



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:16 PM GMT

PDB ID : 3CCS
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
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>

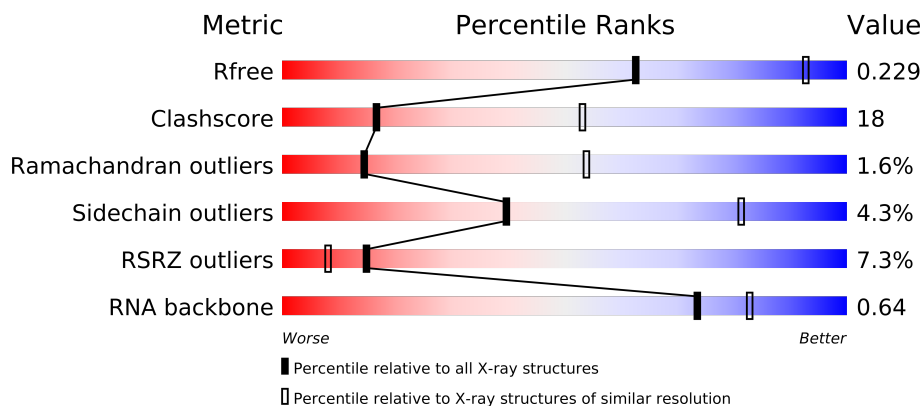
The following versions of software and data (see [references](#)) were used in the production of this report:

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	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8005	-	X
32	MG	0	8009	-	X
32	MG	0	8016	-	X
32	MG	0	8018	-	X
32	MG	0	8020	-	X
32	MG	0	8022	-	X
32	MG	0	8024	-	X
32	MG	0	8027	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8037	-	X
32	MG	0	8040	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8063	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8070	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8080	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	0	8089	-	X
32	MG	0	8092	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
34	NA	0	8502	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8507	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8513	-	X
34	NA	0	8514	-	X
34	NA	0	8519	-	X
34	NA	0	8521	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8527	-	X
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8537	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8550	-	X
34	NA	0	8551	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8571	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
34	NA	9	8572	-	X
34	NA	B	8552	-	X
34	NA	H	8518	-	X
35	CL	0	8805	-	X
35	CL	0	8815	-	X
35	CL	0	8816	-	X
35	CL	0	8822	-	X
35	CL	A	8809	-	X
36	SR	0	8901	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8924	-	X
36	SR	0	8925	-	X
36	SR	0	8926	-	X
36	SR	0	8947	-	X
36	SR	0	8953	-	X
36	SR	0	8957	-	X
36	SR	0	8959	-	X
36	SR	0	8973	-	X
36	SR	0	8976	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8989	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	B	8987	-	X
36	SR	L	8969	-	X
36	SR	R	8912	-	X
37	CD	3	8704	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99121 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
			1753	1072	352	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
			2625	1616	493	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
			1860	1130	345	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
			1094	685	195	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
			1357	840	224	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
			890	551	141	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
			1282	798	240	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
			519	323	81	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
			1120	696	199	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
			994	609	189	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
			1118	670	222	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
			1558	943	333	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
			1445	895	262	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
			865	529	161	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
			1136	683	229	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
			735	450	141	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
			1149	713	209	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
			641	389	111	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
			950	568	180	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
			1196	737	209	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
			654	402	129	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
			573	343	113	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
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59019	26349	10873	19052	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
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	86	Total	Mg	0	0
			86	86		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	0	0
33	M	1	Total K 1 1	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	65	Total Na 65 65	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	B	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	92	Total 92	Sr 92	0	0
36	1	2	Total 2	Sr 2	0	0
36	H	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	2	Total 2	Sr 2	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	L	1	Total 1	Sr 1	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5904	Total 5904	O 5904	0	0
38	9	149	Total 149	O 149	0	0
38	A	119	Total 119	O 119	0	0
38	B	152	Total 152	O 152	0	0
38	C	185	Total 185	O 185	0	0
38	D	42	Total 42	O 42	0	0
38	E	43	Total 43	O 43	0	0
38	F	26	Total 26	O 26	0	0
38	G	19	Total 19	O 19	0	0
38	H	65	Total 65	O 65	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	58	Total 58	O 58	0	0
38	L	85	Total 85	O 85	0	0
38	M	127	Total 127	O 127	0	0

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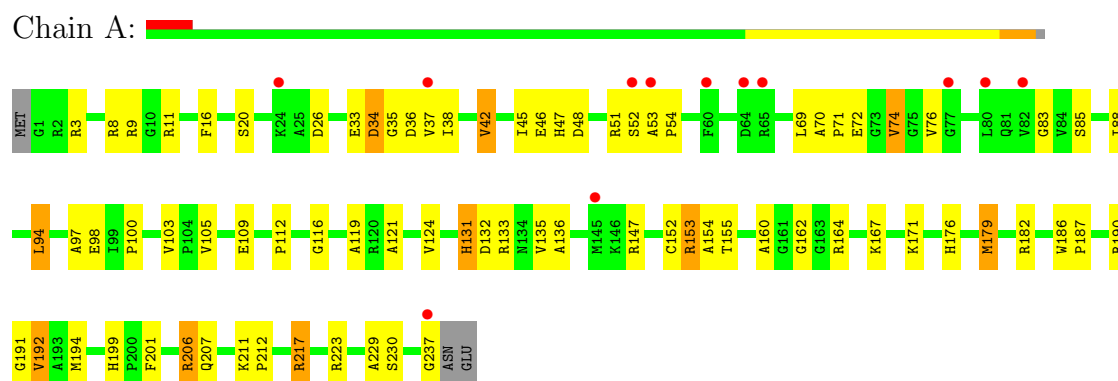
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	N	59	Total 59	O 59	0	0
38	O	39	Total 39	O 39	0	0
38	P	67	Total 67	O 67	0	0
38	Q	48	Total 48	O 48	0	0
38	R	77	Total 77	O 77	0	0
38	S	30	Total 30	O 30	0	0
38	T	36	Total 36	O 36	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	31	Total 31	O 31	0	0
38	1	59	Total 59	O 59	0	0
38	2	43	Total 43	O 43	0	0
38	3	70	Total 70	O 70	0	0

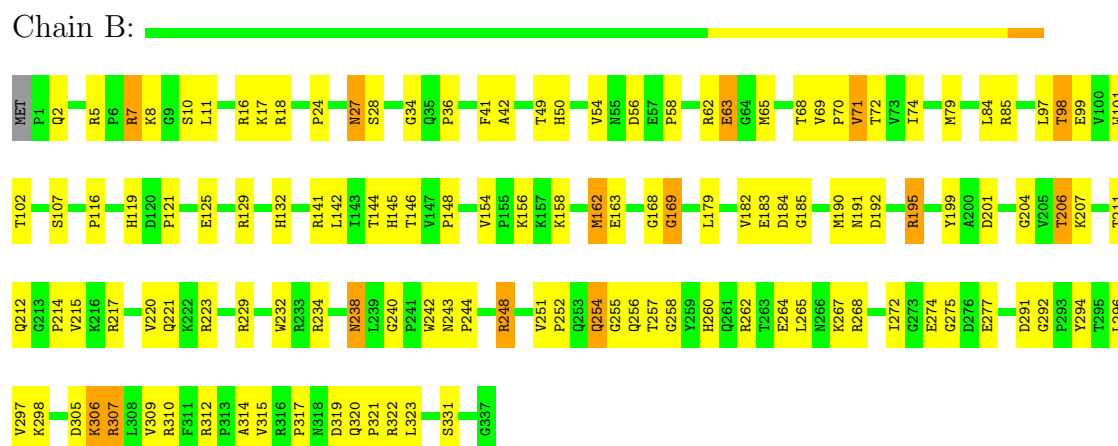
3 Residue-property plots

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.

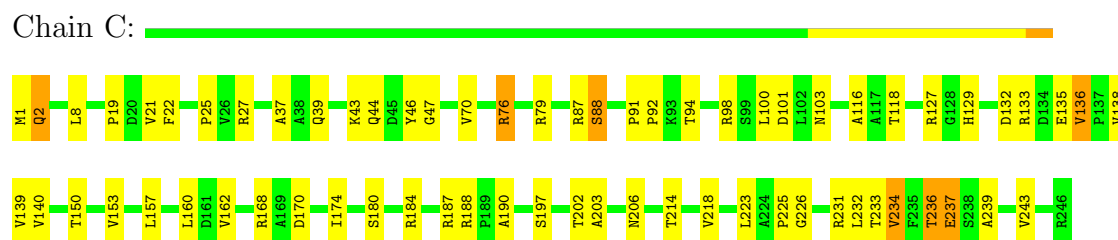
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P

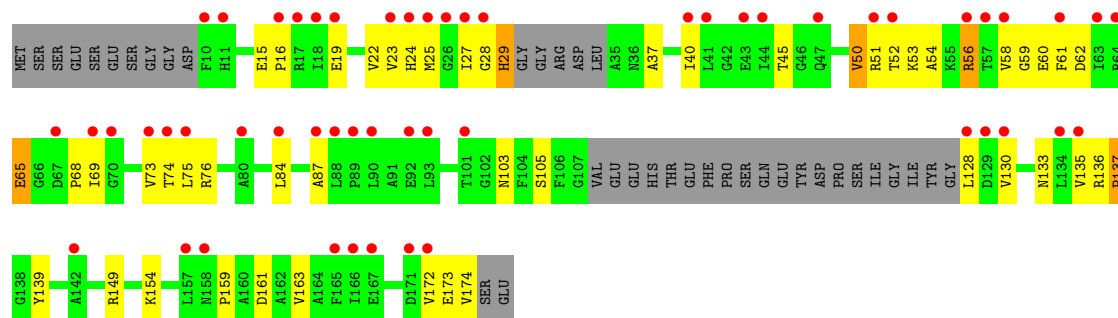


- Molecule 3: 50S ribosomal protein L4P



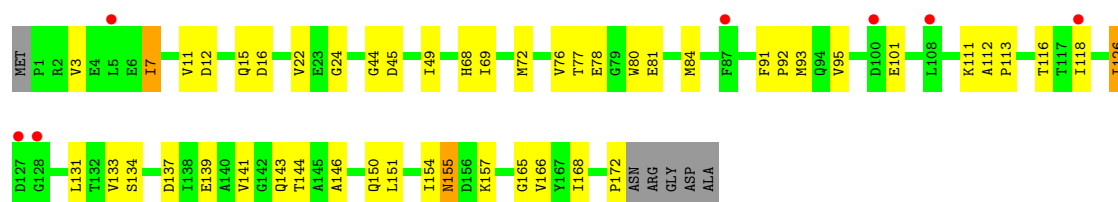
- Molecule 4: 50S ribosomal protein L5P

Chain D:



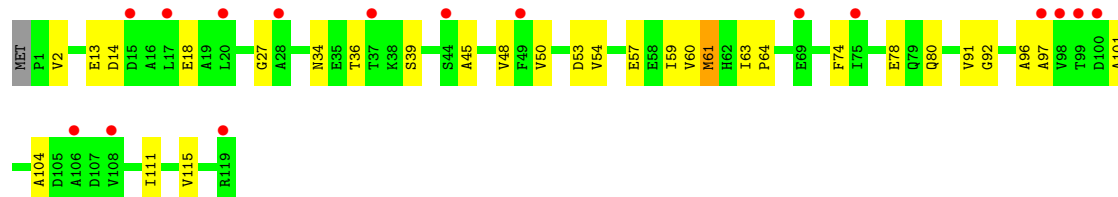
- Molecule 5: 50S ribosomal protein L6P

Chain E:



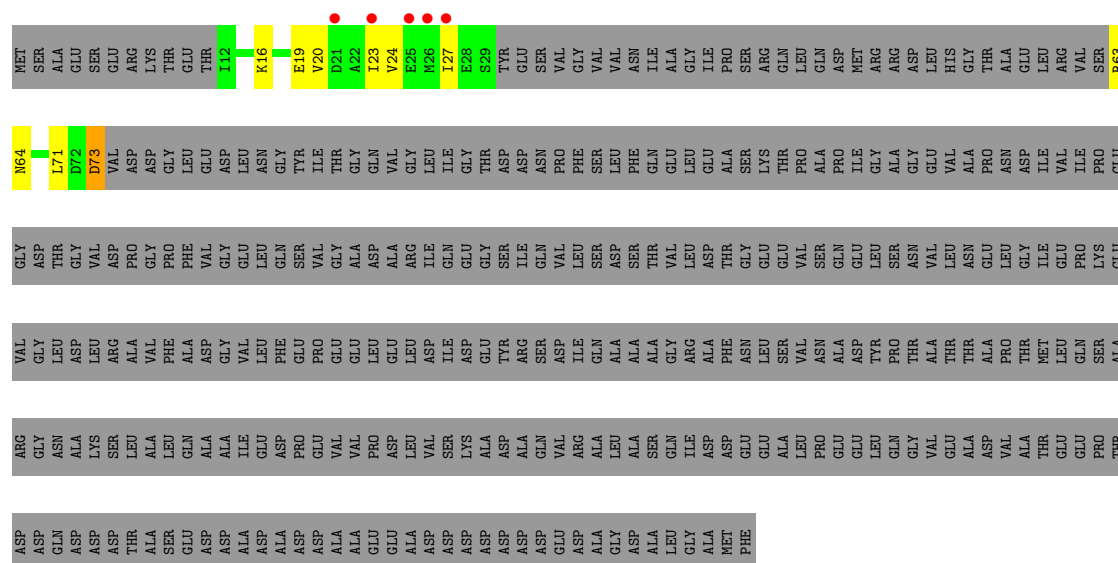
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



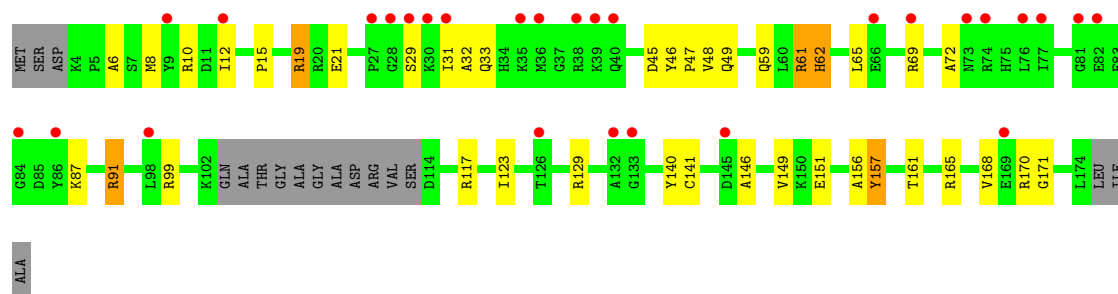
- Molecule 7: 50S ribosomal protein L10E

Chain G:



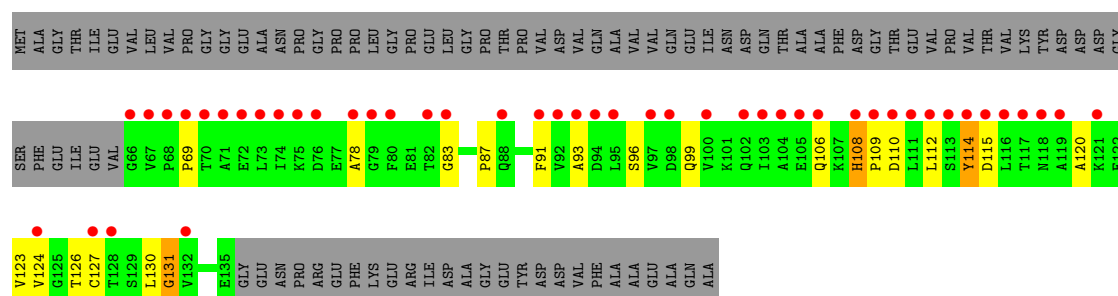
- Molecule 8: 50S ribosomal protein L10e

Chain H:



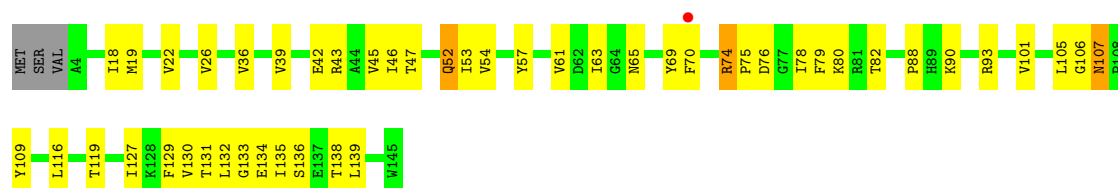
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

Chain J:



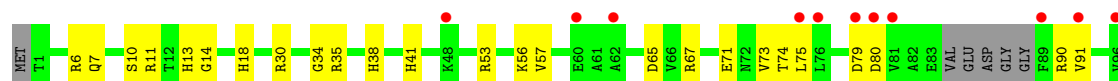
- Molecule 11: 50S ribosomal protein L14P

Chain K:



- Molecule 12: 50S ribosomal protein L15P

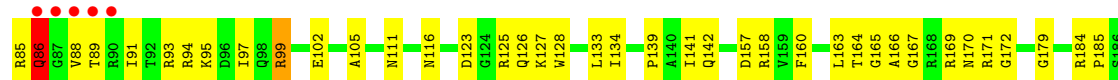
Chain L:





- Molecule 13: 50S ribosomal protein L15e

Chain M:



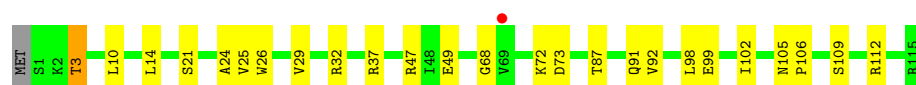
- Molecule 14: 50S ribosomal protein L18P

Chain N:



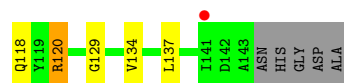
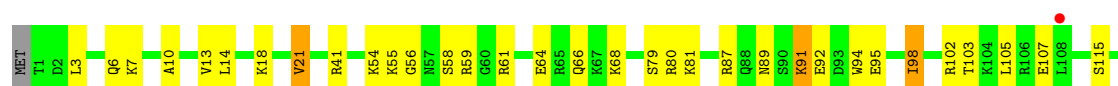
- Molecule 15: 50S ribosomal protein L18e

Chain O:



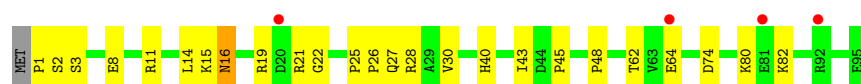
- Molecule 16: 50S ribosomal protein L19e

Chain P:



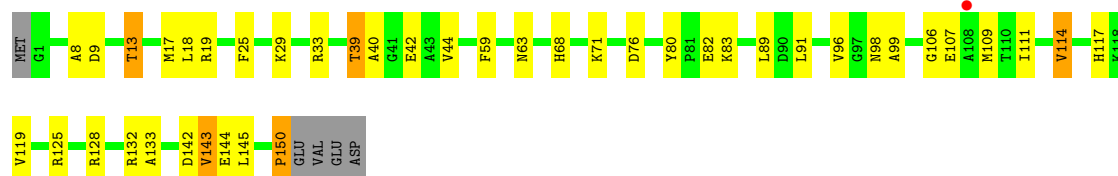
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



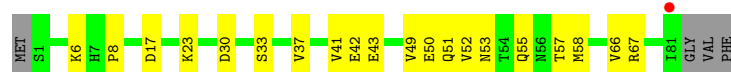
- Molecule 18: 50S ribosomal protein L22P

Chain R:



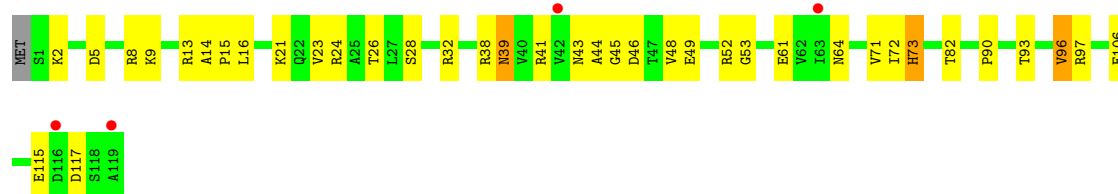
- Molecule 19: 50S ribosomal protein L23P

Chain S:



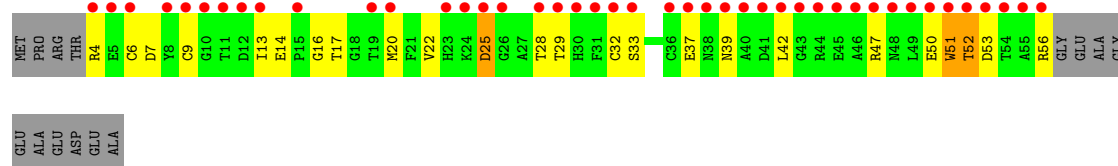
- Molecule 20: 50S ribosomal protein L24P

Chain T:



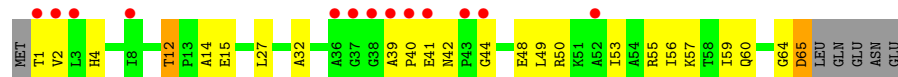
- Molecule 21: 50S ribosomal protein L24e

Chain U:



- Molecule 22: 50S ribosomal protein L29P

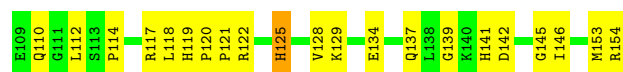
Chain V:



- Molecule 23: 50S ribosomal protein L30P

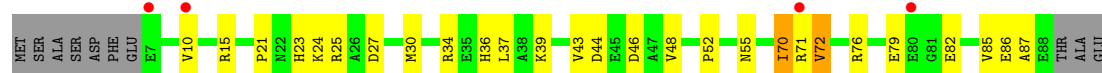
Chain W:





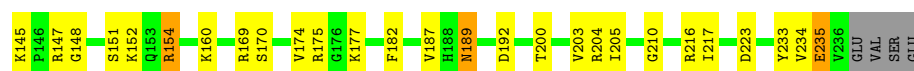
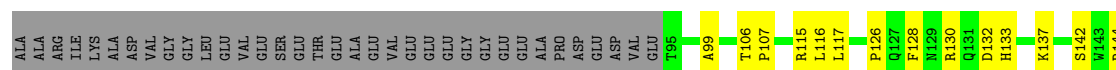
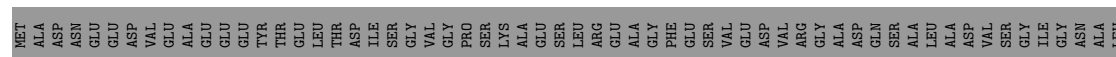
- Molecule 24: 50S ribosomal protein L31e

Chain X:



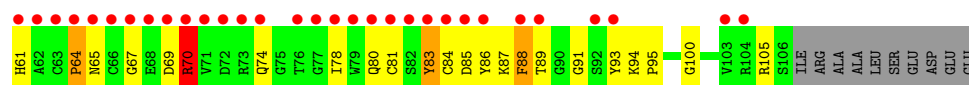
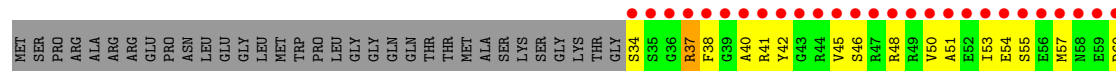
- Molecule 25: 50S ribosomal protein L32e

Chain Y:



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 27: 50S ribosomal protein L37e

Chain 1:



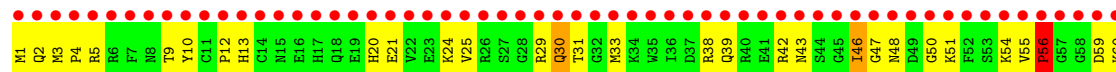
- Molecule 28: 50S ribosomal protein L39e

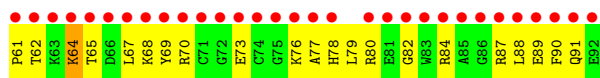
Chain 2:



- Molecule 29: 50S ribosomal protein L44E

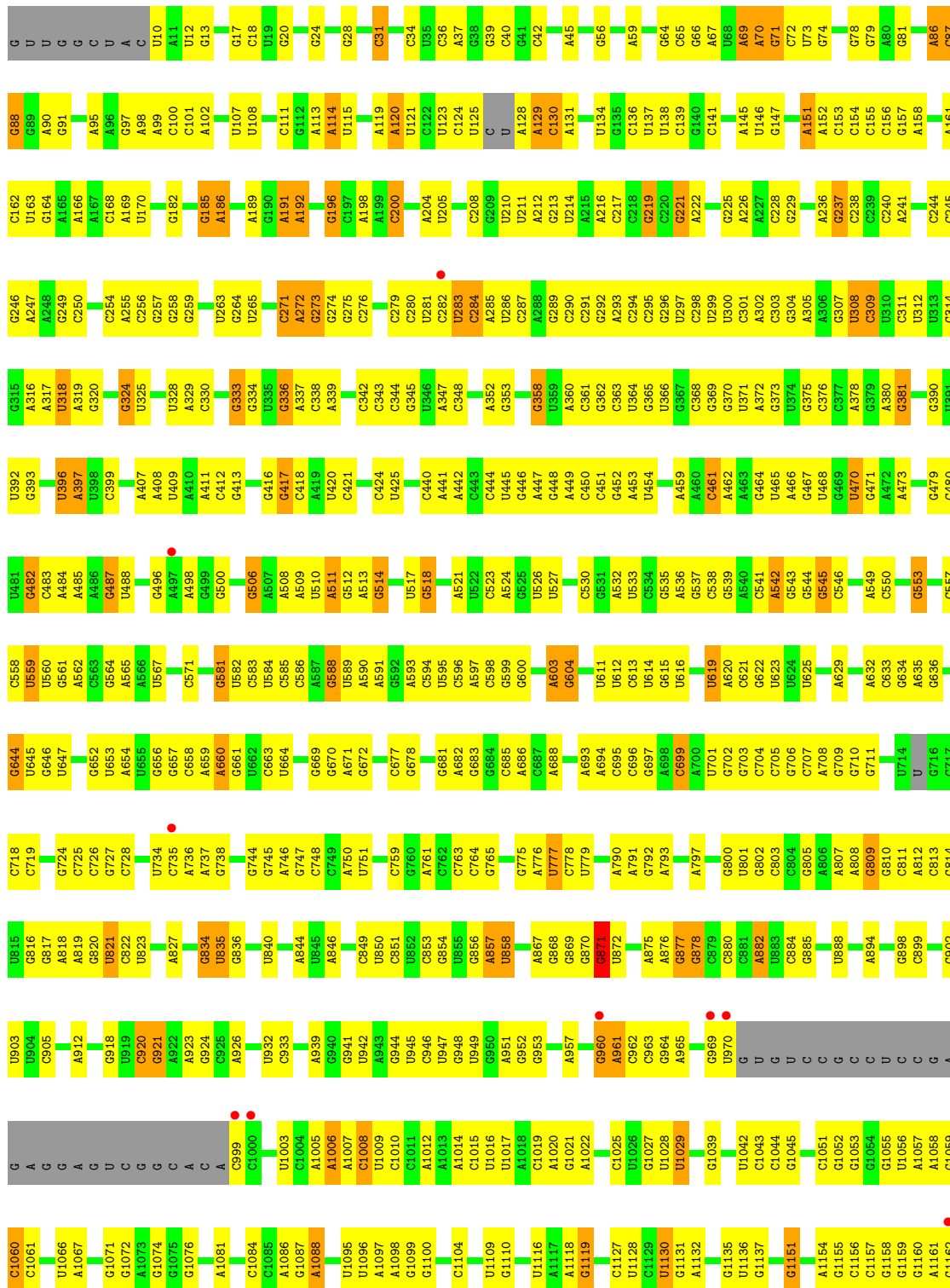
Chain 3:



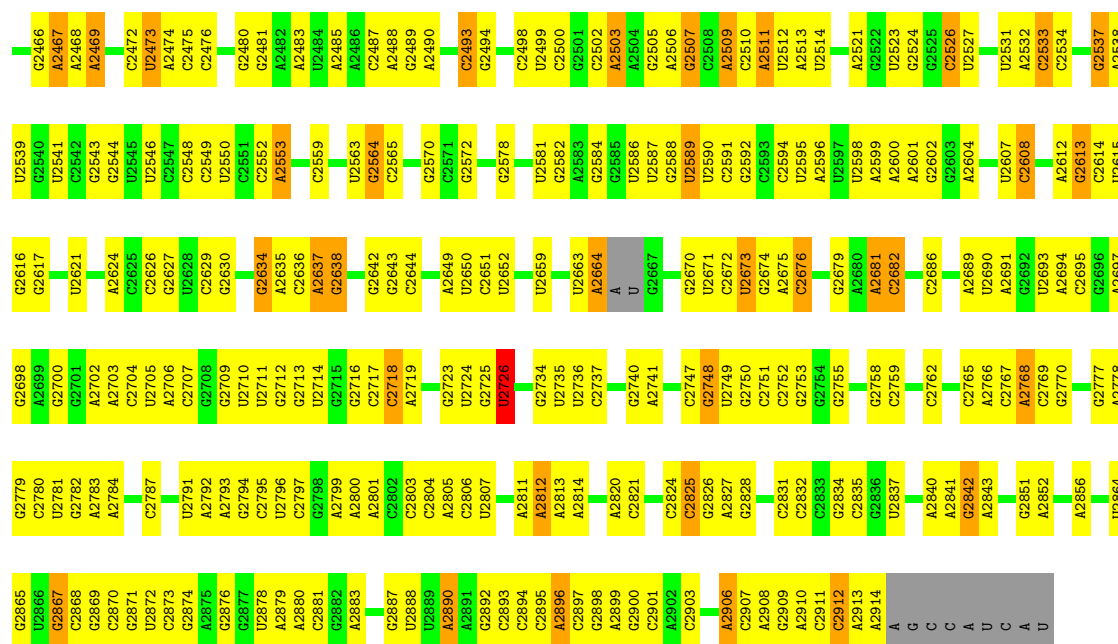


Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

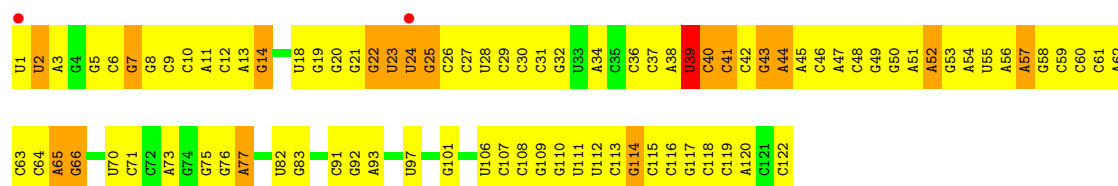


C2376	U2377	U2378	G2379	C2309	A	U	A2096	U1996	G1925	U1831	G1752	U1654	G1567	A1466	A1399	G1315	C1229	G1163
C2313	C2314	C2315	C2316	C2317	C	A	A2099	G1998	G1926	U1832	A1755	G1655	A1572	U1466	U1405	G1316	C1230	G1164
G2314	C2315	C2316	C2317	C	A	A2100	A2101	C2002	G1928	U1833	U1757	A1657	C1574	U1407	U1406	A1317	C1230	G1165
C2316	C2317	C2318	C2319	C2320	C2237	G	G2102	U2003	G1929	A1836	U1758	A1658	C1575	U1408	U1234	U1234	C1234	G1166
C2318	C2319	C2320	C2321	C2322	A2238	G	A2103	U2004	G1933	G1837	G1759	A1661	G1576	U1496	U1236	U1236	C1236	G1167
C2319	C2320	C2321	C2322	C2323	A2239	G	C2104	G2005	A1934	A1838	U1761	A1664	G1760	G1409	U1237	U1237	C1237	U1169
U2387	U2388	U2389	U2390	U2391	U2240	G	C2105	A2007	C1935	A1839	U1762	G1665	C1578	G1410	U1238	U1238	C1238	U1170
C2388	C2389	C2390	C2391	C2392	U2242	A	C2106	U2008	U1937	A1840	C1763	G1666	C1578	U1500	U1239	U1239	C1239	G1171
A2401	A2402	A2403	A2404	A2405	C2243	C	G2110	G2009	G1938	A1845	C1764	U1667	A1581	U1503	U1419	A1242	A1242	A1173
A2402	G2323	G2324	G2325	G2326	C2245	C	G2111	A2010	U1939	U1846	C1765	U1668	C1582	U1504	U1420	C1243	C1243	G1175
A2408	G2324	G2325	G2326	G2327	C2246	G	A2112	A2011	C1940	U1850	U1766	U1677	C1585	U1505	U1422	C1244	C1244	G1176
A2409	U2325	U2326	U2327	U2328	C2248	C	C2119	G2013	A1941	G1851	U1767	U1677	C1585	U1506	U1422	C1245	C1245	A1177
A2410	U2325	U2326	U2327	U2328	C2249	C	U2120	U2017	G1943	G1852	C1769	U1677	C1585	U1506	U1422	C1246	C1246	
A2411	C2329	C2330	C2331	C2332	G2250	G	G2121	A2018	G1947	C1854	U1771	G1683	G1589	U1511	A1424	A1247	A1247	U1180
A2412	U2330	U2331	U2332	U2333	G2251	U	G2128	A2018	U1948	C1855	U1772	A1684	C1592	U1512	U1425	A1248	A1248	A1181
A2413	C2331	C2332	C2333	C2334	G2252	C	U2129	A2022	G1949	C1856	G1773	C1686	C1593	U1516	U1427	U1249	U1249	C1182
A2414	A2332	A2333	A2334	A2335	G2254	C	G2254	G2255	G1950	C1856	G1774	C1687	C1594	U1516	C1428	C1250	C1250	C1183
A2415	C2335	C2336	C2337	C2338	G2255	G	G2134	U2032	G1951	C1864	G1777	C1682	G1595	U1516	U1429	C1254	C1254	U1185
A2416	C2336	C2337	C2338	C2339	G2256	G	A2135	G2033	U	A1865	G1777	C1682	G1595	U1516	U1429	C1254	C1254	C1186
A2417	C2336	C2337	C2338	C2339	G2257	G	G2136	U2034	A	A1866	A1778	C1697	A1597	U1522	A1434	G1260	G1260	U1187
A2418	C2337	C2338	C2339	C2340	A2258	C	A	C2035	C	G1868	A1779	C1697	U1598	G1523	U1435	U1266	U1266	A1188
A2419	C2338	C2339	C2340	C2341	G2263	C	C	C2035	U	G1868	G1780	C1697	U1599	G1523	U1436	U1266	U1266	G1190
A2420	A	C2341	C2342	C2343	G2264	A	G	A2039	A	U1871	C1787	A1701	A1603	G1525	U1436	C1267	C1267	A1191
A2421	C	C2342	C2343	C2344	U2265	C	G	C2040	U	C1872	U1788	U1702	A1604	A1526	U1439	C1268	C1268	A1192
U2422	A	C2345	C2346	C2347	U2266	C	G	U2043	U	G1873	U1788	G1706	G1605	A1527	U1440	G1269	G1269	A1193
A2425	G	C2347	C2348	C2349	A2267	C	U	G2044	G	G1877	G1789	G1707	G1606	A1528	U1441	U1270	U1270	
A2426	A	C2349	C2350	C2351	C2269	G	G	G2044	C	U1878	U1791	G1707	G1607	G1529	A1442	C1273	C1273	U1197
A2427	C2344	C2345	C2346	C2347	G2270	A	C	G2050	C	U1879	C1792	A1710	G1608	U1530	U1446	C1273	C1273	U1198
A2434	C2345	C2346	C2347	C2348	G2271	C	C	A2054	U1964	C1882	C1793	C1714	C1609	G1531	U1447	A1278	A1278	A1199
U2435	C2346	C2347	C2348	C2349	G2272	A	C	A2055	C1965	C1883	G1794	C1715	G1610	G1535	C1451	U1279	U1279	A1200
U2436	C2347	C2348	C2349	C2350	G2273	C	G	A2056	U1966	C1883	G1795	C1715	G1611	C1536	C1451	A1280	A1280	C1201
A2437	C2348	C2349	C2350	C2351	A2274	C	A	C2057	U1967	G1884	A1796	A1716	A1612	C1537	G1452	C1360	C1360	A1202
A2438	C2349	C2350	C2351	C2352	G2275	C	U	U2057	U1967	G1884	A1796	A1716	A1612	C1538	G1452	C1361	C1361	G1203
A2439	C2350	C2351	C2352	C2353	U2276	U	G	G2058	U1968	U1890	C1798	A1717	A1614	C1539	U1454	C1287	C1287	G1204
C2440	C2351	C2352	C2353	C2354	U2277	U	U	U2059	A1969	U1890	C1798	U1722	G1614	C1540	U1455	C1289	C1289	U1205
U2441	C2352	C2353	C2354	C2355	U2278	G	G	A2060	G1970	C1894	A1801	G1723	A1616	U1541	C1456	G1364	G1364	U1206
U2442	C2356	C2357	C2358	C2359	C2281	A	C	C2061	U1971	C1894	A1801	G1723	A1616	U1541	C1456	G1364	G1364	U1207
U2443	C2359	U2282	U2283	U2284	U2281	A	C	C2061	U1971	C1894	A1801	G1723	A1616	U1541	C1456	G1364	G1364	U1207
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G2445	A2361	C2362	C2363	C2364	G2283	U	G	U2063	A1973	U1903	G1805	C1623	G1622	U1544	U1461	A1296	A1296	C1209
G2446	C2362	C2363	C2364	C2365	G2284	C	A	U2064	G1974	A1904	G1806	C1623	G1622	U1544	U1461	A1296	A1296	G1210
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G2449	C2365	C2366	C2367	C2368	G2289	U	A	C2071	U1977	C1913	C1810	A1732	A1626	U1552	A1470	U1304	U1304	
G2450	C2366	C2367	C2368	C2369	G2290	C	G	G2072	U1978	C1913	C1810	A1732	A1626	U1552	A1470	U1304	U1304	
G2451	C2367	C2368	C2369	C2370	U2290	C	G	G2073	U1979	C1914	A1811	C1734	A1627	C1554	A1471	C1305	C1305	
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G2454	C2369	C2370	C2371	C2372	G2296	G	G	G2075	U1981	U1916	A1816	A1736	A1632	U1473	U1306	G1217	G1217	
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U2461	C2373	C2374	C2375	C2376	A2300	G	G	U2088	U1992	C1920	C1818	A1742	U1635	C1561	C1477	U1309	U1309	
U2462	C2374	C2375	C2376	C2377	A2301	C	U	G2092	C1993	A1922	G1820	U1748	A1641	G1563	U1478	U1310	U1310	
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U2466	C2378	C2379	C2380	C2381	A2305	C	C	G2092	C1993	A1922	G1820	U1748	A1641	G1563	U1478	U1310	U1310	
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U2471	C2383	C2384	C2385	C2386	A2310	C	C	G2092	C1993	A1922	G1820	U1748	A1641	G1563	U1478	U1310	U1310	
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U2479	C2391	C2392	C2393	C2394	A2318	C	C	G2092	C1993	A1922	G1820	U1748	A1641	G1563	U1478	U1310	U1310	
U2480	C2392	C2393	C2394	C2395	A2319	C	C	G2092	C1993	A1922	G1820	U1748	A1641	G1563	U1478	U1310	U1310	
U2481	C2393	C2394	C2395	C2396	A2320	C	C	G2092	C1993	A1922	G1820	U1748	A1641	G1563	U1478	U1310	U1310	
U2482	C2394	C2395	C															



