:174:VAL:C	2.58	0.41
2:9:3088:G:N2	2:9:3089:C:C2	2.89	0.41
15:K:1:THR:N	42:K:8583:HOH:O	2.54	0.41
1:0:1972:U:C2'	1:0:1973:A:H5'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2415:A:C2	17:M:25:ARG:HB3	2.56	0.41
16:L:55:LYS:O	16:L:60:ILE:HD12	2.21	0.41
1:0:1086:A:N6	26:V:11:VAL:HG11	2.36	0.41
1:0:1730:G:C5'	1:0:1731:C:H6	2.33	0.41
26:V:119:HIS:CD2	26:V:120:PRO:O	2.73	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.68	0.41
1:0:2842:G:C2'	1:0:2843:A:H5'	2.50	0.41
1:0:2265:U:H2'	1:0:2266:A:C8	2.56	0.41
23:S:23:VAL:HG23	23:S:41:ARG:HG3	2.02	0.41
1:0:1312:G:OP1	28:X:213:LYS:NZ	2.48	0.41
1:0:2039:A:OP2	6:B:234:ARG:NH2	2.54	0.41
1:0:488:U:H2'	42:0:3493:HOH:O	2.21	0.41
1:0:1025:C:H5'	26:V:23:MET:O	2.21	0.41
1:0:963:C:H6	1:0:963:C:O5'	2.04	0.41
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.88	0.41
2:9:3052:A:H2'	2:9:3053:G:O4'	2.21	0.41
1:0:241:A:C2	1:0:378:A:H4'	2.56	0.41
1:0:1613:C:H2'	1:0:1614:G:O4'	2.20	0.41
24:T:50:GLU:CD	42:T:7349:HOH:O	2.58	0.41
29:Y:77:LYS:HA	29:Y:80:MET:CE	2.51	0.41
13:I:116:LEU:HB2	13:I:119:THR:HG21	2.02	0.41
17:M:34:LEU:HD22	17:M:129:ILE:CD1	2.51	0.41
12:H:83:PHE:HD1	12:H:134:ALA:HB2	1.84	0.41
16:L:63:VAL:HG21	16:L:109:PHE:CZ	2.56	0.41
9:E:22:VAL:O	9:E:28:SER:HA	2.21	0.41
27:W:76:ARG:NH1	27:W:76:ARG:CG	2.84	0.41
5:A:94:LEU:N	5:A:94:LEU:CD2	2.84	0.41
17:M:154:LEU:CG	17:M:155:GLU:N	2.83	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
29:Y:13:ARG:NH1	29:Y:14:PHE:CE2	2.88	0.41
8:D:58:VAL:CG1	8:D:59:GLY:N	2.83	0.41
8:D:59:GLY:C	8:D:61:PHE:H	2.19	0.41
1:0:2831:C:H2'	1:0:2832:C:C5'	2.51	0.41
23:S:40:VAL:HA	23:S:119:ALA:O	2.21	0.41
1:0:424:C:H2'	1:0:425:U:H6	1.85	0.41
22:R:25:GLN:HG2	22:R:65:VAL:HG22	2.03	0.41
1:0:794:U:H3	1:0:819:A:H61	1.68	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.41
1:0:1079:A:N1	1:0:2068:G:O2'	2.48	0.41
2:9:3040:C:N4	8:D:51:ARG:HB2	2.36	0.40
26:V:6:GLN:HA	26:V:52:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:32:GLY:N	42:F:3111:HOH:O	2.53	0.40
9:E:98:GLU:N	42:E:4191:HOH:O	2.53	0.40
10:F:100:ASP:O	10:F:101:ALA:O	2.39	0.40
7:C:138:VAL:O	7:C:234:VAL:HA	2.21	0.40
7:C:192:ILE:CG2	7:C:234:VAL:HG12	2.51	0.40
42:O:5726:HOH:O	24:T:56:ARG:HD3	2.20	0.40
21:Q:18:LEU:HB2	21:Q:143:VAL:HG13	2.03	0.40
17:M:149:GLU:O	17:M:152:GLU:HB2	2.21	0.40
5:A:81:GLN:CB	5:A:92:ASN:ND2	2.83	0.40
18:N:96:VAL:CG1	18:N:100:GLN:HB2	2.51	0.40
25:U:23:LEU:HD22	25:U:49:LEU:HD23	2.03	0.40
8:D:170:TYR:N	8:D:170:TYR:CD1	2.89	0.40
1:O:2912:C:H2'	1:O:2913:A:O4'	2.21	0.40
2:9:3105:A:H2'	2:9:3106:C:O4'	2.21	0.40
1:O:941:G:C5	1:O:942:U:C4	3.09	0.40
21:Q:47:LEU:HB2	21:Q:89:LEU:HD21	2.02	0.40
1:O:2610:U:H4'	42:O:8982:HOH:O	2.20	0.40
1:O:1815:A:H4'	1:O:2751:C:O4'	2.22	0.40
1:O:1003:U:H4'	12:H:86:ARG:O	2.21	0.40
1:O:566:A:H2'	1:O:567:U:O4'	2.21	0.40
29:Y:22:ILE:HG22	29:Y:23:ARG:N	2.36	0.40
1:O:67:A:H5''	1:O:69:A:C8	2.57	0.40
1:O:1477:C:H5'	1:O:1868:G:H5'	2.03	0.40
1:O:2474:A:N7	1:O:2621:U:H4'	2.37	0.40
1:O:1268:C:H2'	1:O:1269:G:C8	2.56	0.40
1:O:612:U:H2'	1:O:613:C:C6	2.57	0.40
12:H:129:ASN:N	12:H:129:ASN:HD22	2.18	0.40
16:L:168:ARG:NH1	42:L:8604:HOH:O	2.54	0.40
23:S:14:ALA:HA	23:S:15:PRO:HD3	1.94	0.40
1:O:90:A:H2'	1:O:91:G:O4'	2.21	0.40
1:O:626:U:C4	1:O:627:G:C6	3.08	0.40
12:H:26:LYS:CG	12:H:28:ILE:H	2.23	0.40
1:O:1164:U:N3	1:O:1192:A:H2	2.09	0.40
17:M:91:ARG:HG3	17:M:186:LEU:CD2	2.49	0.40
1:O:544:G:H2'	1:O:545:G:C5'	2.46	0.40
6:B:258:GLY:HA2	42:B:8555:HOH:O	2.20	0.40
17:M:163:PHE:O	17:M:164:ASP:O	2.38	0.40
5:A:130:THR:HG22	5:A:131:HIS:O	2.21	0.40
15:K:61:ALA:HA	42:K:8570:HOH:O	2.21	0.40
28:X:99:ALA:HB2	28:X:233:TYR:CE2	2.56	0.40
1:O:2266:A:H2'	1:O:2267:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:121:ILE:HG12	15:K:141:GLU:HB2	2.02	0.40
1:O:745:G:O6	18:N:68:GLY:HA3	2.22	0.40
1:O:1992:U:H2'	1:O:1994:A:OP2	2.22	0.40
1:O:1815:A:H2'	1:O:1816:C:O4'	2.22	0.40
1:O:1762:C:O2'	1:O:1763:C:H5'	2.21	0.40
1:O:1307:A:H2'	1:O:1308:A:C8	2.56	0.40
1:O:954:U:O2'	1:O:955:A:H5'	2.21	0.40
7:C:84:VAL:O	7:C:85:LYS:HB2	2.21	0.40
1:O:1515:A:H2'	1:O:1516:C:C6	2.56	0.40
1:O:1711:A:O2'	1:O:1712:A:H5'	2.20	0.40
5:A:29:HIS:CE1	5:A:107:ASN:ND2	2.89	0.40
1:O:1881:A:OP1	5:A:199:HIS:HE1	2.05	0.40
1:O:1641:A:C2'	1:O:1642:A:H5'	2.49	0.40
1:O:2851:G:C2'	1:O:2852:A:H5'	2.52	0.40
1:O:2589:U:H2'	1:O:2590:U:C6	2.57	0.40
1:O:1730:G:C5'	1:O:1731:C:C6	3.04	0.40
16:L:59:GLY:HA3	16:L:141:ILE:CD1	2.50	0.40
27:W:30:MET:CE	27:W:58:ALA:HB3	2.51	0.40
20:P:30:VAL:O	20:P:30:VAL:HG12	2.21	0.40
1:O:40:C:H6	1:O:40:C:O5'	2.05	0.40
1:O:2582:G:O3'	14:J:41:LYS:HA	2.21	0.40
1:O:2897:C:H2'	1:O:2898:G:H8	1.85	0.40
8:D:68:PRO:HG3	42:D:1982:HOH:O	2.21	0.40
1:O:1050:G:C6	1:O:1051:C:C4	3.10	0.40
26:V:67:ALA:HB2	26:V:93:ILE:HD13	2.04	0.40
1:O:1624:A:H5'	1:O:1626:A:O4'	2.22	0.40
1:O:39:G:N2	1:O:444:C:C2	2.90	0.40
1:O:825:U:H5''	1:O:826:U:OP1	2.21	0.40
12:H:48:LEU:CD1	12:H:157:ILE:HG21	2.50	0.40
18:N:32:ARG:HB2	42:N:4656:HOH:O	2.20	0.40
26:V:14:HIS:HB2	26:V:17:ILE:HG13	2.04	0.40
8:D:57:THR:HA	8:D:63:ILE:HA	2.03	0.40
11:G:71:LEU:C	11:G:73:ASP:N	2.75	0.40
1:O:187:A:H3'	1:O:188:C:H6	1.86	0.40
8:D:77:ASP:HB3	8:D:78:GLU:H	1.60	0.40
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.35	0.40
1:O:128:A:C8	1:O:128:A:C3'	3.03	0.40
1:O:1804:A:H2'	1:O:1805:G:C8	2.55	0.40
10:F:78:GLU:HG3	42:F:5966:HOH:O	2.20	0.40
1:O:1516:C:H2'	1:O:1517:U:C6	2.57	0.40
26:V:7:LEU:HA	26:V:7:LEU:HD23	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:105:G:O2'	1:0:106:A:H5'	2.21	0.40
1:0:832:U:H2'	1:0:833:G:C8	2.57	0.40
7:C:102:LEU:HD12	42:C:8316:HOH:O	2.21	0.40
5:A:140:LEU:HB3	5:A:141:PRO:HD2	2.04	0.40
1:0:793:A:H5''	19:O:83:LYS:HG2	2.04	0.40
1:0:2364:A:H5''	20:P:15:LYS:HD3	2.03	0.40
6:B:14:GLY:HA2	6:B:15:PRO:C	2.41	0.40
23:S:43:ASN:C	23:S:45:GLY:H	2.24	0.40
7:C:154:VAL:O	7:C:158:GLU:HG3	2.21	0.40
22:R:73:ASP:OD1	22:R:75:GLN:HB2	2.22	0.40
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/239 (98%)	199 (85%)	32 (14%)	4 (2%)	11	43
6	B	335/337 (99%)	299 (89%)	29 (9%)	7 (2%)	9	37
7	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	24	63
8	D	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	1	3
9	E	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
10	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	11	43
11	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
12	H	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	5	26
13	I	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	6	29
14	J	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	13	46
15	K	141/164 (86%)	124 (88%)	16 (11%)	1 (1%)	26	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	L	192/194 (99%)	174 (91%)	17 (9%)	1 (0%)	34	72
17	M	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	4	22
18	N	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
19	O	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	26	65
20	P	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
21	Q	148/154 (96%)	136 (92%)	11 (7%)	1 (1%)	26	65
22	R	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
23	S	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
24	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
25	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	26
26	V	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	15	50
27	W	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	4	22
28	X	140/240 (58%)	140 (100%)	0	0	100	100
29	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	14	48
30	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
31	1	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
32	2	90/92 (98%)	84 (93%)	3 (3%)	3 (3%)	5	26
All	All	3633/4235 (86%)	3293 (91%)	278 (8%)	62 (2%)	11	43

