



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:52 AM GMT

PDB ID : 3CME
Title : The Structure of CA and CCA-PHE-CAP-BIO Bound to the Large Ribosomal Subunit of Haloarcula Marismortui
Authors : Simonovic, M.; Steitz, T.A.
Deposited on : 2008-03-21
Resolution : 2.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

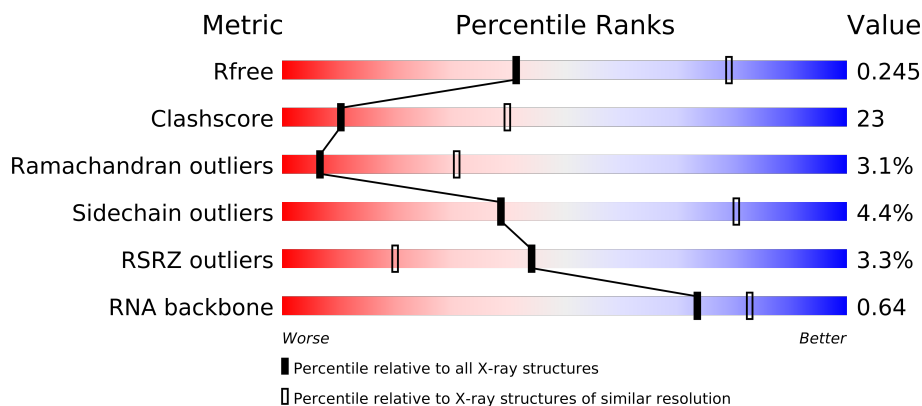
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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Mol	Chain	Length	Quality of chain
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	240	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	
32	5	3	
33	6	3	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
34	PHE	6	77	-	X
34	ACA	6	78	-	X
35	MG	0	8001	-	X
35	MG	0	8002	-	X
35	MG	0	8004	-	X
35	MG	0	8005	-	X
35	MG	0	8006	-	X
35	MG	0	8008	-	X
35	MG	0	8009	-	X
35	MG	0	8010	-	X
35	MG	0	8014	-	X
35	MG	0	8015	-	X
35	MG	0	8016	-	X
35	MG	0	8018	-	X
35	MG	0	8020	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	MG	0	8022	-	X
35	MG	0	8023	-	X
35	MG	0	8024	-	X
35	MG	0	8027	-	X
35	MG	0	8028	-	X
35	MG	0	8029	-	X
35	MG	0	8034	-	X
35	MG	0	8036	-	X
35	MG	0	8037	-	X
35	MG	0	8039	-	X
35	MG	0	8040	-	X
35	MG	0	8041	-	X
35	MG	0	8045	-	X
35	MG	0	8046	-	X
35	MG	0	8047	-	X
35	MG	0	8048	-	X
35	MG	0	8049	-	X
35	MG	0	8050	-	X
35	MG	0	8055	-	X
35	MG	0	8056	-	X
35	MG	0	8058	-	X
35	MG	0	8059	-	X
35	MG	0	8061	-	X
35	MG	0	8062	-	X
35	MG	0	8063	-	X
35	MG	0	8064	-	X
35	MG	0	8065	-	X
35	MG	0	8066	-	X
35	MG	0	8067	-	X
35	MG	0	8070	-	X
35	MG	0	8071	-	X
35	MG	0	8072	-	X
35	MG	0	8076	-	X
35	MG	0	8078	-	X
35	MG	0	8079	-	X
35	MG	0	8081	-	X
35	MG	0	8085	-	X
35	MG	0	8087	-	X
35	MG	0	8088	-	X
35	MG	0	8090	-	X
35	MG	0	8092	-	X
35	MG	2	8060	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	MG	9	8074	-	X
35	MG	A	8025	-	X
35	MG	A	8051	-	X
35	MG	B	8042	-	X
35	MG	B	8043	-	X
35	MG	C	8012	-	X
35	MG	K	8054	-	X
35	MG	Y	8086	-	X
36	NA	0	8501	-	X
36	NA	0	8502	-	X
36	NA	0	8505	-	X
36	NA	0	8507	-	X
36	NA	0	8509	-	X
36	NA	0	8511	-	X
36	NA	0	8512	-	X
36	NA	0	8513	-	X
36	NA	0	8514	-	X
36	NA	0	8516	-	X
36	NA	0	8519	-	X
36	NA	0	8520	-	X
36	NA	0	8521	-	X
36	NA	0	8523	-	X
36	NA	0	8524	-	X
36	NA	0	8525	-	X
36	NA	0	8527	-	X
36	NA	0	8528	-	X
36	NA	0	8530	-	X
36	NA	0	8531	-	X
36	NA	0	8533	-	X
36	NA	0	8534	-	X
36	NA	0	8535	-	X
36	NA	0	8536	-	X
36	NA	0	8541	-	X
36	NA	0	8545	-	X
36	NA	0	8546	-	X
36	NA	0	8547	-	X
36	NA	0	8548	-	X
36	NA	0	8550	-	X
36	NA	0	8552	-	X
36	NA	0	8553	-	X
36	NA	0	8554	-	X
36	NA	0	8555	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	NA	0	8556	-	X
36	NA	0	8557	-	X
36	NA	0	8558	-	X
36	NA	0	8559	-	X
36	NA	0	8560	-	X
36	NA	0	8561	-	X
36	NA	0	8562	-	X
36	NA	0	8563	-	X
36	NA	0	8565	-	X
36	NA	0	8566	-	X
36	NA	0	8567	-	X
36	NA	0	8568	-	X
36	NA	0	8569	-	X
36	NA	0	8570	-	X
36	NA	0	8571	-	X
36	NA	0	8573	-	X
36	NA	0	8574	-	X
36	NA	9	8544	-	X
36	NA	9	8572	-	X
36	NA	H	8518	-	X
36	NA	S	8510	-	X
37	SR	0	8901	-	X
37	SR	0	8903	-	X
37	SR	0	8904	-	X
37	SR	0	8905	-	X
37	SR	0	8906	-	X
37	SR	0	8908	-	X
37	SR	0	8909	-	X
37	SR	0	8910	-	X
37	SR	0	8914	-	X
37	SR	0	8917	-	X
37	SR	0	8918	-	X
37	SR	0	8920	-	X
37	SR	0	8923	-	X
37	SR	0	8924	-	X
37	SR	0	8925	-	X
37	SR	0	8926	-	X
37	SR	0	8927	-	X
37	SR	0	8931	-	X
37	SR	0	8933	-	X
37	SR	0	8936	-	X
37	SR	0	8937	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	0	8938	-	X
37	SR	0	8941	-	X
37	SR	0	8942	-	X
37	SR	0	8944	-	X
37	SR	0	8946	-	X
37	SR	0	8948	-	X
37	SR	0	8949	-	X
37	SR	0	8954	-	X
37	SR	0	8958	-	X
37	SR	0	8961	-	X
37	SR	0	8963	-	X
37	SR	0	8965	-	X
37	SR	0	8966	-	X
37	SR	0	8974	-	X
37	SR	0	8976	-	X
37	SR	0	8979	-	X
37	SR	0	8983	-	X
37	SR	0	8984	-	X
37	SR	0	8985	-	X
37	SR	0	8989	-	X
37	SR	0	8990	-	X
37	SR	0	8994	-	X
37	SR	0	8996	-	X
37	SR	0	8998	-	X
37	SR	0	9000	-	X
37	SR	0	9001	-	X
37	SR	0	9006	-	X
37	SR	0	9007	-	X
37	SR	0	9008	-	X
37	SR	1	8913	-	X
37	SR	1	8952	-	X
37	SR	B	8950	-	X
37	SR	B	8987	-	X
37	SR	L	8969	-	X
37	SR	T	8939	-	X
38	CL	0	8822	-	X
38	CL	J	8816	-	X
39	K	0	8401	-	X
39	K	0	8402	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 99194 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1752	1072	351	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2624	1616	492	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1859	1130	344	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1093	685	194	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1356	840	223	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			889	551	140	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1281	798	239	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			518	323	80	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1119	696	198	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			993	609	188	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O		0	0	0
			1117	670	221	226				

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1557	943	332	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1444	895	261	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			864	529	160	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1135	683	228	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			734	450	140	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1148	713	208	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			640	389	110	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			949	568	179	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1195	737	208	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			653	402	128	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			572	343	112	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			754	458	152	137	7			

- Molecule 30 is a RNA chain called 50S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26345	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2595	1156	471	847	121			

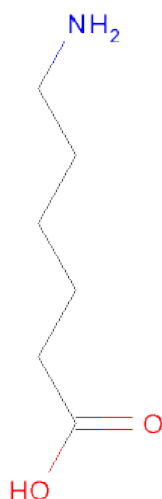
- Molecule 32 is a RNA chain called RNA (5'-R(*C*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	5	2	Total	C	N	O	P	0	0	0
			39	19	8	11	1			

- Molecule 33 is a RNA chain called RNA (5'-R(*CP*CP*(8AN))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	6	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			

- Molecule 34 is PHENYLALANINE (three-letter code: ACA, PHE) (formula: C₆H₁₃NO₂, C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	6	2	Total	C	N	O	0	0
			19	15	2	2		

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	82	Total	Mg	0	0
			82	82		
35	Y	1	Total	Mg	0	0
			1	1		
35	K	1	Total	Mg	0	0
			1	1		
35	B	2	Total	Mg	0	0
			2	2		
35	C	1	Total	Mg	0	0
			1	1		
35	A	3	Total	Mg	0	0
			3	3		
35	T	1	Total	Mg	0	0
			1	1		
35	2	1	Total	Mg	0	0
			1	1		
35	9	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	65	Total Na 65 65	0	0
36	J	1	Total Na 1 1	0	0
36	Q	1	Total Na 1 1	0	0
36	H	1	Total Na 1 1	0	0
36	C	1	Total Na 1 1	0	0
36	R	1	Total Na 1 1	0	0
36	9	3	Total Na 3 3	0	0
36	S	1	Total Na 1 1	0	0
36	M	1	Total Na 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	87	Total Sr 87 87	0	0
37	Y	1	Total Sr 1 1	0	0
37	H	2	Total Sr 2 2	0	0
37	B	2	Total Sr 2 2	0	0
37	1	2	Total Sr 2 2	0	0
37	A	3	Total Sr 3 3	0	0
37	T	2	Total Sr 2 2	0	0
37	R	1	Total Sr 1 1	0	0
37	9	3	Total Sr 3 3	0	0
37	L	1	Total Sr 1 1	0	0
37	3	3	Total Sr 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	1	Total	Sr	0	0
			1	1		

- Molecule 38 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	6	Total	Cl	0	0
			6	6		
38	J	4	Total	Cl	0	0
			4	4		
38	Q	1	Total	Cl	0	0
			1	1		
38	B	1	Total	Cl	0	0
			1	1		
38	A	1	Total	Cl	0	0
			1	1		
38	N	1	Total	Cl	0	0
			1	1		
38	O	1	Total	Cl	0	0
			1	1		
38	R	1	Total	Cl	0	0
			1	1		
38	Y	2	Total	Cl	0	0
			2	2		
38	L	2	Total	Cl	0	0
			2	2		
38	3	1	Total	Cl	0	0
			1	1		
38	M	1	Total	Cl	0	0
			1	1		

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	2	Total	K	0	0
			2	2		

- Molecule 40 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	O	1	Total	Cd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	Z	1	Total 1	Cd 1	0	0
40	1	1	Total 1	Cd 1	0	0
40	3	1	Total 1	Cd 1	0	0
40	U	1	Total 1	Cd 1	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	9	138	Total 138	O 138	0	0
41	A	134	Total 134	O 134	0	0
41	B	156	Total 156	O 156	0	0
41	C	168	Total 168	O 168	0	0
41	D	49	Total 49	O 49	0	0
41	E	49	Total 49	O 49	0	0
41	F	31	Total 31	O 31	0	0
41	G	20	Total 20	O 20	0	0
41	H	78	Total 78	O 78	0	0
41	I	11	Total 11	O 11	0	0
41	J	58	Total 58	O 58	0	0
41	K	57	Total 57	O 57	0	0
41	L	91	Total 91	O 91	0	0
41	M	129	Total 129	O 129	0	0
41	N	68	Total 68	O 68	0	0

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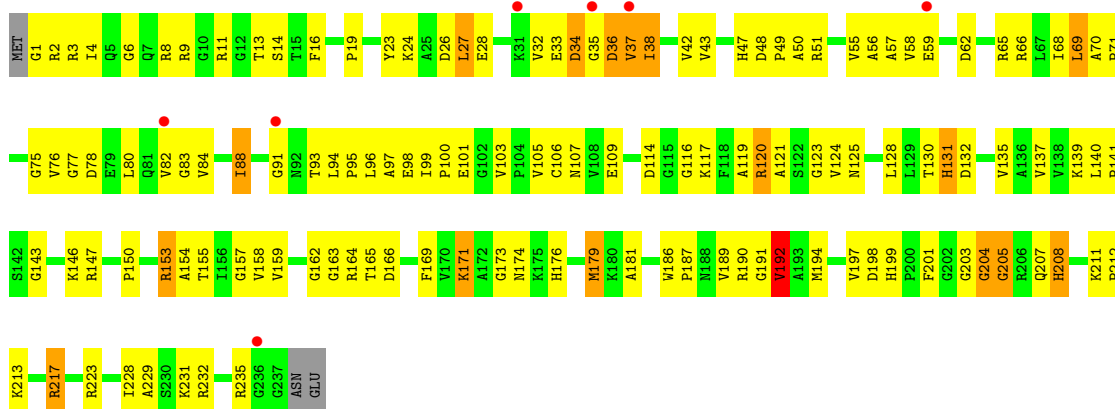
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	O	46	Total 46	O 46	0	0
41	P	72	Total 72	O 72	0	0
41	Q	52	Total 52	O 52	0	0
41	R	89	Total 89	O 89	0	0
41	S	35	Total 35	O 35	0	0
41	T	42	Total 42	O 42	0	0
41	U	29	Total 29	O 29	0	0
41	V	16	Total 16	O 16	0	0
41	W	75	Total 75	O 75	0	0
41	X	31	Total 31	O 31	0	0
41	Y	105	Total 105	O 105	0	0
41	Z	25	Total 25	O 25	0	0
41	0	5775	Total 5775	O 5775	0	0
41	1	57	Total 57	O 57	0	0
41	2	50	Total 50	O 50	0	0
41	3	66	Total 66	O 66	0	0
41	6	6	Total 6	O 6	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.

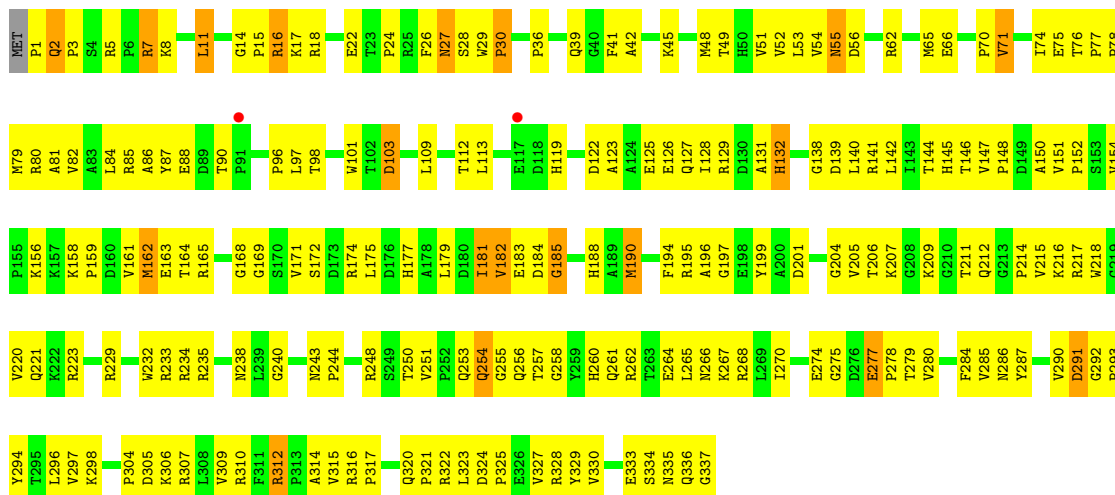
• Molecule 1: 50S ribosomal protein L2P

Chain A: 



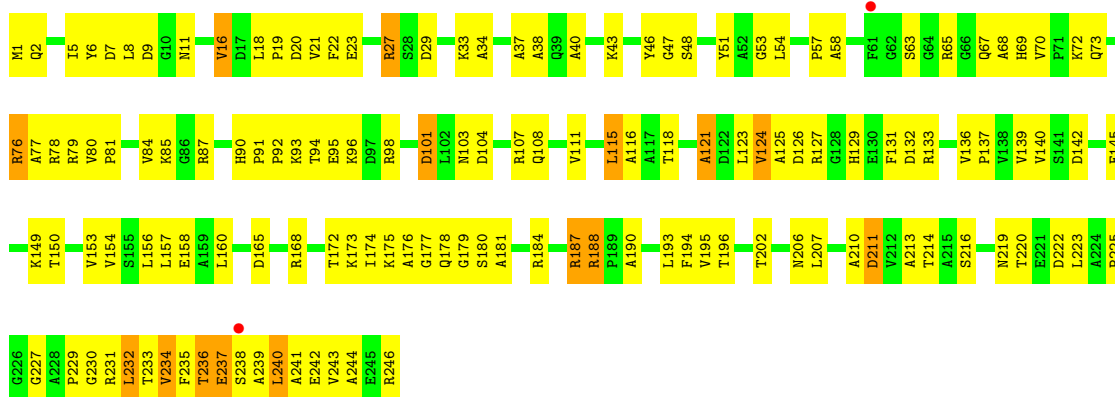
• Molecule 2: 50S ribosomal protein L3P

Chain B: 



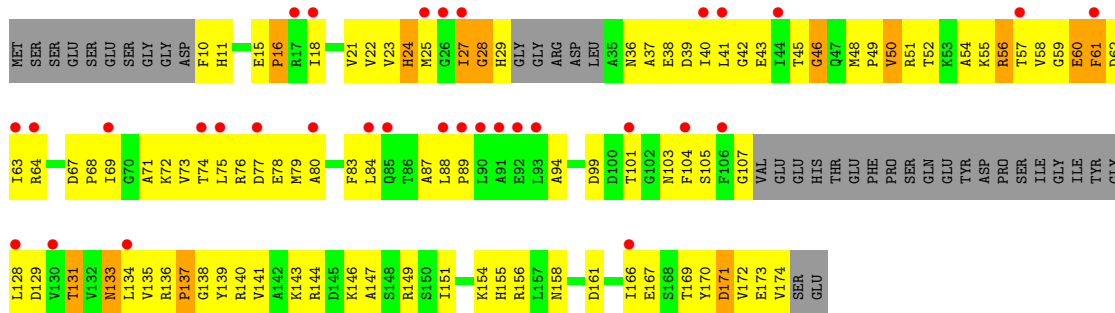
• Molecule 3: 50S ribosomal protein L4P

Chain C: 



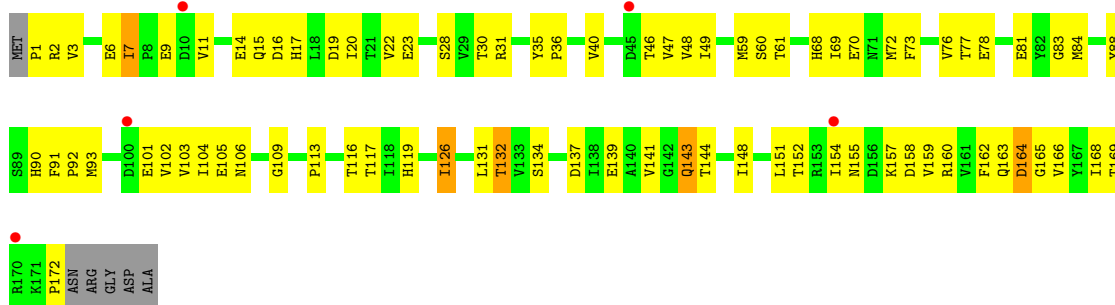
- Molecule 4: 50S ribosomal protein L5P

Chain D: 



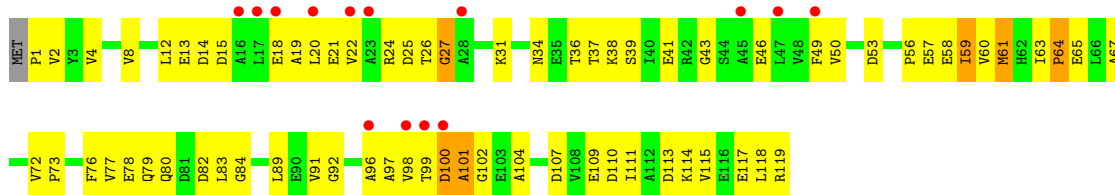
- Molecule 5: 50S ribosomal protein L6P

Chain E:



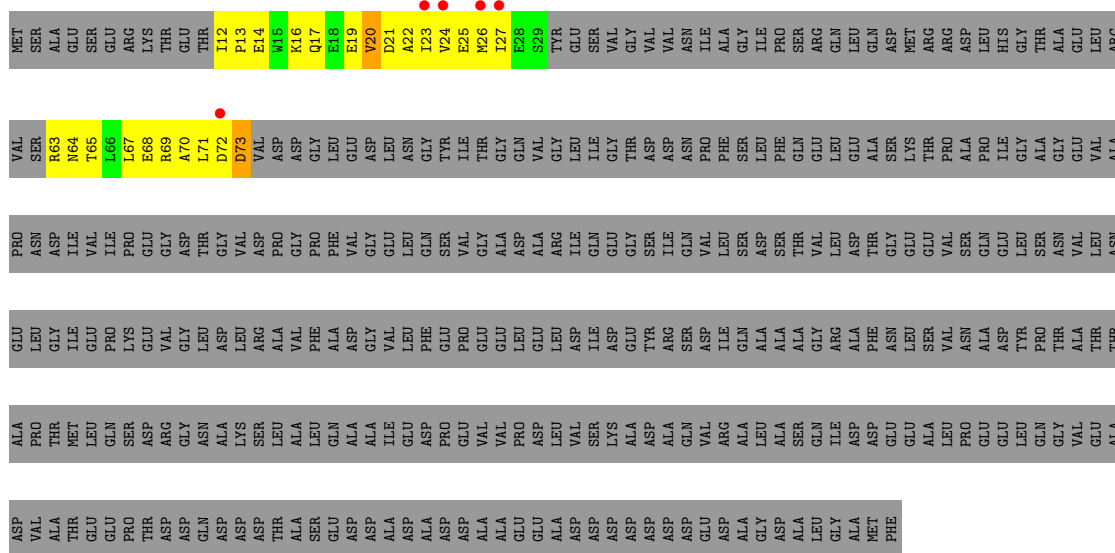
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



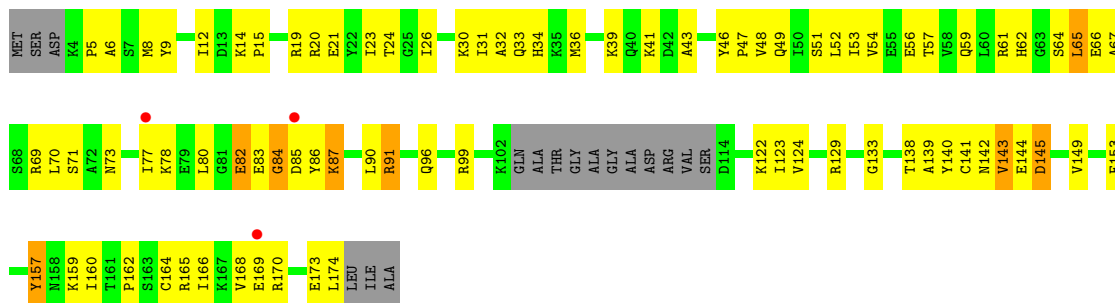
- Molecule 7: 50S ribosomal protein L10E

Chain G:



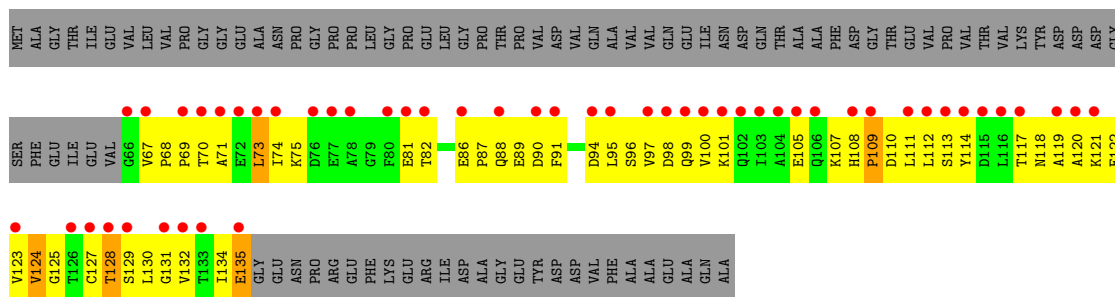
- Molecule 8: 50S ribosomal protein L10e

Chain H:



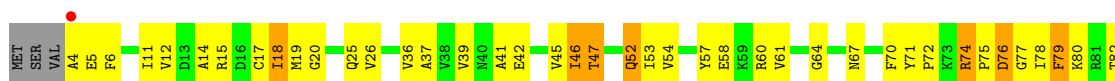
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

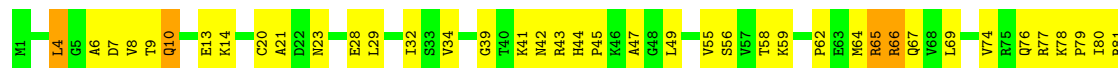
Chain J:





• Molecule 11: 50S ribosomal protein L14P

Chain K:



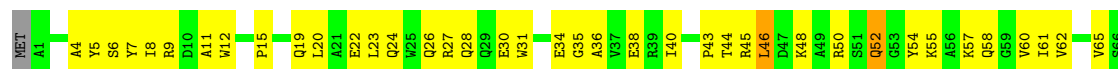
• Molecule 12: 50S ribosomal protein L15P

Chain L:



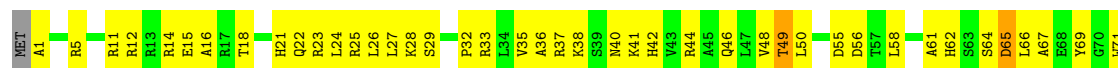
• Molecule 13: 50S ribosomal protein L15e

Chain M:



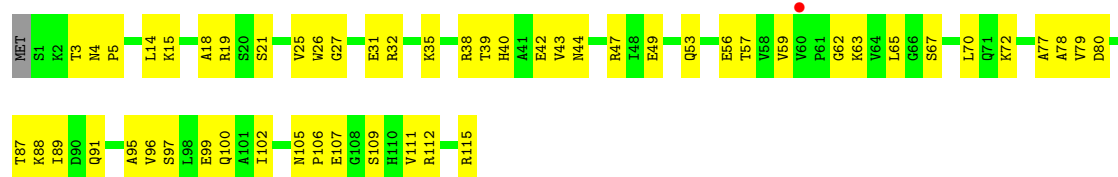
• Molecule 14: 50S ribosomal protein L18P

Chain N:



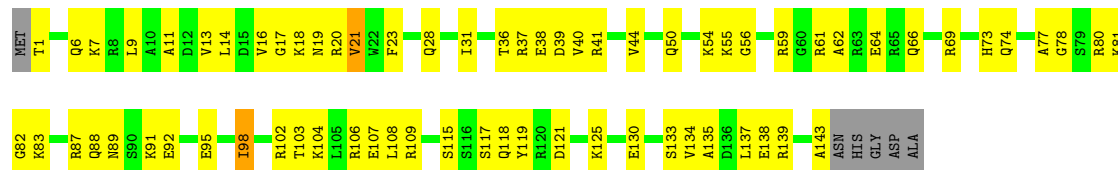
• Molecule 15: 50S ribosomal protein L18e

Chain O: 



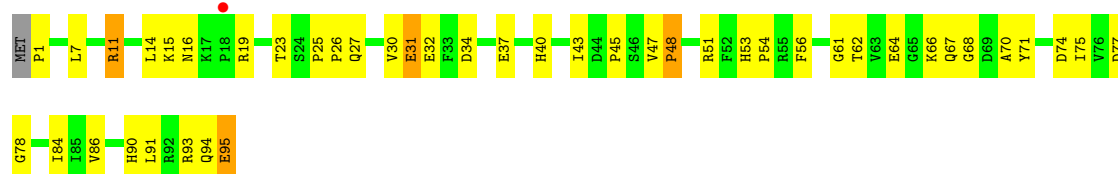
- Molecule 16: 50S ribosomal protein L19e

Chain P: 



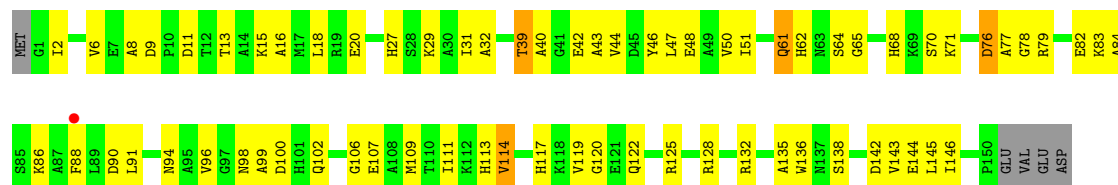
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 



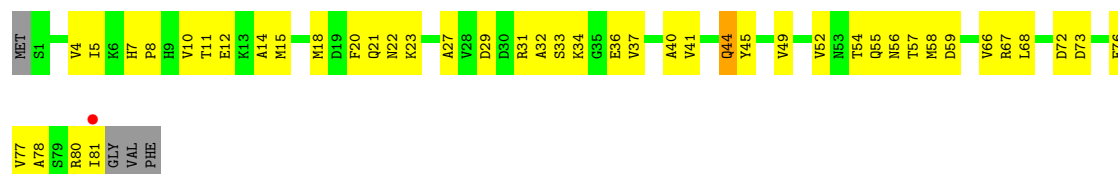
- Molecule 18: 50S ribosomal protein L22P

Chain R: 



- Molecule 19: 50S ribosomal protein L23P

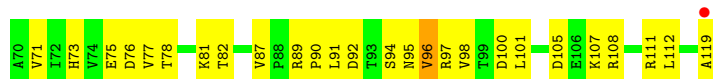
Chain S: 



- Molecule 20: 50S ribosomal protein L24P

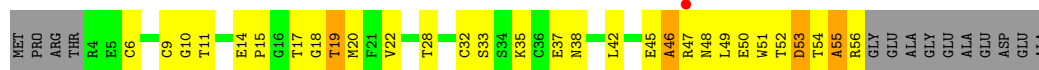
Chain T: 





- Molecule 21: 50S ribosomal protein L24e

Chain U: 



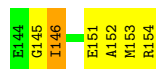
- Molecule 22: 50S ribosomal protein L29P

Chain V:



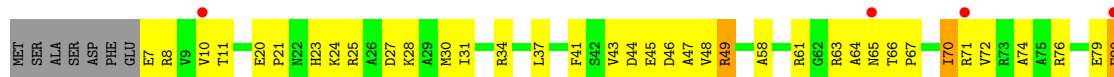
- Molecule 23: 50S ribosomal protein L30P

Chain W: 



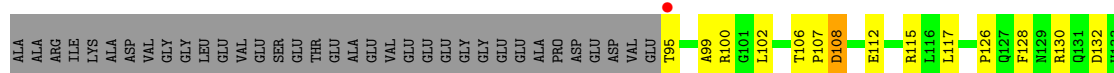
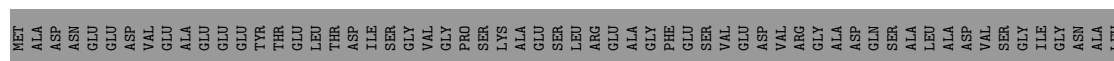
- Molecule 24: 50S ribosomal protein L31e

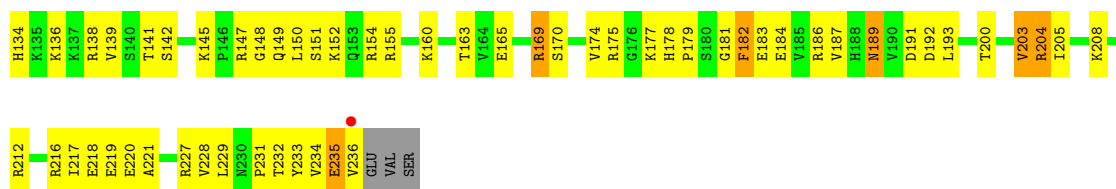
Chain X:



- Molecule 25: 50S ribosomal protein L32e

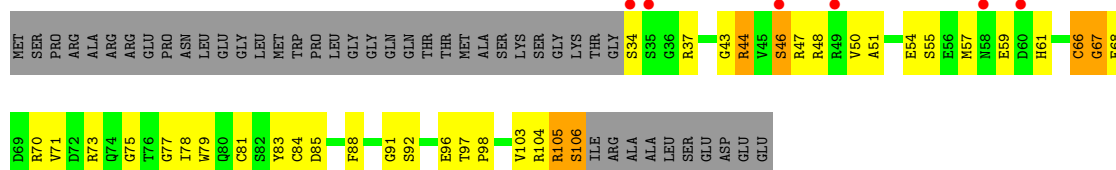
Chain Y: 





- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 27: 50S ribosomal protein L37e

Chain 1:



- Molecule 28: 50S ribosomal protein L39e

Chain 2:



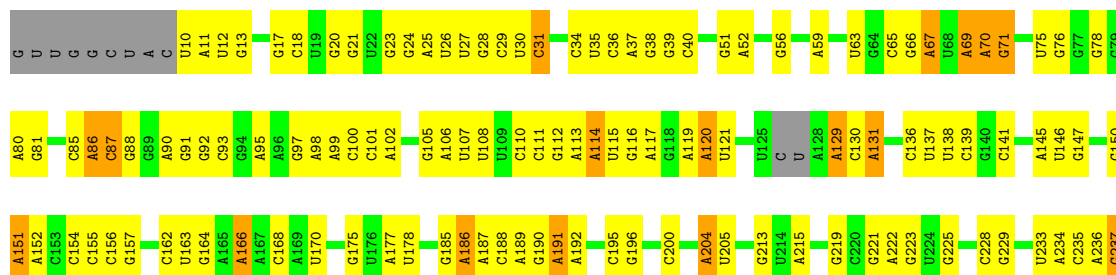
- Molecule 29: 50S ribosomal protein L44E

Chain 3:



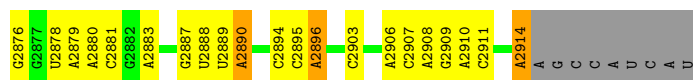
- Molecule 30: 50S RIBOSOMAL RNA

Chain 0:



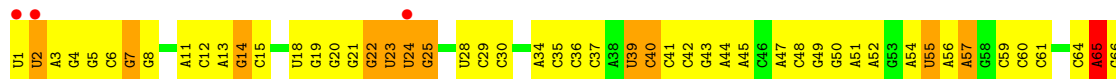
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A1522	U1417	U1333	C1250	A1180	A1097	C	9921	G524	G728	G652	G568	A486	U392	A316	
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U1524	C1420	G1183	G1258	C1183	G1100	A	A923	G834	G730		A575	C491	U396	A248	
G1525	C1421	C1184	G1259	U1185	C1103	C1099	G924	U835	U731	G656	C578	C492	A397	C233	G249
A1526	U1422	U1186	A1261	U1186	C1104	C1000	G925	U835	G732	G657	G579	U493	U397	U325	C254
A1527	C1423	C1187	C1262	U1187	U1001	U1001	A926	C839	G735	G658	A580	C494	C399	A326	A255
A1528	A1424	U1188	C1263	U1188	G1002	G1002	C936	U840	A736	A659	G581	A495	C400	A327	C256
G1529		U1189	U1264	U1189	U1003	U1003	C937	A841	A737	G661	U582	C496	C401	U328	G257
	G1433	A1190		A1190			C938		G738	U662	C583	A497		C258	
A1533		A1191	C1267	A1191	A1006	A1006	G938	A844		C663	U584	A498	A407	G259	
C1534	G1445	A1192	C1268	A1192	A1007	A1007			C741	U664		C499	A408		
	U1446	A1193		A1193	C1008	C1008	G941	G854		A665	G588	C500	A408	G333	U263
C1545	U1447		G1269		U1115	U1115	U942	U855	G744	A666	U589	G506	C412	U335	U264
A1547	C1451	G1351	A1271	C1196	A1117	A1117	U943	G856	G745	C667	U590	A507	C413	U336	U265
U1548	G1452	C1352		U1197	A1118	A1118	G944	U857	A746	C668	A591	A508	G417	A337	C266
		C1353	U1276	U1197	U1119	U1119	U945	U858	G747	G669	G592	A509	C418	C338	G267
		G1354	C1277	U1198	U1120	G1025	U947	C859		A671	A593	U510	C419	A339	U268
G1552	C1456	A1355	U1279	A1200	U1130	U1029	G948	U862	A750		G600	U511	U420	C342	G269
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G1555	A1458	A1357		A1202	A1132	G1032	U950	G863		G678	A603	A513	C421	C344	A272
		A1358	A1287	A1203	A1133	C1033	A951	G868	C757		U603	G514	U425	G345	G273
C1462		C1360	U1288	C1204	A1134	G1034	G952	G869	C758	C681	C605		G426	U346	
U1463	U1463	C1361	U1289	U1205	U1135	U1041	G953	G870	A759		G604		G426	A347	C280
A1559		U1362	G1290	U1206	U1136	U1042	G956	U871		A686	C605		G431	U348	U281
U1561	C1464	G1363	A1291	A1207	U1139	U1043	A957	U872	C764	C687	U611	A519	C432	C349	C282
C1562	A1471	C1364	G1292	C1208	U1139	C1043	G958	U873	G765	A688	U612	A521	C433	U349	U283
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A1573	A1476	C1370	U1298	C1213	U1149	C1051	C962		A776	C696			A442	C355	A288
C1574	C1477	G1371	G1300	A1215	A1150	G1052	G969	A882	G777	U619			U445	G358	C290
G1575		A1372	C1301	G1216	A1152	G1053	U970	U883		A620			G446	U359	C291
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	G1586	C1377	C1303	U1218	G1158	A1057	U	G885	A791	G622			A448	C361	A293
U1587	U1587	G1378	U1304	U1219	U1159	A1058	G	A886	U701	U623			G449	G362	C294
G1588		A1379	C1305	U1220	G1059	G1059	U	G887	U702	U624			C450	C363	C295
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A1590	A1496		A1307		G1161		C	C889	G704	U626			G452	G365	U297
	G1497	U1383	A1308	C1228	G1162	G1065	G	C890		G627					
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G1594		A1393	U1314	U1234	A1166	G1072	C	A894	A708	A631			A460	A371	C303
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A1597		C1396	U1317	C1238	U1169	A1078	G		U714				U470	C376	G307
U1598		U1405	G1318	U1239	U1170	A1079	A	U903	U				G471	A377	U308
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C1602		A1406		A1243	U1172	A1081	C	C905	G817					G379	U310
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G1604		U1408		U1245	A1174	A1086	A	A907	A819				A477	G381	U312
G1605		G1409	G1325	A1246	G1175	G1087	G		C719					U382	
A1606		G1410			C1176	A1088	U		G722						
A1607			A1328	A1247	A1177		C	A912							

G2794	G2698	G2616	G2540	A2311	C2105	G2023	C1946	C1853	G1773	G1687	G1608
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A2800	G2712	G2626	U2544	G2315	U2109	U2032	G1950	G1863	G1777	G1695	
A2801	G2715	G2627	G2545	G2316	G2110	G2033	G1951	C1864	A1778	G1618	
A2802	G2716	G2634	C2548	G2317	G2111	U2034	U	A1865	A1779	G1619	
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C2849	G2772	U2676	U2585	C2356	U2157	U2082	U2004	A1931	U1835		
C2850	U2773	U2677	A2601	G2357	U2158	U2083	U2005	G1932	A1836	U1761	
C2851	G2774	U2678	G2602	A2358	U2159	U2084	G2006	A1932	U1837	U1762	
C2852	U2775	U2679	U2603	G2359	U2160	U2085	U2007	G1933	U1838	U1763	
C2853	G2776	U2680	A2604	A2360	U2161	U2086	U2008	A1933	A1839	U1764	
C2854	U2777	U2681	G2605	G2361	U2162	U2087	U2009	A1934	A1840	G1765	
C2855	G2778	U2682	U2606	A2362	U2163	U2088	U2010	G1935	U1841	U1766	
C2856	U2779	U2683	U2607	G2363	U2164	U2089	A2011	U1936	U1842	U1767	
C2857	G2780	U2684	G2608	A2364	U2165	U2090	U2012	U1937	U1843	G1768	
C2858	U2781	U2685	C2609	G2365	U2166	U2091	G2013	U1938	A1844	C1769	
C2859	G2782	U2686	U2610	U2366	U2167	U2092	A2019	A1941	U1845	U1770	
C2860	U2783	U2687	U2611	U2367	U2168	U2093	U2020	C1942	U1846	C1772	
C2861	G2784	U2688	G2612	G2368	U2169	U2094	U2021	A1943			
C2862	U2785	U2689	U2613	U2369	U2170	U2095	U2022				
C2863	G2786	U2690	A2614	U2370	U2171	U2096	U2023				
C2864	U2787	U2691	U2615	U2371	U2172	U2097	U2024				
C2865	G2788	U2692	G2616	G2372	U2173	U2098	U2025				
C2866	U2789	U2693	U2617	U2373	U2174	U2099	U2026				
C2867	G2790	U2694	A2618	U2374	U2175	U2100	U2027				
C2868	U2791	U2695	G2619	U2375	U2176	U2101	U2028				
C2869	G2792	U2696	U2620	U2376	U2177	U2102	U2029				
C2870	U2793	U2697	G2621	U2377	U2178	U2103	U2030				
C2871	G2794	U2698	U2622	U2378	U2179	U2104	U2031				
C2872	U2795	U2699	A2623	U2379	U2180	U2105	U2032				
C2873	G2796	U2700	G2624	U2380	U2181	U2106	U2033				
C2874	U2797	U2701	U2625	U2381	U2182	U2107	U2034				
C2875	G2798	U2702	G2626	U2382	U2183	U2108	U2035				
C2876	U2799	U2703	U2627	U2383	U2184	U2109	U2036				
C2877	G2800	U2704	A2628	U2384	U2185	U2110	U2037				
C2878	U2801	U2705	G2629	U2385	U2186	U2111	U2038				
C2879	G2802	U2706	U2630	U2386	U2187	U2112	U2039				
C2880	U2803	U2707	G2631	U2387	U2188	U2113	U2040				
C2881	G2804	U2708	U2632	U2388	U2189	U2114	U2041				
C2882	U2805	U2709	A2633	U2389	U2190	U2115	U2042				
C2883	G2806	U2710	G2634	U2390	U2191	U2116	U2043				
C2884	U2807	U2711	U2635	U2391	U2192	U2117	U2044				
C2885	G2808	U2712	G2636	U2392	U2193	U2118	U2045				
C2886	U2809	U2713	U2637	U2393	U2194	U2119	U2046				
C2887	G2810	U2714	A2637	U2394	U2195	U2120	U2047				
C2888	U2811	U2715	G2638	U2395	U2196	U2121	U2048				
C2889	G2812	U2716	U2639	U2396	U2197	U2122	U2049				
C2890	U2813	U2717	G2640	U2397	U2198	U2123	U2050				
C2891	G2814	U2718	U2641	U2398	U2199	U2124	U2051				
C2892	U2815	U2719	G2642	U2399	U2200	U2125	U2052				
C2893	G2816	U2720	U2643	U2400	U2201	U2126	U2053				
C2894	U2817	U2721	G2644	U2401	U2202	U2127	U2054				
C2895	G2818	U2722	U2645	U2402	U2203	U2128	U2055				
C2896	U2819	U2723	G2646	U2403	U2204	U2129	U2056				
C2897	G2820	U2724	U2647	U2404	U2205	U2130	U2057				
C2898	U2821	U2725	G2648	U2405	U2206	U2131	U2058				
C2899	G2822	U2726	U2649	U2406	U2207	U2132	U2059				
C2900	U2823	U2727	G2650	U2407	U2208	U2133	U2060				
C2901	G2824	U2728	U2651	U2408	U2209	U2134	U2061				
C2902	U2825	U2729	G2652	U2409	U2210	U2135	U2062				
C2903	G2826	U2730	U2653	U2410	U2211	U2136	U2063				
C2904	U2827	U2731	G2654	U2411	U2212	U2137	U2064				
C2905	G2828	U2732	U2655	U2412	U2213	U2138	U2065				
C2906	U2829	U2733	A2566	U2413	U2214	U2139	U2066				
C2907	G2830	U2734	G2567	U2414	U2215	U2140	U2067				
C2908	U2831	U2735	U2568	U2415	U2216	U2141	U2068				
C2909	G2832	U2736	G2569	U2416	U2217	U2142	U2069				
C2910	U2833	U2737	U2570	U2417	U2218	U2143	U2070				
C2911	G2834	U2738	G2571	U2418	U2219	U2144	U2071				
C2912	U2835	U2739	U2572	U2419	U2220	U2145	U2072				
C2913	G2836	U2740	A2506	U2420	U2221	U2146	U2073				
C2914	U2837	U2741	G2507	U2421	U2222	U2147	U2074				
C2915	G2838	U2742	U2508	U2422	U2223	U2148	U2075				
C2916	U2839	U2743	G2509	U2423	U2224	U2149	U2076				
C2917	G2840	U2744	U2510	U2424	U2225	U2150	U2077				
C2918	U2841	U2745	A2511	U2425	U2226	U2151	U2078				
C2919	G2842	U2746	U2512	U2426	U2227	U2152	U2079				
C2920	U2843	U2747	G2513	U2427	U2228	U2153	U2080				
C2921	G2844	U2748	U2514	U2428	U2229	U2154	U2081				
C2922	U2845	U2749	A2506	U2429	U2230	U2155	U2082				



- Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



- Molecule 32: RNA (5'-R(*C*CP*A)-3')

Chain 5:



- Molecule 33: RNA (5'-R(*CP*CP*(8AN))-3')

Chain 6:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	210.79Å 297.78Å 572.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.95 85.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.82-2.95) 90.2 (85.07-2.39)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.255 0.193 , 0.245	Depositor DCC
R_{free} test set	3262 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 667135 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99194	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACA, OMG, 8AN, CL, SR, NA, K, MG, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/1784	0.67	0/2403
2	B	0.36	0/2687	0.68	0/3644
3	C	0.38	0/1883	0.65	0/2547
4	D	0.33	0/1109	0.58	0/1493
5	E	0.35	0/1380	0.61	0/1875
6	F	0.36	0/899	0.60	0/1219
7	G	0.30	0/241	0.51	0/324
8	H	0.36	0/1300	0.67	0/1738
9	I	0.29	0/524	0.54	0/711
10	J	0.38	0/1134	0.62	0/1525
11	K	0.39	0/1002	0.68	0/1346
12	L	0.34	0/1128	0.65	0/1504
13	M	0.38	0/1580	0.61	0/2111
14	N	0.31	0/1472	0.66	1/1994 (0.1%)
15	O	0.35	0/872	0.64	0/1176
16	P	0.37	0/1145	0.56	0/1524
17	Q	0.36	0/747	0.68	0/1001
18	R	0.39	0/1170	0.66	0/1574
19	S	0.37	0/646	0.60	1/870 (0.1%)
20	T	0.35	0/956	0.64	0/1284
21	U	0.36	0/417	0.64	0/562
22	V	0.29	0/502	0.57	0/675
23	W	0.39	0/1217	1.24	2/1650 (0.1%)
24	X	0.35	0/662	0.61	0/890
25	Y	0.37	0/1146	0.65	0/1536
26	Z	0.36	0/582	0.62	0/776
27	1	0.41	0/438	0.62	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.40	0/769	0.61	0/1019
30	0	0.42	1/65948 (0.0%)	0.69	18/102852 (0.0%)
31	9	0.37	0/2894	0.71	0/4509
32	5	0.45	0/43	0.61	0/65

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.38	0/40	0.60	0/60
All	All	0.40	1/98718 (0.0%)	0.69	22/147564 (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
23	W	0	1
30	0	0	39
31	9	0	2
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	1942	A	O3'-P	-6.61	1.53	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	36.02	168.52	110.90
23	W	52	VAL	CA-CB-CG2	-23.54	75.59	110.90
30	0	1942	A	C5'-C4'-C3'	7.03	127.25	116.00
30	0	1942	A	OP2-P-O3'	6.73	120.00	105.20
30	0	1942	A	C5'-C4'-O4'	6.64	117.07	109.10
30	0	2467	A	C1'-O4'-C4'	-6.45	104.74	109.90
30	0	2291	A	N9-C1'-C2'	6.25	122.13	114.00
30	0	2726	U	N1-C1'-C2'	5.77	121.51	114.00
30	0	921	G	N9-C1'-C2'	5.53	121.19	114.00
30	0	1979	G	N9-C1'-C2'	5.44	121.07	114.00
30	0	1819	G	C5'-C4'-C3'	5.33	124.53	116.00
30	0	1942	A	C1'-O4'-C4'	-5.31	105.65	109.90
30	0	2313	C	C5'-C4'-C3'	5.24	124.39	116.00
30	0	1979	G	C2'-C3'-O3'	5.19	122.00	113.70
30	0	1701	A	C5'-C4'-C3'	5.18	124.29	116.00
14	N	163	PHE	N-CA-C	-5.18	97.02	111.00
19	S	27	ALA	N-CA-C	-5.17	97.04	111.00
30	0	1941	A	O3'-P-O5'	5.15	113.78	104.00
30	0	1504	A	C1'-O4'-C4'	-5.11	105.81	109.90
30	0	1504	A	N9-C1'-C2'	5.11	120.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	699	C	C1'-O4'-C4'	-5.06	105.85	109.90
30	0	2301	A	N9-C1'-C2'	5.02	120.53	114.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1309	U	Sidechain
30	0	1340	G	Sidechain
30	0	1358	A	Sidechain
30	0	1359	U	Sidechain
30	0	1380	U	Sidechain
30	0	1417	G	Sidechain
30	0	1635	U	Sidechain
30	0	1741	U	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1855	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	2043	U	Sidechain
30	0	2046	G	Sidechain
30	0	2065	C	Sidechain
30	0	2316	G	Sidechain
30	0	2478	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2557	U	Sidechain
30	0	2673	U	Sidechain
30	0	2781	U	Sidechain
30	0	2790	C	Sidechain
30	0	2840	A	Sidechain
30	0	333	G	Sidechain
30	0	471	G	Sidechain
30	0	518	G	Sidechain
30	0	63	U	Sidechain