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.24Å 299.19Å 575.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 85.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 91.7 (85.59-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.238 0.178 , 0.229	Depositor DCC
R_{free} test set	3430 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 667094 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: MG, OMG, CL, SR, NA, K, 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	0.34	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.39	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.57	0/1498
5	E	0.34	0/1382	0.56	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.32	0/241	0.47	0/324
8	H	0.33	0/1302	0.62	0/1743
9	I	0.32	0/526	0.54	0/716
10	J	0.39	0/1136	0.61	0/1530
11	K	0.37	0/1004	0.66	0/1351
12	L	0.34	0/1130	0.61	0/1509
13	M	0.40	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.61	0/1999
15	O	0.37	0/874	0.62	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.64	0/1005
18	R	1.27	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.36	0/648	0.59	0/875
20	T	0.34	0/958	0.66	0/1289
21	U	0.45	0/417	0.60	0/562
22	V	0.34	0/502	0.53	0/675
23	W	0.38	0/1219	0.65	0/1655
24	X	0.36	0/664	0.61	0/895
25	Y	0.38	0/1146	0.62	0/1536
26	Z	0.43	0/584	0.63	0/781
27	1	0.47	0/438	0.64	0/578
28	2	0.36	0/401	0.61	0/529
29	3	0.46	0/771	0.60	0/1024
30	0	0.42	0/65956	0.68	7/102865 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.42	7/98700 (0.0%)	0.67	14/147584 (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
18	R	1	0
23	W	0	1
30	0	0	34
All	All	1	35

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.15	2.85	1.50
18	R	150	PRO	CA-C	-18.51	1.15	1.52
18	R	150	PRO	CG-CD	13.84	1.96	1.50
18	R	150	PRO	C-O	11.87	1.47	1.23
18	R	150	PRO	N-CA	11.57	1.67	1.47
18	R	150	PRO	N-CD	10.73	1.62	1.47
18	R	150	PRO	CA-CB	7.84	1.69	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.43	55.92	112.00
18	R	150	PRO	N-CA-C	-19.45	61.53	112.10
18	R	150	PRO	CA-N-CD	12.27	128.88	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.27	100.34	120.20
18	R	150	PRO	CA-CB-CG	-6.08	92.45	104.00
30	0	871	G	C5'-C4'-O4'	-5.70	102.26	109.10
30	0	1504	A	C1'-O4'-C4'	-5.64	105.39	109.90
30	0	1942	A	C5'-C4'-C3'	5.59	124.94	116.00
30	0	1971	G	N9-C1'-C2'	5.38	121.00	114.00
30	0	1819	G	C5'-C4'-C3'	5.29	124.46	116.00
30	0	2726	U	N1-C1'-C2'	5.20	120.75	114.00
30	0	2313	C	O4'-C4'-C3'	-5.12	98.88	104.00
31	9	39	U	N1-C1'-C2'	5.09	120.62	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1236	A	Sidechain
30	0	1260	G	Sidechain
30	0	1430	G	Sidechain
30	0	1524	U	Sidechain
30	0	1599	U	Sidechain
30	0	1736	A	Sidechain
30	0	1741	U	Sidechain
30	0	1777	G	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1878	G	Sidechain
30	0	196	G	Sidechain
30	0	1993	C	Sidechain
30	0	221	G	Sidechain
30	0	2316	G	Sidechain
30	0	2473	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2552	C	Sidechain
30	0	2599	A	Sidechain
30	0	2630	G	Sidechain
30	0	2673	U	Sidechain
30	0	2726	U	Sidechain
30	0	2842	G	Sidechain
30	0	324	G	Sidechain
30	0	333	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	506	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	888	U	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	1753	0	1766	85	0
2	B	2625	0	2533	108	0
3	C	1860	0	1813	63	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	39	0
6	F	890	0	843	19	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	14	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	34	0
12	L	1118	0	1076	38	0
13	M	1558	0	1573	95	0
14	N	1445	0	1401	73	0
15	O	865	0	873	22	0
16	P	1136	0	1123	34	0
17	Q	735	0	729	28	0
18	R	1149	0	1122	41	0
19	S	641	0	605	15	0
20	T	950	0	924	36	0
21	U	410	0	368	26	0
22	V	499	0	511	21	0
23	W	1196	0	1137	58	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	39	0
26	Z	573	0	535	50	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	732	57	0
30	0	59019	0	29809	1661	0
31	9	2599	0	1325	128	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
33	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	65	0	0	0	0
34	9	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	3	0
35	3	1	0	0	1	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	2	0
36	0	92	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	2	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5904	0	0	251	0
38	1	59	0	0	3	0
38	2	43	0	0	2	0
38	3	70	0	0	3	0
38	9	149	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	119	0	0	7	0
38	B	152	0	0	16	0
38	C	185	0	0	18	0
38	D	42	0	0	4	0
38	E	43	0	0	1	0
38	F	26	0	0	1	0
38	G	19	0	0	1	0
38	H	65	0	0	4	0
38	I	8	0	0	1	0
38	J	53	0	0	1	0
38	K	58	0	0	3	0
38	L	85	0	0	9	0
38	M	127	0	0	13	0
38	N	59	0	0	2	0
38	O	39	0	0	2	0
38	P	67	0	0	3	0
38	Q	48	0	0	1	0
38	R	77	0	0	2	0
38	S	30	0	0	2	0
38	T	36	0	0	3	0
38	U	28	0	0	4	0
38	V	13	0	0	2	0
38	W	67	0	0	3	0
38	X	21	0	0	2	0
38	Y	100	0	0	5	0
38	Z	31	0	0	7	0
All	All	99121	0	59922	2676	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 18.