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
8	D	93	LEU
8	D	95	THR
8	D	173	GLU
10	F	101	ALA
12	H	162	SER
15	K	80	ASP
17	M	154	LEU
17	M	164	ASP
17	M	183	ASP
5	A	34	ASP
5	A	132	ASP
6	B	34	GLY
6	B	107	SER

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Mol	Chain	Res	Type
6	B	169	GLY
7	C	8	LEU
8	D	20	LYS
8	D	36	ASN
8	D	137	PRO
12	H	138	PRO
12	H	164	ALA
13	I	5	GLU
14	J	119	GLN
17	M	162	ASP
32	2	57	GLY
5	A	119	ALA
6	B	184	ASP
8	D	11	HIS
8	D	171	ASP
13	I	7	ASP
16	L	140	ALA
17	M	167	ASP
17	M	181	ASP
19	O	116	SER
25	U	43	PRO
26	V	49	ASN
26	V	77	ALA
27	W	77	PHE
27	W	87	ALA
32	2	56	PRO
6	B	185	GLY
8	D	147	ALA
10	F	64	PRO
13	I	76	ASP
13	I	143	LYS
14	J	126	SER
17	M	155	GLU
29	Y	81	LYS
6	B	2	GLN
8	D	16	PRO
8	D	82	GLU
7	C	79	ARG
8	D	61	PHE
8	D	170	TYR
12	H	40	PRO
12	H	72	VAL

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Mol	Chain	Res	Type
5	A	37	VAL
21	Q	106	GLY
25	U	40	PRO
27	W	52	PRO
32	2	25	VAL
8	D	27	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/181 (99%)	166 (93%)	13 (7%)	17	52
6	B	282/282 (100%)	263 (93%)	19 (7%)	20	56
7	C	193/193 (100%)	177 (92%)	16 (8%)	14	46
8	D	117/147 (80%)	108 (92%)	9 (8%)	16	50
9	E	152/155 (98%)	146 (96%)	6 (4%)	39	75
10	F	92/92 (100%)	92 (100%)	0	100	100
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	122/122 (100%)	111 (91%)	11 (9%)	12	41
13	I	118/121 (98%)	107 (91%)	11 (9%)	11	39
14	J	106/106 (100%)	102 (96%)	4 (4%)	40	76
15	K	112/126 (89%)	108 (96%)	4 (4%)	42	77
16	L	166/166 (100%)	157 (95%)	9 (5%)	27	64
17	M	149/149 (100%)	145 (97%)	4 (3%)	52	82
18	N	93/93 (100%)	91 (98%)	2 (2%)	60	85
19	O	113/116 (97%)	109 (96%)	4 (4%)	43	78
20	P	79/79 (100%)	76 (96%)	3 (4%)	40	76
21	Q	117/121 (97%)	113 (97%)	4 (3%)	44	79
22	R	71/73 (97%)	71 (100%)	0	100	100
23	S	105/105 (100%)	102 (97%)	3 (3%)	50	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	T	44/52 (85%)	43 (98%)	1 (2%)	58	84
25	U	51/56 (91%)	49 (96%)	2 (4%)	39	75
26	V	130/130 (100%)	121 (93%)	9 (7%)	19	55
27	W	66/73 (90%)	61 (92%)	5 (8%)	16	51
28	X	120/195 (62%)	112 (93%)	8 (7%)	20	56
29	Y	56/56 (100%)	49 (88%)	7 (12%)	6	22
30	Z	46/46 (100%)	46 (100%)	0	100	100
31	1	42/44 (96%)	41 (98%)	1 (2%)	57	84
32	2	79/79 (100%)	75 (95%)	4 (5%)	29	66
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	28	64