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Mol	Chain	Res	Type	Group
30	0	688	A	Sidechain
30	0	722	G	Sidechain
30	0	877	G	Sidechain
30	0	888	U	Sidechain
31	9	65	A	Sidechain
31	9	90	G	Sidechain
23	W	90	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1752	0	1764	160	0
2	B	2624	0	2530	225	0
3	C	1859	0	1811	154	0
4	D	1093	0	1083	102	0
5	E	1356	0	1264	81	0
6	F	889	0	841	68	0
7	G	240	0	231	30	0
8	H	1281	0	1290	86	0
9	I	518	0	495	67	0
10	J	1119	0	1096	87	0
11	K	993	0	1025	77	0
12	L	1117	0	1071	85	0
13	M	1557	0	1571	130	0
14	N	1444	0	1399	140	0
15	O	864	0	868	60	0
16	P	1135	0	1120	68	0
17	Q	734	0	726	50	0
18	R	1148	0	1119	81	0
19	S	640	0	600	36	0
20	T	949	0	922	88	0
21	U	410	0	364	38	0
22	V	499	0	511	49	0
23	W	1195	0	1135	118	0
24	X	653	0	651	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	1130	0	1133	82	0
26	Z	572	0	529	35	0
27	1	431	0	426	43	0
28	2	396	0	413	30	0
29	3	754	0	726	58	0
30	0	59017	0	29809	1406	0
31	9	2595	0	1322	96	0
32	5	39	0	24	3	0
33	6	59	0	35	6	0
34	6	19	0	20	0	0
35	0	82	0	0	0	0
35	2	1	0	0	0	0
35	9	1	0	0	0	0
35	A	3	0	0	0	0
35	B	2	0	0	0	0
35	C	1	0	0	0	0
35	K	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	65	0	0	0	0
36	9	3	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	87	0	0	1	0
37	1	2	0	0	0	0
37	3	3	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	2	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	T	2	0	0	0	0
37	Y	1	0	0	0	0
38	0	6	0	0	1	0
38	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	1	0	0	0	0
38	B	1	0	0	0	0
38	J	4	0	0	4	0
38	L	2	0	0	2	0
38	M	1	0	0	1	0
38	N	1	0	0	0	0
38	O	1	0	0	1	0
38	Q	1	0	0	1	0
38	R	1	0	0	0	0
38	Y	2	0	0	0	0
39	0	2	0	0	0	0
40	1	1	0	0	0	0
40	3	1	0	0	0	0
40	O	1	0	0	0	0
40	U	1	0	0	0	0
40	Z	1	0	0	0	0
41	0	5775	0	0	197	0
41	1	57	0	0	3	0
41	2	50	0	0	2	0
41	3	66	0	0	7	0
41	6	6	0	0	4	0
41	9	138	0	0	12	0
41	A	134	0	0	19	0
41	B	156	0	0	21	0
41	C	168	0	0	21	0
41	D	49	0	0	6	0
41	E	49	0	0	5	0
41	F	31	0	0	3	0
41	G	20	0	0	2	0
41	H	78	0	0	9	0
41	I	11	0	0	3	0
41	J	58	0	0	2	0
41	K	57	0	0	3	0
41	L	91	0	0	11	0
41	M	129	0	0	5	0
41	N	68	0	0	14	0
41	O	46	0	0	6	0
41	P	72	0	0	7	0
41	Q	52	0	0	3	0
41	R	89	0	0	5	0
41	S	35	0	0	1	0
41	T	42	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	U	29	0	0	3	0
41	V	16	0	0	2	0
41	W	75	0	0	10	0
41	X	31	0	0	5	0
41	Y	105	0	0	5	0
41	Z	25	0	0	6	0
All	All	99194	0	59924	3515	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (3515) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.27	1.15
3:C:236:THR:HG22	3:C:239:ALA:H	1.00	1.13
37:O:8979:SR:SR	41:O:4399:HOH:O	0.84	1.13
14:N:37:ARG:HH12	31:9:6:C:H5''	1.10	1.09
30:O:870:G:H2'	30:O:871:G:H5''	1.30	1.08
14:N:37:ARG:NH1	31:9:6:C:H5''	1.69	1.07
31:9:76:G:H3'	31:9:77:A:H5''	1.29	1.07
10:J:52:GLN:HE22	30:O:1119:G:H2'	0.96	1.05
30:O:871:G:H5'	30:O:871:G:H8	1.17	1.05
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.39	1.05
6:F:91:VAL:HG12	6:F:92:GLY:H	1.18	1.05
30:O:1160:G:H5'	30:O:1161:A:H5'	1.39	1.04
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.39	1.04
22:V:1:THR:HG23	22:V:2:VAL:H	1.18	1.04
10:J:52:GLN:NE2	30:O:1119:G:H2'	1.73	1.03
24:X:28:LYS:HD2	24:X:31:ILE:HD12	1.41	1.03
13:M:164:THR:HG22	13:M:166:ALA:H	1.18	1.03
10:J:82:THR:HG23	30:O:1242:A:H5'	1.40	1.03
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.41	1.03
30:O:871:G:C8	30:O:871:G:H5'	1.93	1.02
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.37	1.02
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.18	1.02
30:O:541:C:H2'	30:O:542:A:H5''	1.42	1.02
11:K:10:GLN:NE2	11:K:10:GLN:H	1.58	1.01
3:C:1:MET:HG2	3:C:2:GLN:H	1.25	0.99
16:P:115:SER:H	16:P:118:GLN:HE21	1.05	0.98
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.42	0.98
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.45	0.98
30:O:2586:U:H3	30:O:2592:G:H22	1.12	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.06	0.96
30:0:542:A:H5'	30:0:542:A:H8	1.29	0.96
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.48	0.96
2:B:36:PRO:HG3	2:B:169:GLY:H	1.30	0.95
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.43	0.95
30:0:2717:C:H2'	30:0:2718:C:H5''	1.47	0.95
14:N:144:GLY:O	14:N:147:ILE:HG22	1.66	0.95
30:0:1451:C:H5'	30:0:1505:U:C5	2.01	0.95
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.44	0.94
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.49	0.94
4:D:57:THR:HG23	4:D:63:ILE:HA	1.50	0.94
4:D:172:VAL:HG12	4:D:173:GLU:H	1.32	0.94
31:9:56:A:H2'	31:9:57:A:H5''	1.49	0.93
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.51	0.93
30:0:541:C:C2'	30:0:542:A:H5''	1.97	0.93
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.49	0.93
30:0:2506:A:HO2'	30:0:2507:G:H8	1.04	0.93
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.49	0.92
3:C:236:THR:HG22	3:C:239:ALA:N	1.85	0.92
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.52	0.91
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.50	0.91
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.04	0.91
18:R:39:THR:HB	18:R:42:GLU:HG3	1.50	0.90
2:B:179:LEU:O	2:B:183:GLU:HG2	1.71	0.90
30:0:506:G:H22	30:0:509:A:H5'	1.34	0.90
2:B:206:THR:HG21	30:0:2716:G:H5''	1.51	0.90
8:H:30:LYS:H	8:H:62:HIS:HD2	1.17	0.89
30:0:1667:A:H8	30:0:1667:A:H5'	1.36	0.88
11:K:39:GLY:HA2	41:K:4183:HOH:O	1.73	0.88
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.53	0.88
3:C:233:THR:HG22	3:C:234:VAL:H	1.38	0.88
30:0:2005:G:H3'	30:0:2005:G:OP2	1.74	0.88
11:K:87:ARG:HB2	21:U:19:THR:HG23	1.53	0.88
11:K:10:GLN:H	11:K:10:GLN:HE21	1.19	0.88
3:C:236:THR:HG21	41:C:8580:HOH:O	1.74	0.88
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.54	0.87
13:M:164:THR:HG22	13:M:166:ALA:N	1.89	0.87
30:0:2291:A:C8	30:0:2309:C:H5'	2.09	0.87
5:E:15:GLN:HG2	5:E:19:ASP:O	1.74	0.87
1:A:153:ARG:CB	1:A:153:ARG:HH11	1.86	0.87
15:O:3:THR:HB	30:0:656:G:H5'	1.57	0.87
3:C:27:ARG:HG2	3:C:27:ARG:HH11	1.37	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:9:CYS:HA	21:U:52:THR:HG23	1.57	0.86
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.57	0.86
3:C:72:LYS:HG2	3:C:77:ALA:HA	1.56	0.86
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.05	0.86
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.56	0.86
30:0:1451:C:H5'	30:0:1505:U:H5	1.34	0.86
30:0:1559:A:H1'	41:0:6702:HOH:O	1.74	0.86
30:0:870:G:C2'	30:0:871:G:H5''	2.05	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD3	1.40	0.86
16:P:103:THR:HA	16:P:106:ARG:NH1	1.91	0.85
30:0:681:G:N3	30:0:681:G:H5'	1.91	0.85
30:0:545:G:H8	30:0:545:G:H5'	1.40	0.85
1:A:109:GLU:HG2	1:A:116:GLY:H	1.42	0.85
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.56	0.85
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.58	0.85
4:D:25:MET:HE1	4:D:41:LEU:HG	1.57	0.85
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.58	0.85
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.73	0.85
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.58	0.85
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.55	0.85
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.40	0.84
20:T:28:SER:HA	20:T:97:ARG:HD3	1.59	0.84
12:L:55:GLN:HA	12:L:58:GLN:HE21	1.38	0.84
19:S:10:VAL:HG11	22:V:36:ALA:HB2	1.59	0.84
1:A:153:ARG:NH1	1:A:153:ARG:HB2	1.93	0.84
30:0:2717:C:C2'	30:0:2718:C:H5''	2.07	0.84
28:2:41:HIS:H	28:2:45:ASN:HD22	1.20	0.84
24:X:49:ARG:HG3	24:X:49:ARG:O	1.75	0.84
30:0:2812:A:H2	30:0:2814:A:H62	1.22	0.84
15:O:42:GLU:HB2	41:O:2176:HOH:O	1.77	0.84
30:0:1474:C:H6	30:0:1474:C:H5'	1.41	0.84
31:9:29:C:H2'	31:9:30:C:H5'	1.59	0.84
30:0:1603:A:H5'	30:0:1605:G:O4'	1.77	0.84
30:0:1116:U:O2'	30:0:1118:A:H2	1.61	0.83
6:F:12:LEU:HD21	6:F:111:ILE:HG23	1.58	0.83
41:Z:8705:HOH:O	30:0:1886:A:H4'	1.78	0.83
12:L:35:ARG:HH11	12:L:35:ARG:HB2	1.41	0.83
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.60	0.83
30:0:1160:G:C5'	30:0:1161:A:H5'	2.07	0.83
32:5:75:C:H3'	32:5:76:A:H8	1.42	0.83
21:U:52:THR:HG22	21:U:54:THR:H	1.44	0.83
30:0:1184:C:H1'	41:0:9264:HOH:O	1.79	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:91:VAL:HG12	6:F:92:GLY:N	1.94	0.82
14:N:113:SER:HB2	41:N:8857:HOH:O	1.79	0.82
29:3:6:ARG:NH1	29:3:21:GLU:HG3	1.94	0.82
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.62	0.82
30:0:1116:U:HO2'	30:0:1118:A:H2	0.83	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.78	0.81
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.62	0.81
29:3:48:ASN:HD21	30:0:2468:A:H61	1.28	0.81
10:J:52:GLN:HG3	10:J:53:ILE:N	1.94	0.81
2:B:162:MET:HE1	2:B:310:ARG:HD2	1.63	0.81
15:O:21:SER:OG	15:O:106:PRO:HB2	1.80	0.81
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.43	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:1679:C:H5'	41:0:3235:HOH:O	1.78	0.81
16:P:38:GLU:HA	16:P:41:ARG:HD2	1.63	0.81
27:1:20:ARG:HG2	30:0:111:C:O2'	1.81	0.81
9:I:73:LEU:HD12	9:I:107:LYS:NZ	1.96	0.81
30:0:271:C:H41	30:0:378:A:H2	1.27	0.81
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.62	0.81
18:R:18:LEU:HB2	18:R:143:VAL:HG12	1.63	0.80
30:0:877:G:H5'	30:0:878:G:OP1	1.81	0.80
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.63	0.80
7:G:23:ILE:HD13	7:G:67:LEU:HD23	1.63	0.80
3:C:225:PRO:O	30:0:1308:A:H4'	1.82	0.80
18:R:99:ALA:HB1	18:R:109:MET:CE	2.12	0.80
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.64	0.80
30:0:1625:U:H4'	41:0:5524:HOH:O	1.80	0.80
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.61	0.80
3:C:103:ASN:ND2	30:0:663:C:H5''	1.95	0.80
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.63	0.80
30:0:1160:G:H5'	30:0:1161:A:C5'	2.12	0.80
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.64	0.80
18:R:18:LEU:HD12	18:R:143:VAL:HG11	1.63	0.80
30:0:2420:G:O2'	30:0:2421:G:H5'	1.82	0.79
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.62	0.79
1:A:26:ASP:HB2	41:0:4577:HOH:O	1.81	0.79
8:H:30:LYS:H	8:H:62:HIS:CD2	2.01	0.79
27:1:16:HIS:HD2	30:0:470:U:O2'	1.65	0.79
19:S:73:ASP:OD1	19:S:76:GLU:HG3	1.83	0.79
18:R:114:VAL:HB	18:R:145:LEU:HD12	1.64	0.79
30:0:1377:C:H6	30:0:1377:C:H5'	1.45	0.79
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.63	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:132:ARG:NH2	30:0:2055:A:H4'	1.98	0.79
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.64	0.79
21:U:14:GLU:O	21:U:17:THR:HB	1.83	0.78
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.23	0.78
30:0:2042:U:H1'	41:0:9124:HOH:O	1.82	0.78
23:W:80:ASP:O	23:W:84:VAL:HG23	1.84	0.78
1:A:33:GLU:H	1:A:33:GLU:CD	1.86	0.78
30:0:1205:U:H2'	30:0:1206:U:H5''	1.66	0.78
14:N:164:ASP:CG	14:N:167:ASP:HA	2.04	0.78
13:M:171:ARG:HD3	30:0:156:C:H5''	1.64	0.78
22:V:50:ARG:NH1	30:0:56:G:H5''	1.99	0.78
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.66	0.78
16:P:115:SER:OG	16:P:118:GLN:HG3	1.84	0.78
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.64	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.63	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.78
6:F:58:GLU:CD	13:M:27:ARG:HH22	1.87	0.78
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.64	0.78
12:L:92:ASP:HA	12:L:121:ILE:HB	1.66	0.78
1:A:199:HIS:CD2	1:A:201:PHE:H	2.02	0.78
18:R:39:THR:HG23	18:R:107:GLU:O	1.83	0.78
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.82	0.77
2:B:162:MET:CE	2:B:310:ARG:HD2	2.14	0.77
14:N:40:ASN:HD21	31:9:28:U:H5''	1.49	0.77
14:N:40:ASN:ND2	31:9:28:U:H5''	2.00	0.77
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.15	0.77
1:A:179:MET:HA	1:A:179:MET:CE	2.14	0.77
2:B:275:GLY:O	2:B:291:ASP:HA	1.84	0.77
23:W:137:GLN:HE21	23:W:141:HIS:CE1	1.98	0.77
3:C:27:ARG:HG2	3:C:27:ARG:NH1	1.95	0.77
1:A:191:GLY:HA2	1:A:194:MET:CE	2.14	0.77
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.48	0.77
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.67	0.77
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.67	0.76
22:V:12:THR:HG22	22:V:15:GLU:CG	2.16	0.76
1:A:66:ARG:HH11	1:A:66:ARG:HB2	1.50	0.76
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.66	0.76
30:0:541:C:H2'	30:0:542:A:C5'	2.13	0.76
30:0:1835:U:H5	30:0:1840:A:N7	1.83	0.76
7:G:64:ASN:O	7:G:68:GLU:HG3	1.86	0.76
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.65	0.76
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.19	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.49	0.76
2:B:267:LYS:HD3	41:O:3465:HOH:O	1.85	0.76
12:L:90:ARG:HA	12:L:119:THR:HB	1.67	0.76
10:J:131:THR:HG22	10:J:134:GLU:H	1.51	0.76
30:O:2661:U:H3	30:O:2812:A:H62	1.32	0.76
3:C:236:THR:H	3:C:239:ALA:HB3	1.51	0.76
30:O:1116:U:H3	30:O:1246:A:H62	1.32	0.76
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.21	0.76
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.69	0.75
13:M:80:GLY:O	13:M:81:ARG:HD2	1.86	0.75
30:O:871:G:C5'	30:O:871:G:H8	1.95	0.75
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.07	0.75
30:O:1118:A:H8	30:O:1119:G:H5''	1.51	0.75
32:5:75:C:H3'	32:5:76:A:C8	2.21	0.75
24:X:43:VAL:HG12	24:X:44:ASP:H	1.51	0.75
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.16	0.75
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.66	0.75
30:O:1730:G:H5'	30:O:1731:C:C5	2.22	0.75
1:A:203:GLY:HA2	41:O:3401:HOH:O	1.87	0.75
30:O:2578:G:H5'	30:O:2578:G:H8	1.50	0.75
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.69	0.75
30:O:542:A:H5'	30:O:542:A:C8	2.18	0.74
4:D:170:TYR:O	4:D:171:ASP:HB3	1.87	0.74
22:V:1:THR:HG23	22:V:2:VAL:N	1.99	0.74
15:O:57:THR:O	15:O:111:VAL:HG23	1.87	0.74
11:K:87:ARG:HG3	30:O:2721:U:H4'	1.68	0.74
3:C:180:SER:HB2	41:C:8643:HOH:O	1.86	0.74
4:D:105:SER:HB2	4:D:131:THR:HG23	1.70	0.74
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.69	0.74
30:O:530:C:H4'	30:O:612:U:H4'	1.69	0.74
30:O:625:U:H3'	41:O:4150:HOH:O	1.87	0.74
9:I:101:LYS:O	9:I:105:GLU:HG3	1.87	0.74
22:V:12:THR:HG22	22:V:15:GLU:OE2	1.87	0.74
24:X:61:ARG:HB2	24:X:65:ASN:HB2	1.69	0.74
30:O:1206:U:H5'	30:O:1206:U:H6	1.51	0.74
14:N:169:PRO:O	14:N:172:PHE:HB3	1.88	0.74
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.02	0.74
30:O:292:G:H2'	30:O:358:G:N2	2.02	0.74
25:Y:189:ASN:CA	25:Y:217:ILE:HD11	2.16	0.74
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.22	0.74
7:G:12:ILE:HG23	41:O:6301:HOH:O	1.88	0.74
14:N:119:GLN:O	14:N:123:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:86:LEU:O	14:N:90:LEU:HG	1.88	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.52	0.74
30:0:1878:G:H5'	41:0:5236:HOH:O	1.87	0.73
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.18	0.73
30:0:1452:G:H1'	38:0:8803:CL:CL	2.25	0.73
30:0:2073:G:H5''	41:0:4699:HOH:O	1.88	0.73
2:B:27:ASN:HD21	30:0:2807:U:P	2.11	0.73
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.71	0.73
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.52	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.87	0.73
18:R:82:GLU:HG3	18:R:83:LYS:N	2.04	0.73
30:0:1119:G:N2	30:0:1246:A:C2	2.56	0.73
41:M:8871:HOH:O	30:0:381:G:H5''	1.89	0.73
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.53	0.73
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.71	0.73
24:X:72:VAL:HG22	24:X:85:VAL:CG1	2.19	0.72
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.70	0.72
4:D:57:THR:HA	41:D:5728:HOH:O	1.89	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.70	0.72
31:9:50:G:H2'	31:9:51:A:C8	2.24	0.72
18:R:39:THR:HB	18:R:42:GLU:CG	2.18	0.72
14:N:110:THR:HB	14:N:113:SER:OG	1.89	0.72
14:N:112:GLY:HA2	14:N:137:ALA:H	1.54	0.72
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.71	0.72
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.24	0.72
30:0:78:G:N3	30:0:78:G:N2	2.37	0.72
10:J:77:GLY:HA2	10:J:80:LYS:H	1.54	0.72
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.54	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.38	0.72
20:T:2:LYS:HG2	30:0:447:A:OP1	1.90	0.72
30:0:558:C:H2'	30:0:559:U:H5''	1.71	0.72
27:1:1:THR:HA	41:1:435:HOH:O	1.89	0.72
12:L:143:THR:HG22	12:L:145:LEU:H	1.55	0.72
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.72
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72
2:B:140:LEU:HA	41:B:9050:HOH:O	1.90	0.72
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.72	0.71
30:0:855:U:H3'	41:0:4510:HOH:O	1.89	0.71
30:0:558:C:C2'	30:0:559:U:H5''	2.19	0.71
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.71	0.71
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.70	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:96:ALA:HA	41:F:3111:HOH:O	1.88	0.71
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.73	0.71
30:0:2356:A:H2'	30:0:2357:G:O4'	1.91	0.71
10:J:74:ARG:CB	10:J:74:ARG:HH11	2.04	0.71
30:0:2296:C:H2'	30:0:2297:U:H6	1.55	0.71
22:V:12:THR:CG2	22:V:15:GLU:HG3	2.20	0.71
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.71
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.36	0.71
30:0:1838:U:O2'	30:0:2644:C:H5'	1.90	0.71
30:0:1667:A:H5'	30:0:1667:A:C8	2.25	0.71
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.70	0.71
18:R:82:GLU:HG3	18:R:83:LYS:H	1.55	0.71
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.56	0.71
22:V:39:ALA:N	22:V:40:PRO:HD2	2.05	0.71
22:V:1:THR:CG2	22:V:2:VAL:H	2.00	0.70
6:F:58:GLU:HA	6:F:61:MET:CE	2.21	0.70
24:X:49:ARG:HG2	24:X:84:ILE:HG12	1.72	0.70
18:R:6:VAL:HG21	18:R:113:HIS:CD2	2.25	0.70
30:0:1701:A:H4'	30:0:1702:U:H5''	1.72	0.70
3:C:194:PHE:HA	3:C:234:VAL:HG13	1.73	0.70
1:A:36:ASP:O	1:A:38:ILE:N	2.23	0.70
30:0:1372:A:H3'	41:0:7993:HOH:O	1.91	0.70
17:Q:66:LYS:HB2	17:Q:70:ALA:O	1.91	0.70
30:0:1474:C:C6	30:0:1474:C:H5'	2.24	0.70
14:N:164:ASP:OD1	14:N:167:ASP:HA	1.91	0.70
29:3:68:LYS:HE2	30:0:2436:U:H5'	1.71	0.70
14:N:11:ARG:HD3	31:9:114:G:O6	1.91	0.70
14:N:132:ASN:O	14:N:135:VAL:HG12	1.92	0.70
3:C:1:MET:HG2	3:C:2:GLN:N	2.04	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.89	0.70
30:0:2851:G:O2'	30:0:2852:A:H5'	1.90	0.70
20:T:54:ASP:OD2	30:0:316:A:H5'	1.90	0.70
30:0:2908:A:H2'	30:0:2909:G:O4'	1.92	0.70
5:E:84:MET:HG2	5:E:168:ILE:HA	1.73	0.70
27:1:9:GLY:HA2	30:0:1687:C:O2	1.91	0.70
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.73	0.70
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.72	0.70
18:R:128:ARG:NH2	30:0:2054:A:N3	2.39	0.70
3:C:27:ARG:CG	3:C:27:ARG:HH11	2.05	0.70
13:M:164:THR:CG2	13:M:166:ALA:H	2.02	0.69
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.73	0.69
31:9:56:A:C2'	31:9:57:A:H5''	2.20	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:57:LYS:HE2	13:M:140:ALA:O	1.92	0.69
3:C:84:VAL:HG12	3:C:85:LYS:HG2	1.72	0.69
8:H:36:MET:HB3	8:H:73:ASN:ND2	2.07	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.27	0.69
30:0:1829:A:H2'	30:0:1830:C:H5'	1.74	0.69
30:0:236:A:H4'	30:0:237:G:H5'	1.74	0.69
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.69
30:0:1634:G:H3'	41:0:4766:HOH:O	1.92	0.69
3:C:233:THR:HG22	3:C:234:VAL:N	2.07	0.69
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.23	0.69
8:H:31:ILE:HA	8:H:66:GLU:OE1	1.93	0.69
26:Z:46:SER:O	26:Z:50:VAL:HG23	1.92	0.69
31:9:75:G:H1	31:9:106:U:H3	1.39	0.69
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.74	0.69
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.23	0.69
25:Y:117:LEU:HD13	25:Y:174:VAL:HG11	1.73	0.69
30:0:2637:A:H4'	30:0:2638:G:C5'	2.23	0.69
30:0:1205:U:H2'	30:0:1206:U:C5'	2.22	0.69
13:M:24:GLN:NE2	13:M:27:ARG:HD2	2.07	0.69
2:B:175:LEU:O	2:B:175:LEU:HD23	1.93	0.69
25:Y:234:VAL:HG12	25:Y:235:GLU:H	1.56	0.69
30:0:2102:G:H2'	41:0:9555:HOH:O	1.93	0.69
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.74	0.69
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.08	0.69
30:0:2004:U:H2'	30:0:2004:U:O2	1.93	0.69
30:0:2387:U:H2'	30:0:2388:C:C6	2.28	0.69
23:W:52:VAL:HG23	23:W:53:ALA:N	1.64	0.69
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.22	0.69
22:V:11:MET:HB3	22:V:15:GLU:HB2	1.73	0.68
1:A:199:HIS:HD2	1:A:201:PHE:H	1.38	0.68
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.09	0.68
24:X:25:ARG:HD3	24:X:64:ALA:O	1.93	0.68
17:Q:16:ASN:HD21	17:Q:45:PRO:HD2	1.58	0.68
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
2:B:229:ARG:HD2	41:B:8991:HOH:O	1.93	0.68
3:C:193:LEU:HD13	3:C:222:ASP:HB2	1.76	0.68
30:0:2247:C:H2'	30:0:2248:C:H6	1.59	0.68
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.76	0.68
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.23	0.68
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.23	0.68
23:W:38:THR:HG22	23:W:39:ASP:N	2.09	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:LYS:HE2	1:A:143:GLY:HA2	1.76	0.68
10:J:4:ALA:O	10:J:5:GLU:HB2	1.94	0.68
16:P:139:ARG:HH11	16:P:139:ARG:HG3	1.58	0.68
30:0:1300:G:H1'	41:0:5541:HOH:O	1.91	0.68
30:0:304:G:H1'	30:0:347:A:N6	2.08	0.68
16:P:115:SER:H	16:P:118:GLN:NE2	1.86	0.68
14:N:5:ARG:NH1	30:0:962:C:H1'	2.09	0.68
8:H:6:ALA:HB3	30:0:2521:A:OP2	1.94	0.68
4:D:135:VAL:HG21	4:D:139:TYR:CG	2.28	0.68
6:F:14:ASP:O	6:F:18:GLU:HG3	1.94	0.68
30:0:2851:G:C2'	30:0:2852:A:H5'	2.24	0.68
23:W:13:MET:CE	23:W:17:ILE:HG22	2.24	0.68
30:0:558:C:H2'	30:0:559:U:C5'	2.24	0.68
3:C:153:VAL:O	3:C:157:LEU:HG	1.94	0.68
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.87	0.68
30:0:282:C:O2'	30:0:283:U:H5'	1.93	0.68
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.75	0.68
2:B:214:PRO:HD2	41:0:2996:HOH:O	1.92	0.68
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.67
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.67
25:Y:170:SER:OG	25:Y:175:ARG:HG3	1.94	0.67
23:W:84:VAL:HG12	41:W:6679:HOH:O	1.94	0.67
30:0:2588:OMG:HN21	32:5:76:A:H2	1.40	0.67
30:0:1182:C:H1'	30:0:1192:A:H8	1.59	0.67
6:F:83:LEU:HD11	6:F:96:ALA:HB3	1.76	0.67
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.76	0.67
7:G:27:ILE:HD13	7:G:71:LEU:HD23	1.76	0.67
22:V:1:THR:HB	30:0:93:C:H5''	1.77	0.67
29:3:25:VAL:HG13	29:3:68:LYS:HE3	1.75	0.67
12:L:6:ARG:HD3	30:0:1299:G:O6	1.94	0.67
22:V:56:ILE:O	22:V:60:GLN:HG3	1.93	0.67
10:J:54:VAL:O	10:J:58:GLU:HG3	1.95	0.67
18:R:117:HIS:HD2	30:0:20:G:H21	1.40	0.67
4:D:27:ILE:HD11	4:D:37:ALA:CB	2.25	0.67
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
21:U:11:THR:HG22	21:U:53:ASP:HB2	1.77	0.67
3:C:211:ASP:HB2	3:C:231:ARG:HH22	1.60	0.67
2:B:74:ILE:HG22	2:B:76:THR:HG23	1.76	0.67
1:A:201:PHE:HA	41:A:9065:HOH:O	1.94	0.67
30:0:2073:G:OP2	30:0:2490:A:H5'	1.94	0.67
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:18:U:H2'	31:9:19:G:H8	1.59	0.67
2:B:321:PRO:HA	41:B:9136:HOH:O	1.94	0.67
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.25	0.67
8:H:48:VAL:HA	8:H:170:ARG:O	1.94	0.67
5:E:101:GLU:HB3	5:E:117:THR:HA	1.75	0.67
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.23	0.67
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.77	0.67
31:9:49:G:H5''	41:9:9086:HOH:O	1.95	0.67
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.67
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.67
11:K:41:LYS:HE2	11:K:42:ASN:HD21	1.60	0.67
30:0:1058:A:H2'	30:0:1060:C:C5'	2.25	0.67
1:A:103:VAL:O	1:A:105:VAL:HG23	1.95	0.67
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.41	0.67
30:0:1730:G:H5'	30:0:1731:C:C6	2.30	0.67
3:C:174:ILE:CD1	30:0:338:C:H4'	2.25	0.67
30:0:1834:C:H2'	30:0:1840:A:N6	2.10	0.67
30:0:451:C:O2'	30:0:452:G:H5'	1.95	0.67
30:0:2047:C:H5'	41:0:3722:HOH:O	1.95	0.67
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.25	0.66
30:0:2102:G:H1'	41:0:6120:HOH:O	1.94	0.66
23:W:122:ARG:NH2	23:W:154:ARG:HB3	2.10	0.66
5:E:23:GLU:HG2	5:E:28:SER:CB	2.25	0.66
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.76	0.66
18:R:16:ALA:HB1	18:R:94:ASN:HD22	1.60	0.66
30:0:1766:U:O2	30:0:1778:A:H5'	1.95	0.66
2:B:235:ARG:HD3	30:0:2091:G:O3'	1.95	0.66
12:L:55:GLN:HA	12:L:58:GLN:NE2	2.07	0.66
27:1:16:HIS:HE1	30:0:775:G:OP1	1.79	0.66
30:0:1461:U:H2'	30:0:1462:C:C6	2.31	0.66
3:C:236:THR:CG2	3:C:239:ALA:H	1.93	0.66
30:0:1666:C:O2'	30:0:1667:A:H5''	1.96	0.66
20:T:9:LYS:HD2	41:0:4631:HOH:O	1.96	0.66
4:D:131:THR:HG21	30:0:2348:C:H1'	1.77	0.66
18:R:68:HIS:CD2	18:R:76:ASP:HB2	2.30	0.66
22:V:26:GLU:OE2	22:V:45:ARG:HD3	1.95	0.66
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.10	0.66
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.66
6:F:26:THR:HG21	6:F:102:GLY:C	2.16	0.66
13:M:31:TRP:HA	13:M:34:GLU:HG3	1.78	0.66
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.75	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.66
30:0:2769:C:H2'	30:0:2770:G:O4'	1.95	0.66
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.76	0.66
30:0:1666:C:H2'	30:0:1667:A:H5'	1.78	0.66
21:U:45:GLU:HB2	21:U:48:ASN:HD22	1.60	0.66
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.78	0.66
24:X:80:GLU:HB3	41:X:5564:HOH:O	1.96	0.66
2:B:211:THR:HG23	30:0:2840:A:OP1	1.96	0.66
14:N:36:ALA:HB1	14:N:118:ILE:HD12	1.77	0.66
30:0:1171:A:H2'	30:0:1172:G:H5'	1.78	0.66
30:0:1118:A:H3'	30:0:1118:A:C8	2.30	0.66
20:T:48:VAL:HG23	20:T:98:VAL:HA	1.78	0.66
30:0:946:C:H2'	30:0:947:U:H6	1.61	0.66
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.77	0.66
3:C:246:ARG:NH1	3:C:246:ARG:HB3	2.11	0.66
18:R:39:THR:CB	18:R:42:GLU:HG3	2.24	0.65
1:A:33:GLU:O	1:A:34:ASP:HB2	1.95	0.65
25:Y:235:GLU:CD	25:Y:235:GLU:H	1.98	0.65
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.77	0.65
33:6:76:8AN:C2	41:6:82:HOH:O	2.44	0.65
3:C:111:VAL:HB	41:C:8521:HOH:O	1.95	0.65
10:J:25:GLN:HE22	10:J:116:LEU:HB3	1.61	0.65
1:A:88:ILE:HG22	1:A:88:ILE:O	1.96	0.65
3:C:156:LEU:O	3:C:160:LEU:HG	1.96	0.65
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.19	0.65
4:D:173:GLU:O	4:D:174:VAL:O	2.13	0.65
10:J:19:MET:HE2	10:J:79:PHE:HA	1.77	0.65
21:U:45:GLU:HB2	21:U:48:ASN:ND2	2.11	0.65
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.27	0.65
8:H:5:PRO:O	8:H:8:MET:HB2	1.95	0.65
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.94	0.65
31:9:23:U:O2'	31:9:24:U:H4'	1.95	0.65
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.79	0.65
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.79	0.65
31:9:76:G:C3'	31:9:77:A:H5''	2.16	0.65
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.27	0.65
1:A:207:GLN:HA	41:A:9036:HOH:O	1.95	0.65
19:S:22:ASN:ND2	19:S:68:LEU:HB2	2.12	0.65
3:C:242:GLU:HG3	41:C:8587:HOH:O	1.95	0.65
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.25	0.65
10:J:76:ASP:HA	41:J:5907:HOH:O	1.97	0.65
6:F:84:GLY:O	6:F:89:LEU:HB2	1.95	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1201:C:H5''	41:0:7064:HOH:O	1.96	0.65
23:W:139:GLY:O	23:W:141:HIS:HD2	1.79	0.65
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.11	0.65
16:P:121:ASP:O	16:P:125:LYS:HG3	1.96	0.65
30:0:168:C:H5''	41:0:3347:HOH:O	1.96	0.65
14:N:78:MET:HB2	14:N:146:HIS:CE1	2.32	0.65
9:I:127:CYS:C	9:I:129:SER:H	2.00	0.65
30:0:2387:U:H2'	30:0:2388:C:H6	1.61	0.65
9:I:82:THR:HG23	30:0:1168:C:H5''	1.79	0.65
6:F:27:GLY:HA3	6:F:101:ALA:O	1.97	0.65
6:F:46:GLU:O	6:F:73:PRO:HD2	1.97	0.65
30:0:506:G:H22	30:0:509:A:C5'	2.07	0.64
31:9:13:A:O2'	31:9:14:G:H5''	1.97	0.64
30:0:545:G:C8	30:0:545:G:H5'	2.29	0.64
2:B:77:PRO:HA	2:B:293:PRO:HB2	1.79	0.64
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.79	0.64
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.79	0.64
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.79	0.64
30:0:1118:A:H3'	30:0:1118:A:H8	1.62	0.64
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.64
28:2:41:HIS:CD2	28:2:44:ARG:H	2.14	0.64
21:U:6:CYS:O	21:U:10:GLY:HA2	1.98	0.64
30:0:1136:U:H2'	41:0:5826:HOH:O	1.96	0.64
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.28	0.64
20:T:48:VAL:CG2	20:T:96:VAL:HG13	2.28	0.64
30:0:2637:A:H4'	30:0:2638:G:H5'	1.79	0.64
3:C:5:ILE:HD11	3:C:16:VAL:HG22	1.79	0.64
27:1:28:HIS:HD2	27:1:30:LYS:H	1.45	0.64
30:0:660:A:H4'	30:0:661:G:O5'	1.98	0.64
17:Q:95:GLU:HA	30:0:949:U:H4'	1.79	0.64
6:F:37:THR:O	6:F:41:GLU:HG3	1.97	0.64
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.80	0.64
14:N:182:GLY:O	14:N:184:ILE:HG22	1.97	0.64
6:F:57:GLU:O	6:F:61:MET:HG3	1.98	0.64
15:O:65:LEU:HD13	30:0:746:A:C6	2.32	0.64
30:0:2540:G:O2'	30:0:2541:U:H5''	1.98	0.64
14:N:160:SER:HB3	31:9:51:A:H5'	1.80	0.64
16:P:7:LYS:HD3	16:P:23:PHE:CZ	2.32	0.64
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.80	0.64
19:S:33:SER:O	19:S:37:VAL:HG23	1.97	0.64
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.45	0.64
13:M:68:ARG:HD3	13:M:68:ARG:O	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:14:LYS:HE2	41:0:4718:HOH:O	1.98	0.64
21:U:9:CYS:SG	21:U:11:THR:HG23	2.38	0.64
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	1.79	0.64
2:B:211:THR:HG21	41:0:9253:HOH:O	1.98	0.64
19:S:52:VAL:HG22	19:S:66:VAL:HG22	1.79	0.64
31:9:2:U:OP2	31:9:3:A:H5'	1.96	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.56	0.64
9:I:110:ASP:O	30:0:1163:G:H5'	1.98	0.64
30:0:316:A:N3	30:0:336:G:O2'	2.31	0.64
16:P:1:THR:O	30:0:1396:C:H1'	1.97	0.64
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.11	0.64
22:V:50:ARG:HH12	30:0:56:G:H5''	1.60	0.64
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.63	0.64
2:B:62:ARG:HA	2:B:65:MET:CE	2.28	0.64
3:C:246:ARG:HH11	3:C:246:ARG:HB3	1.63	0.63
20:T:16:LEU:HB2	30:0:100:C:H4'	1.80	0.63
9:I:96:SER:HB3	9:I:99:GLN:HE21	1.61	0.63
31:9:59:C:H2'	31:9:60:C:C6	2.33	0.63
10:J:90:LYS:HB2	38:J:8802:CL:CL	2.35	0.63
6:F:91:VAL:CG1	6:F:92:GLY:H	2.02	0.63
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.62	0.63
6:F:58:GLU:HA	6:F:61:MET:HE2	1.79	0.63
31:9:29:C:C2'	31:9:30:C:H5'	2.29	0.63
29:3:73:GLU:HB3	41:3:9050:HOH:O	1.97	0.63
18:R:51:ILE:HD13	18:R:86:LYS:HG2	1.79	0.63
1:A:11:ARG:NH1	41:A:9044:HOH:O	2.31	0.63
29:3:62:THR:HB	41:3:9041:HOH:O	1.98	0.63
2:B:139:ASP:OD2	2:B:165:ARG:HD2	1.97	0.63
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.63
15:O:32:ARG:HD3	15:O:32:ARG:O	1.98	0.63
12:L:67:ARG:O	12:L:71:GLU:HG3	1.99	0.63
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.80	0.63
30:0:1042:U:O2'	30:0:1043:C:H5'	1.98	0.63
11:K:125:ALA:C	11:K:127:ALA:H	2.02	0.63
30:0:1189:A:H3'	41:0:9471:HOH:O	1.98	0.63
23:W:88:THR:HB	41:W:6679:HOH:O	1.99	0.63
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.81	0.63
21:U:14:GLU:OE1	21:U:15:PRO:HD2	1.98	0.63
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.61	0.63
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.29	0.63
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.34	0.63
1:A:8:ARG:HG2	41:A:9031:HOH:O	1.96	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:104:ASP:O	3:C:108:GLN:HG3	1.98	0.63
7:G:16:LYS:O	7:G:20:VAL:HG23	1.98	0.63
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.34	0.63
30:0:1183:C:H2'	41:0:7072:HOH:O	1.99	0.63
1:A:179:MET:HA	1:A:179:MET:HE3	1.80	0.63
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.64	0.63
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	1.98	0.63
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.81	0.63
1:A:121:ALA:O	1:A:124:VAL:HG22	1.99	0.63
30:0:2106:C:H5'	30:0:2284:G:H21	1.64	0.63
20:T:50:VAL:HG12	20:T:56:ALA:HA	1.81	0.63
30:0:463:A:H5'	30:0:465:U:O4'	1.99	0.63
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.63
30:0:95:A:H5''	30:0:97:G:O4'	1.99	0.62
30:0:151:A:H2'	30:0:152:A:O4'	1.99	0.62
7:G:69:ARG:NH2	30:0:1150:A:N7	2.47	0.62
30:0:858:U:H2'	30:0:859:C:H6	1.64	0.62
2:B:150:ALA:O	2:B:152:PRO:HD3	1.98	0.62
2:B:97:LEU:O	2:B:98:THR:HG23	1.99	0.62
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.17	0.62
20:T:49:GLU:OE2	20:T:97:ARG:NH1	2.32	0.62
12:L:35:ARG:HD3	12:L:35:ARG:C	2.20	0.62
13:M:171:ARG:CD	30:0:156:C:H5''	2.28	0.62
23:W:46:ALA:O	23:W:49:ASN:HB2	1.99	0.62
22:V:13:PRO:HA	22:V:16:ARG:NH1	2.14	0.62
30:0:871:G:C8	30:0:871:G:C5'	2.74	0.62
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.81	0.62
10:J:130:VAL:HG12	10:J:131:THR:N	2.15	0.62
30:0:281:U:H2'	30:0:282:C:O4'	1.98	0.62
30:0:2362:A:H2'	30:0:2363:G:C8	2.34	0.62
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.78	0.62
12:L:7:GLN:HG3	38:L:8814:CL:CL	2.37	0.62
30:0:603:A:H4'	30:0:604:G:O5'	2.00	0.62
20:T:48:VAL:HG21	20:T:96:VAL:HG13	1.80	0.62
30:0:280:C:H2'	30:0:281:U:O4'	1.99	0.62
27:1:9:GLY:HA3	30:0:1695:G:H1'	1.79	0.62
30:0:1058:A:H2'	30:0:1060:C:H5''	1.80	0.62
30:0:726:C:H2'	30:0:727:G:O4'	2.00	0.62
31:9:98:C:H2'	31:9:99:U:H6	1.64	0.62
30:0:1218:U:H2'	30:0:1219:U:C6	2.34	0.62
30:0:2266:A:H2'	30:0:2267:G:C8	2.35	0.62
30:0:790:A:H1'	30:0:1710:A:H2'	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.29	0.62
31:9:73:A:H61	31:9:108:C:H42	1.48	0.62
20:T:19:ARG:HD3	20:T:67:LEU:O	2.00	0.62
4:D:64:ARG:NE	4:D:67:ASP:HB3	2.15	0.62
16:P:143:ALA:HA	41:P:5521:HOH:O	1.99	0.62
12:L:66:VAL:HG23	12:L:67:ARG:N	2.14	0.62
30:0:204:A:H2'	30:0:205:U:H5'	1.82	0.62
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.80	0.62
30:0:241:A:C2	30:0:378:A:H4'	2.35	0.62
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.82	0.62
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.35	0.62
30:0:1406:A:H4'	30:0:1407:A:H5''	1.82	0.62
4:D:25:MET:CE	4:D:37:ALA:HB1	2.23	0.62
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.81	0.62
30:0:2106:C:H1'	30:0:2484:U:O2	2.00	0.62
30:0:59:A:H5'	41:0:5197:HOH:O	1.98	0.62
3:C:214:THR:HG22	3:C:216:SER:H	1.64	0.62
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.65	0.62
5:E:131:LEU:HD12	5:E:166:VAL:HG11	1.81	0.62
27:1:25:LYS:O	27:1:25:LYS:HG2	2.00	0.62
16:P:9:LEU:O	16:P:13:VAL:HG12	2.00	0.62
5:E:36:PRO:HD3	10:J:127:ILE:CD1	2.30	0.62
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.80	0.61
5:E:144:THR:O	5:E:148:ILE:HG13	1.99	0.61
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.35	0.61
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.00	0.61
29:3:6:ARG:HH11	29:3:21:GLU:HG3	1.65	0.61
30:0:2766:A:H5'	41:0:3465:HOH:O	1.99	0.61
31:9:14:G:C8	31:9:14:G:H5'	2.35	0.61
30:0:951:A:H2'	30:0:952:G:H5'	1.81	0.61
30:0:564:G:H1'	41:0:7141:HOH:O	1.99	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.29	0.61
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.61
30:0:946:C:H2'	30:0:947:U:C6	2.34	0.61
30:0:2866:U:H4'	30:0:2867:G:H5'	1.81	0.61
31:9:64:C:H2'	31:9:65:A:H5'	1.82	0.61
14:N:147:ILE:HD12	41:9:9086:HOH:O	2.00	0.61
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.33	0.61
30:0:2533:C:H5'	30:0:2533:C:H6	1.65	0.61
30:0:589:U:H2'	30:0:590:A:H8	1.64	0.61
12:L:53:ARG:HD2	30:0:2441:U:H4'	1.82	0.61
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:101:ASP:HB2	30:0:750:A:O3'	2.01	0.61
30:0:1976:G:O2'	30:0:1977:U:H5'	2.01	0.61
12:L:125:PHE:CZ	12:L:140:VAL:HG22	2.35	0.61
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.00	0.61
30:0:1461:U:H2'	30:0:1462:C:H6	1.65	0.61
16:P:121:ASP:OD1	16:P:125:LYS:HE3	1.99	0.61
30:0:494:C:H2'	30:0:496:G:OP2	2.00	0.61
18:R:29:LYS:HB3	41:R:8939:HOH:O	1.99	0.61
30:0:247:A:H2'	41:0:4794:HOH:O	2.00	0.61
30:0:1205:U:C2'	30:0:1206:U:H5''	2.30	0.61
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.35	0.61
13:M:61:ILE:N	13:M:61:ILE:HD12	2.15	0.61
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.64	0.61
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.66	0.61
1:A:19:PRO:HG2	1:A:23:TYR:CE2	2.35	0.61
29:3:65:THR:CG2	29:3:67:LEU:HG	2.31	0.61
18:R:46:TYR:HD2	18:R:47:LEU:HD23	1.65	0.61
13:M:9:ARG:HD2	30:0:380:A:OP2	2.00	0.61
3:C:121:ALA:N	3:C:136:VAL:HG11	2.15	0.61
30:0:185:G:H4'	30:0:186:A:H4'	1.81	0.61
25:Y:148:GLY:O	25:Y:154:ARG:HD3	2.01	0.61
7:G:12:ILE:HG22	7:G:17:GLN:NE2	2.16	0.61
14:N:112:GLY:HA2	14:N:137:ALA:N	2.15	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.31	0.61
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.81	0.61
30:0:2896:A:N3	30:0:2896:A:H2'	2.16	0.61
30:0:2735:U:H2'	30:0:2736:U:C6	2.36	0.61
30:0:1528:A:H2'	30:0:1529:G:O4'	2.00	0.61
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.82	0.61
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.65	0.61
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.30	0.61
30:0:120:A:H2'	30:0:120:A:N3	2.15	0.61
3:C:51:TYR:CE1	27:1:56:GLU:HB2	2.35	0.61
30:0:2795:C:O2'	30:0:2796:U:H5'	2.00	0.61
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.83	0.61
10:J:127:ILE:N	38:J:8801:CL:CL	2.66	0.61
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.29	0.61
15:O:14:LEU:HG	15:O:102:ILE:HD11	1.83	0.61
23:W:48:VAL:HG12	23:W:48:VAL:O	2.00	0.60
21:U:9:CYS:HA	21:U:52:THR:CG2	2.30	0.60
5:E:35:TYR:HA	10:J:127:ILE:HD11	1.83	0.60
11:K:66:ARG:HH12	30:0:1992:U:H3'	1.66	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:42:ALA:HB2	2:B:162:MET:HE1	1.83	0.60
5:E:166:VAL:HG12	41:E:3134:HOH:O	2.00	0.60
14:N:48:VAL:HG13	14:N:55:ASP:HB3	1.83	0.60
30:0:2534:C:H1'	41:0:4385:HOH:O	2.00	0.60
13:M:22:GLU:O	13:M:26:GLN:HG3	2.01	0.60
30:0:536:A:H3'	41:0:5901:HOH:O	2.00	0.60
30:0:664:U:O4	30:0:681:G:H5''	2.00	0.60
2:B:75:GLU:C	2:B:77:PRO:HD3	2.22	0.60
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.65	0.60
7:G:67:LEU:O	7:G:71:LEU:HG	2.01	0.60
11:K:113:ILE:HG22	11:K:114:ALA:N	2.16	0.60
2:B:279:THR:HG22	2:B:280:VAL:H	1.64	0.60
2:B:16:ARG:HD3	41:B:9081:HOH:O	2.01	0.60
30:0:1206:U:H2'	30:0:1207:A:O4'	2.01	0.60
15:O:59:VAL:CG2	15:O:111:VAL:HG21	2.32	0.60
23:W:13:MET:HE2	23:W:17:ILE:HG22	1.83	0.60
19:S:37:VAL:O	19:S:41:VAL:HG23	2.01	0.60
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.15	0.60
1:A:130:THR:HB	1:A:137:VAL:HB	1.84	0.60
21:U:17:THR:CG2	21:U:18:GLY:N	2.64	0.60
1:A:84:VAL:O	1:A:98:GLU:HG3	2.01	0.60
30:0:1931:A:H2'	30:0:1932:G:H5'	1.83	0.60
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	1.84	0.60
30:0:1249:U:H2'	30:0:1250:C:C6	2.36	0.60
23:W:85:ALA:HB2	23:W:91:ASP:O	2.00	0.60
13:M:165:GLY:O	13:M:169:ARG:HB2	2.02	0.60
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.60
31:9:20:G:O2'	31:9:21:G:H5'	2.02	0.60
7:G:20:VAL:O	7:G:24:VAL:HG23	2.02	0.60
3:C:7:ASP:OD2	3:C:9:ASP:HB2	2.01	0.60
30:0:1209:C:H2'	30:0:1210:G:H8	1.66	0.60
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.16	0.60
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.32	0.60
30:0:2296:C:H2'	30:0:2297:U:C6	2.37	0.60
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.83	0.60
30:0:1909:A:N1	30:0:2128:G:H1'	2.17	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.83	0.60
30:0:1416:G:C2'	30:0:1417:G:H5'	2.32	0.60
21:U:11:THR:HG22	21:U:53:ASP:CB	2.31	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.32	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.17	0.60
22:V:29:ASN:O	22:V:33:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:238:ASN:HD22	2:B:240:GLY:H	1.49	0.60
30:0:2472:C:O2'	30:0:2634:G:H4'	2.00	0.60
3:C:211:ASP:HB2	3:C:231:ARG:NH2	2.17	0.60
2:B:175:LEU:C	2:B:175:LEU:HD23	2.22	0.60
22:V:5:VAL:HG12	22:V:9:ARG:NH1	2.17	0.60
30:0:2816:A:H5''	30:0:2817:G:H5'	1.83	0.60
25:Y:208:LYS:NZ	30:0:1343:C:H1'	2.17	0.60
2:B:162:MET:HE3	2:B:310:ARG:HH11	1.67	0.59
21:U:17:THR:HG22	21:U:18:GLY:N	2.16	0.59
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.01	0.59
14:N:152:GLU:C	14:N:154:LEU:H	2.05	0.59
30:0:2748:G:H2'	41:0:9338:HOH:O	2.01	0.59
5:E:132:THR:HB	41:E:2227:HOH:O	2.03	0.59
2:B:26:PHE:HD1	2:B:310:ARG:HH21	1.50	0.59
11:K:41:LYS:HE2	11:K:42:ASN:ND2	2.17	0.59
20:T:8:ARG:NH1	30:0:31:C:OP2	2.35	0.59
9:I:120:ALA:O	9:I:124:VAL:HG23	2.02	0.59
30:0:2626:C:H2'	30:0:2627:G:C8	2.37	0.59
1:A:33:GLU:CD	1:A:33:GLU:N	2.55	0.59
20:T:76:ASP:C	20:T:78:THR:HG23	2.23	0.59
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.67	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.67	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.83	0.59
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.85	0.59
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.84	0.59
12:L:148:GLU:HA	41:L:9037:HOH:O	2.00	0.59
30:0:336:G:H5''	41:0:4601:HOH:O	2.02	0.59
30:0:1883:U:H5''	30:0:2013:G:OP2	2.01	0.59
30:0:969:G:H1	30:0:999:C:H42	1.50	0.59
14:N:77:ASN:C	14:N:80:SER:HB3	2.23	0.59
30:0:530:C:C4'	30:0:612:U:H4'	2.32	0.59
30:0:1172:G:H1'	41:0:5831:HOH:O	2.01	0.59
30:0:1545:C:H2'	30:0:1546:G:O4'	2.02	0.59
30:0:459:A:H4'	41:0:3355:HOH:O	2.03	0.59
1:A:82:VAL:HG22	1:A:93:THR:HB	1.83	0.59
30:0:248:A:H5'	30:0:249:G:OP2	2.03	0.59
24:X:72:VAL:HG22	24:X:85:VAL:HG11	1.84	0.59
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.00	0.59
30:0:2326:C:H4'	30:0:2412:G:C4'	2.33	0.59
9:I:108:HIS:N	9:I:109:PRO:HD2	2.17	0.59
3:C:154:VAL:O	3:C:158:GLU:HG3	2.03	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1416:G:H2'	30:0:1417:G:H5'	1.85	0.59
14:N:149:GLU:HA	14:N:152:GLU:HB2	1.83	0.59
30:0:1555:G:H4'	30:0:1630:A:H2	1.67	0.59
8:H:54:VAL:HG13	8:H:162:PRO:CG	2.32	0.59
5:E:152:THR:HG21	5:E:165:GLY:HA2	1.84	0.59
30:0:834:G:H3'	30:0:835:U:H4'	1.83	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.18	0.59
12:L:27:ARG:NH2	12:L:30:ARG:HG2	2.17	0.59
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.02	0.59
12:L:35:ARG:NH1	12:L:35:ARG:HB2	2.13	0.59
25:Y:117:LEU:HD13	25:Y:174:VAL:CG1	2.33	0.59
12:L:71:GLU:HG2	30:0:700:A:C2	2.38	0.59
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.03	0.59
30:0:625:U:H5''	30:0:1044:C:N4	2.17	0.59
30:0:1634:G:H2'	30:0:1635:U:C6	2.38	0.59
30:0:1735:C:O2'	30:0:1736:A:H5'	2.02	0.59
9:I:121:LYS:HD3	30:0:1185:U:OP1	2.02	0.59
18:R:77:ALA:O	18:R:78:GLY:CA	2.51	0.59
30:0:213:G:N2	30:0:225:G:H2'	2.18	0.59
4:D:38:GLU:OE2	4:D:51:ARG:NE	2.35	0.59
11:K:10:GLN:N	11:K:10:GLN:NE2	2.37	0.58
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.18	0.58
18:R:106:GLY:HA2	18:R:109:MET:CE	2.33	0.58
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.32	0.58
17:Q:25:PRO:HB2	41:9:9077:HOH:O	2.03	0.58
30:0:559:U:H6	30:0:559:U:H5'	1.66	0.58
20:T:43:ASN:C	20:T:45:GLY:H	2.06	0.58
28:2:25:VAL:O	28:2:29:THR:HG23	2.02	0.58
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.03	0.58
8:H:80:LEU:HD21	8:H:145:ASP:HB3	1.85	0.58
14:N:71:TRP:HB2	41:N:8838:HOH:O	2.04	0.58
14:N:86:LEU:HD21	14:N:180:LEU:HD12	1.85	0.58
23:W:122:ARG:NH1	23:W:152:ALA:O	2.35	0.58
25:Y:165:GLU:HB3	41:0:7515:HOH:O	2.03	0.58
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.58
11:K:43:ARG:NH1	30:0:2712:G:OP1	2.35	0.58
1:A:66:ARG:NH1	1:A:66:ARG:HB2	2.16	0.58
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.03	0.58
30:0:958:G:O2'	30:0:959:C:H5'	2.03	0.58
30:0:1187:U:O2'	30:0:1189:A:H2	1.86	0.58
24:X:47:ALA:HB1	24:X:82:GLU:CB	2.32	0.58
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.17	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1829:A:C2'	30:0:1830:C:H5'	2.33	0.58
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.33	0.58
16:P:16:VAL:HG13	16:P:20:ARG:NH1	2.18	0.58
1:A:55:VAL:HG23	1:A:68:ILE:O	2.03	0.58
30:0:2392:C:H4'	41:0:5133:HOH:O	2.03	0.58
14:N:139:TRP:CE3	14:N:139:TRP:HA	2.37	0.58
30:0:65:C:O2'	30:0:66:G:H5'	2.03	0.58
14:N:96:GLY:O	14:N:98:GLU:HG3	2.04	0.58
30:0:1067:A:H5'	41:0:5212:HOH:O	2.04	0.58
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.86	0.58
2:B:177:HIS:O	2:B:181:ILE:HG13	2.03	0.58
9:I:129:SER:O	9:I:130:LEU:HD23	2.03	0.58
22:V:50:ARG:HD3	41:V:2826:HOH:O	2.03	0.58
12:L:140:VAL:HB	41:L:9020:HOH:O	2.03	0.58
30:0:1527:A:H1'	30:0:1528:A:C8	2.38	0.58
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.86	0.58
13:M:159:VAL:HG12	38:M:8818:CL:CL	2.41	0.58
3:C:2:GLN:HB3	41:C:8589:HOH:O	2.02	0.58
30:0:1180:U:H1'	41:0:4130:HOH:O	2.04	0.58
5:E:84:MET:SD	5:E:168:ILE:HD13	2.43	0.58
30:0:459:A:H5"	41:0:2968:HOH:O	2.03	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58
30:0:2667:G:H1'	30:0:2914:A:N3	2.19	0.58
12:L:59:GLU:HA	12:L:104:ASP:OD2	2.04	0.58
2:B:262:ARG:HD2	30:0:2715:G:O2'	2.03	0.58
15:O:31:GLU:O	15:O:35:LYS:HG3	2.04	0.58
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.69	0.58
2:B:3:PRO:HG2	41:0:9686:HOH:O	2.02	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.86	0.58
4:D:52:THR:HG21	30:0:2346:C:O2'	2.03	0.58
4:D:99:ASP:HB3	4:D:103:ASN:H	1.69	0.58
4:D:18:ILE:HG12	4:D:134:LEU:HD23	1.84	0.58
30:0:221:G:H2'	30:0:222:A:C8	2.39	0.58
30:0:264:G:H1'	30:0:265:U:H5	1.69	0.58
14:N:67:ALA:HA	14:N:71:TRP:CB	2.34	0.58
2:B:16:ARG:HB3	2:B:217:ARG:NH2	2.19	0.58
22:V:64:GLY:O	22:V:65:ASP:HB2	2.04	0.58
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.04	0.58
30:0:2670:G:O2'	30:0:2671:U:H5'	2.03	0.58
27:1:45:ARG:HB3	41:1:988:HOH:O	2.02	0.58
30:0:2608:C:H2'	41:0:4456:HOH:O	2.04	0.58
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:150:G:H1'	41:0:4496:HOH:O	2.04	0.58
30:0:157:G:H3'	41:0:4827:HOH:O	2.03	0.58
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.03	0.58
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.19	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.04	0.58
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.86	0.58
30:0:2314:G:C2'	30:0:2315:C:H5'	2.34	0.58
13:M:71:SER:HB2	13:M:92:THR:HG22	1.86	0.58
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.58
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.04	0.58
8:H:165:ARG:HD3	41:H:9040:HOH:O	2.03	0.58
1:A:107:ASN:OD1	1:A:120:ARG:HD2	2.04	0.58
30:0:1615:A:H5'	41:0:5049:HOH:O	2.04	0.58
11:K:77:ARG:C	11:K:78:LYS:CA	2.72	0.58
23:W:130:HIS:O	23:W:136:GLY:HA3	2.04	0.58
30:0:23:G:H1'	30:0:520:A:N6	2.19	0.58
4:D:40:ILE:HG13	4:D:41:LEU:N	2.19	0.58
30:0:31:C:H2'	41:0:9479:HOH:O	2.03	0.58
23:W:90:TYR:CD1	23:W:90:TYR:N	2.71	0.58
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.68	0.57
6:F:83:LEU:HD11	6:F:96:ALA:CB	2.34	0.57
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.19	0.57
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.86	0.57
30:0:2251:G:H2'	30:0:2252:A:C8	2.38	0.57
7:G:23:ILE:HG22	7:G:27:ILE:HD11	1.85	0.57
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.37	0.57
3:C:20:ASP:O	3:C:23:GLU:HB2	2.03	0.57
30:0:2312:G:H2'	30:0:2313:C:H5'	1.85	0.57
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.69	0.57
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.04	0.57
24:X:20:GLU:CD	24:X:21:PRO:HD2	2.24	0.57
28:2:11:LEU:HD22	30:0:1417:G:O2'	2.04	0.57
28:2:20:ARG:HG2	41:2:5444:HOH:O	2.04	0.57
3:C:184:ARG:NH2	30:0:450:C:OP1	2.37	0.57
29:3:15:ASN:O	30:0:2408:A:H4'	2.05	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
30:0:137:U:H2'	30:0:139:C:C5	2.38	0.57
6:F:4:VAL:HG13	6:F:76:PHE:CD1	2.38	0.57
23:W:55:GLY:HA3	23:W:146:ILE:HG13	1.86	0.57
21:U:52:THR:CG2	21:U:54:THR:HB	2.34	0.57
23:W:110:GLN:HA	23:W:110:GLN:NE2	2.20	0.57
30:0:2896:A:H5"	41:0:6932:HOH:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:136:C:H2'	30:0:137:U:O4'	2.04	0.57
30:0:757:C:H2'	30:0:758:A:C8	2.39	0.57
10:J:107:ASN:ND2	10:J:109:TYR:H	2.02	0.57
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.04	0.57
3:C:168:ARG:NH2	3:C:190:ALA:O	2.37	0.57
10:J:52:GLN:HG3	10:J:53:ILE:H	1.67	0.57
30:0:380:A:H2'	41:0:9039:HOH:O	2.03	0.57
2:B:86:ALA:HA	41:B:9050:HOH:O	2.05	0.57
23:W:154:ARG:NH1	30:0:588:G:O6	2.37	0.57
2:B:85:ARG:NH1	41:B:9110:HOH:O	2.37	0.57
23:W:35:VAL:HG22	23:W:36:PRO:O	2.05	0.57
16:P:77:ALA:O	16:P:78:GLY:CA	2.52	0.57
4:D:25:MET:CE	4:D:41:LEU:HG	2.30	0.57
11:K:74:VAL:HG13	11:K:113:ILE:CG2	2.29	0.57
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.70	0.57
12:L:92:ASP:OD1	12:L:94:ARG:HB2	2.04	0.57
33:6:76:8AN:N3	41:6:80:HOH:O	2.32	0.57
30:0:1097:A:H2'	30:0:1098:A:C8	2.39	0.57
30:0:1249:U:H2'	30:0:1250:C:H6	1.68	0.57
26:Z:73:ARG:HG2	26:Z:75:GLY:H	1.69	0.57
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.38	0.57
23:W:108:ARG:HG3	23:W:114:PRO:HG3	1.85	0.57
30:0:619:U:H3'	41:0:4175:HOH:O	2.05	0.57
14:N:23:ARG:NH1	14:N:27:LEU:HD11	2.18	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.85	0.57
1:A:105:VAL:HG12	1:A:106:CYS:N	2.20	0.57
2:B:42:ALA:HB2	2:B:162:MET:CE	2.35	0.57
2:B:77:PRO:C	2:B:78:PRO:HG3	2.25	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
13:M:92:THR:HB	30:0:401:C:O2'	2.05	0.57
30:0:2032:U:H2'	30:0:2033:G:H5''	1.87	0.57
30:0:1946:C:H2'	30:0:1971:G:C8	2.40	0.57
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.87	0.57
23:W:64:THR:O	23:W:68:THR:HG22	2.05	0.57
14:N:176:ARG:HG2	14:N:180:LEU:HD13	1.86	0.57
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.87	0.57
30:0:1165:G:O2'	30:0:1174:A:H4'	2.05	0.57
2:B:87:TYR:OH	2:B:163:GLU:OE2	2.16	0.57
1:A:117:LYS:HA	41:A:9015:HOH:O	2.05	0.57
6:F:13:GLU:OE1	6:F:77:VAL:HG13	2.04	0.57
9:I:69:PRO:HA	30:0:1164:U:OP1	2.05	0.57
30:0:447:A:O2'	30:0:448:G:H5'	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:36:ILE:HG23	29:3:37:ASP:N	2.19	0.57
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.19	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.20	0.57
30:0:2301:A:H5''	30:0:2302:A:H5'	1.86	0.57
30:0:941:G:O2'	30:0:942:U:H5'	2.04	0.57
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.05	0.57
23:W:60:GLU:O	23:W:63:GLU:HB2	2.05	0.57
30:0:1624:A:H4'	30:0:1626:A:H5''	1.86	0.57
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.33	0.56
23:W:122:ARG:HH12	23:W:154:ARG:N	2.03	0.56
15:O:14:LEU:CG	15:O:102:ILE:HD11	2.35	0.56
30:0:1342:C:O2'	30:0:1343:C:H5'	2.05	0.56
30:0:2011:A:H5'	30:0:2013:G:H1'	1.85	0.56
3:C:181:ALA:HA	41:T:2331:HOH:O	2.04	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.56
30:0:1482:A:O2'	30:0:1483:C:H5'	2.04	0.56
30:0:699:C:H2'	30:0:744:G:O4'	2.05	0.56
23:W:115:THR:HG22	23:W:116:LEU:N	2.20	0.56
30:0:710:G:O2'	30:0:711:G:H5'	2.05	0.56
30:0:1118:A:C8	30:0:1119:G:H5''	2.37	0.56
6:F:50:VAL:HG21	6:F:63:ILE:HG21	1.86	0.56
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.58	0.56
27:1:15:THR:HG1	30:0:777:U:H5	1.53	0.56
30:0:1364:G:H1'	41:0:5657:HOH:O	2.05	0.56
7:G:63:ARG:O	7:G:67:LEU:HG	2.04	0.56
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.05	0.56
2:B:162:MET:HB2	2:B:310:ARG:NH1	2.21	0.56
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.41	0.56
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.87	0.56
30:0:255:A:H2'	30:0:256:C:C6	2.41	0.56
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.05	0.56
19:S:57:THR:HG22	19:S:58:MET:N	2.21	0.56
15:O:77:ALA:HA	15:O:96:VAL:O	2.05	0.56
30:0:1419:U:H2'	30:0:1685:A:C2	2.39	0.56
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.88	0.56
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.33	0.56
4:D:167:GLU:OE2	4:D:173:GLU:HB3	2.05	0.56
29:3:77:ALA:C	29:3:78:HIS:CA	2.74	0.56
23:W:5:VAL:HG11	23:W:153:MET:CE	2.35	0.56
30:0:499:G:O2'	30:0:500:G:H5'	2.05	0.56
30:0:1279:U:O2	30:0:1279:U:H2'	2.06	0.56
16:P:91:LYS:O	16:P:95:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:83:LYS:HG2	30:0:793:A:H5''	1.88	0.56
13:M:82:ARG:O	13:M:84:LYS:N	2.38	0.56
20:T:26:THR:HG23	20:T:97:ARG:HG3	1.87	0.56
30:0:1730:G:C5'	30:0:1731:C:C6	2.89	0.56
14:N:23:ARG:NH2	31:9:7:G:H4'	2.21	0.56
8:H:23:ILE:HG22	8:H:123:ILE:HD11	1.88	0.56
30:0:334:G:H2'	30:0:335:U:O4'	2.05	0.56
16:P:82:GLY:O	30:0:1761:U:H4'	2.04	0.56
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.88	0.56
12:L:55:GLN:CA	12:L:58:GLN:HE21	2.17	0.56
23:W:13:MET:HE1	23:W:18:GLN:HA	1.88	0.56
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.88	0.56
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.05	0.56
30:0:69:A:H5'	30:0:69:A:C8	2.40	0.56
30:0:706:G:N2	30:0:707:C:H41	2.04	0.56
30:0:1346:U:H2'	30:0:1347:U:C6	2.41	0.56
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.05	0.56
18:R:40:ALA:O	18:R:43:ALA:HB3	2.05	0.56
3:C:127:ARG:HD2	3:C:229:PRO:O	2.05	0.56
13:M:60:VAL:HG22	13:M:134:ILE:HD12	1.87	0.56
30:0:119:A:H2'	30:0:120:A:C5'	2.36	0.56
18:R:99:ALA:HB1	18:R:109:MET:HE3	1.87	0.56
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.86	0.56
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.88	0.56
2:B:206:THR:CG2	30:0:2716:G:H5''	2.30	0.56
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.36	0.56
25:Y:208:LYS:HZ3	30:0:1343:C:H1'	1.71	0.56
30:0:137:U:OP1	30:0:259:G:O2'	2.24	0.56
13:M:58:GLN:NE2	30:0:259:G:H21	2.03	0.56
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.41	0.56
3:C:149:LYS:NZ	30:0:327:A:OP1	2.38	0.56
31:9:54:A:O2'	31:9:55:U:H5'	2.06	0.56
30:0:622:G:O2'	30:0:623:U:H5'	2.05	0.56
2:B:144:THR:HB	41:B:9099:HOH:O	2.03	0.56
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.86	0.56
2:B:62:ARG:HA	2:B:65:MET:HE2	1.87	0.56
12:L:108:VAL:HB	12:L:125:PHE:CD2	2.41	0.56
12:L:91:VAL:CG1	12:L:120:LEU:HD23	2.36	0.56
30:0:2353:A:H4'	30:0:2354:A:O5'	2.05	0.56
10:J:93:ARG:O	10:J:96:GLU:HB2	2.06	0.56
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:25:GLN:NE2	10:J:116:LEU:HB3	2.20	0.56
1:A:204:GLY:N	30:0:2634:G:OP2	2.38	0.56
30:0:637:C:H2'	30:0:638:C:C6	2.41	0.56
20:T:81:LYS:HG3	20:T:87:VAL:HG13	1.88	0.56
1:A:32:VAL:HG12	1:A:34:ASP:H	1.70	0.55
25:Y:187:VAL:CG1	25:Y:205:ILE:HA	2.36	0.55
30:0:612:U:H2'	30:0:613:C:C6	2.41	0.55
17:Q:16:ASN:HB2	41:0:7765:HOH:O	2.06	0.55
10:J:19:MET:CE	10:J:132:LEU:HD11	2.36	0.55
18:R:77:ALA:C	18:R:78:GLY:CA	2.75	0.55
12:L:120:LEU:HD12	12:L:133:VAL:HG21	1.87	0.55
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.21	0.55
8:H:34:HIS:HD2	8:H:90:LEU:O	1.88	0.55
30:0:2439:C:H5'	41:0:6330:HOH:O	2.06	0.55
19:S:11:THR:O	19:S:14:ALA:HB3	2.06	0.55
30:0:2507:G:H2'	30:0:2510:C:H42	1.71	0.55
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.73	0.55
13:M:12:TRP:O	13:M:15:PRO:HD3	2.06	0.55
12:L:13:HIS:HB3	41:L:9060:HOH:O	2.05	0.55
16:P:36:THR:O	16:P:40:VAL:HG23	2.05	0.55
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.07	0.55
7:G:63:ARG:N	41:G:2569:HOH:O	2.39	0.55
24:X:74:ALA:CA	24:X:85:VAL:HG13	2.37	0.55
29:3:70:ARG:HB3	41:3:9062:HOH:O	2.06	0.55
1:A:211:LYS:O	30:0:1943:C:H4'	2.06	0.55
11:K:87:ARG:NH2	30:0:2720:C:O2	2.39	0.55
5:E:36:PRO:HD3	10:J:127:ILE:HG13	1.89	0.55
29:3:22:VAL:HG11	29:3:67:LEU:HD13	1.88	0.55
4:D:60:GLU:O	4:D:60:GLU:HG3	2.07	0.55
5:E:7:ILE:HD11	5:E:11:VAL:O	2.07	0.55
8:H:30:LYS:N	8:H:62:HIS:HD2	1.96	0.55
10:J:12:VAL:HG21	10:J:116:LEU:HD11	1.88	0.55
23:W:91:ASP:HB2	41:W:5425:HOH:O	2.06	0.55
21:U:20:MET:HE2	21:U:28:THR:HG21	1.88	0.55
1:A:43:VAL:HG21	1:A:59:GLU:HG3	1.87	0.55
30:0:553:G:H5'	41:0:4389:HOH:O	2.06	0.55
2:B:254:GLN:HG2	2:B:255:GLY:N	2.21	0.55
8:H:69:ARG:HD3	41:H:9037:HOH:O	2.05	0.55
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.55
25:Y:174:VAL:HG13	25:Y:177:LYS:HD2	1.88	0.55
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.36	0.55
4:D:60:GLU:O	4:D:61:PHE:C	2.45	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:274:GLU:HA	2:B:292:GLY:O	2.06	0.55
14:N:74:PRO:HG2	14:N:159:TYR:CE1	2.42	0.55
3:C:207:LEU:HB2	3:C:210:ALA:HB2	1.87	0.55
13:M:178:LYS:HB2	41:O:7686:HOH:O	2.06	0.55
6:F:65:GLU:HB3	41:F:5163:HOH:O	2.06	0.55
30:O:624:U:H3'	41:O:5060:HOH:O	2.07	0.55
4:D:25:MET:SD	4:D:40:ILE:HD11	2.47	0.55
13:M:12:TRP:CD2	13:M:45:ARG:HD2	2.41	0.55
30:O:292:G:H1'	30:O:360:A:H61	1.72	0.55
8:H:96:GLN:NE2	8:H:129:ARG:NH2	2.55	0.55
27:I:1:THR:O	30:O:1836:A:H1'	2.07	0.55
18:R:113:HIS:HB3	18:R:146:ILE:HD12	1.89	0.55
23:W:4:LEU:HD22	23:W:52:VAL:HB	1.88	0.55
30:O:2828:G:H8	30:O:2828:G:O5'	1.90	0.55
2:B:98:THR:HG21	2:B:127:GLN:OE1	2.06	0.55
16:P:11:ALA:HB1	16:P:16:VAL:O	2.06	0.55
4:D:24:HIS:HB2	4:D:72:LYS:HA	1.88	0.55
6:F:19:ALA:O	6:F:22:VAL:HG22	2.07	0.55
30:O:2562:G:H4'	41:O:5081:HOH:O	2.07	0.55