All (2676) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.41
30:0:871:G:C8	30:0:871:G:H5'	1.77	1.19
10:J:82:THR:HG23	30:0:1242:A:H5'	1.23	1.16
30:0:1165:G:H1'	30:0:1174:A:H1'	1.17	1.14
31:9:56:A:H2'	31:9:57:A:H5''	1.19	1.13
30:0:1559:A:H1'	38:0:5849:HOH:O	1.45	1.13
30:0:1160:G:C5'	30:0:1161:A:H5'	1.78	1.13
31:9:29:C:H2'	31:9:30:C:H5'	1.32	1.10
15:O:3:THR:HG22	30:0:656:G:H5'	1.19	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:171:ARG:HD3	30:0:156:C:H5''	1.28	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.80	1.09
30:0:871:G:H8	30:0:871:G:H5'	0.99	1.08
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.17	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.69	1.07
31:9:76:G:H3'	31:9:77:A:H5''	1.33	1.05
30:0:545:G:H8	30:0:545:G:H5'	1.22	1.05
14:N:37:ARG:NH1	31:9:6:C:H5''	1.71	1.03
30:0:1603:A:H5'	30:0:1605:G:O4'	1.60	1.02
30:0:1641:A:H2'	30:0:1642:A:H5'	1.44	0.99
21:U:56:ARG:HD2	30:0:2890:A:C8	1.98	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.63	0.98
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.43	0.98
11:K:10:GLN:H	11:K:10:GLN:HE21	0.99	0.97
30:0:1979:G:H2'	38:0:9283:HOH:O	1.65	0.97
30:0:871:G:H8	30:0:871:G:C5'	1.78	0.96
30:0:381:G:H5''	38:0:4317:HOH:O	1.64	0.96
30:0:1165:G:H21	30:0:1173:A:H5''	1.30	0.96
13:M:70:GLY:HA3	13:M:73:ARG:NH2	1.80	0.96
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.47	0.96
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.05	0.95
31:9:56:A:C2'	31:9:57:A:H5''	1.95	0.95
30:0:1474:C:H6	30:0:1474:C:H5'	1.30	0.95
31:9:14:G:H5'	31:9:14:G:H8	1.32	0.94
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.50	0.94
30:0:236:A:H4'	30:0:237:G:H5'	1.49	0.94
2:B:264:GLU:HG2	2:B:267:LYS:HE3	1.50	0.94
30:0:1165:G:H21	30:0:1173:A:C5'	1.81	0.93
16:P:115:SER:H	16:P:118:GLN:HE21	1.11	0.93
30:0:2505:G:H2'	30:0:2506:A:H5'	1.50	0.93
30:0:2717:C:C2'	30:0:2718:C:H5''	1.99	0.93
30:0:2502:C:H2'	30:0:2503:A:H5'	1.52	0.92
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.35	0.92
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.52	0.91
3:C:27:ARG:HG2	3:C:27:ARG:HH11	1.36	0.91
30:0:2321:A:H2	30:0:2378:U:H3	1.14	0.91
15:O:3:THR:CG2	30:0:656:G:H5'	2.00	0.91
30:0:2710:U:H1'	38:0:7613:HOH:O	1.71	0.90
30:0:282:C:O2'	30:0:283:U:H5'	1.71	0.90
30:0:1118:A:H62	30:0:1244:U:H3	1.14	0.90
3:C:236:THR:HG22	3:C:239:ALA:H	1.35	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2506:A:HO2'	30:0:2507:G:H8	0.90	0.90
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.53	0.90
30:0:2812:A:H2	30:0:2814:A:H62	1.19	0.90
30:0:1116:U:O2'	30:0:1118:A:H2	1.54	0.90
30:0:545:G:C8	30:0:545:G:H5'	2.06	0.89
30:0:2321:A:H8	30:0:2322:U:HO2'	1.13	0.89
30:0:2502:C:C2'	30:0:2503:A:H5'	2.03	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.88
35:Y:8820:CL:CL	38:0:4953:HOH:O	2.27	0.88
30:0:1119:G:H22	30:0:1246:A:H2	1.16	0.88
30:0:2700:G:H3'	38:0:3569:HOH:O	1.73	0.88
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.20	0.88
13:M:79:ALA:HB3	13:M:81:ARG:HH12	1.38	0.88
31:9:92:G:H2'	31:9:93:A:C8	2.07	0.88
30:0:1118:A:H3'	30:0:1118:A:C8	2.08	0.88
30:0:1206:U:H5'	30:0:1206:U:H6	1.39	0.88
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.35	0.88
30:0:506:G:H22	30:0:509:A:C5'	1.85	0.87
30:0:1474:C:C6	30:0:1474:C:H5'	2.10	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.73	0.87
30:0:542:A:H5'	30:0:542:A:H8	1.39	0.87
30:0:1118:A:H3'	30:0:1118:A:H8	1.39	0.87
30:0:2321:A:H4'	30:0:2322:U:OP1	1.73	0.87
30:0:363:C:H1'	38:0:5273:HOH:O	1.75	0.86
30:0:2505:G:C2'	30:0:2506:A:H5'	2.04	0.86
30:0:1278:A:H4'	30:0:1279:U:C4	2.10	0.86
1:A:70:ALA:HB1	26:Z:89:THR:HG21	1.57	0.86
30:0:1701:A:H4'	30:0:1702:U:H5''	1.55	0.86
13:M:70:GLY:HA2	30:0:2263:G:H4'	1.59	0.85
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.58	0.85
30:0:506:G:H22	30:0:509:A:H5''	1.42	0.85
30:0:1641:A:C2'	30:0:1642:A:H5'	2.06	0.85
30:0:1205:U:H2'	30:0:1206:U:H5'	1.58	0.85
26:Z:70:ARG:NH1	26:Z:83:TYR:HB2	1.91	0.85
30:0:2717:C:H2'	30:0:2718:C:H5''	1.59	0.85
30:0:1666:C:H2'	30:0:1667:A:H5'	1.58	0.84
30:0:2717:C:O2'	30:0:2718:C:H5''	1.76	0.84
29:3:68:LYS:HE2	30:0:2436:U:H5'	1.60	0.84
30:0:2637:A:H4'	38:0:4923:HOH:O	1.78	0.83
30:0:2043:U:H3'	38:0:6696:HOH:O	1.76	0.83
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.58	0.83
30:0:2010:A:H2'	38:0:5942:HOH:O	1.77	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:125:HIS:NE2	30:0:1097:A:H5''	1.93	0.83
1:A:167:LYS:HE2	26:Z:50:VAL:HG13	1.61	0.83
13:M:68:ARG:NH2	13:M:73:ARG:HD3	1.94	0.83
30:0:380:A:H2'	38:0:7216:HOH:O	1.77	0.83
29:3:64:LYS:HA	29:3:84:ARG:HA	1.57	0.83
11:K:10:GLN:H	11:K:10:GLN:NE2	1.77	0.83
11:K:39:GLY:HA2	38:0:5215:HOH:O	1.76	0.83
30:0:2454:C:H5''	38:0:7719:HOH:O	1.79	0.82
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.61	0.82
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:1667:A:H8	30:0:1667:A:H5'	1.44	0.82
13:M:27:ARG:HH22	13:M:44:THR:HG23	1.44	0.82
30:0:541:C:C2'	30:0:542:A:H5''	2.09	0.82
30:0:541:C:H2'	30:0:542:A:C5'	2.08	0.82
30:0:1300:G:H1'	38:0:4678:HOH:O	1.80	0.81
29:3:31:THR:O	30:0:1923:G:H4'	1.79	0.81
30:0:1184:C:H1'	38:0:7461:HOH:O	1.80	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.81
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.62	0.81
30:0:2769:C:O2'	30:0:2770:G:H5'	1.81	0.81
31:9:29:C:C2'	31:9:30:C:H5'	2.08	0.81
30:0:559:U:H5'	30:0:559:U:H6	1.45	0.81
3:C:139:VAL:HG13	38:C:8658:HOH:O	1.79	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.80	0.81
30:0:1174:A:C6	30:0:1201:C:H4'	2.14	0.81
18:R:39:THR:HG22	18:R:42:GLU:H	1.46	0.81
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.25	0.81
30:0:1119:G:N2	30:0:1246:A:C2	2.47	0.81
30:0:1205:U:H2'	30:0:1206:U:C5'	2.10	0.81
30:0:681:G:N3	30:0:681:G:H5'	1.96	0.81
30:0:1641:A:H2'	30:0:1642:A:C5'	2.09	0.81
30:0:1801:A:H3'	38:0:7607:HOH:O	1.81	0.80
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.47	0.80
30:0:2748:G:H2'	38:0:7534:HOH:O	1.81	0.80
28:2:41:HIS:H	28:2:45:ASN:HD22	1.27	0.80
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.96	0.80
30:0:1593:C:H1'	38:0:6089:HOH:O	1.80	0.80
15:O:3:THR:HG22	30:0:656:G:C5'	2.09	0.80
30:0:2783:A:H3'	38:0:5225:HOH:O	1.81	0.80
31:9:39:U:H1'	31:9:44:A:H61	1.45	0.80
25:Y:115:ARG:NH2	30:0:1266:U:H4'	1.97	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:14:G:H5'	31:9:14:G:C8	2.16	0.80
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.62	0.80
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.63	0.80
30:0:586:C:H5''	38:0:7275:HOH:O	1.81	0.80
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.63	0.79
13:M:27:ARG:NH2	13:M:44:THR:HG23	1.96	0.79
6:F:91:VAL:HG12	6:F:92:GLY:H	1.46	0.79
38:N:8842:HOH:O	31:9:49:G:H5''	1.83	0.79
10:J:82:THR:CG2	30:0:1242:A:H5'	2.09	0.79
30:0:2586:U:H3	30:0:2592:G:H22	1.28	0.79
30:0:2419:U:H5''	30:0:2420:G:H5'	1.65	0.79
30:0:1183:C:H2'	38:0:6224:HOH:O	1.82	0.79
30:0:255:A:H2'	30:0:256:C:H6	1.48	0.79
3:C:1:MET:HG2	3:C:2:GLN:H	1.47	0.78
30:0:2635:A:O2'	30:0:2636:C:H5'	1.82	0.78
30:0:308:U:H5'	30:0:309:C:OP1	1.82	0.78
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.48	0.78
30:0:659:A:H5''	38:0:7089:HOH:O	1.83	0.78
30:0:1372:A:H3'	38:0:7180:HOH:O	1.81	0.78
4:D:154:LYS:HD2	4:D:154:LYS:H	1.48	0.78
30:0:123:U:H5'	38:0:6637:HOH:O	1.82	0.78
30:0:2485:A:H3'	38:0:5838:HOH:O	1.82	0.78
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.31	0.78
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.80	0.78
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.66	0.78
30:0:960:G:H4'	38:0:7423:HOH:O	1.83	0.78
30:0:1595:G:O2'	30:0:1596:U:H5'	1.84	0.78
30:0:2291:A:C8	30:0:2309:C:H5'	2.19	0.78
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.82	0.78
30:0:541:C:H2'	30:0:542:A:H5''	1.65	0.77
30:0:2469:A:H1'	38:0:3229:HOH:O	1.83	0.77
30:0:871:G:C8	30:0:871:G:C5'	2.58	0.77
30:0:1189:A:H3'	38:0:7669:HOH:O	1.83	0.77
30:0:2420:G:O2'	30:0:2421:G:H5'	1.85	0.77
30:0:1116:U:H3	30:0:1246:A:H62	1.33	0.77
30:0:558:C:C2'	30:0:559:U:H5''	2.14	0.77
30:0:564:G:H1'	38:0:6295:HOH:O	1.84	0.77
30:0:2769:C:C2'	30:0:2770:G:H5'	2.15	0.77
30:0:558:C:O2'	30:0:559:U:H5''	1.85	0.77
30:0:2703:A:H2'	30:0:2704:C:H6	1.50	0.76
30:0:1973:A:H5'	30:0:1973:A:H8	1.48	0.76
30:0:1632:A:H2'	30:0:1633:C:H5'	1.67	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:283:U:H5	30:0:284:C:C4	2.02	0.76
30:0:1175:G:H1'	30:0:1193:A:H2'	1.65	0.76
31:9:1:U:H4'	31:9:3:A:OP1	1.84	0.76
30:0:2468:A:H3'	38:0:5449:HOH:O	1.84	0.76
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.33	0.76
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.68	0.76
30:0:2506:A:O2'	30:0:2507:G:H8	1.68	0.76
30:0:969:G:H1	30:0:999:C:H42	1.34	0.76
38:C:8633:HOH:O	30:0:338:C:H5''	1.86	0.76
13:M:71:SER:HB3	30:0:2264:A:OP1	1.85	0.75
30:0:899:C:H5'	38:0:3190:HOH:O	1.85	0.75
4:D:105:SER:OG	30:0:2338:G:H1'	1.85	0.75
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.66	0.75
30:0:2505:G:H2'	30:0:2506:A:C5'	2.17	0.75
30:0:282:C:H1'	30:0:368:C:N4	2.01	0.75
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.52	0.75
30:0:1170:U:H2'	30:0:1172:G:OP2	1.87	0.75
26:Z:70:ARG:HB2	26:Z:70:ARG:HH11	1.51	0.74
30:0:2908:A:H2'	30:0:2909:G:O4'	1.87	0.74
30:0:544:G:H2'	30:0:545:G:H5''	1.68	0.74
30:0:1741:U:O2'	30:0:2723:G:H4'	1.87	0.74
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.52	0.74
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.52	0.74
3:C:218:VAL:HG12	38:C:8637:HOH:O	1.87	0.74
30:0:1834:C:H2'	30:0:1840:A:N6	2.02	0.74
35:0:8813:CL:CL	38:0:4678:HOH:O	2.43	0.74
30:0:2781:U:C2'	30:0:2782:G:H5'	2.18	0.74
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.69	0.74
30:0:2793:A:H1'	38:0:6312:HOH:O	1.88	0.74
14:N:11:ARG:HD3	31:9:114:G:O6	1.88	0.74
25:Y:235:GLU:H	25:Y:235:GLU:CD	1.92	0.73
3:C:140:VAL:HB	38:C:8660:HOH:O	1.86	0.73
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.70	0.73
18:R:98:ASN:HD21	30:0:500:G:H21	1.36	0.73
31:9:92:G:H2'	31:9:93:A:H8	1.50	0.73
30:0:2578:G:H5'	30:0:2578:G:H8	1.52	0.73
30:0:1525:G:H5'	30:0:1526:A:OP2	1.89	0.73
21:U:56:ARG:HH11	21:U:56:ARG:HG3	1.54	0.73
2:B:56:ASP:HB2	2:B:322:ARG:HE	1.52	0.73
30:0:2748:G:H1'	38:0:7889:HOH:O	1.88	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.70	0.73
30:0:1279:U:O2	30:0:1279:U:H2'	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2768:A:O2'	30:0:2769:C:H5'	1.89	0.72
30:0:619:U:H3'	38:0:3270:HOH:O	1.88	0.72
14:N:37:ARG:HH12	31:9:6:C:H5''	1.55	0.72
30:0:2871:G:H2'	30:0:2872:U:H6	1.54	0.72
30:0:2524:G:H21	30:0:2526:C:N4	1.85	0.72
30:0:558:C:H2'	30:0:559:U:C5'	2.20	0.72
30:0:271:C:H41	30:0:378:A:H2	1.33	0.72
30:0:1921:A:O2'	30:0:1922:A:H5'	1.89	0.72
2:B:179:LEU:O	2:B:183:GLU:HG2	1.89	0.72
30:0:2766:A:H5'	38:0:9565:HOH:O	1.88	0.72
30:0:1166:A:P	30:0:1174:A:H4'	2.29	0.72
31:9:29:C:H2'	31:9:30:C:C5'	2.17	0.72
30:0:877:G:H5'	30:0:878:G:OP1	1.89	0.72
30:0:2533:C:H6	30:0:2533:C:H5'	1.53	0.72
30:0:544:G:C2'	30:0:545:G:H5''	2.20	0.72
13:M:79:ALA:H	13:M:81:ARG:HH22	1.37	0.72
30:0:2712:G:H5'	38:0:5215:HOH:O	1.90	0.72
30:0:836:G:H5''	38:0:9285:HOH:O	1.89	0.72
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.70	0.72
31:9:54:A:O2'	31:9:55:U:H5'	1.89	0.71
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.24	0.71
2:B:145:HIS:HD2	2:B:146:THR:O	1.73	0.71
29:3:2:GLN:O	30:0:2320:U:H2'	1.90	0.71
14:N:159:TYR:HE1	31:9:50:G:H5''	1.55	0.71
30:0:281:U:H2'	30:0:282:C:O4'	1.90	0.71
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.72	0.71
30:0:702:G:O2'	30:0:703:G:H5'	1.90	0.71
30:0:2534:C:H1'	38:0:3477:HOH:O	1.91	0.71
30:0:821:U:H3'	38:0:3759:HOH:O	1.90	0.71
30:0:2426:G:H1'	38:0:6075:HOH:O	1.90	0.71
30:0:1165:G:N2	30:0:1173:A:C5'	2.53	0.71
30:0:221:G:H5''	38:0:5725:HOH:O	1.90	0.71
38:I:6825:HOH:O	30:0:1166:A:H2	1.73	0.71
30:0:1835:U:C5	30:0:1840:A:N7	2.57	0.71
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.55	0.71
30:0:1132:A:N6	30:0:1229:C:H2'	2.06	0.71
30:0:1589:G:N2	30:0:1605:G:H1'	2.05	0.71
30:0:1979:G:H3'	38:0:3282:HOH:O	1.88	0.71
14:N:5:ARG:HH11	14:N:5:ARG:HB2	1.56	0.71
30:0:2487:C:H5	38:0:4880:HOH:O	1.73	0.70
30:0:2514:U:OP1	30:0:2572:G:H1'	1.90	0.70
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.56	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2505:G:O2'	30:0:2506:A:H5'	1.90	0.70
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.55	0.70
30:0:1666:C:H2'	30:0:1667:A:C5'	2.21	0.70
26:Z:70:ARG:HH12	26:Z:83:TYR:HB2	1.55	0.70
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.20	0.70
17:Q:11:ARG:NH2	30:0:2297:U:H4'	2.07	0.70
30:0:1189:A:H1'	30:0:1209:C:C1'	2.21	0.70
30:0:1209:C:H2'	30:0:1210:G:H8	1.57	0.70
30:0:2237:G:H1'	30:0:2238:A:C8	2.27	0.70
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.06	0.70
13:M:188:ARG:HD3	30:0:155:C:OP2	1.92	0.70
26:Z:80:GLN:HG3	26:Z:81:CYS:H	1.56	0.70
30:0:31:C:H2'	38:0:7677:HOH:O	1.90	0.70
38:Q:6286:HOH:O	30:0:1019:C:H5'	1.91	0.69
30:0:2251:G:H2'	30:0:2252:A:C8	2.27	0.69
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.07	0.69
30:0:1562:C:O2	30:0:1562:C:H2'	1.91	0.69
2:B:36:PRO:HG3	2:B:169:GLY:H	1.57	0.69
30:0:42:C:H3'	38:0:4166:HOH:O	1.92	0.69
30:0:138:U:H5''	30:0:139:C:OP2	1.93	0.69
30:0:1451:C:H5'	30:0:1505:U:C5	2.27	0.69
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.57	0.69
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.74	0.69
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.55	0.69
14:N:49:THR:HB	14:N:58:LEU:HD11	1.74	0.69
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.69
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.06	0.69
30:0:287:C:H42	30:0:365:G:H1	1.41	0.69
30:0:2102:G:H4'	38:0:5631:HOH:O	1.92	0.69
30:0:2102:G:N2	30:0:2103:A:N1	2.40	0.69
30:0:2871:G:H2'	30:0:2872:U:C6	2.28	0.69
30:0:961:A:H4'	38:0:6759:HOH:O	1.91	0.69
30:0:407:A:H2'	30:0:408:A:C8	2.28	0.69
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.72	0.69
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.75	0.69
14:N:141:ARG:HH21	31:9:48:C:H4'	1.57	0.69
31:9:39:U:H3'	31:9:40:C:H5''	1.75	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.73	0.69
12:L:91:VAL:HG13	12:L:120:LEU:HD23	1.75	0.69
30:0:2511:A:H2'	30:0:2512:U:O4'	1.93	0.69
30:0:2781:U:H2'	30:0:2782:G:H5'	1.73	0.69
2:B:18:ARG:HE	2:B:256:GLN:HE21	1.41	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1589:G:H22	30:0:1605:G:H1'	1.55	0.69
13:M:68:ARG:HD3	13:M:68:ARG:O	1.93	0.69
30:0:969:G:H1	30:0:999:C:N4	1.91	0.69
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.92	0.68
22:V:50:ARG:HH12	30:0:56:G:H5''	1.58	0.68
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.59	0.68
30:0:317:A:H5'	38:0:3761:HOH:O	1.91	0.68
30:0:1474:C:C5'	30:0:1474:C:H6	2.06	0.68
30:0:2781:U:O2'	30:0:2782:G:H5'	1.93	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.22	0.68
14:N:40:ASN:ND2	31:9:28:U:H5''	2.08	0.68
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.87	0.68
29:3:59:ASP:HA	30:0:2460:A:H5''	1.74	0.68
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.75	0.68
30:0:962:C:H2'	30:0:963:C:H5'	1.74	0.68
2:B:254:GLN:HG3	38:0:9697:HOH:O	1.92	0.68
30:0:255:A:H2'	30:0:256:C:C6	2.29	0.68
30:0:390:G:H5'	38:0:7539:HOH:O	1.94	0.68
28:2:35:ARG:HB2	38:2:2691:HOH:O	1.92	0.68
10:J:131:THR:HB	10:J:134:GLU:HG3	1.75	0.68
30:0:283:U:H5	30:0:284:C:N3	1.91	0.68
30:0:1702:U:H1'	38:0:5758:HOH:O	1.93	0.68
30:0:1527:A:H1'	30:0:1528:A:C8	2.28	0.68
30:0:1634:G:H2'	30:0:1635:U:H6	1.57	0.68
13:M:171:ARG:CD	30:0:156:C:H5''	2.15	0.68
30:0:2374:G:H2'	30:0:2375:A:C8	2.29	0.68
12:L:6:ARG:HD3	30:0:1299:G:O6	1.94	0.68
30:0:440:C:H2'	30:0:441:A:C8	2.29	0.68
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.91	0.68
13:M:83:SER:HA	38:M:8877:HOH:O	1.94	0.68
26:Z:70:ARG:HB3	38:Z:8728:HOH:O	1.93	0.68
30:0:1666:C:C2'	30:0:1667:A:H5''	2.23	0.67
2:B:264:GLU:CG	2:B:267:LYS:HE3	2.24	0.67
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.93	0.67
30:0:1158:G:C2'	30:0:1159:G:H5'	2.24	0.67
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.08	0.67
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.75	0.67
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.31	0.67
30:0:1634:G:H2'	30:0:1635:U:C6	2.29	0.67
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.76	0.67
31:9:24:U:H3'	31:9:25:G:H5'	1.75	0.67
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:283:U:C5	30:0:284:C:C4	2.83	0.67
20:T:2:LYS:HG2	30:0:447:A:OP1	1.95	0.67
31:9:91:C:H1'	38:9:9143:HOH:O	1.95	0.67
30:0:1632:A:C2'	30:0:1633:C:H5'	2.24	0.67
30:0:735:C:C5	30:0:736:A:C4	2.82	0.67
30:0:1762:C:O2'	30:0:1763:C:H5'	1.95	0.67
30:0:541:C:H2'	30:0:542:A:H5'	1.75	0.67
30:0:1268:C:H2'	30:0:1269:G:H8	1.59	0.67
18:R:150:PRO:O	18:R:150:PRO:CG	2.42	0.67
30:0:221:G:H2'	30:0:222:A:C8	2.30	0.67
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.95	0.67
1:A:72:GLU:HG2	26:Z:100:GLY:HA3	1.76	0.67
30:0:603:A:H5''	30:0:604:G:OP1	1.94	0.67
9:I:96:SER:H	9:I:99:GLN:NE2	1.93	0.66
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.77	0.66
30:0:2073:G:OP2	30:0:2490:A:H5'	1.95	0.66
30:0:506:G:H22	30:0:509:A:H5'	1.60	0.66
23:W:44:MET:CE	30:0:944:G:H21	2.09	0.66
30:0:613:C:H2'	30:0:614:U:H6	1.61	0.66
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.78	0.66
30:0:2488:A:C2	38:0:7265:HOH:O	2.48	0.66
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.77	0.66
30:0:451:C:O2'	30:0:452:G:H5'	1.95	0.66
30:0:1158:G:O2'	30:0:1159:G:H5'	1.96	0.66
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.76	0.66
31:9:55:U:H4'	31:9:56:A:C8	2.31	0.66
22:V:50:ARG:NH1	30:0:56:G:H5''	2.10	0.66
30:0:849:C:H1'	38:0:6602:HOH:O	1.95	0.66
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.96	0.66
30:0:2461:U:O2	30:0:2466:G:H1'	1.96	0.66
30:0:2321:A:C2	30:0:2378:U:N3	2.57	0.66
30:0:735:C:H2'	30:0:736:A:O4'	1.96	0.66
9:I:87:PRO:HD2	30:0:1180:U:H1'	1.77	0.66
30:0:558:C:H2'	30:0:559:U:H5'	1.78	0.66
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.61	0.66
9:I:110:ASP:O	30:0:1163:G:H5'	1.96	0.65
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.10	0.65
4:D:103:ASN:HD22	4:D:133:ASN:HA	1.60	0.65
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.11	0.65
3:C:233:THR:HG22	3:C:234:VAL:H	1.61	0.65
21:U:56:ARG:NE	30:0:2890:A:H1'	2.11	0.65
30:0:567:U:H5''	38:0:5280:HOH:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:635:A:H2'	30:0:636:G:H5''	1.77	0.65
30:0:1940:C:H1'	38:0:9376:HOH:O	1.96	0.65
30:0:1950:G:H2'	30:0:1951:G:C8	2.32	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.26	0.65
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.27	0.65
30:0:1925:G:O2'	30:0:1926:G:H5'	1.96	0.65
30:0:625:U:H5''	30:0:1044:C:N4	2.11	0.65
5:E:139:GLU:OE2	30:0:2781:U:H1'	1.97	0.65
30:0:2869:G:H2'	30:0:2870:C:C6	2.31	0.65
30:0:1165:G:H1'	30:0:1174:A:C1'	2.11	0.65
14:N:144:GLY:O	14:N:147:ILE:HG22	1.97	0.65
22:V:39:ALA:N	22:V:40:PRO:HD2	2.12	0.65
30:0:1972:U:H2'	30:0:1973:A:C5'	2.27	0.65
30:0:2458:U:H3'	38:0:3239:HOH:O	1.96	0.64
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.78	0.64
17:Q:19:ARG:HH21	31:9:11:A:P	2.19	0.64
30:0:1165:G:H21	30:0:1173:A:H5'	1.63	0.64
30:0:583:C:H2'	30:0:584:U:H6	1.62	0.64
30:0:2896:A:H5''	38:0:6082:HOH:O	1.96	0.64
30:0:128:A:O2'	30:0:129:A:H5'	1.97	0.64
30:0:2672:C:O2'	30:0:2673:U:H5'	1.97	0.64
30:0:369:G:O2'	30:0:370:G:H5'	1.98	0.64
30:0:660:A:H4'	30:0:661:G:O5'	1.98	0.64
30:0:69:A:H5'	30:0:69:A:C8	2.32	0.64
30:0:125:U:H2'	38:0:3755:HOH:O	1.97	0.64
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.79	0.64
30:0:2488:A:H2	38:0:7265:HOH:O	1.81	0.64
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.79	0.64
30:0:200:C:H2'	38:0:3428:HOH:O	1.96	0.64
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.79	0.64
30:0:1167:G:H2'	30:0:1168:C:O4'	1.98	0.64
13:M:70:GLY:CA	30:0:2263:G:H4'	2.28	0.64
31:9:36:C:H5'	38:9:9047:HOH:O	1.98	0.64
30:0:285:A:H2'	30:0:286:U:O4'	1.97	0.64
30:0:1119:G:N2	30:0:1246:A:H2	1.89	0.64
30:0:2781:U:H2'	30:0:2782:G:C5'	2.27	0.64
30:0:1181:A:H2'	30:0:1182:C:H5'	1.78	0.64
31:9:5:G:O2'	31:9:6:C:H5'	1.97	0.64
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.12	0.64
30:0:441:A:H1'	30:0:442:A:N7	2.13	0.64
30:0:2436:U:H2'	30:0:2437:A:C8	2.33	0.64
18:R:132:ARG:HH21	30:0:2055:A:H4'	1.61	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2878:U:H5''	38:0:4165:HOH:O	1.98	0.64
30:0:2887:G:H2'	30:0:2888:U:C6	2.32	0.64
30:0:1213:C:O2'	30:0:1214:G:H5'	1.98	0.64
30:0:2377:U:O2'	30:0:2378:U:H5'	1.98	0.63
31:9:24:U:H3'	31:9:25:G:C5'	2.28	0.63
12:L:143:THR:HG22	12:L:144:ASP:H	1.62	0.63
30:0:2613:G:O2'	30:0:2614:C:H5'	1.99	0.63
30:0:2281:C:C2'	30:0:2282:U:H5'	2.28	0.63
30:0:2831:C:C2'	30:0:2832:C:H5'	2.28	0.63
14:N:141:ARG:NH2	31:9:48:C:H4'	2.13	0.63
30:0:585:C:H5''	38:0:4864:HOH:O	1.98	0.63
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.81	0.63
21:U:4:ARG:O	21:U:13:ILE:HG22	1.98	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.97	0.63
13:M:99:ARG:HE	13:M:170:ASN:ND2	1.96	0.63
30:0:1170:U:H1'	30:0:1172:G:N7	2.13	0.63
30:0:2869:G:H5'	38:0:5487:HOH:O	1.97	0.63
13:M:81:ARG:HB3	13:M:85:ARG:HB2	1.80	0.63
30:0:1204:C:H1'	38:0:4741:HOH:O	1.98	0.63
30:0:1268:C:H2'	30:0:1269:G:C8	2.34	0.63
30:0:2336:G:H2'	38:0:6280:HOH:O	1.98	0.63
30:0:2868:C:H1'	38:0:7114:HOH:O	1.97	0.63
30:0:1904:A:C2	30:0:1905:U:H1'	2.34	0.63
3:C:174:ILE:CD1	30:0:338:C:H4'	2.29	0.63
30:0:820:G:H5'	30:0:821:U:H5'	1.80	0.63
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.79	0.63
29:3:55:VAL:HB	29:3:56:PRO:HD2	1.81	0.63
30:0:2321:A:H8	30:0:2322:U:O2'	1.80	0.63
30:0:2831:C:H2'	30:0:2832:C:H5'	1.79	0.63
30:0:1528:A:H2'	30:0:1529:G:O4'	1.98	0.63
30:0:424:C:H2'	30:0:425:U:H6	1.64	0.63
30:0:280:C:H2'	30:0:281:U:O4'	1.99	0.63
31:9:2:U:OP2	31:9:3:A:H5'	1.99	0.63
30:0:1950:G:H2'	30:0:1951:G:H8	1.64	0.63
31:9:36:C:C5	31:9:37:C:C5	2.87	0.63
4:D:25:MET:SD	4:D:40:ILE:HD11	2.39	0.63
30:0:2401:A:H2'	30:0:2402:A:C8	2.34	0.63
18:R:9:ASP:O	18:R:13:THR:HB	1.99	0.62
30:0:558:C:C2'	30:0:559:U:C5'	2.77	0.62
18:R:39:THR:HG23	18:R:107:GLU:O	1.99	0.62
30:0:834:G:H4'	30:0:835:U:OP2	1.99	0.62
30:0:2594:C:O2'	30:0:2595:U:H5'	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2894:C:O2'	30:0:2895:C:H5'	1.99	0.62
13:M:179:GLY:O	30:0:399:C:H5'	1.98	0.62
2:B:238:ASN:HD22	2:B:240:GLY:H	1.45	0.62
30:0:2827:A:H2'	30:0:2828:G:O4'	1.99	0.62
2:B:272:ILE:HG22	38:B:9132:HOH:O	2.00	0.62
12:L:79:ASP:HB3	38:L:9022:HOH:O	1.98	0.62
30:0:2505:G:C2'	30:0:2506:A:C5'	2.76	0.62
30:0:308:U:C4	30:0:342:C:H1'	2.34	0.62
30:0:1829:A:H2'	30:0:1830:C:H5'	1.81	0.62
11:K:66:ARG:HH22	30:0:1994:A:P	2.21	0.62
30:0:256:C:H2'	30:0:257:G:O4'	2.00	0.62
30:0:1797:A:H4'	30:0:1798:C:C5	2.33	0.62
30:0:249:G:O2'	30:0:250:C:H5'	1.99	0.62
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.82	0.62
30:0:506:G:N2	30:0:509:A:H5''	2.14	0.62
25:Y:204:ARG:HH22	30:0:553:G:P	2.22	0.62
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.81	0.62
17:Q:11:ARG:HH21	30:0:2297:U:H4'	1.62	0.62
30:0:2705:U:H2'	30:0:2706:A:C8	2.35	0.62
30:0:1230:A:H8	30:0:1230:A:OP1	1.83	0.62
30:0:1087:G:H4'	30:0:1088:A:OP1	2.00	0.62
30:0:418:C:H5	38:0:5765:HOH:O	1.82	0.62
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.48	0.62
17:Q:27:GLN:HE21	31:9:8:G:C5'	2.11	0.62
30:0:2248:C:H3'	38:0:5435:HOH:O	1.98	0.62
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.35	0.62
30:0:1625:U:H5''	38:0:6005:HOH:O	2.00	0.62
30:0:1165:G:N2	30:0:1173:A:H5''	2.09	0.62
15:O:37:ARG:HD2	30:0:656:G:OP2	2.00	0.62
30:0:303:C:O2'	30:0:304:G:H5'	2.00	0.62
13:M:79:ALA:H	13:M:81:ARG:NH2	1.96	0.62
30:0:1477:C:H5'	30:0:1868:G:H5'	1.81	0.62
8:H:168:VAL:HG13	38:H:9006:HOH:O	2.00	0.62
30:0:289:G:O2'	30:0:290:C:H5'	1.98	0.62
23:W:44:MET:HE2	30:0:944:G:H21	1.63	0.61
31:9:110:G:C6	31:9:111:U:C5	2.88	0.61
30:0:545:G:H8	30:0:545:G:C5'	2.08	0.61
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.34	0.61
19:S:52:VAL:HG22	19:S:66:VAL:HG22	1.82	0.61
30:0:807:A:O2'	30:0:808:A:H5'	1.99	0.61
3:C:27:ARG:HG2	3:C:27:ARG:NH1	2.12	0.61
20:T:9:LYS:HD2	38:0:3744:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.31	0.61
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.82	0.61
12:L:90:ARG:HA	12:L:119:THR:HB	1.82	0.61
28:2:41:HIS:HE1	30:0:1439:C:H5'	1.65	0.61
30:0:2102:G:N2	30:0:2104:C:C2	2.69	0.61
30:0:1596:U:H2'	30:0:1598:A:OP2	2.00	0.61
31:9:107:C:O2'	31:9:108:C:H5'	2.00	0.61
30:0:39:G:N2	30:0:444:C:C2	2.68	0.61
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.35	0.61
30:0:1245:C:O5'	30:0:1245:C:H6	1.84	0.61
30:0:1015:C:H2'	30:0:1016:U:H6	1.64	0.61
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.00	0.61
30:0:2717:C:H2'	30:0:2718:C:C5'	2.30	0.61
30:0:2502:C:H2'	30:0:2503:A:C5'	2.29	0.61
3:C:236:THR:HG22	3:C:239:ALA:N	2.12	0.61
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	0.61
30:0:138:U:OP2	30:0:139:C:H5	1.84	0.61
26:Z:40:ALA:HA	30:0:1773:G:C8	2.35	0.61
29:3:60:LYS:CG	29:3:61:PRO:HD2	2.29	0.61
30:0:559:U:H5'	30:0:559:U:C6	2.32	0.61
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.83	0.61
30:0:24:G:N2	30:0:518:G:H1'	2.16	0.61
26:Z:78:ILE:HD12	38:Z:8714:HOH:O	2.01	0.61
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.16	0.61
30:0:272:A:H5'	30:0:273:G:OP2	2.01	0.61
30:0:2766:A:O2'	30:0:2767:C:H5'	2.00	0.61
30:0:735:C:H5	30:0:736:A:C4	2.18	0.61
30:0:424:C:H2'	30:0:425:U:C6	2.35	0.61
30:0:1015:C:H2'	30:0:1016:U:C6	2.36	0.61
30:0:946:C:H2'	30:0:947:U:H6	1.65	0.61
30:0:657:G:H2'	30:0:658:C:H6	1.64	0.61
29:3:4:PRO:HA	29:3:91:GLN:HB2	1.82	0.61
30:0:1741:U:H5'	30:0:1742:A:OP1	2.01	0.60
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.49	0.60
30:0:1165:G:N2	30:0:1173:A:H5'	2.15	0.60
30:0:2769:C:H2'	30:0:2770:G:H5'	1.82	0.60
30:0:1972:U:H2'	30:0:1973:A:H5'	1.83	0.60
15:O:32:ARG:HD3	15:O:32:ARG:O	2.01	0.60
30:0:1181:A:C2'	30:0:1182:C:H5'	2.30	0.60
30:0:1603:A:C5'	30:0:1605:G:H5'	2.29	0.60
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.01	0.60
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:2:10:ARG:NH2	30:0:121:U:OP2	2.34	0.60
30:0:1183:C:N4	30:0:1184:C:H41	1.98	0.60
31:9:76:G:C3'	31:9:77:A:H5''	2.21	0.60
30:0:1603:A:C5'	30:0:1605:G:O4'	2.45	0.60
30:0:2102:G:C8	30:0:2538:A:O4'	2.54	0.60
31:9:20:G:O2'	31:9:21:G:H5'	2.02	0.60
30:0:272:A:H3'	38:0:7522:HOH:O	2.00	0.60
30:0:2281:C:H2'	30:0:2282:U:H5'	1.83	0.60
30:0:192:A:H5'	38:0:7634:HOH:O	1.99	0.60
8:H:29:SER:HA	8:H:62:HIS:HD2	1.66	0.60
30:0:1622:G:H2'	30:0:1623:C:H5'	1.83	0.60
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.84	0.60
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.84	0.60
10:J:107:ASN:HD22	10:J:109:TYR:H	1.48	0.60
30:0:396:U:H3'	38:0:3920:HOH:O	2.00	0.60
13:M:84:LYS:HA	29:3:46:ILE:O	2.01	0.60
30:0:851:C:O2	30:0:2022:A:H2	1.85	0.60
30:0:282:C:O2'	30:0:283:U:C5'	2.48	0.60
13:M:77:HIS:HB2	13:M:81:ARG:HH21	1.66	0.60
30:0:946:C:H2'	30:0:947:U:C6	2.35	0.60
29:3:3:MET:SD	29:3:88:LEU:HD11	2.41	0.60
30:0:333:G:O2'	30:0:334:G:H5'	2.01	0.60
30:0:2659:U:H5''	38:0:4122:HOH:O	2.02	0.60
30:0:182:G:H5'	38:0:5152:HOH:O	2.01	0.60
16:P:115:SER:N	16:P:118:GLN:HE21	1.92	0.60
30:0:228:C:H2'	30:0:229:G:H5'	1.82	0.60
5:E:24:GLY:HA3	5:E:76:VAL:HB	1.82	0.60
30:0:671:A:O2'	30:0:672:G:H2'	2.02	0.60
30:0:90:A:H2'	30:0:91:G:O4'	2.01	0.60
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.30	0.60
30:0:2793:A:H2'	38:0:4488:HOH:O	2.02	0.60
30:0:293:A:O2'	30:0:294:C:H5'	2.02	0.60
19:S:33:SER:O	19:S:37:VAL:HG23	2.02	0.60
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.84	0.60
30:0:1183:C:H42	30:0:1184:C:H41	1.50	0.60
30:0:2769:C:H2'	30:0:2770:G:C5'	2.31	0.60
26:Z:37:ARG:HB2	30:0:819:A:C4'	2.32	0.60
3:C:184:ARG:NH2	30:0:450:C:OP1	2.29	0.60
30:0:453:A:H5''	38:0:3254:HOH:O	2.02	0.60
26:Z:53:ILE:O	26:Z:57:MET:HB2	2.02	0.60
27:1:9:GLY:HA2	30:0:1687:C:O2	2.02	0.59
1:A:35:GLY:O	1:A:36:ASP:HB3	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.83	0.59
21:U:39:ASN:HB3	38:U:3805:HOH:O	2.02	0.59
30:0:2812:A:H1'	38:0:5773:HOH:O	2.01	0.59
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.31	0.59
31:9:63:C:O2'	31:9:64:C:H5'	2.02	0.59
2:B:258:GLY:H	2:B:260:HIS:CE1	2.20	0.59
14:N:159:TYR:CE1	31:9:50:G:H5''	2.37	0.59
30:0:1973:A:H5'	30:0:1973:A:C8	2.35	0.59
27:1:1:THR:HB	38:0:7134:HOH:O	2.02	0.59
30:0:1058:A:H2'	30:0:1060:C:H5''	1.83	0.59
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.01	0.59
30:0:1819:G:H2'	30:0:1820:G:H4'	1.82	0.59
30:0:2321:A:H2	30:0:2378:U:N3	1.92	0.59
31:9:39:U:H1'	31:9:44:A:N6	2.15	0.59
30:0:747:G:H5'	38:0:4947:HOH:O	2.02	0.59
30:0:2472:C:O2'	30:0:2634:G:H4'	2.02	0.59
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.32	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
30:0:2498:C:O2'	30:0:2499:U:H5'	2.03	0.59
30:0:2689:A:H2'	30:0:2690:U:H5'	1.85	0.59
30:0:247:A:H2'	38:0:3921:HOH:O	2.02	0.59
13:M:9:ARG:HD2	30:0:380:A:OP2	2.02	0.59
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.59
17:Q:11:ARG:NH2	30:0:2363:G:H4'	2.18	0.59
21:U:6:CYS:SG	21:U:32:CYS:HB3	2.43	0.59
30:0:468:U:H3'	38:0:7561:HOH:O	2.03	0.59
26:Z:64:PRO:HB2	26:Z:86:TYR:CE2	2.38	0.59
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.17	0.59
29:3:51:LYS:HB3	30:0:219:G:O2'	2.03	0.59
30:0:1201:C:H5''	38:0:6132:HOH:O	2.02	0.59
30:0:1904:A:H2'	30:0:1905:U:O4'	2.02	0.59
30:0:1116:U:HO2'	30:0:1118:A:H2	0.72	0.59
30:0:1377:C:H6	30:0:1377:C:H5'	1.67	0.59
17:Q:26:PRO:O	17:Q:30:VAL:HG22	2.02	0.59
30:0:214:U:H5'	38:0:6123:HOH:O	2.01	0.59
30:0:1187:U:H2'	38:0:6882:HOH:O	2.02	0.59
30:0:319:A:H4'	30:0:338:C:C4	2.38	0.59
30:0:2250:G:H2'	30:0:2251:G:O4'	2.03	0.59
30:0:1634:G:H3'	38:0:3889:HOH:O	2.02	0.59
4:D:62:ASP:HA	38:D:4233:HOH:O	2.03	0.59
30:0:827:A:H1'	38:0:6196:HOH:O	2.02	0.59
15:O:25:VAL:HG12	30:0:709:G:O2'	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1118:A:C8	30:0:1118:A:C3'	2.74	0.58
30:0:1175:G:H1'	30:0:1193:A:C2'	2.31	0.58
29:3:3:MET:O	29:3:90:PHE:HA	2.03	0.58
18:R:40:ALA:O	18:R:44:VAL:HG23	2.03	0.58
2:B:68:THR:HG21	21:U:16:GLY:HA3	1.85	0.58
20:T:48:VAL:HG11	20:T:96:VAL:HG13	1.85	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:542:A:H5'	30:0:542:A:C8	2.29	0.58
30:0:2353:A:H4'	30:0:2354:A:O5'	2.02	0.58
2:B:195:ARG:HE	2:B:323:LEU:HD13	1.68	0.58
31:9:54:A:C2'	31:9:55:U:H5'	2.33	0.58
30:0:482:G:H4'	30:0:508:A:N1	2.18	0.58
2:B:256:GLN:HG2	38:B:9129:HOH:O	2.03	0.58
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.84	0.58
30:0:669:G:O2'	30:0:670:G:H5'	2.03	0.58
30:0:918:G:H5''	38:0:9099:HOH:O	2.01	0.58
30:0:1393:A:H2'	30:0:1394:C:C6	2.38	0.58
30:0:1929:G:H1'	38:0:5153:HOH:O	2.03	0.58
30:0:1161:A:O5'	30:0:1161:A:H8	1.85	0.58
30:0:657:G:H2'	30:0:658:C:C6	2.38	0.58
30:0:1127:C:C5	30:0:1128:U:C4	2.91	0.58
1:A:199:HIS:CD2	1:A:201:PHE:H	2.21	0.58
13:M:68:ARG:HH21	13:M:73:ARG:HD3	1.65	0.58
3:C:2:GLN:HB3	38:C:8594:HOH:O	2.04	0.58
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.19	0.58
30:0:962:C:H2'	30:0:963:C:C5'	2.33	0.58
12:L:30:ARG:HD2	30:0:164:G:H5''	1.85	0.58
30:0:812:A:H2'	30:0:813:C:C6	2.38	0.58
12:L:133:VAL:HA	38:L:9035:HOH:O	2.04	0.58
30:0:69:A:H5'	30:0:69:A:H8	1.69	0.58
30:0:2878:U:H2'	30:0:2879:A:O4'	2.02	0.58
12:L:80:ASP:HB2	12:L:90:ARG:O	2.03	0.58
7:G:64:ASN:HD22	7:G:64:ASN:N	1.99	0.58
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.39	0.58
30:0:858:U:H5	38:0:5421:HOH:O	1.86	0.58
30:0:2900:G:H2'	30:0:2901:C:O4'	2.03	0.58
30:0:2256:G:O2'	30:0:2257:G:H5'	2.04	0.58
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.68	0.58
30:0:696:C:O2'	30:0:697:G:H5'	2.03	0.58
30:0:416:G:H3'	38:0:9910:HOH:O	2.02	0.58
30:0:814:G:H4'	38:0:3124:HOH:O	2.03	0.58
3:C:236:THR:HA	38:C:8660:HOH:O	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:541:C:O2'	30:0:542:A:H5''	2.03	0.58
28:2:41:HIS:CD2	28:2:43:ARG:H	2.22	0.58
30:0:244:C:H6	30:0:244:C:O5'	1.87	0.58
2:B:125:GLU:O	2:B:129:ARG:HG3	2.03	0.58
30:0:2276:U:H1'	38:0:9608:HOH:O	2.04	0.58
25:Y:133:HIS:HD2	38:Y:8886:HOH:O	1.85	0.58
13:M:81:ARG:HG3	30:0:161:A:OP1	2.04	0.58
31:9:1:U:C4'	31:9:3:A:OP1	2.52	0.58
30:0:1819:G:H2'	30:0:1820:G:C5'	2.34	0.58
1:A:109:GLU:HG2	1:A:116:GLY:H	1.69	0.58
30:0:1221:G:H8	38:0:5971:HOH:O	1.87	0.58
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.58
30:0:2064:U:H5'	30:0:2652:U:H4'	1.86	0.58
29:3:60:LYS:HB2	30:0:2460:A:OP1	2.04	0.58
31:9:64:C:C2'	31:9:65:A:H5'	2.33	0.58
30:0:1205:U:C2'	30:0:1206:U:C5'	2.81	0.58
30:0:2867:G:H2'	30:0:2868:C:C6	2.39	0.58
22:V:1:THR:HG23	22:V:2:VAL:H	1.69	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.35	0.58
13:M:28:GLN:O	13:M:32:ARG:HG3	2.02	0.58
23:W:64:THR:O	23:W:68:THR:HG22	2.04	0.58
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.04	0.57
5:E:143:GLN:NE2	30:0:2779:G:H21	2.01	0.57
26:Z:80:GLN:HG3	26:Z:81:CYS:N	2.20	0.57
30:0:1829:A:C2'	30:0:1830:C:H5'	2.34	0.57
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.57
3:C:25:PRO:HG2	38:C:8522:HOH:O	2.03	0.57
30:0:553:G:H5'	38:0:3481:HOH:O	2.04	0.57
31:9:108:C:H2'	31:9:109:G:C8	2.38	0.57
30:0:2499:U:H2'	30:0:2500:C:H6	1.69	0.57
30:0:695:C:O2'	30:0:696:C:H5'	2.04	0.57
30:0:1664:A:OP1	30:0:1664:A:H8	1.87	0.57
30:0:1626:A:H2'	30:0:1627:G:C5'	2.35	0.57
30:0:1197:G:H1'	30:0:1203:G:N2	2.19	0.57
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.86	0.57
30:0:1494:A:C4	30:0:1495:C:C5	2.93	0.57
12:L:14:GLY:O	30:0:1295:G:H5''	2.04	0.57
30:0:544:G:C3'	30:0:545:G:H5''	2.35	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.81	0.57
31:9:49:G:O2'	31:9:50:G:H5'	2.05	0.57
30:0:1395:C:H2'	30:0:1396:C:C6	2.39	0.57
30:0:2269:C:C2'	30:0:2270:G:H5'	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:81:LYS:O	30:0:1761:U:H5'	2.04	0.57
20:T:26:THR:HA	20:T:39:ASN:HB3	1.86	0.57
29:3:69:TYR:HD1	29:3:78:HIS:O	1.87	0.57
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.19	0.57
30:0:2840:A:H3'	38:0:7638:HOH:O	2.04	0.57
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.57
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.34	0.57
30:0:2563:U:H2'	30:0:2565:C:O5'	2.04	0.57
30:0:2300:A:H4'	30:0:2301:A:O5'	2.05	0.57
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.52	0.57
30:0:1919:A:H4'	38:0:4844:HOH:O	2.04	0.57
30:0:1165:G:O3'	30:0:1174:A:H4'	2.04	0.57
30:0:1201:C:H2'	30:0:1202:A:H5'	1.85	0.57
30:0:957:A:H8	30:0:957:A:O5'	1.88	0.57
9:I:126:THR:O	9:I:130:LEU:HG	2.03	0.57
25:Y:130:ARG:HD2	38:Y:8857:HOH:O	2.04	0.57
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.85	0.57
31:9:114:G:H2'	31:9:115:C:C6	2.39	0.57
14:N:4:PRO:HD2	38:0:6759:HOH:O	2.04	0.57
3:C:101:ASP:HB2	30:0:750:A:O3'	2.05	0.57
8:H:146:ALA:O	8:H:149:VAL:HG12	2.04	0.57
30:0:2531:U:O2'	30:0:2532:A:H5'	2.05	0.57
30:0:1200:A:H3'	38:0:5738:HOH:O	2.05	0.57
30:0:1482:A:H1'	38:0:9425:HOH:O	2.04	0.57
30:0:2032:U:H2'	30:0:2033:G:C5'	2.35	0.57
15:O:73:ASP:HA	15:O:92:VAL:O	2.05	0.57
4:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.57
5:E:69:ILE:HA	5:E:72:MET:HE3	1.86	0.57
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.05	0.57
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.04	0.57
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.99	0.57
30:0:2437:A:H2'	30:0:2438:G:C8	2.40	0.57
29:3:25:VAL:HG12	38:0:9267:HOH:O	2.04	0.57
30:0:2768:A:H2'	30:0:2769:C:O4'	2.05	0.57
30:0:2831:C:H2'	30:0:2832:C:C5'	2.35	0.57
30:0:1697:G:H4'	38:0:9342:HOH:O	2.05	0.57
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.85	0.57
30:0:1202:A:H2'	30:0:1203:G:C5'	2.34	0.56
2:B:307:ARG:HB3	38:B:9126:HOH:O	2.04	0.56
30:0:2324:G:H1'	38:0:6095:HOH:O	2.04	0.56
30:0:1748:U:C5	30:0:1749:U:C5	2.92	0.56
30:0:589:U:H2'	30:0:590:A:H8	1.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:39:ALA:H	22:V:40:PRO:HD2	1.69	0.56
30:0:2032:U:O2'	30:0:2033:G:H5''	2.04	0.56
2:B:297:VAL:HB	38:B:9075:HOH:O	2.03	0.56
2:B:229:ARG:HD2	38:0:9111:HOH:O	2.04	0.56
3:C:214:THR:HG23	38:C:8649:HOH:O	2.04	0.56
30:0:1511:U:O2'	30:0:1512:G:H5'	2.05	0.56
30:0:2824:C:O3'	30:0:2825:C:H6	1.88	0.56
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.56
26:Z:45:VAL:HA	26:Z:48:ARG:HB3	1.87	0.56
30:0:2758:G:H2'	30:0:2759:C:C6	2.40	0.56
21:U:56:ARG:HD2	30:0:2890:A:N9	2.20	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.14	0.56
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.87	0.56
31:9:38:A:H2'	31:9:39:U:C6	2.41	0.56
30:0:962:C:C2'	30:0:963:C:H5'	2.35	0.56
30:0:708:A:H2'	30:0:709:G:O4'	2.05	0.56
2:B:244:PRO:HB3	30:0:1234:U:N3	2.20	0.56
30:0:1426:C:H2'	38:0:9592:HOH:O	2.04	0.56
3:C:138:VAL:HG11	3:C:160:LEU:HD13	1.87	0.56
31:9:18:U:H2'	31:9:19:G:C8	2.40	0.56
30:0:594:C:O2'	30:0:595:U:H5'	2.05	0.56
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.40	0.56
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.88	0.56
3:C:88:SER:HB3	3:C:91:PRO:HB3	1.87	0.56
24:X:71:ARG:HD3	38:X:2171:HOH:O	2.04	0.56
8:H:31:ILE:HD11	8:H:65:LEU:HD23	1.87	0.56
30:0:1202:A:C2'	30:0:1203:G:H5'	2.35	0.56
30:0:31:C:H4'	38:0:7417:HOH:O	2.04	0.56
30:0:1236:A:C2'	30:0:1237:U:H5'	2.36	0.56
30:0:28:G:H1'	38:0:4676:HOH:O	2.04	0.56
30:0:2703:A:H2'	30:0:2704:C:C6	2.37	0.56
30:0:2248:C:H2'	30:0:2249:G:H8	1.70	0.56
29:3:67:LEU:HD21	29:3:88:LEU:HD21	1.86	0.56
5:E:93:MET:HE1	5:E:165:GLY:N	2.21	0.56
30:0:941:G:C5	30:0:942:U:C4	2.94	0.56
30:0:1523:G:H2'	30:0:1524:U:C6	2.41	0.56
30:0:1559:A:OP2	30:0:1559:A:H8	1.87	0.56
14:N:58:LEU:N	14:N:58:LEU:HD12	2.20	0.56
38:B:9106:HOH:O	30:0:2672:C:H1'	2.05	0.56
26:Z:37:ARG:HD3	26:Z:37:ARG:H	1.71	0.56
22:V:55:ARG:O	22:V:59:ILE:HG12	2.06	0.56
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:24:GLN:HE21	13:M:27:ARG:NH1	2.03	0.56
30:0:1504:A:H5'	38:0:4410:HOH:O	2.06	0.56
31:9:52:A:O2'	31:9:53:G:H5'	2.06	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.35	0.56
30:0:711:G:C2	30:0:718:C:C2	2.93	0.56
21:U:56:ARG:NH1	21:U:56:ARG:HG3	2.18	0.56
19:S:37:VAL:O	19:S:41:VAL:HG23	2.04	0.56
30:0:1574:C:H2'	30:0:1575:C:H6	1.70	0.56
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.56
30:0:2559:C:H4'	38:0:7245:HOH:O	2.06	0.56
30:0:1537:C:H1'	38:0:6573:HOH:O	2.05	0.56
26:Z:51:ALA:O	26:Z:55:SER:HB2	2.05	0.56
30:0:1202:A:H2'	30:0:1203:G:O4'	2.06	0.56
28:2:41:HIS:CE1	30:0:1439:C:H5''	2.41	0.56
30:0:1622:G:C2'	30:0:1623:C:H5'	2.36	0.56
30:0:1574:C:H2'	30:0:1575:C:C6	2.41	0.56
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.04	0.56
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.40	0.56
30:0:1850:U:O4'	30:0:1941:A:C2	2.59	0.56
30:0:2795:C:O2'	30:0:2796:U:H5'	2.05	0.56
30:0:2897:C:O2'	30:0:2898:G:H5'	2.06	0.56
30:0:1159:G:H21	30:0:1189:A:H8	1.53	0.56
30:0:2004:U:H2'	30:0:2004:U:O2	2.05	0.56
30:0:2291:A:N9	30:0:2309:C:H5'	2.21	0.56
30:0:290:C:O2'	30:0:291:C:H5'	2.05	0.56
30:0:1060:C:H6	30:0:1060:C:H5'	1.71	0.56
30:0:1778:A:H2'	30:0:1779:A:H5'	1.87	0.56
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.01	0.55
26:Z:34:SER:HA	30:0:797:A:H4'	1.88	0.55
30:0:2316:G:H4'	38:0:6075:HOH:O	2.06	0.55
29:3:12:PRO:HD3	38:3:9032:HOH:O	2.05	0.55
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.46	0.55
30:0:2906:A:H5'	30:0:2907:C:O4'	2.07	0.55
13:M:77:HIS:HB2	13:M:81:ARG:HE	1.72	0.55
14:N:49:THR:HG22	14:N:56:ASP:HB3	1.88	0.55
30:0:304:G:H1'	30:0:347:A:N6	2.21	0.55
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.75	0.55
30:0:595:U:O2'	30:0:596:C:H5'	2.05	0.55
30:0:485:A:N3	30:0:487:G:H5''	2.20	0.55
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.06	0.55
30:0:299:U:C2	30:0:300:U:C6	2.95	0.55
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1594:C:O2'	30:0:1607:A:H4'	2.07	0.55
30:0:2718:C:H6	30:0:2718:C:H5'	1.71	0.55
30:0:1972:U:C2'	30:0:1973:A:H5''	2.36	0.55
30:0:2887:G:H2'	30:0:2888:U:O4'	2.07	0.55
12:L:30:ARG:HD3	30:0:164:G:H4'	1.87	0.55
26:Z:81:CYS:O	26:Z:85:ASP:HA	2.05	0.55
22:V:4:HIS:HB3	38:V:6622:HOH:O	2.06	0.55
30:0:12:U:H2'	30:0:13:G:H5'	1.88	0.55
30:0:1361:C:H2'	30:0:1362:U:H6	1.72	0.55
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.32	0.55
29:3:2:GLN:HA	29:3:89:GLU:O	2.07	0.55
13:M:82:ARG:H	13:M:82:ARG:HD3	1.72	0.55
23:W:38:THR:HG22	23:W:39:ASP:H	1.72	0.55
30:0:136:C:H2'	30:0:137:U:O4'	2.07	0.55
30:0:699:C:C2	30:0:744:G:C2	2.95	0.55
30:0:536:A:H3'	38:0:5040:HOH:O	2.06	0.55
30:0:1809:G:H1'	38:0:7682:HOH:O	2.06	0.55
30:0:1913:C:H2'	30:0:1914:C:C6	2.41	0.55
30:0:2812:A:C2	30:0:2814:A:N6	2.71	0.55
14:N:17:ARG:NH1	14:N:17:ARG:HB3	2.21	0.55
30:0:1762:C:H2'	30:0:1763:C:H6	1.71	0.55
13:M:164:THR:HG22	13:M:166:ALA:H	1.71	0.55
29:3:48:ASN:O	30:0:170:U:H4'	2.07	0.55
30:0:1342:C:O2'	30:0:1343:C:H5'	2.06	0.55
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.88	0.55
30:0:2451:G:H8	38:0:5174:HOH:O	1.90	0.55
1:A:54:PRO:HG2	1:A:160:ALA:HB3	1.89	0.55
8:H:29:SER:HA	8:H:62:HIS:CD2	2.41	0.55
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.89	0.55
30:0:876:A:N3	30:0:876:A:H2'	2.22	0.55
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.89	0.55
30:0:2480:G:H3'	38:0:4182:HOH:O	2.07	0.55
30:0:1174:A:C5	30:0:1201:C:H4'	2.41	0.55
30:0:1202:A:C8	30:0:1203:G:C8	2.95	0.55
30:0:1667:A:C8	30:0:1667:A:H5'	2.34	0.55
30:0:1204:C:H2'	30:0:1205:U:O4'	2.06	0.55