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	33	GLU
5	A	36	ASP
5	A	55	VAL
5	A	68	ILE
5	A	69	LEU
5	A	78	ASP
5	A	94	LEU
5	A	120	ARG
5	A	131	HIS
5	A	153	ARG
5	A	179	MET
5	A	217	ARG
6	B	7	ARG
6	B	11	LEU
6	B	27	ASN
6	B	33	ASP
6	B	63	GLU
6	B	97	LEU
6	B	98	THR
6	B	103	ASP
6	B	162	MET
6	B	195	ARG
6	B	245	SER
6	B	251	VAL

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Mol	Chain	Res	Type
6	B	254	GLN
6	B	256	GLN
6	B	257	THR
6	B	264	GLU
6	B	304	PRO
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	27	ARG
7	C	67	GLN
7	C	76	ARG
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
8	D	24	HIS
8	D	61	PHE
8	D	99	ASP
8	D	100	ASP
8	D	131	THR
8	D	133	ASN
8	D	136	ARG
8	D	137	PRO
8	D	149	ARG
9	E	7	ILE
9	E	12	ASP
9	E	15	GLN
9	E	54	ASP
9	E	102	VAL
9	E	164	ASP
12	H	30	GLN
12	H	59	ASN
12	H	61	LEU
12	H	72	VAL

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Mol	Chain	Res	Type
12	H	73	GLN
12	H	82	LYS
12	H	85	ILE
12	H	86	ARG
12	H	94	ARG
12	H	142	VAL
12	H	150	LYS
13	I	46	ILE
13	I	52	GLN
13	I	74	ARG
13	I	76	ASP
13	I	79	PHE
13	I	107	ASN
13	I	112	ASP
13	I	120	SER
13	I	125	SER
13	I	127	ILE
13	I	131	THR
14	J	7	ASP
14	J	10	GLN
14	J	49	LEU
14	J	98	VAL
15	K	30	ARG
15	K	35	ARG
15	K	80	ASP
15	K	117	GLU
16	L	38	VAL
16	L	46	LEU
16	L	48	ARG
16	L	68	ARG
16	L	81	ARG
16	L	87	MET
16	L	93	ARG
16	L	99	ARG
16	L	164	THR
17	M	26	LEU
17	M	128	ASP
17	M	152	GLU
17	M	163	PHE
18	N	3	THR
18	N	67	SER
19	O	52	LYS

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Mol	Chain	Res	Type
19	O	91	LYS
19	O	94	TRP
19	O	98	ILE
20	P	11	ARG
20	P	57	ASP
20	P	95	GLU
21	Q	13	THR
21	Q	39	THR
21	Q	82	GLU
21	Q	132	ARG
23	S	39	ASN
23	S	73	HIS
23	S	96	VAL
24	T	9	CYS
25	U	43	PRO
25	U	65	ASP
26	V	4	LEU
26	V	26	ILE
26	V	35	VAL
26	V	52	VAL
26	V	73	LEU
26	V	122	ARG
26	V	142	ASP
26	V	146	ILE
26	V	154	ARG
27	W	15	ARG
27	W	27	ASP
27	W	44	ASP
27	W	52	PRO
27	W	72	VAL
28	X	154	ARG
28	X	163	THR
28	X	172	THR
28	X	186	ARG
28	X	189	ASN
28	X	200	THR
28	X	203	VAL
28	X	235	GLU
29	Y	11	THR
29	Y	32	LYS
29	Y	42	CYS
29	Y	49	ARG

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Mol	Chain	Res	Type
29	Y	60	CYS
29	Y	64	ILE
29	Y	68	CYS
31	1	18	ASN
32	2	14	CYS
32	2	42	ARG
32	2	56	PRO
32	2	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	47	HIS
5	A	92	ASN
5	A	127	GLN
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	221	GLN
6	B	238	ASN
6	B	256	GLN
6	B	260	HIS
6	B	332	ASN
7	C	2	GLN
7	C	39	GLN
7	C	129	HIS
8	D	47	GLN
8	D	85	GLN
8	D	103	ASN
9	E	90	HIS
9	E	106	ASN
9	E	119	HIS
9	E	143	GLN
11	G	17	GLN
11	G	64	ASN
12	H	35	ASN
12	H	36	ASN
12	H	55	GLN
12	H	58	HIS
12	H	59	ASN
12	H	69	ASN
12	H	74	ASN

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Mol	Chain	Res	Type
12	H	91	HIS
12	H	129	ASN
12	H	130	HIS
12	H	166	ASN
13	I	52	GLN
13	I	107	ASN
13	I	126	ASN
14	J	10	GLN
15	K	18	HIS
15	K	41	HIS
15	K	42	ASN
15	K	55	GLN
15	K	58	GLN
15	K	116	HIS
16	L	26	HIS
16	L	58	GLN
16	L	78	ASN
16	L	176	GLN
17	M	107	ASN
17	M	140	GLN
17	M	153	GLN
19	O	50	GLN
19	O	66	GLN
19	O	73	HIS
19	O	118	GLN
20	P	16	ASN
20	P	40	HIS
21	Q	61	GLN
21	Q	94	ASN
21	Q	98	ASN
21	Q	113	HIS
21	Q	117	HIS
22	R	53	ASN
23	S	39	ASN
23	S	43	ASN
23	S	73	HIS
24	T	39	ASN
24	T	48	ASN
25	U	60	GLN
26	V	27	HIS
26	V	28	HIS
26	V	59	GLN

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Mol	Chain	Res	Type
26	V	87	HIS
26	V	110	GLN
26	V	119	HIS
26	V	125	HIS
26	V	141	HIS
27	W	23	HIS
28	X	133	HIS
28	X	134	HIS
28	X	149	GLN
28	X	189	ASN
29	Y	33	HIS
29	Y	70	GLN
30	Z	8	GLN
30	Z	16	HIS
30	Z	28	HIS
31	1	16	ASN
31	1	18	ASN
31	1	37	HIS
31	1	41	HIS
31	1	45	ASN
32	2	15	ASN
32	2	30	GLN
32	2	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	244 (8%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	4 (3%)
3	3	2/3 (66%)	1 (50%)	0
4	4	1/2 (50%)	0	0
All	All	2871/3049 (94%)	259 (9%)	38 (1%)

All (259) 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

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Mol	Chain	Res	Type
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	169	A
1	0	185	G
1	0	186	A
1	0	187	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	317	A
1	0	318	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U

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Mol	Chain	Res	Type
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	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

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Mol	Chain	Res	Type
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1171	A
1	0	1174	A
1	0	1175	G
1	0	1177	A
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1451	C
1	0	1460	G
1	0	1474	C

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Mol	Chain	Res	Type
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	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	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1904	A
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U

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Mol	Chain	Res	Type
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	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2466	G
1	0	2467	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G

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Mol	Chain	Res	Type
1	0	2608	C
1	0	2613	G
1	0	2619	U
1	0	2620	U
1	0	2637	A
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	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3024	U
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G

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Mol	Chain	Res	Type
2	9	3122	C
3	3	76	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	716	G
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1164	U
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1563	G
1	0	1692	C
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2466	G
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
2	9	3002	U
2	9	3023	U