31:9:76:G:H3'	31:9:77:A:C5'	2.20	0.55
41:C:8562:HOH:O	15:O:3:THR:HG21	2.06	0.55
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.55
29:3:11:CYS:HB2	29:3:20:HIS:NE2	2.21	0.55
3:C:246:ARG:HD2	41:C:8576:HOH:O	2.07	0.55
24:X:23:HIS:NE2	24:X:24:LYS:HD2	2.21	0.55
30:O:2032:U:H2'	30:O:2033:G:C5'	2.37	0.55
30:O:2115:U:H2'	30:O:2116:U:C6	2.41	0.55
13:M:146:ASP:O	13:M:147:LEU:HD23	2.06	0.55
16:P:74:GLN:HG2	30:O:1786:C:OP1	2.06	0.55
14:N:21:HIS:HB2	41:N:8831:HOH:O	2.07	0.55
5:E:77:THR:O	5:E:78:GLU:CA	2.55	0.55
1:A:2:ARG:HD3	1:A:198:ASP:OD1	2.06	0.55
30:O:1260:G:H3'	30:O:1261:A:N7	2.21	0.55
1:A:66:ARG:CB	1:A:66:ARG:NH1	2.69	0.55
30:O:2401:A:H2'	30:O:2402:A:C8	2.42	0.55
22:V:20:LEU:HD22	22:V:60:GLN:HE22	1.71	0.55
2:B:36:PRO:HA	2:B:168:GLY:CA	2.25	0.55
1:A:32:VAL:HG12	1:A:34:ASP:N	2.22	0.55
1:A:189:VAL:HA	30:O:1845:A:OP1	2.07	0.55
1:A:82:VAL:HA	1:A:93:THR:O	2.07	0.55
1:A:69:LEU:HD21	1:A:120:ARG:HB3	1.88	0.55
6:F:4:VAL:HG13	6:F:76:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:23:ILE:CG2	8:H:123:ILE:HD11	2.37	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.42	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.55
4:D:172:VAL:HG12	4:D:173:GLU:N	2.13	0.55
3:C:227:GLY:O	3:C:229:PRO:HD3	2.07	0.55
25:Y:149:GLN:HE22	30:0:1293:U:H4'	1.72	0.55
30:0:1529:G:H5'	41:0:9193:HOH:O	2.05	0.55
18:R:120:GLY:HA3	41:R:8961:HOH:O	2.07	0.55
30:0:841:A:H5''	41:0:7724:HOH:O	2.07	0.55
30:0:307:G:H3'	30:0:342:C:OP2	2.07	0.55
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.88	0.55
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.55
14:N:37:ARG:NE	41:N:8833:HOH:O	2.39	0.54
2:B:75:GLU:OE2	2:B:151:VAL:HG13	2.07	0.54
18:R:82:GLU:O	18:R:86:LYS:HG3	2.07	0.54
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.87	0.54
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.36	0.54
10:J:80:LYS:HE2	10:J:98:PHE:CZ	2.43	0.54
23:W:4:LEU:HD22	23:W:52:VAL:HG11	1.89	0.54
30:0:945:U:H2'	30:0:946:C:C6	2.42	0.54
13:M:84:LYS:HE2	41:0:5258:HOH:O	2.08	0.54
30:0:905:C:H3'	41:0:6033:HOH:O	2.06	0.54
30:0:107:U:H2'	30:0:108:U:H5'	1.89	0.54
30:0:2502:C:C2'	30:0:2503:A:H5'	2.37	0.54
30:0:1681:G:H5''	30:0:1682:A:H5'	1.88	0.54
12:L:14:GLY:O	30:0:1295:G:H5''	2.06	0.54
1:A:95:PRO:HA	1:A:153:ARG:HA	1.90	0.54
30:0:1730:G:C5'	30:0:1731:C:H6	2.20	0.54
30:0:2072:G:C6	30:0:2533:C:H1'	2.43	0.54
22:V:39:ALA:N	22:V:40:PRO:CD	2.70	0.54
3:C:165:ASP:O	3:C:168:ARG:HB3	2.06	0.54
30:0:1198:U:H2'	30:0:1200:A:OP2	2.07	0.54
15:O:63:LYS:HG3	15:O:80:ASP:O	2.07	0.54
2:B:80:ARG:HB2	2:B:145:HIS:CE1	2.42	0.54
30:0:2783:A:H3'	41:0:6077:HOH:O	2.08	0.54
5:E:81:GLU:O	5:E:172:PRO:HD3	2.07	0.54
13:M:60:VAL:C	13:M:61:ILE:HD12	2.27	0.54
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.23	0.54
20:T:48:VAL:HG21	20:T:96:VAL:CG1	2.37	0.54
9:I:70:THR:HG21	41:I:5331:HOH:O	2.08	0.54
22:V:5:VAL:HG23	41:V:2271:HOH:O	2.07	0.54
30:0:2326:C:H4'	30:0:2412:G:H4'	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.72	0.54
30:0:1632:A:H2'	30:0:1633:C:H5'	1.90	0.54
30:0:2697:A:H2'	30:0:2698:G:O4'	2.08	0.54
30:0:666:A:H2'	30:0:667:C:O4'	2.08	0.54
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.38	0.54
3:C:206:ASN:HB2	30:0:329:A:OP2	2.07	0.54
19:S:15:MET:O	19:S:18:MET:HB3	2.07	0.54
3:C:80:VAL:HA	41:C:8554:HOH:O	2.08	0.54
30:0:1447:U:H3'	30:0:1506:U:O2	2.07	0.54
24:X:71:ARG:HD3	41:X:7542:HOH:O	2.07	0.54
3:C:235:PHE:CE2	3:C:243:VAL:HG21	2.41	0.54
31:9:30:C:H42	31:9:50:G:H1	1.55	0.54
28:2:48:ASP:O	28:2:49:GLU:HB2	2.08	0.54
30:0:589:U:H2'	30:0:590:A:C8	2.41	0.54
30:0:1647:G:O2'	30:0:1648:G:H5'	2.08	0.54
4:D:36:ASN:HA	41:D:7500:HOH:O	2.07	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
30:0:1839:A:H5'	30:0:2643:G:H4'	1.89	0.54
30:0:631:A:C6	30:0:2074:A:H5'	2.43	0.54
15:O:99:GLU:HG3	41:O:6044:HOH:O	2.07	0.54
2:B:2:GLN:NE2	30:0:2545:U:OP2	2.41	0.54
30:0:1189:A:H1'	30:0:1209:C:H1'	1.90	0.54
8:H:59:GLN:HE21	8:H:129:ARG:HG2	1.73	0.54
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.88	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.22	0.54
3:C:58:ALA:HA	3:C:73:GLN:NE2	2.22	0.54
2:B:98:THR:HG22	30:0:2820:A:OP1	2.07	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
3:C:77:ALA:C	3:C:78:ARG:CA	2.76	0.54
30:0:2042:U:H2'	30:0:2043:U:C6	2.42	0.54
30:0:1298:U:H2'	30:0:1299:G:C8	2.42	0.54
30:0:304:G:H1'	30:0:347:A:H61	1.73	0.54
26:Z:54:GLU:HG2	26:Z:57:MET:HE2	1.90	0.54
18:R:98:ASN:HD22	18:R:98:ASN:N	2.06	0.54
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.88	0.54
30:0:2281:C:C2'	30:0:2282:U:H5'	2.37	0.54
25:Y:136:LYS:HB3	25:Y:139:VAL:HG23	1.90	0.54
14:N:37:ARG:HH12	31:9:6:C:C5'	2.00	0.54
18:R:39:THR:HB	18:R:42:GLU:CD	2.27	0.54
30:0:1666:C:H2'	30:0:1667:A:C5'	2.37	0.54
30:0:2502:C:N3	30:0:2518:C:N4	2.55	0.54
23:W:27:HIS:CD2	30:0:1288:U:H4'	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:407:A:H2'	30:0:408:A:C8	2.43	0.54
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
20:T:28:SER:CA	20:T:97:ARG:HD3	2.35	0.54
18:R:132:ARG:HH21	30:0:2055:A:H4'	1.69	0.54
30:0:187:A:H3'	30:0:188:C:H6	1.73	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.07	0.54
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.87	0.54
9:I:127:CYS:C	9:I:129:SER:N	2.62	0.54
30:0:1834:C:H2'	30:0:1840:A:H62	1.72	0.54
10:J:77:GLY:C	10:J:78:ILE:CA	2.77	0.54
29:3:84:ARG:HB3	41:3:9041:HOH:O	2.08	0.54
27:1:46:ARG:HA	41:0:3919:HOH:O	2.07	0.54
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.07	0.54
31:9:78:G:N3	31:9:78:G:H1'	2.22	0.54
30:0:877:G:H1'	41:0:3080:HOH:O	2.07	0.53
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.09	0.53
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.08	0.53
30:0:2332:A:H3'	30:0:2333:G:H8	1.73	0.53
30:0:2526:C:O2'	30:0:2527:U:H5'	2.09	0.53
9:I:88:GLN:HA	9:I:91:PHE:HE2	1.73	0.53
30:0:2824:C:O3'	30:0:2825:C:H6	1.91	0.53
19:S:34:LYS:HG2	19:S:54:THR:HG23	1.89	0.53
8:H:66:GLU:HA	41:H:9037:HOH:O	2.07	0.53
2:B:244:PRO:HB3	30:0:1234:U:N3	2.23	0.53
13:M:84:LYS:HB2	30:0:170:U:OP1	2.08	0.53
25:Y:138:ARG:NH1	30:0:638:C:OP2	2.38	0.53
30:0:812:A:H2'	30:0:813:C:C6	2.43	0.53
30:0:1940:C:H4'	41:0:9153:HOH:O	2.07	0.53
8:H:174:LEU:HD11	30:0:1220:U:H4'	1.90	0.53
1:A:173:GLY:O	1:A:176:HIS:HB3	2.07	0.53
23:W:137:GLN:HG3	23:W:137:GLN:O	2.08	0.53
18:R:9:ASP:O	18:R:13:THR:HG22	2.08	0.53
2:B:53:LEU:HD21	2:B:270:ILE:HG23	1.91	0.53
30:0:138:U:H5''	30:0:139:C:OP2	2.08	0.53
23:W:65:VAL:HA	23:W:68:THR:HG22	1.90	0.53
30:0:705:C:H3'	30:0:706:G:H8	1.73	0.53
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.72	0.53
5:E:81:GLU:HG2	5:E:134:SER:CB	2.33	0.53
23:W:115:THR:HB	41:W:6871:HOH:O	2.09	0.53
30:0:690:G:H4'	30:0:741:C:O2	2.09	0.53
30:0:1947:G:H2'	30:0:1948:G:H8	1.71	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:139:VAL:HG12	41:C:8645:HOH:O	2.08	0.53
2:B:14:GLY:HA2	2:B:15:PRO:C	2.28	0.53
30:0:1118:A:C3'	30:0:1118:A:C8	2.91	0.53
30:0:1160:G:H5'	30:0:1161:A:C4'	2.38	0.53
1:A:212:PRO:HA	30:0:1943:C:O4'	2.08	0.53
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.89	0.53
6:F:20:LEU:HB2	6:F:49:PHE:CZ	2.43	0.53
23:W:39:ASP:HB2	41:W:3580:HOH:O	2.09	0.53
30:0:2802:C:H2'	30:0:2803:C:C6	2.44	0.53
30:0:708:A:H2'	30:0:709:G:O4'	2.08	0.53
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
30:0:2761:A:H2'	41:0:6484:HOH:O	2.08	0.53
16:P:89:ASN:HB3	16:P:92:GLU:HB2	1.91	0.53
3:C:1:MET:HG2	3:C:2:GLN:HE21	1.74	0.53
23:W:55:GLY:CA	23:W:146:ILE:HG13	2.38	0.53
14:N:80:SER:HB2	41:N:8835:HOH:O	2.07	0.53
3:C:233:THR:CG2	3:C:234:VAL:H	2.16	0.53
6:F:58:GLU:OE2	13:M:27:ARG:NH2	2.40	0.53
30:0:2420:G:H4'	41:0:4965:HOH:O	2.09	0.53
1:A:194:MET:SD	30:0:875:A:C2	3.02	0.53
30:0:78:G:N1	30:0:78:G:N2	2.56	0.53
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.56	0.53
30:0:2748:G:H4'	30:0:2749:U:C5'	2.39	0.53
30:0:2239:C:H2'	30:0:2240:U:H6	1.74	0.53
26:Z:54:GLU:HB2	41:Z:8712:HOH:O	2.09	0.53
13:M:91:ILE:HD13	41:0:4059:HOH:O	2.08	0.53
30:0:354:A:H2'	30:0:355:C:C6	2.43	0.53
2:B:36:PRO:HB3	2:B:174:ARG:HB3	1.90	0.53
19:S:10:VAL:HG11	22:V:36:ALA:CB	2.36	0.53
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.91	0.53
1:A:38:ILE:O	1:A:38:ILE:HG22	2.08	0.53
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.24	0.53
1:A:179:MET:HG2	1:A:186:TRP:CB	2.38	0.53
15:O:59:VAL:HG23	15:O:111:VAL:HG21	1.91	0.53
30:0:855:U:H4'	30:0:856:G:O4'	2.08	0.53
23:W:151:GLU:O	23:W:154:ARG:HB2	2.08	0.53
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.39	0.53
30:0:2698:G:H2'	30:0:2699:A:C8	2.44	0.53
11:K:76:GLN:HA	11:K:93:ASN:HA	1.90	0.53
20:T:105:ASP:OD2	20:T:107:LYS:HB2	2.08	0.53
19:S:23:LYS:HE2	41:0:5526:HOH:O	2.09	0.53
8:H:168:VAL:HG13	41:H:9015:HOH:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:37:ARG:NH1	31:9:6:C:OP1	2.42	0.53
1:A:211:LYS:NZ	1:A:223:ARG:HH21	2.07	0.53
1:A:190:ARG:HD2	30:0:1884:G:O6	2.09	0.53
1:A:207:GLN:O	1:A:208:HIS:HB3	2.07	0.53
30:0:78:G:N3	30:0:78:G:N9	2.57	0.53
30:0:820:G:O2'	30:0:856:G:H4'	2.09	0.53
13:M:107:ARG:NH1	13:M:107:ARG:HG3	2.23	0.53
23:W:39:ASP:OD1	23:W:42:ARG:NH2	2.42	0.53
2:B:8:LYS:HB3	2:B:218:TRP:O	2.08	0.53
25:Y:152:LYS:CB	25:Y:160:LYS:HG3	2.38	0.53
2:B:56:ASP:HB3	2:B:322:ARG:HH21	1.74	0.53
30:0:839:C:H1'	41:0:6899:HOH:O	2.07	0.53
41:N:8841:HOH:O	17:Q:19:ARG:HD2	2.09	0.53
23:W:21:LEU:HD13	23:W:26:ILE:HD11	1.91	0.53
3:C:142:ASP:OD1	3:C:236:THR:HG23	2.08	0.53
15:O:3:THR:CB	30:0:656:G:H5'	2.34	0.53
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.91	0.53
10:J:131:THR:HG22	10:J:133:GLY:N	2.24	0.53
30:0:1165:G:H4'	30:0:1174:A:O2'	2.08	0.53
30:0:858:U:H2'	30:0:859:C:C6	2.43	0.53
2:B:171:VAL:HG23	2:B:172:SER:N	2.24	0.53
41:P:6012:HOH:O	30:0:1548:U:H4'	2.07	0.53
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.90	0.53
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.23	0.53
30:0:482:G:H4'	30:0:508:A:N1	2.23	0.53
23:W:117:ARG:HB3	23:W:117:ARG:HH11	1.74	0.53
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.09	0.53
4:D:172:VAL:CG1	4:D:173:GLU:H	2.15	0.53
16:P:103:THR:HA	16:P:106:ARG:HH12	1.68	0.53
30:0:1181:A:H2'	30:0:1182:C:H5'	1.91	0.53
1:A:34:ASP:C	1:A:36:ASP:H	2.12	0.53
1:A:199:HIS:CD2	1:A:201:PHE:HB2	2.44	0.53
2:B:5:ARG:HD2	2:B:8:LYS:HE2	1.91	0.53
12:L:54:PRO:HG2	12:L:57:VAL:HG21	1.89	0.53
19:S:33:SER:OG	19:S:36:GLU:HG3	2.09	0.53
30:0:2562:G:H1'	41:0:6532:HOH:O	2.09	0.53
13:M:67:VAL:HG11	13:M:97:ILE:HG23	1.91	0.53
18:R:15:LYS:HE3	41:R:8986:HOH:O	2.09	0.53
30:0:2274:A:O2'	30:0:2275:G:H5'	2.09	0.53
1:A:37:VAL:HG23	41:A:9074:HOH:O	2.09	0.53
30:0:1160:G:HO2'	30:0:1190:G:H8	1.57	0.52
5:E:84:MET:CG	5:E:168:ILE:HD13	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:558:C:O2'	30:0:559:U:H5''	2.09	0.52
8:H:14:LYS:HB3	41:H:9007:HOH:O	2.09	0.52
30:0:1218:U:H2'	30:0:1219:U:H6	1.73	0.52
30:0:2414:A:H2'	30:0:2415:A:C8	2.43	0.52
14:N:27:LEU:HD22	14:N:50:LEU:HD22	1.91	0.52
29:3:80:ARG:O	30:0:2457:U:H4'	2.10	0.52
30:0:2880:A:H2'	30:0:2881:C:H5'	1.91	0.52
30:0:1445:G:N2	30:0:1678:A:H1'	2.23	0.52
2:B:122:ASP:O	2:B:126:GLU:HB2	2.09	0.52
16:P:55:LYS:HG2	16:P:56:GLY:N	2.23	0.52
6:F:99:THR:HG23	6:F:99:THR:O	2.09	0.52
24:X:45:GLU:HG3	41:X:6178:HOH:O	2.09	0.52
25:Y:193:LEU:CD1	25:Y:221:ALA:HB2	2.39	0.52
30:0:2786:G:H2'	41:0:7991:HOH:O	2.10	0.52
13:M:115:LEU:HD13	13:M:116:ASN:HB2	1.91	0.52
20:T:30:ASP:O	20:T:33:GLU:HB3	2.10	0.52
3:C:236:THR:HA	41:C:8648:HOH:O	2.07	0.52
9:I:98:ASP:OD1	9:I:101:LYS:HD2	2.09	0.52
8:H:33:GLN:H	8:H:69:ARG:NH1	2.07	0.52
30:0:948:G:O2'	30:0:949:U:H5'	2.08	0.52
25:Y:208:LYS:HZ1	30:0:1343:C:C2'	2.22	0.52
30:0:2584:G:H8	41:0:5461:HOH:O	1.91	0.52
5:E:106:ASN:ND2	5:E:109:GLY:HA2	2.25	0.52
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.08	0.52
1:A:186:TRP:CG	1:A:187:PRO:HA	2.44	0.52
10:J:130:VAL:HG12	10:J:131:THR:H	1.72	0.52
2:B:171:VAL:HG23	2:B:172:SER:H	1.74	0.52
30:0:1902:G:H2'	30:0:1903:U:O4'	2.10	0.52
30:0:1496:A:H2'	30:0:1497:G:O4'	2.09	0.52
30:0:2613:G:O2'	30:0:2614:C:H5'	2.09	0.52
3:C:18:LEU:HD12	3:C:19:PRO:HD2	1.91	0.52
13:M:77:HIS:C	13:M:78:LYS:CA	2.78	0.52
11:K:96:VAL:HG21	11:K:109:LEU:HD22	1.92	0.52
30:0:2505:G:C2'	30:0:2506:A:H5'	2.39	0.52
5:E:14:GLU:O	5:E:15:GLN:HB2	2.09	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.92	0.52
18:R:114:VAL:HB	18:R:145:LEU:CD1	2.36	0.52
4:D:136:ARG:NH1	4:D:156:ARG:O	2.41	0.52
30:0:2634:G:O2'	30:0:2635:A:H5'	2.09	0.52
4:D:99:ASP:HB3	4:D:103:ASN:HB2	1.90	0.52
19:S:57:THR:HG22	19:S:59:ASP:H	1.73	0.52
10:J:14:ALA:O	10:J:17:CYS:HB2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:195:C:H2'	30:0:196:G:H5'	1.92	0.52
30:0:583:C:H2'	30:0:584:U:H6	1.75	0.52
30:0:2432:C:O2'	30:0:2433:A:H5'	2.10	0.52
3:C:123:LEU:O	3:C:126:ASP:N	2.42	0.52
4:D:21:VAL:HG23	4:D:80:ALA:HB1	1.91	0.52
1:A:96:LEU:CD2	1:A:128:LEU:HD22	2.39	0.52
25:Y:107:PRO:HD3	25:Y:182:PHE:CD1	2.44	0.52
13:M:139:PRO:HA	13:M:142:GLN:HB2	1.92	0.52
14:N:82:TYR:OH	14:N:176:ARG:NH1	2.43	0.52
30:0:2768:A:O2'	30:0:2769:C:H5'	2.10	0.52
4:D:99:ASP:OD2	4:D:101:THR:HB	2.08	0.52
2:B:145:HIS:HD2	2:B:146:THR:O	1.92	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.52
30:0:462:A:N6	30:0:477:A:C2	2.77	0.52
30:0:578:C:H2'	30:0:579:G:O4'	2.10	0.52
20:T:66:ASP:OD1	20:T:69:LYS:N	2.34	0.52
2:B:336:GLN:O	30:0:2862:G:H4'	2.10	0.52
30:0:1244:U:H4'	30:0:1246:A:O4'	2.10	0.52
24:X:74:ALA:HA	24:X:85:VAL:HG13	1.92	0.52
4:D:49:PRO:HA	4:D:73:VAL:HG22	1.90	0.52
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.10	0.52
30:0:1183:C:H5	30:0:1192:A:OP1	1.91	0.52
1:A:217:ARG:NH1	1:A:217:ARG:CG	2.70	0.52
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.90	0.52
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.45	0.52
30:0:25:A:O2'	30:0:640:G:H5'	2.10	0.52
30:0:830:G:H5''	41:0:9420:HOH:O	2.09	0.52
8:H:91:ARG:O	30:0:1003:U:H4'	2.10	0.52
30:0:1314:U:H2'	41:0:6711:HOH:O	2.08	0.52
30:0:1783:A:O2'	30:0:1784:U:H5'	2.08	0.52
10:J:46:ILE:HA	41:0:3802:HOH:O	2.09	0.52
30:0:2649:A:H2'	41:0:6965:HOH:O	2.08	0.52
2:B:36:PRO:HB3	2:B:174:ARG:CB	2.40	0.52
30:0:35:U:O2'	30:0:36:C:H5'	2.09	0.52
30:0:336:G:H2'	41:0:4601:HOH:O	2.08	0.52
13:M:158:ARG:HA	13:M:163:LEU:HD12	1.90	0.52
19:S:57:THR:CG2	19:S:58:MET:N	2.73	0.52
1:A:176:HIS:CD2	30:0:857:A:H4'	2.45	0.52
20:T:66:ASP:OD1	20:T:68:ASP:N	2.42	0.52
30:0:1809:G:N2	30:0:1811:A:H3'	2.24	0.52
14:N:163:PHE:HZ	14:N:171:HIS:HD1	1.56	0.52
30:0:1117:A:H2'	41:0:5754:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:123:VAL:C	9:I:125:GLY:H	2.13	0.52
1:A:14:SER:HB2	41:A:9016:HOH:O	2.09	0.52
3:C:93:LYS:O	3:C:98:ARG:NH2	2.42	0.52
3:C:124:VAL:HG12	3:C:131:PHE:HE2	1.74	0.52
24:X:66:THR:CG2	24:X:67:PRO:HD2	2.40	0.52
30:0:37:A:H2'	30:0:38:G:C8	2.45	0.52
15:O:32:ARG:HB2	41:O:4656:HOH:O	2.10	0.52
30:0:625:U:H5'	41:0:4081:HOH:O	2.10	0.52
23:W:38:THR:CG2	23:W:39:ASP:N	2.73	0.52
30:0:204:A:C2'	30:0:205:U:H5'	2.39	0.52
30:0:1406:A:H4'	30:0:1407:A:C5'	2.39	0.52
14:N:33:ARG:HH21	14:N:48:VAL:HG11	1.74	0.52
14:N:23:ARG:NH1	41:N:8868:HOH:O	2.42	0.52
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.91	0.52
14:N:115:VAL:HG13	41:9:9103:HOH:O	2.10	0.52
2:B:258:GLY:H	2:B:260:HIS:CE1	2.28	0.52
23:W:120:PRO:HG2	30:0:1095:U:O2	2.10	0.52
15:O:44:ASN:HB2	38:O:8808:CL:CL	2.47	0.52
30:0:627:G:H1'	41:0:5293:HOH:O	2.08	0.52
41:K:4183:HOH:O	30:0:2712:G:H5'	2.10	0.52
30:0:2765:C:H2'	30:0:2766:A:C8	2.45	0.52
30:0:78:G:N3	30:0:78:G:N1	2.58	0.52
17:Q:15:LYS:NZ	41:Q:5620:HOH:O	2.43	0.52
30:0:951:A:O2'	30:0:952:G:H5'	2.10	0.52
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.91	0.52
9:I:108:HIS:N	9:I:109:PRO:CD	2.72	0.52
30:0:2314:G:H2'	30:0:2315:C:H5'	1.92	0.52
30:0:2253:G:O2'	30:0:2254:G:H5'	2.09	0.52
3:C:175:LYS:NZ	3:C:184:ARG:HB3	2.25	0.52
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.39	0.52
31:9:78:G:N1	31:9:78:G:N3	2.58	0.52
3:C:124:VAL:HG12	3:C:131:PHE:CE2	2.45	0.52
12:L:11:ARG:NH1	30:0:903:U:OP2	2.41	0.52
30:0:1574:C:H6	30:0:1574:C:O5'	1.92	0.52
30:0:396:U:O2'	30:0:418:C:H4'	2.09	0.52
30:0:1748:U:H4'	41:0:9318:HOH:O	2.10	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.09	0.52
18:R:96:VAL:O	18:R:99:ALA:HB3	2.09	0.52
27:1:28:HIS:ND1	27:1:31:LYS:HE2	2.25	0.52
30:0:2426:G:H1'	41:0:6925:HOH:O	2.09	0.52
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.10	0.52
3:C:33:LYS:HE2	41:C:8564:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:49:LEU:HG	41:U:3805:HOH:O	2.10	0.52
7:G:22:ALA:O	7:G:25:GLU:HB3	2.10	0.52
2:B:28:SER:HB3	30:0:2807:U:OP1	2.11	0.51
20:T:43:ASN:O	20:T:45:GLY:N	2.41	0.51
25:Y:150:LEU:HB2	41:0:6295:HOH:O	2.09	0.51
22:V:27:LEU:HA	22:V:49:LEU:HD13	1.92	0.51
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.26	0.51
14:N:157:PRO:HA	41:N:8823:HOH:O	2.09	0.51
2:B:41:PHE:CE1	2:B:79:MET:HG3	2.44	0.51
7:G:64:ASN:N	7:G:64:ASN:HD22	2.07	0.51
1:A:132:ASP:HB3	1:A:135:VAL:H	1.75	0.51
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.11	0.51
24:X:87:ALA:O	24:X:88:GLU:HB3	2.10	0.51
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.81	0.51
30:0:432:G:H2'	30:0:433:C:H6	1.75	0.51
7:G:27:ILE:HD12	7:G:70:ALA:HB1	1.92	0.51
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.92	0.51
15:O:32:ARG:NE	15:O:35:LYS:HD3	2.18	0.51
6:F:58:GLU:HA	6:F:61:MET:HE1	1.91	0.51
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.93	0.51
30:0:2247:C:H2'	30:0:2248:C:C6	2.43	0.51
10:J:90:LYS:HE2	30:0:2083:A:N6	2.26	0.51
1:A:16:PHE:HB3	41:A:9032:HOH:O	2.09	0.51
2:B:145:HIS:CD2	2:B:159:PRO:HB3	2.45	0.51
12:L:79:ASP:HB3	41:L:9021:HOH:O	2.10	0.51
30:0:105:G:O2'	30:0:106:A:H5'	2.10	0.51
1:A:77:GLY:C	1:A:78:ASP:CA	2.79	0.51
4:D:23:VAL:CG2	4:D:73:VAL:HB	2.40	0.51
13:M:133:LEU:O	13:M:134:ILE:HD13	2.10	0.51
2:B:243:ASN:HA	2:B:244:PRO:C	2.29	0.51
29:3:84:ARG:HD3	41:3:9041:HOH:O	2.11	0.51
24:X:87:ALA:O	24:X:88:GLU:CB	2.57	0.51
30:0:1190:G:H4'	30:0:1207:A:N1	2.24	0.51
4:D:75:LEU:HD13	4:D:79:MET:O	2.10	0.51
25:Y:148:GLY:HA3	30:0:622:G:P	2.51	0.51
30:0:2765:C:H2'	30:0:2766:A:H8	1.75	0.51
16:P:139:ARG:NH1	16:P:139:ARG:HG3	2.21	0.51
16:P:125:LYS:HB3	16:P:130:GLU:HG3	1.92	0.51
1:A:96:LEU:HD22	1:A:128:LEU:HD22	1.93	0.51
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.51
23:W:142:ASP:O	23:W:145:GLY:N	2.43	0.51
3:C:140:VAL:HB	41:C:8648:HOH:O	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1161:A:H1'	41:0:4752:HOH:O	2.11	0.51
7:G:23:ILE:HG22	7:G:27:ILE:CD1	2.39	0.51
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.10	0.51
25:Y:177:LYS:HE2	25:Y:183:GLU:OE2	2.09	0.51
9:I:96:SER:OG	9:I:99:GLN:HG3	2.10	0.51
22:V:64:GLY:O	22:V:65:ASP:CB	2.58	0.51
10:J:6:PHE:HB3	10:J:109:TYR:OH	2.10	0.51
16:P:37:ARG:NH2	30:0:1502:A:OP1	2.43	0.51
2:B:145:HIS:HD2	2:B:159:PRO:HB3	1.76	0.51
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.25	0.51
12:L:18:HIS:HB3	41:L:8973:HOH:O	2.09	0.51
30:0:2850:C:H1'	41:0:9168:HOH:O	2.10	0.51
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.92	0.51
30:0:1746:A:H5''	41:0:6929:HOH:O	2.10	0.51
30:0:1471:A:H2'	30:0:1472:C:C6	2.45	0.51
30:0:1790:C:H2'	30:0:1791:U:H6	1.75	0.51
30:0:146:U:O2'	30:0:147:G:H5'	2.11	0.51
11:K:101:ASN:O	11:K:102:GLU:HB2	2.10	0.51
20:T:40:VAL:HG23	20:T:119:ALA:OXT	2.10	0.51
2:B:316:ARG:HG3	2:B:316:ARG:O	2.11	0.51
20:T:24:ARG:HH11	20:T:24:ARG:HG2	1.75	0.51
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.93	0.51
30:0:1705:C:O2	30:0:2735:U:H5''	2.11	0.51
16:P:14:LEU:O	16:P:16:VAL:HG23	2.10	0.51
15:O:97:SER:H	15:O:100:GLN:NE2	2.08	0.51
25:Y:203:VAL:CG1	25:Y:228:VAL:HG22	2.41	0.51
9:I:91:PHE:HA	9:I:131:GLY:HA3	1.93	0.51
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.51
25:Y:112:GLU:CD	25:Y:115:ARG:HH12	2.13	0.51
31:9:96:C:H2'	31:9:97:U:C6	2.46	0.51
29:3:31:THR:O	30:0:1923:G:H4'	2.11	0.51
23:W:77:ALA:HB3	41:W:5763:HOH:O	2.11	0.51
30:0:1700:C:OP2	41:0:6868:HOH:O	2.19	0.51
30:0:1303:C:O2	30:0:1353:C:H1'	2.09	0.51
3:C:65:ARG:HG3	3:C:67:GLN:HB2	1.93	0.51
4:D:40:ILE:HA	4:D:43:GLU:OE1	2.11	0.51
1:A:109:GLU:HG2	1:A:116:GLY:N	2.20	0.51
20:T:43:ASN:HD22	20:T:108:ARG:CZ	2.24	0.51
30:0:2566:A:H61	30:0:2699:A:H61	1.59	0.51
23:W:117:ARG:CB	23:W:117:ARG:HH11	2.23	0.51
12:L:73:VAL:HG23	12:L:74:THR:H	1.75	0.51
21:U:35:LYS:HE2	21:U:51:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:159:VAL:O	5:E:163:GLN:HG2	2.11	0.51
30:0:1979:G:H2'	41:0:3192:HOH:O	2.10	0.51
1:A:66:ARG:CB	1:A:66:ARG:HH11	2.21	0.51
30:0:1835:U:C5	30:0:1840:A:N7	2.71	0.51
31:9:3:A:H2	31:9:21:G:N3	2.09	0.51
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.51
3:C:175:LYS:HZ3	3:C:184:ARG:HB3	1.76	0.51
30:0:2502:C:H2'	30:0:2503:A:H5'	1.92	0.51
31:9:97:U:H3'	41:9:9104:HOH:O	2.11	0.51
4:D:154:LYS:HD2	4:D:154:LYS:H	1.75	0.51
8:H:87:LYS:HB2	8:H:87:LYS:NZ	2.26	0.51
9:I:134:ILE:HG22	9:I:135:GLU:N	2.26	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
2:B:11:LEU:HD21	2:B:250:THR:HG22	1.93	0.51
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.46	0.51
14:N:11:ARG:NH1	31:9:8:G:O6	2.43	0.51
31:9:92:G:H2'	31:9:93:A:H8	1.75	0.51
17:Q:7:LEU:HD12	30:0:2424:U:C1'	2.41	0.51
30:0:2735:U:H2'	30:0:2736:U:H6	1.76	0.51
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.41	0.51
20:T:107:LYS:O	20:T:111:ARG:HB2	2.09	0.51
23:W:142:ASP:HB3	41:W:2729:HOH:O	2.11	0.51
4:D:10:PHE:CE1	4:D:11:HIS:HB3	2.46	0.51
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.93	0.51
2:B:216:LYS:HA	41:0:5933:HOH:O	2.11	0.51
30:0:1477:C:H5'	30:0:1868:G:C5'	2.40	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51
30:0:2911:C:H3'	41:0:6395:HOH:O	2.11	0.51
8:H:20:ARG:HD3	8:H:26:ILE:HD12	1.92	0.51
17:Q:1:PRO:HA	30:0:2299:G:O6	2.11	0.51
3:C:236:THR:HB	3:C:239:ALA:HB2	1.93	0.50
25:Y:189:ASN:HD22	25:Y:191:ASP:N	2.10	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.62	0.50
20:T:49:GLU:OE2	20:T:51:LEU:HD21	2.11	0.50
12:L:80:ASP:HB2	12:L:90:ARG:O	2.11	0.50
14:N:86:LEU:HD21	14:N:180:LEU:CD1	2.41	0.50
8:H:49:GLN:OE1	8:H:169:GLU:HG2	2.11	0.50
30:0:566:A:H2'	30:0:567:U:H5'	1.91	0.50
23:W:122:ARG:CZ	23:W:154:ARG:HB3	2.40	0.50
29:3:84:ARG:HD2	30:0:2427:C:OP2	2.10	0.50
5:E:35:TYR:HA	10:J:127:ILE:CD1	2.41	0.50
30:0:2251:G:H2'	30:0:2252:A:H8	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:354:A:H2'	30:0:355:C:H6	1.76	0.50
23:W:117:ARG:CB	23:W:117:ARG:NH1	2.74	0.50
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.46	0.50
4:D:135:VAL:HG22	4:D:136:ARG:N	2.26	0.50
20:T:43:ASN:OD1	30:0:80:A:H3'	2.11	0.50
30:0:314:G:N2	30:0:316:A:H3'	2.26	0.50
2:B:214:PRO:HB2	2:B:220:VAL:HG21	1.93	0.50
30:0:2819:C:H2'	30:0:2820:A:C8	2.46	0.50
5:E:36:PRO:HD3	10:J:127:ILE:CG1	2.42	0.50
30:0:213:G:H22	30:0:225:G:H2'	1.76	0.50
30:0:1595:G:O2'	30:0:1596:U:H5'	2.11	0.50
2:B:125:GLU:O	2:B:129:ARG:HG3	2.11	0.50
30:0:561:G:O2'	30:0:562:A:H5'	2.11	0.50
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.92	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.50
2:B:279:THR:HG22	2:B:280:VAL:N	2.26	0.50
6:F:46:GLU:OE2	6:F:100:ASP:HA	2.10	0.50
3:C:168:ARG:NH1	30:0:1310:U:OP2	2.44	0.50
25:Y:112:GLU:OE1	25:Y:115:ARG:NH1	2.44	0.50
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.47	0.50
10:J:71:TYR:CD1	10:J:72:PRO:HD2	2.46	0.50
25:Y:102:LEU:HG	41:Y:8887:HOH:O	2.11	0.50
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.50
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.75	0.50
14:N:1:ALA:HB2	31:9:14:G:O2'	2.11	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.69	0.50
31:9:106:U:O2'	31:9:107:C:H5'	2.11	0.50
16:P:134:VAL:O	16:P:138:GLU:HG3	2.11	0.50
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.92	0.50
25:Y:170:SER:HG	25:Y:175:ARG:HG3	1.76	0.50
29:3:38:ARG:NH1	30:0:396:U:OP2	2.43	0.50
30:0:2324:G:N2	30:0:2377:U:H1'	2.26	0.50
1:A:146:LYS:NZ	30:0:1855:G:O3'	2.44	0.50
23:W:73:LEU:HD22	23:W:111:GLY:HA2	1.94	0.50
9:I:97:VAL:O	9:I:101:LYS:HG3	2.12	0.50
11:K:74:VAL:HG13	11:K:113:ILE:HG12	1.93	0.50
22:V:39:ALA:O	22:V:41:GLU:N	2.43	0.50
8:H:49:GLN:O	8:H:169:GLU:HB3	2.11	0.50
14:N:183:ASP:O	14:N:184:ILE:O	2.28	0.50
12:L:13:HIS:ND1	38:L:8814:CL:CL	2.77	0.50
3:C:7:ASP:O	3:C:9:ASP:N	2.44	0.50
24:X:10:VAL:HG12	24:X:11:THR:N	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:83:GLY:O	5:E:169:THR:N	2.35	0.50
14:N:78:MET:HB2	14:N:146:HIS:HE1	1.76	0.50
30:0:506:G:N1	30:0:509:A:OP2	2.43	0.50
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.50
20:T:52:ARG:HB2	20:T:95:ASN:HB3	1.94	0.50
4:D:170:TYR:O	4:D:171:ASP:CB	2.59	0.50
23:W:7:LEU:HD12	23:W:53:ALA:HB2	1.93	0.50
20:T:16:LEU:HB2	30:0:100:C:C4'	2.41	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50
1:A:69:LEU:HD11	1:A:159:VAL:HG13	1.94	0.50
30:0:1309:U:H2'	30:0:1310:U:O4'	2.12	0.50
30:0:553:G:H2'	30:0:554:G:H5'	1.94	0.50
30:0:823:U:H3'	41:0:5310:HOH:O	2.12	0.50
30:0:371:U:H2'	30:0:372:A:H8	1.76	0.50
30:0:1649:G:O2'	30:0:1650:C:H5'	2.11	0.50
30:0:1301:C:O2'	30:0:1331:G:H4'	2.11	0.50
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.50
3:C:27:ARG:NH2	30:0:657:G:OP1	2.44	0.50
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.94	0.50
30:0:303:C:H2'	30:0:304:G:O4'	2.12	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
20:T:20:HIS:O	20:T:23:VAL:HG23	2.11	0.50
29:3:22:VAL:CG1	29:3:67:LEU:HD13	2.42	0.50
30:0:1980:U:H5'	30:0:2626:C:H1'	1.93	0.50
19:S:56:ASN:O	28:2:8:LYS:NZ	2.45	0.50
19:S:77:VAL:C	19:S:78:ALA:CA	2.80	0.50
30:0:1659:A:H2'	30:0:1660:G:O4'	2.11	0.50
30:0:1755:A:H2'	30:0:1756:G:O4'	2.11	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
9:I:86:GLU:HB2	9:I:90:ASP:OD2	2.12	0.50
11:K:64:MET:O	11:K:67:GLN:HB2	2.12	0.50
30:0:1805:G:O2'	30:0:1806:G:H5'	2.12	0.50
22:V:1:THR:C	22:V:3:LEU:N	2.65	0.50
5:E:40:VAL:HB	41:E:2857:HOH:O	2.11	0.50
30:0:1992:U:H2'	30:0:1994:A:OP2	2.12	0.50
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.76	0.50
30:0:1200:A:H3'	41:0:6592:HOH:O	2.11	0.50
8:H:41:LYS:O	8:H:87:LYS:HE2	2.11	0.50
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.50
22:V:6:GLN:HB2	41:0:7782:HOH:O	2.11	0.50
30:0:1590:A:H1'	30:0:1606:A:C2	2.47	0.50
2:B:197:GLY:HA3	2:B:323:LEU:HA	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:1:PRO:HG2	5:E:59:MET:SD	2.52	0.50
11:K:55:VAL:HG12	11:K:56:SER:N	2.27	0.50
25:Y:189:ASN:HD22	25:Y:191:ASP:H	1.59	0.50
5:E:22:VAL:O	5:E:28:SER:HA	2.11	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.50
30:0:2836:G:O2'	30:0:2838:A:N7	2.34	0.50
3:C:5:ILE:HG22	3:C:6:TYR:N	2.27	0.50
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.11	0.50
30:0:1503:U:C2'	30:0:1504:A:H5'	2.42	0.50
3:C:124:VAL:HA	3:C:230:GLY:O	2.11	0.50
30:0:445:U:O2'	30:0:446:G:H5'	2.12	0.50
12:L:10:SER:O	12:L:11:ARG:HB3	2.12	0.50
30:0:1641:A:H2'	30:0:1642:A:H5'	1.93	0.50
15:O:43:VAL:CG1	15:O:47:ARG:HD2	2.42	0.50
29:3:40:ARG:HD2	41:3:9047:HOH:O	2.12	0.50
30:0:1985:U:C5	30:0:1996:U:C2	3.00	0.50
12:L:4:LYS:HE2	30:0:645:U:OP2	2.12	0.50
30:0:162:C:H2'	30:0:163:U:H5'	1.94	0.50
13:M:46:LEU:HD22	13:M:50:ARG:CD	2.42	0.50
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.30	0.49
29:3:68:LYS:HE2	30:0:2436:U:C5'	2.40	0.49
1:A:26:ASP:O	1:A:28:GLU:N	2.45	0.49
30:0:875:A:H5'	30:0:876:A:N7	2.27	0.49
21:U:56:ARG:O	21:U:56:ARG:CD	2.60	0.49
17:Q:16:ASN:ND2	17:Q:45:PRO:HB2	2.27	0.49
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.42	0.49
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.49
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.45	0.49
30:0:2114:C:O2'	30:0:2115:U:H5'	2.11	0.49
12:L:89:PHE:CD1	12:L:89:PHE:N	2.80	0.49
23:W:29:VAL:O	23:W:30:ASN:HB2	2.10	0.49
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.46	0.49
30:0:412:C:H2'	30:0:413:G:O4'	2.11	0.49
18:R:44:VAL:O	18:R:48:GLU:HG3	2.12	0.49
30:0:2001:G:O2'	30:0:2002:C:H5'	2.12	0.49
18:R:9:ASP:OD1	18:R:11:ASP:HB2	2.12	0.49
5:E:31:ARG:NH1	41:E:5919:HOH:O	2.46	0.49
30:0:1878:G:H1'	41:0:6953:HOH:O	2.11	0.49
30:0:2839:C:H2'	30:0:2840:A:H5''	1.95	0.49
31:9:98:C:H2'	31:9:99:U:C6	2.44	0.49
30:0:2314:G:O2'	30:0:2315:C:H5'	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2252:A:H2'	30:0:2253:G:O4'	2.11	0.49
30:0:1773:G:H4'	41:0:4407:HOH:O	2.12	0.49
30:0:1270:U:H2'	30:0:1271:A:C8	2.46	0.49
20:T:53:GLY:HA3	41:0:7613:HOH:O	2.12	0.49
2:B:1:PRO:HG3	30:0:2591:C:OP1	2.11	0.49
3:C:195:VAL:HA	3:C:213:ALA:O	2.12	0.49
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.45	0.49
30:0:1714:C:O2'	30:0:1715:C:H5'	2.12	0.49
4:D:57:THR:HG23	4:D:63:ILE:CA	2.32	0.49
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.40	0.49
41:Z:8722:HOH:O	30:0:1886:A:H5'	2.11	0.49
9:I:87:PRO:HD3	41:0:4130:HOH:O	2.12	0.49
1:A:65:ARG:C	1:A:66:ARG:HG3	2.32	0.49
30:0:283:U:H5''	30:0:284:C:OP2	2.12	0.49
20:T:1:SER:HB2	30:0:447:A:P	2.53	0.49
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.59	0.49
30:0:1165:G:H1'	30:0:1174:A:H1'	1.95	0.49
30:0:1201:C:H2'	30:0:1202:A:H5'	1.94	0.49
6:F:38:LYS:HA	6:F:41:GLU:OE1	2.12	0.49
14:N:154:LEU:O	14:N:155:GLU:HB3	2.12	0.49
3:C:202:THR:HG22	30:0:328:U:O4'	2.12	0.49
26:Z:105:ARG:O	26:Z:106:SER:C	2.50	0.49
22:V:12:THR:HG22	22:V:15:GLU:CD	2.31	0.49
13:M:133:LEU:N	13:M:133:LEU:HD12	2.26	0.49
14:N:15:GLU:O	14:N:16:ALA:HB3	2.13	0.49
12:L:108:VAL:HB	12:L:125:PHE:HD2	1.77	0.49
11:K:77:ARG:O	11:K:78:LYS:CA	2.60	0.49
31:9:78:G:N2	31:9:102:G:H2'	2.27	0.49
26:Z:77:GLY:O	26:Z:78:ILE:CA	2.61	0.49
4:D:151:ILE:CG2	4:D:155:HIS:HB3	2.43	0.49
25:Y:212:ARG:HD2	41:Y:8907:HOH:O	2.12	0.49
41:X:4132:HOH:O	30:0:2895:C:H4'	2.12	0.49
14:N:64:SER:C	14:N:66:LEU:H	2.15	0.49
4:D:77:ASP:C	4:D:78:GLU:CA	2.81	0.49
29:3:55:VAL:HB	29:3:56:PRO:HD2	1.94	0.49
19:S:40:ALA:O	19:S:44:GLN:HB2	2.12	0.49
20:T:27:LEU:HB2	20:T:32:ARG:CG	2.42	0.49
14:N:176:ARG:O	14:N:180:LEU:HD13	2.12	0.49
30:0:2296:C:H4'	30:0:2362:A:H2	1.78	0.49
30:0:568:G:C6	30:0:588:G:H1'	2.48	0.49
30:0:945:U:H2'	30:0:946:C:H6	1.78	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:88:TYR:CE1	5:E:92:PRO:HA	2.47	0.49
30:0:695:C:H2'	30:0:696:C:H6	1.77	0.49
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.77	0.49
2:B:277:GLU:N	2:B:278:PRO:HD2	2.27	0.49
30:0:764:C:H2'	30:0:765:G:O4'	2.13	0.49
30:0:772:G:H2'	30:0:773:A:O4'	2.12	0.49
14:N:141:ARG:HH12	31:9:35:C:H2'	1.77	0.49
16:P:64:GLU:HG2	41:P:2495:HOH:O	2.13	0.49
1:A:169:PHE:O	1:A:171:LYS:N	2.43	0.49
30:0:2289:G:H21	30:0:2291:A:H2	1.57	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
20:T:26:THR:CG2	20:T:97:ARG:HG3	2.42	0.49
2:B:161:VAL:HG12	2:B:162:MET:N	2.28	0.49
30:0:285:A:H2'	30:0:286:U:O4'	2.12	0.49
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.49
13:M:57:LYS:HZ3	13:M:144:ASP:HB2	1.78	0.49
20:T:77:VAL:C	20:T:78:THR:CA	2.81	0.49
31:9:18:U:H2'	31:9:19:G:C8	2.44	0.49
9:I:96:SER:HB3	9:I:99:GLN:NE2	2.27	0.49
13:M:58:GLN:HG3	41:M:8907:HOH:O	2.12	0.49
15:O:26:TRP:CE3	15:O:26:TRP:HA	2.48	0.49
15:O:77:ALA:C	15:O:78:ALA:CA	2.81	0.49
30:0:816:G:H5'	30:0:1598:A:H4'	1.95	0.49
16:P:6:GLN:HG2	16:P:31:ILE:HG22	1.93	0.49
15:O:38:ARG:NH1	41:O:7674:HOH:O	2.45	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
30:0:300:U:O2'	30:0:301:C:H5'	2.12	0.49
23:W:62:LEU:HD21	23:W:100:LEU:HD12	1.94	0.49
1:A:165:THR:HG22	41:A:9096:HOH:O	2.11	0.49
30:0:98:A:C2'	30:0:99:A:H5'	2.42	0.49
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.13	0.49
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.43	0.49
18:R:46:TYR:O	18:R:50:VAL:HG23	2.13	0.49
11:K:87:ARG:HD2	41:K:4066:HOH:O	2.12	0.49
31:9:29:C:H2'	31:9:30:C:C5'	2.38	0.49
2:B:279:THR:HG23	2:B:290:VAL:H	1.77	0.49
30:0:2909:G:O2'	30:0:2910:A:H5'	2.13	0.49
24:X:25:ARG:HD2	41:X:5356:HOH:O	2.13	0.49
13:M:40:ILE:HD11	13:M:62:VAL:HG12	1.94	0.49
9:I:118:ASN:HA	9:I:121:LYS:HD2	1.95	0.49
30:0:2566:A:H2	30:0:2695:C:O2	1.95	0.49
30:0:2583:A:H3'	41:O:5461:HOH:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1314:U:H5''	30:0:1316:G:O4'	2.12	0.49
19:S:5:ILE:HD12	19:S:44:GLN:HG3	1.93	0.49
30:0:98:A:H2'	30:0:99:A:H5'	1.95	0.49
30:0:1230:A:OP1	30:0:1230:A:H8	1.95	0.49
29:3:16:GLU:HB2	41:0:6515:HOH:O	2.12	0.49
2:B:29:TRP:CZ3	2:B:164:THR:HG23	2.48	0.49
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.12	0.49
11:K:9:THR:O	11:K:10:GLN:C	2.51	0.49
30:0:2718:C:H6	30:0:2718:C:H5'	1.78	0.49
13:M:144:ASP:O	13:M:148:SER:HB3	2.12	0.49
30:0:2426:G:H5''	30:0:2427:C:O4'	2.11	0.49
30:0:565:A:OP2	30:0:592:G:N1	2.42	0.49
15:O:26:TRP:HA	15:O:26:TRP:HE3	1.78	0.49
19:S:56:ASN:HD22	30:0:1676:G:P	2.34	0.49
26:Z:54:GLU:HA	26:Z:57:MET:HB3	1.93	0.49
4:D:80:ALA:O	4:D:83:PHE:HB3	2.13	0.49
30:0:1367:A:H2'	30:0:1368:U:O4'	2.12	0.49
30:0:669:G:O2'	30:0:670:G:H5'	2.13	0.49
10:J:67:ASN:OD1	30:0:2082:G:H1'	2.12	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.49
14:N:140:GLN:O	14:N:143:ARG:HB2	2.13	0.49
30:0:1666:C:C2'	30:0:1667:A:C5'	2.91	0.49
30:0:658:C:O2'	30:0:662:U:OP1	2.25	0.49
2:B:52:VAL:C	2:B:53:LEU:HD12	2.33	0.49
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.48	0.49
23:W:129:LYS:HE2	30:0:1098:A:O3'	2.12	0.49
28:2:20:ARG:HG3	28:2:21:VAL:N	2.28	0.49
30:0:222:A:H2'	30:0:223:G:O4'	2.12	0.49
30:0:690:G:H1'	30:0:731:U:H1'	1.95	0.49
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.48	0.49
3:C:131:PHE:CD2	3:C:232:LEU:HD22	2.47	0.49
23:W:34:LEU:HD13	23:W:100:LEU:HD13	1.94	0.49
30:0:737:A:H2'	30:0:738:G:O4'	2.12	0.49
3:C:188:ARG:NH2	41:C:8523:HOH:O	2.44	0.49
24:X:63:ARG:HG2	24:X:63:ARG:O	2.13	0.49
30:0:1393:A:H2'	30:0:1394:C:C6	2.48	0.49
29:3:51:LYS:HB2	41:0:5348:HOH:O	2.12	0.49
41:A:9044:HOH:O	30:0:871:G:H4'	2.12	0.49
1:A:211:LYS:HB2	41:A:9098:HOH:O	2.13	0.49
20:T:101:LEU:HD22	20:T:108:ARG:NH2	2.27	0.49
23:W:42:ARG:HA	23:W:45:VAL:HG22	1.95	0.49
1:A:204:GLY:O	1:A:205:GLY:C	2.51	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:2:43:ARG:HH21	30:0:1685:A:H4'	1.78	0.49
30:0:2642:G:H2'	30:0:2643:G:O4'	2.13	0.49
12:L:4:LYS:HD2	41:0:5885:HOH:O	2.13	0.49
30:0:1774:G:H1'	41:0:5405:HOH:O	2.13	0.49
2:B:128:ILE:O	2:B:131:ALA:HB3	2.12	0.49
30:0:71:G:H8	41:0:4782:HOH:O	1.96	0.49
30:0:883:U:C5	30:0:888:U:H5'	2.48	0.49
3:C:87:ARG:NH2	30:0:894:A:C2	2.80	0.49
17:Q:77:ASP:C	17:Q:78:GLY:CA	2.82	0.49
30:0:17:G:H2'	30:0:18:C:C6	2.48	0.49
10:J:52:GLN:NE2	30:0:1119:G:C2'	2.63	0.48
30:0:2073:G:H2'	41:0:4699:HOH:O	2.13	0.48
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.43	0.48
30:0:2387:U:O2	30:0:2402:A:C2	2.66	0.48
30:0:1175:G:H1'	30:0:1193:A:H2'	1.94	0.48
6:F:100:ASP:O	6:F:101:ALA:O	2.31	0.48
14:N:155:GLU:O	14:N:156:GLU:HG3	2.13	0.48
4:D:52:THR:CG2	30:0:2346:C:H4'	2.43	0.48
5:E:137:ASP:O	5:E:141:VAL:HG23	2.13	0.48
23:W:117:ARG:HB2	23:W:117:ARG:NH1	2.28	0.48
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.48
30:0:1139:U:H2'	30:0:1140:C:C6	2.48	0.48
20:T:44:ALA:HA	20:T:62:VAL:HG12	1.95	0.48
30:0:2473:U:O3'	30:0:2474:A:H3'	2.13	0.48
14:N:37:ARG:HH11	14:N:37:ARG:HG3	1.78	0.48
31:9:28:U:H2'	31:9:29:C:C6	2.48	0.48
16:P:41:ARG:O	16:P:44:VAL:HB	2.13	0.48
2:B:280:VAL:HG13	2:B:333:GLU:O	2.14	0.48
12:L:6:ARG:NH2	41:L:9012:HOH:O	2.45	0.48
4:D:59:GLY:O	4:D:61:PHE:N	2.46	0.48
30:0:2312:G:C2'	30:0:2313:C:H5'	2.43	0.48
26:Z:54:GLU:HG2	26:Z:57:MET:CE	2.43	0.48
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.48	0.48
2:B:285:VAL:O	2:B:286:ASN:HB2	2.13	0.48
30:0:2688:U:H2'	30:0:2689:A:H8	1.79	0.48
30:0:1121:G:H4'	41:0:6381:HOH:O	2.13	0.48
7:G:14:GLU:HB3	41:G:4173:HOH:O	2.13	0.48
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.13	0.48
14:N:143:ARG:HA	14:N:172:PHE:CD2	2.49	0.48
30:0:1666:C:C2'	30:0:1667:A:H5''	2.42	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.12	0.48
2:B:316:ARG:HB2	30:0:2768:A:C8	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:102:ILE:HB	41:O:7481:HOH:O	2.13	0.48
8:H:23:ILE:HG22	8:H:123:ILE:CD1	2.43	0.48
41:J:2219:HOH:O	30:O:1103:C:H5''	2.13	0.48
27:1:50:TRP:O	30:O:890:C:O2'	2.28	0.48
28:2:28:LYS:O	30:O:87:C:H2'	2.13	0.48
30:O:1505:U:H4'	41:O:6027:HOH:O	2.12	0.48
21:U:52:THR:HG22	21:U:54:THR:HB	1.95	0.48
30:O:380:A:O4'	30:O:382:U:H1'	2.13	0.48
1:A:179:MET:C	1:A:181:ALA:H	2.17	0.48
30:O:2607:U:H4'	41:O:3343:HOH:O	2.12	0.48
41:B:9059:HOH:O	30:O:2819:C:H5'	2.13	0.48
30:O:2780:C:H2'	30:O:2781:U:C6	2.49	0.48
16:P:77:ALA:C	16:P:78:GLY:CA	2.81	0.48
28:2:42:TRP:CZ3	28:2:43:ARG:HB2	2.48	0.48
2:B:45:LYS:HG2	2:B:305:ASP:HA	1.94	0.48
3:C:37:ALA:O	3:C:38:ALA:C	2.51	0.48
14:N:100:ALA:HB3	14:N:129:ILE:HG12	1.95	0.48
8:H:122:LYS:O	8:H:124:VAL:HG13	2.13	0.48
30:O:441:A:H1'	30:O:442:A:N7	2.28	0.48
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.43	0.48
11:K:98:VAL:CG1	11:K:99:ASP:N	2.76	0.48
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.77	0.48
8:H:24:THR:O	8:H:123:ILE:HD12	2.13	0.48
1:A:4:ILE:HG22	1:A:198:ASP:O	2.14	0.48
25:Y:193:LEU:HD13	25:Y:221:ALA:HB2	1.95	0.48
9:I:81:GLU:N	9:I:81:GLU:OE1	2.46	0.48
25:Y:108:ASP:OD1	25:Y:108:ASP:N	2.47	0.48
30:O:1475:G:N3	30:O:1866:A:H2	2.11	0.48
30:O:1405:U:H2'	41:O:7653:HOH:O	2.14	0.48
28:2:5:LYS:HD2	30:O:1675:C:H5''	1.95	0.48
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.96	0.48
4:D:23:VAL:O	4:D:23:VAL:HG23	2.13	0.48
4:D:45:THR:HB	4:D:75:LEU:HD11	1.96	0.48
30:O:368:C:C2'	30:O:369:G:H5'	2.44	0.48
29:3:64:LYS:HA	29:3:84:ARG:HA	1.94	0.48
20:T:21:LYS:HA	20:T:24:ARG:CG	2.42	0.48
30:O:694:A:H2'	30:O:695:C:H5'	1.95	0.48
22:V:27:LEU:O	22:V:30:ALA:HB3	2.13	0.48
30:O:887:G:H2'	30:O:888:U:C6	2.48	0.48
30:O:2755:G:H1'	41:O:5540:HOH:O	2.12	0.48
4:D:50:VAL:O	4:D:71:ALA:HA	2.13	0.48
30:O:1409:G:H5'	41:O:4602:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:61:VAL:HA	41:O:3397:HOH:O	2.13	0.48
30:O:1876:C:H4'	30:O:1877:G:OP2	2.14	0.48
17:Q:53:HIS:CD2	30:O:2389:U:H4'	2.48	0.48
12:L:150:GLN:HB3	41:L:9035:HOH:O	2.14	0.48
5:E:81:GLU:OE2	5:E:132:THR:OG1	2.31	0.48
2:B:16:ARG:NH1	41:B:9091:HOH:O	2.45	0.48
20:T:20:HIS:HB3	20:T:41:ARG:HD2	1.95	0.48
14:N:25:ARG:HG2	30:O:2416:G:O2'	2.13	0.48
30:O:333:G:O2'	30:O:334:G:H5'	2.13	0.48
25:Y:182:PHE:HD2	25:Y:200:THR:O	1.95	0.48
30:O:1394:C:H3'	30:O:1433:G:H22	1.78	0.48
5:E:162:PHE:CD1	5:E:162:PHE:N	2.81	0.48
12:L:97:VAL:HB	12:L:100:ALA:HB2	1.96	0.48
30:O:2351:C:H2'	30:O:2352:G:O4'	2.14	0.48
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.96	0.48
18:R:100:ASP:C	18:R:102:GLN:H	2.16	0.48
30:O:1189:A:H1'	30:O:1209:C:C1'	2.43	0.48
28:2:46:ASP:OD1	28:2:47:THR:O	2.32	0.48
30:O:111:C:C2'	30:O:112:G:H5'	2.44	0.48
30:O:746:A:H4'	30:O:747:G:H5'	1.95	0.48
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.78	0.48
12:L:77:ALA:C	12:L:79:ASP:H	2.17	0.48
30:O:1353:C:H5''	41:O:7423:HOH:O	2.12	0.48
13:M:46:LEU:HD22	13:M:50:ARG:HD2	1.96	0.48
22:V:42:ASN:O	22:V:44:GLY:N	2.47	0.48
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.13	0.48
9:I:127:CYS:O	9:I:129:SER:N	2.47	0.48
1:A:57:ALA:HB1	1:A:65:ARG:HE	1.78	0.48
25:Y:117:LEU:CD1	25:Y:174:VAL:HG11	2.40	0.48
13:M:95:LYS:CE	30:O:157:G:H4'	2.44	0.48
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.44	0.48
20:T:81:LYS:HE3	30:O:486:A:O5'	2.13	0.48
26:Z:51:ALA:HA	41:Z:8712:HOH:O	2.13	0.48
30:O:696:C:O2'	30:O:731:U:OP1	2.30	0.48
30:O:1819:G:H2'	30:O:1820:G:H5'	1.96	0.48
13:M:5:TYR:CE2	13:M:50:ARG:HD3	2.49	0.48
30:O:670:G:H2'	30:O:671:A:C8	2.48	0.48
30:O:1490:G:H4'	30:O:1533:A:OP1	2.14	0.48
17:Q:77:ASP:O	17:Q:78:GLY:C	2.51	0.48
21:U:37:GLU:HB3	41:U:408:HOH:O	2.12	0.48
28:2:5:LYS:O	28:2:9:LYS:HG3	2.14	0.48
17:Q:86:VAL:HG11	17:Q:91:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:294:TYR:CD1	2:B:294:TYR:C	2.87	0.48
30:0:419:A:H1'	30:0:1921:A:C2	2.49	0.48
23:W:128:VAL:O	23:W:138:LEU:HD11	2.14	0.48
30:0:349:U:O2'	30:0:350:G:H5'	2.14	0.48
21:U:11:THR:CG2	21:U:53:ASP:HB2	2.42	0.48
22:V:50:ARG:HH12	30:0:56:G:C5'	2.26	0.48
20:T:9:LYS:CE	20:T:13:ARG:NH1	2.76	0.48
16:P:104:LYS:HE2	16:P:138:GLU:HG2	1.95	0.48
11:K:66:ARG:NH2	30:0:1994:A:P	2.87	0.48
14:N:151:ASP:O	14:N:154:LEU:HD13	2.13	0.48
30:0:2253:G:H2'	30:0:2254:G:H8	1.78	0.48
26:Z:73:ARG:HB2	26:Z:79:TRP:CZ3	2.49	0.48
31:9:78:G:N3	31:9:78:G:N2	2.62	0.48
30:0:1819:G:C2'	30:0:1820:G:H5'	2.43	0.48
30:0:1457:U:O2'	30:0:1458:A:H5'	2.13	0.48
30:0:2045:G:H5''	41:0:9032:HOH:O	2.14	0.48
3:C:107:ARG:NH2	30:0:678:G:OP2	2.46	0.48
13:M:150:ILE:HA	13:M:155:GLN:HG3	1.95	0.48
2:B:264:GLU:HG3	41:B:9010:HOH:O	2.13	0.48
11:K:49:LEU:HD22	11:K:80:ILE:HD13	1.96	0.48
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.20	0.47
10:J:60:ARG:NH2	30:0:1242:A:OP2	2.37	0.47
9:I:87:PRO:HG3	30:0:1181:A:H1'	1.96	0.47
14:N:82:TYR:HE1	14:N:120:GLU:HG2	1.77	0.47
30:0:559:U:C6	30:0:559:U:H5'	2.48	0.47
12:L:53:ARG:NH2	12:L:57:VAL:CG1	2.76	0.47
15:O:26:TRP:N	41:O:3062:HOH:O	2.47	0.47
30:0:1346:U:H2'	30:0:1347:U:H6	1.79	0.47
2:B:123:ALA:O	2:B:126:GLU:HB3	2.14	0.47
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.72	0.47
30:0:1057:A:H1'	30:0:2492:U:O2'	2.14	0.47
30:0:635:A:H2'	30:0:636:G:H5''	1.96	0.47
30:0:1159:G:H1	30:0:1208:C:H42	1.62	0.47
11:K:8:VAL:HG12	11:K:9:THR:N	2.29	0.47
21:U:11:THR:HG22	21:U:53:ASP:CG	2.34	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.14	0.47
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.54	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:567:U:O5'	30:0:567:U:H6	1.96	0.47
23:W:43:GLY:HA3	30:0:945:U:O2'	2.15	0.47
30:0:100:C:H2'	30:0:101:C:H6	1.80	0.47
30:0:1248:A:H2'	30:0:1249:U:C6	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.44	0.47
30:0:1278:A:H2'	30:0:1280:A:C8	2.49	0.47
2:B:132:HIS:CE1	2:B:171:VAL:HG21	2.50	0.47
26:Z:54:GLU:HA	26:Z:57:MET:HE2	1.95	0.47
18:R:98:ASN:ND2	18:R:98:ASN:N	2.62	0.47
30:0:1948:G:H2'	30:0:1949:G:H8	1.79	0.47
30:0:1948:G:H2'	30:0:1949:G:C8	2.49	0.47
23:W:117:ARG:HB3	30:0:1263:C:OP1	2.14	0.47
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.47
30:0:364:U:H2'	30:0:365:G:O4'	2.14	0.47
8:H:52:LEU:HD13	8:H:153:PHE:HB3	1.96	0.47
18:R:136:TRP:CE2	30:0:2053:G:H4'	2.50	0.47
30:0:1033:C:H2'	30:0:1034:G:H5'	1.96	0.47
5:E:103:VAL:HG12	5:E:104:ILE:N	2.29	0.47
8:H:32:ALA:C	8:H:33:GLN:HG3	2.34	0.47
30:0:1067:A:H3'	41:0:5158:HOH:O	2.14	0.47
30:0:1383:U:O2'	30:0:1384:C:H5'	2.14	0.47
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.96	0.47
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.47
30:0:425:U:O2'	30:0:426:G:H5'	2.14	0.47
3:C:53:GLY:O	3:C:79:ARG:HA	2.14	0.47
9:I:129:SER:HB3	30:0:1192:A:N6	2.29	0.47
30:0:876:A:H2'	30:0:876:A:N3	2.29	0.47
30:0:2578:G:C8	30:0:2578:G:H5'	2.40	0.47
18:R:82:GLU:CG	18:R:83:LYS:N	2.77	0.47
27:1:4:GLY:O	27:1:8:GLN:HG2	2.14	0.47
11:K:115:ARG:HG3	11:K:116:GLU:N	2.29	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.96	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
5:E:60:SER:OG	30:0:2784:A:H1'	2.15	0.47
30:0:1819:G:H2'	30:0:1820:G:H4'	1.96	0.47
30:0:1816:C:H2'	30:0:1817:U:O4'	2.15	0.47
30:0:514:G:H3'	30:0:514:G:OP1	2.15	0.47
8:H:77:ILE:C	8:H:78:LYS:CA	2.83	0.47
1:A:80:LEU:HD22	1:A:91:GLY:O	2.13	0.47
8:H:143:VAL:HG21	8:H:173:GLU:HG2	1.96	0.47
30:0:1079:A:N3	30:0:2078:U:H1'	2.30	0.47
24:X:72:VAL:HG23	24:X:86:GLU:O	2.15	0.47
6:F:56:PRO:HG3	13:M:44:THR:HA	1.95	0.47
18:R:106:GLY:O	18:R:109:MET:HB2	2.14	0.47
1:A:58:VAL:O	1:A:65:ARG:HA	2.15	0.47
8:H:96:GLN:HE21	8:H:129:ARG:HH21	1.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:78:G:N1	30:0:78:G:N7	2.62	0.47
30:0:1973:A:C8	30:0:1973:A:H5'	2.42	0.47
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.29	0.47
30:0:2520:G:O2'	30:0:2521:A:H5'	2.14	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.95	0.47
30:0:1736:A:H5'	41:0:5472:HOH:O	2.14	0.47
9:I:118:ASN:HA	9:I:121:LYS:CD	2.44	0.47
30:0:1259:A:N1	30:0:1261:A:H1'	2.29	0.47
4:D:21:VAL:CG2	4:D:80:ALA:HB1	2.45	0.47
2:B:17:LYS:O	2:B:260:HIS:HD2	1.97	0.47
7:G:65:THR:HG23	41:0:6310:HOH:O	2.15	0.47
41:N:8812:HOH:O	31:9:36:C:H4'	2.13	0.47
30:0:323:C:O2'	30:0:324:G:H5'	2.14	0.47
30:0:1051:C:H2'	30:0:1052:G:O4'	2.15	0.47
30:0:344:C:H2'	30:0:345:G:O4'	2.13	0.47
6:F:117:GLU:C	6:F:119:ARG:H	2.17	0.47
1:A:212:PRO:HB2	41:A:9041:HOH:O	2.14	0.47
30:0:544:G:H2'	30:0:545:G:H5''	1.97	0.47
23:W:110:GLN:HA	23:W:110:GLN:HE21	1.78	0.47
30:0:1180:U:H2'	30:0:1181:A:C8	2.50	0.47
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.43	0.47
30:0:590:A:H2'	30:0:591:A:H5'	1.97	0.47
30:0:1976:G:O2'	30:0:1977:U:C5'	2.63	0.47
30:0:264:G:H1'	30:0:265:U:C5	2.49	0.47
30:0:695:C:H2'	30:0:696:C:C6	2.50	0.47
23:W:142:ASP:O	23:W:143:THR:C	2.53	0.47
27:1:13:THR:HG22	27:1:14:THR:N	2.30	0.47
30:0:270:U:H5''	41:0:5432:HOH:O	2.14	0.47
6:F:21:GLU:O	6:F:24:ARG:CG	2.63	0.47
13:M:137:ASN:ND2	30:0:145:A:H4'	2.29	0.47
2:B:248:ARG:NH2	41:B:8995:HOH:O	2.47	0.47
21:U:52:THR:HG21	21:U:54:THR:HB	1.96	0.47
30:0:1730:G:H5'	30:0:1731:C:H5	1.75	0.47
17:Q:27:GLN:NE2	31:9:8:G:H4'	2.30	0.47
14:N:24:LEU:HG	14:N:28:LYS:HE3	1.97	0.47
30:0:1972:U:H2'	30:0:1973:A:C5'	2.44	0.47
13:M:57:LYS:NZ	13:M:144:ASP:HB2	2.30	0.47
2:B:214:PRO:C	2:B:220:VAL:HG22	2.35	0.47
1:A:83:GLY:O	1:A:94:LEU:HB3	2.14	0.47
3:C:34:ALA:CB	3:C:220:THR:HG21	2.44	0.47
14:N:152:GLU:C	14:N:154:LEU:N	2.67	0.47
30:0:1309:U:O2'	30:0:1310:U:H5'	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:25:VAL:HG12	30:0:709:G:O2'	2.14	0.47
18:R:98:ASN:ND2	18:R:98:ASN:H	2.12	0.47
31:9:78:G:N1	31:9:78:G:N7	2.62	0.47
30:0:352:A:H2'	30:0:353:G:C8	2.50	0.47
8:H:39:LYS:HA	8:H:87:LYS:HZ1	1.78	0.47
30:0:1333:U:H2'	30:0:1334:C:H6	1.79	0.47
30:0:636:G:H5'	30:0:2059:U:OP2	2.14	0.47
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.72	0.47
8:H:85:ASP:OD2	8:H:142:ASN:ND2	2.37	0.47
10:J:39:VAL:HG13	10:J:106:GLY:O	2.14	0.47
13:M:149:TRP:C	13:M:151:CYS:H	2.18	0.47
30:0:970:U:H6	30:0:970:U:O5'	1.98	0.47
31:9:100:G:H3'	41:9:9133:HOH:O	2.14	0.47
30:0:1158:G:O2'	30:0:1159:G:H5'	2.15	0.47
4:D:166:ILE:O	4:D:169:THR:N	2.48	0.47
1:A:26:ASP:O	1:A:26:ASP:CG	2.52	0.47
14:N:49:THR:HB	14:N:58:LEU:HD13	1.97	0.47
30:0:187:A:H3'	30:0:188:C:C6	2.50	0.47
30:0:1309:U:C2'	30:0:1310:U:H5'	2.45	0.47
30:0:2517:A:C2'	30:0:2518:C:H5'	2.44	0.47
13:M:69:LYS:HG2	13:M:127:LYS:HE3	1.95	0.47
30:0:1809:G:H2'	30:0:1811:A:OP2	2.15	0.47
30:0:366:U:H2'	30:0:367:G:O4'	2.15	0.47
6:F:79:GLN:HB2	6:F:82:ASP:OD2	2.14	0.47
11:K:28:GLU:HB3	11:K:59:LYS:HB2	1.95	0.47
1:A:231:LYS:HG3	30:0:1853:C:OP1	2.15	0.47
30:0:1519:U:H2'	30:0:1520:G:C8	2.50	0.47
15:O:35:LYS:O	15:O:40:HIS:NE2	2.47	0.47
14:N:86:LEU:HA	14:N:121:GLY:O	2.14	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG1	2.45	0.47
30:0:1203:G:O2'	30:0:1204:C:H5'	2.15	0.47
30:0:185:G:C4'	30:0:186:A:H4'	2.45	0.47
4:D:60:GLU:O	4:D:62:ASP:HB2	2.14	0.47
11:K:13:GLU:OE2	11:K:44:HIS:HB2	2.14	0.47
30:0:1745:G:H22	30:0:2033:G:H5'	1.80	0.47
30:0:1682:A:H2'	41:0:3704:HOH:O	2.15	0.47
1:A:6:GLY:HA3	41:0:5481:HOH:O	2.15	0.47
30:0:2515:C:H2'	30:0:2516:G:O4'	2.14	0.47
16:P:69:ARG:HA	16:P:73:HIS:O	2.14	0.47
2:B:36:PRO:CG	2:B:169:GLY:H	2.16	0.47
4:D:40:ILE:HG13	4:D:41:LEU:H	1.79	0.47
24:X:7:GLU:HG3	24:X:74:ALA:O	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:77:ALA:O	29:3:78:HIS:CA	2.63	0.47
30:0:1665:G:H2'	30:0:1666:C:O4'	2.14	0.47
30:0:308:U:H5'	30:0:309:C:OP1	2.14	0.47
14:N:164:ASP:OD2	14:N:167:ASP:HA	2.15	0.47
30:0:400:C:H2'	30:0:401:C:C6	2.51	0.47
30:0:1347:U:H2'	30:0:1348:A:C8	2.50	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
30:0:1503:U:H2'	30:0:1504:A:H5'	1.96	0.47
19:S:44:GLN:HB3	19:S:45:TYR:CD1	2.50	0.47
30:0:2499:U:O2'	30:0:2500:C:H5'	2.14	0.47
3:C:173:LYS:HB3	3:C:187:ARG:HG3	1.96	0.47
2:B:147:VAL:O	2:B:147:VAL:HG12	2.15	0.47
23:W:106:THR:OG1	23:W:109:GLU:HG3	2.14	0.47
13:M:170:ASN:HB2	41:M:8837:HOH:O	2.15	0.47
3:C:238:SER:O	3:C:241:ALA:HB3	2.14	0.46
25:Y:100:ARG:HD2	25:Y:218:GLU:OE1	2.15	0.46
13:M:68:ARG:HG2	13:M:73:ARG:CZ	2.45	0.46
30:0:1909:A:H2'	30:0:1910:A:C8	2.50	0.46
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.46
8:H:12:ILE:HD12	8:H:57:THR:CG2	2.45	0.46
14:N:108:SER:HA	14:N:109:PRO:HD3	1.79	0.46
31:9:11:A:O2'	31:9:12:C:H3'	2.15	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.03	0.46
15:O:112:ARG:HD2	41:0:3570:HOH:O	2.15	0.46
30:0:512:G:H1'	41:0:7627:HOH:O	2.15	0.46
30:0:2554:U:H1'	41:0:6968:HOH:O	2.15	0.46
30:0:615:G:H2'	30:0:616:U:C6	2.50	0.46
30:0:2511:A:H2'	30:0:2512:U:O4'	2.15	0.46
30:0:2102:G:H5''	30:0:2538:A:C2	2.51	0.46
6:F:15:ASP:O	6:F:18:GLU:HB2	2.16	0.46
12:L:24:ALA:CB	12:L:30:ARG:HG3	2.46	0.46
15:O:25:VAL:CG1	30:0:710:G:H5'	2.45	0.46
12:L:136:ALA:HB3	41:L:9038:HOH:O	2.15	0.46
25:Y:204:ARG:HH22	30:0:553:G:P	2.37	0.46
3:C:67:GLN:O	30:0:1359:U:C4	2.68	0.46
30:0:1131:G:C6	30:0:1230:A:C4	3.03	0.46
30:0:1361:C:H2'	30:0:1362:U:H6	1.80	0.46
30:0:824:G:N2	41:0:6935:HOH:O	2.48	0.46
12:L:134:GLU:HA	12:L:138:GLY:O	2.15	0.46
10:J:36:VAL:CG1	10:J:37:ALA:N	2.78	0.46
30:0:652:G:H2'	30:0:653:U:O4'	2.16	0.46
30:0:2568:A:H2'	30:0:2569:A:O4'	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:48:SER:OG	3:C:91:PRO:HB2	2.16	0.46
30:0:1077:G:H2'	30:0:1080:C:H42	1.79	0.46
30:0:177:A:H2'	30:0:178:U:O4'	2.16	0.46
4:D:167:GLU:C	4:D:169:THR:H	2.19	0.46
3:C:51:TYR:HA	3:C:54:LEU:HD12	1.97	0.46
30:0:1931:A:C2'	30:0:1932:G:H5'	2.44	0.46
16:P:91:LYS:NZ	30:0:816:G:OP1	2.39	0.46
30:0:107:U:C2'	30:0:108:U:H5'	2.45	0.46
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.80	0.46
29:3:42:ARG:HH11	29:3:42:ARG:HG3	1.79	0.46
30:0:1477:C:H5'	30:0:1868:G:H5'	1.97	0.46
30:0:920:C:H2'	30:0:2109:U:C2	2.51	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.48	0.46
30:0:1149:U:C5	30:0:1215:A:C5	3.03	0.46
2:B:148:PRO:HG2	2:B:158:LYS:O	2.15	0.46
11:K:21:ALA:HB1	11:K:110:LYS:O	2.14	0.46
30:0:2651:C:H2'	30:0:2652:U:O4'	2.15	0.46
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.97	0.46
1:A:109:GLU:HG2	1:A:114:ASP:OD1	2.15	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.15	0.46
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.16	0.46
30:0:292:G:H1'	30:0:360:A:N6	2.29	0.46
30:0:2296:C:H4'	30:0:2362:A:C2	2.51	0.46
31:9:3:A:H2'	41:9:9043:HOH:O	2.15	0.46
29:3:36:ILE:CG2	29:3:37:ASP:N	2.79	0.46
8:H:149:VAL:HG22	41:H:9034:HOH:O	2.13	0.46
8:H:87:LYS:HB2	8:H:87:LYS:HZ2	1.81	0.46
11:K:62:PRO:HA	11:K:65:ARG:NH2	2.31	0.46
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.30	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.14	0.46
2:B:251:VAL:HG23	2:B:253:GLN:HG3	1.97	0.46
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.46
18:R:135:ALA:O	30:0:2054:A:H4'	2.16	0.46
23:W:10:GLU:O	23:W:13:MET:HB3	2.16	0.46
14:N:29:SER:HB3	30:0:2415:A:O2'	2.16	0.46
3:C:176:ALA:HB2	30:0:1343:C:C5	2.50	0.46
4:D:18:ILE:HG12	4:D:134:LEU:CD2	2.45	0.46
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.15	0.46
13:M:52:GLN:HG2	13:M:116:ASN:CG	2.36	0.46
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.97	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.64	0.46
1:A:42:VAL:O	1:A:76:VAL:HG13	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1410:G:H3'	41:0:6433:HOH:O	2.15	0.46
16:P:88:GLN:HE22	30:0:1799:G:H21	1.63	0.46
3:C:90:HIS:HB2	41:C:8544:HOH:O	2.14	0.46
30:0:2453:G:H5'	41:0:5549:HOH:O	2.15	0.46
3:C:241:ALA:O	3:C:244:ALA:HB3	2.14	0.46
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.41	0.46
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.46
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.97	0.46
16:P:134:VAL:O	16:P:137:LEU:HB3	2.16	0.46
30:0:2838:A:H2'	30:0:2839:C:C6	2.51	0.46
1:A:27:LEU:HD11	1:A:51:ARG:HE	1.79	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.16	0.46
30:0:1971:G:H5''	41:0:7875:HOH:O	2.14	0.46
30:0:699:C:H6	30:0:744:G:O4'	1.98	0.46
5:E:7:ILE:HD11	5:E:11:VAL:C	2.36	0.46
15:O:44:ASN:CG	15:O:67:SER:HB3	2.36	0.46
30:0:1791:U:H2'	30:0:1792:C:C6	2.51	0.46
3:C:178:GLN:O	3:C:179:GLY:C	2.54	0.46
30:0:1001:U:O2'	30:0:1002:G:H5'	2.15	0.46
30:0:574:G:H2'	30:0:575:A:O4'	2.16	0.46
4:D:39:ASP:HB2	41:D:5583:HOH:O	2.15	0.46
1:A:75:GLY:HA2	26:Z:88:PHE:HA	1.98	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.96	0.46
30:0:129:A:O2'	30:0:131:A:OP1	2.32	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:791:A:H2'	30:0:792:G:O4'	2.16	0.46
13:M:45:ARG:HB2	13:M:118:TYR:CE1	2.51	0.46
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.31	0.46
30:0:558:C:H2'	30:0:559:U:H5'	1.97	0.46
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.98	0.46
30:0:566:A:C2'	30:0:567:U:H5'	2.46	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
16:P:36:THR:O	16:P:39:ASP:HB2	2.16	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.51	0.46
22:V:49:LEU:O	22:V:53:ILE:HG13	2.15	0.46
30:0:2842:G:C2'	30:0:2843:A:H5'	2.45	0.46
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.98	0.46
30:0:1130:U:H2'	30:0:1131:G:O4'	2.16	0.46
13:M:98:GLN:HB2	13:M:129:HIS:CD2	2.51	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
11:K:81:ARG:HG3	11:K:85:GLY:O	2.15	0.46
9:I:82:THR:CG2	30:0:1168:C:H5''	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:284:PHE:HB2	2:B:287:TYR:HB3	1.96	0.46
18:R:119:VAL:HG23	18:R:142:ASP:HB2	1.98	0.46
30:0:612:U:H2'	30:0:613:C:H6	1.80	0.46
30:0:1202:A:H2'	30:0:1203:G:O4'	2.16	0.46
19:S:49:VAL:HG13	19:S:66:VAL:HG13	1.96	0.46
30:0:1098:A:H2'	30:0:1099:G:O4'	2.15	0.46
2:B:238:ASN:ND2	2:B:240:GLY:H	2.11	0.46
2:B:109:LEU:HD22	2:B:145:HIS:CE1	2.51	0.46
31:9:39:U:H1'	31:9:44:A:H61	1.81	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
30:0:535:G:C5	30:0:2063:U:C4	3.04	0.46
16:P:107:GLU:C	16:P:109:ARG:H	2.19	0.46
30:0:1135:G:H5'	41:0:6761:HOH:O	2.16	0.46
30:0:111:C:O2'	30:0:112:G:H5'	2.16	0.46
14:N:164:ASP:OD1	14:N:167:ASP:OD1	2.34	0.46
17:Q:25:PRO:HB3	41:9:9006:HOH:O	2.15	0.46
6:F:49:PHE:HB2	6:F:96:ALA:HB3	1.98	0.46
31:9:74:G:C6	31:9:75:G:N7	2.84	0.46
19:S:68:LEU:HB3	19:S:72:ASP:HB2	1.97	0.46
13:M:40:ILE:HD11	13:M:130:GLU:HG2	1.97	0.46
30:0:1260:G:H3'	30:0:1261:A:C8	2.51	0.46
3:C:139:VAL:HG13	3:C:240:LEU:HD12	1.98	0.46
10:J:45:VAL:HG23	10:J:129:PHE:HD1	1.81	0.46
11:K:64:MET:HA	11:K:67:GLN:HE21	1.80	0.46
2:B:305:ASP:O	2:B:306:LYS:CB	2.63	0.46
20:T:38:ARG:HH21	30:0:306:A:P	2.38	0.46
30:0:956:G:H5'	31:9:81:C:H4'	1.98	0.46
11:K:23:ASN:HD21	11:K:107:THR:HB	1.80	0.46
30:0:1304:U:H2'	30:0:1305:C:C6	2.51	0.46
30:0:2371:G:H5'	41:0:5865:HOH:O	2.14	0.46
15:O:19:ARG:HH11	30:0:1276:U:H3'	1.81	0.46
30:0:1206:U:C6	30:0:1206:U:H5'	2.42	0.46
18:R:39:THR:O	18:R:40:ALA:C	2.55	0.46
2:B:76:THR:O	2:B:77:PRO:C	2.53	0.46
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.30	0.46
8:H:49:GLN:NE2	8:H:140:TYR:CE2	2.84	0.46
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.80	0.46
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.80	0.46
14:N:26:LEU:HD21	14:N:103:ASP:HA	1.97	0.46
30:0:2748:G:H4'	30:0:2749:U:H5'	1.98	0.46
30:0:25:A:H2'	30:0:26:U:H5'	1.98	0.46
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2760:C:H5''	41:0:6171:HOH:O	2.16	0.46
5:E:158:ASP:OD1	5:E:160:ARG:HB2	2.15	0.46
22:V:23:LEU:O	22:V:24:LYS:C	2.54	0.46
8:H:86:TYR:C	8:H:86:TYR:CD1	2.90	0.46
2:B:337:GLY:N	41:B:9013:HOH:O	2.49	0.46
30:0:1607:A:H2'	30:0:1608:G:O4'	2.16	0.46
30:0:1209:C:O2'	30:0:1210:G:H5'	2.15	0.45
16:P:115:SER:N	16:P:118:GLN:HE21	1.89	0.45
30:0:2506:A:O2'	30:0:2507:G:O5'	2.35	0.45
18:R:8:ALA:HB1	18:R:13:THR:CG2	2.35	0.45
28:2:45:ASN:HB3	28:2:46:ASP:H	1.58	0.45
6:F:8:VAL:HG13	6:F:12:LEU:HD13	1.98	0.45
1:A:135:VAL:HG13	1:A:135:VAL:O	2.16	0.45
16:P:104:LYS:HG2	16:P:137:LEU:HD23	1.98	0.45