30:0:945:U:H2'	30:0:946:C:C6	2.42	0.55
30:0:1236:A:O2'	30:0:1237:U:H5'	2.07	0.55
18:R:114:VAL:HA	18:R:144:GLU:O	2.06	0.55
30:0:2240:U:O2'	30:0:2241:C:H5'	2.06	0.55
6:F:59:ILE:CD1	30:0:263:U:C2	2.90	0.55
30:0:154:C:H2'	30:0:155:C:H6	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2416:G:H2'	30:0:2417:C:C6	2.42	0.55
25:Y:182:PHE:HD2	25:Y:200:THR:O	1.89	0.55
31:9:59:C:H4'	38:9:9127:HOH:O	2.06	0.55
19:S:57:THR:HG22	19:S:58:MET:N	2.21	0.55
30:0:2102:G:N3	30:0:2103:A:C6	2.75	0.55
30:0:807:A:H2'	30:0:808:A:C8	2.41	0.55
2:B:41:PHE:HA	2:B:79:MET:HE2	1.89	0.55
1:A:192:VAL:HG12	38:A:9012:HOH:O	2.06	0.55
22:V:64:GLY:O	22:V:65:ASP:HB2	2.07	0.55
30:0:368:C:H2'	30:0:369:G:H5'	1.88	0.54
30:0:2869:G:H2'	30:0:2870:C:H6	1.73	0.54
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.37	0.54
30:0:1377:C:H5'	30:0:1377:C:C6	2.42	0.54
3:C:188:ARG:HD3	38:C:8571:HOH:O	2.07	0.54
30:0:204:A:H2'	30:0:205:U:H5'	1.89	0.54
1:A:237:GLY:O	30:0:1939:U:H5''	2.06	0.54
26:Z:46:SER:O	26:Z:50:VAL:HB	2.07	0.54
3:C:233:THR:HG22	3:C:234:VAL:N	2.21	0.54
30:0:1878:G:C4'	38:0:6104:HOH:O	2.55	0.54
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.90	0.54
18:R:150:PRO:CG	18:R:150:PRO:CB	2.85	0.54
30:0:1183:C:N3	30:0:1184:C:N4	2.55	0.54
30:0:2872:U:H2'	30:0:2873:C:H6	1.73	0.54
30:0:963:C:O2	30:0:1005:A:N1	2.39	0.54
30:0:1334:C:O2'	30:0:1335:C:H5'	2.07	0.54
30:0:2372:A:H2'	30:0:2373:U:C6	2.43	0.54
30:0:1188:A:C5	30:0:1189:A:C2	2.95	0.54
25:Y:169:ARG:NE	35:Y:8820:CL:CL	2.73	0.54
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.88	0.54
30:0:1902:G:N2	30:0:1936:C:C2	2.75	0.54
30:0:561:G:H2'	30:0:562:A:H8	1.73	0.54
20:T:52:ARG:HD2	30:0:317:A:H5''	1.90	0.54
30:0:951:A:C2'	30:0:952:G:H5'	2.37	0.54
25:Y:216:ARG:HD2	38:Y:8874:HOH:O	2.06	0.54
30:0:1969:A:O2'	30:0:1970:G:H5'	2.08	0.54
4:D:76:ARG:NE	31:9:44:A:O4'	2.41	0.54
30:0:2102:G:C2	30:0:2103:A:C6	2.95	0.54
30:0:703:G:O2'	30:0:704:C:H5'	2.07	0.54
14:N:5:ARG:NH1	14:N:5:ARG:HB2	2.21	0.54
30:0:314:G:N2	30:0:317:A:C8	2.75	0.54
1:A:199:HIS:HD2	1:A:201:PHE:H	1.55	0.54
14:N:43:VAL:CG1	14:N:118:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:80:TYR:O	30:0:2050:G:H5''	2.08	0.54
31:9:55:U:H4'	31:9:56:A:H8	1.73	0.54
16:P:115:SER:H	16:P:118:GLN:NE2	1.92	0.54
1:A:211:LYS:HG2	38:0:7019:HOH:O	2.08	0.54
30:0:2321:A:H2'	30:0:2321:A:N3	2.22	0.54
29:3:79:LEU:HD13	30:0:2457:U:H1'	1.88	0.54
30:0:255:A:C5	30:0:256:C:C5	2.96	0.54
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.36	0.54
27:1:42:SER:HB2	38:1:354:HOH:O	2.08	0.54
7:G:20:VAL:O	7:G:24:VAL:HG23	2.07	0.54
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.06	0.54
15:O:14:LEU:HG	15:O:102:ILE:HD11	1.89	0.54
27:1:1:THR:HA	38:0:9360:HOH:O	2.07	0.54
12:L:41:HIS:H	12:L:41:HIS:CD2	2.25	0.54
30:0:120:A:H2'	30:0:120:A:N3	2.22	0.54
30:0:535:G:C5	30:0:2063:U:C4	2.95	0.54
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.54
30:0:1202:A:O2'	30:0:1203:G:H5'	2.08	0.54
23:W:26:ILE:HB	38:W:5420:HOH:O	2.06	0.54
30:0:2638:G:H5'	38:0:4923:HOH:O	2.07	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.54
1:A:190:ARG:HD2	30:0:1884:G:O6	2.08	0.54
30:0:2589:U:H2'	30:0:2590:U:C6	2.42	0.54
10:J:39:VAL:HG13	10:J:106:GLY:O	2.08	0.54
30:0:2326:C:H4'	30:0:2412:G:C4'	2.38	0.54
1:A:176:HIS:CD2	30:0:857:A:H4'	2.43	0.54
30:0:1163:G:H1	30:0:1184:C:N4	2.06	0.54
14:N:147:ILE:HD11	31:9:49:G:O3'	2.07	0.54
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.89	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.22	0.54
30:0:2344:G:H8	38:0:6641:HOH:O	1.91	0.54
3:C:237:GLU:HA	38:C:8643:HOH:O	2.08	0.54
2:B:98:THR:HG22	2:B:99:GLU:H	1.73	0.54
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.89	0.54
30:0:1714:C:O2'	30:0:1715:C:H5'	2.08	0.54
30:0:1176:C:H5	38:0:5727:HOH:O	1.91	0.54
14:N:37:ARG:NH1	31:9:6:C:C5'	2.60	0.53
14:N:67:ALA:HA	14:N:71:TRP:CB	2.37	0.53
30:0:2335:C:H2'	30:0:2336:G:C8	2.43	0.53
6:F:96:ALA:HA	38:F:3111:HOH:O	2.08	0.53
3:C:135:GLU:HB3	38:C:8586:HOH:O	2.08	0.53
29:3:33:MET:SD	30:0:2450:C:H4'	2.48	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.08	0.53
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.08	0.53
30:0:1706:G:C6	30:0:1707:G:C6	2.96	0.53
21:U:33:SER:O	21:U:37:GLU:HG3	2.08	0.53
21:U:51:TRP:HA	21:U:56:ARG:HE	1.72	0.53
30:0:2712:G:H1'	38:0:5829:HOH:O	2.08	0.53
30:0:962:C:H5''	38:0:4907:HOH:O	2.06	0.53
29:3:48:ASN:HB3	30:0:170:U:H5'	1.91	0.53
30:0:1379:A:H1'	38:0:9690:HOH:O	2.08	0.53
30:0:480:C:H4'	38:0:7715:HOH:O	2.08	0.53
30:0:2347:C:H2'	30:0:2348:C:H6	1.73	0.53
30:0:1506:U:H6	30:0:1506:U:H5'	1.73	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.90	0.53
23:W:88:THR:HG22	23:W:89:ASP:H	1.74	0.53
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.74	0.53
1:A:36:ASP:HB2	1:A:85:SER:H	1.73	0.53
3:C:180:SER:HB2	38:C:8656:HOH:O	2.06	0.53
30:0:311:C:H2'	30:0:312:U:C6	2.43	0.53
30:0:2546:U:H4'	38:0:6160:HOH:O	2.09	0.53
31:9:13:A:O2'	31:9:14:G:H5''	2.09	0.53
31:9:39:U:H3'	31:9:40:C:C5'	2.39	0.53
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.72	0.53
1:A:109:GLU:HG2	1:A:116:GLY:N	2.23	0.53
14:N:55:ASP:OD2	31:9:7:G:H4'	2.08	0.53
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.91	0.53
31:9:60:C:O2'	31:9:61:C:H5'	2.08	0.53
31:9:117:G:H2'	31:9:118:C:C6	2.44	0.53
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.89	0.53
30:0:185:G:H4'	30:0:186:A:OP1	2.08	0.53
30:0:1205:U:H2'	30:0:1206:U:H5''	1.88	0.53
13:M:164:THR:HG22	13:M:166:ALA:N	2.23	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.90	0.53
30:0:2265:U:H2'	30:0:2266:A:C8	2.43	0.53
30:0:363:C:O2'	30:0:364:U:H5'	2.09	0.53
30:0:1269:G:H2'	30:0:1270:U:C6	2.44	0.53
30:0:1014:A:H5''	31:9:101:G:O2'	2.09	0.53
30:0:517:U:H2'	30:0:518:G:H5'	1.90	0.53
30:0:1523:G:C6	30:0:1524:U:O4	2.62	0.53
30:0:1553:C:H2'	30:0:1554:C:H6	1.74	0.53
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.09	0.53
30:0:2112:A:C8	38:0:6930:HOH:O	2.54	0.53
13:M:68:ARG:HG3	30:0:1469:C:OP1	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:39:THR:HB	18:R:42:GLU:HG3	1.91	0.53
30:0:2371:G:H5'	38:0:5000:HOH:O	2.07	0.53
30:0:10:U:O4	30:0:532:A:OP2	2.27	0.53
31:9:76:G:H3'	31:9:77:A:C5'	2.23	0.53
31:9:39:U:H3	31:9:42:C:H5''	1.72	0.53
30:0:2578:G:C8	30:0:2578:G:H5'	2.40	0.53
30:0:734:U:O2'	30:0:736:A:N7	2.35	0.53
2:B:102:THR:HG21	2:B:182:VAL:O	2.09	0.53
16:P:134:VAL:O	16:P:137:LEU:HB3	2.09	0.53
14:N:132:ASN:O	14:N:135:VAL:HG12	2.09	0.53
30:0:1940:C:H4'	38:0:7336:HOH:O	2.08	0.53
30:0:312:U:C2	30:0:320:G:N2	2.77	0.53
30:0:1224:G:H2'	30:0:1225:C:C6	2.43	0.53
30:0:454:U:C2	38:0:9033:HOH:O	2.53	0.53
30:0:279:C:O2'	30:0:280:C:H5'	2.09	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.73	0.53
29:3:70:ARG:HA	29:3:77:ALA:HB2	1.91	0.53
30:0:10:U:C4	30:0:532:A:C8	2.97	0.53
30:0:1515:A:H2'	30:0:1516:U:C6	2.43	0.53
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	1.91	0.53
23:W:13:MET:HE1	23:W:18:GLN:HA	1.90	0.53
14:N:160:SER:CB	31:9:51:A:H5'	2.39	0.53
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.74	0.53
14:N:42:HIS:HB3	14:N:62:HIS:HE1	1.73	0.53
2:B:62:ARG:HA	2:B:65:MET:CE	2.39	0.53
30:0:2438:G:H2'	30:0:2439:C:O4'	2.09	0.52
2:B:211:THR:HG23	30:0:2840:A:OP1	2.08	0.52
26:Z:61:HIS:HB3	38:Z:8710:HOH:O	2.07	0.52
30:0:853:C:H3'	38:0:4548:HOH:O	2.08	0.52
30:0:72:C:H5'	38:0:5876:HOH:O	2.10	0.52
1:A:51:ARG:NH2	1:A:53:ALA:HB3	2.25	0.52
30:0:1180:U:H2'	30:0:1181:A:O4'	2.10	0.52
30:0:1201:C:H6	38:0:5738:HOH:O	1.93	0.52
30:0:2506:A:N6	30:0:2511:A:O2'	2.42	0.52
30:0:2748:G:H5'	38:0:7534:HOH:O	2.08	0.52
9:I:108:HIS:H	9:I:109:PRO:HD2	1.74	0.52
27:1:2:GLY:O	27:1:6:PRO:HG2	2.09	0.52
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.74	0.52
24:X:30:MET:HE1	24:X:55:ASN:HA	1.91	0.52
3:C:94:THR:HG22	38:C:8687:HOH:O	2.09	0.52
1:A:33:GLU:O	1:A:34:ASP:HB2	2.09	0.52
30:0:960:G:H2'	30:0:960:G:N3	2.23	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.74	0.52
30:0:2499:U:H2'	30:0:2500:C:C6	2.44	0.52
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.91	0.52
2:B:298:LYS:HD3	38:B:9095:HOH:O	2.08	0.52
30:0:705:C:H2'	30:0:705:C:O2	2.08	0.52
30:0:1311:G:C2	30:0:1312:G:C8	2.96	0.52
12:L:145:LEU:O	12:L:148:GLU:HG3	2.09	0.52
30:0:1441:G:O2'	30:0:1442:A:H5'	2.09	0.52
14:N:32:PRO:HD2	14:N:99:GLU:O	2.10	0.52
13:M:73:ARG:HD2	13:M:73:ARG:N	2.24	0.52
30:0:506:G:N2	30:0:509:A:C5'	2.66	0.52
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.06	0.52
30:0:1928:C:H2'	30:0:1929:G:O4'	2.09	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.10	0.52
30:0:324:G:O2'	30:0:325:U:H5'	2.09	0.52
30:0:2864:U:O2'	30:0:2865:G:H5'	2.09	0.52
30:0:2295:G:N3	30:0:2361:A:C2	2.77	0.52
31:9:56:A:C3'	31:9:57:A:H5''	2.39	0.52
30:0:2831:C:O2'	30:0:2832:C:H5'	2.10	0.52
1:A:94:LEU:N	1:A:94:LEU:HD23	2.24	0.52
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.40	0.52
5:E:80:TRP:O	5:E:134:SER:HA	2.10	0.52
30:0:2032:U:H2'	30:0:2033:G:H5'	1.91	0.52
23:W:38:THR:O	23:W:42:ARG:HB2	2.09	0.52
30:0:1375:A:C2'	30:0:1376:G:H5'	2.39	0.52
30:0:107:U:H2'	30:0:108:U:H5'	1.92	0.52
20:T:28:SER:O	20:T:32:ARG:HG3	2.10	0.52
23:W:52:VAL:HG22	23:W:53:ALA:H	1.75	0.52
21:U:6:CYS:SG	21:U:13:ILE:HD12	2.49	0.52
5:E:118:ILE:HG23	5:E:144:THR:HG21	1.92	0.52
30:0:297:U:H2'	30:0:298:C:C6	2.43	0.52
30:0:1183:C:O2	30:0:1183:C:H2'	2.08	0.52
30:0:1182:C:H1'	30:0:1192:A:H8	1.74	0.52
30:0:1667:A:H2'	30:0:1668:U:C6	2.44	0.52
13:M:77:HIS:CE1	13:M:86:GLN:HG3	2.44	0.52
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.40	0.52
13:M:91:ILE:HG12	38:0:7539:HOH:O	2.10	0.52
30:0:1269:G:H2'	30:0:1270:U:H6	1.75	0.52
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.52
3:C:70:VAL:HG21	30:0:1361:C:H5'	1.91	0.52
30:0:2326:C:H4'	30:0:2412:G:H4'	1.91	0.52
2:B:49:THR:HG21	2:B:331:SER:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:64:G:H2'	30:0:65:C:O4'	2.10	0.52
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.10	0.52
30:0:506:G:N2	30:0:508:A:H3'	2.25	0.52
30:0:2420:G:C2'	30:0:2421:G:H5'	2.39	0.52
30:0:1972:U:H2'	30:0:1973:A:H5''	1.90	0.52
30:0:1992:U:H2'	30:0:1994:A:OP2	2.10	0.52
30:0:2689:A:C2'	30:0:2690:U:H5'	2.40	0.52
30:0:1845:A:O2'	30:0:1846:U:H5'	2.10	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.25	0.52
30:0:2584:G:H4'	38:0:7109:HOH:O	2.08	0.52
30:0:101:C:H2'	30:0:102:A:C8	2.45	0.52
13:M:46:LEU:HG	38:M:8918:HOH:O	2.08	0.52
13:M:89:THR:HA	38:M:8851:HOH:O	2.10	0.52
30:0:2111:G:H1'	38:0:9051:HOH:O	2.09	0.52
30:0:553:G:O4'	30:0:1325:G:H5'	2.10	0.52
29:3:51:LYS:HA	29:3:54:LYS:HD2	1.92	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
30:0:208:C:H3'	38:0:6388:HOH:O	2.10	0.52
30:0:2549:C:O2'	30:0:2550:U:H5'	2.09	0.52
30:0:541:C:C2'	30:0:542:A:C5'	2.75	0.52
30:0:365:G:C6	30:0:366:U:C4	2.98	0.52
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.91	0.52
23:W:4:LEU:O	23:W:32:CYS:HA	2.10	0.52
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.24	0.52
30:0:293:A:C4	30:0:360:A:C2	2.98	0.52
31:9:18:U:H2'	31:9:19:G:H8	1.74	0.52
14:N:119:GLN:O	14:N:123:ILE:HG13	2.10	0.52
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.91	0.52
7:G:27:ILE:HD13	7:G:71:LEU:HD23	1.92	0.52
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.91	0.52
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.31	0.52
30:0:1189:A:H1'	30:0:1209:C:H1'	1.92	0.51
29:3:64:LYS:HD2	30:0:2459:G:OP2	2.11	0.51
30:0:960:G:N3	30:0:960:G:C2'	2.73	0.51
30:0:2526:C:O2'	30:0:2527:U:H5'	2.10	0.51
26:Z:42:TYR:HA	30:0:1829:A:H61	1.74	0.51
30:0:1495:C:H1'	30:0:1573:A:H1'	1.93	0.51
2:B:214:PRO:HD2	38:0:9078:HOH:O	2.10	0.51
30:0:523:C:H2'	30:0:524:A:C8	2.45	0.51
31:9:22:G:H5'	31:9:23:U:OP1	2.10	0.51
14:N:4:PRO:CB	30:0:1010:C:H4'	2.40	0.51
29:3:42:ARG:NH1	30:0:396:U:H5'	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:226:GLY:HA3	30:0:1308:A:O4'	2.10	0.51
30:0:1682:A:O2'	30:0:1683:G:H5''	2.10	0.51
17:Q:45:PRO:O	30:0:2365:G:H4'	2.10	0.51
30:0:1185:U:H5'	38:0:7461:HOH:O	2.10	0.51
30:0:2004:U:H4'	38:0:5299:HOH:O	2.09	0.51
11:K:41:LYS:HA	30:0:2582:G:O3'	2.11	0.51
5:E:22:VAL:O	5:E:76:VAL:HG11	2.10	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.24	0.51
14:N:102:LEU:HD13	14:N:119:GLN:HB2	1.92	0.51
22:V:44:GLY:O	22:V:48:GLU:HG2	2.10	0.51
30:0:78:G:C6	30:0:79:G:C6	2.99	0.51
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.51
30:0:282:C:C2'	30:0:283:U:H5'	2.40	0.51
13:M:81:ARG:HG2	38:M:8926:HOH:O	2.11	0.51
30:0:2769:C:C2'	30:0:2770:G:C5'	2.88	0.51
30:0:255:A:C4	30:0:256:C:C6	2.98	0.51
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.26	0.51
30:0:2269:C:O2'	30:0:2270:G:H5'	2.10	0.51
30:0:2239:C:H2'	30:0:2240:U:C6	2.46	0.51
15:O:105:ASN:HD21	15:O:109:SER:H	1.58	0.51
30:0:2088:C:H1'	30:0:2841:A:N1	2.25	0.51
30:0:2269:C:H2'	30:0:2270:G:O4'	2.09	0.51
30:0:1361:C:H2'	30:0:1362:U:C6	2.45	0.51
30:0:1788:U:C2	30:0:1805:G:N2	2.79	0.51
30:0:1563:G:H4'	38:0:4227:HOH:O	2.10	0.51
8:H:141:CYS:HB2	38:H:8991:HOH:O	2.10	0.51
28:2:2:LYS:HG3	30:0:1486:A:C5	2.45	0.51
3:C:150:THR:HA	3:C:203:ALA:O	2.11	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
26:Z:37:ARG:HB2	30:0:819:A:H4'	1.92	0.51
30:0:646:G:H2'	30:0:647:U:C6	2.46	0.51
30:0:466:A:H2'	30:0:467:G:O4'	2.10	0.51
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.26	0.51
30:0:1304:U:H2'	30:0:1305:C:C6	2.46	0.51
30:0:1061:C:H1'	30:0:2283:G:O6	2.10	0.51
30:0:343:C:O2'	30:0:344:C:H5'	2.11	0.51
30:0:2851:G:O2'	30:0:2852:A:H5'	2.11	0.51
30:0:2507:G:H2'	30:0:2510:C:H42	1.75	0.51
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.74	0.51
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.58	0.51
31:9:3:A:OP2	31:9:25:G:N2	2.43	0.51
24:X:76:ARG:NH1	24:X:76:ARG:HG3	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:56:ILE:O	22:V:60:GLN:HG3	2.10	0.51
30:0:42:C:H1'	38:0:4670:HOH:O	2.09	0.51
30:0:2899:A:O2'	30:0:2900:G:H5'	2.10	0.51
30:0:1878:G:H1'	38:0:6104:HOH:O	2.11	0.51
31:9:117:G:H2'	31:9:118:C:H6	1.75	0.51
21:U:47:ARG:HG3	38:U:4381:HOH:O	2.10	0.51
30:0:1855:G:H4'	30:0:1856:C:O5'	2.10	0.51
31:9:45:A:C5	31:9:46:C:C5	2.98	0.51
14:N:163:PHE:HB3	38:N:8829:HOH:O	2.11	0.51
30:0:2099:A:H2	38:0:3918:HOH:O	1.93	0.51
3:C:21:VAL:HG13	38:C:8606:HOH:O	2.09	0.51
5:E:137:ASP:O	5:E:141:VAL:HG23	2.10	0.51
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.93	0.51
30:0:703:G:H2'	30:0:704:C:H6	1.76	0.51
30:0:2354:A:H5'	30:0:2355:G:N7	2.26	0.51
2:B:162:MET:HG3	2:B:310:ARG:HH11	1.75	0.51
30:0:1626:A:O2'	30:0:1627:G:H5'	2.10	0.51
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.46	0.51
14:N:114:LYS:O	14:N:118:ILE:HG13	2.10	0.51
30:0:1020:A:H1'	38:0:7218:HOH:O	2.11	0.51
30:0:1581:A:C5	30:0:1582:C:C5	2.99	0.51
30:0:124:C:H3'	38:0:7649:HOH:O	2.10	0.51
30:0:1056:U:H2'	30:0:1057:A:O4'	2.10	0.51
6:F:39:SER:OG	6:F:45:ALA:HB2	2.11	0.51
30:0:2842:G:H2'	30:0:2843:A:H5'	1.92	0.51
30:0:1562:C:O2	30:0:1562:C:C2'	2.59	0.51
30:0:1279:U:O2	30:0:1279:U:C2'	2.58	0.51
30:0:1701:A:H5''	30:0:1702:U:H3'	1.93	0.51
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.11	0.51
3:C:76:ARG:NH2	30:0:1363:G:OP1	2.44	0.51
1:A:223:ARG:HG3	38:A:9021:HOH:O	2.11	0.51
1:A:132:ASP:CG	1:A:133:ARG:H	2.14	0.51
30:0:920:C:H5'	30:0:921:G:C4	2.46	0.51
30:0:615:G:H2'	30:0:616:U:C6	2.46	0.51
29:3:10:TYR:HD1	30:0:2408:A:HO2'	1.52	0.51
30:0:1202:A:H2'	30:0:1203:G:H5'	1.92	0.51
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.38	0.51
30:0:255:A:C5	30:0:256:C:C4	2.99	0.51
30:0:1972:U:C2'	30:0:1973:A:C5'	2.89	0.51
17:Q:28:ARG:HG2	38:9:9082:HOH:O	2.11	0.51
1:A:207:GLN:HA	38:A:8981:HOH:O	2.10	0.51
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:168:C:O5'	30:0:168:C:H6	1.92	0.51
30:0:1218:U:H2'	30:0:1219:U:C6	2.46	0.51
30:0:2345:A:H3'	30:0:2346:C:C6	2.45	0.51
20:T:72:ILE:HD13	20:T:93:THR:HG22	1.92	0.50
17:Q:11:ARG:HH22	30:0:2363:G:C5'	2.24	0.50
26:Z:80:GLN:CG	26:Z:81:CYS:H	2.22	0.50
30:0:407:A:H5'	38:0:6009:HOH:O	2.11	0.50
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.50
30:0:1626:A:C2'	30:0:1627:G:H5'	2.41	0.50
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.93	0.50
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.11	0.50
30:0:2506:A:O2'	30:0:2507:G:C8	2.49	0.50
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.20	0.50
30:0:1213:C:C2'	30:0:1214:G:H5'	2.42	0.50
3:C:46:TYR:CE1	30:0:450:C:H4'	2.45	0.50
2:B:72:THR:HB	38:B:9075:HOH:O	2.10	0.50
1:A:179:MET:HG2	1:A:186:TRP:CB	2.41	0.50
35:0:8812:CL:CL	38:0:5117:HOH:O	2.57	0.50
30:0:151:A:H2'	30:0:152:A:O4'	2.11	0.50
30:0:1589:G:H4'	38:0:6843:HOH:O	2.10	0.50
30:0:1934:A:C8	30:0:1935:C:C5	3.00	0.50
2:B:238:ASN:HD22	2:B:240:GLY:N	2.10	0.50
30:0:396:U:O2'	30:0:397:A:P	2.70	0.50
30:0:2758:G:H2'	30:0:2759:C:H6	1.76	0.50
30:0:1189:A:O2'	30:0:1208:C:H2'	2.12	0.50
25:Y:115:ARG:HH22	30:0:1266:U:H4'	1.72	0.50
23:W:5:VAL:HG22	23:W:32:CYS:HB2	1.94	0.50
30:0:2533:C:C6	30:0:2533:C:H5'	2.42	0.50
30:0:2896:A:N3	30:0:2896:A:H2'	2.26	0.50
5:E:81:GLU:O	5:E:172:PRO:HD3	2.12	0.50
30:0:99:A:C8	30:0:100:C:C5	2.99	0.50
21:U:9:CYS:HB2	38:U:6796:HOH:O	2.12	0.50
13:M:139:PRO:HA	13:M:142:GLN:HB2	1.93	0.50
1:A:162:GLY:N	26:Z:91:GLY:HA2	2.26	0.50
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.93	0.50
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.50
38:C:8676:HOH:O	30:0:2100:A:H5'	2.12	0.50
30:0:549:A:O2'	30:0:550:C:H5'	2.11	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.75	0.50
30:0:693:A:H2'	30:0:694:A:C8	2.46	0.50
30:0:920:C:H4'	30:0:921:G:C2	2.46	0.50
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.94	0.50
30:0:1180:U:O2'	30:0:1181:A:H5'	2.11	0.50
30:0:1183:C:N3	30:0:1184:C:C5	2.79	0.50
30:0:2072:G:C6	30:0:2533:C:H1'	2.47	0.50
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.50
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.94	0.50
30:0:1759:A:N3	30:0:1818:C:H2'	2.27	0.50
30:0:216:A:O2'	30:0:217:C:H5'	2.12	0.50
16:P:41:ARG:HH22	30:0:1500:U:P	2.34	0.50
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.93	0.50
3:C:197:SER:HB3	38:C:8583:HOH:O	2.12	0.50
13:M:72:ALA:HB3	38:M:8944:HOH:O	2.12	0.50
30:0:1158:G:H2'	30:0:1159:G:H5'	1.93	0.50
30:0:559:U:H6	30:0:559:U:C5'	2.20	0.50
10:J:75:PRO:HD3	10:J:136:SER:OG	2.12	0.50
30:0:2781:U:C2'	30:0:2782:G:C5'	2.89	0.50
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.39	0.50
30:0:820:G:H5'	30:0:821:U:C5'	2.41	0.50
30:0:39:G:C2	30:0:444:C:C2	3.00	0.50
30:0:1819:G:H2'	30:0:1820:G:C4'	2.42	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1395:C:H2'	30:0:1396:C:H6	1.77	0.50
30:0:2416:G:H2'	30:0:2417:C:H6	1.76	0.50
5:E:11:VAL:HG12	5:E:12:ASP:N	2.27	0.50
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.94	0.50
2:B:158:LYS:HB2	38:0:4101:HOH:O	2.11	0.50
10:J:82:THR:HG23	30:0:1242:A:C5'	2.17	0.50
30:0:441:A:C2	30:0:442:A:N6	2.80	0.50
30:0:2354:A:H5'	30:0:2355:G:C5	2.46	0.50
30:0:204:A:C2'	30:0:205:U:H5'	2.41	0.50
31:9:61:C:H2'	31:9:62:A:H8	1.76	0.50
14:N:160:SER:HB3	31:9:51:A:H5'	1.93	0.50
30:0:523:C:H2'	30:0:524:A:H8	1.77	0.50
30:0:1765:G:H1'	30:0:1780:G:N2	2.26	0.50
30:0:2598:U:O2	30:0:2600:A:H8	1.95	0.50
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.50
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.94	0.50
30:0:1610:G:H2'	30:0:1611:G:O4'	2.12	0.50
23:W:121:PRO:CA	23:W:153:MET:HG2	2.42	0.50
30:0:1160:G:H5'	30:0:1161:A:H5'	0.83	0.50
14:N:169:PRO:O	14:N:172:PHE:HB3	2.12	0.50
10:J:22:VAL:O	10:J:26:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2269:C:H2'	30:0:2270:G:C5'	2.42	0.50
31:9:58:G:C8	31:9:59:C:C5	3.00	0.50
27:1:28:HIS:HE1	30:0:776:A:OP1	1.95	0.50
30:0:932:U:H2'	30:0:933:C:C6	2.47	0.50
30:0:1398:G:H2'	30:0:1399:A:C8	2.47	0.50
30:0:1947:G:H2'	30:0:1948:G:H8	1.77	0.50
30:0:2330:U:H4'	30:0:2331:C:OP1	2.11	0.50
30:0:1226:G:H5'	38:0:4526:HOH:O	2.11	0.50
10:J:76:ASP:HA	38:J:8863:HOH:O	2.11	0.50
30:0:2502:C:O2'	30:0:2503:A:H5'	2.12	0.49
30:0:299:U:N3	30:0:300:U:C5	2.80	0.49
27:1:28:HIS:HD2	27:1:30:LYS:H	1.58	0.49
30:0:88:G:H5'	30:0:88:G:H8	1.76	0.49
30:0:1791:U:O2'	30:0:1792:C:H5'	2.12	0.49
30:0:1541:G:O2'	30:0:1542:G:H5'	2.11	0.49
30:0:1365:C:H4'	38:0:4606:HOH:O	2.12	0.49
30:0:1188:A:C6	30:0:1189:A:C6	3.00	0.49
31:9:114:G:H2'	31:9:115:C:H6	1.76	0.49
30:0:249:G:N2	30:0:250:C:C2	2.80	0.49
30:0:2705:U:H2'	30:0:2706:A:H8	1.73	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.12	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.12	0.49
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.77	0.49
30:0:1964:U:O2	30:0:1964:U:H2'	2.10	0.49
13:M:94:ARG:HD2	30:0:158:A:OP2	2.11	0.49
18:R:117:HIS:HD2	30:0:20:G:H21	1.61	0.49
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.41	0.49
4:D:76:ARG:NH1	31:9:42:C:O2	2.45	0.49
31:9:49:G:H2'	31:9:50:G:O4'	2.12	0.49
31:9:20:G:H3'	38:9:9055:HOH:O	2.12	0.49
30:0:699:C:O2'	30:0:744:G:H1'	2.12	0.49
30:0:876:A:N3	30:0:876:A:C2'	2.75	0.49
11:K:8:VAL:HG12	11:K:9:THR:N	2.26	0.49
5:E:15:GLN:HG2	5:E:16:ASP:N	2.28	0.49
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.94	0.49
30:0:2002:C:H2'	30:0:2003:U:H5'	1.94	0.49
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.94	0.49
30:0:1191:A:H2'	30:0:1193:A:H5'	1.95	0.49
30:0:816:G:H5'	30:0:1598:A:H4'	1.94	0.49
30:0:2316:G:H8	38:0:5642:HOH:O	1.95	0.49
26:Z:38:PHE:HB3	26:Z:42:TYR:HD1	1.78	0.49
23:W:90:TYR:N	23:W:90:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:11:VAL:HG11	30:0:1086:A:C6	2.48	0.49
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.94	0.49
30:0:1453:G:H2'	30:0:1454:U:O4'	2.13	0.49
30:0:1206:U:H5'	30:0:1206:U:C6	2.31	0.49
2:B:212:GLN:HA	30:0:1733:A:H4'	1.94	0.49
30:0:1526:A:H4'	30:0:1527:A:H5'	1.95	0.49
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.95	0.49
30:0:1942:A:O2'	30:0:1943:C:H5'	2.11	0.49
29:3:38:ARG:CB	29:3:42:ARG:HH12	2.25	0.49
15:O:25:VAL:HG23	15:O:26:TRP:N	2.27	0.49
14:N:18:THR:HG21	38:9:9099:HOH:O	2.12	0.49
30:0:514:G:OP1	30:0:514:G:H2'	2.12	0.49
11:K:22:ASP:HB2	38:K:5264:HOH:O	2.13	0.49
30:0:2612:A:H4'	38:0:3666:HOH:O	2.13	0.49
23:W:119:HIS:HE1	38:0:9557:HOH:O	1.96	0.49
30:0:445:U:O2'	30:0:446:G:H5'	2.12	0.49
30:0:1159:G:H2'	30:0:1160:G:O4'	2.11	0.49
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.94	0.49
30:0:314:G:C2	30:0:317:A:C8	3.01	0.49
31:9:7:G:H5'	38:9:9099:HOH:O	2.11	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.27	0.49
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.48	0.49
30:0:1375:A:H2'	30:0:1376:G:H5'	1.95	0.49
2:B:28:SER:HB2	30:0:2807:U:OP2	2.13	0.49
30:0:352:A:H2'	30:0:353:G:C8	2.48	0.49
30:0:128:A:H3'	30:0:128:A:C8	2.47	0.49
29:3:48:ASN:ND2	30:0:169:A:H1'	2.27	0.49
30:0:2820:A:H2'	30:0:2821:C:C6	2.46	0.49
30:0:2265:U:H2'	30:0:2266:A:H8	1.77	0.49
30:0:2135:A:O4'	30:0:2243:C:N4	2.45	0.49
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.13	0.49
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.78	0.49
27:1:16:HIS:HD2	30:0:470:U:O2'	1.95	0.49
30:0:1181:A:C2	30:0:1192:A:C8	3.00	0.49
30:0:1209:C:H2'	30:0:1210:G:C8	2.42	0.49
30:0:1976:G:H1'	30:0:2005:G:N2	2.28	0.49
30:0:2237:G:H1'	30:0:2238:A:H8	1.77	0.49
30:0:661:G:C5	30:0:686:A:C2	3.01	0.49
30:0:1572:A:H3'	38:0:4098:HOH:O	2.13	0.49
31:9:52:A:H2'	31:9:53:G:H8	1.76	0.49
7:G:16:LYS:O	7:G:20:VAL:HG23	2.13	0.49
21:U:9:CYS:HA	21:U:52:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1765:G:O2'	30:0:1766:U:H5'	2.12	0.49
30:0:2707:C:H2'	30:0:2707:C:O2	2.13	0.49
30:0:2805:A:C8	30:0:2806:C:C5	3.01	0.49
30:0:2635:A:C2'	30:0:2636:C:H5'	2.41	0.49
13:M:133:LEU:O	13:M:134:ILE:HD13	2.13	0.49
30:0:2254:G:H1'	38:0:5527:HOH:O	2.12	0.49
30:0:264:G:H1'	30:0:265:U:H5	1.78	0.49
38:L:9036:HOH:O	30:0:196:G:H2'	2.12	0.49
30:0:2359:G:H3'	38:0:5674:HOH:O	2.13	0.49
30:0:1521:C:H2'	30:0:1522:A:H8	1.78	0.49
30:0:1118:A:C8	30:0:1119:G:H5''	2.47	0.49
30:0:1118:A:N6	30:0:1244:U:H3	1.95	0.49
29:3:68:LYS:HE3	30:0:2435:U:O2'	2.12	0.49
30:0:2289:G:O2'	30:0:2291:A:N6	2.45	0.49
10:J:19:MET:HE1	10:J:132:LEU:HD21	1.93	0.49
14:N:132:ASN:HD22	30:0:2413:A:C4'	2.25	0.49
19:S:49:VAL:HG13	19:S:66:VAL:HG13	1.95	0.49
26:Z:64:PRO:HB2	26:Z:86:TYR:HE2	1.78	0.49
30:0:1913:C:H2'	30:0:1914:C:H6	1.76	0.49
30:0:1586:G:O2'	30:0:1587:U:H5'	2.13	0.49
30:0:1566:C:O2'	30:0:1567:G:H5'	2.12	0.49
30:0:2911:C:H2'	30:0:2912:C:C6	2.48	0.49
30:0:526:U:H2'	30:0:527:U:C6	2.48	0.49
30:0:727:G:H3'	30:0:728:C:H6	1.78	0.49
6:F:91:VAL:HG12	6:F:92:GLY:N	2.22	0.48
17:Q:11:ARG:HH22	30:0:2363:G:H5''	1.78	0.48
30:0:2269:C:H2'	30:0:2270:G:H5'	1.95	0.48
30:0:10:U:O4	30:0:532:A:H8	1.96	0.48
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.48
30:0:146:U:O2'	30:0:147:G:H5'	2.12	0.48
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.95	0.48
30:0:59:A:H5'	38:0:4330:HOH:O	2.13	0.48
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.94	0.48
30:0:1641:A:O2'	30:0:1642:A:H5'	2.13	0.48
21:U:50:GLU:O	21:U:56:ARG:HG2	2.13	0.48
30:0:2710:U:O2'	30:0:2711:U:H5'	2.13	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.65	0.48
30:0:2073:G:C6	30:0:2489:G:H4'	2.48	0.48
30:0:1447:U:H3'	30:0:1506:U:O2	2.12	0.48
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.95	0.48
30:0:2061:C:C2'	30:0:2062:A:H5'	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:64:GLU:HG2	38:P:169:HOH:O	2.13	0.48
29:3:5:ARG:O	29:3:21:GLU:HA	2.12	0.48
13:M:70:GLY:HA3	13:M:73:ARG:CZ	2.42	0.48
30:0:2509:A:H2'	30:0:2510:C:O4'	2.13	0.48
30:0:2512:U:H4'	30:0:2514:U:O4	2.13	0.48
1:A:212:PRO:HB2	38:A:8985:HOH:O	2.13	0.48
30:0:1922:A:N1	30:0:2449:G:O2'	2.46	0.48
20:T:8:ARG:NH1	30:0:31:C:OP2	2.46	0.48
11:K:74:VAL:HG21	11:K:96:VAL:HG23	1.95	0.48
13:M:164:THR:CG2	13:M:165:GLY:N	2.75	0.48
30:0:311:C:H2'	30:0:312:U:H6	1.77	0.48
2:B:49:THR:HG22	2:B:50:HIS:H	1.79	0.48
30:0:344:C:H2'	30:0:345:G:O4'	2.12	0.48
30:0:1566:C:H2'	30:0:1567:G:H8	1.78	0.48
30:0:1461:U:H2'	30:0:1462:C:C6	2.48	0.48
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.13	0.48
30:0:305:A:C5	30:0:329:A:C2	3.02	0.48
30:0:682:A:H2'	30:0:683:G:O4'	2.13	0.48
30:0:598:C:H2'	30:0:599:G:H8	1.77	0.48
30:0:2616:G:H1'	38:0:9428:HOH:O	2.12	0.48
30:0:370:G:O2'	30:0:371:U:H5'	2.14	0.48
12:L:143:THR:HG22	12:L:144:ASP:N	2.28	0.48
30:0:1706:G:C6	30:0:1707:G:N1	2.81	0.48
30:0:2271:G:N3	30:0:2271:G:H2'	2.27	0.48
30:0:1188:A:H5'	38:0:7418:HOH:O	2.12	0.48
30:0:2511:A:H2'	30:0:2512:U:C6	2.47	0.48
30:0:1835:U:H3'	38:0:5569:HOH:O	2.12	0.48
29:3:64:LYS:HA	29:3:84:ARG:CA	2.38	0.48
30:0:816:G:C6	30:0:817:G:N1	2.82	0.48
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.95	0.48
30:0:2673:U:C4	30:0:2674:G:C6	3.01	0.48
26:Z:37:ARG:HB2	30:0:819:A:O4'	2.14	0.48
30:0:2651:C:H2'	30:0:2652:U:O4'	2.13	0.48
30:0:1626:A:H2'	30:0:1627:G:H5'	1.96	0.48
30:0:645:U:O2	30:0:761:A:H2	1.97	0.48
30:0:2626:C:H2'	30:0:2627:G:C8	2.49	0.48
13:M:48:LYS:HE3	13:M:52:GLN:HE21	1.78	0.48
30:0:809:G:H2'	30:0:810:G:H8	1.78	0.48
30:0:1187:U:O2'	30:0:1188:A:C8	2.64	0.48
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.36	0.48
29:3:64:LYS:HD3	29:3:82:GLY:O	2.13	0.48
30:0:1684:A:O2'	30:0:1685:A:H5''	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:Z:74:GLN:HG2	26:Z:80:GLN:HB2	1.95	0.48
30:0:1905:U:H2'	30:0:1906:C:H6	1.79	0.48
20:T:48:VAL:HG12	20:T:49:GLU:N	2.29	0.48
30:0:421:C:H4'	30:0:1919:A:C6	2.49	0.48
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.43	0.48
13:M:74:LYS:O	13:M:88:VAL:HG13	2.13	0.48
30:0:2713:G:O2'	30:0:2714:U:H5'	2.13	0.48
11:K:130:MET:SD	21:U:25:ASP:O	2.71	0.48
31:9:23:U:H2'	31:9:23:U:O2	2.14	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.49	0.48
30:0:154:C:H2'	30:0:155:C:C6	2.49	0.48
1:A:72:GLU:HG2	26:Z:100:GLY:CA	2.40	0.48
30:0:696:C:HO2'	30:0:697:G:H5'	1.78	0.48
2:B:74:ILE:HG13	38:B:9075:HOH:O	2.13	0.48
30:0:1343:C:H2'	30:0:1344:G:O5'	2.12	0.48
5:E:101:GLU:HB2	5:E:116:THR:O	2.13	0.48
30:0:2608:C:H2'	38:0:3561:HOH:O	2.13	0.48
18:R:33:ARG:NH1	38:R:8944:HOH:O	2.47	0.48
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.14	0.48
12:L:65:ASP:HA	12:L:109:LEU:O	2.14	0.48
13:M:73:ARG:HH22	30:0:2263:G:H5''	1.77	0.48
30:0:284:C:H4'	30:0:285:A:H8	1.79	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.44	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.96	0.48
17:Q:27:GLN:HE21	31:9:8:G:H5''	1.75	0.48
30:0:2524:G:N2	30:0:2526:C:N4	2.57	0.48
30:0:1168:C:H5	38:0:7488:HOH:O	1.96	0.48
30:0:228:C:C2'	30:0:229:G:H5'	2.44	0.48
30:0:589:U:H2'	30:0:590:A:C8	2.47	0.48
2:B:84:LEU:HD23	2:B:142:LEU:HD23	1.96	0.48
23:W:107:LEU:O	23:W:112:LEU:HB2	2.13	0.48
30:0:1422:U:H2'	30:0:1423:C:C6	2.49	0.48
10:J:135:ILE:O	10:J:139:LEU:HG	2.14	0.48
30:0:533:U:H3'	38:0:3736:HOH:O	2.13	0.48
31:9:38:A:H2	31:9:43:G:H5''	1.77	0.48
30:0:2614:C:O2'	30:0:2615:U:H5'	2.13	0.48
30:0:1965:C:H2'	30:0:1966:U:C6	2.49	0.48
30:0:581:G:O2'	30:0:582:U:H5'	2.13	0.48
38:2:3526:HOH:O	30:0:1413:A:H5''	2.14	0.48
30:0:1795:G:H2'	30:0:1796:A:O4'	2.13	0.48
31:9:5:G:C2'	31:9:6:C:H5'	2.43	0.48
30:0:542:A:H2'	30:0:543:G:O4'	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.40	0.48
30:0:1592:G:C4	30:0:1593:C:C5	3.02	0.48
24:X:85:VAL:HG12	24:X:86:GLU:N	2.29	0.48
30:0:2296:C:H2'	30:0:2297:U:H6	1.79	0.48
30:0:138:U:OP2	30:0:139:C:C5	2.67	0.48
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.96	0.48
30:0:1706:G:C5	30:0:1707:G:C6	3.02	0.48
20:T:38:ARG:NH1	38:0:6667:HOH:O	2.47	0.48
30:0:2842:G:C2'	30:0:2843:A:H5'	2.44	0.48
4:D:52:THR:HG21	30:0:2346:C:O2'	2.13	0.48
30:0:1790:C:H2'	30:0:1791:U:H6	1.79	0.48
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.44	0.48
3:C:206:ASN:HB2	30:0:329:A:OP2	2.13	0.48
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.49	0.48
30:0:113:A:C8	30:0:114:A:C8	3.02	0.48
23:W:134:GLU:OE2	31:9:97:U:H1'	2.14	0.48
13:M:40:ILE:HG21	13:M:64:ARG:NH2	2.29	0.48
18:R:39:THR:HB	18:R:42:GLU:CG	2.44	0.47
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.96	0.47
1:A:36:ASP:O	1:A:38:ILE:N	2.44	0.47
14:N:22:GLN:O	14:N:26:LEU:HB2	2.14	0.47
30:0:1878:G:C1'	38:0:6104:HOH:O	2.62	0.47
11:K:37:TYR:HB3	38:K:7169:HOH:O	2.14	0.47
23:W:11:VAL:O	23:W:12:ASN:HB2	2.14	0.47
30:0:1735:C:H2'	30:0:1736:A:C8	2.49	0.47
30:0:764:C:H2'	30:0:765:G:O4'	2.14	0.47
30:0:2074:A:H2'	38:0:3520:HOH:O	2.13	0.47
1:A:42:VAL:HG21	1:A:74:VAL:CG1	2.44	0.47
16:P:102:ARG:NH2	30:0:1596:U:C5	2.82	0.47
30:0:24:G:H22	30:0:518:G:H1'	1.79	0.47
10:J:107:ASN:ND2	10:J:109:TYR:H	2.11	0.47
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.79	0.47
30:0:2864:U:C2'	30:0:2865:G:H5'	2.44	0.47
30:0:45:A:N6	30:0:147:G:C4	2.83	0.47
30:0:844:A:C6	30:0:882:A:C6	3.02	0.47
30:0:2890:A:H2'	30:0:2890:A:N3	2.29	0.47
30:0:1205:U:C2'	30:0:1206:U:H5''	2.44	0.47
30:0:703:G:H2'	30:0:704:C:C6	2.49	0.47
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.96	0.47
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.96	0.47
2:B:41:PHE:HB3	2:B:190:MET:CE	2.44	0.47
31:9:52:A:H2'	31:9:53:G:O4'	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2241:C:O2'	30:0:2242:U:H5'	2.14	0.47
27:1:20:ARG:HG2	30:0:111:C:O2'	2.14	0.47
26:Z:65:ASN:HD22	26:Z:84:CYS:HB2	1.80	0.47
2:B:54:VAL:HB	38:B:9084:HOH:O	2.13	0.47
28:2:29:THR:HG22	30:0:86:A:O4'	2.14	0.47
30:0:301:C:H2'	30:0:302:A:H8	1.79	0.47
30:0:1787:C:H4'	30:0:2883:A:O4'	2.14	0.47
30:0:1603:A:H5''	30:0:1604:G:H3'	1.96	0.47
31:9:108:C:H2'	31:9:109:G:H8	1.79	0.47
20:T:48:VAL:HG13	20:T:97:ARG:O	2.14	0.47
30:0:2032:U:C2'	30:0:2033:G:C5'	2.93	0.47
29:3:10:TYR:HE2	30:0:2382:A:H1'	1.80	0.47
30:0:2784:A:H8	30:0:2784:A:O5'	1.98	0.47
2:B:305:ASP:O	2:B:306:LYS:HB2	2.15	0.47
16:P:55:LYS:HG3	16:P:56:GLY:N	2.29	0.47
30:0:1561:U:H5'	38:0:7421:HOH:O	2.13	0.47
30:0:95:A:H5''	30:0:97:G:O4'	2.14	0.47
3:C:153:VAL:O	3:C:157:LEU:HG	2.15	0.47
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	1.96	0.47
1:A:45:ILE:HG22	26:Z:78:ILE:HG12	1.96	0.47
30:0:2908:A:O5'	30:0:2908:A:H8	1.97	0.47
30:0:1942:A:H3'	38:0:7336:HOH:O	2.14	0.47
30:0:2336:G:C2'	38:0:6280:HOH:O	2.60	0.47
30:0:292:G:H2'	30:0:358:G:N2	2.30	0.47
30:0:1217:G:C2	30:0:1218:U:C2	3.03	0.47
30:0:599:G:H2'	30:0:600:G:H8	1.79	0.47
30:0:810:G:H2'	30:0:811:C:C6	2.49	0.47
13:M:75:ARG:HB2	38:M:8905:HOH:O	2.14	0.47
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.96	0.47
30:0:2697:A:H2'	30:0:2698:G:O4'	2.15	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.95	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.47
30:0:2510:C:H5'	30:0:2511:A:OP2	2.13	0.47
30:0:371:U:H2'	30:0:372:A:C8	2.49	0.47
29:3:79:LEU:HB2	38:0:6581:HOH:O	2.14	0.47
30:0:960:G:H3'	30:0:960:G:N3	2.30	0.47
13:M:91:ILE:HD11	38:M:8830:HOH:O	2.15	0.47
10:J:131:THR:HG22	10:J:133:GLY:H	1.79	0.47
6:F:50:VAL:HG21	6:F:63:ILE:HG21	1.97	0.47
29:3:46:ILE:HG12	38:0:3138:HOH:O	2.14	0.47
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.47
30:0:1318:A:H4'	30:0:1343:C:H4'	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:TRP:CG	1:A:187:PRO:HA	2.50	0.47
23:W:120:PRO:HG2	30:0:1095:U:O2	2.14	0.47
23:W:119:HIS:HD2	23:W:120:PRO:O	1.97	0.47
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.47	0.47
30:0:1359:U:C5	30:0:2101:A:C8	3.03	0.47
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.97	0.47
30:0:1173:A:H4'	30:0:1174:A:C8	2.49	0.47
30:0:2686:C:C2	30:0:2709:G:N2	2.82	0.47
30:0:282:C:H1'	30:0:368:C:H41	1.78	0.47
30:0:484:A:N1	30:0:506:G:H4'	2.30	0.47
23:W:88:THR:HB	38:W:6679:HOH:O	2.14	0.47
30:0:1882:C:H2'	30:0:1883:U:H6	1.80	0.47
30:0:1523:G:C6	30:0:1524:U:C4	3.03	0.47
2:B:98:THR:HG23	30:0:2820:A:OP1	2.15	0.47
18:R:68:HIS:CD2	18:R:76:ASP:HB2	2.50	0.47
23:W:121:PRO:HA	23:W:153:MET:HG2	1.96	0.47
30:0:2598:U:O2	30:0:2600:A:C8	2.68	0.47
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.47
30:0:1769:C:O2'	30:0:1770:U:H5'	2.15	0.47
30:0:677:C:O2'	30:0:678:G:H5'	2.14	0.47
30:0:1042:U:O2'	30:0:1043:C:H5'	2.15	0.47
30:0:512:G:O3'	30:0:513:A:H8	1.97	0.47
30:0:1864:C:H2'	30:0:1865:A:O4'	2.14	0.47
29:3:50:GLY:HA3	38:0:9164:HOH:O	2.14	0.47
30:0:1183:C:C2	30:0:1184:C:C5	3.03	0.47
30:0:1187:U:O2'	30:0:1189:A:H2	1.98	0.47
30:0:2253:G:H2'	30:0:2254:G:H8	1.80	0.47
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.80	0.47
22:V:39:ALA:N	22:V:40:PRO:CD	2.77	0.47
30:0:304:G:H8	30:0:304:G:O5'	1.98	0.47
29:3:24:LYS:HE3	29:3:90:PHE:CE1	2.50	0.47
30:0:1377:C:C5'	30:0:1377:C:H6	2.28	0.47
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.63	0.47
30:0:2134:G:N2	30:0:2242:U:C2	2.83	0.47
30:0:2329:C:O2'	30:0:2330:U:H5'	2.14	0.47
23:W:29:VAL:O	23:W:30:ASN:HB2	2.13	0.47
17:Q:14:LEU:HD21	17:Q:43:ILE:HD12	1.97	0.47
1:A:121:ALA:O	1:A:124:VAL:HG22	2.14	0.47
30:0:2383:G:C6	30:0:2384:U:C4	3.03	0.47
30:0:2752:C:O2'	30:0:2753:G:H5'	2.15	0.47
30:0:371:U:H2'	30:0:372:A:H8	1.80	0.47
30:0:2769:C:H2'	30:0:2770:G:O4'	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:36:C:C2	30:0:447:A:C2	3.03	0.47
30:0:447:A:O2'	30:0:448:G:H5'	2.15	0.47
30:0:1966:U:O5'	30:0:1966:U:H6	1.98	0.47
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.47
8:H:91:ARG:HB2	30:0:1003:U:OP1	2.15	0.47
30:0:2096:A:H2'	30:0:2539:U:O4'	2.14	0.47
25:Y:137:LYS:HD2	30:0:521:A:H5''	1.97	0.47
17:Q:11:ARG:CZ	30:0:2363:G:H4'	2.44	0.47
30:0:613:C:H2'	30:0:614:U:C6	2.46	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:805:G:N2	30:0:807:A:H3'	2.30	0.47
30:0:1878:G:O2'	30:0:1879:U:C5	2.66	0.47
3:C:103:ASN:ND2	30:0:663:C:H5''	2.29	0.47
30:0:2604:A:H5'	38:0:5775:HOH:O	2.14	0.47
18:R:82:GLU:HG3	18:R:83:LYS:N	2.29	0.47
13:M:111:ASN:HB2	38:M:8849:HOH:O	2.14	0.47
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.44	0.46
30:0:1477:C:C5'	30:0:1868:G:H5''	2.45	0.46
30:0:1477:C:H4'	30:0:1868:G:OP1	2.15	0.46
5:E:93:MET:HE1	5:E:165:GLY:H	1.79	0.46
30:0:1969:A:C2'	30:0:1970:G:H5'	2.45	0.46
5:E:7:ILE:HG23	5:E:45:ASP:O	2.15	0.46
30:0:1350:U:H4'	38:0:5115:HOH:O	2.15	0.46
30:0:1163:G:N1	30:0:1184:C:N4	2.64	0.46
30:0:1116:U:C2	30:0:1246:A:N6	2.83	0.46
30:0:877:G:C5'	30:0:878:G:OP1	2.62	0.46
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.46
30:0:1634:G:H2'	38:0:3889:HOH:O	2.15	0.46
30:0:735:C:H3'	30:0:736:A:C8	2.50	0.46
2:B:79:MET:HE1	38:B:9096:HOH:O	2.15	0.46
29:3:69:TYR:O	29:3:77:ALA:HA	2.15	0.46
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.14	0.46
30:0:921:G:H4'	30:0:924:G:N1	2.30	0.46
11:K:34:VAL:HB	38:K:7169:HOH:O	2.15	0.46
30:0:1949:G:H22	30:0:1964:U:H1'	1.79	0.46
30:0:629:A:C2	30:0:2074:A:C2	3.03	0.46
30:0:1838:U:O2'	30:0:2644:C:H5'	2.15	0.46
30:0:1197:G:H1'	30:0:1203:G:C2	2.51	0.46
30:0:1545:C:H1'	30:0:1641:A:N6	2.29	0.46
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.46
30:0:2102:G:C2	30:0:2103:A:N6	2.83	0.46
30:0:2526:C:H5'	30:0:2526:C:C6	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.77	0.46
30:0:530:C:H4'	30:0:612:U:H4'	1.97	0.46
30:0:1797:A:O3'	30:0:1798:C:C6	2.69	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.45	0.46
30:0:2256:G:H2'	30:0:2257:G:C5'	2.46	0.46
30:0:790:A:H2'	30:0:791:A:O4'	2.16	0.46
30:0:2347:C:H2'	30:0:2348:C:C6	2.50	0.46
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.13	0.46
30:0:1617:C:C5	30:0:1643:C:H4'	2.50	0.46
22:V:27:LEU:HA	22:V:49:LEU:HD13	1.98	0.46
30:0:130:C:O2'	30:0:131:A:N7	2.46	0.46
16:P:87:ARG:HG2	38:P:186:HOH:O	2.15	0.46
7:G:63:ARG:N	38:G:2569:HOH:O	2.48	0.46
30:0:238:C:H4'	30:0:287:C:OP1	2.16	0.46
30:0:2438:G:H2'	30:0:2439:C:C6	2.50	0.46
30:0:2297:U:H1'	38:0:5172:HOH:O	2.16	0.46
21:U:13:ILE:HG13	38:U:3194:HOH:O	2.15	0.46
30:0:834:G:C4'	30:0:835:U:OP2	2.61	0.46
29:3:47:GLY:HA2	30:0:2121:G:H4'	1.97	0.46
4:D:29:HIS:N	4:D:29:HIS:ND1	2.61	0.46
5:E:84:MET:HG2	5:E:168:ILE:HA	1.98	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
27:1:25:LYS:O	27:1:25:LYS:HG2	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
21:U:56:ARG:HD2	30:0:2890:A:C1'	2.46	0.46
30:0:2434:A:H2'	30:0:2435:U:O4'	2.15	0.46
1:A:171:LYS:HB2	30:0:820:G:C6	2.50	0.46
13:M:102:GLU:CD	13:M:164:THR:HG21	2.36	0.46
12:L:10:SER:O	12:L:11:ARG:HB3	2.16	0.46
10:J:80:LYS:HE3	10:J:101:VAL:O	2.14	0.46
6:F:111:ILE:O	6:F:115:VAL:HG23	2.15	0.46
31:9:14:G:H8	31:9:14:G:C5'	2.16	0.46
30:0:660:A:N6	30:0:746:A:O4'	2.49	0.46
30:0:100:C:H2'	30:0:101:C:H6	1.80	0.46
30:0:101:C:H2'	30:0:102:A:H8	1.80	0.46
30:0:461:C:N3	30:0:479:G:H5'	2.31	0.46
30:0:1154:A:H2'	30:0:1155:G:C8	2.50	0.46
30:0:1434:A:H2'	30:0:1436:C:C5	2.51	0.46
29:3:1:MET:HG2	29:3:87:ARG:O	2.16	0.46
16:P:115:SER:OG	16:P:118:GLN:HG3	2.16	0.46
30:0:365:G:C5	30:0:366:U:C5	3.04	0.46
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.25	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:11:ARG:NH1	31:9:8:G:O6	2.48	0.46
2:B:144:THR:HG22	2:B:145:HIS:N	2.31	0.46
30:0:517:U:C2'	30:0:518:G:H5'	2.46	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.46
30:0:1878:G:O2'	30:0:1879:U:OP2	2.33	0.46
30:0:561:G:O2'	30:0:562:A:H5'	2.15	0.46
27:1:16:HIS:HE1	30:0:775:G:OP1	1.97	0.46
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.50	0.46
30:0:134:U:C2	30:0:145:A:C2	3.04	0.46
8:H:48:VAL:HA	8:H:170:ARG:O	2.15	0.46
30:0:17:G:H2'	30:0:18:C:C6	2.51	0.46
30:0:2812:A:N7	38:0:7508:HOH:O	2.36	0.46
30:0:2537:G:H5''	30:0:2538:A:H5''	1.98	0.46
31:9:3:A:H2	31:9:21:G:N3	2.14	0.46
30:0:1526:A:H4'	30:0:1527:A:C5'	2.45	0.46
30:0:241:A:C2	30:0:378:A:H4'	2.51	0.46
26:Z:41:ARG:HH12	30:0:821:U:H4'	1.81	0.46
31:9:47:A:C2	31:9:48:C:C2	3.04	0.46
2:B:85:ARG:NH1	38:B:9106:HOH:O	2.47	0.46
2:B:232:TRP:CZ3	30:0:2614:C:H5''	2.51	0.46
30:0:1845:A:C2'	30:0:1846:U:H5'	2.45	0.46
30:0:1894:C:N4	30:0:1939:U:H2'	2.30	0.46
30:0:1764:C:O2'	30:0:1765:G:H5'	2.15	0.46
13:M:47:ASP:CG	13:M:48:LYS:N	2.70	0.46
29:3:30:GLN:HB3	38:3:9051:HOH:O	2.16	0.46
30:0:1871:U:O4'	30:0:1873:G:C8	2.69	0.46
12:L:34:GLY:HA2	38:L:9017:HOH:O	2.16	0.46
19:S:43:GLU:HB3	38:S:7106:HOH:O	2.16	0.46
30:0:545:G:C8	30:0:545:G:C5'	2.88	0.46
30:0:1132:A:H61	30:0:1229:C:H2'	1.80	0.46
30:0:1634:G:C4	30:0:1635:U:C5	3.03	0.46
30:0:1294:A:H2'	30:0:1295:G:O4'	2.16	0.46
30:0:594:C:C2'	30:0:595:U:H5'	2.46	0.46
14:N:22:GLN:HG3	30:0:2415:A:C2	2.51	0.46
20:T:16:LEU:HB2	30:0:100:C:H4'	1.98	0.46
3:C:43:LYS:HG2	30:0:449:A:N7	2.31	0.46
30:0:1021:G:O2'	30:0:1022:A:H5'	2.16	0.46
1:A:230:SER:HB2	30:0:1852:A:H4'	1.97	0.46
30:0:2624:A:H1'	38:0:9764:HOH:O	2.14	0.46
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.97	0.46
30:0:1346:U:H2'	30:0:1347:U:C6	2.50	0.46
30:0:1166:A:C6	30:0:1181:A:C2	3.04	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1588:G:C6	30:0:1589:G:N1	2.84	0.46
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.46
30:0:483:C:C4	30:0:484:A:C6	3.04	0.46
38:C:8575:HOH:O	20:T:2:LYS:HE2	2.15	0.46
30:0:603:A:H4'	30:0:604:G:O5'	2.15	0.46
30:0:2488:A:H1'	38:0:9096:HOH:O	2.16	0.46
30:0:2017:U:O2'	30:0:2018:A:C8	2.66	0.46
31:9:65:A:C2'	31:9:66:G:OP2	2.64	0.46
30:0:2276:U:H2'	30:0:2277:U:C6	2.51	0.46
30:0:1012:A:O5'	30:0:1012:A:H8	1.99	0.46
13:M:169:ARG:HD2	38:M:8885:HOH:O	2.16	0.46
30:0:1615:A:H4'	38:0:5868:HOH:O	2.16	0.46
30:0:1615:A:H5'	38:0:4181:HOH:O	2.15	0.46
30:0:1119:G:C5	30:0:1243:C:C4	3.04	0.45
30:0:1890:U:H4'	30:0:2010:A:C6	2.51	0.45
30:0:255:A:C4	30:0:256:C:C5	3.05	0.45
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.98	0.45
30:0:1520:G:C6	30:0:1521:C:C4	3.05	0.45
30:0:1756:G:H1'	38:0:6244:HOH:O	2.15	0.45