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Mol	Chain	Res	Type
2	9	3065	A
2	9	3103	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 236 ligands modelled in this entry, 232 are monoatomic - leaving 4 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	$\# Z  > 2$
37	PPU	4	76	38,4	30,40,41	2.47	3 (10%)	37,57,60	1.23	3 (8%)
38	PHA	4	77	39,37	10,11,11	0.99	0	10,13,13	0.78	0
39	ACA	4	78	38,40	7,7,8	2.23	2 (28%)	5,6,8	1.30	1 (20%)
40	BTN	4	79	39	14,16,17	2.02	4 (28%)	13,21,23	1.24	1 (7%)

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
37	PPU	4	76	38,4	-	0/21/43/44	0/4/4/4
38	PHA	4	77	39,37	-	0/4/6/6	0/1/1/1
39	ACA	4	78	38,40	-	0/4/5/6	0/0/0/0
40	BTN	4	79	39	-	0/5/27/28	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	78	ACA	C3-C2	-5.26	1.32	1.52
37	4	76	PPU	OC-CM	-5.23	1.26	1.42
40	4	79	BTN	C9-C10	-4.04	1.36	1.52
40	4	79	BTN	C8-C7	-4.03	1.33	1.52
40	4	79	BTN	C3-N1	-3.39	1.30	1.35
37	4	76	PPU	C3'-N3'	-2.45	1.41	1.45
39	4	78	ACA	C2-C1	-2.10	1.43	1.49
40	4	79	BTN	O3-C3	2.48	1.28	1.23
37	4	76	PPU	C-N3'	11.67	1.61	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	76	PPU	C4'-C3'-N3'	-4.09	105.07	113.61
40	4	79	BTN	O3-C3-N2	-2.46	123.05	125.90
39	4	78	ACA	C4-C3-C2	-2.16	105.42	113.86
37	4	76	PPU	C-CA-N	2.20	118.52	108.73
37	4	76	PPU	C2-N1-C6	3.48	118.83	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	4	76	PPU	2	0
38	4	77	PHA	1	0
40	4	79	BTN	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2754/2922 (94%)	-0.18	61 (2%) 65 42	11, 39, 86, 141	0
2	9	122/122 (100%)	0.28	6 (4%) 33 14	28, 60, 91, 145	0
3	3	3/3 (100%)	1.49	0 100 100	44, 44, 46, 52	3 (100%)
4	4	2/2 (100%)	0.06	0 100 100	48, 48, 48, 56	0
5	A	237/239 (99%)	-0.17	5 (2%) 67 44	21, 53, 94, 113	0
6	B	337/337 (100%)	-0.33	1 (0%) 94 88	19, 45, 71, 81	0
7	C	246/246 (100%)	-0.39	1 (0%) 93 85	12, 37, 63, 71	0
8	D	140/176 (79%)	1.18	32 (22%) 1 0	55, 94, 120, 127	0
9	E	172/177 (97%)	0.19	2 (1%) 81 64	32, 56, 81, 87	0
10	F	119/119 (100%)	0.14	2 (1%) 73 52	41, 66, 94, 104	0
11	G	29/348 (8%)	1.58	8 (27%) 1 0	60, 79, 84, 89	0
12	H	156/167 (93%)	-0.00	1 (0%) 90 80	30, 48, 74, 81	0
13	I	142/145 (97%)	-0.41	0 100 100	26, 38, 60, 77	0
14	J	132/132 (100%)	-0.31	0 100 100	24, 44, 72, 76	0
15	K	145/164 (88%)	0.34	12 (8%) 14 5	16, 68, 97, 109	0
16	L	194/194 (100%)	0.06	19 (9%) 10 3	23, 39, 118, 128	0
17	M	186/186 (100%)	0.41	19 (10%) 9 3	36, 65, 109, 120	0
18	N	115/115 (100%)	-0.21	0 100 100	31, 47, 65, 69	0
19	O	143/148 (96%)	-0.05	1 (0%) 89 78	27, 47, 67, 77	0
20	P	95/95 (100%)	-0.26	1 (1%) 82 66	27, 40, 57, 79	0
21	Q	150/154 (97%)	-0.52	0 100 100	22, 35, 54, 65	0
22	R	81/84 (96%)	-0.03	2 (2%) 61 37	35, 53, 73, 80	0
23	S	119/119 (100%)	0.13	6 (5%) 32 13	33, 47, 75, 91	0
24	T	53/66 (80%)	3.01	37 (69%) 0 0	101, 113, 122, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	U	65/70 (92%)	0.72	6 (9%) 11 4	45, 69, 106, 112	0
26	V	154/154 (100%)	-0.41	0 100 100	25, 38, 56, 69	0
27	W	82/91 (90%)	0.18	3 (3%) 45 22	32, 49, 69, 89	0
28	X	142/240 (59%)	-0.27	1 (0%) 89 78	17, 36, 58, 77	0
29	Y	73/73 (100%)	4.11	49 (67%) 0 0	89, 118, 129, 133	0
30	Z	56/56 (100%)	-0.73	0 100 100	14, 26, 32, 39	0
31	1	46/48 (95%)	-0.02	1 (2%) 65 42	23, 52, 84, 96	0
32	2	92/92 (100%)	7.49	92 (100%) 0 0	122, 136, 142, 146	0
All	All	6582/7284 (90%)	0.08	368 (5%) 28 11	11, 45, 105, 146	3 (0%)

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2	37	ASP	17.5
32	2	78	HIS	17.4
32	2	82	GLY	17.2
32	2	11	CYS	14.7
29	Y	11	THR	13.7
32	2	65	THR	12.7
32	2	83	TRP	12.5
32	2	9	THR	12.4
32	2	59	ASP	12.1
32	2	67	LEU	11.9
32	2	20	HIS	11.7
32	2	14	CYS	11.2
32	2	15	ASN	11.0
32	2	16	GLU	10.7
32	2	66	ASP	10.4
32	2	71	CYS	10.4
32	2	33	MET	10.4
32	2	18	GLN	10.3
32	2	10	TYR	10.3
32	2	62	THR	10.3
32	2	77	ALA	10.3
32	2	34	LYS	10.1
29	Y	30	GLU	10.0
32	2	39	GLN	9.7
32	2	68	LYS	9.5
32	2	22	VAL	9.3