41:N:8846:HOH:O	31:9:7:G:H5'	2.16	0.45
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.17	0.45
30:0:37:A:C2	30:0:446:G:C2	3.04	0.45
31:9:39:U:HO2'	31:9:42:C:H5	1.57	0.45
30:0:1393:A:N1	30:0:1725:C:O2'	2.43	0.45
15:O:19:ARG:NH1	30:0:1276:U:H3'	2.30	0.45
30:0:1463:U:H2'	30:0:1464:C:C6	2.51	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.45
30:0:2269:C:H2'	30:0:2270:G:O4'	2.15	0.45
30:0:1739:G:H1'	30:0:2726:U:O4	2.16	0.45
22:V:1:THR:O	22:V:3:LEU:N	2.50	0.45
3:C:2:GLN:HB2	41:C:8534:HOH:O	2.16	0.45
30:0:2507:G:H2'	30:0:2510:C:N4	2.31	0.45
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.31	0.45
30:0:544:G:C2'	30:0:545:G:H5''	2.45	0.45
30:0:820:G:H5'	30:0:821:U:C5'	2.47	0.45
25:Y:174:VAL:HA	25:Y:177:LYS:HE3	1.97	0.45
20:T:23:VAL:O	20:T:42:VAL:HG23	2.16	0.45
25:Y:106:THR:CG2	25:Y:107:PRO:HD2	2.46	0.45
30:0:425:U:H4'	41:0:7746:HOH:O	2.16	0.45
20:T:29:ALA:HA	41:T:7653:HOH:O	2.16	0.45
30:0:2087:C:C2	30:0:2658:G:C2	3.04	0.45
4:D:27:ILE:HD11	4:D:37:ALA:HB2	1.98	0.45
1:A:105:VAL:HG13	1:A:155:THR:O	2.16	0.45
3:C:193:LEU:HD23	3:C:233:THR:HG23	1.99	0.45
30:0:1183:C:H41	30:0:1192:A:P	2.39	0.45
4:D:149:ARG:HH12	14:N:15:GLU:HA	1.79	0.45
30:0:2004:U:O2	30:0:2004:U:C2'	2.64	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
33:6:76:8AN:H2	41:6:82:HOH:O	2.15	0.45
11:K:115:ARG:O	11:K:118:ALA:HB3	2.16	0.45
23:W:31:HIS:HB3	23:W:115:THR:HG21	1.98	0.45
30:0:710:G:C2'	30:0:711:G:H5'	2.47	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.98	0.45
23:W:117:ARG:HH22	30:0:1264:U:P	2.39	0.45
30:0:584:U:H3'	41:0:6928:HOH:O	2.17	0.45
25:Y:112:GLU:CD	25:Y:115:ARG:NH1	2.69	0.45
22:V:44:GLY:HA3	30:0:92:G:H4'	1.98	0.45
30:0:1361:C:H2'	30:0:1362:U:C6	2.51	0.45
30:0:1588:G:H1'	30:0:1607:A:H61	1.81	0.45
30:0:644:G:H1'	41:0:7230:HOH:O	2.16	0.45
30:0:1864:C:H2'	30:0:1865:A:O4'	2.16	0.45
30:0:228:C:H2'	30:0:229:G:H5'	1.97	0.45
30:0:1619:G:H2'	30:0:1620:C:O4'	2.15	0.45
18:R:64:SER:OG	30:0:1369:A:H5''	2.16	0.45
30:0:2560:C:H4'	41:0:7451:HOH:O	2.17	0.45
7:G:23:ILE:CD1	7:G:67:LEU:HD23	2.42	0.45
20:T:52:ARG:HD2	30:0:317:A:H5''	1.97	0.45
2:B:279:THR:HA	2:B:284:PHE:HE1	1.81	0.45
23:W:52:VAL:CG2	23:W:53:ALA:N	2.49	0.45
12:L:6:ARG:NH1	30:0:1299:G:N7	2.65	0.45
11:K:125:ALA:O	11:K:127:ALA:N	2.50	0.45
2:B:88:GLU:HB3	2:B:97:LEU:HD12	1.99	0.45
3:C:101:ASP:HA	41:C:8646:HOH:O	2.16	0.45
12:L:125:PHE:CE1	12:L:140:VAL:HG22	2.52	0.45
20:T:41:ARG:NH1	20:T:42:VAL:O	2.50	0.45
16:P:16:VAL:HG12	16:P:17:GLY:N	2.31	0.45
1:A:48:ASP:OD2	1:A:51:ARG:HG3	2.17	0.45
9:I:91:PHE:CD2	9:I:131:GLY:HA2	2.50	0.45
24:X:87:ALA:O	24:X:88:GLU:HG2	2.16	0.45
30:0:2842:G:H2'	30:0:2843:A:C5'	2.46	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
13:M:8:ILE:O	13:M:11:ALA:HB3	2.17	0.45
30:0:2894:C:O2'	30:0:2895:C:H5'	2.16	0.45
18:R:100:ASP:C	18:R:102:GLN:N	2.68	0.45
16:P:73:HIS:HE1	30:0:1789:G:O6	2.00	0.45
31:9:12:C:H4'	31:9:69:U:O2	2.17	0.45
30:0:652:G:C2	30:0:653:U:H1'	2.51	0.45
30:0:27:U:H2'	30:0:28:G:O4'	2.17	0.45
30:0:2846:C:H2'	30:0:2847:G:H8	1.80	0.45
6:F:67:ALA:HB1	6:F:72:VAL:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:82:THR:HA	41:O:4859:HOH:O	2.15	0.45
8:H:141:CYS:HB2	41:H:8997:HOH:O	2.15	0.45
11:K:132:VAL:HG11	21:U:22:VAL:HG22	1.98	0.45
30:O:1181:A:H2'	30:O:1182:C:C5'	2.47	0.45
2:B:140:LEU:HD13	2:B:175:LEU:HA	1.98	0.45
30:O:1165:G:H21	30:O:1173:A:H5''	1.82	0.45
30:O:604:G:H2'	41:O:9543:HOH:O	2.16	0.45
1:A:23:TYR:CD1	1:A:50:ALA:HB2	2.51	0.45
19:S:11:THR:H	19:S:14:ALA:HB3	1.82	0.45
14:N:73:ALA:HB1	14:N:74:PRO:HD2	1.97	0.45
26:Z:51:ALA:O	26:Z:55:SER:HB2	2.16	0.45
30:O:731:U:H2'	30:O:732:C:C6	2.52	0.45
30:O:1810:C:H2'	30:O:1811:A:O4'	2.17	0.45
14:N:72:GLU:HB3	14:N:163:PHE:CE1	2.52	0.45
30:O:1394:C:H3'	30:O:1433:G:N2	2.32	0.45
6:F:21:GLU:O	6:F:24:ARG:HG2	2.17	0.45
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.98	0.45
30:O:1889:C:H2'	30:O:1890:U:O4'	2.17	0.45
30:O:1787:C:H4'	30:O:2883:A:O4'	2.17	0.45
14:N:77:ASN:C	14:N:78:MET:CA	2.84	0.45
30:O:2506:A:O2'	30:O:2507:G:P	2.75	0.45
5:E:20:ILE:O	5:E:30:THR:HG23	2.16	0.45
11:K:101:ASN:O	11:K:102:GLU:CB	2.63	0.45
30:O:2419:U:H5''	30:O:2420:G:H5'	1.97	0.45
19:S:73:ASP:HB3	19:S:76:GLU:OE1	2.17	0.45
1:A:199:HIS:N	41:A:9110:HOH:O	2.49	0.45
30:O:1833:U:O2'	30:O:1834:C:H5'	2.16	0.45
7:G:64:ASN:OD1	30:O:1211:G:H5''	2.16	0.45
31:9:13:A:H3'	31:9:14:G:H5'	1.99	0.45
20:T:43:ASN:ND2	20:T:108:ARG:CZ	2.79	0.45
30:O:168:C:H5'	30:O:2277:U:OP1	2.16	0.45
27:1:15:THR:O	27:1:29:THR:N	2.46	0.45
30:O:24:G:N2	30:O:518:G:H1'	2.31	0.45
2:B:185:GLY:HA2	41:B:9109:HOH:O	2.15	0.45
30:O:1484:G:H2'	41:O:3021:HOH:O	2.17	0.45
30:O:116:G:H2'	30:O:117:A:C8	2.52	0.45
3:C:76:ARG:HB3	3:C:78:ARG:NH1	2.32	0.45
30:O:1831:U:O4	30:O:1845:A:H2	1.99	0.45
15:O:59:VAL:HG23	15:O:111:VAL:CG2	2.46	0.45
20:T:17:HIS:HB3	30:O:100:C:O2	2.17	0.45
12:L:66:VAL:CG2	12:L:67:ARG:N	2.78	0.45
14:N:151:ASP:OD1	14:N:154:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:69:LYS:O	30:0:2263:G:H4'	2.17	0.45
30:0:2081:A:H2'	30:0:2082:G:O4'	2.17	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.17	0.45
30:0:343:C:O2'	30:0:344:C:H5'	2.16	0.45
14:N:102:LEU:HG	14:N:104:ILE:HG23	1.98	0.45
30:0:1741:U:H5''	41:0:3669:HOH:O	2.17	0.45
22:V:43:PRO:O	22:V:46:ILE:HG22	2.16	0.45
17:Q:14:LEU:HB3	41:Q:3971:HOH:O	2.16	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.16	0.45
1:A:211:LYS:HZ2	1:A:223:ARG:HH21	1.64	0.45
3:C:193:LEU:HA	3:C:211:ASP:O	2.17	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.17	0.45
23:W:122:ARG:NH2	41:0:6133:HOH:O	2.50	0.45
31:9:1:U:H5'	31:9:121:C:O2	2.16	0.45
31:9:60:C:H2'	31:9:61:C:H6	1.80	0.45
2:B:141:ARG:CG	2:B:165:ARG:HA	2.47	0.45
17:Q:62:THR:O	17:Q:64:GLU:HG2	2.16	0.45
30:0:750:A:H2'	30:0:751:U:C6	2.51	0.45
12:L:130:ARG:HA	41:L:9020:HOH:O	2.17	0.45
29:3:65:THR:HG23	29:3:67:LEU:HG	1.99	0.45
30:0:2011:A:H5'	30:0:2013:G:C1'	2.46	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.46	0.45
30:0:12:U:C2'	30:0:13:G:H5'	2.47	0.45
20:T:27:LEU:HB2	20:T:32:ARG:HG3	1.99	0.45
8:H:9:TYR:HE2	8:H:99:ARG:O	2.00	0.45
2:B:188:HIS:HD1	2:B:188:HIS:H	1.64	0.45
30:0:325:U:H2'	30:0:326:G:H8	1.79	0.45
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.45
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.45
3:C:219:ASN:O	3:C:223:LEU:HB2	2.16	0.45
23:W:80:ASP:H	23:W:83:TRP:HB3	1.82	0.45
2:B:74:ILE:HG13	41:B:9078:HOH:O	2.16	0.45
13:M:30:GLU:O	13:M:34:GLU:HG3	2.16	0.45
30:0:2443:C:H3'	41:0:4363:HOH:O	2.17	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.45
10:J:36:VAL:HG12	10:J:37:ALA:N	2.32	0.45
30:0:2135:A:O4'	30:0:2243:C:N4	2.50	0.45
15:O:49:GLU:OE1	15:O:70:LEU:HD12	2.16	0.45
30:0:2887:G:H2'	30:0:2888:U:C6	2.52	0.45
18:R:27:HIS:O	18:R:31:ILE:HG13	2.17	0.45
26:Z:37:ARG:HD3	41:Z:8713:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:236:THR:O	3:C:237:GLU:C	2.55	0.45
29:3:73:GLU:C	29:3:75:GLY:N	2.69	0.45
2:B:113:LEU:HD21	2:B:161:VAL:HG21	1.97	0.45
2:B:297:VAL:HB	41:B:9078:HOH:O	2.17	0.45
30:0:290:C:O2'	30:0:291:C:H5'	2.16	0.45
30:0:2361:A:H2'	30:0:2362:A:C8	2.51	0.45
30:0:191:A:C4	30:0:237:G:N7	2.85	0.45
16:P:138:GLU:O	16:P:139:ARG:C	2.54	0.45
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.52	0.45
17:Q:95:GLU:HA	30:0:949:U:C4'	2.46	0.45
24:X:20:GLU:CG	24:X:21:PRO:HD2	2.45	0.45
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.49	0.45
30:0:1985:U:C2	30:0:1996:U:O4'	2.70	0.45
2:B:294:TYR:HE2	41:B:9128:HOH:O	1.99	0.45
2:B:66:GLU:OE1	2:B:328:ARG:HD2	2.17	0.45
23:W:25:ASN:OD1	30:0:1025:C:H5''	2.17	0.45
30:0:2088:C:H1'	30:0:2841:A:C2	2.52	0.45
14:N:22:GLN:HB3	41:N:8873:HOH:O	2.17	0.45
4:D:141:VAL:HG13	4:D:144:ARG:NH2	2.32	0.45
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.87	0.44
13:M:80:GLY:C	13:M:81:ARG:HD2	2.37	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.44
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.25	0.44
13:M:72:ALA:HB1	13:M:93:ARG:NE	2.32	0.44
31:9:73:A:H61	31:9:108:C:N4	2.13	0.44
1:A:94:LEU:N	1:A:94:LEU:HD23	2.31	0.44
30:0:1165:G:O2'	30:0:1174:A:C4'	2.65	0.44
30:0:1477:C:H4'	30:0:1868:G:OP1	2.17	0.44
30:0:2335:C:H2'	30:0:2336:G:H8	1.82	0.44
30:0:1031:G:O3'	30:0:1032:A:H8	2.00	0.44
30:0:2435:U:H1'	41:0:6273:HOH:O	2.17	0.44
5:E:9:GLU:HG2	41:E:7544:HOH:O	2.17	0.44
30:0:1291:A:H2	41:0:6136:HOH:O	2.00	0.44
30:0:297:U:H1'	41:0:4807:HOH:O	2.16	0.44
18:R:62:HIS:HB3	30:0:1370:G:O5'	2.16	0.44
8:H:67:ALA:HB1	8:H:159:LYS:HD3	1.98	0.44
14:N:37:ARG:HH21	14:N:105:GLY:CA	2.30	0.44
27:1:42:SER:HB3	30:0:1473:U:O4'	2.17	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.57	0.44
29:3:24:LYS:HE3	29:3:90:PHE:CE1	2.52	0.44
12:L:54:PRO:HG2	12:L:57:VAL:CG2	2.47	0.44
17:Q:61:GLY:HA3	17:Q:74:ASP:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:44:HIS:O	11:K:45:PRO:C	2.56	0.44
23:W:126:ASP:O	23:W:136:GLY:HA2	2.16	0.44
30:0:23:G:C6	30:0:24:G:N1	2.85	0.44
23:W:115:THR:HG23	41:W:5420:HOH:O	2.17	0.44
26:Z:77:GLY:C	26:Z:78:ILE:CA	2.86	0.44
23:W:56:GLU:O	23:W:143:THR:HG23	2.17	0.44
30:0:2394:A:H4'	41:0:9457:HOH:O	2.16	0.44
2:B:195:ARG:HG3	2:B:196:ALA:N	2.31	0.44
30:0:2869:G:H2'	30:0:2870:C:C6	2.52	0.44
25:Y:95:THR:O	25:Y:95:THR:HG22	2.16	0.44
25:Y:95:THR:N	25:Y:236:VAL:O	2.51	0.44
27:1:54:ALA:HB2	30:0:892:G:H5''	1.98	0.44
15:O:62:GLY:O	15:O:79:VAL:HG23	2.18	0.44
23:W:9:GLY:N	30:0:1086:A:OP1	2.50	0.44
3:C:145:GLU:CD	3:C:196:THR:HB	2.38	0.44
2:B:261:GLN:HG2	30:0:2808:U:OP1	2.17	0.44
30:0:1187:U:HO2'	30:0:1188:A:H8	1.65	0.44
24:X:41:PHE:HD2	24:X:76:ARG:HB2	1.81	0.44
30:0:2592:G:H2'	30:0:2593:C:C6	2.52	0.44
10:J:70:PHE:HE1	30:0:2676:C:C4'	2.19	0.44
18:R:39:THR:CG2	18:R:42:GLU:HG3	2.48	0.44
30:0:877:G:C2	30:0:885:G:O4'	2.70	0.44
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.33	0.44
30:0:34:C:H2'	30:0:35:U:C6	2.52	0.44
30:0:1298:U:H2'	30:0:1299:G:H8	1.81	0.44
30:0:254:C:H2'	30:0:255:A:O4'	2.18	0.44
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.44
2:B:274:GLU:HG3	2:B:292:GLY:C	2.38	0.44
30:0:812:A:H2'	30:0:813:C:O4'	2.17	0.44
19:S:67:ARG:HD3	41:0:5526:HOH:O	2.16	0.44
12:L:73:VAL:HG23	12:L:74:THR:N	2.31	0.44
10:J:57:TYR:O	10:J:61:VAL:HG23	2.18	0.44
13:M:98:GLN:HB2	13:M:129:HIS:NE2	2.32	0.44
2:B:209:LYS:HE2	41:B:9040:HOH:O	2.15	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.47	0.44
30:0:2323:G:H5'	41:0:7829:HOH:O	2.17	0.44
30:0:1021:G:O2'	30:0:1022:A:H5'	2.18	0.44
25:Y:186:ARG:HD2	41:0:5056:HOH:O	2.17	0.44
30:0:1617:C:C5	30:0:1643:C:H4'	2.53	0.44
5:E:73:PHE:O	5:E:76:VAL:HG22	2.18	0.44
30:0:1803:C:H2'	30:0:1804:A:C8	2.52	0.44
30:0:542:A:H1'	41:0:5534:HOH:O	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:77:ALA:O	3:C:78:ARG:CA	2.65	0.44
2:B:79:MET:HE3	2:B:144:THR:CG2	2.47	0.44
2:B:41:PHE:HB3	2:B:190:MET:CE	2.42	0.44
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
13:M:28:GLN:HA	13:M:31:TRP:HB2	1.98	0.44
15:O:65:LEU:HD13	30:0:746:A:N6	2.33	0.44
23:W:12:ASN:HA	30:0:1067:A:O2'	2.17	0.44
23:W:65:VAL:HA	23:W:68:THR:CG2	2.47	0.44
30:0:941:G:C5	30:0:942:U:C4	3.06	0.44
13:M:122:GLN:HB2	13:M:126:GLN:O	2.18	0.44
2:B:22:GLU:HA	2:B:205:VAL:HG21	1.98	0.44
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.82	0.44
11:K:65:ARG:C	11:K:67:GLN:H	2.19	0.44
30:0:166:A:H2'	30:0:2109:U:H5	1.83	0.44
30:0:2846:C:H4'	41:0:5931:HOH:O	2.16	0.44
30:0:1558:C:O2	30:0:1563:G:N2	2.45	0.44
12:L:98:GLU:O	12:L:99:GLU:HB2	2.16	0.44
12:L:36:ASP:HB2	41:0:5147:HOH:O	2.18	0.44
30:0:1238:C:H5'	30:0:1239:G:OP2	2.17	0.44
26:Z:34:SER:OG	30:0:797:A:H4'	2.18	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44
1:A:212:PRO:HA	30:0:1943:C:C4'	2.48	0.44
20:T:52:ARG:O	30:0:317:A:OP1	2.36	0.44
24:X:49:ARG:NH1	30:0:1385:G:O3'	2.51	0.44
18:R:88:PHE:O	18:R:91:LEU:HB3	2.17	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.63	0.44
29:3:24:LYS:HE3	29:3:90:PHE:HE1	1.83	0.44
30:0:255:A:C5	30:0:256:C:C4	3.05	0.44
2:B:217:ARG:CG	2:B:257:THR:HG22	2.44	0.44
20:T:92:ASP:OD2	30:0:335:U:H4'	2.18	0.44
9:I:91:PHE:HA	9:I:131:GLY:CA	2.47	0.44
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.32	0.44
2:B:84:LEU:HB2	2:B:182:VAL:HG21	2.00	0.44
30:0:1913:C:H2'	30:0:1914:C:C6	2.52	0.44
30:0:376:C:O5'	30:0:376:C:H6	2.00	0.44
19:S:20:PHE:CD2	19:S:20:PHE:N	2.85	0.44
17:Q:56:PHE:HE2	38:Q:8811:CL:CL	2.38	0.44
30:0:2285:G:H1	33:6:74:C:H42	1.65	0.44
10:J:41:ALA:HB2	10:J:103:VAL:CG1	2.47	0.44
6:F:31:LYS:HD2	41:0:5661:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:179:GLY:O	30:0:399:C:H5'	2.18	0.44
13:M:188:ARG:HD3	30:0:155:C:OP2	2.18	0.44
9:I:98:ASP:C	9:I:100:VAL:H	2.21	0.44
1:A:192:VAL:HG12	41:A:9070:HOH:O	2.18	0.44
30:0:1878:G:O2'	30:0:1879:U:H6	2.01	0.44
31:9:107:C:H2'	31:9:108:C:H6	1.82	0.44
23:W:4:LEU:CD2	23:W:52:VAL:HB	2.47	0.44
30:0:2889:U:H4'	30:0:2890:A:H5'	1.98	0.44
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.28	0.44
5:E:35:TYR:HB2	5:E:61:THR:HG21	2.00	0.44
30:0:2415:A:C2'	30:0:2416:G:H5'	2.47	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
15:O:96:VAL:HG13	15:O:100:GLN:CD	2.37	0.44
30:0:462:A:N6	30:0:477:A:H2	2.15	0.44
30:0:1457:U:H5	41:0:9660:HOH:O	2.00	0.44
30:0:1636:G:O2'	30:0:1637:A:H5'	2.17	0.44
30:0:362:G:O2'	30:0:363:C:H5'	2.18	0.44
30:0:1644:C:O2'	30:0:1645:U:H5'	2.18	0.44
15:O:87:THR:O	15:O:88:LYS:C	2.55	0.44
30:0:522:U:O2'	30:0:1366:C:H5'	2.17	0.44
14:N:35:VAL:HG11	31:9:6:C:H4'	1.99	0.44
1:A:88:ILE:HG21	1:A:100:PRO:HG3	1.99	0.44
4:D:104:PHE:CE2	4:D:166:ILE:HD13	2.53	0.44
20:T:48:VAL:HG22	20:T:97:ARG:C	2.37	0.44
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.18	0.44
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.51	0.44
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.44
23:W:122:ARG:NH2	41:W:5817:HOH:O	2.44	0.44
30:0:1174:A:C5	30:0:1201:C:H4'	2.52	0.44
9:I:124:VAL:O	9:I:124:VAL:HG12	2.18	0.44
8:H:54:VAL:HG12	8:H:56:GLU:O	2.17	0.44
29:3:10:TYR:CD1	30:0:2408:A:H1'	2.52	0.44
30:0:553:G:O4'	30:0:1325:G:H5'	2.18	0.44
25:Y:102:LEU:O	25:Y:227:ARG:HG3	2.18	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.52	0.44
13:M:46:LEU:HD11	30:0:263:U:O3'	2.17	0.44
25:Y:212:ARG:HB3	41:Y:8835:HOH:O	2.18	0.44
30:0:970:U:H2'	41:0:7156:HOH:O	2.16	0.44
3:C:177:GLY:HA2	41:0:3551:HOH:O	2.17	0.44
30:0:1826:C:O2'	30:0:1827:G:H5'	2.17	0.44
1:A:157:GLY:HA2	26:Z:103:VAL:CG1	2.48	0.44
13:M:74:LYS:HG3	41:M:8878:HOH:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1894:C:N4	30:0:1939:U:H2'	2.33	0.44
9:I:71:ALA:O	9:I:75:LYS:HE3	2.17	0.44
30:0:844:A:C6	30:0:882:A:C6	3.06	0.44
9:I:97:VAL:CG1	9:I:101:LYS:HE3	2.28	0.44
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.44
4:D:45:THR:OG1	4:D:46:GLY:N	2.48	0.44
3:C:225:PRO:CD	3:C:231:ARG:HD2	2.48	0.44
1:A:190:ARG:NE	41:A:9070:HOH:O	2.51	0.44
7:G:64:ASN:ND2	7:G:64:ASN:N	2.65	0.44
30:0:236:A:H8	30:0:236:A:OP1	2.00	0.44
17:Q:16:ASN:HD21	17:Q:45:PRO:CD	2.29	0.44
2:B:141:ARG:CB	2:B:165:ARG:HA	2.47	0.44
30:0:2634:G:H5'	41:0:3070:HOH:O	2.16	0.44
30:0:1318:A:H4'	30:0:1343:C:H4'	2.00	0.44
30:0:834:G:H4'	30:0:835:U:OP2	2.18	0.44
4:D:99:ASP:CB	4:D:103:ASN:HB2	2.48	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.01	0.44
14:N:21:HIS:CD2	30:0:2369:A:H5''	2.53	0.44
5:E:90:HIS:CD2	30:0:2694:A:H5''	2.53	0.44
2:B:109:LEU:HA	2:B:159:PRO:HG2	1.99	0.44
1:A:71:PRO:HA	1:A:158:VAL:O	2.18	0.44
30:0:70:A:H4'	41:0:4782:HOH:O	2.17	0.44
30:0:349:U:H2'	30:0:350:G:O4'	2.17	0.44
8:H:77:ILE:O	8:H:78:LYS:C	2.55	0.44
2:B:251:VAL:HG22	41:0:5183:HOH:O	2.18	0.44
30:0:2344:G:N3	30:0:2344:G:H2'	2.32	0.44
30:0:1586:G:O2'	30:0:1587:U:H5'	2.17	0.44
30:0:1534:C:O2'	30:0:1656:A:OP1	2.24	0.44
19:S:21:GLN:NE2	30:0:1508:C:H5'	2.32	0.44
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.90	0.44
13:M:36:ALA:O	13:M:65:VAL:HG13	2.18	0.44
5:E:105:GLU:HG2	5:E:113:PRO:HB3	2.00	0.44
22:V:1:THR:C	22:V:3:LEU:H	2.20	0.44
14:N:79:PRO:HG3	14:N:143:ARG:C	2.38	0.44
31:9:56:A:C3'	31:9:57:A:H5''	2.48	0.44
13:M:9:ARG:NH2	30:0:378:A:OP1	2.42	0.44
30:0:1845:A:O2'	30:0:1846:U:H5'	2.17	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HB3	2.00	0.44
28:2:48:ASP:O	28:2:49:GLU:CB	2.65	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
22:V:5:VAL:CG1	22:V:9:ARG:NH1	2.80	0.44
13:M:163:LEU:O	13:M:168:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:132:HIS:CE1	2:B:171:VAL:CG2	3.01	0.44
2:B:17:LYS:O	2:B:260:HIS:CD2	2.71	0.44
1:A:171:LYS:NZ	41:A:8996:HOH:O	2.51	0.44
12:L:149:ARG:O	12:L:150:GLN:HB2	2.17	0.44
16:P:107:GLU:O	16:P:109:ARG:N	2.50	0.44
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.18	0.44
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.18	0.44
30:0:491:C:H2'	30:0:492:C:C6	2.53	0.44
30:0:2379:G:N3	30:0:2418:G:H2'	2.33	0.44
7:G:63:ARG:HG2	30:0:1210:G:OP1	2.18	0.43
14:N:79:PRO:HG3	14:N:144:GLY:CA	2.47	0.43
21:U:45:GLU:O	21:U:46:ALA:C	2.56	0.43
26:Z:70:ARG:NH2	30:0:1602:C:OP2	2.50	0.43
28:2:14:LEU:HD13	28:2:47:THR:CG2	2.48	0.43
5:E:119:HIS:HB2	5:E:144:THR:OG1	2.17	0.43
2:B:74:ILE:CD1	2:B:309:VAL:HG21	2.39	0.43
1:A:194:MET:CE	1:A:199:HIS:HB2	2.48	0.43
30:0:1267:C:O2'	30:0:1268:C:H5'	2.18	0.43
8:H:19:ARG:HG2	41:H:8976:HOH:O	2.18	0.43
30:0:2907:C:H2'	30:0:2908:A:O4'	2.17	0.43
14:N:5:ARG:HB2	41:0:7582:HOH:O	2.18	0.43
30:0:1776:A:C8	30:0:1778:A:O4'	2.71	0.43
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.83	0.43
12:L:66:VAL:HG23	12:L:67:ARG:H	1.80	0.43
30:0:2106:C:H2'	30:0:2107:U:C6	2.53	0.43
3:C:51:TYR:HE1	27:1:55:GLY:O	2.00	0.43
4:D:103:ASN:OD1	4:D:133:ASN:ND2	2.51	0.43
30:0:23:G:H1'	30:0:520:A:H61	1.83	0.43
10:J:11:ILE:HD13	10:J:109:TYR:CD1	2.52	0.43
30:0:619:U:H2'	30:0:629:A:O4'	2.18	0.43
30:0:2031:C:H2'	30:0:2032:U:C6	2.53	0.43
3:C:181:ALA:HB2	30:0:30:U:OP2	2.18	0.43
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.17	0.43
30:0:1902:G:N2	30:0:1936:C:C2	2.86	0.43
12:L:18:HIS:HB2	30:0:903:U:O4	2.18	0.43
15:O:47:ARG:NH1	15:O:47:ARG:HG3	2.32	0.43
30:0:2059:U:H2'	30:0:2060:A:C8	2.53	0.43
30:0:2616:G:N3	30:0:2616:G:H2'	2.33	0.43
27:1:5:THR:N	27:1:6:PRO:HD2	2.32	0.43
30:0:1096:U:H5''	30:0:1258:G:O6	2.17	0.43
12:L:5:LYS:HE3	30:0:1354:G:O6	2.17	0.43
4:D:146:LYS:NZ	14:N:38:LYS:HE2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:21:LEU:HD22	23:W:26:ILE:HD13	2.01	0.43
31:9:5:G:O2'	31:9:6:C:H5'	2.18	0.43
1:A:11:ARG:HH12	1:A:13:THR:CG2	2.31	0.43
11:K:96:VAL:CG2	11:K:109:LEU:HD22	2.48	0.43
30:0:2361:A:H8	30:0:2361:A:H5'	1.83	0.43
8:H:36:MET:HB3	8:H:73:ASN:HD21	1.83	0.43
30:0:2402:A:H1'	41:0:4055:HOH:O	2.17	0.43
3:C:7:ASP:OD1	3:C:11:ASN:O	2.36	0.43
30:0:2346:C:H6	30:0:2346:C:O5'	2.02	0.43
30:0:637:C:H2'	30:0:638:C:H6	1.83	0.43
30:0:697:G:H4'	30:0:730:G:O3'	2.19	0.43
1:A:128:LEU:HG	41:A:9054:HOH:O	2.18	0.43
30:0:2019:A:H5'	41:0:5405:HOH:O	2.17	0.43
6:F:119:ARG:HD3	6:F:119:ARG:OXT	2.18	0.43
22:V:4:HIS:O	22:V:8:ILE:HG13	2.17	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.18	0.43
30:0:2619:UR3:H2'	30:0:2620:U:C6	2.53	0.43
30:0:702:G:O2'	30:0:703:G:H5'	2.18	0.43
14:N:46:GLN:NE2	31:9:5:G:N3	2.65	0.43
30:0:1667:A:H2'	30:0:1668:U:C6	2.52	0.43
12:L:35:ARG:NE	12:L:46:LEU:CD2	2.81	0.43
2:B:51:VAL:HG13	2:B:53:LEU:CD1	2.49	0.43
14:N:82:TYR:CD2	14:N:82:TYR:C	2.92	0.43
30:0:1878:G:O2'	30:0:1879:U:C6	2.65	0.43
30:0:603:A:H5''	30:0:604:G:OP1	2.18	0.43
12:L:56:LYS:CE	30:0:2443:C:H1'	2.48	0.43
14:N:155:GLU:O	14:N:156:GLU:CG	2.66	0.43
15:O:25:VAL:HG23	15:O:26:TRP:N	2.33	0.43
27:1:36:SER:O	27:1:46:ARG:HD3	2.17	0.43
30:0:2332:A:H3'	30:0:2333:G:C8	2.51	0.43
13:M:5:TYR:O	13:M:8:ILE:N	2.51	0.43
30:0:1914:C:H2'	30:0:1915:U:H6	1.82	0.43
30:0:923:A:H2'	41:0:6521:HOH:O	2.17	0.43
20:T:47:THR:HB	20:T:100:ASP:HB3	2.00	0.43
30:0:1768:C:H2'	30:0:1769:C:O4'	2.18	0.43
31:9:70:U:H2'	31:9:71:C:O4'	2.19	0.43
1:A:123:GLY:HA3	1:A:162:GLY:HA2	2.01	0.43
30:0:1119:G:N2	30:0:1246:A:N1	2.66	0.43
13:M:24:GLN:HE21	13:M:27:ARG:HD2	1.83	0.43
3:C:7:ASP:C	3:C:9:ASP:H	2.21	0.43
1:A:43:VAL:HG21	1:A:59:GLU:CG	2.48	0.43
29:3:42:ARG:HD2	41:3:9003:HOH:O	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:21:ASP:O	7:G:22:ALA:C	2.56	0.43
25:Y:150:LEU:HB3	41:Y:8857:HOH:O	2.17	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:2120:U:H2'	30:0:2121:G:O4'	2.18	0.43
30:0:2345:A:N6	41:0:6637:HOH:O	2.49	0.43
18:R:65:GLY:HA3	41:R:9001:HOH:O	2.18	0.43
29:3:69:TYR:O	29:3:77:ALA:HA	2.17	0.43
30:0:657:G:H2'	30:0:658:C:C6	2.54	0.43
23:W:110:GLN:NE2	23:W:110:GLN:CA	2.81	0.43
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.18	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.17	0.43
18:R:114:VAL:HA	18:R:144:GLU:O	2.18	0.43
2:B:77:PRO:O	2:B:78:PRO:CA	2.67	0.43
10:J:131:THR:CG2	10:J:133:GLY:H	2.31	0.43
30:0:292:G:H8	30:0:292:G:O5'	2.01	0.43
2:B:27:ASN:ND2	2:B:27:ASN:C	2.71	0.43
30:0:2852:A:H4'	30:0:2853:U:H5	1.83	0.43
30:0:235:C:O2'	30:0:236:A:H2'	2.18	0.43
25:Y:100:ARG:HE	25:Y:234:VAL:HG21	1.84	0.43
23:W:38:THR:HG22	23:W:39:ASP:H	1.81	0.43
3:C:174:ILE:HD11	30:0:338:C:H4'	2.00	0.43
9:I:96:SER:H	9:I:99:GLN:CD	2.21	0.43
30:0:463:A:H3'	41:0:7246:HOH:O	2.19	0.43
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.48	0.43
12:L:30:ARG:HD3	30:0:164:G:H4'	2.00	0.43
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.81	0.43
31:9:95:C:O2'	31:9:96:C:H5'	2.19	0.43
30:0:1359:U:O5'	30:0:1360:C:H5''	2.17	0.43
31:9:39:U:H3'	31:9:40:C:H5''	2.00	0.43
2:B:277:GLU:N	2:B:278:PRO:CD	2.81	0.43
30:0:957:A:H8	30:0:957:A:O5'	2.01	0.43
30:0:960:G:N3	30:0:960:G:H3'	2.33	0.43
30:0:1006:A:N1	30:0:2311:A:H1'	2.34	0.43
1:A:213:LYS:CE	30:0:1942:A:H5''	2.48	0.43
28:2:35:ARG:N	41:2:2691:HOH:O	2.50	0.43
9:I:98:ASP:HA	9:I:101:LYS:HD2	2.01	0.43
9:I:111:LEU:HD22	9:I:122:GLU:OE1	2.18	0.43
7:G:12:ILE:HG22	7:G:17:GLN:HE21	1.81	0.43
22:V:19:GLU:HG3	22:V:56:ILE:HD11	2.01	0.43
30:0:1171:A:N6	30:0:1172:G:C2	2.87	0.43
27:1:15:THR:O	27:1:28:HIS:HA	2.18	0.43
5:E:93:MET:CE	5:E:165:GLY:H	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:29:C:O2'	30:0:30:U:H5'	2.19	0.43
12:L:18:HIS:CD2	30:0:902:G:N7	2.87	0.43
30:0:1359:U:O4	30:0:2101:A:H5''	2.19	0.43
13:M:50:ARG:HH11	13:M:50:ARG:HG2	1.84	0.43
4:D:107:GLY:O	30:0:2338:G:O3'	2.37	0.43
12:L:72:ASN:O	12:L:76:LEU:HG	2.19	0.43
18:R:125:ARG:HG2	41:R:8948:HOH:O	2.18	0.43
21:U:38:ASN:O	21:U:42:LEU:HG	2.18	0.43
24:X:70:ILE:O	24:X:70:ILE:HG23	2.18	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
3:C:236:THR:HB	3:C:239:ALA:CB	2.48	0.43
24:X:85:VAL:HG12	24:X:86:GLU:N	2.34	0.43
30:0:1167:G:H1	30:0:1179:C:H42	1.67	0.43
15:O:106:PRO:HG2	15:O:107:GLU:OE2	2.18	0.43
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.18	0.43
12:L:144:ASP:O	12:L:147:GLU:HB2	2.18	0.43
30:0:854:G:H5''	30:0:855:U:OP1	2.18	0.43
30:0:1299:G:N2	41:0:5541:HOH:O	2.52	0.43
30:0:1766:U:H2'	30:0:1776:A:N6	2.34	0.43
33:6:75:C:H5''	33:6:76:8AN:O1P	2.18	0.43
2:B:87:TYR:CE2	2:B:96:PRO:HG3	2.54	0.43
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
5:E:93:MET:HE3	5:E:93:MET:HB2	1.81	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.17	0.43
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.82	0.43
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.84	0.43
3:C:240:LEU:O	3:C:240:LEU:HD23	2.18	0.43
6:F:99:THR:HA	41:F:3461:HOH:O	2.18	0.43
9:I:119:ALA:O	9:I:123:VAL:HG23	2.18	0.43
10:J:88:PRO:O	10:J:94:GLY:HA3	2.18	0.43
2:B:29:TRP:CH2	2:B:164:THR:HA	2.53	0.43
30:0:936:C:H42	30:0:1034:G:H1	1.66	0.43
30:0:1077:G:H2'	30:0:1080:C:N4	2.34	0.43
15:O:15:LYS:HD3	15:O:19:ARG:NH2	2.34	0.43
14:N:41:LYS:HD3	41:9:9061:HOH:O	2.18	0.43
30:0:581:G:O2'	30:0:582:U:H5'	2.18	0.43
26:Z:97:THR:O	26:Z:98:PRO:C	2.56	0.43
4:D:140:ARG:NH1	31:9:45:A:OP1	2.50	0.43
7:G:71:LEU:O	7:G:73:ASP:N	2.52	0.43
5:E:2:ARG:HH21	5:E:48:VAL:HG21	1.82	0.43
20:T:48:VAL:HG22	20:T:97:ARG:O	2.19	0.43
2:B:51:VAL:HG22	2:B:327:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:101:LEU:HD13	20:T:112:LEU:HD11	2.01	0.43
10:J:74:ARG:CG	10:J:74:ARG:HH11	2.31	0.43
31:9:73:A:N6	31:9:108:C:H42	2.15	0.43
22:V:45:ARG:C	22:V:47:LYS:N	2.72	0.43
20:T:21:LYS:HA	20:T:24:ARG:CD	2.49	0.43
30:0:790:A:H1'	30:0:1710:A:C2'	2.49	0.43
6:F:1:PRO:HB2	41:M:8924:HOH:O	2.17	0.43
30:0:758:A:H2'	30:0:759:C:O4'	2.19	0.43
14:N:72:GLU:HG2	14:N:163:PHE:HD1	1.84	0.43
27:1:48:TYR:CZ	30:0:773:A:H4'	2.54	0.43
30:0:2569:A:H2'	30:0:2570:G:O4'	2.18	0.43
30:0:2752:C:O2'	30:0:2753:G:H5'	2.19	0.43
2:B:103:ASP:HB2	41:B:9064:HOH:O	2.17	0.43
30:0:234:A:H4'	30:0:437:A:O4'	2.19	0.43
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.43
30:0:2005:G:N2	30:0:2008:U:H1'	2.34	0.43
30:0:1473:U:O2'	30:0:1474:C:H5''	2.18	0.43
9:I:112:LEU:HG	41:I:6070:HOH:O	2.19	0.43
14:N:11:ARG:HG2	14:N:15:GLU:OE2	2.18	0.43
30:0:2073:G:N1	30:0:2607:U:C6	2.86	0.43
2:B:87:TYR:O	2:B:138:GLY:N	2.42	0.43
30:0:710:G:N2	30:0:719:C:C2	2.87	0.43
25:Y:184:GLU:HG2	25:Y:229:LEU:HD11	2.01	0.43
6:F:22:VAL:HG23	6:F:104:ALA:HB2	2.00	0.43
2:B:145:HIS:CD2	2:B:146:THR:O	2.72	0.43
30:0:1503:U:H2'	30:0:1504:A:O4'	2.18	0.43
30:0:812:A:H2'	30:0:813:C:H6	1.83	0.43
10:J:123:ARG:NH1	10:J:129:PHE:HZ	2.16	0.43
22:V:27:LEU:CA	22:V:49:LEU:HD13	2.48	0.43
30:0:1476:A:O2'	30:0:1477:C:H5'	2.18	0.43
27:1:53:LYS:O	27:1:54:ALA:C	2.57	0.43
30:0:1616:A:H5''	30:0:1617:C:OP1	2.18	0.43
4:D:48:MET:HE2	4:D:48:MET:HB3	1.89	0.43
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.19	0.43
24:X:85:VAL:HG12	24:X:86:GLU:H	1.83	0.43
18:R:46:TYR:CD2	18:R:47:LEU:HD23	2.50	0.43
20:T:48:VAL:HG22	20:T:96:VAL:HG13	2.00	0.43
4:D:156:ARG:HH11	4:D:156:ARG:HG3	1.84	0.43
10:J:130:VAL:CG1	10:J:131:THR:N	2.82	0.43
14:N:24:LEU:CD1	17:Q:26:PRO:HB3	2.49	0.43
30:0:1217:G:O2'	30:0:1218:U:H5'	2.19	0.43
16:P:20:ARG:HD2	30:0:1718:G:OP2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:462:A:H2'	41:0:5741:HOH:O	2.19	0.43
1:A:171:LYS:HG3	1:A:174:ASN:ND2	2.33	0.43
1:A:231:LYS:O	1:A:232:ARG:HB3	2.19	0.43
30:0:228:C:C2'	30:0:229:G:H5'	2.49	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.43
25:Y:216:ARG:O	25:Y:219:GLU:HG2	2.19	0.43
16:P:50:GLN:HG2	41:P:6904:HOH:O	2.19	0.43
14:N:37:ARG:HA	14:N:37:ARG:HD3	1.90	0.42
30:0:542:A:H2'	30:0:543:G:O4'	2.19	0.42
12:L:145:LEU:O	12:L:145:LEU:HD23	2.19	0.42
30:0:1972:U:H2'	30:0:1973:A:H5'	2.01	0.42
31:9:107:C:H2'	31:9:108:C:C6	2.54	0.42
33:6:75:C:H2'	41:6:80:HOH:O	2.19	0.42
3:C:149:LYS:NZ	30:0:328:U:OP1	2.52	0.42
30:0:1819:G:H2'	30:0:1820:G:C4'	2.49	0.42
30:0:431:G:O2'	30:0:432:G:H5'	2.19	0.42
8:H:87:LYS:CB	8:H:87:LYS:NZ	2.82	0.42
15:O:49:GLU:O	15:O:72:LYS:HE3	2.19	0.42
30:0:1724:U:H5''	41:0:4609:HOH:O	2.19	0.42
30:0:2029:C:H2'	30:0:2030:A:O4'	2.19	0.42
30:0:1245:C:H6	30:0:1245:C:O5'	2.01	0.42
30:0:1767:A:H3'	41:0:5918:HOH:O	2.19	0.42
8:H:83:GLU:O	8:H:84:GLY:C	2.58	0.42
30:0:2241:C:O2'	30:0:2242:U:H5'	2.19	0.42
30:0:1925:G:O2'	30:0:1926:G:H5'	2.19	0.42
30:0:51:G:O2'	30:0:52:A:H5'	2.19	0.42
10:J:20:GLY:HA3	30:0:1242:A:O3'	2.20	0.42
1:A:95:PRO:C	1:A:97:ALA:H	2.23	0.42
11:K:8:VAL:CG1	11:K:9:THR:N	2.81	0.42
2:B:280:VAL:HG11	2:B:335:ASN:OD1	2.19	0.42
10:J:93:ARG:HH11	10:J:93:ARG:CB	2.27	0.42
12:L:144:ASP:HA	12:L:147:GLU:HG3	2.01	0.42
17:Q:43:ILE:O	17:Q:45:PRO:HD3	2.20	0.42
16:P:104:LYS:HA	16:P:104:LYS:HD2	1.91	0.42
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.42
23:W:125:HIS:CD2	23:W:125:HIS:H	2.37	0.42
30:0:1632:A:C2'	30:0:1633:C:H5'	2.48	0.42
30:0:1503:U:H2'	30:0:1504:A:C5'	2.48	0.42
30:0:639:A:H2'	30:0:640:G:C8	2.54	0.42
17:Q:86:VAL:HG13	17:Q:91:LEU:HD11	2.00	0.42
15:O:39:THR:O	15:O:115:ARG:NH2	2.51	0.42
23:W:66:LEU:HD23	23:W:66:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:105:ASN:HD21	15:O:109:SER:H	1.66	0.42
30:0:67:A:H2'	41:0:5002:HOH:O	2.19	0.42
23:W:47:LYS:HE2	30:0:944:G:O3'	2.19	0.42
12:L:16:GLY:HA2	30:0:1294:A:O3'	2.19	0.42
29:3:63:LYS:NZ	30:0:2460:A:OP1	2.51	0.42
3:C:142:ASP:CG	3:C:238:SER:HG	2.23	0.42
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.53	0.42
7:G:12:ILE:HG22	7:G:12:ILE:O	2.17	0.42
31:9:14:G:C6	31:9:68:G:C2	3.07	0.42
14:N:14:ARG:NH2	31:9:13:A:N3	2.66	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.81	0.42
13:M:57:LYS:HZ2	13:M:144:ASP:CG	2.23	0.42
23:W:52:VAL:HG22	23:W:52:VAL:H	1.45	0.42
8:H:61:ARG:O	8:H:64:SER:N	2.43	0.42
3:C:246:ARG:NH2	30:0:677:C:H4'	2.34	0.42
27:1:8:GLN:HE22	27:1:11:LYS:HZ1	1.66	0.42
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.54	0.42
14:N:179:LEU:HD23	14:N:184:ILE:HD12	2.01	0.42
7:G:19:GLU:O	7:G:20:VAL:C	2.57	0.42
27:1:45:ARG:NH2	41:1:2086:HOH:O	2.50	0.42
13:M:163:LEU:HD21	30:0:188:C:H5''	2.00	0.42
13:M:95:LYS:HE2	30:0:157:G:H4'	2.01	0.42
30:0:1971:G:N2	30:0:2009:G:H2'	2.34	0.42
30:0:699:C:C6	30:0:744:G:O4'	2.73	0.42
10:J:45:VAL:CG2	10:J:129:PHE:CD1	3.02	0.42
30:0:432:G:O2'	30:0:433:C:H5'	2.19	0.42
4:D:10:PHE:CD1	4:D:11:HIS:N	2.87	0.42
6:F:24:ARG:HG3	6:F:25:ASP:N	2.34	0.42
30:0:1362:U:O2'	30:0:1363:G:H5'	2.19	0.42
4:D:143:LYS:O	31:9:45:A:H4'	2.19	0.42
2:B:48:MET:O	2:B:49:THR:HG23	2.19	0.42
8:H:157:TYR:CD1	8:H:157:TYR:C	2.92	0.42
5:E:16:ASP:O	5:E:17:HIS:HB2	2.19	0.42
30:0:1566:C:H2'	30:0:1567:G:C8	2.54	0.42
30:0:2647:C:H1'	41:0:7245:HOH:O	2.19	0.42
30:0:2464:C:H5''	30:0:2465:A:OP1	2.20	0.42
12:L:101:ASP:C	12:L:103:ALA:H	2.23	0.42
6:F:109:GLU:O	6:F:113:ASP:OD2	2.37	0.42
3:C:27:ARG:HG2	3:C:29:ASP:OD1	2.19	0.42
9:I:130:LEU:HA	41:I:7210:HOH:O	2.19	0.42
2:B:162:MET:CE	2:B:310:ARG:HH11	2.31	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:611:U:H2'	30:0:612:U:C6	2.54	0.42
14:N:119:GLN:HG2	14:N:123:ILE:HD11	2.01	0.42
2:B:243:ASN:ND2	30:0:2607:U:OP2	2.45	0.42
1:A:135:VAL:HG21	1:A:147:ARG:NH1	2.35	0.42
10:J:77:GLY:O	10:J:78:ILE:CA	2.68	0.42
21:U:56:ARG:HD2	21:U:56:ARG:O	2.20	0.42
30:0:1058:A:H2'	30:0:1060:C:H5'	2.00	0.42
11:K:4:LEU:HD23	11:K:4:LEU:HA	1.86	0.42
30:0:564:G:H2'	30:0:592:G:C6	2.54	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
9:I:114:TYR:CD1	9:I:114:TYR:N	2.87	0.42
13:M:71:SER:CB	13:M:92:THR:HG22	2.47	0.42
1:A:120:ARG:HD3	41:A:9015:HOH:O	2.19	0.42
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.92	0.42
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.38	0.42
30:0:640:G:C6	30:0:641:G:N7	2.87	0.42
3:C:40:ALA:O	3:C:43:LYS:HB2	2.19	0.42
11:K:28:GLU:OE2	11:K:58:THR:HG21	2.19	0.42
15:O:18:ALA:HB2	15:O:27:GLY:N	2.34	0.42
9:I:67:VAL:HG13	9:I:68:PRO:HD2	2.00	0.42
17:Q:34:ASP:HB2	17:Q:37:GLU:HG3	2.00	0.42
30:0:2067:A:H2'	30:0:2068:G:O4'	2.18	0.42
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.52	0.42
24:X:76:ARG:NH1	24:X:76:ARG:HG3	2.31	0.42
18:R:119:VAL:CG1	18:R:119:VAL:O	2.67	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:559:U:H2'	30:0:560:U:O4'	2.20	0.42
30:0:1299:G:H2'	30:0:1300:G:O4'	2.20	0.42
3:C:174:ILE:HD12	30:0:338:C:H4'	1.99	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
12:L:27:ARG:HH22	12:L:30:ARG:HG2	1.81	0.42
13:M:84:LYS:HZ1	30:0:391:U:P	2.42	0.42
21:U:20:MET:CG	21:U:28:THR:HG23	2.50	0.42
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.19	0.42
8:H:77:ILE:O	8:H:78:LYS:CA	2.68	0.42
30:0:1821:A:O2'	30:0:1822:A:H5'	2.20	0.42
28:2:18:ASN:ND2	28:2:18:ASN:O	2.52	0.42
30:0:2604:A:H4'	41:0:9401:HOH:O	2.20	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
23:W:82:GLU:O	23:W:86:GLU:HG3	2.19	0.42
30:0:2470:A:H5''	41:0:4137:HOH:O	2.19	0.42
41:Y:8878:HOH:O	30:0:1355:A:H5''	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:74:VAL:HG21	11:K:96:VAL:HG23	2.01	0.42
14:N:40:ASN:HB2	41:9:9062:HOH:O	2.20	0.42
17:Q:27:GLN:HB2	41:9:9006:HOH:O	2.19	0.42
31:9:24:U:H3'	31:9:25:G:H5'	2.01	0.42
3:C:46:TYR:CE1	3:C:92:PRO:HB3	2.55	0.42
28:2:43:ARG:HH21	30:0:1685:A:C4'	2.32	0.42
30:0:2611:G:H5'	30:0:2613:G:C8	2.55	0.42
25:Y:231:PRO:HG2	25:Y:233:TYR:CE1	2.55	0.42
30:0:370:G:O2'	30:0:371:U:H5'	2.19	0.42
2:B:112:THR:HG23	2:B:158:LYS:NZ	2.35	0.42
30:0:2039:A:H4'	30:0:2760:C:O2'	2.20	0.42
13:M:193:LYS:HB3	30:0:392:U:H5''	2.01	0.42
30:0:2791:U:C4	30:0:2794:G:O6	2.73	0.42
8:H:53:ILE:HG23	8:H:133:GLY:O	2.20	0.42
3:C:68:ALA:O	3:C:70:VAL:N	2.52	0.42
12:L:65:ASP:CG	12:L:111:ALA:HB3	2.39	0.42
13:M:78:LYS:HE2	30:0:870:G:OP1	2.19	0.42
13:M:61:ILE:N	13:M:61:ILE:CD1	2.81	0.42
2:B:52:VAL:O	2:B:53:LEU:HD12	2.19	0.42
30:0:2355:G:H5''	30:0:2356:A:OP2	2.20	0.42
25:Y:100:ARG:HE	25:Y:234:VAL:CG2	2.32	0.42
23:W:13:MET:HA	41:W:4944:HOH:O	2.20	0.42
22:V:45:ARG:HA	22:V:48:GLU:HB2	2.01	0.42
30:0:2819:C:H2'	30:0:2820:A:H8	1.84	0.42
14:N:103:ASP:OD1	14:N:103:ASP:C	2.57	0.42
2:B:238:ASN:HD21	30:0:2609:G:N2	2.17	0.42
30:0:1684:A:H5'	30:0:1692:C:OP1	2.19	0.42
5:E:88:TYR:CD1	5:E:91:PHE:O	2.71	0.42
30:0:353:G:O2'	30:0:354:A:H5'	2.19	0.42
30:0:1548:U:O2'	30:0:1798:C:O2	2.32	0.42
2:B:205:VAL:O	2:B:307:ARG:NE	2.53	0.42
20:T:30:ASP:O	20:T:33:GLU:N	2.53	0.42
2:B:7:ARG:CZ	2:B:11:LEU:HD13	2.49	0.42
16:P:109:ARG:NH1	16:P:119:TYR:CE2	2.88	0.42
3:C:21:VAL:HG22	41:C:8598:HOH:O	2.20	0.42
30:0:2673:U:C4	30:0:2674:G:C6	3.07	0.42
1:A:163:GLY:CA	1:A:166:ASP:OD2	2.68	0.42
30:0:2079:G:H2'	30:0:2080:G:O4'	2.19	0.42
15:O:89:ILE:HG21	15:O:95:ALA:HB2	2.01	0.42
16:P:81:LYS:HG2	41:O:3439:HOH:O	2.19	0.42
22:V:1:THR:CB	30:0:93:C:H5''	2.46	0.42
16:P:115:SER:O	16:P:117:SER:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:175:LEU:HA	14:N:175:LEU:HD12	1.86	0.42
4:D:94:ALA:HA	4:D:174:VAL:C	2.40	0.42
30:0:2506:A:H2'	30:0:2506:A:O5'	2.20	0.42
9:I:87:PRO:HB3	9:I:129:SER:O	2.19	0.42
13:M:171:ARG:HD3	30:0:156:C:C5'	2.43	0.42
20:T:9:LYS:HE3	20:T:13:ARG:NH2	2.34	0.42
31:9:14:G:O2'	31:9:15:C:H5'	2.19	0.42
18:R:82:GLU:CG	18:R:83:LYS:H	2.29	0.42
31:9:72:C:H2'	31:9:73:A:H8	1.85	0.42
24:X:30:MET:HG2	30:0:1384:C:H5'	2.00	0.42
30:0:1504:A:O2'	30:0:1506:U:OP2	2.38	0.42
29:3:42:ARG:NH1	30:0:396:U:H5'	2.35	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.50	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.42
29:3:1:MET:N	29:3:87:ARG:O	2.49	0.42
2:B:54:VAL:O	2:B:55:ASN:C	2.56	0.42
30:0:312:U:O5'	30:0:312:U:H6	2.02	0.42
22:V:59:ILE:HA	22:V:62:GLU:HB2	2.02	0.42
26:Z:96:GLU:OE1	26:Z:104:ARG:NH2	2.53	0.42
4:D:55:LYS:O	4:D:56:ARG:HB2	2.20	0.42
11:K:69:LEU:HD12	11:K:97:ILE:HD13	2.02	0.42
30:0:2510:C:H5'	30:0:2511:A:OP2	2.20	0.42
24:X:49:ARG:O	24:X:49:ARG:CG	2.58	0.42
30:0:1603:A:H5'	30:0:1605:G:C4'	2.49	0.42
29:3:71:CYS:O	29:3:75:GLY:HA2	2.20	0.42
1:A:34:ASP:O	1:A:36:ASP:N	2.53	0.42
14:N:165:ALA:C	14:N:167:ASP:H	2.22	0.42
10:J:75:PRO:HD3	10:J:136:SER:CB	2.50	0.42
30:0:1044:C:H5	41:0:7418:HOH:O	2.03	0.42
2:B:244:PRO:HB3	30:0:1234:U:C2	2.55	0.42
8:H:59:GLN:HE21	8:H:129:ARG:CG	2.32	0.42
18:R:82:GLU:HB2	18:R:86:LYS:HE3	2.02	0.42
30:0:1972:U:C2'	30:0:1973:A:H5''	2.50	0.42
30:0:1165:G:N2	30:0:1173:A:H5''	2.35	0.42
20:T:24:ARG:NH1	20:T:24:ARG:HG2	2.35	0.42
30:0:2106:C:H1'	30:0:2484:U:C2	2.55	0.42
11:K:66:ARG:NH2	30:0:1994:A:OP2	2.42	0.42
2:B:56:ASP:HB3	2:B:322:ARG:NH2	2.35	0.42
3:C:150:THR:OG1	30:0:327:A:H2'	2.19	0.42
12:L:18:HIS:HD2	30:0:902:G:N7	2.18	0.42
3:C:63:SER:OG	30:0:2101:A:H2'	2.20	0.42
25:Y:212:ARG:HB2	30:0:1315:G:C4	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:51:LYS:C	29:3:53:SER:H	2.23	0.42
6:F:118:LEU:O	6:F:119:ARG:OXT	2.38	0.42
16:P:107:GLU:C	16:P:109:ARG:N	2.73	0.42
30:0:644:G:N3	30:0:644:G:H5'	2.34	0.42
26:Z:34:SER:HB3	41:Z:8723:HOH:O	2.18	0.42
14:N:111:PRO:HD2	31:9:37:C:H4'	2.02	0.42
16:P:18:LYS:O	16:P:21:VAL:HG13	2.20	0.42
30:0:912:A:H4'	41:0:6799:HOH:O	2.19	0.42
30:0:461:C:H2'	41:0:4868:HOH:O	2.20	0.42
21:U:47:ARG:HG3	41:U:4381:HOH:O	2.20	0.42
30:0:1664:A:OP1	30:0:1664:A:H8	2.03	0.42
30:0:75:U:H2'	30:0:76:G:C8	2.55	0.42
25:Y:178:HIS:CG	25:Y:179:PRO:HD2	2.55	0.42
30:0:1141:U:O2'	30:0:1142:C:H5'	2.19	0.42
14:N:44:ARG:NH2	31:9:4:G:O2'	2.52	0.42
6:F:39:SER:O	6:F:43:GLY:N	2.53	0.42
19:S:29:ASP:OD1	19:S:31:ARG:HG3	2.20	0.42
10:J:47:THR:HB	30:0:1244:U:C6	2.55	0.42
14:N:79:PRO:HA	14:N:142:THR:O	2.20	0.42
5:E:69:ILE:O	5:E:72:MET:HB2	2.19	0.42
20:T:51:LEU:O	20:T:52:ARG:HG2	2.20	0.42
4:D:138:GLY:HA2	31:9:29:C:O3'	2.20	0.42
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.42
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.55	0.42
23:W:4:LEU:O	23:W:32:CYS:HA	2.19	0.42
30:0:2519:C:O2'	30:0:2520:G:H5'	2.20	0.42
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.01	0.42
11:K:66:ARG:HH22	30:0:1994:A:P	2.40	0.42
9:I:117:THR:O	9:I:120:ALA:HB3	2.19	0.42
12:L:133:VAL:HA	41:L:9038:HOH:O	2.20	0.42
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.85	0.42
13:M:122:GLN:HB3	13:M:127:LYS:HG2	2.02	0.42
9:I:88:GLN:HE21	9:I:128:THR:CG2	2.33	0.42
30:0:696:C:O2'	30:0:697:G:H5'	2.20	0.42
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.01	0.42
30:0:432:G:H2'	30:0:433:C:C6	2.55	0.42
3:C:94:THR:C	3:C:96:LYS:H	2.22	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
26:Z:37:ARG:HD2	30:0:818:A:O2'	2.20	0.42
2:B:66:GLU:HG2	41:B:9125:HOH:O	2.20	0.42
8:H:157:TYR:C	8:H:157:TYR:HD1	2.24	0.42
30:0:2462:G:O4'	30:0:2464:C:C2	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2133:U:H4'	30:0:2134:G:H5'	2.02	0.42
2:B:334:SER:HG	30:0:2861:G:HO2'	1.62	0.42
30:0:2467:A:H5'	41:0:5160:HOH:O	2.19	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
3:C:236:THR:N	3:C:239:ALA:HB3	2.28	0.41
9:I:94:ASP:O	9:I:95:LEU:HD23	2.20	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.20	0.41
15:O:21:SER:CB	15:O:106:PRO:HB2	2.50	0.41
30:0:271:C:N4	30:0:378:A:H2	2.06	0.41
13:M:9:ARG:HG3	41:0:4079:HOH:O	2.20	0.41
2:B:190:MET:CE	2:B:194:PHE:CD1	3.02	0.41
10:J:42:GLU:O	10:J:131:THR:HG23	2.20	0.41
30:0:289:G:O2'	30:0:290:C:H5'	2.19	0.41
2:B:175:LEU:C	2:B:175:LEU:CD2	2.88	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.20	0.41
13:M:31:TRP:CA	13:M:34:GLU:HG3	2.48	0.41
2:B:217:ARG:HB2	2:B:257:THR:HG21	2.01	0.41
14:N:182:GLY:O	14:N:183:ASP:C	2.59	0.41
18:R:29:LYS:HD3	41:0:5581:HOH:O	2.20	0.41
30:0:2896:A:C2'	30:0:2896:A:N3	2.83	0.41
1:A:56:ALA:O	1:A:68:ILE:N	2.53	0.41
2:B:274:GLU:HG3	2:B:292:GLY:HA2	2.02	0.41
3:C:81:PRO:HD3	41:C:8554:HOH:O	2.20	0.41
30:0:1153:C:N3	30:0:2786:G:O6	2.52	0.41
20:T:68:ASP:HB2	41:T:4787:HOH:O	2.20	0.41
30:0:25:A:C2'	30:0:26:U:H5'	2.50	0.41
25:Y:112:GLU:HA	25:Y:112:GLU:OE1	2.20	0.41
30:0:163:U:O3'	30:0:896:C:H4'	2.20	0.41
18:R:61:GLN:HG2	18:R:62:HIS:CD2	2.55	0.41
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.84	0.41
18:R:122:GLN:HB3	18:R:138:SER:HB2	2.01	0.41
30:0:1844:C:H6	30:0:1844:C:O5'	2.03	0.41
14:N:127:LEU:HB2	41:N:8856:HOH:O	2.19	0.41
30:0:310:U:H2'	30:0:311:C:C6	2.54	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.53	0.41
8:H:160:ILE:HD11	8:H:164:CYS:SG	2.60	0.41
16:P:133:SER:HA	41:P:1882:HOH:O	2.20	0.41
23:W:92:ASP:OD2	23:W:94:SER:HB2	2.19	0.41
31:9:77:A:N1	31:9:103:A:H5''	2.35	0.41
13:M:102:GLU:CD	13:M:164:THR:HG21	2.41	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:116:PHE:O	14:N:119:GLN:HB3	2.20	0.41
17:Q:30:VAL:O	17:Q:31:GLU:C	2.59	0.41
30:0:2072:G:O2'	30:0:2489:G:N2	2.52	0.41
23:W:10:GLU:HG2	41:0:3876:HOH:O	2.19	0.41
3:C:7:ASP:C	3:C:9:ASP:N	2.74	0.41
4:D:101:THR:HG22	4:D:101:THR:O	2.21	0.41
13:M:157:ASP:O	13:M:158:ARG:C	2.58	0.41
13:M:99:ARG:NE	13:M:167:GLY:HA2	2.35	0.41
3:C:184:ARG:HD2	30:0:1306:U:H5''	2.02	0.41
13:M:82:ARG:O	13:M:83:SER:C	2.59	0.41
30:0:2281:C:O2'	30:0:2282:U:H5'	2.20	0.41
30:0:432:G:H3'	41:0:8000:HOH:O	2.18	0.41
30:0:1131:G:H5'	31:9:91:C:O4'	2.21	0.41
8:H:153:PHE:HD1	8:H:166:ILE:HG23	1.84	0.41
9:I:67:VAL:CG1	9:I:68:PRO:HD2	2.50	0.41
17:Q:68:GLY:HA3	30:0:2404:G:C5'	2.50	0.41
10:J:52:GLN:HE21	30:0:1119:G:H5'	1.84	0.41
14:N:77:ASN:O	14:N:78:MET:CA	2.68	0.41
3:C:223:LEU:HA	3:C:223:LEU:HD12	1.94	0.41
30:0:506:G:N2	30:0:509:A:H5'	2.16	0.41
4:D:23:VAL:HG22	4:D:73:VAL:HB	2.02	0.41
2:B:335:ASN:HA	41:0:4561:HOH:O	2.20	0.41
1:A:38:ILE:HD11	1:A:62:ASP:OD1	2.21	0.41
1:A:208:HIS:O	1:A:208:HIS:CG	2.74	0.41
31:9:3:A:N6	31:9:22:G:H1'	2.35	0.41
1:A:35:GLY:C	1:A:37:VAL:H	2.23	0.41
30:0:2649:A:C8	30:0:2649:A:H5'	2.55	0.41
3:C:93:LYS:HD2	30:0:646:G:O4'	2.20	0.41
30:0:1741:U:O2'	30:0:2723:G:H4'	2.20	0.41
30:0:1741:U:H5'	30:0:1742:A:OP1	2.20	0.41
30:0:2398:A:O2'	30:0:2428:G:H4'	2.20	0.41
3:C:22:PHE:HA	3:C:116:ALA:HA	2.01	0.41
30:0:11:A:N3	30:0:11:A:H2'	2.36	0.41
30:0:921:G:H4'	30:0:924:G:C6	2.55	0.41
4:D:42:GLY:N	41:D:5828:HOH:O	2.53	0.41
30:0:497:A:H2'	30:0:498:A:C5'	2.51	0.41
14:N:91:ARG:HD3	41:N:8811:HOH:O	2.20	0.41
30:0:600:G:N2	30:0:601:G:H1'	2.35	0.41
11:K:79:PRO:HG3	11:K:89:LYS:HB3	2.01	0.41
16:P:115:SER:C	16:P:117:SER:N	2.73	0.41
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.01	0.41
30:0:558:C:C2'	30:0:559:U:C5'	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:246:ARG:CB	3:C:246:ARG:HH11	2.32	0.41
19:S:32:ALA:HA	19:S:36:GLU:OE1	2.20	0.41
11:K:125:ALA:C	11:K:127:ALA:N	2.69	0.41
30:0:2265:U:H2'	30:0:2266:A:C8	2.56	0.41
10:J:126:ASN:HA	38:J:8801:CL:CL	2.57	0.41
14:N:33:ARG:NH1	14:N:103:ASP:OD2	2.53	0.41
30:0:1526:A:H4'	30:0:1527:A:C5'	2.50	0.41
30:0:1416:G:H2'	30:0:1417:G:C5'	2.50	0.41
2:B:266:ASN:OD1	2:B:317:PRO:HA	2.20	0.41
30:0:553:G:C2'	30:0:554:G:H5'	2.50	0.41
30:0:2783:A:H2'	30:0:2784:A:C8	2.55	0.41
10:J:45:VAL:HG22	10:J:46:ILE:N	2.35	0.41
30:0:1588:G:C6	30:0:1589:G:C6	3.08	0.41
10:J:64:GLY:HA3	38:J:8821:CL:CL	2.57	0.41
30:0:287:C:H2'	30:0:288:A:C8	2.55	0.41
12:L:41:HIS:CD2	30:0:926:A:O2'	2.73	0.41
30:0:2095:A:OP1	30:0:2096:A:H4'	2.20	0.41
16:P:135:ALA:HB2	41:P:4754:HOH:O	2.20	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.51	0.41
13:M:139:PRO:C	13:M:141:ILE:N	2.71	0.41
20:T:51:LEU:O	20:T:52:ARG:NH1	2.52	0.41
30:0:111:C:H2'	30:0:112:G:H5'	2.03	0.41
30:0:1212:C:H2'	30:0:1213:C:H5'	2.02	0.41
30:0:282:C:H2'	30:0:283:U:O4'	2.20	0.41
17:Q:11:ARG:HD3	41:Q:5620:HOH:O	2.20	0.41
14:N:5:ARG:HD3	41:0:7778:HOH:O	2.20	0.41
17:Q:94:GLN:HG2	17:Q:95:GLU:OE1	2.21	0.41
2:B:141:ARG:HG2	2:B:165:ARG:CA	2.49	0.41
30:0:2669:U:H2'	30:0:2670:G:C8	2.55	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.86	0.41
30:0:407:A:H5'	41:0:6858:HOH:O	2.20	0.41
3:C:98:ARG:NH1	41:C:8560:HOH:O	2.53	0.41
17:Q:47:VAL:HB	17:Q:90:HIS:CE1	2.55	0.41
30:0:2847:G:O2'	30:0:2848:G:H5'	2.20	0.41
2:B:195:ARG:HD2	2:B:324:ASP:OD1	2.20	0.41
23:W:9:GLY:H	30:0:1086:A:P	2.42	0.41
30:0:154:C:H2'	30:0:155:C:C6	2.55	0.41
30:0:390:G:H5'	41:0:3451:HOH:O	2.20	0.41
10:J:143:LYS:HG3	10:J:145:TRP:CE2	2.56	0.41
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.41
2:B:321:PRO:HG3	41:B:9072:HOH:O	2.19	0.41
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:1:26:SER:CB	27:1:36:SER:HB2	2.51	0.41
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.20	0.41
11:K:64:MET:HA	11:K:67:GLN:NE2	2.36	0.41
30:0:1033:C:H2'	30:0:1034:G:C5'	2.51	0.41
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.51	0.41
12:L:98:GLU:O	12:L:99:GLU:CB	2.67	0.41
30:0:581:G:H2'	30:0:582:U:H6	1.85	0.41
30:0:75:U:H2'	30:0:76:G:H8	1.86	0.41
30:0:2133:U:H4'	30:0:2134:G:C5'	2.51	0.41
30:0:2758:G:H2'	30:0:2759:C:C6	2.56	0.41
30:0:2022:A:H5''	30:0:2023:G:OP2	2.21	0.41
30:0:1576:G:H2'	30:0:1577:U:C6	2.55	0.41
4:D:29:HIS:HB2	41:D:2768:HOH:O	2.20	0.41
30:0:1513:C:H2'	30:0:1514:C:H6	1.85	0.41
30:0:1205:U:H2'	30:0:1206:U:H5'	2.00	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
11:K:113:ILE:HG22	11:K:114:ALA:H	1.86	0.41
5:E:2:ARG:NH2	5:E:48:VAL:HG21	2.36	0.41
30:0:111:C:H2'	30:0:112:G:C5'	2.50	0.41
18:R:132:ARG:HD3	41:0:3121:HOH:O	2.20	0.41
18:R:119:VAL:HG21	18:R:142:ASP:OD1	2.20	0.41
30:0:293:A:P	30:0:358:G:H22	2.44	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.19	0.41
8:H:48:VAL:O	8:H:140:TYR:HA	2.21	0.41
1:A:228:ILE:O	1:A:229:ALA:C	2.58	0.41
3:C:51:TYR:CD1	27:1:56:GLU:HB2	2.56	0.41
30:0:400:C:H2'	30:0:401:C:H6	1.86	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
30:0:1684:A:O2'	30:0:1685:A:H5''	2.20	0.41
20:T:94:SER:OG	30:0:334:G:N2	2.54	0.41
30:0:1839:A:C5'	30:0:2643:G:H4'	2.51	0.41
30:0:2332:A:H5'	30:0:2333:G:OP2	2.21	0.41
20:T:32:ARG:NH1	20:T:38:ARG:NH1	2.69	0.41
8:H:143:VAL:CG2	8:H:173:GLU:HG2	2.51	0.41
17:Q:47:VAL:O	17:Q:51:ARG:NE	2.48	0.41
14:N:69:TYR:CD1	14:N:69:TYR:N	2.89	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.55	0.41
19:S:80:ARG:HA	41:S:8538:HOH:O	2.21	0.41
30:0:1065:G:H2'	30:0:1066:U:C6	2.56	0.41
24:X:41:PHE:CZ	24:X:74:ALA:HB3	2.56	0.41
5:E:40:VAL:HA	5:E:48:VAL:O	2.21	0.41
21:U:52:THR:HB	21:U:55:ALA:H	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.41
29:3:20:HIS:CD2	29:3:71:CYS:HA	2.56	0.41
27:1:20:ARG:HH21	30:0:120:A:H5'	1.85	0.41
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	2.02	0.41
10:J:131:THR:HG22	10:J:134:GLU:N	2.28	0.41
27:1:25:LYS:CG	27:1:25:LYS:O	2.67	0.41
30:0:1170:U:O2'	30:0:1172:G:N7	2.49	0.41
17:Q:40:HIS:HE1	30:0:949:U:O2'	2.04	0.41
24:X:23:HIS:C	24:X:24:LYS:HG3	2.41	0.41
30:0:727:G:H5'	30:0:728:C:OP2	2.21	0.41
30:0:2867:G:H2'	30:0:2868:C:C6	2.56	0.41
12:L:27:ARG:NE	41:L:8980:HOH:O	2.39	0.41
30:0:1736:A:H1'	41:0:9381:HOH:O	2.21	0.41
30:0:537:G:H4'	30:0:538:C:O5'	2.21	0.41
30:0:705:C:H3'	30:0:706:G:C8	2.55	0.41
3:C:123:LEU:HD11	41:C:8660:HOH:O	2.20	0.41
30:0:240:C:H1'	30:0:431:G:N2	2.35	0.41
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.35	0.41
29:3:47:GLY:HA2	30:0:2121:G:H4'	2.01	0.41
30:0:52:A:C2	30:0:110:C:C2	3.08	0.41
30:0:215:A:N1	30:0:393:G:H1'	2.36	0.41
4:D:128:LEU:HB2	41:D:6007:HOH:O	2.19	0.41
30:0:1522:A:H2'	30:0:1523:G:H5'	2.03	0.41
10:J:91:LYS:O	10:J:92:GLN:C	2.58	0.41
30:0:1118:A:H3'	30:0:1119:G:H5''	2.03	0.41
1:A:105:VAL:HG12	1:A:106:CYS:H	1.83	0.41
3:C:194:PHE:HA	3:C:234:VAL:CG1	2.47	0.41
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.61	0.41
13:M:20:LEU:HA	13:M:23:LEU:HB2	2.03	0.41
20:T:52:ARG:HH22	30:0:308:U:H2'	1.85	0.41
9:I:130:LEU:HB2	9:I:132:VAL:HG23	2.03	0.41
30:0:1211:G:H2'	30:0:1212:C:H6	1.85	0.41
17:Q:31:GLU:OE1	17:Q:31:GLU:HA	2.21	0.41
20:T:1:SER:H3	20:T:7:GLN:HE21	1.69	0.41
12:L:145:LEU:O	12:L:148:GLU:HG3	2.20	0.41
30:0:1973:A:H2'	30:0:1974:G:O4'	2.21	0.41
29:3:60:LYS:HG3	41:0:9354:HOH:O	2.21	0.41
18:R:94:ASN:ND2	30:0:500:G:O2'	2.47	0.41
30:0:1343:C:H2'	30:0:1344:G:O5'	2.21	0.41
30:0:2305:A:H4'	30:0:2392:C:C6	2.56	0.41
23:W:130:HIS:C	23:W:136:GLY:HA3	2.40	0.41
10:J:107:ASN:HD22	10:J:108:PRO:N	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:31:HIS:HB3	23:W:115:THR:CG2	2.51	0.41
15:O:25:VAL:HG23	15:O:26:TRP:CE3	2.56	0.41
3:C:123:LEU:O	3:C:125:ALA:N	2.54	0.41
30:0:1573:A:N7	30:0:1574:C:C2	2.89	0.41
30:0:2531:U:C2'	30:0:2532:A:H5'	2.51	0.41
30:0:1358:A:N7	30:0:1360:C:C2	2.89	0.41
30:0:1421:C:H2'	30:0:1422:U:H6	1.86	0.41
30:0:1423:C:O2'	30:0:1424:A:H5'	2.21	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.52	0.41
6:F:59:ILE:HD13	30:0:263:U:O4'	2.20	0.41
2:B:286:ASN:O	2:B:306:LYS:HE3	2.21	0.41
30:0:2474:A:H4'	30:0:2475:C:O5'	2.21	0.41
30:0:1456:C:H2'	30:0:1457:U:C6	2.56	0.41
6:F:24:ARG:HG3	6:F:25:ASP:H	1.86	0.41
30:0:116:G:H2'	30:0:117:A:H8	1.86	0.41
23:W:23:MET:C	23:W:25:ASN:H	2.22	0.41
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.41
30:0:491:C:H2'	30:0:492:C:H6	1.86	0.41
16:P:98:ILE:HG21	30:0:1597:A:H5''	2.02	0.41
30:0:919:U:H5'	30:0:2465:A:O2'	2.21	0.41
30:0:2397:G:H2'	30:0:2398:A:C8	2.56	0.41
30:0:2096:A:H2'	30:0:2539:U:O4'	2.21	0.41
30:0:1757:U:H6	30:0:1757:U:O5'	2.03	0.41
1:A:235:ARG:NH1	41:A:9014:HOH:O	2.53	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
30:0:10:U:O4	30:0:532:A:OP2	2.39	0.41
30:0:2573:G:O2'	30:0:2574:G:H5'	2.20	0.41
30:0:2111:G:H2'	30:0:2112:A:O4'	2.21	0.41
4:D:158:ASN:HB2	4:D:161:ASP:HB2	2.02	0.41
16:P:28:GLN:HB2	41:P:6051:HOH:O	2.20	0.41
30:0:113:A:H3'	30:0:114:A:C5'	2.50	0.41
30:0:1207:A:H5'	30:0:1208:C:OP2	2.21	0.41
30:0:544:G:H2'	30:0:545:G:C5'	2.51	0.41
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.56	0.41
9:I:95:LEU:HG	9:I:132:VAL:CG1	2.51	0.41
18:R:84:ALA:O	18:R:88:PHE:HD1	2.04	0.41
14:N:165:ALA:HA	41:N:8823:HOH:O	2.21	0.41
16:P:59:ARG:O	16:P:62:ALA:HB3	2.20	0.41
30:0:907:A:H4'	30:0:1328:A:C2	2.56	0.41
17:Q:15:LYS:HD3	30:0:2364:A:H5''	2.02	0.41
2:B:221:GLN:HB2	41:B:9055:HOH:O	2.21	0.41
11:K:6:ALA:HB3	11:K:116:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:S:41:VAL:HG21	19:S:66:VAL:HG21	2.03	0.41
31:9:3:A:C2	31:9:21:G:N3	2.89	0.41
24:X:20:GLU:HG3	24:X:21:PRO:HD2	2.03	0.41
30:0:2326:C:H4'	30:0:2412:G:O4'	2.21	0.41
28:2:21:VAL:O	28:2:22:PRO:C	2.59	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:2032:U:O2'	30:0:2033:G:H5''	2.21	0.41
30:0:1220:U:O2'	30:0:1221:G:H5'	2.20	0.41
1:A:141:PRO:HG2	30:0:1855:G:O6	2.20	0.41
13:M:5:TYR:O	13:M:7:TYR:N	2.54	0.41
30:0:574:G:O2'	30:0:575:A:H5'	2.21	0.41
30:0:287:C:H2'	30:0:288:A:H8	1.86	0.41
2:B:71:VAL:HG11	2:B:296:LEU:HD22	2.02	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
1:A:164:ARG:HB2	26:Z:92:SER:OG	2.21	0.41
3:C:133:ARG:HD2	41:C:8613:HOH:O	2.21	0.41
19:S:7:HIS:HA	19:S:8:PRO:HD3	1.92	0.41
13:M:54:TYR:CG	13:M:55:LYS:N	2.89	0.41
5:E:15:GLN:CG	5:E:20:ILE:HG12	2.48	0.40
3:C:78:ARG:O	3:C:79:ARG:HB3	2.21	0.40
13:M:72:ALA:CB	13:M:93:ARG:NE	2.84	0.40
30:0:820:G:H5'	30:0:821:U:H5'	2.03	0.40
20:T:43:ASN:C	20:T:45:GLY:N	2.72	0.40
30:0:2851:G:H2'	30:0:2852:A:H5'	2.00	0.40
3:C:136:VAL:HG22	3:C:137:PRO:HA	2.03	0.40
2:B:215:VAL:N	2:B:220:VAL:HG22	2.36	0.40
8:H:170:ARG:HD2	41:H:8992:HOH:O	2.21	0.40
2:B:223:ARG:NE	2:B:232:TRP:HB3	2.35	0.40
26:Z:48:ARG:O	26:Z:51:ALA:HB3	2.21	0.40
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.40
30:0:1359:U:C5	30:0:2101:A:C8	3.10	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.89	0.40
30:0:1797:A:H2'	30:0:1799:G:O5'	2.21	0.40
30:0:1588:G:H1'	30:0:1607:A:N6	2.37	0.40
30:0:1739:G:O2'	30:0:1740:U:H5'	2.21	0.40
30:0:1065:G:H2'	30:0:1066:U:O4'	2.21	0.40
30:0:2057:U:O5'	30:0:2057:U:H6	2.03	0.40
20:T:75:GLU:HB3	41:T:4772:HOH:O	2.21	0.40
30:0:85:C:H3'	30:0:86:A:H2'	2.03	0.40
2:B:233:ARG:HD2	41:0:9321:HOH:O	2.21	0.40
23:W:59:GLN:NE2	23:W:97:ALA:HB3	2.36	0.40
30:0:2656:G:O2'	30:0:2657:G:H5'	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:267:G:H2'	30:0:268:U:O4'	2.20	0.40
13:M:191:GLY:O	30:0:175:G:H5''	2.21	0.40
9:I:132:VAL:HG12	9:I:132:VAL:O	2.21	0.40
9:I:70:THR:O	9:I:74:ILE:HG13	2.22	0.40
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.56	0.40
30:0:1552:G:N2	30:0:1634:G:H1'	2.36	0.40
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.19	0.40
8:H:43:ALA:HB1	8:H:140:TYR:CE2	2.56	0.40
30:0:451:C:C2'	30:0:452:G:H5'	2.51	0.40
20:T:21:LYS:HA	20:T:24:ARG:HD2	2.03	0.40
30:0:632:A:OP2	30:0:2534:C:O2'	2.34	0.40
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.40
23:W:115:THR:CG2	23:W:116:LEU:N	2.84	0.40
30:0:69:A:C3'	30:0:69:A:C8	3.04	0.40
30:0:2831:C:H2'	30:0:2832:C:C5'	2.51	0.40
30:0:1041:U:H4'	30:0:1295:G:H5'	2.02	0.40
29:3:42:ARG:NH1	29:3:42:ARG:HG3	2.36	0.40
30:0:297:U:H6	30:0:297:U:O5'	2.03	0.40
30:0:233:U:H2'	30:0:234:A:O4'	2.21	0.40
30:0:1724:U:H2'	41:0:5552:HOH:O	2.21	0.40
29:3:86:GLY:HA3	30:0:2318:C:OP1	2.21	0.40
30:0:2800:A:H5'	30:0:2801:A:OP2	2.21	0.40
30:0:2563:U:H2'	30:0:2565:C:O5'	2.21	0.40
10:J:47:THR:HB	30:0:1244:U:H6	1.85	0.40
14:N:143:ARG:NH2	14:N:169:PRO:HB2	2.35	0.40
30:0:36:C:C2	30:0:447:A:C2	3.10	0.40
20:T:2:LYS:HE2	41:T:2822:HOH:O	2.21	0.40
30:0:80:A:H4'	30:0:81:G:O5'	2.22	0.40
2:B:215:VAL:HG11	2:B:234:ARG:NH2	2.36	0.40
30:0:745:G:H5''	30:0:746:A:OP1	2.20	0.40
30:0:190:G:O2'	30:0:204:A:N3	2.46	0.40
5:E:36:PRO:CD	10:J:127:ILE:HG13	2.52	0.40
30:0:1445:G:H21	30:0:1678:A:H1'	1.84	0.40
30:0:1270:U:H2'	30:0:1271:A:H8	1.87	0.40
30:0:426:G:H5''	41:0:9419:HOH:O	2.21	0.40
8:H:142:ASN:O	8:H:144:GLU:N	2.53	0.40
30:0:653:U:H3	30:0:752:G:H1	1.70	0.40
5:E:70:GLU:O	5:E:73:PHE:HB2	2.21	0.40
15:O:87:THR:O	15:O:91:GLN:HG3	2.20	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.21	0.40
2:B:70:PRO:HG3	30:0:2719:A:C2	2.57	0.40
30:0:2685:C:O2'	30:0:2686:C:H5'	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:26:MET:HE1	41:0:9290:HOH:O	2.20	0.40
7:G:23:ILE:O	7:G:27:ILE:HG13	2.21	0.40
29:3:6:ARG:HB3	29:3:20:HIS:O	2.21	0.40
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.11	0.40
2:B:267:LYS:HA	41:0:3465:HOH:O	2.22	0.40
4:D:170:TYR:CD1	4:D:170:TYR:N	2.89	0.40
30:0:2852:A:H4'	30:0:2853:U:C5	2.57	0.40
2:B:229:ARG:NH2	30:0:1753:C:O2	2.38	0.40
6:F:26:THR:HG21	6:F:102:GLY:O	2.20	0.40
30:0:168:C:H6	30:0:168:C:O5'	2.05	0.40
30:0:661:G:C5	30:0:686:A:C2	3.10	0.40
12:L:130:ARG:O	12:L:132:LYS:N	2.54	0.40
19:S:45:TYR:HE2	19:S:81:ILE:HG12	1.86	0.40
30:0:17:G:H2'	30:0:18:C:H6	1.85	0.40
8:H:82:GLU:O	8:H:83:GLU:HG3	2.22	0.40
15:O:4:ASN:HA	15:O:5:PRO:HD3	1.88	0.40
30:0:2325:U:O2'	30:0:2411:C:H1'	2.21	0.40
30:0:1114:A:H2'	30:0:1115:U:H6	1.86	0.40
18:R:43:ALA:O	18:R:46:TYR:HB3	2.22	0.40
2:B:51:VAL:HG23	2:B:329:TYR:O	2.21	0.40
25:Y:100:ARG:HD2	25:Y:232:THR:HB	2.03	0.40
23:W:54:PHE:CZ	23:W:140:LYS:HB2	2.57	0.40
17:Q:16:ASN:ND2	17:Q:45:PRO:CG	2.84	0.40
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.54	0.40
31:9:1:U:O3'	31:9:3:A:H5''	2.21	0.40
20:T:16:LEU:HD12	30:0:100:C:H5'	2.02	0.40
30:0:1228:C:H2'	30:0:1229:C:O4'	2.21	0.40
12:L:104:ASP:O	12:L:105:TYR:HB3	2.21	0.40
30:0:1688:G:C6	30:0:1692:C:C6	3.09	0.40
30:0:69:A:H3'	30:0:69:A:C8	2.56	0.40
1:A:2:ARG:HG3	1:A:197:VAL:HG22	2.03	0.40
26:Z:54:GLU:HA	26:Z:57:MET:CE	2.50	0.40
30:0:2824:C:H5''	30:0:2825:C:H5'	2.04	0.40
10:J:71:TYR:HA	10:J:72:PRO:HD2	1.89	0.40
29:3:40:ARG:HG3	29:3:52:PHE:CD2	2.57	0.40
14:N:41:LYS:HE3	41:9:9020:HOH:O	2.22	0.40
30:0:2604:A:H5'	41:0:6629:HOH:O	2.22	0.40
29:3:91:GLN:O	29:3:92:GLU:HB2	2.22	0.40
2:B:298:LYS:HG2	41:0:6362:HOH:O	2.21	0.40
30:0:862:U:O2'	30:0:863:G:H5'	2.21	0.40
18:R:2:ILE:HG22	30:0:21:G:H4'	2.03	0.40
30:0:2551:C:O2'	30:0:2552:C:H5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	
1	A	233/240 (97%)	198 (85%)	25 (11%)	10 (4%)	4	21
2	B	333/338 (98%)	285 (86%)	41 (12%)	7 (2%)	11	45
3	C	242/246 (98%)	202 (84%)	32 (13%)	8 (3%)	6	29
4	D	132/177 (75%)	87 (66%)	35 (26%)	10 (8%)	2	6
5	E	168/178 (94%)	150 (89%)	17 (10%)	1 (1%)	33	79
6	F	115/120 (96%)	94 (82%)	15 (13%)	6 (5%)	3	16
7	G	25/348 (7%)	15 (60%)	7 (28%)	3 (12%)	1	2
8	H	154/177 (87%)	125 (81%)	23 (15%)	6 (4%)	5	23
9	I	66/162 (41%)	43 (65%)	18 (27%)	5 (8%)	2	6
10	J	138/145 (95%)	120 (87%)	15 (11%)	3 (2%)	10	43
11	K	128/132 (97%)	115 (90%)	8 (6%)	5 (4%)	5	23
12	L	139/165 (84%)	106 (76%)	27 (19%)	6 (4%)	4	21
13	M	190/196 (97%)	170 (90%)	16 (8%)	4 (2%)	11	45
14	N	182/187 (97%)	153 (84%)	19 (10%)	10 (6%)	3	14
15	O	111/116 (96%)	92 (83%)	19 (17%)	0	100	100
16	P	139/149 (93%)	129 (93%)	8 (6%)	2 (1%)	16	58
17	Q	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	4	20
18	R	146/155 (94%)	131 (90%)	12 (8%)	3 (2%)	11	45
19	S	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	18	60
20	T	115/120 (96%)	95 (83%)	17 (15%)	3 (3%)	8	37
21	U	51/67 (76%)	45 (88%)	4 (8%)	2 (4%)	5	23
22	V	63/71 (89%)	53 (84%)	9 (14%)	1 (2%)	14	54
23	W	150/154 (97%)	131 (87%)	19 (13%)	0	100	100
24	X	78/92 (85%)	68 (87%)	7 (9%)	3 (4%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	140/240 (58%)	128 (91%)	11 (8%)	1 (1%)	30	76
26	Z	69/116 (60%)	51 (74%)	13 (19%)	5 (7%)	2	7
27	1	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	12	49
28	2	42/50 (84%)	34 (81%)	8 (19%)	0	100	100
29	3	88/92 (96%)	77 (88%)	9 (10%)	2 (2%)	10	41
All	All	3659/4471 (82%)	3087 (84%)	460 (13%)	112 (3%)	7	31