30:0:71:G:H8	38:0:3908:HOH:O	1.98	0.45
30:0:1409:G:C2	30:0:1410:G:C8	3.04	0.45
30:0:1052:G:H2'	30:0:1052:G:N3	2.31	0.45
30:0:2740:G:H2'	30:0:2741:A:O4'	2.15	0.45
30:0:1029:U:O2'	30:0:1273:C:OP1	2.31	0.45
14:N:37:ARG:NH1	31:9:6:C:OP1	2.48	0.45
30:0:2717:C:C2'	30:0:2718:C:C5'	2.84	0.45
30:0:1625:U:H4'	38:0:4661:HOH:O	2.15	0.45
30:0:293:A:C5	30:0:360:A:C2	3.04	0.45
30:0:810:G:H2'	30:0:811:C:H6	1.81	0.45
30:0:1768:C:H2'	30:0:1769:C:O4'	2.16	0.45
30:0:2057:U:O5'	30:0:2057:U:H6	1.98	0.45
28:2:28:LYS:O	30:0:87:C:H2'	2.17	0.45
30:0:633:C:O2'	30:0:634:G:H5'	2.15	0.45
31:9:28:U:O2	31:9:57:A:N6	2.50	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.04	0.45
27:1:11:LYS:HG2	30:0:777:U:O2'	2.17	0.45
30:0:612:U:H2'	30:0:613:C:C6	2.52	0.45
30:0:1902:G:O2'	30:0:1903:U:H5'	2.16	0.45
30:0:1131:G:C6	30:0:1230:A:C4	3.04	0.45
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.65	0.45
29:3:70:ARG:NH2	29:3:77:ALA:HB3	2.31	0.45
30:0:1882:C:H2'	30:0:1883:U:C6	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1310:U:C2'	30:0:1311:G:O5'	2.64	0.45
30:0:1856:C:H1'	38:0:5858:HOH:O	2.17	0.45
30:0:2298:C:O2'	30:0:2299:G:H5'	2.17	0.45
30:0:1730:G:H4'	30:0:1731:C:H6	1.82	0.45
30:0:2438:G:H2'	30:0:2439:C:H6	1.81	0.45
26:Z:34:SER:HA	30:0:797:A:C4'	2.46	0.45
30:0:670:G:H2'	30:0:671:A:C8	2.51	0.45
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.99	0.45
30:0:1342:C:H2'	30:0:1343:C:H5'	1.99	0.45
13:M:88:VAL:HG13	38:M:8902:HOH:O	2.16	0.45
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.98	0.45
18:R:128:ARG:NH2	30:0:2054:A:C2	2.84	0.45
12:L:142:LEU:HG	12:L:146:GLY:HA3	1.99	0.45
2:B:275:GLY:O	2:B:291:ASP:HA	2.16	0.45
14:N:40:ASN:HD22	31:9:28:U:H5''	1.82	0.45
30:0:1187:U:C2	30:0:1189:A:OP2	2.70	0.45
3:C:236:THR:CG2	3:C:239:ALA:H	2.17	0.45
30:0:169:A:HO2'	30:0:170:U:H6	1.63	0.45
11:K:115:ARG:HG3	11:K:116:GLU:N	2.32	0.45
30:0:2032:U:C2'	30:0:2033:G:H5''	2.46	0.45
30:0:1758:U:O2'	30:0:1759:A:H5'	2.15	0.45
30:0:1540:G:C4	30:0:1541:G:C8	3.05	0.45
30:0:2315:C:H4'	30:0:2425:A:C6	2.51	0.45
29:3:9:THR:HG23	29:3:20:HIS:ND1	2.32	0.45
30:0:1613:C:H2'	30:0:1614:G:O4'	2.15	0.45
30:0:1603:A:H5''	30:0:1605:G:C5'	2.39	0.45
30:0:2505:G:H3'	38:0:5626:HOH:O	2.17	0.45
30:0:1278:A:H4'	30:0:1279:U:C5	2.49	0.45
30:0:2591:C:H2'	30:0:2592:G:O4'	2.16	0.45
30:0:2104:C:O2	30:0:2485:A:N1	2.49	0.45
30:0:1016:U:H2'	30:0:1017:U:O4'	2.17	0.45
8:H:170:ARG:HD2	38:H:8987:HOH:O	2.15	0.45
8:H:123:ILE:HD12	8:H:123:ILE:N	2.32	0.45
10:J:42:GLU:HG2	10:J:43:ARG:HG3	1.98	0.45
25:Y:142:SER:HB2	38:Y:8903:HOH:O	2.16	0.45
15:O:87:THR:O	15:O:91:GLN:HG3	2.17	0.45
8:H:165:ARG:HD2	38:H:9029:HOH:O	2.16	0.45
21:U:14:GLU:O	21:U:17:THR:HB	2.16	0.45
30:0:1535:G:H2'	30:0:1536:C:C6	2.52	0.45
12:L:75:LEU:HD21	38:O:7543:HOH:O	2.17	0.45
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.52	0.45
30:0:2321:A:C4	30:0:2323:G:C8	3.05	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.47	0.45
2:B:254:GLN:HG2	2:B:255:GLY:N	2.31	0.45
21:U:6:CYS:SG	21:U:13:ILE:HB	2.57	0.45
30:0:212:A:O4'	30:0:214:U:C6	2.70	0.45
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.45
30:0:352:A:H2'	30:0:353:G:H8	1.79	0.45
30:0:2778:A:C2	30:0:2797:C:O2	2.70	0.45
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.50	0.45
31:9:26:C:H5''	38:9:9049:HOH:O	2.17	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45
1:A:47:HIS:HD2	30:0:1654:U:C2'	2.30	0.45
30:0:921:G:H4'	30:0:924:G:C6	2.52	0.45
30:0:727:G:C2	30:0:728:C:C2	3.05	0.45
30:0:1346:U:H2'	30:0:1347:U:H6	1.82	0.45
30:0:644:G:H1'	38:0:6390:HOH:O	2.16	0.45
30:0:2679:G:H2'	30:0:2681:A:OP2	2.17	0.45
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.99	0.45
30:0:213:G:N2	30:0:225:G:H2'	2.31	0.45
30:0:867:A:H2	30:0:880:C:O2	2.00	0.45
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.47	0.45
30:0:2071:C:H5'	38:0:9532:HOH:O	2.17	0.45
30:0:226:A:H1'	30:0:393:G:C5	2.51	0.45
30:0:1151:G:H2'	38:0:5008:HOH:O	2.17	0.45
23:W:129:LYS:HE2	30:0:1098:A:O3'	2.17	0.45
14:N:110:THR:HB	14:N:113:SER:OG	2.17	0.45
3:C:170:ASP:OD2	30:0:330:C:H5	2.00	0.45
13:M:68:ARG:HD3	13:M:68:ARG:C	2.37	0.45
3:C:27:ARG:CG	3:C:27:ARG:HH11	2.15	0.45
30:0:282:C:H2'	30:0:283:U:O4'	2.16	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.45
30:0:559:U:H2'	30:0:560:U:O4'	2.17	0.45
4:D:154:LYS:HD2	4:D:154:LYS:N	2.22	0.45
30:0:2691:A:H5'	30:0:2693:U:H1'	1.99	0.45
12:L:136:ALA:HB3	38:L:9035:HOH:O	2.17	0.45
30:0:2650:U:O2'	30:0:2651:C:H5'	2.16	0.45
30:0:941:G:C6	30:0:942:U:C4	3.05	0.45
30:0:2596:A:H2	35:0:8812:CL:CL	2.37	0.45
30:0:113:A:H3'	30:0:114:A:H5''	1.98	0.45
2:B:252:PRO:HD2	30:0:2548:C:H5'	1.99	0.45
30:0:1755:A:H2'	30:0:1756:G:O4'	2.16	0.45
30:0:2735:U:H2'	30:0:2736:U:C6	2.52	0.45
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.17	0.45
31:9:82:U:H2'	31:9:83:G:C8	2.52	0.45
30:0:2010:A:C2'	38:0:5942:HOH:O	2.51	0.45
30:0:2252:A:C5	30:0:2253:G:H1'	2.51	0.45
30:0:1878:G:O2'	30:0:1879:U:P	2.74	0.45
2:B:5:ARG:HD2	2:B:8:LYS:HE2	1.99	0.45
3:C:39:GLN:O	3:C:43:LYS:HD3	2.17	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.32	0.45
1:A:76:VAL:HG23	26:Z:87:LYS:O	2.17	0.45
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.51	0.45
30:0:792:G:O2'	30:0:793:A:H5'	2.16	0.45
30:0:1249:U:H2'	30:0:1250:C:H6	1.82	0.45
30:0:1209:C:C2	30:0:1210:G:C8	3.04	0.44
28:2:41:HIS:H	28:2:45:ASN:ND2	2.04	0.44
30:0:797:A:N6	30:0:816:G:H1'	2.32	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.65	0.44
30:0:1268:C:O2'	30:0:1269:G:H5'	2.16	0.44
30:0:2335:C:H2'	30:0:2336:G:H8	1.80	0.44
30:0:2301:A:H5''	30:0:2302:A:H5'	1.99	0.44
30:0:699:C:C2	30:0:744:G:N2	2.85	0.44
18:R:114:VAL:HG13	18:R:114:VAL:O	2.18	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
15:O:98:LEU:O	15:O:102:ILE:HG13	2.17	0.44
30:0:65:C:O2'	30:0:66:G:H5'	2.16	0.44
30:0:152:A:H2'	30:0:153:C:C6	2.52	0.44
13:M:72:ALA:C	13:M:74:LYS:H	2.20	0.44
16:P:68:LYS:HE2	30:0:1787:C:OP1	2.16	0.44
30:0:2837:U:H2'	38:0:6825:HOH:O	2.15	0.44
30:0:365:G:C5	30:0:366:U:C4	3.05	0.44
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.99	0.44
31:9:1:U:O3'	31:9:3:A:H5''	2.16	0.44
30:0:2250:G:C2	30:0:2251:G:H1'	2.52	0.44
1:A:51:ARG:C	1:A:53:ALA:H	2.20	0.44
30:0:1310:U:H2'	30:0:1311:G:O5'	2.17	0.44
30:0:1949:G:N2	30:0:1964:U:H1'	2.32	0.44
30:0:598:C:H2'	30:0:599:G:C8	2.51	0.44
30:0:2074:A:H1'	38:0:9875:HOH:O	2.16	0.44
30:0:2734:G:O2'	30:0:2735:U:H5'	2.17	0.44
1:A:206:ARG:HH21	30:0:2629:C:N4	2.16	0.44
30:0:2493:C:O2	30:0:2493:C:H2'	2.17	0.44
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.52	0.44
21:U:42:LEU:O	30:0:1810:C:H5'	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.81	0.44
30:0:1206:U:C3'	30:0:1206:U:C6	3.01	0.44
30:0:1279:U:C5'	30:0:1280:A:OP2	2.65	0.44
23:W:24:LEU:O	23:W:26:ILE:HG22	2.18	0.44
30:0:2004:U:H2'	30:0:2005:G:OP1	2.17	0.44
30:0:307:G:C2	30:0:309:C:C4	3.05	0.44
14:N:11:ARG:HG3	14:N:14:ARG:HH12	1.82	0.44
30:0:734:U:H2'	30:0:736:A:OP2	2.17	0.44
7:G:64:ASN:N	7:G:64:ASN:ND2	2.65	0.44
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.44
30:0:1461:U:H2'	30:0:1462:C:H6	1.83	0.44
30:0:1735:C:O2'	30:0:1736:A:H5'	2.17	0.44
26:Z:65:ASN:HB2	26:Z:84:CYS:SG	2.58	0.44
38:B:9136:HOH:O	21:U:17:THR:HG21	2.16	0.44
30:0:2777:G:O2'	30:0:2778:A:H5'	2.17	0.44
30:0:40:C:O5'	30:0:40:C:H6	2.01	0.44
30:0:2410:G:O2'	30:0:2411:C:H5'	2.18	0.44
5:E:3:VAL:HG22	5:E:49:ILE:HB	2.00	0.44
30:0:970:U:H2'	38:0:6313:HOH:O	2.16	0.44
30:0:2642:G:H2'	30:0:2643:G:O4'	2.16	0.44
13:M:73:ARG:NH2	30:0:2263:G:H5''	2.32	0.44
30:0:161:A:H2'	30:0:162:C:C6	2.52	0.44
20:T:71:VAL:HG12	20:T:72:ILE:N	2.32	0.44
30:0:664:U:O4	30:0:681:G:H5''	2.16	0.44
4:D:154:LYS:H	4:D:154:LYS:CD	2.24	0.44
4:D:22:VAL:HA	4:D:73:VAL:O	2.17	0.44
30:0:1928:C:O2'	30:0:1929:G:H5'	2.17	0.44
30:0:711:G:C2	30:0:718:C:O2	2.70	0.44
3:C:226:GLY:HA3	30:0:1308:A:C4'	2.48	0.44
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.98	0.44
30:0:2755:G:H1'	38:0:4677:HOH:O	2.17	0.44
30:0:2663:U:N3	30:0:2664:A:N6	2.65	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	1.98	0.44
3:C:162:VAL:CG2	3:C:232:LEU:HD21	2.47	0.44
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.44
31:9:82:U:H2'	31:9:83:G:H8	1.82	0.44
30:0:2245:C:H6	30:0:2245:C:O5'	2.00	0.44
1:A:11:ARG:HD3	38:0:9221:HOH:O	2.17	0.44
30:0:1076:G:C2	30:0:1084:C:C2	3.06	0.44
5:E:95:VAL:HG11	5:E:131:LEU:HD11	1.99	0.44
20:T:23:VAL:HG23	20:T:41:ARG:HG3	2.00	0.44
18:R:125:ARG:HG2	38:R:8942:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:159:PRO:O	4:D:163:VAL:HG23	2.17	0.44
30:0:1116:U:C2'	30:0:1118:A:H2	2.28	0.44
1:A:46:GLU:C	26:Z:78:ILE:HD11	2.38	0.44
30:0:2887:G:H2'	30:0:2888:U:H6	1.79	0.44
12:L:129:ALA:O	12:L:133:VAL:HG23	2.17	0.44
10:J:63:ILE:CD1	30:0:1236:A:C8	3.01	0.44
19:S:57:THR:CG2	19:S:58:MET:N	2.79	0.44
30:0:549:A:C2	30:0:550:C:C2	3.06	0.44
30:0:2325:U:O2'	30:0:2411:C:H1'	2.18	0.44
21:U:7:ASP:HB2	21:U:29:THR:HG23	2.00	0.44
30:0:737:A:H2'	30:0:738:G:O4'	2.18	0.44
30:0:2119:C:O2'	30:0:2120:U:H5'	2.18	0.44
9:I:114:TYR:N	9:I:114:TYR:CD1	2.86	0.44
14:N:93:GLN:HA	14:N:93:GLN:HE21	1.82	0.44
13:M:97:ILE:HD13	13:M:127:LYS:HD2	2.00	0.44
3:C:37:ALA:HA	3:C:100:LEU:HD12	2.00	0.44
30:0:1028:U:H1'	38:0:3631:HOH:O	2.18	0.44
16:P:18:LYS:O	16:P:21:VAL:HG13	2.18	0.44
15:O:49:GLU:OE1	15:O:72:LYS:HG3	2.17	0.44
30:0:81:G:N3	30:0:98:A:C2	2.85	0.44
30:0:1067:A:H5'	38:0:4344:HOH:O	2.18	0.44
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.18	0.44
30:0:2313:C:H4'	38:0:6558:HOH:O	2.18	0.44
13:M:171:ARG:NH2	30:0:189:A:OP1	2.50	0.44
30:0:1597:A:C4	30:0:1598:A:C8	3.05	0.44
30:0:1014:A:H2'	30:0:1015:C:H5'	1.99	0.44
27:1:1:THR:O	30:0:1836:A:H1'	2.17	0.44
30:0:912:A:C4	30:0:1294:A:C2	3.05	0.44
30:0:1883:U:C2'	30:0:1884:G:H5'	2.48	0.44
30:0:615:G:H2'	30:0:616:U:H6	1.83	0.44
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.49	0.44
30:0:1249:U:H2'	30:0:1250:C:C6	2.53	0.44
30:0:462:A:H2'	38:0:4875:HOH:O	2.18	0.44
25:Y:116:LEU:HA	25:Y:116:LEU:HD23	1.80	0.44
4:D:56:ARG:NH2	30:0:2332:A:H5'	2.32	0.44
17:Q:3:SER:O	17:Q:8:GLU:HG3	2.18	0.44
12:L:149:ARG:O	12:L:150:GLN:HB2	2.17	0.44
29:3:62:THR:HG21	30:0:2317:C:H5'	1.98	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.18	0.44
30:0:725:C:H2'	30:0:726:C:O5'	2.18	0.44
30:0:1246:A:C4	30:0:1248:A:C8	3.06	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.96	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:368:C:C2'	30:0:369:G:H5'	2.48	0.44
30:0:2457:U:O2'	30:0:2458:U:H5'	2.17	0.44
30:0:2793:A:H2'	30:0:2794:G:H5'	2.00	0.44
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.33	0.44
23:W:122:ARG:NH2	23:W:154:ARG:HG2	2.33	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.50	0.44
30:0:1773:G:C2'	30:0:1774:G:H5'	2.48	0.44
30:0:2276:U:O2'	30:0:2277:U:H5'	2.18	0.44
30:0:1307:A:H2'	30:0:1308:A:C8	2.53	0.44
30:0:1730:G:H4'	30:0:1731:C:C6	2.52	0.44
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.53	0.44
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.48	0.44
15:O:21:SER:OG	15:O:106:PRO:HB2	2.18	0.44
2:B:119:HIS:O	2:B:121:PRO:HD3	2.18	0.44
30:0:2128:G:C5	30:0:2129:U:C5	3.06	0.44
30:0:2105:C:H2'	30:0:2106:C:C6	2.53	0.44
3:C:27:ARG:HD2	38:O:327:HOH:O	2.17	0.44
30:0:559:U:C3'	30:0:559:U:C6	3.01	0.44
14:N:147:ILE:HD11	31:9:50:G:OP1	2.18	0.44
13:M:95:LYS:HE2	30:0:157:G:H4'	1.99	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.48	0.44
30:0:416:G:H2'	38:0:9910:HOH:O	2.16	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.53	0.44
8:H:157:TYR:HD1	8:H:157:TYR:C	2.21	0.44
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.06	0.44
30:0:1657:A:H2'	30:0:1658:A:C8	2.53	0.44
1:A:26:ASP:OD2	30:0:1872:C:H4'	2.18	0.44
17:Q:62:THR:O	17:Q:64:GLU:HG2	2.18	0.44
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.57	0.44
30:0:1254:C:O2'	30:0:1255:A:H5'	2.18	0.44
30:0:2473:U:O2'	30:0:2474:A:H5''	2.18	0.44
30:0:1198:U:C6	30:0:1200:A:OP2	2.71	0.43
30:0:1592:G:H1'	30:0:1593:C:C6	2.53	0.43
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.42	0.43
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.00	0.43
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.17	0.43
20:T:48:VAL:CG1	20:T:49:GLU:N	2.81	0.43
30:0:2256:G:C2'	30:0:2257:G:H5'	2.48	0.43
30:0:590:A:H2'	30:0:591:A:O4'	2.18	0.43
30:0:297:U:H2'	30:0:298:C:H6	1.83	0.43
4:D:59:GLY:HA3	38:D:4886:HOH:O	2.17	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:117:GLU:HB3	38:L:9018:HOH:O	2.18	0.43
30:0:1973:A:H2'	30:0:1974:G:O4'	2.17	0.43
30:0:1477:C:O2'	30:0:1478:U:H5'	2.17	0.43
2:B:223:ARG:HG3	2:B:232:TRP:O	2.17	0.43
31:9:64:C:O2'	31:9:65:A:H5'	2.18	0.43
5:E:111:LYS:HE3	30:0:2690:U:H4'	1.99	0.43
12:L:41:HIS:CD2	30:0:926:A:O2'	2.71	0.43
2:B:41:PHE:HB3	2:B:190:MET:HE2	2.00	0.43
30:0:596:C:H2'	30:0:597:A:C8	2.53	0.43
20:T:38:ARG:HG3	20:T:38:ARG:HH11	1.83	0.43
30:0:549:A:C6	30:0:550:C:C4	3.07	0.43
2:B:305:ASP:O	2:B:306:LYS:CB	2.66	0.43
17:Q:1:PRO:HA	30:0:2299:G:O6	2.18	0.43
1:A:182:ARG:HH11	1:A:182:ARG:HG2	1.83	0.43
3:C:118:THR:O	3:C:136:VAL:HG13	2.18	0.43
4:D:45:THR:HB	4:D:75:LEU:HD21	1.99	0.43
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.52	0.43
19:S:50:GLU:HB3	19:S:67:ARG:NH2	2.33	0.43
16:P:10:ALA:HA	16:P:13:VAL:HG12	2.01	0.43
1:A:211:LYS:HB2	38:A:9038:HOH:O	2.18	0.43
30:0:2321:A:N1	30:0:2378:U:O2	2.52	0.43
30:0:1702:U:H5''	38:0:7207:HOH:O	2.19	0.43
14:N:67:ALA:CA	14:N:71:TRP:HB3	2.44	0.43
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.00	0.43
20:T:48:VAL:HG11	20:T:96:VAL:CG1	2.46	0.43
30:0:1362:U:H5'	38:0:3253:HOH:O	2.18	0.43
30:0:107:U:C2'	30:0:108:U:H5'	2.48	0.43
25:Y:144:ARG:NH1	38:Y:8882:HOH:O	2.51	0.43
25:Y:148:GLY:HA3	30:0:622:G:P	2.59	0.43
30:0:1183:C:H41	30:0:1192:A:P	2.42	0.43
22:V:50:ARG:HH12	30:0:56:G:C5'	2.30	0.43
2:B:42:ALA:CB	2:B:162:MET:HE3	2.48	0.43
30:0:1878:G:O2'	30:0:1879:U:C6	2.60	0.43
2:B:199:TYR:HE1	2:B:319:ASP:HB2	1.83	0.43
30:0:853:C:H2'	30:0:854:G:O4'	2.17	0.43
30:0:920:C:H5''	30:0:921:G:O5'	2.18	0.43
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.17	0.43
8:H:157:TYR:CD1	8:H:157:TYR:C	2.90	0.43
30:0:2474:A:H4'	30:0:2475:C:O5'	2.18	0.43
30:0:275:G:N2	30:0:376:C:C2	2.87	0.43
30:0:496:G:H3'	38:0:7658:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:Z:94:LYS:HA	38:Z:8719:HOH:O	2.18	0.43
14:N:154:LEU:C	14:N:156:GLU:H	2.20	0.43
30:0:2834:G:H2'	30:0:2835:C:O5'	2.18	0.43
30:0:2355:G:H5''	30:0:2356:A:OP2	2.19	0.43
30:0:1809:G:H2'	30:0:1811:A:OP2	2.19	0.43
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.99	0.43
23:W:118:LEU:HD12	23:W:153:MET:HE3	2.00	0.43
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.52	0.43
30:0:40:C:H4'	38:0:6993:HOH:O	2.18	0.43
29:3:39:GLN:HG2	29:3:43:ASN:OD1	2.19	0.43
30:0:1185:U:H2'	30:0:1186:C:C6	2.54	0.43
30:0:2718:C:H5'	30:0:2718:C:C6	2.52	0.43
30:0:557:C:O2'	30:0:558:C:H5'	2.19	0.43
30:0:2102:G:N2	30:0:2104:C:N3	2.67	0.43
10:J:19:MET:HE2	10:J:79:PHE:HA	2.01	0.43
30:0:2346:C:O5'	30:0:2346:C:C6	2.72	0.43
30:0:2039:A:H2'	30:0:2040:C:C6	2.53	0.43
22:V:49:LEU:O	22:V:53:ILE:HG13	2.18	0.43
14:N:86:LEU:O	14:N:90:LEU:HG	2.19	0.43
6:F:14:ASP:O	6:F:18:GLU:HG3	2.18	0.43
30:0:1471:A:H2'	30:0:1472:C:C6	2.54	0.43
13:M:49:ALA:C	13:M:54:TYR:HB3	2.38	0.43
20:T:43:ASN:C	20:T:45:GLY:H	2.22	0.43
30:0:1173:A:H4'	30:0:1174:A:H8	1.83	0.43
30:0:878:G:H4'	30:0:1835:U:H4'	2.00	0.43
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.48	0.43
30:0:2103:A:N3	30:0:2103:A:H2'	2.33	0.43
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.51	0.43
11:K:66:ARG:NH2	30:0:1994:A:OP1	2.52	0.43
30:0:1773:G:H4'	38:0:3505:HOH:O	2.19	0.43
10:J:107:ASN:HD22	10:J:107:ASN:C	2.22	0.43
1:A:217:ARG:HG2	1:A:229:ALA:CB	2.48	0.43
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.52	0.43
30:0:2564:G:OP2	30:0:2565:C:H5''	2.18	0.43
30:0:750:A:H2'	30:0:751:U:C6	2.54	0.43
1:A:51:ARG:HH21	1:A:53:ALA:HB3	1.82	0.43
31:9:45:A:N7	31:9:46:C:C5	2.87	0.43
30:0:1566:C:H2'	30:0:1567:G:C8	2.54	0.43
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	1.99	0.43
28:2:20:ARG:NH1	28:2:39:ARG:HH21	2.17	0.43
20:T:82:THR:HG21	30:0:488:U:O2'	2.19	0.43
30:0:1427:A:C2'	30:0:1428:C:H5'	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2379:G:N3	30:0:2418:G:H2'	2.34	0.43
30:0:328:U:C2	30:0:348:C:H4'	2.53	0.43
30:0:459:A:H4'	38:0:9455:HOH:O	2.17	0.43
14:N:109:PRO:HB3	30:0:2413:A:N7	2.34	0.43
14:N:49:THR:HG22	14:N:56:ASP:CB	2.49	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.17	0.43
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.84	0.43
31:9:110:G:C5	31:9:111:U:C5	3.07	0.43
31:9:110:G:C2	31:9:111:U:C6	3.07	0.43
1:A:192:VAL:O	1:A:207:GLN:HG2	2.18	0.43
30:0:119:A:H2'	30:0:120:A:C5'	2.49	0.43
30:0:2681:A:H4'	30:0:2682:C:OP1	2.19	0.43
26:Z:95:PRO:HD2	38:Z:8719:HOH:O	2.18	0.43
30:0:2694:A:H3'	30:0:2695:C:H6	1.84	0.43
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.83	0.43
38:M:8865:HOH:O	30:0:2244:A:H1'	2.18	0.43
3:C:132:ASP:O	3:C:133:ARG:HG3	2.19	0.43
18:R:59:PHE:O	18:R:63:ASN:HB3	2.18	0.43
30:0:361:C:H2'	30:0:362:G:O4'	2.19	0.43
30:0:1592:G:HO2'	30:0:1593:C:H6	1.67	0.43
30:0:2523:U:H2'	30:0:2524:G:O4'	2.18	0.43
30:0:2487:C:C5	38:0:4880:HOH:O	2.57	0.43
30:0:636:G:H5'	30:0:2059:U:OP2	2.19	0.43
30:0:1937:U:O2'	30:0:1938:G:H5'	2.18	0.43
26:Z:40:ALA:O	30:0:2018:A:H2	2.02	0.43
2:B:116:PRO:HG3	30:0:2821:C:H4'	2.01	0.43
30:0:920:C:C5	30:0:2467:A:OP1	2.72	0.43
2:B:215:VAL:HB	38:B:9090:HOH:O	2.19	0.43
30:0:2581:U:H1'	38:0:4466:HOH:O	2.17	0.43
26:Z:88:PHE:N	26:Z:88:PHE:CD2	2.86	0.43
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.19	0.43
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.34	0.43
30:0:1156:C:O2'	30:0:1157:C:H5'	2.19	0.43
9:I:69:PRO:HA	30:0:1164:U:OP1	2.19	0.43
30:0:802:G:H2'	30:0:803:C:C6	2.54	0.43
30:0:1099:G:H2'	30:0:1100:G:O4'	2.19	0.43
30:0:236:A:H8	30:0:236:A:OP1	2.02	0.43
30:0:1923:G:H2'	30:0:1924:A:H8	1.83	0.43
30:0:308:U:C4	30:0:342:C:C1'	3.01	0.43
31:9:3:A:N6	31:9:22:G:H1'	2.34	0.43
30:0:2252:A:H2'	30:0:2253:G:O4'	2.19	0.43
23:W:122:ARG:NH2	38:0:5280:HOH:O	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.52	0.43
1:A:48:ASP:HB3	1:A:51:ARG:HG3	2.00	0.43
30:0:1758:U:H2'	30:0:1759:A:O4'	2.19	0.43
30:0:301:C:H2'	30:0:302:A:C8	2.54	0.43
30:0:1561:U:C5'	38:0:7421:HOH:O	2.67	0.43
1:A:230:SER:CB	30:0:1852:A:H4'	2.49	0.43
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.86	0.43
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.84	0.43
16:P:58:SER:HB3	38:0:5616:HOH:O	2.18	0.43
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.43
16:P:129:GLY:HA2	38:P:153:HOH:O	2.18	0.43
4:D:136:ARG:HA	4:D:137:PRO:HD3	1.84	0.43
29:3:13:HIS:HD2	29:3:76:LYS:HB3	1.83	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.53	0.43
30:0:2070:G:H2'	30:0:2072:G:OP1	2.19	0.42
10:J:131:THR:HG22	10:J:133:GLY:N	2.34	0.42
30:0:1552:G:C6	30:0:1634:G:C6	3.07	0.42
30:0:612:U:H2'	30:0:613:C:H6	1.84	0.42
30:0:290:C:C2'	30:0:291:C:H5'	2.49	0.42
31:9:65:A:N6	31:9:112:U:C6	2.86	0.42
30:0:2499:U:H1'	38:0:9433:HOH:O	2.19	0.42
30:0:1882:C:O2'	30:0:2012:U:OP2	2.32	0.42
30:0:1748:U:C5	30:0:1749:U:C4	3.07	0.42
30:0:2587:OMU:H2'	30:0:2589:U:H5''	2.01	0.42
30:0:1095:U:H2'	30:0:1096:U:O4'	2.18	0.42
12:L:150:GLN:HB3	38:L:9032:HOH:O	2.18	0.42
12:L:117:GLU:HG3	12:L:117:GLU:O	2.19	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.34	0.42
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.19	0.42
30:0:412:C:O2'	30:0:413:G:H5'	2.18	0.42
30:0:1562:C:N4	38:0:5849:HOH:O	2.49	0.42
30:0:271:C:C2	30:0:273:G:O4'	2.73	0.42
30:0:706:G:N2	30:0:707:C:H41	2.17	0.42
30:0:696:C:H4'	38:0:7268:HOH:O	2.19	0.42
30:0:2415:A:H2'	30:0:2416:G:H5'	2.01	0.42
30:0:1878:G:H4'	38:0:6104:HOH:O	2.19	0.42
30:0:1878:G:H5''	38:0:5160:HOH:O	2.18	0.42
15:O:105:ASN:HD21	15:O:109:SER:N	2.17	0.42
30:0:2842:G:H2'	30:0:2843:A:C5'	2.48	0.42
1:A:135:VAL:HG22	1:A:136:ALA:N	2.35	0.42
30:0:2061:C:H2'	30:0:2062:A:H5'	1.99	0.42
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:146:ALA:O	5:E:150:GLN:HG2	2.19	0.42
15:O:112:ARG:NH2	30:0:719:C:O2'	2.52	0.42
30:0:1544:U:O2'	30:0:1545:C:H5'	2.19	0.42
30:0:1206:U:C6	30:0:1206:U:H3'	2.55	0.42
2:B:217:ARG:HG3	2:B:257:THR:CG2	2.41	0.42
30:0:128:A:C8	30:0:128:A:C3'	2.99	0.42
13:M:84:LYS:HB2	30:0:170:U:OP1	2.18	0.42
2:B:17:LYS:O	2:B:260:HIS:HD2	2.02	0.42
16:P:105:LEU:HD21	16:P:137:LEU:HD11	2.01	0.42
2:B:62:ARG:HA	2:B:65:MET:HE2	2.01	0.42
30:0:113:A:H3'	30:0:114:A:C5'	2.48	0.42
2:B:8:LYS:HG3	2:B:220:VAL:HG12	2.01	0.42
27:1:25:LYS:HD2	28:2:48:ASP:HA	2.02	0.42
12:L:11:ARG:O	30:0:903:U:C2	2.72	0.42
30:0:1345:A:H2'	30:0:1346:U:C6	2.54	0.42
30:0:2035:C:H6	30:0:2035:C:O5'	2.02	0.42
30:0:276:C:O5'	30:0:276:C:H6	2.02	0.42
30:0:2787:C:H5	38:0:4627:HOH:O	2.02	0.42
30:0:1757:U:H6	30:0:1757:U:O5'	2.03	0.42
30:0:1407:A:O2'	30:0:1408:U:H3'	2.20	0.42
17:Q:2:SER:HA	38:0:6711:HOH:O	2.19	0.42
31:9:75:G:N2	31:9:106:U:O2	2.43	0.42
23:W:142:ASP:HB3	23:W:145:GLY:H	1.83	0.42
1:A:8:ARG:HG2	38:A:8978:HOH:O	2.20	0.42
30:0:1173:A:C2	30:0:1177:A:C8	3.07	0.42
30:0:2709:G:N2	38:0:7613:HOH:O	2.53	0.42
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.73	0.42
30:0:1902:G:C2	30:0:1936:C:C2	3.07	0.42
30:0:2828:G:H8	30:0:2828:G:O5'	2.03	0.42
29:3:3:MET:HA	29:3:4:PRO:HD2	1.86	0.42
30:0:707:C:C2	30:0:708:A:C8	3.07	0.42
30:0:1393:A:N1	30:0:1725:C:O2'	2.44	0.42
30:0:1804:A:H2'	30:0:1805:G:C8	2.53	0.42
18:R:68:HIS:O	30:0:2842:G:H5'	2.19	0.42
4:D:54:ALA:HB2	30:0:2346:C:H5'	2.01	0.42
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.34	0.42
30:0:1585:C:H2'	30:0:1586:G:H8	1.84	0.42
5:E:126:ILE:HA	5:E:131:LEU:HD23	2.00	0.42
13:M:97:ILE:HG21	13:M:127:LYS:HD2	2.01	0.42
12:L:7:GLN:HB3	12:L:13:HIS:CE1	2.54	0.42
4:D:50:VAL:HG13	31:9:41:C:O4'	2.19	0.42
11:K:79:PRO:HB3	11:K:87:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:407:A:H3'	38:0:4452:HOH:O	2.19	0.42
30:0:849:C:H2'	30:0:850:U:O4'	2.20	0.42
2:B:310:ARG:HB3	38:B:9121:HOH:O	2.19	0.42
30:0:1933:G:O2'	30:0:1934:A:H5'	2.19	0.42
30:0:2480:G:O2'	30:0:2481:G:H5'	2.19	0.42
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.42
30:0:727:G:H3'	30:0:728:C:C6	2.54	0.42
23:W:128:VAL:HG22	30:0:1098:A:OP1	2.19	0.42
30:0:1420:C:O2	30:0:1420:C:H2'	2.19	0.42
30:0:420:U:O4'	30:0:1920:C:C4	2.73	0.42
30:0:939:A:N1	30:0:1027:G:O2'	2.45	0.42
16:P:103:THR:O	16:P:107:GLU:HG3	2.19	0.42
30:0:1321:A:H2'	30:0:1322:G:C8	2.55	0.42
10:J:45:VAL:CG2	10:J:129:PHE:HD1	2.32	0.42
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.42
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.34	0.42
19:S:6:LYS:HD3	38:S:2519:HOH:O	2.20	0.42
30:0:1559:A:OP2	30:0:1559:A:C8	2.70	0.42
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.19	0.42
30:0:273:G:H2'	30:0:274:G:O4'	2.20	0.42
2:B:145:HIS:CD2	2:B:146:THR:O	2.63	0.42
30:0:154:C:O2'	30:0:155:C:H5'	2.18	0.42
13:M:188:ARG:NH1	30:0:154:C:H3'	2.35	0.42
30:0:299:U:C2	30:0:300:U:C5	3.08	0.42
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.53	0.42
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.00	0.42
29:3:29:ARG:HG2	29:3:30:GLN:N	2.35	0.42
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.54	0.42
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.85	0.42
30:0:571:C:H6	30:0:571:C:O5'	2.02	0.42
30:0:1006:A:H2'	30:0:1007:A:C8	2.55	0.42
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.77	0.42
30:0:2321:A:C5	30:0:2323:G:C8	3.07	0.42
30:0:2274:A:H2'	30:0:2275:G:C8	2.54	0.42
30:0:1924:A:H1'	38:0:5731:HOH:O	2.19	0.42
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.54	0.42
30:0:1168:C:C5	30:0:1169:U:C4	3.08	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.53	0.42
30:0:1883:U:O2'	30:0:1884:G:H5'	2.19	0.42
30:0:137:U:OP1	30:0:259:G:O2'	2.36	0.42
13:M:46:LEU:HD22	13:M:50:ARG:CD	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1454:U:H5''	30:0:1455:C:OP2	2.19	0.42
30:0:17:G:H2'	30:0:18:C:H6	1.84	0.42
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.02	0.42
13:M:172:GLY:HA2	38:0:9086:HOH:O	2.19	0.42
8:H:117:ARG:HH12	30:0:2287:C:N4	2.17	0.42
30:0:1188:A:C5	30:0:1189:A:N1	2.88	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.02	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.18	0.42
29:3:64:LYS:HB3	29:3:82:GLY:O	2.20	0.42
30:0:2354:A:C2	30:0:2367:A:C8	3.08	0.42
22:V:39:ALA:C	22:V:41:GLU:H	2.22	0.42
30:0:2671:U:C2'	30:0:2672:C:O5'	2.68	0.42
30:0:2673:U:O2'	30:0:2674:G:H5'	2.20	0.42
26:Z:42:TYR:HA	30:0:1829:A:N6	2.35	0.42
30:0:2690:U:C4	30:0:2691:A:C5	3.07	0.42
30:0:918:G:C2	30:0:926:A:C2	3.08	0.42
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.53	0.42
31:9:116:C:O2'	31:9:117:G:H5'	2.20	0.42
13:M:74:LYS:HB3	38:M:8944:HOH:O	2.20	0.42
30:0:1539:U:O2'	30:0:1540:G:H5'	2.20	0.42
2:B:252:PRO:HD3	38:0:9818:HOH:O	2.18	0.42
30:0:644:G:N3	30:0:644:G:H5'	2.35	0.42
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.20	0.42
8:H:151:GLU:HA	8:H:151:GLU:OE1	2.19	0.42
24:X:70:ILE:O	24:X:70:ILE:HG23	2.20	0.42
30:0:1576:G:H2'	30:0:1577:U:C6	2.54	0.42
19:S:8:PRO:HD2	22:V:32:ALA:HA	2.02	0.42
11:K:132:VAL:HG11	21:U:22:VAL:HG22	2.02	0.42
30:0:1815:A:H2'	30:0:1816:C:O4'	2.20	0.42
30:0:1198:U:H2'	30:0:1200:A:OP2	2.20	0.42
30:0:1200:A:H4'	38:0:7330:HOH:O	2.19	0.42
30:0:1474:C:C5'	30:0:1474:C:C6	2.89	0.42
30:0:2458:U:O2'	30:0:2459:G:H5'	2.20	0.42
28:2:43:ARG:HH22	30:0:1684:A:C1'	2.26	0.42
30:0:820:G:O2'	30:0:856:G:H4'	2.20	0.42
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.42
30:0:1573:A:H2'	30:0:1574:C:O4'	2.20	0.42
30:0:710:G:O2'	30:0:711:G:H5'	2.20	0.42
25:Y:160:LYS:HA	25:Y:160:LYS:HD3	1.87	0.42
30:0:151:A:H2'	30:0:152:A:C8	2.55	0.42
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.34	0.42
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.23	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2332:A:H2'	38:0:5623:HOH:O	2.19	0.42
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.34	0.42
10:J:74:ARG:O	10:J:78:ILE:HG12	2.20	0.42
8:H:10:ARG:HD2	8:H:161:THR:HG21	2.01	0.42
13:M:187:LEU:HD22	13:M:194:GLY:HA3	2.01	0.42
30:0:1181:A:N1	30:0:1192:A:O2'	2.45	0.42
30:0:1158:G:H2'	30:0:1159:G:C5'	2.50	0.42
31:9:29:C:C5	31:9:30:C:C6	3.08	0.42
10:J:52:GLN:HE21	30:0:1119:G:H5'	1.84	0.42
30:0:191:A:H2'	30:0:237:G:O6	2.20	0.42
23:W:139:GLY:O	23:W:141:HIS:CD2	2.73	0.42
30:0:364:U:H2'	30:0:365:G:O4'	2.20	0.42
18:R:98:ASN:ND2	30:0:500:G:H21	2.11	0.42
1:A:94:LEU:HD12	1:A:98:GLU:CB	2.47	0.42
20:T:48:VAL:CG1	20:T:96:VAL:HG13	2.50	0.42
30:0:1538:C:O2'	30:0:1539:U:H5'	2.19	0.42
30:0:1585:C:H2'	30:0:1586:G:C8	2.54	0.42
30:0:1794:G:N2	30:0:1796:A:H3'	2.35	0.42
18:R:89:LEU:HA	18:R:89:LEU:HD23	1.82	0.42
24:X:10:VAL:HG11	24:X:36:HIS:HE1	1.85	0.42
30:0:1314:U:H5''	30:0:1316:G:O4'	2.19	0.42
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.48	0.41
26:Z:41:ARG:HD3	38:Z:8717:HOH:O	2.19	0.41
9:I:91:PHE:CD2	9:I:131:GLY:HA2	2.44	0.41
31:9:73:A:N1	31:9:108:C:O2	2.53	0.41
30:0:299:U:H2'	30:0:300:U:H6	1.85	0.41
6:F:54:VAL:HG13	30:0:263:U:C4	2.55	0.41
2:B:49:THR:HG22	2:B:331:SER:HB3	2.02	0.41
30:0:1359:U:C5	30:0:2101:A:H8	2.38	0.41
30:0:1345:A:H2'	30:0:1346:U:H6	1.85	0.41
10:J:42:GLU:HG2	10:J:43:ARG:N	2.34	0.41
1:A:20:SER:HB3	30:0:1872:C:H5	1.85	0.41
30:0:1316:G:H5''	38:0:5311:HOH:O	2.20	0.41
30:0:1734:C:H6	30:0:1734:C:O5'	2.03	0.41
30:0:1135:G:H5'	38:0:5913:HOH:O	2.19	0.41
30:0:1531:U:O2	30:0:1661:A:C2	2.73	0.41
30:0:559:U:C4	30:0:560:U:C4	3.08	0.41
30:0:257:G:N2	30:0:258:G:C4	2.88	0.41
31:9:3:A:C8	31:9:26:C:O2	2.72	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.21	0.41
30:0:820:G:N3	30:0:1831:U:H1'	2.35	0.41
20:T:52:ARG:O	30:0:317:A:OP1	2.37	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:567:U:H5''	38:0:6387:HOH:O	2.19	0.41
30:0:1926:G:C4	30:0:1927:A:C8	3.08	0.41
30:0:1572:A:C2	30:0:1573:A:C4	3.08	0.41
30:0:1333:U:H2'	30:0:1334:C:C6	2.54	0.41
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.36	0.41
30:0:1441:G:H1'	38:0:7755:HOH:O	2.19	0.41
1:A:135:VAL:HG11	1:A:147:ARG:HH21	1.85	0.41
26:Z:65:ASN:ND2	26:Z:84:CYS:SG	2.91	0.41
30:0:1832:G:H5''	38:0:9044:HOH:O	2.19	0.41
30:0:1405:U:H2'	38:0:6827:HOH:O	2.20	0.41
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.45	0.41
30:0:1997:A:C6	30:0:1998:G:C5	3.09	0.41
30:0:34:C:H1'	38:0:9175:HOH:O	2.18	0.41
30:0:1116:U:C2'	30:0:1118:A:C2	3.04	0.41
30:0:282:C:O2'	30:0:283:U:C4'	2.69	0.41
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.40	0.41
28:2:40:ARG:HD2	28:2:47:THR:HG22	2.01	0.41
31:9:39:U:C2'	31:9:40:C:OP1	2.68	0.41
30:0:2909:G:H2'	30:0:2910:A:H8	1.85	0.41
30:0:1168:C:C4	30:0:1169:U:C4	3.08	0.41
30:0:1168:C:C5	30:0:1169:U:C5	3.09	0.41
30:0:818:A:C6	30:0:819:A:C2	3.07	0.41
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.02	0.41
1:A:51:ARG:NH2	1:A:69:LEU:HD11	2.36	0.41
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.01	0.41
30:0:778:C:C4	30:0:779:U:C4	3.08	0.41
31:9:119:C:H2'	31:9:120:A:C8	2.55	0.41
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.56	0.41
30:0:2675:A:H1'	30:0:2813:A:C2	2.56	0.41
14:N:40:ASN:HD21	31:9:28:U:H5''	1.83	0.41
30:0:1246:A:C5	30:0:1248:A:C5	3.09	0.41
30:0:271:C:N4	30:0:378:A:C2	2.76	0.41
30:0:820:G:C5'	30:0:821:U:H5'	2.46	0.41
30:0:2092:G:H5''	30:0:2613:G:OP1	2.21	0.41
30:0:1015:C:C2	30:0:1016:U:C5	3.09	0.41
29:3:69:TYR:CE1	29:3:80:ARG:HB2	2.55	0.41
30:0:1607:A:C4	30:0:1608:G:C8	3.08	0.41
31:9:7:G:C5'	38:9:9099:HOH:O	2.68	0.41
14:N:42:HIS:CB	14:N:62:HIS:HE1	2.33	0.41
30:0:2874:G:H3'	38:0:9578:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:546:C:H6	30:0:546:C:O5'	2.03	0.41
31:9:31:C:O2'	31:9:32:G:H5'	2.20	0.41
30:0:2011:A:H5'	30:0:2013:G:H1'	2.01	0.41
30:0:1183:C:O2	30:0:1183:C:C2'	2.68	0.41
30:0:1545:C:H2'	30:0:1546:G:O4'	2.20	0.41
13:M:68:ARG:CZ	13:M:73:ARG:HD3	2.51	0.41
30:0:1191:A:H3'	30:0:1191:A:H8	1.84	0.41
22:V:12:THR:H	22:V:15:GLU:HB2	1.85	0.41
31:9:1:U:O3'	31:9:3:A:OP1	2.39	0.41
17:Q:21:ARG:HG2	17:Q:22:GLY:H	1.86	0.41
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	2.02	0.41
30:0:293:A:P	30:0:358:G:H22	2.43	0.41
29:3:46:ILE:HA	38:0:7897:HOH:O	2.20	0.41
31:9:112:U:H2'	31:9:113:C:H5'	2.02	0.41
30:0:1335:C:H2'	30:0:1336:U:C6	2.56	0.41
30:0:932:U:H1'	30:0:1296:A:H1'	2.02	0.41
30:0:488:U:H2'	38:0:4003:HOH:O	2.20	0.41
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.20	0.41
31:9:9:C:H2'	31:9:10:C:H5'	2.03	0.41
16:P:3:LEU:HA	16:P:6:GLN:OE1	2.21	0.41
30:0:652:G:H8	38:0:3003:HOH:O	2.03	0.41
9:I:123:VAL:O	9:I:127:CYS:SG	2.78	0.41
30:0:2799:A:N6	30:0:2801:A:C2	2.89	0.41
10:J:116:LEU:HB2	10:J:119:THR:HG21	2.02	0.41
3:C:27:ARG:CG	3:C:27:ARG:NH1	2.79	0.41
13:M:77:HIS:CG	13:M:81:ARG:HB2	2.56	0.41
23:W:24:LEU:HD21	23:W:44:MET:SD	2.61	0.41
30:0:1915:U:H2'	30:0:1916:C:O4'	2.21	0.41
30:0:822:C:C2	30:0:823:U:C5	3.08	0.41
12:L:6:ARG:NH1	30:0:1299:G:N7	2.68	0.41
30:0:69:A:C2'	30:0:70:A:OP2	2.69	0.41
30:0:69:A:H2'	30:0:70:A:OP2	2.20	0.41
30:0:2092:G:H2'	30:0:2613:G:OP1	2.21	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.73	0.41
18:R:17:MET:HE3	18:R:19:ARG:HH21	1.86	0.41
1:A:194:MET:CE	1:A:199:HIS:HB2	2.50	0.41
30:0:1362:U:H2'	30:0:1363:G:C8	2.55	0.41
7:G:71:LEU:C	7:G:73:ASP:H	2.23	0.41
30:0:1563:G:H4'	30:0:1564:C:H5'	2.01	0.41
28:2:2:LYS:HG3	30:0:1486:A:C4	2.55	0.41
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.51	0.41
27:1:16:HIS:CD2	30:0:470:U:O2'	2.72	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.50	0.41
30:0:1427:A:O2'	30:0:1428:C:H5'	2.21	0.41
30:0:1757:U:H5	38:0:3211:HOH:O	2.03	0.41
17:Q:16:ASN:HA	17:Q:16:ASN:HD22	1.67	0.41
14:N:23:ARG:O	14:N:27:LEU:HG	2.21	0.41
29:3:73:GLU:HB3	38:3:9056:HOH:O	2.21	0.41
30:0:2409:C:H5''	38:0:4005:HOH:O	2.20	0.41
30:0:2872:U:C2	30:0:2873:C:C6	3.08	0.41
30:0:396:U:H1'	30:0:397:A:OP1	2.20	0.41
31:9:70:U:H2'	31:9:71:C:O4'	2.20	0.41
23:W:38:THR:HG22	38:W:3580:HOH:O	2.21	0.41
30:0:536:A:N1	30:0:2075:G:O2'	2.50	0.41
30:0:186:A:OP1	30:0:186:A:H4'	2.21	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.55	0.41
30:0:130:C:H2'	38:0:3150:HOH:O	2.21	0.41
30:0:1051:C:H2'	30:0:1052:G:O4'	2.20	0.41
23:W:23:MET:O	30:0:1025:C:H5'	2.21	0.41
16:P:13:VAL:HG13	16:P:14:LEU:N	2.36	0.41
5:E:155:ASN:H	5:E:155:ASN:ND2	2.17	0.41
30:0:2880:A:H2'	30:0:2881:C:H5'	2.02	0.41
30:0:964:G:C4	30:0:965:A:C8	3.08	0.41
4:D:84:LEU:HA	4:D:87:ALA:HB3	2.02	0.41
30:0:1339:G:C6	30:0:1340:G:N1	2.89	0.41
5:E:77:THR:OG1	5:E:78:GLU:N	2.52	0.41
30:0:2780:C:C4	30:0:2781:U:C4	3.09	0.41
30:0:2892:G:C6	30:0:2893:C:C4	3.09	0.41
30:0:397:A:H1'	30:0:417:G:H1'	2.03	0.41
30:0:706:G:O2'	30:0:707:C:H6	2.03	0.41
30:0:1682:A:H5''	38:0:9458:HOH:O	2.20	0.41
3:C:22:PHE:HA	3:C:116:ALA:HA	2.02	0.41
30:0:240:C:O2	30:0:240:C:H2'	2.20	0.41
30:0:73:U:O2'	30:0:74:G:H5'	2.21	0.41
30:0:1215:A:O3'	30:0:1216:G:C4'	2.69	0.41
30:0:1337:G:C6	30:0:1338:U:C4	3.09	0.41
30:0:800:G:H2'	30:0:801:U:C6	2.56	0.41
30:0:1244:U:H4'	30:0:1246:A:O4'	2.21	0.41
30:0:1834:C:H2'	30:0:1840:A:H62	1.82	0.41
1:A:45:ILE:HD12	26:Z:89:THR:HG23	2.02	0.41
30:0:2438:G:C6	30:0:2439:C:C4	3.08	0.41
30:0:2296:C:H2'	30:0:2297:U:C6	2.56	0.41
11:K:75:ARG:HD2	11:K:90:PHE:CD2	2.55	0.41
29:3:88:LEU:HD22	35:3:8804:CL:CL	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1819:G:C2'	30:0:1820:G:H5'	2.50	0.41
30:0:1523:G:C5	30:0:1524:U:C4	3.08	0.41
6:F:57:GLU:O	6:F:61:MET:HG3	2.21	0.41
14:N:48:VAL:HG11	14:N:55:ASP:HB3	2.02	0.41
20:T:32:ARG:NH1	20:T:38:ARG:NH1	2.68	0.41
30:0:99:A:C8	30:0:100:C:C6	3.09	0.41
30:0:2345:A:H3'	30:0:2346:C:C5	2.56	0.41
30:0:37:A:C2	30:0:446:G:C2	3.09	0.41
2:B:27:ASN:HD21	30:0:2807:U:P	2.43	0.41
30:0:1423:C:O2'	30:0:1424:A:H5'	2.20	0.41
31:9:75:G:H1	31:9:106:U:H3	1.69	0.41
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.56	0.41
12:L:53:ARG:HD2	30:0:2441:U:H4'	2.02	0.41
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.73	0.41
30:0:210:U:O2'	30:0:211:U:H5'	2.21	0.41
30:0:565:A:N6	30:0:593:A:C8	2.88	0.41
3:C:44:GLN:HA	38:C:8614:HOH:O	2.21	0.41
2:B:274:GLU:HA	2:B:292:GLY:O	2.21	0.41
26:Z:54:GLU:HB3	38:Z:8731:HOH:O	2.21	0.41
2:B:58:PRO:HA	2:B:63:GLU:CD	2.40	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.82	0.41
3:C:87:ARG:NH2	30:0:894:A:C2	2.89	0.41
30:0:1351:G:H1'	38:0:4673:HOH:O	2.21	0.41
30:0:1193:A:C2	30:0:1194:A:N6	2.89	0.41
30:0:1419:U:H2'	30:0:1685:A:C2	2.56	0.41
4:D:53:LYS:HE3	31:9:40:C:H42	1.85	0.41
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.56	0.41
30:0:407:A:H8	38:0:4452:HOH:O	2.04	0.41
1:A:47:HIS:CD2	30:0:1654:U:C2'	3.02	0.41
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.56	0.41
30:0:39:G:C2	30:0:444:C:N3	2.89	0.41
1:A:191:GLY:HA2	1:A:194:MET:HE2	2.02	0.41
30:0:2064:U:H5'	30:0:2652:U:O3'	2.21	0.41
16:P:81:LYS:HG2	38:0:9540:HOH:O	2.20	0.41
2:B:243:ASN:HA	2:B:244:PRO:C	2.41	0.41
2:B:244:PRO:HG3	2:B:248:ARG:NH2	2.35	0.41
14:N:22:GLN:HG3	30:0:2415:A:H2	1.85	0.41
24:X:43:VAL:HG12	24:X:44:ASP:H	1.84	0.41
1:A:33:GLU:CD	1:A:33:GLU:H	2.24	0.41
30:0:2002:C:C2'	30:0:2003:U:H5'	2.50	0.41
30:0:1769:C:C2'	30:0:1770:U:H5'	2.51	0.41
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:193:LYS:HB3	30:0:392:U:C5'	2.51	0.41
15:O:68:GLY:HA3	30:0:745:G:O6	2.20	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.02	0.41
30:0:685:C:O2	30:0:748:C:H4'	2.21	0.41
30:0:375:G:C4	30:0:411:A:C6	3.09	0.41
27:1:38:GLY:HA3	38:1:6935:HOH:O	2.20	0.41
21:U:20:MET:HG3	21:U:28:THR:HG23	2.03	0.41
31:9:14:G:C8	31:9:14:G:C5'	2.95	0.40
8:H:12:ILE:HG12	8:H:59:GLN:HG3	2.02	0.40
13:M:95:LYS:HA	13:M:170:ASN:HD21	1.86	0.40
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.40
19:S:42:GLU:HG2	19:S:49:VAL:HG23	2.03	0.40
4:D:172:VAL:HG12	4:D:173:GLU:N	2.36	0.40
26:Z:53:ILE:HG23	26:Z:93:TYR:HB3	2.02	0.40
13:M:46:LEU:HD22	13:M:50:ARG:HD2	2.03	0.40
30:0:1008:C:H2'	30:0:1009:U:C6	2.56	0.40
26:Z:65:ASN:HD22	26:Z:84:CYS:CB	2.33	0.40
30:0:1327:G:C6	30:0:1331:G:C6	3.09	0.40
30:0:1656:A:H2'	30:0:1657:A:O4'	2.21	0.40
30:0:375:G:C2	30:0:411:A:C2	3.08	0.40
10:J:47:THR:O	10:J:53:ILE:HD11	2.21	0.40
30:0:1589:G:C2	30:0:1605:G:N3	2.89	0.40
30:0:1543:G:N1	30:0:1641:A:OP2	2.41	0.40
30:0:559:U:H3'	30:0:559:U:C6	2.57	0.40
30:0:1972:U:O2'	30:0:1973:A:H5''	2.22	0.40
10:J:19:MET:HE3	10:J:132:LEU:HD11	2.03	0.40
5:E:139:GLU:OE2	30:0:2781:U:C1'	2.68	0.40
23:W:4:LEU:HD23	23:W:4:LEU:HA	1.88	0.40
30:0:2526:C:H6	30:0:2526:C:H3'	1.86	0.40
30:0:2319:C:H2'	30:0:2320:U:H5'	2.03	0.40
11:K:74:VAL:HG12	11:K:75:ARG:HG3	2.02	0.40
1:A:47:HIS:HA	38:A:9024:HOH:O	2.20	0.40
30:0:1497:G:H4'	30:0:1627:G:O2'	2.21	0.40
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.40
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.56	0.40
30:0:1398:G:H2'	30:0:1399:A:H8	1.85	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.89	0.40
16:P:7:LYS:HD3	16:P:21:VAL:HG22	2.03	0.40
30:0:1576:G:H2'	30:0:1577:U:H6	1.87	0.40
30:0:1577:U:O2'	30:0:1578:C:H5'	2.21	0.40
30:0:1531:U:C2	30:0:1661:A:C2	3.10	0.40
5:E:166:VAL:HB	38:E:6341:HOH:O	2.19	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:19:GLU:O	7:G:23:ILE:HG13	2.21	0.40
30:0:245:C:N4	30:0:246:G:C6	2.89	0.40
17:Q:80:LYS:HG2	17:Q:82:LYS:HE3	2.02	0.40
12:L:73:VAL:HG23	12:L:74:THR:H	1.86	0.40
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.58	0.40
30:0:372:A:H2'	30:0:373:G:H8	1.86	0.40
31:9:2:U:OP2	31:9:2:U:H4'	2.22	0.40
30:0:1926:G:H2'	30:0:1927:A:H8	1.86	0.40
30:0:2867:G:H2'	30:0:2868:C:H6	1.86	0.40
30:0:1749:U:O2	30:0:1751:G:C8	2.75	0.40
30:0:1333:U:H2'	30:0:1334:C:H6	1.86	0.40
13:M:74:LYS:O	13:M:88:VAL:HG22	2.21	0.40
30:0:727:G:N2	30:0:728:C:H1'	2.36	0.40
30:0:1461:U:H1'	38:0:7457:HOH:O	2.21	0.40
13:M:64:ARG:HD2	38:M:8879:HOH:O	2.21	0.40
26:Z:65:ASN:CB	26:Z:84:CYS:SG	3.08	0.40
12:L:117:GLU:HG2	38:L:9025:HOH:O	2.20	0.40
30:0:464:G:HO2'	30:0:465:U:P	2.44	0.40
30:0:611:U:O5'	30:0:611:U:H6	2.05	0.40
9:I:78:ALA:HB1	9:I:93:ALA:CB	2.51	0.40
9:I:120:ALA:O	9:I:124:VAL:HG23	2.21	0.40
10:J:57:TYR:O	10:J:61:VAL:HG23	2.21	0.40
2:B:148:PRO:HD2	38:B:9047:HOH:O	2.21	0.40
3:C:168:ARG:NH2	3:C:190:ALA:O	2.55	0.40
30:0:1074:G:H4'	30:0:1260:G:C6	2.57	0.40
31:9:27:C:C4	31:9:28:U:C5	3.09	0.40
14:N:58:LEU:HD12	14:N:58:LEU:H	1.85	0.40
30:0:1936:C:H2'	30:0:1937:U:C6	2.56	0.40
30:0:2248:C:H2'	30:0:2249:G:C8	2.54	0.40
12:L:56:LYS:NZ	38:L:9036:HOH:O	2.54	0.40
30:0:113:A:OP2	30:0:114:A:H2'	2.21	0.40
8:H:91:ARG:O	30:0:1003:U:H4'	2.22	0.40
1:A:105:VAL:HG13	1:A:155:THR:O	2.21	0.40
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.22	0.40
8:H:8:MET:SD	30:0:2494:G:H4'	2.61	0.40
2:B:294:TYR:HE2	38:B:9123:HOH:O	2.03	0.40
25:Y:210:GLY:N	30:0:1313:A:H5''	2.36	0.40
30:0:2803:C:H2'	30:0:2804:C:H6	1.86	0.40
30:0:1982:C:H2'	30:0:1983:C:O4'	2.21	0.40
30:0:2826:G:C6	30:0:2913:A:C6	3.10	0.40
16:P:89:ASN:HB3	16:P:92:GLU:HB2	2.03	0.40
12:L:67:ARG:O	12:L:71:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1163:G:C2	30:0:1184:C:N3	2.89	0.40
30:0:1589:G:H5'	38:0:6843:HOH:O	2.20	0.40
16:P:59:ARG:HD3	38:0:6252:HOH:O	2.22	0.40
30:0:2321:A:H1'	30:0:2322:U:H3'	2.04	0.40
23:W:139:GLY:O	23:W:141:HIS:HD2	2.04	0.40
30:0:1191:A:H3'	30:0:1191:A:C8	2.56	0.40
30:0:506:G:N2	30:0:509:A:H5'	2.31	0.40
30:0:1130:U:H4'	38:0:6109:HOH:O	2.21	0.40
13:M:34:GLU:HB3	13:M:38:GLU:HG3	2.02	0.40
20:T:21:LYS:HA	20:T:24:ARG:HD2	2.04	0.40
1:A:88:ILE:HG22	1:A:88:ILE:O	2.20	0.40
30:0:2295:G:N3	30:0:2361:A:H2	2.17	0.40
30:0:1397:C:O2'	30:0:1398:G:H5'	2.22	0.40
30:0:763:C:O2'	30:0:764:C:H5'	2.21	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.21	0.40
30:0:2694:A:C6	30:0:2702:A:C8	3.09	0.40
30:0:1815:A:H4'	30:0:2751:C:O4'	2.22	0.40
30:0:1135:G:O2'	30:0:1136:U:H5'	2.22	0.40
30:0:2803:C:C4	30:0:2804:C:C5	3.10	0.40
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.53	0.40
2:B:10:SER:O	2:B:16:ARG:NH1	2.45	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	235/240 (98%)	202 (86%)	27 (12%)	6 (3%)	8	37
2	B	335/338 (99%)	309 (92%)	17 (5%)	9 (3%)	8	36
3	C	244/246 (99%)	222 (91%)	20 (8%)	2 (1%)	27	74
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	7	32
5	E	170/178 (96%)	157 (92%)	12 (7%)	1 (1%)	33	79
6	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	18	60
9	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	2	12
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	30	76
11	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	27	74
12	L	141/165 (86%)	120 (85%)	21 (15%)	0	100	100
13	M	192/196 (98%)	179 (93%)	9 (5%)	4 (2%)	11	45
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	10	43
15	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	21	66
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	30	76
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
20	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	14	52
21	U	51/67 (76%)	42 (82%)	8 (16%)	1 (2%)	11	47
22	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
23	W	152/154 (99%)	140 (92%)	10 (7%)	2 (1%)	18	60
24	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	9	38
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	58 (82%)	8 (11%)	5 (7%)	2	8
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	9	40
29	3	90/92 (98%)	74 (82%)	13 (14%)	3 (3%)	6	29
All	All	3705/4472 (83%)	3359 (91%)	286 (8%)	60 (2%)	14	54