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Mol	Chain	Res	Type	RSRZ
32	2	17	HIS	9.3
29	Y	26	VAL	9.2
29	Y	34	LYS	9.2
32	2	8	ASN	9.1
32	2	35	TRP	9.0
32	2	27	SER	9.0
32	2	31	THR	8.9
32	2	23	GLU	8.9
29	Y	12	GLY	8.8
32	2	12	PRO	8.7
29	Y	44	PHE	8.7
29	Y	39	CYS	8.7
32	2	80	ARG	8.6
32	2	69	TYR	8.5
32	2	32	GLY	8.4
32	2	74	CYS	8.3
32	2	76	LYS	8.2
32	2	1	MET	8.1
32	2	38	ARG	8.0
32	2	75	GLY	8.0
32	2	13	HIS	8.0
32	2	21	GLU	7.9
16	L	70	GLY	7.9
32	2	81	GLU	7.8
32	2	3	MET	7.8
2	9	3001	U	7.6
32	2	84	ARG	7.5
32	2	36	ILE	7.5
32	2	72	GLY	7.5
29	Y	45	LYS	7.1
32	2	19	GLU	7.1
32	2	60	LYS	7.1
32	2	6	ARG	7.0
1	0	735	C	7.0
29	Y	29	VAL	7.0
32	2	41	GLU	6.9
32	2	70	ARG	6.9
32	2	4	PRO	6.9
25	U	1	THR	6.8
29	Y	42	CYS	6.8
29	Y	20	LEU	6.8
29	Y	43	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
29	Y	57	CYS	6.6
29	Y	33	HIS	6.6
32	2	91	GLN	6.6
29	Y	22	ILE	6.6
32	2	56	PRO	6.6
32	2	61	PRO	6.5
29	Y	19	GLY	6.4
29	Y	35	LYS	6.4
29	Y	31	ILE	6.4
32	2	79	LEU	6.4
32	2	2	GLN	6.1
29	Y	40	PRO	6.1
24	T	51	TRP	6.0
29	Y	41	VAL	6.0
24	T	55	ALA	6.0
29	Y	28	ASP	6.0
29	Y	32	LYS	5.9
24	T	54	THR	5.9
16	L	89	ASN	5.8
24	T	52	THR	5.8
32	2	26	ARG	5.8
16	L	80	GLY	5.7
16	L	71	SER	5.7
1	0	1198	U	5.7
29	Y	24	VAL	5.7
24	T	9	CYS	5.6
24	T	39	ASN	5.6
29	Y	25	ARG	5.6
32	2	5	ARG	5.6
29	Y	14	PHE	5.6
32	2	25	VAL	5.6
32	2	47	GLY	5.5
32	2	53	SER	5.5
32	2	58	GLY	5.5
32	2	85	ALA	5.4
25	U	40	PRO	5.4
32	2	30	GLN	5.2
32	2	52	PHE	5.2
24	T	48	ASN	5.2
29	Y	23	ARG	5.1
8	D	57	THR	5.1
29	Y	37	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
24	T	36	CYS	5.0
29	Y	27	ALA	5.0
16	L	81	ARG	5.0
32	2	63	LYS	4.9
29	Y	16	PRO	4.9
2	9	3023	U	4.9
25	U	39	ALA	4.9
32	2	28	GLY	4.9
24	T	11	THR	4.9
24	T	53	ASP	4.8
32	2	42	ARG	4.8
8	D	171	ASP	4.7
32	2	73	GLU	4.7
24	T	47	ARG	4.7
32	2	40	ARG	4.7
8	D	63	ILE	4.6
29	Y	38	LYS	4.6
24	T	25	ASP	4.6
29	Y	21	LYS	4.6
32	2	48	ASN	4.6
32	2	86	GLY	4.6
17	M	138	ASP	4.5
32	2	88	LEU	4.5
32	2	43	ASN	4.5
29	Y	15	GLY	4.5
24	T	43	GLY	4.5
32	2	57	GLY	4.5
16	L	78	ASN	4.3
24	T	6	CYS	4.3
32	2	44	SER	4.3
29	Y	47	LEU	4.3
29	Y	10	ARG	4.3
5	A	237	GLY	4.2
24	T	4	ARG	4.2
29	Y	13	ARG	4.2
11	G	23	ILE	4.1
16	L	83	SER	4.1
24	T	50	GLU	4.1
16	L	75	THR	4.1
1	0	1173	A	4.1
24	T	40	ALA	4.1
1	0	1175	G	4.1

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Mol	Chain	Res	Type	RSRZ
29	Y	53	GLY	4.1
2	9	3002	U	4.0
27	W	80	GLU	4.0
22	R	81	ILE	3.9
15	K	60	GLU	3.9
1	0	1199	A	3.9
24	T	10	GLY	3.9
32	2	29	ARG	3.8
32	2	24	LYS	3.8
8	D	62	ASP	3.8
8	D	92	GLU	3.8
24	T	29	THR	3.8
1	0	1171	A	3.8
32	2	51	LYS	3.8
29	Y	58	GLY	3.8
8	D	69	ILE	3.8
16	L	72	SER	3.7
29	Y	18	TYR	3.7
29	Y	55	TRP	3.7
8	D	66	GLY	3.7
1	0	1172	G	3.7
1	0	1177	A	3.7
29	Y	79	VAL	3.6
1	0	282	C	3.6
8	D	56	ARG	3.6
16	L	74	ARG	3.5
8	D	26	GLY	3.5
29	Y	56	MET	3.5
16	L	77	PHE	3.5
32	2	49	ASP	3.5
32	2	7	PHE	3.5
29	Y	80	MET	3.5
32	2	87	ARG	3.5
11	G	27	ILE	3.5
10	F	106	THR	3.4
15	K	80	ASP	3.4
17	M	186	LEU	3.4
29	Y	61	GLY	3.4
2	9	3024	U	3.4
29	Y	59	HIS	3.4
32	2	50	GLY	3.4
1	0	960	G	3.3

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Mol	Chain	Res	Type	RSRZ
24	T	41	ASP	3.3
8	D	10	PHE	3.3
32	2	46	ILE	3.3
24	T	49	LEU	3.2
8	D	172	VAL	3.2
32	2	90	PHE	3.2
11	G	26	MET	3.2
1	0	1951	G	3.2
8	D	67	ASP	3.2
8	D	27	ILE	3.2
2	9	3122	C	3.1
8	D	25	MET	3.1
1	0	10	U	3.1
24	T	46	ALA	3.1
24	T	12	ASP	3.1
27	W	88	GLU	3.1
15	K	104	ASP	3.1
17	M	160	SER	3.1
23	S	119	ALA	3.1
23	S	82	THR	3.0
32	2	64	LYS	3.0
24	T	28	THR	3.0
8	D	44	ILE	3.0
32	2	92	GLU	3.0
23	S	116	ASP	3.0
16	L	82	ARG	3.0
1	0	2237	G	3.0
1	0	1200	A	3.0
16	L	87	MET	3.0
29	Y	46	LYS	3.0
24	T	7	ASP	3.0
24	T	22	VAL	3.0
10	F	119	ARG	2.9
25	U	38	GLY	2.9
16	L	90	ARG	2.9
24	T	33	SER	2.9
1	0	1913	C	2.9
8	D	61	PHE	2.9
5	A	85	ASP	2.9
8	D	88	LEU	2.9
1	0	736	A	2.9
16	L	73	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
11	G	24	VAL	2.9
17	M	147	ILE	2.8
1	0	371	U	2.8
17	M	162	ASP	2.8
1	0	1525	G	2.8
8	D	58	VAL	2.8
24	T	8	TYR	2.8
32	2	45	GLY	2.8
1	0	970	U	2.8
1	0	1168	C	2.8
1	0	370	G	2.8
24	T	23	HIS	2.7
8	D	65	GLU	2.7
1	0	1190	G	2.7
8	D	54	ALA	2.7
29	Y	36	LYS	2.7
15	K	36	ASP	2.7
1	0	2884	G	2.7
1	0	1192	A	2.7
24	T	19	THR	2.7
17	M	167	ASP	2.7
17	M	139	TRP	2.7
16	L	76	ARG	2.6
9	E	100	ASP	2.6
1	0	1204	C	2.6
29	Y	62	TYR	2.6
17	M	179	LEU	2.6
32	2	89	GLU	2.6
1	0	1167	G	2.6
24	T	5	GLU	2.6
8	D	90	LEU	2.5
32	2	54	LYS	2.5
5	A	36	ASP	2.5
8	D	170	TYR	2.5
17	M	166	ALA	2.5
8	D	49	PRO	2.5
1	0	1202	A	2.5
24	T	13	ILE	2.5
20	P	95	GLU	2.5
29	Y	60	CYS	2.5
1	0	2508	C	2.5
8	D	64	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
17	M	172	PHE	2.4
1	0	1925	G	2.4
1	0	1163	G	2.4
1	0	1197	G	2.4
17	M	152	GLU	2.4
32	2	55	VAL	2.4
15	K	105	TYR	2.4
1	0	1169	U	2.4
1	0	368	C	2.4
1	0	2249	G	2.4
5	A	133	ARG	2.4
19	O	77	ALA	2.4
1	0	805	G	2.3
1	0	1165	G	2.3
28	X	235	GLU	2.3
8	D	87	ALA	2.3
15	K	44	GLU	2.3
17	M	157	PRO	2.3
1	0	1203	G	2.3
22	R	77	VAL	2.3
15	K	133	VAL	2.3
1	0	367	G	2.3
12	H	114	PRO	2.3
8	D	45	THR	2.3
1	0	1605	G	2.3
24	T	45	GLU	2.3
1	0	1193	A	2.3
8	D	166	ILE	2.3
25	U	2	VAL	2.3
15	K	130	ARG	2.3
1	0	284	C	2.3
29	Y	17	ARG	2.3
15	K	101	ASP	2.3
1	0	999	C	2.2
5	A	37	VAL	2.2
8	D	93	LEU	2.2
17	M	155	GLU	2.2
9	E	118	ILE	2.2
17	M	163	PHE	2.2
17	M	146	HIS	2.2
23	S	37	GLN	2.2
15	K	102	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
23	S	112	LEU	2.2
15	K	106	VAL	2.2
8	D	86	THR	2.2
11	G	64	ASN	2.2
23	S	80	GLU	2.2
1	0	1166	A	2.2
17	M	151	ASP	2.2
1	0	1000	C	2.2
1	0	1170	U	2.1
24	T	44	ARG	2.1
1	0	1948	G	2.1
1	0	2769	C	2.1
2	9	3073	G	2.1
16	L	86	MET	2.1
24	T	27	ALA	2.1
1	0	1912	A	2.1
17	M	148	ALA	2.1
11	G	68	GLU	2.1
16	L	68	ARG	2.1
17	M	159	TYR	2.1
31	1	35	ARG	2.1
16	L	88	VAL	2.1
27	W	82	GLU	2.1
1	0	2004	U	2.1
8	D	75	LEU	2.1
8	D	89	PRO	2.1
15	K	59	GLU	2.1
8	D	83	PHE	2.1
24	T	38	ASN	2.1
1	0	806	A	2.1
1	0	298	C	2.1
25	U	52	ALA	2.1
11	G	71	LEU	2.1
1	0	807	A	2.1
1	0	1174	A	2.1
1	0	1181	A	2.1
1	0	254	C	2.1
7	C	132	ASP	2.1
11	G	72	ASP	2.1
1	0	2436	U	2.0
17	M	150	TYR	2.0
1	0	1919	A	2.0