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	ASP
1	A	37	VAL
1	A	208	HIS
2	B	181	ILE
4	D	16	PRO
4	D	27	ILE
4	D	171	ASP
6	F	101	ALA
9	I	113	SER
12	L	80	ASP
13	M	83	SER
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
24	X	87	ALA
26	Z	44	ARG
26	Z	105	ARG
29	3	56	PRO
1	A	205	GLY
2	B	291	ASP
3	C	69	HIS
6	F	27	GLY
8	H	84	GLY
9	I	124	VAL
12	L	82	ALA
14	N	165	ALA
20	T	44	ALA
20	T	53	GLY
21	U	55	ALA

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Mol	Chain	Res	Type
22	V	43	PRO
24	X	81	GLY
26	Z	59	GLU
1	A	24	LYS
1	A	119	ALA
3	C	8	LEU
3	C	121	ALA
4	D	28	GLY
4	D	60	GLU
4	D	61	PHE
4	D	137	PRO
4	D	147	ALA
5	E	164	ASP
6	F	100	ASP
7	G	72	ASP
8	H	71	SER
8	H	82	GLU
9	I	128	THR
10	J	15	ARG
10	J	76	ASP
11	K	65	ARG
11	K	126	SER
12	L	21	ARG
14	N	65	ASP
14	N	74	PRO
14	N	164	ASP
14	N	167	ASP
14	N	182	GLY
16	P	19	ASN
16	P	108	LEU
17	Q	23	THR
17	Q	48	PRO
19	S	4	VAL
21	U	46	ALA
24	X	70	ILE
2	B	55	ASN
2	B	185	GLY
4	D	56	ARG
6	F	61	MET
6	F	64	PRO
8	H	70	LEU
8	H	143	VAL