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	37	VAL
1	A	74	VAL
4	D	65	GLU
4	D	137	PRO
8	H	19	ARG

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Mol	Chain	Res	Type
11	K	127	ALA
13	M	82	ARG
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
26	Z	105	ARG
29	3	64	LYS
2	B	306	LYS
6	F	61	MET
6	F	101	ALA
13	M	71	SER
21	U	51	TRP
24	X	70	ILE
26	Z	70	ARG
2	B	184	ASP
3	C	8	LEU
5	E	44	GLY
6	F	27	GLY
9	I	83	GLY
20	T	44	ALA
23	W	36	PRO
23	W	49	ASN
24	X	87	ALA
26	Z	67	GLY
29	3	46	ILE
2	B	2	GLN
2	B	107	SER
4	D	56	ARG
9	I	106	GLN
13	M	86	GLN
20	T	46	ASP
26	Z	83	TYR
28	2	37	HIS
1	A	52	SER
1	A	119	ALA
2	B	206	THR
3	C	79	ARG
10	J	65	ASN
13	M	79	ALA
18	R	114	VAL
29	3	56	PRO
2	B	63	GLU

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Mol	Chain	Res	Type
6	F	104	ALA
8	H	171	GLY
14	N	164	ASP
4	D	27	ILE
17	Q	48	PRO
2	B	34	GLY
2	B	169	GLY
26	Z	64	PRO
2	B	185	GLY
9	I	108	HIS
9	I	131	GLY
1	A	42	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	38	80
2	B	282/283 (100%)	264 (94%)	18 (6%)	25	64
3	C	193/193 (100%)	182 (94%)	11 (6%)	29	70
4	D	117/148 (79%)	110 (94%)	7 (6%)	27	67
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	91
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	85
8	H	134/145 (92%)	126 (94%)	8 (6%)	27	67
9	I	58/130 (45%)	56 (97%)	2 (3%)	49	86
10	J	118/121 (98%)	113 (96%)	5 (4%)	40	82
11	K	106/106 (100%)	104 (98%)	2 (2%)	69	94
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	80
13	M	158/160 (99%)	148 (94%)	10 (6%)	25	65
14	N	149/150 (99%)	144 (97%)	5 (3%)	49	86
15	O	93/94 (99%)	92 (99%)	1 (1%)	84	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	113/117 (97%)	107 (95%)	6 (5%)	32	73
17	Q	79/80 (99%)	78 (99%)	1 (1%)	80	96
18	R	117/122 (96%)	114 (97%)	3 (3%)	59	91
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	96
20	T	105/106 (99%)	99 (94%)	6 (6%)	29	70
21	U	44/53 (83%)	41 (93%)	3 (7%)	22	61
22	V	51/57 (90%)	49 (96%)	2 (4%)	43	83
23	W	130/130 (100%)	124 (95%)	6 (5%)	37	79
24	X	66/74 (89%)	61 (92%)	5 (8%)	19	55
25	Y	120/196 (61%)	115 (96%)	5 (4%)	40	82
26	Z	60/94 (64%)	57 (95%)	3 (5%)	34	75
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	92
29	3	79/79 (100%)	76 (96%)	3 (4%)	44	84
All	All	3095/3646 (85%)	2963 (96%)	132 (4%)	40	81