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Mol	Chain	Res	Type	RSRZ
6	B	32	ASP	2.0
24	T	32	CYS	2.0
1	0	288	A	2.0
1	0	969	G	2.0
1	0	2507	G	2.0
1	0	281	U	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8356	1/1	0.95	0.65	41.33	59,59,59,59	0
34	K	0	8201	1/1	0.96	0.65	36.09	80,80,80,80	0
35	NA	0	8325	1/1	0.96	0.38	33.22	29,29,29,29	0
36	CL	0	8515	1/1	0.90	0.68	30.55	72,72,72,72	0
35	NA	Q	8386	1/1	0.42	0.80	24.66	62,62,62,62	0
35	NA	0	8332	1/1	0.84	0.38	19.43	57,57,57,57	0
35	NA	0	8361	1/1	0.97	0.46	18.20	40,40,40,40	0
35	NA	0	8350	1/1	0.94	0.42	17.84	26,26,26,26	0
35	NA	0	8374	1/1	0.91	0.52	16.49	49,49,49,49	0
35	NA	0	8371	1/1	0.76	0.47	14.89	47,47,47,47	0
35	NA	0	8372	1/1	0.74	0.38	14.80	73,73,73,73	0
35	NA	0	8340	1/1	0.86	0.26	12.84	48,48,48,48	0
35	NA	9	8383	1/1	0.71	0.65	12.76	57,57,57,57	0
35	NA	0	8323	1/1	0.98	0.26	12.50	34,34,34,34	0
40	BTN	4	79	15/16	0.88	0.31	12.31	91,104,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8364	1/1	0.90	0.26	11.73	47,47,47,47	0
35	NA	0	8362	1/1	0.95	0.27	9.98	63,63,63,63	0
35	NA	0	8379	1/1	0.93	0.23	9.95	25,25,25,25	0
35	NA	0	8321	1/1	0.97	0.33	9.30	58,58,58,58	0
35	NA	0	8308	1/1	0.92	0.21	9.26	44,44,44,44	0
35	NA	0	8310	1/1	0.89	0.31	9.22	16,16,16,16	0
36	CL	B	8519	1/1	0.96	0.24	8.51	51,51,51,51	0
36	CL	0	8505	1/1	0.95	0.33	8.41	57,57,57,57	0
33	MG	0	8064	1/1	0.98	0.28	8.40	17,17,17,17	0
39	ACA	4	78	8/9	0.95	0.24	8.32	67,73,85,88	0
35	NA	0	8331	1/1	0.89	0.32	7.94	69,69,69,69	0
35	NA	0	8381	1/1	0.95	0.24	6.94	71,71,71,71	0
35	NA	0	8376	1/1	0.97	0.22	5.33	50,50,50,50	0
35	NA	0	8382	1/1	0.79	0.30	5.14	57,57,57,57	0
33	MG	0	8053	1/1	0.93	0.20	5.13	38,38,38,38	0
35	NA	0	8326	1/1	0.83	0.27	3.47	38,38,38,38	0
35	NA	0	8303	1/1	0.94	0.17	3.06	33,33,33,33	0
36	CL	N	8508	1/1	0.96	0.31	2.66	82,82,82,82	0
35	NA	0	8373	1/1	0.85	0.23	2.27	51,51,51,51	0
41	CD	T	8401	1/1	0.80	0.77	2.01	200,200,200,200	0
35	NA	0	8365	1/1	0.85	0.30	1.83	42,42,42,42	0
34	K	0	8202	1/1	0.83	0.46	1.56	69,69,69,69	0
33	MG	X	8109	1/1	0.99	0.20	1.51	35,35,35,35	0
33	MG	0	8044	1/1	0.98	0.16	1.46	35,35,35,35	0
38	PHA	4	77	11/11	0.91	0.27	1.44	64,67,71,71	0
35	NA	0	8378	1/1	0.95	0.17	1.16	31,31,31,31	0
37	PPU	4	76	37/38	0.96	0.21	1.09	48,55,62,63	0
33	MG	Y	8105	1/1	0.55	0.63	0.91	67,67,67,67	0
35	NA	Q	8337	1/1	0.88	0.19	0.40	41,41,41,41	0
35	NA	0	8368	1/1	0.92	0.14	0.24	41,41,41,41	0
35	NA	0	8324	1/1	0.88	0.18	0.17	39,39,39,39	0
35	NA	0	8366	1/1	0.92	0.17	0.13	20,20,20,20	0
33	MG	0	8067	1/1	0.95	0.15	-0.56	31,31,31,31	0
35	NA	C	8304	1/1	0.96	0.16	-0.61	25,25,25,25	0
36	CL	I	8521	1/1	0.95	0.13	-0.64	39,39,39,39	0
35	NA	0	8327	1/1	0.97	0.13	-0.76	16,16,16,16	0
35	NA	K	8380	1/1	0.96	0.17	-0.77	69,69,69,69	0
41	CD	Y	8403	1/1	0.85	0.52	-0.91	200,200,200,200	0
35	NA	0	8339	1/1	0.94	0.13	-1.06	8,8,8,8	0
35	NA	0	8333	1/1	0.91	0.11	-1.08	25,25,25,25	0
35	NA	P	8348	1/1	0.93	0.13	-1.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8055	1/1	0.93	0.12	-1.17	82,82,82,82	0
35	NA	0	8309	1/1	0.96	0.11	-1.17	24,24,24,24	0
33	MG	0	8052	1/1	0.97	0.13	-1.40	36,36,36,36	0
35	NA	0	8335	1/1	0.98	0.13	-1.43	47,47,47,47	0
41	CD	2	8404	1/1	0.77	0.87	-1.61	200,200,200,200	0
35	NA	0	8302	1/1	0.95	0.12	-1.72	18,18,18,18	0
33	MG	S	8073	1/1	0.95	0.21	-1.78	36,36,36,36	0
35	NA	0	8317	1/1	0.97	0.10	-1.78	23,23,23,23	0
36	CL	2	8504	1/1	0.74	0.43	-1.79	104,104,104,104	0
33	MG	0	8112	1/1	0.96	0.12	-1.79	34,34,34,34	0
35	NA	0	8305	1/1	0.99	0.11	-2.07	19,19,19,19	0
35	NA	I	8346	1/1	0.92	0.09	-2.07	20,20,20,20	0
33	MG	0	8059	1/1	0.95	0.13	-2.07	59,59,59,59	0
33	MG	2	8078	1/1	0.84	0.42	-2.16	73,73,73,73	0
33	MG	A	8065	1/1	0.95	0.09	-2.16	44,44,44,44	0
33	MG	0	8074	1/1	0.96	0.05	-2.25	27,27,27,27	0
36	CL	0	8512	1/1	0.99	0.10	-2.35	34,34,34,34	0