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Mol	Chain	Res	Type
8	H	145	ASP
12	L	50	GLY
12	L	102	ASP
13	M	6	SER
13	M	35	GLY
18	R	114	VAL
20	T	30	ASP
29	3	52	PHE
2	B	2	GLN
3	C	232	LEU
3	C	234	VAL
4	D	46	GLY
9	I	73	LEU
11	K	66	ARG
12	L	131	GLU
17	Q	31	GLU
18	R	20	GLU
26	Z	66	CYS
27	1	54	ALA
1	A	204	GLY
2	B	182	VAL
3	C	95	GLU
6	F	59	ILE
11	K	102	GLU
13	M	88	VAL
17	Q	54	PRO
18	R	32	ALA
25	Y	182	PHE
1	A	192	VAL
3	C	124	VAL
10	J	18	ILE
26	Z	67	GLY
2	B	30	PRO
1	A	88	ILE
3	C	57	PRO
7	G	13	PRO
11	K	83	PRO
14	N	157	PRO
7	G	20	VAL
9	I	109	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/182 (98%)	167 (94%)	11 (6%)	26	66
2	B	281/283 (99%)	266 (95%)	15 (5%)	32	73
3	C	192/193 (100%)	179 (93%)	13 (7%)	22	61
4	D	116/148 (78%)	111 (96%)	5 (4%)	40	81
5	E	151/156 (97%)	144 (95%)	7 (5%)	37	79
6	F	92/94 (98%)	92 (100%)	0	100	100
7	G	27/283 (10%)	26 (96%)	1 (4%)	45	85
8	H	133/145 (92%)	127 (96%)	6 (4%)	38	80
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	94
10	J	117/121 (97%)	109 (93%)	8 (7%)	22	61
11	K	105/106 (99%)	102 (97%)	3 (3%)	55	89
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	80
13	M	157/160 (98%)	149 (95%)	8 (5%)	33	75
14	N	148/150 (99%)	143 (97%)	5 (3%)	49	86
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	94
17	Q	79/80 (99%)	77 (98%)	2 (2%)	60	91
18	R	117/122 (96%)	112 (96%)	5 (4%)	40	81
19	S	71/74 (96%)	69 (97%)	2 (3%)	56	90
20	T	104/106 (98%)	99 (95%)	5 (5%)	35	77
21	U	44/53 (83%)	42 (96%)	2 (4%)	38	80
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	129/130 (99%)	122 (95%)	7 (5%)	31	72
24	X	65/74 (88%)	58 (89%)	7 (11%)	9	33
25	Y	120/195 (62%)	111 (92%)	9 (8%)	19	56
26	Z	59/94 (63%)	56 (95%)	3 (5%)	33	75
27	1	46/47 (98%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	2	42/46 (91%)	40 (95%)	2 (5%)	35	77
29	3	78/79 (99%)	76 (97%)	2 (3%)	59	91
All	All	3079/3646 (84%)	2943 (96%)	136 (4%)	39	80