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	192	VAL
1	A	206	ARG
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	162	MET
2	B	191	ASN
2	B	192	ASP

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Mol	Chain	Res	Type
2	B	195	ARG
2	B	238	ASN
2	B	248	ARG
2	B	251	VAL
2	B	254	GLN
2	B	265	LEU
2	B	277	GLU
2	B	307	ARG
3	C	2	GLN
3	C	76	ARG
3	C	88	SER
3	C	136	VAL
3	C	187	ARG
3	C	202	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	29	HIS
4	D	50	VAL
4	D	61	PHE
4	D	149	ARG
4	D	161	ASP
5	E	7	ILE
5	E	68	HIS
5	E	126	ILE
5	E	155	ASN
7	G	73	ASP
8	H	21	GLU
8	H	33	GLN
8	H	45	ASP
8	H	61	ARG
8	H	62	HIS
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	114	TYR
9	I	115	ASP
10	J	46	ILE

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Mol	Chain	Res	Type
10	J	52	GLN
10	J	74	ARG
10	J	107	ASN
10	J	130	VAL
11	K	10	GLN
11	K	55	VAL
12	L	35	ARG
12	L	99	GLU
12	L	101	ASP
12	L	104	ASP
12	L	114	VAL
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	73	ARG
13	M	82	ARG
13	M	86	GLN
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	125	ARG
14	N	5	ARG
14	N	17	ARG
14	N	49	THR
14	N	56	ASP
14	N	80	SER
15	O	3	THR
16	P	21	VAL
16	P	79	SER
16	P	91	LYS
16	P	94	TRP
16	P	98	ILE
16	P	120	ARG
17	Q	16	ASN
18	R	13	THR
18	R	39	THR
18	R	143	VAL
19	S	30	ASP
20	T	5	ASP
20	T	39	ASN
20	T	73	HIS
20	T	96	VAL

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Mol	Chain	Res	Type
20	T	115	GLU
20	T	117	ASP
21	U	25	ASP
21	U	52	THR
21	U	53	ASP
22	V	12	THR
22	V	65	ASP
23	W	1	MET
23	W	4	LEU
23	W	35	VAL
23	W	88	THR
23	W	125	HIS
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
25	Y	223	ASP
25	Y	235	GLU
26	Z	37	ARG
26	Z	70	ARG
26	Z	88	PHE
28	2	18	ASN
29	3	30	GLN
29	3	56	PRO
29	3	65	THR

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

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS

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Mol	Chain	Res	Type
2	B	320	GLN
3	C	2	GLN
3	C	73	GLN
3	C	103	ASN
3	C	129	HIS
4	D	103	ASN
5	E	55	ASN
5	E	90	HIS
5	E	143	GLN
5	E	150	GLN
7	G	64	ASN
8	H	59	GLN
9	I	99	GLN
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	29	GLN
13	M	170	ASN
14	N	40	ASN
14	N	53	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	27	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN

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Mol	Chain	Res	Type
18	R	117	HIS
18	R	123	GLN
19	S	7	HIS
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	38	ASN
21	U	39	ASN
22	V	34	GLN
22	V	60	GLN
23	W	2	HIS
23	W	12	ASN
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
26	Z	80	GLN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	30	GLN
29	3	48	ASN
29	3	91	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	250 (9%)	21 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	269 (9%)	23 (0%)

All (269) 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	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
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	409	U
30	0	417	G
30	0	461	C
30	0	473	A
30	0	487	G
30	0	498	A
30	0	510	U

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Mol	Chain	Res	Type
30	0	511	A
30	0	514	G
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	581	G
30	0	588	G
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	699	C
30	0	701	U
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	846	A
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A

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Mol	Chain	Res	Type
30	0	953	G
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	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G
30	0	1164	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	1205	U
30	0	1206	U
30	0	1216	G
30	0	1234	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A

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Mol	Chain	Res	Type
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1559	A
30	0	1562	C
30	0	1592	G
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	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1710	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
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	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G

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Mol	Chain	Res	Type
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	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	2110	G
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	2322	U
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2422	U
30	0	2462	G
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2533	C
30	0	2537	G

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Mol	Chain	Res	Type
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
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	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
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	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2906	A
30	0	2912	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G

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Mol	Chain	Res	Type
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	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	396	U
30	0	603	A
30	0	644	G
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	1377	C
30	0	1474	C
30	0	1506	U
30	0	2011	A
30	0	2321	A
30	0	2467	A
30	0	2526	C
30	0	2718	C
30	0	2726	U
30	0	2791	U
31	9	43	G