33	MG	0	8107	1/1	0.99	0.03	-2.72	24,24,24,24	0
33	MG	0	8101	1/1	0.92	0.12	-3.03	40,40,40,40	0
35	NA	Q	8338	1/1	1.00	0.07	-3.03	57,57,57,57	0
35	NA	L	8347	1/1	0.96	0.10	-3.15	7,7,7,7	0
36	CL	L	8518	1/1	0.96	0.12	-3.22	36,36,36,36	0
33	MG	0	8008	1/1	0.97	0.06	-3.25	42,42,42,42	0
33	MG	0	8032	1/1	0.99	0.06	-3.26	29,29,29,29	0
33	MG	0	8056	1/1	0.98	0.06	-3.32	35,35,35,35	0
33	MG	0	8110	1/1	0.98	0.09	-3.43	22,22,22,22	0
33	MG	0	8077	1/1	0.99	0.05	-3.46	21,21,21,21	0
35	NA	A	8345	1/1	0.97	0.11	-3.49	40,40,40,40	0
33	MG	0	8033	1/1	0.99	0.10	-3.93	18,18,18,18	0
33	MG	0	8039	1/1	0.98	0.06	-4.10	31,31,31,31	0
33	MG	0	8012	1/1	0.98	0.07	-4.17	26,26,26,26	0
35	NA	0	8353	1/1	0.98	0.07	-4.24	34,34,34,34	0
33	MG	0	8021	1/1	0.98	0.09	-4.29	26,26,26,26	0
33	MG	0	8014	1/1	0.98	0.07	-4.31	22,22,22,22	0
33	MG	0	8004	1/1	0.98	0.06	-4.34	30,30,30,30	0
35	NA	0	8344	1/1	0.97	0.06	-4.54	9,9,9,9	0
33	MG	0	8071	1/1	0.98	0.08	-4.82	66,66,66,66	0
33	MG	0	8091	1/1	0.98	0.06	-4.88	40,40,40,40	0
33	MG	0	8027	1/1	0.97	0.05	-5.00	37,37,37,37	0
33	MG	0	8108	1/1	0.98	0.06	-5.13	61,61,61,61	0
33	MG	0	8035	1/1	0.98	0.05	-5.15	39,39,39,39	0
41	CD	Z	8402	1/1	1.00	0.06	-5.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8320	1/1	0.98	0.07	-5.23	15,15,15,15	0
33	MG	0	8006	1/1	0.98	0.09	-5.25	28,28,28,28	0
33	MG	0	8038	1/1	0.99	0.04	-5.26	23,23,23,23	0
35	NA	0	8343	1/1	0.98	0.07	-5.54	17,17,17,17	0
33	MG	0	8017	1/1	0.99	0.03	-5.60	15,15,15,15	0
33	MG	0	8015	1/1	0.98	0.07	-5.74	29,29,29,29	0
33	MG	0	8084	1/1	0.98	0.07	-5.83	38,38,38,38	0
33	MG	0	8096	1/1	0.98	0.05	-6.39	33,33,33,33	0
33	MG	0	8057	1/1	0.98	0.10	-6.40	30,30,30,30	0
33	MG	0	8060	1/1	0.98	0.07	-6.80	32,32,32,32	0
33	MG	0	8062	1/1	0.98	0.04	-6.90	37,37,37,37	0
33	MG	0	8054	1/1	0.99	0.05	-7.00	28,28,28,28	0
33	MG	0	8010	1/1	0.97	0.05	-7.10	20,20,20,20	0
33	MG	0	8001	1/1	0.99	0.08	-7.31	21,21,21,21	0
33	MG	0	8058	1/1	0.96	0.06	-7.49	28,28,28,28	0
33	MG	0	8003	1/1	0.98	0.08	-7.56	22,22,22,22	0
33	MG	0	8020	1/1	1.00	0.07	-8.27	16,16,16,16	0
33	MG	0	8013	1/1	0.98	0.08	-8.37	25,25,25,25	0
33	MG	0	8080	1/1	0.99	0.07	-9.58	42,42,42,42	0
33	MG	0	8018	1/1	0.98	0.04	-9.65	32,32,32,32	0
33	MG	0	8002	1/1	0.99	0.05	-10.04	33,33,33,33	0
33	MG	0	8019	1/1	0.99	0.03	-10.72	13,13,13,13	0
33	MG	0	8007	1/1	0.99	0.05	-11.33	18,18,18,18	0
33	MG	0	8089	1/1	0.98	0.12	-	50,50,50,50	0
33	MG	0	8042	1/1	0.98	0.12	-	40,40,40,40	0
33	MG	0	8045	1/1	0.98	0.10	-	44,44,44,44	0
33	MG	0	8025	1/1	0.96	0.08	-	17,17,17,17	0
36	CL	X	8520	1/1	0.95	0.13	-	35,35,35,35	0
33	MG	0	8093	1/1	0.99	0.07	-	43,43,43,43	0
33	MG	0	8005	1/1	0.99	0.05	-	26,26,26,26	0
33	MG	0	8100	1/1	0.96	0.10	-	65,65,65,65	0
36	CL	0	8516	1/1	0.96	0.18	-	44,44,44,44	0
33	MG	0	8063	1/1	0.99	0.06	-	68,68,68,68	0
33	MG	0	8088	1/1	0.95	0.09	-	23,23,23,23	0
35	NA	0	8358	1/1	0.91	0.31	-	98,98,98,98	0
35	NA	0	8341	1/1	0.94	0.15	-	40,40,40,40	0
35	NA	0	8311	1/1	0.91	0.14	-	38,38,38,38	0
35	NA	9	8351	1/1	0.81	0.72	-	112,112,112,112	0
35	NA	0	8334	1/1	0.97	0.12	-	29,29,29,29	0
33	MG	0	8048	1/1	0.98	0.08	-	34,34,34,34	0
33	MG	0	8103	1/1	0.92	0.20	-	34,34,34,34	0
33	MG	0	8117	1/1	0.99	0.09	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8342	1/1	0.96	0.22	-	19,19,19,19	0
33	MG	0	8023	1/1	0.99	0.07	-	28,28,28,28	0
35	NA	0	8349	1/1	0.96	0.14	-	37,37,37,37	0
36	CL	I	8502	1/1	0.95	0.09	-	56,56,56,56	0
33	MG	0	8022	1/1	0.99	0.05	-	30,30,30,30	0
33	MG	0	8047	1/1	0.98	0.10	-	48,48,48,48	0
36	CL	0	8517	1/1	0.92	0.22	-	57,57,57,57	0
36	CL	0	8511	1/1	0.96	0.23	-	63,63,63,63	0
33	MG	0	8016	1/1	0.97	0.09	-	25,25,25,25	0
33	MG	0	8031	1/1	0.99	0.03	-	18,18,18,18	0
33	MG	0	8092	1/1	0.94	0.34	-	71,71,71,71	0
33	MG	0	8114	1/1	0.78	0.73	-	161,161,161,161	0
35	NA	0	8360	1/1	0.96	0.65	-	39,39,39,39	0