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	38	ILE
1	A	69	LEU
1	A	120	ARG
1	A	131	HIS
1	A	153	ARG
1	A	171	LYS
1	A	179	MET
1	A	192	VAL
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	71	VAL
2	B	82	VAL
2	B	90	THR
2	B	103	ASP
2	B	132	HIS
2	B	162	MET
2	B	184	ASP
2	B	190	MET
2	B	254	GLN
2	B	277	GLU
2	B	312	ARG
3	C	16	VAL
3	C	27	ARG
3	C	76	ARG
3	C	101	ASP
3	C	115	LEU
3	C	132	ASP
3	C	172	THR
3	C	187	ARG

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Mol	Chain	Res	Type
3	C	188	ARG
3	C	211	ASP
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
4	D	24	HIS
4	D	50	VAL
4	D	131	THR
4	D	133	ASN
4	D	137	PRO
5	E	7	ILE
5	E	102	VAL
5	E	126	ILE
5	E	132	THR
5	E	143	GLN
5	E	155	ASN
5	E	164	ASP
7	G	73	ASP
8	H	21	GLU
8	H	51	SER
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	135	GLU
10	J	46	ILE
10	J	47	THR
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	112	ASP
10	J	131	THR
11	K	4	LEU
11	K	7	ASP
11	K	10	GLN
12	L	35	ARG
12	L	43	HIS
12	L	89	PHE
12	L	101	ASP
12	L	140	VAL
13	M	46	LEU

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Mol	Chain	Res	Type
13	M	52	GLN
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	130	GLU
13	M	154	ASP
14	N	49	THR
14	N	103	ASP
14	N	110	THR
14	N	124	ASP
14	N	139	TRP
16	P	21	VAL
16	P	98	ILE
17	Q	11	ARG
17	Q	95	GLU
18	R	39	THR
18	R	61	GLN
18	R	70	SER
18	R	76	ASP
18	R	90	ASP
19	S	12	GLU
19	S	44	GLN
20	T	23	VAL
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
21	U	19	THR
21	U	53	ASP
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	88	THR
23	W	125	HIS
23	W	146	ILE
24	X	8	ARG
24	X	27	ASP
24	X	46	ASP
24	X	49	ARG
24	X	79	GLU

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Mol	Chain	Res	Type
24	X	80	GLU
24	X	82	GLU
25	Y	108	ASP
25	Y	141	THR
25	Y	163	THR
25	Y	169	ARG
25	Y	189	ASN
25	Y	203	VAL
25	Y	204	ARG
25	Y	220	GLU
25	Y	235	GLU
26	Z	46	SER
26	Z	68	GLU
26	Z	106	SER
28	2	16	ASN
28	2	18	ASN
29	3	15	ASN
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	11	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
4	D	47	GLN
4	D	103	ASN
4	D	133	ASN
4	D	155	HIS
5	E	74	HIS
5	E	90	HIS
5	E	106	ASN
5	E	143	GLN

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Mol	Chain	Res	Type
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	148	HIS
9	I	88	GLN
9	I	99	GLN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	42	ASN
12	L	18	HIS
12	L	20	ASN
12	L	41	HIS
12	L	42	ASN
12	L	43	HIS
12	L	58	GLN
13	M	24	GLN
13	M	52	GLN
13	M	58	GLN
13	M	137	ASN
14	N	21	HIS
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
14	N	153	GLN
15	O	100	GLN
16	P	50	GLN
16	P	66	GLN
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
17	Q	67	GLN
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS

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Mol	Chain	Res	Type
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	44	GLN
19	S	51	GLN
19	S	53	ASN
20	T	7	GLN
20	T	11	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	49	ASN
23	W	59	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	240 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	2 (1%)
32	5	1/3 (33%)	0	0
33	6	1/3 (33%)	0	0
All	All	2868/3051 (94%)	258 (8%)	32 (1%)

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	511	A
30	0	514	G

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Mol	Chain	Res	Type
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	593	A
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	702	G
30	0	735	C
30	0	746	A
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	938	G
30	0	953	G

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Mol	Chain	Res	Type
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1351	G
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U

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Mol	Chain	Res	Type
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1559	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1873	G
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U

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Mol	Chain	Res	Type
30	0	2013	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2527	U
30	0	2533	C
30	0	2536	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A

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Mol	Chain	Res	Type
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2648	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2786	G
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A

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Mol	Chain	Res	Type
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1474	C
30	0	1684	A
30	0	1692	C
30	0	1730	G
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2011	A
30	0	2103	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2637	A
30	0	2649	A
30	0	2681	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2852	A
31	9	55	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	20,22,23	0.76	1 (5%)	24,31,34	0.77	0
30	OMG	0	2588	32,30	24,26,27	0.90	1 (4%)	32,38,41	5.10	4 (12%)
30	UR3	0	2619	30	20,22,23	0.79	1 (5%)	23,32,35	0.83	0
30	PSU	0	2621	30	19,21,22	1.20	3 (15%)	23,30,33	1.12	2 (8%)
30	1MA	0	628	30,36	23,25,26	0.88	1 (4%)	32,37,40	1.15	2 (6%)
33	8AN	6	76	33,30	24,24,25	1.02	1 (4%)	34,35,38	1.88	6 (17%)

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
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	32,30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,36	-	1/8/25/26	0/1/3/3
33	8AN	6	76	33,30	-	0/9/25/26	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	3.24	1.43	1.37
30	0	2621	PSU	C6-N1	2.48	1.34	1.32
30	0	2587	OMU	P-OP1	2.39	1.49	1.46
30	0	2588	OMG	P-OP1	2.18	1.49	1.46
30	0	2619	UR3	P-OP1	2.15	1.49	1.46
30	0	2621	PSU	P-OP1	2.09	1.49	1.46
30	0	628	1MA	P-OP1	2.07	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	76	8AN	C3'-N3'	-2.04	1.44	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.17	130.35	134.14
33	6	76	8AN	C4'-C3'-N3'	-5.54	101.69	113.46
33	6	76	8AN	C2'-C3'-N3'	-5.05	102.55	113.57
33	6	76	8AN	O2'-C2'-C3'	4.01	121.22	110.90
30	0	2588	OMG	C6-N1-C2	3.52	125.67	119.51
33	6	76	8AN	O4'-C4'-C3'	3.48	109.19	104.00
30	0	628	1MA	CM1-N1-C6	3.40	125.29	120.56
30	0	628	1MA	C2-N3-C4	-3.31	110.58	116.23
33	6	76	8AN	C2'-C1'-N9	2.42	119.47	113.27
33	6	76	8AN	C8-N9-C4	-2.39	105.08	106.90
30	0	2588	OMG	C2-N3-C4	-2.36	111.77	115.09
30	0	2621	PSU	C5-C1'-C2'	-2.23	111.68	115.61
30	0	2621	PSU	C5-C4-N3	-2.16	114.92	118.86
30	0	2588	OMG	C5-C4-N3	2.03	128.88	125.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 307 ligands modelled in this entry, 305 are monoatomic - leaving 2 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	$\# Z > 2$
34	PHE	6	77	-	11,11,12	5.52	3 (27%)	11,13,15	2.92	1 (9%)
34	ACA	6	78	-	7,7,8	8.85	3 (42%)	4,6,8	1.41	1 (25%)

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
34	PHE	6	77	-	-	0/4/6/8	0/1/1/1
34	ACA	6	78	-	-	0/4/5/6	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	6	78	ACA	O1-C1	23.03	1.27	1.11
34	6	77	PHE	O-C	17.45	1.23	1.11
34	6	77	PHE	CA-C	4.57	1.57	1.48
34	6	78	ACA	C3-C2	-3.33	1.36	1.51
34	6	77	PHE	CE1-CD1	2.24	1.44	1.39
34	6	78	ACA	C5-C6	2.12	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	6	77	PHE	C-CA-N	9.45	123.27	113.83
34	6	78	ACA	C5-C4-C3	-2.23	102.56	114.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	-0.26	7 (2%) 48 21	24, 46, 80, 105	0
2	B	337/338 (99%)	-0.48	2 (0%) 86 47	26, 49, 75, 88	0
3	C	246/246 (100%)	-0.42	2 (0%) 83 42	24, 45, 69, 80	0
4	D	140/177 (79%)	1.21	32 (22%) 1 1	64, 93, 124, 135	0
5	E	172/178 (96%)	-0.08	5 (2%) 49 22	41, 62, 84, 92	0
6	F	119/120 (99%)	0.58	14 (11%) 5 3	50, 73, 100, 114	0
7	G	29/348 (8%)	1.26	5 (17%) 2 2	75, 95, 109, 113	0
8	H	160/177 (90%)	-0.08	3 (1%) 64 28	39, 58, 93, 99	0
9	I	70/162 (43%)	3.72	51 (72%) 0 0	141, 152, 166, 168	0
10	J	142/145 (97%)	-0.42	1 (0%) 84 44	35, 47, 66, 86	0
11	K	132/132 (100%)	-0.70	1 (0%) 83 42	28, 41, 63, 73	0
12	L	145/165 (87%)	0.03	7 (4%) 29 15	22, 67, 105, 121	0
13	M	194/196 (98%)	-0.42	1 (0%) 88 50	25, 46, 68, 82	0
14	N	186/187 (99%)	0.03	10 (5%) 25 12	42, 63, 116, 124	0
15	O	115/116 (99%)	-0.24	1 (0%) 81 39	39, 55, 67, 75	0
16	P	143/149 (95%)	-0.49	0 100 100	35, 51, 62, 68	0
17	Q	95/96 (98%)	-0.32	1 (1%) 77 36	35, 49, 66, 75	0
18	R	150/155 (96%)	-0.49	1 (0%) 84 44	22, 42, 62, 69	0
19	S	81/85 (95%)	-0.15	1 (1%) 75 36	44, 56, 81, 94	0
20	T	119/120 (99%)	-0.12	1 (0%) 83 42	38, 54, 84, 116	0
21	U	53/67 (79%)	-0.28	1 (1%) 64 28	38, 49, 73, 86	0
22	V	65/71 (91%)	1.05	10 (15%) 3 2	55, 78, 115, 122	0
23	W	154/154 (100%)	-0.25	1 (0%) 86 47	37, 48, 72, 86	0
24	X	82/92 (89%)	-0.06	6 (7%) 15 8	39, 55, 80, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/240 (59%)	-0.48	2 (1%) 72 34	25, 44, 64, 90	0
26	Z	73/116 (62%)	0.26	6 (8%) 12 6	48, 67, 87, 96	0
27	1	56/57 (98%)	-0.62	0 100 100	22, 32, 39, 51	0
28	2	46/50 (92%)	-0.03	2 (4%) 34 16	29, 61, 76, 89	0
29	3	92/92 (100%)	-0.19	0 100 100	33, 58, 71, 81	0
30	0	2754/2923 (94%)	-0.38	35 (1%) 74 35	16, 45, 92, 179	0
31	9	122/122 (100%)	-0.39	4 (3%) 44 20	36, 65, 92, 148	0
32	5	2/3 (66%)	2.75	2 (100%) 0 0	100, 100, 100, 102	0
33	6	3/3 (100%)	1.71	1 (33%) 1 0	92, 92, 96, 104	0
All	All	6656/7522 (88%)	-0.22	216 (3%) 44 20	16, 50, 99, 179	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	66	GLY	14.4
22	V	40	PRO	10.9
9	I	113	SER	9.7
9	I	132	VAL	9.5
9	I	72	GLU	7.9
9	I	74	ILE	7.6
4	D	57	THR	7.4
22	V	1	THR	7.3
4	D	63	ILE	7.1
22	V	38	GLY	6.8
9	I	70	THR	6.5
9	I	97	VAL	6.5
9	I	103	ILE	6.4
9	I	108	HIS	6.4
9	I	100	VAL	6.3
9	I	98	ASP	6.3
9	I	111	LEU	6.2
9	I	71	ALA	6.1
4	D	90	LEU	6.0
26	Z	35	SER	5.8
26	Z	46	SER	5.8
9	I	99	GLN	5.7
7	G	23	ILE	5.6
22	V	39	ALA	5.6
9	I	121	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
4	D	93	LEU	5.4
9	I	69	PRO	5.4
28	2	49	GLU	5.3
9	I	76	ASP	5.2
9	I	101	LYS	5.2
6	F	16	ALA	5.1
26	Z	34	SER	5.1
19	S	81	ILE	5.1
9	I	112	LEU	5.1
30	0	1172	G	4.9
9	I	104	ALA	4.9
9	I	119	ALA	4.8
6	F	28	ALA	4.8
4	D	26	GLY	4.8
31	9	2	U	4.7
30	0	1199	A	4.7
9	I	123	VAL	4.7
9	I	109	PRO	4.6
30	0	735	C	4.5
9	I	116	LEU	4.4
9	I	73	LEU	4.4
9	I	80	PHE	4.4
14	N	166	ALA	4.3
9	I	120	ALA	4.2
4	D	106	PHE	4.1
9	I	128	THR	4.1
24	X	71	ARG	4.1
4	D	84	LEU	4.0
1	A	37	VAL	4.0
9	I	105	GLU	3.9
4	D	134	LEU	3.9
9	I	94	ASP	3.9
4	D	91	ALA	3.9
9	I	133	THR	3.9
31	9	1	U	3.8
6	F	17	LEU	3.8
26	Z	58	ASN	3.8
4	D	88	LEU	3.8
9	I	106	GLN	3.7
30	0	1169	U	3.7
9	I	129	SER	3.7
23	W	86	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	92	GLU	3.6
12	L	60	GLU	3.6
22	V	46	ILE	3.6
9	I	127	CYS	3.6
7	G	27	ILE	3.5
4	D	27	ILE	3.5
4	D	74	THR	3.5
4	D	40	ILE	3.5
6	F	47	LEU	3.4
30	0	1196	C	3.4
9	I	102	GLN	3.4
7	G	24	VAL	3.4
14	N	180	LEU	3.3
4	D	44	ILE	3.3
20	T	119	ALA	3.3
4	D	41	LEU	3.3
4	D	166	ILE	3.3
30	0	1200	A	3.3
32	5	76	A	3.3
30	0	514	G	3.2
4	D	61	PHE	3.2
33	6	75	C	3.2
6	F	45	ALA	3.1
30	0	1198	U	3.1
9	I	82	THR	3.1
6	F	49	PHE	3.1
22	V	37	GLY	3.1
21	U	47	ARG	3.1
5	E	154	ILE	3.1
30	0	1202	A	3.1
4	D	85	GLN	3.0
24	X	88	GLU	3.0
30	0	2637	A	3.0
9	I	77	GLU	3.0
30	0	1177	A	3.0
22	V	8	ILE	3.0
3	C	61	PHE	3.0
14	N	179	LEU	2.9
6	F	22	VAL	2.9
31	9	24	U	2.9
30	0	1165	G	2.9
9	I	78	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
15	O	60	VAL	2.9
1	A	236	GLY	2.9
12	L	80	ASP	2.9
30	0	1180	U	2.9
12	L	100	ALA	2.8
9	I	131	GLY	2.8
12	L	105	TYR	2.8
7	G	72	ASP	2.8
26	Z	60	ASP	2.8
30	0	282	C	2.8
30	0	1203	G	2.8
8	H	169	GLU	2.8
9	I	117	THR	2.8
5	E	100	ASP	2.8
4	D	130	VAL	2.8
12	L	91	VAL	2.7
30	0	960	G	2.7
14	N	147	ILE	2.7
6	F	23	ALA	2.7
4	D	18	ILE	2.7
7	G	26	MET	2.7
17	Q	18	PRO	2.7
4	D	104	PHE	2.7
14	N	160	SER	2.7
13	M	70	GLY	2.7
22	V	36	ALA	2.7
9	I	81	GLU	2.7
9	I	115	ASP	2.7
30	0	1173	A	2.7
14	N	155	GLU	2.6
30	0	1163	G	2.6
6	F	99	THR	2.6
30	0	999	C	2.6
30	0	1179	C	2.6
30	0	1168	C	2.6
1	A	35	GLY	2.6
22	V	3	LEU	2.6
9	I	67	VAL	2.6
22	V	41	GLU	2.6
24	X	80	GLU	2.6
24	X	85	VAL	2.6
28	2	35	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	89	PRO	2.5
1	A	91	GLY	2.5
4	D	17	ARG	2.5
24	X	65	ASN	2.5
5	E	45	ASP	2.5
6	F	100	ASP	2.5
4	D	75	LEU	2.5
4	D	64	ARG	2.5
9	I	114	TYR	2.5
9	I	126	THR	2.5
2	B	117	GLU	2.5
6	F	98	VAL	2.5
31	9	122	C	2.5
30	0	970	U	2.4
9	I	88	GLN	2.4
5	E	10	ASP	2.4
1	A	31	LYS	2.4
25	Y	95	THR	2.4
4	D	80	ALA	2.4
30	0	1965	C	2.4
30	0	497	A	2.4
30	0	1190	G	2.4
18	R	88	PHE	2.4
6	F	96	ALA	2.4
2	B	91	PRO	2.3
25	Y	236	VAL	2.3
30	0	1171	A	2.3
6	F	18	GLU	2.3
1	A	82	VAL	2.3
9	I	91	PHE	2.3
30	0	1966	U	2.3
8	H	77	ILE	2.3
9	I	135	GLU	2.3
4	D	69	ILE	2.3
30	0	2238	A	2.3
9	I	95	LEU	2.2
32	5	75	C	2.2
30	0	1181	A	2.2
14	N	178	THR	2.2
14	N	183	ASP	2.2
30	0	280	C	2.2
30	0	1197	G	2.2

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Mol	Chain	Res	Type	RSRZ
12	L	106	VAL	2.2
30	0	1170	U	2.2
14	N	181	ASP	2.2
4	D	77	ASP	2.2
4	D	101	THR	2.2
14	N	185	GLU	2.2
4	D	25	MET	2.1
30	0	1164	U	2.1
9	I	90	ASP	2.1
26	Z	49	ARG	2.1
6	F	20	LEU	2.1
8	H	85	ASP	2.1
3	C	238	SER	2.1
4	D	128	LEU	2.1
1	A	59	GLU	2.1
9	I	86	GLU	2.1
11	K	118	ALA	2.0
24	X	10	VAL	2.0
30	0	1182	C	2.0
5	E	170	ARG	2.0
10	J	4	ALA	2.0
12	L	61	ALA	2.0
30	0	288	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	8AN	6	76	22/23	0.27	1.10	87,92,94,95	0
30	UR3	0	2619	21/22	0.14	0.57	40,41,44,47	0
30	1MA	0	628	23/24	0.15	0.44	36,40,42,42	0
30	OMU	0	2587	21/22	0.11	-0.61	30,33,38,38	0
30	OMG	0	2588	24/25	0.12	-0.67	30,34,35,37	0
30	PSU	0	2621	20/21	0.13	-1.46	36,38,42,42	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	8979	1/1	1.70	1060.33	184,184,184,184	0
37	SR	0	8920	1/1	0.92	826.00	200,200,200,200	0
37	SR	0	9000	1/1	0.28	295.00	147,147,147,147	0
37	SR	0	9006	1/1	0.47	109.20	198,198,198,198	0
35	MG	0	8087	1/1	0.96	91.38	107,107,107,107	0
35	MG	0	8049	1/1	0.97	90.42	103,103,103,103	0
35	MG	0	8081	1/1	0.55	85.70	91,91,91,91	0
37	SR	0	8994	1/1	0.98	82.82	200,200,200,200	0
36	NA	0	8547	1/1	0.58	76.81	78,78,78,78	0
35	MG	0	8056	1/1	0.38	61.64	94,94,94,94	0
35	MG	0	8045	1/1	0.65	59.75	119,119,119,119	0
35	MG	0	8066	1/1	0.79	53.87	98,98,98,98	0
36	NA	0	8558	1/1	1.00	53.64	67,67,67,67	0
36	NA	0	8505	1/1	0.52	53.43	29,29,29,29	0
36	NA	0	8519	1/1	0.71	49.43	71,71,71,71	0
36	NA	0	8535	1/1	0.81	49.29	75,75,75,75	0
35	MG	0	8018	1/1	0.24	48.78	3,3,3,3	0
35	MG	0	8078	1/1	0.75	45.72	115,115,115,115	0
38	CL	0	8822	1/1	0.32	45.22	66,66,66,66	0
35	MG	0	8092	1/1	0.54	43.80	76,76,76,76	0
36	NA	0	8571	1/1	0.29	43.00	85,85,85,85	0
35	MG	0	8085	1/1	0.67	39.66	92,92,92,92	0
36	NA	9	8544	1/1	0.52	38.88	73,73,73,73	0
35	MG	0	8079	1/1	0.33	33.77	64,64,64,64	0
35	MG	0	8050	1/1	0.32	32.20	152,152,152,152	0
35	MG	0	8047	1/1	0.47	32.18	92,92,92,92	0
36	NA	0	8514	1/1	0.29	31.41	83,83,83,83	0
39	K	0	8402	1/1	1.51	29.78	117,117,117,117	0
36	NA	0	8566	1/1	0.50	27.46	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	MG	0	8065	1/1	0.39	25.73	102,102,102,102	0
36	NA	0	8516	1/1	0.46	25.00	65,65,65,65	0
37	SR	0	8925	1/1	0.17	24.37	70,70,70,70	0
35	MG	0	8016	1/1	0.48	23.14	131,131,131,131	0
35	MG	0	8090	1/1	0.89	23.12	130,130,130,130	0
37	SR	0	9007	1/1	0.48	23.05	195,195,195,195	0
36	NA	0	8527	1/1	0.43	21.47	73,73,73,73	0
36	NA	0	8555	1/1	0.37	19.78	52,52,52,52	0
37	SR	0	8990	1/1	0.56	19.07	177,177,177,177	0
35	MG	0	8071	1/1	0.47	18.79	88,88,88,88	0
36	NA	0	8509	1/1	0.37	18.46	80,80,80,80	0
36	NA	0	8523	1/1	0.25	17.84	61,61,61,61	0
36	NA	0	8562	1/1	0.32	17.62	55,55,55,55	0
39	K	0	8401	1/1	0.58	17.21	82,82,82,82	0
37	SR	L	8969	1/1	0.50	16.66	175,175,175,175	0
35	MG	0	8010	1/1	0.56	16.09	78,78,78,78	0
37	SR	0	9001	1/1	0.33	14.32	190,190,190,190	0
36	NA	0	8512	1/1	0.40	14.14	46,46,46,46	0
35	MG	0	8046	1/1	0.42	14.10	72,72,72,72	0
35	MG	0	8028	1/1	0.23	14.10	1,1,1,1	0
35	MG	0	8076	1/1	0.32	13.87	72,72,72,72	0
35	MG	0	8029	1/1	0.28	13.65	83,83,83,83	0
36	NA	0	8520	1/1	0.22	13.60	58,58,58,58	0
36	NA	0	8548	1/1	0.18	13.12	26,26,26,26	0
36	NA	9	8572	1/1	0.27	12.77	96,96,96,96	0
36	NA	0	8546	1/1	0.73	12.59	97,97,97,97	0
37	SR	0	8917	1/1	0.18	12.55	67,67,67,67	0
35	MG	0	8009	1/1	0.32	12.51	1,1,1,1	0
36	NA	0	8502	1/1	0.23	12.28	60,60,60,60	0
35	MG	0	8058	1/1	0.20	11.82	1,1,1,1	0
36	NA	0	8574	1/1	0.31	11.79	43,43,43,43	0
36	NA	0	8528	1/1	0.25	11.58	55,55,55,55	0
35	MG	0	8036	1/1	0.15	11.57	50,50,50,50	0
36	NA	0	8507	1/1	0.24	11.57	29,29,29,29	0
34	ACA	6	78	8/9	0.43	11.49	88,90,91,91	0
36	NA	S	8510	1/1	0.61	11.10	80,80,80,80	0
36	NA	0	8553	1/1	0.26	10.99	100,100,100,100	0
35	MG	0	8001	1/1	0.23	10.83	7,7,7,7	0
36	NA	0	8521	1/1	0.33	10.82	51,51,51,51	0
37	SR	0	8989	1/1	0.29	10.61	200,200,200,200	0
36	NA	0	8556	1/1	0.79	10.34	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	MG	0	8064	1/1	0.26	10.03	53,53,53,53	0
35	MG	0	8072	1/1	0.20	10.00	55,55,55,55	0
37	SR	0	8927	1/1	0.19	9.82	70,70,70,70	0
36	NA	0	8557	1/1	0.22	9.75	82,82,82,82	0
35	MG	A	8025	1/1	0.28	9.75	39,39,39,39	0
36	NA	0	8533	1/1	0.29	9.74	64,64,64,64	0
37	SR	0	8905	1/1	0.25	9.66	61,61,61,61	0
35	MG	A	8051	1/1	1.00	9.60	82,82,82,82	0
37	SR	0	8926	1/1	0.17	9.36	87,87,87,87	0
36	NA	0	8568	1/1	0.39	9.32	18,18,18,18	0
35	MG	0	8037	1/1	0.18	9.26	64,64,64,64	0
36	NA	0	8550	1/1	0.27	9.22	51,51,51,51	0
35	MG	0	8040	1/1	0.26	9.09	70,70,70,70	0
35	MG	9	8074	1/1	0.22	9.09	52,52,52,52	0
37	SR	0	8942	1/1	0.30	8.90	155,155,155,155	0
36	NA	0	8536	1/1	0.18	8.86	63,63,63,63	0
36	NA	0	8567	1/1	0.28	8.81	61,61,61,61	0
36	NA	0	8545	1/1	0.27	8.68	64,64,64,64	0
36	NA	0	8561	1/1	0.23	8.55	66,66,66,66	0
37	SR	T	8939	1/1	0.14	8.22	70,70,70,70	0
38	CL	J	8816	1/1	0.31	8.21	80,80,80,80	0
35	MG	0	8063	1/1	0.31	8.14	69,69,69,69	0
35	MG	0	8048	1/1	0.27	7.98	49,49,49,49	0
36	NA	0	8525	1/1	0.17	7.91	53,53,53,53	0
35	MG	0	8024	1/1	0.33	7.80	69,69,69,69	0
37	SR	B	8987	1/1	0.39	7.71	199,199,199,199	0
37	SR	0	8949	1/1	0.16	7.69	62,62,62,62	0
35	MG	0	8061	1/1	0.23	7.67	17,17,17,17	0
37	SR	0	8937	1/1	0.21	7.47	69,69,69,69	0
37	SR	0	8903	1/1	0.21	7.39	55,55,55,55	0
36	NA	0	8559	1/1	0.18	7.37	64,64,64,64	0
37	SR	0	8983	1/1	0.22	7.31	169,169,169,169	0
36	NA	0	8541	1/1	0.23	7.17	103,103,103,103	0
37	SR	0	8958	1/1	0.15	7.17	77,77,77,77	0
35	MG	0	8023	1/1	0.24	7.11	25,25,25,25	0
36	NA	0	8531	1/1	0.14	7.09	41,41,41,41	0
37	SR	0	8976	1/1	0.21	7.07	117,117,117,117	0
35	MG	0	8002	1/1	0.27	7.01	19,19,19,19	0
36	NA	0	8552	1/1	0.27	7.00	86,86,86,86	0
37	SR	0	8914	1/1	0.26	6.83	88,88,88,88	0
37	SR	0	9008	1/1	0.22	6.73	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	MG	0	8059	1/1	0.17	6.68	88,88,88,88	0
37	SR	0	8961	1/1	0.15	6.48	185,185,185,185	0
36	NA	0	8511	1/1	0.16	6.35	35,35,35,35	0
35	MG	0	8014	1/1	0.20	6.34	16,16,16,16	0
35	MG	0	8062	1/1	0.29	6.22	41,41,41,41	0
37	SR	0	8938	1/1	0.14	6.20	95,95,95,95	0
37	SR	0	8901	1/1	0.19	6.15	48,48,48,48	0
35	MG	0	8020	1/1	0.20	6.10	24,24,24,24	0
37	SR	0	8944	1/1	0.18	5.84	155,155,155,155	0
35	MG	0	8022	1/1	0.21	5.76	11,11,11,11	0
34	PHE	6	77	11/12	0.34	5.72	88,88,90,90	0
36	NA	0	8569	1/1	0.23	5.64	32,32,32,32	0
37	SR	0	8931	1/1	0.18	5.59	80,80,80,80	0
36	NA	0	8563	1/1	0.22	5.57	51,51,51,51	0
37	SR	0	8904	1/1	0.21	5.43	55,55,55,55	0
35	MG	0	8055	1/1	0.27	5.43	26,26,26,26	0
35	MG	0	8041	1/1	0.20	5.19	33,33,33,33	0
35	MG	0	8070	1/1	0.19	5.09	63,63,63,63	0
35	MG	C	8012	1/1	0.27	5.08	17,17,17,17	0
35	MG	0	8015	1/1	0.17	4.92	41,41,41,41	0
35	MG	B	8042	1/1	0.28	4.90	103,103,103,103	0
37	SR	0	8923	1/1	0.20	4.73	72,72,72,72	0
36	NA	0	8534	1/1	0.35	4.68	68,68,68,68	0
36	NA	H	8518	1/1	0.28	4.48	69,69,69,69	0
37	SR	0	8924	1/1	0.22	4.37	80,80,80,80	0
37	SR	0	8933	1/1	0.28	4.34	126,126,126,126	0
35	MG	2	8060	1/1	0.21	4.23	45,45,45,45	0
37	SR	0	8998	1/1	0.23	4.22	113,113,113,113	0
37	SR	1	8952	1/1	0.19	4.16	67,67,67,67	0
37	SR	0	8966	1/1	0.15	3.99	85,85,85,85	0
36	NA	0	8560	1/1	0.32	3.82	134,134,134,134	0
36	NA	0	8565	1/1	0.20	3.80	48,48,48,48	0
37	SR	0	8948	1/1	0.17	3.79	65,65,65,65	0
36	NA	0	8573	1/1	0.36	3.55	79,79,79,79	0
35	MG	0	8034	1/1	0.21	3.55	30,30,30,30	0
36	NA	0	8570	1/1	0.15	3.50	48,48,48,48	0
35	MG	Y	8086	1/1	0.16	3.45	48,48,48,48	0
36	NA	0	8530	1/1	0.18	3.43	49,49,49,49	0
37	SR	0	8946	1/1	0.19	3.41	98,98,98,98	0
37	SR	0	8996	1/1	0.21	3.37	158,158,158,158	0
35	MG	0	8039	1/1	0.20	3.36	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8985	1/1	0.15	3.25	142,142,142,142	0
35	MG	B	8043	1/1	0.17	3.11	29,29,29,29	0
35	MG	0	8067	1/1	0.29	3.09	33,33,33,33	0
37	SR	0	8918	1/1	0.19	3.02	53,53,53,53	0
36	NA	0	8501	1/1	0.16	3.01	107,107,107,107	0
35	MG	K	8054	1/1	0.17	2.99	15,15,15,15	0
36	NA	0	8554	1/1	0.20	2.96	42,42,42,42	0
37	SR	0	8936	1/1	0.17	2.92	67,67,67,67	0
35	MG	0	8008	1/1	0.16	2.90	9,9,9,9	0
36	NA	0	8513	1/1	0.20	2.89	53,53,53,53	0
35	MG	0	8004	1/1	0.20	2.82	21,21,21,21	0
37	SR	0	8954	1/1	0.16	2.82	82,82,82,82	0
37	SR	0	8941	1/1	0.20	2.81	77,77,77,77	0
35	MG	0	8027	1/1	0.12	2.71	28,28,28,28	0
37	SR	0	8906	1/1	0.21	2.69	56,56,56,56	0
35	MG	0	8005	1/1	0.22	2.58	25,25,25,25	0
35	MG	0	8006	1/1	0.17	2.52	8,8,8,8	0
37	SR	0	8963	1/1	0.15	2.45	74,74,74,74	0
37	SR	0	8984	1/1	0.14	2.38	92,92,92,92	0
35	MG	0	8088	1/1	0.17	2.36	40,40,40,40	0
37	SR	0	8910	1/1	0.16	2.27	47,47,47,47	0
37	SR	0	8908	1/1	0.15	2.18	64,64,64,64	0
37	SR	1	8913	1/1	0.19	2.17	54,54,54,54	0
36	NA	0	8524	1/1	0.13	2.12	52,52,52,52	0
37	SR	0	8909	1/1	0.16	2.07	56,56,56,56	0
37	SR	0	8965	1/1	0.14	2.04	95,95,95,95	0
37	SR	B	8950	1/1	0.16	2.01	98,98,98,98	0
37	SR	0	8974	1/1	0.21	2.00	125,125,125,125	0
37	SR	0	8916	1/1	0.14	1.91	64,64,64,64	0
38	CL	A	8809	1/1	0.16	1.85	51,51,51,51	0
35	MG	0	8003	1/1	0.18	1.81	14,14,14,14	0
37	SR	0	8964	1/1	0.14	1.67	102,102,102,102	0
37	SR	R	8912	1/1	0.18	1.57	64,64,64,64	0
35	MG	0	8030	1/1	0.23	1.57	167,167,167,167	0
37	SR	0	8915	1/1	0.14	1.57	84,84,84,84	0
36	NA	0	8522	1/1	0.13	1.35	72,72,72,72	0
37	SR	0	8928	1/1	0.11	1.34	92,92,92,92	0
37	SR	0	8978	1/1	0.14	1.33	71,71,71,71	0
37	SR	0	8922	1/1	0.17	1.31	61,61,61,61	0
35	MG	0	8011	1/1	0.18	1.29	4,4,4,4	0
37	SR	0	8902	1/1	0.18	1.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8504	1/1	0.16	1.23	31,31,31,31	0
36	NA	0	8517	1/1	0.16	1.23	36,36,36,36	0
37	SR	0	8981	1/1	0.17	1.21	117,117,117,117	0
36	NA	C	8503	1/1	0.19	1.17	31,31,31,31	0
37	SR	3	8932	1/1	0.17	1.16	74,74,74,74	0
37	SR	0	8921	1/1	0.14	1.13	58,58,58,58	0
37	SR	A	8930	1/1	0.17	0.99	78,78,78,78	0
37	SR	0	8935	1/1	0.14	0.97	73,73,73,73	0
37	SR	H	8907	1/1	0.13	0.88	48,48,48,48	0
38	CL	Y	8817	1/1	0.16	0.80	55,55,55,55	0
35	MG	0	8035	1/1	0.14	0.76	84,84,84,84	0
37	SR	0	8973	1/1	0.11	0.74	98,98,98,98	0
35	MG	0	8068	1/1	0.14	0.73	50,50,50,50	0
35	MG	0	8077	1/1	0.17	0.67	41,41,41,41	0
37	SR	0	8934	1/1	0.16	0.65	71,71,71,71	0
37	SR	Y	9002	1/1	0.11	0.64	124,124,124,124	0
35	MG	0	8017	1/1	0.19	0.58	123,123,123,123	0
38	CL	Q	8811	1/1	0.21	0.57	86,86,86,86	0
36	NA	R	8532	1/1	0.12	0.55	25,25,25,25	0
38	CL	J	8801	1/1	0.15	0.54	62,62,62,62	0
36	NA	0	8515	1/1	0.16	0.49	26,26,26,26	0
35	MG	0	8052	1/1	0.14	0.43	42,42,42,42	0
36	NA	0	8549	1/1	0.15	0.43	36,36,36,36	0
37	SR	0	8943	1/1	0.12	0.40	88,88,88,88	0
37	SR	0	8940	1/1	0.17	0.39	51,51,51,51	0
35	MG	0	8053	1/1	0.15	0.26	33,33,33,33	0
38	CL	O	8808	1/1	0.17	0.20	75,75,75,75	0
37	SR	T	8911	1/1	0.11	0.08	58,58,58,58	0
37	SR	0	8947	1/1	0.14	0.07	91,91,91,91	0
36	NA	0	8575	1/1	0.14	0.07	44,44,44,44	0
38	CL	J	8821	1/1	0.15	0.04	64,64,64,64	0
35	MG	0	8019	1/1	0.15	-0.03	1,1,1,1	0
37	SR	9	8968	1/1	0.11	-0.05	117,117,117,117	0
35	MG	A	8044	1/1	0.13	-0.05	51,51,51,51	0
37	SR	0	8956	1/1	0.14	-0.14	111,111,111,111	0
38	CL	L	8814	1/1	0.14	-0.15	62,62,62,62	0
36	NA	0	8542	1/1	0.15	-0.16	31,31,31,31	0
37	SR	0	8919	1/1	0.15	-0.19	92,92,92,92	0
37	SR	0	9004	1/1	0.16	-0.22	121,121,121,121	0
37	SR	3	8953	1/1	0.16	-0.24	110,110,110,110	0
36	NA	0	8564	1/1	0.09	-0.29	35,35,35,35	0
37	SR	A	8977	1/1	0.16	-0.32	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	8986	1/1	0.11	-0.43	108,108,108,108	0
37	SR	0	8957	1/1	0.11	-0.44	124,124,124,124	0
38	CL	0	8812	1/1	0.11	-0.44	50,50,50,50	0
35	MG	0	8069	1/1	0.16	-0.44	120,120,120,120	0
36	NA	J	8538	1/1	0.12	-0.64	31,31,31,31	0
35	MG	0	8084	1/1	0.10	-0.66	27,27,27,27	0
37	SR	A	8929	1/1	0.12	-0.68	114,114,114,114	0
36	NA	Q	8540	1/1	0.12	-0.81	66,66,66,66	0
37	SR	0	8951	1/1	0.10	-0.83	105,105,105,105	0
37	SR	F	9005	1/1	0.11	-0.84	98,98,98,98	0
37	SR	0	8967	1/1	0.09	-0.88	103,103,103,103	0
38	CL	0	8815	1/1	0.10	-0.88	69,69,69,69	0
38	CL	M	8818	1/1	0.12	-0.90	46,46,46,46	0
36	NA	0	8508	1/1	0.11	-0.92	27,27,27,27	0
35	MG	0	8083	1/1	0.09	-0.95	29,29,29,29	0
37	SR	0	8995	1/1	0.12	-0.97	98,98,98,98	0
35	MG	0	8080	1/1	0.07	-1.00	45,45,45,45	0
40	CD	1	8702	1/1	0.11	-1.01	57,57,57,57	0
40	CD	Z	8703	1/1	0.10	-1.02	55,55,55,55	0
37	SR	0	8962	1/1	0.13	-1.02	104,104,104,104	0
37	SR	0	8993	1/1	0.04	-1.10	146,146,146,146	0
36	NA	0	8537	1/1	0.09	-1.11	21,21,21,21	0
36	NA	0	8529	1/1	0.07	-1.16	24,24,24,24	0
36	NA	M	8539	1/1	0.10	-1.22	33,33,33,33	0
35	MG	T	8057	1/1	0.15	-1.26	31,31,31,31	0
35	MG	0	8082	1/1	0.12	-1.27	70,70,70,70	0
40	CD	U	8701	1/1	0.08	-1.37	57,57,57,57	0
36	NA	9	8543	1/1	0.13	-1.38	65,65,65,65	0
37	SR	0	8960	1/1	0.09	-1.40	98,98,98,98	0
37	SR	3	8999	1/1	0.12	-1.43	69,69,69,69	0
37	SR	0	8955	1/1	0.09	-1.47	127,127,127,127	0
36	NA	0	8551	1/1	0.10	-1.50	32,32,32,32	0
38	CL	L	8810	1/1	0.07	-1.50	56,56,56,56	0
37	SR	0	8991	1/1	0.09	-1.64	148,148,148,148	0
35	MG	0	8073	1/1	0.08	-1.70	58,58,58,58	0
37	SR	0	8970	1/1	0.08	-1.72	99,99,99,99	0
35	MG	0	8007	1/1	0.14	-1.79	30,30,30,30	0
35	MG	0	8075	1/1	0.09	-1.79	38,38,38,38	0
37	SR	0	8945	1/1	0.09	-1.80	104,104,104,104	0
37	SR	H	8972	1/1	0.08	-1.83	132,132,132,132	0
35	MG	0	8033	1/1	0.09	-1.96	44,44,44,44	0
38	CL	J	8802	1/1	0.08	-2.06	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
40	CD	3	8704	1/1	0.08	-2.15	52,52,52,52	0
38	CL	Y	8820	1/1	0.06	-2.16	48,48,48,48	0
38	CL	B	8819	1/1	0.10	-2.17	62,62,62,62	0
35	MG	0	8026	1/1	0.09	-2.18	43,43,43,43	0
37	SR	0	8959	1/1	0.06	-2.20	120,120,120,120	0
36	NA	0	8506	1/1	0.07	-2.23	50,50,50,50	0
40	CD	O	8705	1/1	0.04	-2.27	111,111,111,111	0
37	SR	0	8988	1/1	0.09	-2.41	114,114,114,114	0
38	CL	N	8807	1/1	0.07	-2.58	70,70,70,70	0
38	CL	R	8806	1/1	0.11	-2.83	44,44,44,44	0
35	MG	0	8021	1/1	0.07	-2.93	24,24,24,24	0
37	SR	0	8992	1/1	0.06	-3.06	122,122,122,122	0
37	SR	0	8975	1/1	0.04	-3.25	125,125,125,125	0
38	CL	0	8805	1/1	0.08	-3.28	60,60,60,60	0
38	CL	3	8804	1/1	0.10	-3.62	60,60,60,60	0
38	CL	0	8813	1/1	0.08	-4.07	63,63,63,63	0
38	CL	0	8803	1/1	0.05	-4.47	51,51,51,51	0
35	MG	0	8032	1/1	0.04	-4.86	21,21,21,21	0
35	MG	0	8093	1/1	0.06	-6.07	27,27,27,27	0
37	SR	0	8982	1/1	0.08	-6.33	116,116,116,116	0
35	MG	0	8013	1/1	0.04	-6.84	20,20,20,20	0
37	SR	9	8980	1/1	0.08	-7.33	132,132,132,132	0
36	NA	0	8526	1/1	0.10	-7.87	55,55,55,55	0
37	SR	9	9003	1/1	0.04	-8.00	144,144,144,144	0
35	MG	0	8089	1/1	0.09	-9.07	31,31,31,31	0
37	SR	0	8997	1/1	0.06	-9.25	116,116,116,116	0
35	MG	0	8031	1/1	0.05	-9.61	41,41,41,41	0
35	MG	0	8091	1/1	0.14	-	76,76,76,76	0
35	MG	0	8038	1/1	0.25	-	97,97,97,97	0
37	SR	0	8971	1/1	0.12	-	191,191,191,191	0

6.5 Other polymers ⓘ

There are no such residues in this entry.