36	CL	Q	8506	1/1	0.99	0.11	-	43,43,43,43	0
33	MG	0	8076	1/1	0.84	0.18	-	70,70,70,70	0
33	MG	0	8113	1/1	0.96	0.20	-	36,36,36,36	0
36	CL	0	8513	1/1	0.95	0.11	-	52,52,52,52	0
35	NA	0	8330	1/1	0.98	0.19	-	21,21,21,21	0
33	MG	0	8079	1/1	0.98	0.05	-	27,27,27,27	0
36	CL	M	8507	1/1	0.93	0.15	-	54,54,54,54	0
33	MG	0	8082	1/1	0.94	0.13	-	43,43,43,43	0
35	NA	H	8322	1/1	0.86	0.25	-	48,48,48,48	0
35	NA	0	8377	1/1	0.83	0.28	-	59,59,59,59	0
33	MG	0	8036	1/1	0.97	0.10	-	32,32,32,32	0
35	NA	0	8385	1/1	0.65	0.39	-	52,52,52,52	0
33	MG	0	8043	1/1	0.96	0.07	-	34,34,34,34	0
35	NA	0	8319	1/1	0.96	0.09	-	50,50,50,50	0
33	MG	0	8086	1/1	0.95	0.10	-	41,41,41,41	0
33	MG	0	8097	1/1	0.98	0.14	-	30,30,30,30	0
33	MG	0	8085	1/1	0.97	0.30	-	103,103,103,103	0
33	MG	0	8081	1/1	0.98	0.08	-	36,36,36,36	0
35	NA	0	8306	1/1	0.90	0.68	-	21,21,21,21	0
35	NA	0	8359	1/1	0.98	0.18	-	42,42,42,42	0
33	MG	J	8069	1/1	0.98	0.08	-	47,47,47,47	0
33	MG	0	8099	1/1	0.94	0.18	-	37,37,37,37	0
35	NA	0	8355	1/1	0.93	0.60	-	60,60,60,60	0
33	MG	0	8116	1/1	0.91	0.10	-	64,64,64,64	0
33	MG	0	8090	1/1	0.97	0.11	-	65,65,65,65	0
36	CL	0	8514	1/1	0.98	0.12	-	44,44,44,44	0
33	MG	0	8111	1/1	0.91	0.10	-	49,49,49,49	0
33	MG	0	8046	1/1	0.92	0.09	-	40,40,40,40	0
33	MG	0	8104	1/1	0.95	0.16	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	9	8095	1/1	0.93	0.14	-	72,72,72,72	0
35	NA	0	8328	1/1	0.89	0.49	-	41,41,41,41	0
35	NA	0	8315	1/1	0.98	0.15	-	32,32,32,32	0
35	NA	0	8313	1/1	0.99	0.15	-	59,59,59,59	0
33	MG	0	8098	1/1	0.98	0.29	-	24,24,24,24	0
33	MG	0	8040	1/1	0.98	0.09	-	107,107,107,107	0
33	MG	0	8009	1/1	0.99	0.04	-	18,18,18,18	0
33	MG	0	8068	1/1	0.98	0.08	-	58,58,58,58	0
35	NA	0	8384	1/1	0.35	1.14	-	87,87,87,87	0
33	MG	0	8102	1/1	0.85	1.14	-	135,135,135,135	0
35	NA	0	8357	1/1	0.93	0.11	-	53,53,53,53	0
33	MG	0	8050	1/1	0.95	0.23	-	78,78,78,78	0
35	NA	0	8336	1/1	0.93	0.08	-	30,30,30,30	0
33	MG	0	8011	1/1	0.98	0.20	-	1,1,1,1	0
35	NA	0	8363	1/1	0.64	0.74	-	40,40,40,40	0
33	MG	0	8034	1/1	0.99	0.03	-	22,22,22,22	0
35	NA	0	8301	1/1	0.94	0.11	-	28,28,28,28	0
33	MG	0	8066	1/1	0.94	0.14	-	60,60,60,60	0
33	MG	0	8029	1/1	0.98	0.05	-	23,23,23,23	0
33	MG	0	8087	1/1	0.94	0.10	-	36,36,36,36	0
36	CL	0	8503	1/1	0.94	0.18	-	49,49,49,49	0
33	MG	0	8028	1/1	0.97	0.06	-	23,23,23,23	0
35	NA	0	8316	1/1	0.97	0.19	-	28,28,28,28	0
35	NA	0	8369	1/1	0.89	0.36	-	67,67,67,67	0
35	NA	0	8329	1/1	0.23	0.56	-	62,62,62,62	0
35	NA	0	8370	1/1	0.96	0.28	-	48,48,48,48	0
33	MG	0	8049	1/1	0.87	0.29	-	73,73,73,73	0
33	MG	0	8051	1/1	0.89	0.17	-	70,70,70,70	0
33	MG	0	8106	1/1	0.95	0.09	-	64,64,64,64	0
33	MG	0	8030	1/1	0.99	0.11	-	29,29,29,29	0
36	CL	A	8509	1/1	0.90	0.25	-	76,76,76,76	0
36	CL	K	8510	1/1	0.84	0.23	-	70,70,70,70	0
35	NA	0	8318	1/1	0.99	0.08	-	22,22,22,22	0
33	MG	0	8075	1/1	0.97	0.06	-	50,50,50,50	0
36	CL	0	8522	1/1	0.85	0.37	-	76,76,76,76	0
33	MG	0	8072	1/1	0.97	0.10	-	43,43,43,43	0
35	NA	0	8367	1/1	0.96	0.20	-	36,36,36,36	0
35	NA	0	8307	1/1	0.92	0.23	-	40,40,40,40	0
35	NA	0	8354	1/1	0.81	0.37	-	29,29,29,29	0
33	MG	0	8024	1/1	0.86	0.68	-	109,109,109,109	0
35	NA	0	8314	1/1	0.94	0.16	-	33,33,33,33	0
41	CD	N	8405	1/1	0.92	0.06	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8375	1/1	0.97	0.20	-	40,40,40,40	0
35	NA	R	8312	1/1	0.55	0.65	-	84,84,84,84	0
33	MG	0	8083	1/1	0.99	0.05	-	38,38,38,38	0
33	MG	0	8061	1/1	0.99	0.07	-	28,28,28,28	0
33	MG	0	8037	1/1	0.99	0.05	-	34,34,34,34	0
36	CL	I	8501	1/1	0.98	0.13	-	60,60,60,60	0
33	MG	0	8115	1/1	0.94	0.12	-	58,58,58,58	0
33	MG	0	8094	1/1	0.97	0.06	-	54,54,54,54	0
33	MG	0	8026	1/1	0.99	0.08	-	25,25,25,25	0
33	MG	0	8041	1/1	0.95	0.28	-	50,50,50,50	0
35	NA	0	8352	1/1	0.85	0.26	-	28,28,28,28	0
33	MG	0	8070	1/1	0.98	0.44	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.