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Mol	Chain	Res	Type
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	OMU	0	2587	30	20,22,23	0.70	0	24,31,34	0.76	0
30	OMG	0	2588	30	24,26,27	0.74	0	32,38,41	5.16	3 (9%)
30	UR3	0	2619	30	20,22,23	0.81	1 (5%)	23,32,35	0.80	0
30	PSU	0	2621	30	19,21,22	1.18	3 (15%)	23,30,33	1.09	2 (8%)
30	1MA	0	628	30	23,25,26	0.80	0	32,37,40	1.00	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	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	-	0/8/25/26	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.83	1.42	1.37
30	0	2621	PSU	P-OP1	2.29	1.49	1.46
30	0	2621	PSU	C6-N1	2.28	1.34	1.32
30	0	2619	UR3	P-OP1	2.02	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.58	130.29	134.14
30	0	2588	OMG	C6-N1-C2	3.31	125.31	119.51
30	0	628	1MA	C2-N3-C4	-3.20	110.76	116.23
30	0	2588	OMG	C2-N3-C4	-2.37	111.76	115.09
30	0	2621	PSU	C5-C4-N3	-2.22	114.81	118.86
30	0	2621	PSU	C5-C1'-C2'	-2.17	111.77	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	-0.11	12 (5%) 27 13	36, 71, 108, 128	0
2	B	337/338 (99%)	-0.40	0 100 100	38, 67, 98, 112	0
3	C	246/246 (100%)	-0.37	0 100 100	32, 56, 80, 91	0
4	D	140/177 (79%)	1.61	53 (37%) 1 0	89, 121, 144, 151	0
5	E	172/178 (96%)	-0.05	7 (4%) 35 17	57, 83, 104, 113	0
6	F	119/120 (99%)	0.58	16 (13%) 4 2	64, 88, 121, 131	0
7	G	29/348 (8%)	1.18	5 (17%) 2 2	92, 107, 116, 118	0
8	H	160/177 (90%)	0.72	28 (17%) 2 2	65, 89, 118, 127	0
9	I	70/162 (43%)	3.44	47 (67%) 0 0	145, 162, 177, 179	0
10	J	142/145 (97%)	-0.37	1 (0%) 84 44	47, 63, 86, 105	0
11	K	132/132 (100%)	-0.47	0 100 100	45, 63, 91, 100	0
12	L	145/165 (87%)	0.54	21 (14%) 3 2	41, 88, 131, 140	0
13	M	194/196 (98%)	0.28	21 (10%) 6 4	37, 53, 115, 122	0
14	N	186/187 (99%)	0.82	33 (17%) 2 2	70, 90, 134, 139	0
15	O	115/116 (99%)	-0.34	1 (0%) 81 39	46, 64, 81, 87	0
16	P	143/149 (95%)	-0.30	2 (1%) 72 34	48, 67, 85, 96	0
17	Q	95/96 (98%)	-0.00	4 (4%) 35 17	57, 69, 89, 97	0
18	R	150/155 (96%)	-0.52	1 (0%) 84 44	39, 56, 79, 95	0
19	S	81/85 (95%)	-0.23	1 (1%) 75 36	52, 70, 89, 104	0
20	T	119/120 (99%)	-0.07	4 (3%) 43 19	48, 67, 95, 125	0
21	U	53/67 (79%)	4.70	43 (81%) 0 0	112, 125, 131, 134	0
22	V	65/71 (91%)	0.95	13 (20%) 2 1	51, 83, 131, 135	0
23	W	154/154 (100%)	-0.36	1 (0%) 86 47	45, 62, 79, 92	0
24	X	82/92 (89%)	0.02	4 (4%) 28 14	54, 72, 95, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.55	0 100 100	30, 53, 78, 97	0
26	Z	73/116 (62%)	8.27	58 (79%) 0 0	111, 130, 139, 142	0
27	1	56/57 (98%)	-0.52	0 100 100	30, 39, 47, 65	0
28	2	46/50 (92%)	-0.14	2 (4%) 34 16	39, 72, 104, 110	0
29	3	92/92 (100%)	9.07	91 (98%) 0 0	123, 135, 142, 148	0
30	0	2754/2923 (94%)	-0.41	23 (0%) 83 42	25, 58, 106, 183	0
31	9	122/122 (100%)	-0.59	2 (1%) 68 32	51, 90, 111, 159	0
All	All	6651/7517 (88%)	0.12	494 (7%) 15 8	25, 66, 129, 183	0

All (494) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	58	ASN	29.0
29	3	41	GLU	22.2
29	3	35	TRP	21.5
26	Z	36	GLY	21.5
26	Z	35	SER	21.5
26	Z	55	SER	21.0
29	3	39	GLN	21.0
26	Z	43	GLY	20.8
26	Z	46	SER	20.5
29	3	47	GLY	19.3
29	3	48	ASN	18.6
29	3	36	ILE	18.4
26	Z	38	PHE	18.3
26	Z	50	VAL	18.2
26	Z	39	GLY	18.1
26	Z	59	GLU	18.0
29	3	32	GLY	17.7
29	3	40	ARG	17.2
29	3	45	GLY	16.1
29	3	44	SER	16.0
29	3	82	GLY	15.8
26	Z	44	ARG	15.6
26	Z	34	SER	15.4
29	3	38	ARG	15.2
26	Z	69	ASP	15.2
26	Z	45	VAL	15.0
29	3	42	ARG	14.8
13	M	87	GLY	14.6

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Mol	Chain	Res	Type	RSRZ
26	Z	56	GLU	14.0
13	M	80	GLY	14.0
26	Z	42	TYR	14.0
29	3	37	ASP	13.9
29	3	81	GLU	13.7
29	3	43	ASN	13.5
26	Z	54	GLU	13.1
29	3	11	CYS	13.1
29	3	33	MET	12.5
29	3	55	VAL	12.4
29	3	34	LYS	12.3
29	3	15	ASN	12.2
26	Z	53	ILE	12.1
29	3	57	GLY	12.1
29	3	53	SER	12.1
29	3	56	PRO	12.0
29	3	62	THR	11.9
26	Z	82	SER	11.6
29	3	83	TRP	11.4
26	Z	57	MET	11.4
21	U	43	GLY	11.2
21	U	40	ALA	11.2
29	3	51	LYS	10.9
29	3	30	GLN	10.7
26	Z	68	GLU	10.5
26	Z	77	GLY	10.5
26	Z	60	ASP	10.5
26	Z	48	ARG	10.4
29	3	71	CYS	10.2
9	I	66	GLY	10.0
29	3	20	HIS	9.9
29	3	27	SER	9.9
26	Z	47	ARG	9.9
29	3	31	THR	9.7
9	I	70	THR	9.6
29	3	18	GLN	9.5
26	Z	49	ARG	9.4
21	U	54	THR	9.4
22	V	39	ALA	9.4
29	3	14	CYS	9.2
29	3	52	PHE	9.1
13	M	90	ARG	9.0

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Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	9.0
13	M	70	GLY	9.0
21	U	41	ASP	9.0
26	Z	37	ARG	8.9
29	3	19	GLU	8.9
9	I	104	ALA	8.9
29	3	16	GLU	8.7
29	3	1	MET	8.7
26	Z	78	ILE	8.6
26	Z	40	ALA	8.5
29	3	80	ARG	8.5
12	L	60	GLU	8.3
26	Z	71	VAL	8.3
29	3	46	ILE	8.3
26	Z	51	ALA	8.2
13	M	82	ARG	8.2
21	U	9	CYS	8.1
21	U	46	ALA	8.1
29	3	10	TYR	8.1
21	U	38	ASN	7.9
9	I	128	THR	7.9
21	U	52	THR	7.9
29	3	50	GLY	7.8
26	Z	52	GLU	7.8
29	3	59	ASP	7.7
29	3	78	HIS	7.6
21	U	42	LEU	7.5
13	M	83	SER	7.5
29	3	13	HIS	7.4
29	3	29	ARG	7.3
29	3	17	HIS	7.3
29	3	84	ARG	7.2
29	3	9	THR	7.2
21	U	31	PHE	7.2
29	3	91	GLN	7.2
26	Z	61	HIS	7.1
29	3	22	VAL	7.1
29	3	12	PRO	7.0
29	3	61	PRO	7.0
29	3	49	ASP	7.0
26	Z	67	GLY	7.0
29	3	8	ASN	7.0

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Mol	Chain	Res	Type	RSRZ
13	M	81	ARG	6.9
21	U	55	ALA	6.9
21	U	12	ASP	6.9
29	3	85	ALA	6.8
21	U	36	CYS	6.8
4	D	63	ILE	6.8
9	I	113	SER	6.7
26	Z	81	CYS	6.7
29	3	77	ALA	6.6
21	U	51	TRP	6.6
26	Z	65	ASN	6.6
4	D	69	ILE	6.6
4	D	57	THR	6.6
29	3	86	GLY	6.6
29	3	3	MET	6.6
9	I	71	ALA	6.6
29	3	69	TYR	6.5
9	I	106	GLN	6.5
26	Z	79	TRP	6.5
29	3	74	CYS	6.4
29	3	5	ARG	6.3
31	9	1	U	6.3
13	M	74	LYS	6.3
22	V	1	THR	6.3
13	M	89	THR	6.3
29	3	64	LYS	6.3
29	3	90	PHE	6.2
29	3	54	LYS	6.2
26	Z	41	ARG	6.2
29	3	28	GLY	6.2
13	M	79	ALA	6.2
29	3	88	LEU	6.1
26	Z	66	CYS	6.1
26	Z	62	ALA	6.1
26	Z	70	ARG	6.1
21	U	53	ASP	6.1
29	3	4	PRO	6.1
9	I	97	VAL	6.1
9	I	111	LEU	6.0
9	I	117	THR	6.0
29	3	92	GLU	6.0
21	U	4	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
21	U	48	ASN	5.9
21	U	39	ASN	5.9
29	3	58	GLY	5.9
26	Z	74	GLN	5.9
9	I	132	VAL	5.8
4	D	75	LEU	5.7
26	Z	76	THR	5.7
13	M	71	SER	5.7
21	U	45	GLU	5.7
29	3	2	GLN	5.6
14	N	166	ALA	5.6
29	3	23	GLU	5.6
13	M	78	LYS	5.6
29	3	66	ASP	5.6
22	V	38	GLY	5.6
4	D	135	VAL	5.6
21	U	47	ARG	5.5
14	N	179	LEU	5.5
26	Z	63	CYS	5.5
29	3	6	ARG	5.4
29	3	65	THR	5.4
9	I	116	LEU	5.3
21	U	30	HIS	5.3
22	V	43	PRO	5.3
9	I	72	GLU	5.3
29	3	68	LYS	5.3
9	I	73	LEU	5.3
13	M	76	ARG	5.2
9	I	109	PRO	5.2
21	U	24	LYS	5.2
26	Z	85	ASP	5.1
4	D	18	ILE	5.1
30	0	735	C	5.1
22	V	40	PRO	5.1
4	D	27	ILE	5.1
22	V	37	GLY	4.9
19	S	81	ILE	4.9
29	3	7	PHE	4.9
29	3	70	ARG	4.9
9	I	103	ILE	4.9
29	3	25	VAL	4.8
21	U	5	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
13	M	73	ARG	4.8
9	I	110	ASP	4.8
21	U	13	ILE	4.8
9	I	69	PRO	4.8
9	I	118	ASN	4.7
26	Z	89	THR	4.7
21	U	25	ASP	4.7
29	3	67	LEU	4.7
29	3	76	LYS	4.7
4	D	25	MET	4.7
9	I	100	VAL	4.7
8	H	82	GLU	4.6
8	H	133	GLY	4.6
29	3	72	GLY	4.6
26	Z	93	TYR	4.6
7	G	27	ILE	4.5
29	3	21	GLU	4.5
26	Z	92	SER	4.5
26	Z	80	GLN	4.5
21	U	44	ARG	4.5
13	M	75	ARG	4.5
21	U	8	TYR	4.5
9	I	108	HIS	4.4
14	N	181	ASP	4.4
29	3	75	GLY	4.4
26	Z	88	PHE	4.3
13	M	86	GLN	4.3
30	0	1172	G	4.3
9	I	67	VAL	4.3
29	3	24	LYS	4.3
24	X	10	VAL	4.3
4	D	40	ILE	4.3
13	M	88	VAL	4.3
6	F	28	ALA	4.2
4	D	26	GLY	4.2
12	L	106	VAL	4.2
21	U	28	THR	4.2
14	N	182	GLY	4.2
30	0	1199	A	4.2
4	D	44	ILE	4.1
1	A	65	ARG	4.1
29	3	73	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
21	U	29	THR	4.1
29	3	60	LYS	4.1
30	0	970	U	4.1
26	Z	83	TYR	4.1
29	3	89	GLU	4.1
29	3	63	LYS	4.1
9	I	112	LEU	4.1
29	3	87	ARG	4.1
1	A	64	ASP	4.1
1	A	237	GLY	4.0
29	3	26	ARG	4.0
9	I	80	PHE	4.0
4	D	90	LEU	4.0
14	N	155	GLU	4.0
7	G	23	ILE	4.0
30	0	1198	U	4.0
21	U	11	THR	4.0
8	H	77	ILE	3.9
6	F	99	THR	3.9
14	N	185	GLU	3.9
12	L	105	TYR	3.9
21	U	32	CYS	3.9
26	Z	72	ASP	3.8
1	A	37	VAL	3.8
14	N	178	THR	3.8
9	I	102	GLN	3.8
9	I	94	ASP	3.8
9	I	105	GLU	3.8
21	U	37	GLU	3.7
21	U	19	THR	3.7
26	Z	86	TYR	3.7
28	2	49	GLU	3.7
28	2	48	ASP	3.7
8	H	66	GLU	3.7
9	I	68	PRO	3.7
21	U	10	GLY	3.7
21	U	33	SER	3.7
21	U	56	ARG	3.6
26	Z	73	ARG	3.6
4	D	166	ILE	3.6
8	H	81	GLY	3.6
8	H	84	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
12	L	48	LYS	3.5
13	M	77	HIS	3.5
9	I	78	ALA	3.4
22	V	36	ALA	3.4
9	I	82	THR	3.4
4	D	41	LEU	3.4
8	H	31	ILE	3.4
14	N	75	THR	3.4
9	I	75	LYS	3.4
4	D	130	VAL	3.4
21	U	6	CYS	3.3
26	Z	84	CYS	3.3
4	D	70	GLY	3.3
4	D	84	LEU	3.3
9	I	98	ASP	3.3
21	U	23	HIS	3.3
8	H	132	ALA	3.3
8	H	69	ARG	3.3
24	X	71	ARG	3.3
30	0	1000	C	3.3
22	V	44	GLY	3.3
9	I	119	ALA	3.3
4	D	93	LEU	3.3
6	F	106	ALA	3.2
4	D	129	ASP	3.2
9	I	91	PHE	3.2
4	D	157	LEU	3.2
9	I	93	ALA	3.2
4	D	134	LEU	3.2
6	F	17	LEU	3.2
4	D	11	HIS	3.2
4	D	171	ASP	3.2
30	0	1177	A	3.2
14	N	78	MET	3.2
30	0	1951	G	3.2
20	T	119	ALA	3.2
30	0	1171	A	3.2
4	D	64	ARG	3.2
4	D	73	VAL	3.1
26	Z	104	ARG	3.1
6	F	44	SER	3.1
4	D	88	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	58	VAL	3.1
30	O	1163	G	3.1
6	F	75	ILE	3.1
22	V	2	VAL	3.1
7	G	25	GLU	3.1
14	N	95	ALA	3.1
12	L	123	ASP	3.1
17	Q	20	ASP	3.1
21	U	49	LEU	3.0
14	N	153	GLN	3.0
30	O	999	C	3.0
4	D	67	ASP	3.0
4	D	23	VAL	3.0
6	F	97	ALA	3.0
4	D	172	VAL	3.0
17	Q	64	GLU	3.0
9	I	95	LEU	2.9
13	M	84	LYS	2.9
12	L	80	ASP	2.9
12	L	75	LEU	2.9
4	D	16	PRO	2.9
9	I	76	ASP	2.9
14	N	180	LEU	2.9
4	D	74	THR	2.9
6	F	108	VAL	2.8
9	I	92	VAL	2.8
9	I	127	CYS	2.8
9	I	88	GLN	2.8
14	N	92	ALA	2.8
14	N	145	ALA	2.8
4	D	51	ARG	2.8
14	N	149	GLU	2.8
4	D	128	LEU	2.8
12	L	96	VAL	2.8
31	9	24	U	2.8
8	H	86	TYR	2.8
5	E	100	ASP	2.8
12	L	79	ASP	2.8
4	D	19	GLU	2.8
20	T	42	VAL	2.8
4	D	87	ALA	2.8
14	N	159	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
14	N	156	GLU	2.7
1	A	82	VAL	2.7
8	H	40	GLN	2.7
4	D	17	ARG	2.7
14	N	97	VAL	2.7
14	N	128	ASP	2.7
12	L	81	VAL	2.7
4	D	165	PHE	2.7
30	O	1170	U	2.7
12	L	124	ASP	2.7
22	V	41	GLU	2.6
12	L	120	LEU	2.6
12	L	142	LEU	2.6
26	Z	103	VAL	2.6
4	D	92	GLU	2.6
30	O	282	C	2.6
9	I	83	GLY	2.6
1	A	52	SER	2.6
9	I	121	LYS	2.6
4	D	52	THR	2.6
13	M	72	ALA	2.6
9	I	124	VAL	2.6
17	Q	81	GLU	2.5
30	O	1162	G	2.5
4	D	56	ARG	2.5
5	E	5	LEU	2.5
4	D	142	ALA	2.5
20	T	116	ASP	2.5
1	A	145	MET	2.5
8	H	126	THR	2.5
17	Q	92	ARG	2.5
12	L	76	LEU	2.5
30	O	1185	U	2.5
9	I	114	TYR	2.5
6	F	37	THR	2.5
30	O	1173	A	2.5
30	O	960	G	2.4
1	A	53	ALA	2.4
12	L	130	ARG	2.4
8	H	169	GLU	2.4
30	O	497	A	2.4
30	O	1200	A	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	24	HIS	2.4
6	F	20	LEU	2.4
4	D	101	THR	2.4
4	D	158	ASN	2.4
12	L	91	VAL	2.4
4	D	61	PHE	2.4
21	U	50	GLU	2.4
30	O	1190	G	2.4
14	N	152	GLU	2.4
14	N	183	ASP	2.4
8	H	29	SER	2.3
4	D	28	GLY	2.3
6	F	100	ASP	2.3
8	H	36	MET	2.3
22	V	3	LEU	2.3
4	D	43	GLU	2.3
14	N	115	VAL	2.3
18	R	108	ALA	2.3
6	F	49	PHE	2.3
9	I	79	GLY	2.3
4	D	10	PHE	2.3
12	L	125	PHE	2.3
7	G	21	ASP	2.3
24	X	80	GLU	2.3
1	A	60	PHE	2.3
21	U	15	PRO	2.3
12	L	62	ALA	2.3
1	A	80	LEU	2.2
8	H	28	GLY	2.2
4	D	80	ALA	2.2
22	V	52	ALA	2.2
15	O	69	VAL	2.2
8	H	76	LEU	2.2
8	H	145	ASP	2.2
1	A	24	LYS	2.2
6	F	98	VAL	2.2
13	M	1	ALA	2.2
30	O	1279	U	2.2
14	N	7	LYS	2.2
5	E	128	GLY	2.2
24	X	7	GLU	2.2
9	I	115	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	87	PHE	2.2
21	U	20	MET	2.2
6	F	119	ARG	2.2
6	F	69	GLU	2.2
8	H	27	PRO	2.2
14	N	150	TYR	2.2
12	L	141	GLU	2.2
12	L	89	PHE	2.1
30	O	969	G	2.1
4	D	167	GLU	2.1
6	F	15	ASP	2.1
8	H	12	ILE	2.1
22	V	8	ILE	2.1
14	N	84	THR	2.1
20	T	63	ILE	2.1
10	J	70	PHE	2.1
5	E	108	LEU	2.1
23	W	96	LEU	2.1
1	A	77	GLY	2.1
14	N	81	ALA	2.1
14	N	137	ALA	2.1
16	P	108	LEU	2.1
8	H	38	ARG	2.1
12	L	114	VAL	2.1
14	N	138	ASP	2.1
5	E	118	ILE	2.1
8	H	35	LYS	2.1
8	H	39	LYS	2.1
8	H	30	LYS	2.1
14	N	158	LEU	2.1
26	Z	64	PRO	2.0
21	U	26	GLY	2.0
5	E	127	ASP	2.0
8	H	74	ARG	2.0
4	D	89	PRO	2.0
14	N	142	THR	2.0
16	P	141	ILE	2.0
30	O	1186	C	2.0
8	H	98	LEU	2.0
14	N	50	LEU	2.0
14	N	127	LEU	2.0
4	D	47	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
7	G	26	MET	2.0
14	N	88	ALA	2.0
8	H	9	TYR	2.0
8	H	73	ASN	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
30	PSU	0	2621	20/21	0.17	0.81	39,41,53,53	0
30	UR3	0	2619	21/22	0.13	-0.13	47,49,51,54	0
30	OMU	0	2587	21/22	0.11	-0.56	43,47,50,51	0
30	1MA	0	628	23/24	0.14	-1.01	38,44,47,47	0
30	OMG	0	2588	24/25	0.12	-1.35	41,43,46,50	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
36	SR	0	9007	1/1	1.81	199.06	200,200,200,200	0
34	NA	0	8549	1/1	0.67	169.41	56,56,56,56	0
36	SR	0	8982	1/1	2.34	119.04	200,200,200,200	0
36	SR	0	9006	1/1	0.69	105.36	200,200,200,200	0
34	NA	0	8545	1/1	0.82	62.44	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8562	1/1	0.93	51.50	82,82,82,82	0
34	NA	0	8547	1/1	0.88	48.75	67,67,67,67	0
35	CL	0	8822	1/1	0.45	48.55	88,88,88,88	0
34	NA	0	8551	1/1	0.67	45.33	63,63,63,63	0
32	MG	0	8089	1/1	0.27	44.00	65,65,65,65	0
34	NA	0	8505	1/1	0.78	39.77	53,53,53,53	0
34	NA	0	8565	1/1	0.39	32.94	78,78,78,78	0
34	NA	0	8554	1/1	1.02	31.89	69,69,69,69	0
34	NA	0	8574	1/1	0.53	28.22	60,60,60,60	0
36	SR	0	8996	1/1	0.50	27.21	200,200,200,200	0
34	NA	0	8564	1/1	0.34	25.99	69,69,69,69	0
34	NA	0	8524	1/1	0.54	24.82	73,73,73,73	0
36	SR	0	9004	1/1	0.89	24.30	200,200,200,200	0
36	SR	0	8994	1/1	0.60	24.22	200,200,200,200	0
34	NA	0	8509	1/1	0.17	20.58	69,69,69,69	0
36	SR	0	8983	1/1	0.40	19.51	197,197,197,197	0
34	NA	0	8536	1/1	0.21	17.67	64,64,64,64	0
34	NA	0	8566	1/1	0.35	17.46	63,63,63,63	0
34	NA	0	8528	1/1	0.56	16.75	76,76,76,76	0
36	SR	0	8986	1/1	0.80	16.64	200,200,200,200	0
36	SR	0	8909	1/1	0.15	16.00	93,93,93,93	0
32	MG	0	8040	1/1	0.36	15.79	86,86,86,86	0
32	MG	0	8030	1/1	0.48	15.78	90,90,90,90	0
34	NA	0	8530	1/1	0.50	15.53	74,74,74,74	0
36	SR	B	8987	1/1	0.62	14.32	200,200,200,200	0
32	MG	0	8031	1/1	0.31	13.91	83,83,83,83	0
36	SR	0	8997	1/1	0.25	13.65	189,189,189,189	0
34	NA	0	8508	1/1	0.31	13.60	52,52,52,52	0
34	NA	0	8542	1/1	0.51	13.43	58,58,58,58	0
34	NA	0	8556	1/1	0.96	12.79	71,71,71,71	0
34	NA	0	8546	1/1	0.64	12.71	94,94,94,94	0
33	K	0	8401	1/1	0.59	12.58	139,139,139,139	0
34	NA	H	8518	1/1	0.54	12.54	91,91,91,91	0
34	NA	0	8525	1/1	0.18	11.92	75,75,75,75	0
36	SR	0	8957	1/1	0.34	11.89	200,200,200,200	0
34	NA	0	8571	1/1	0.17	11.12	79,79,79,79	0
34	NA	0	8561	1/1	0.32	11.05	65,65,65,65	0
34	NA	0	8567	1/1	0.28	10.91	78,78,78,78	0
34	NA	9	8572	1/1	0.32	10.77	88,88,88,88	0
35	CL	0	8815	1/1	0.19	10.61	89,89,89,89	0
36	SR	L	8969	1/1	0.24	9.01	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8905	1/1	0.25	8.98	72,72,72,72	0
35	CL	A	8809	1/1	0.31	8.86	104,104,104,104	0
34	NA	0	8555	1/1	0.42	8.84	52,52,52,52	0
32	MG	0	8078	1/1	0.30	8.71	65,65,65,65	0
36	SR	0	8924	1/1	0.19	8.52	124,124,124,124	0
32	MG	0	8022	1/1	0.19	7.88	33,33,33,33	0
34	NA	0	8559	1/1	0.18	7.62	77,77,77,77	0
32	MG	0	8092	1/1	0.17	7.56	76,76,76,76	0
32	MG	0	8047	1/1	0.35	7.41	66,66,66,66	0
36	SR	0	8959	1/1	0.24	7.27	200,200,200,200	0
34	NA	0	8521	1/1	0.28	7.26	64,64,64,64	0
36	SR	0	8976	1/1	0.25	7.16	193,193,193,193	0
32	MG	0	8063	1/1	0.29	7.00	116,116,116,116	0
34	NA	0	8507	1/1	0.21	7.00	43,43,43,43	0
34	NA	0	8527	1/1	0.29	6.94	72,72,72,72	0
34	NA	B	8552	1/1	0.29	6.93	89,89,89,89	0
34	NA	0	8514	1/1	0.32	6.79	55,55,55,55	0
34	NA	0	8575	1/1	0.27	6.73	103,103,103,103	0
34	NA	0	8558	1/1	0.31	6.32	58,58,58,58	0
36	SR	0	8914	1/1	0.28	5.92	133,133,133,133	0
36	SR	0	8903	1/1	0.18	5.92	57,57,57,57	0
34	NA	0	8513	1/1	0.36	5.91	68,68,68,68	0
34	NA	0	8544	1/1	0.18	5.83	79,79,79,79	0
35	CL	0	8805	1/1	0.17	5.74	98,98,98,98	0
34	NA	0	8535	1/1	0.23	5.70	67,67,67,67	0
34	NA	0	8548	1/1	0.16	5.70	56,56,56,56	0
32	MG	0	8048	1/1	0.23	5.46	29,29,29,29	0
36	SR	0	8973	1/1	0.16	5.09	146,146,146,146	0
36	SR	0	8926	1/1	0.14	5.07	122,122,122,122	0
32	MG	0	8049	1/1	0.25	4.88	64,64,64,64	0
35	CL	0	8816	1/1	0.41	4.85	85,85,85,85	0
34	NA	0	8550	1/1	0.25	4.73	71,71,71,71	0
32	MG	0	8082	1/1	0.21	4.65	76,76,76,76	0
36	SR	0	8925	1/1	0.13	4.64	98,98,98,98	0
32	MG	0	8018	1/1	0.19	4.48	33,33,33,33	0
32	MG	0	8037	1/1	0.14	4.37	77,77,77,77	0
36	SR	0	8989	1/1	0.20	4.37	178,178,178,178	0
32	MG	0	8085	1/1	0.15	4.17	76,76,76,76	0
34	NA	0	8553	1/1	0.25	4.12	89,89,89,89	0
32	MG	0	8009	1/1	0.24	3.92	34,34,34,34	0
36	SR	0	8901	1/1	0.17	3.55	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8947	1/1	0.23	3.22	200,200,200,200	0
34	NA	0	8506	1/1	0.18	3.13	83,83,83,83	0
36	SR	R	8912	1/1	0.18	3.08	95,95,95,95	0
32	MG	0	8079	1/1	0.17	3.07	66,66,66,66	0
32	MG	0	8027	1/1	0.12	2.67	47,47,47,47	0
32	MG	0	8005	1/1	0.22	2.63	42,42,42,42	0
32	MG	0	8016	1/1	0.18	2.61	40,40,40,40	0
32	MG	0	8070	1/1	0.17	2.56	66,66,66,66	0
34	NA	0	8502	1/1	0.17	2.50	69,69,69,69	0
34	NA	0	8541	1/1	0.22	2.39	64,64,64,64	0
32	MG	0	8024	1/1	0.17	2.35	62,62,62,62	0
36	SR	0	8992	1/1	0.18	2.35	159,159,159,159	0
32	MG	0	8029	1/1	0.15	2.25	59,59,59,59	0
34	NA	0	8519	1/1	0.21	2.23	52,52,52,52	0
34	NA	0	8537	1/1	0.17	2.23	50,50,50,50	0
32	MG	0	8020	1/1	0.14	2.20	41,41,41,41	0
32	MG	A	8051	1/1	0.32	2.00	94,94,94,94	0
36	SR	0	8904	1/1	0.19	1.94	57,57,57,57	0
36	SR	0	8975	1/1	0.13	1.94	149,149,149,149	0
32	MG	0	8003	1/1	0.19	1.87	38,38,38,38	0
32	MG	0	8091	1/1	0.13	1.75	56,56,56,56	0
32	MG	0	8014	1/1	0.18	1.67	37,37,37,37	0
32	MG	0	8011	1/1	0.20	1.67	25,25,25,25	0
34	NA	0	8501	1/1	0.14	1.61	39,39,39,39	0
36	SR	0	8922	1/1	0.20	1.56	168,168,168,168	0
32	MG	0	8028	1/1	0.17	1.55	34,34,34,34	0
32	MG	0	8064	1/1	0.17	1.54	45,45,45,45	0
36	SR	0	8998	1/1	0.17	1.39	178,178,178,178	0
36	SR	0	8943	1/1	0.12	1.34	84,84,84,84	0
35	CL	J	8801	1/1	0.20	1.26	95,95,95,95	0
32	MG	0	8036	1/1	0.12	1.25	48,48,48,48	0
36	SR	0	8946	1/1	0.18	1.23	137,137,137,137	0
32	MG	K	8054	1/1	0.17	1.23	57,57,57,57	0
35	CL	R	8806	1/1	0.17	1.21	58,58,58,58	0
35	CL	0	8814	1/1	0.16	1.18	79,79,79,79	0
34	NA	0	8568	1/1	0.22	1.14	54,54,54,54	0
32	MG	0	8023	1/1	0.16	1.04	28,28,28,28	0
34	NA	0	8523	1/1	0.17	1.03	54,54,54,54	0
32	MG	0	8008	1/1	0.13	0.98	31,31,31,31	0
32	MG	0	8061	1/1	0.19	0.95	36,36,36,36	0
32	MG	0	8066	1/1	0.16	0.95	69,69,69,69	0
36	SR	0	8906	1/1	0.21	0.91	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8084	1/1	0.16	0.89	35,35,35,35	0
34	NA	0	8526	1/1	0.09	0.83	46,46,46,46	0
32	MG	0	8080	1/1	0.64	0.79	83,83,83,83	0
35	CL	0	8817	1/1	0.14	0.70	72,72,72,72	0
32	MG	0	8015	1/1	0.13	0.56	45,45,45,45	0
32	MG	0	8007	1/1	0.17	0.53	36,36,36,36	0
35	CL	N	8807	1/1	0.27	0.46	87,87,87,87	0
32	MG	0	8043	1/1	0.13	0.46	52,52,52,52	0
36	SR	0	8964	1/1	0.11	0.45	134,134,134,134	0
32	MG	0	8039	1/1	0.19	0.43	84,84,84,84	0
32	MG	0	8019	1/1	0.18	0.43	29,29,29,29	0
36	SR	1	8952	1/1	0.15	0.42	90,90,90,90	0
34	NA	R	8532	1/1	0.13	0.38	50,50,50,50	0
34	NA	0	8516	1/1	0.16	0.37	39,39,39,39	0
32	MG	0	8081	1/1	0.13	0.37	88,88,88,88	0
35	CL	0	8811	1/1	0.21	0.35	81,81,81,81	0
32	MG	0	8062	1/1	0.18	0.34	56,56,56,56	0
36	SR	0	8917	1/1	0.14	0.33	114,114,114,114	0
32	MG	0	8041	1/1	0.16	0.31	36,36,36,36	0
36	SR	0	9002	1/1	0.12	0.22	193,193,193,193	0
34	NA	0	8560	1/1	0.54	0.22	118,118,118,118	0
36	SR	0	8931	1/1	0.10	0.20	111,111,111,111	0
34	NA	0	8569	1/1	0.16	0.14	50,50,50,50	0
36	SR	9	8980	1/1	0.11	0.12	183,183,183,183	0
36	SR	A	8929	1/1	0.15	0.02	139,139,139,139	0
36	SR	0	8949	1/1	0.13	0.00	117,117,117,117	0
32	MG	0	8045	1/1	0.11	-0.03	31,31,31,31	0
36	SR	0	8951	1/1	0.09	-0.07	155,155,155,155	0
36	SR	0	8921	1/1	0.12	-0.11	83,83,83,83	0
36	SR	3	8999	1/1	0.26	-0.12	187,187,187,187	0
32	MG	0	8012	1/1	0.16	-0.15	25,25,25,25	0
34	NA	0	8512	1/1	0.16	-0.22	56,56,56,56	0
32	MG	0	8006	1/1	0.12	-0.22	44,44,44,44	0
34	NA	0	8529	1/1	0.08	-0.23	48,48,48,48	0
34	NA	0	8573	1/1	0.15	-0.25	73,73,73,73	0
35	CL	O	8808	1/1	0.19	-0.30	86,86,86,86	0
36	SR	0	8953	1/1	0.56	-0.32	200,200,200,200	0
32	MG	0	8083	1/1	0.09	-0.33	55,55,55,55	0
36	SR	0	8995	1/1	0.15	-0.35	150,150,150,150	0
34	NA	0	8511	1/1	0.11	-0.38	81,81,81,81	0
36	SR	0	8907	1/1	0.11	-0.44	63,63,63,63	0
37	CD	U	8701	1/1	0.43	-0.48	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	Q	8540	1/1	0.14	-0.49	79,79,79,79	0
34	NA	C	8503	1/1	0.15	-0.50	46,46,46,46	0
36	SR	0	8981	1/1	0.12	-0.53	161,161,161,161	0
36	SR	0	8911	1/1	0.11	-0.54	88,88,88,88	0
34	NA	J	8538	1/1	0.14	-0.54	78,78,78,78	0
33	K	M	8402	1/1	0.13	-0.55	87,87,87,87	0
32	MG	0	8090	1/1	0.16	-0.55	97,97,97,97	0
34	NA	0	8522	1/1	0.10	-0.56	82,82,82,82	0
32	MG	0	8010	1/1	0.15	-0.60	72,72,72,72	0
36	SR	H	8972	1/1	0.13	-0.60	164,164,164,164	0
36	SR	A	8930	1/1	0.13	-0.64	142,142,142,142	0
37	CD	3	8704	1/1	0.72	-0.67	200,200,200,200	0
36	SR	0	8935	1/1	0.10	-0.69	103,103,103,103	0
36	SR	0	8993	1/1	0.11	-0.71	167,167,167,167	0
37	CD	Z	8703	1/1	0.45	-0.71	200,200,200,200	0
36	SR	0	8936	1/1	0.11	-0.72	95,95,95,95	0
36	SR	0	8956	1/1	0.11	-0.74	169,169,169,169	0
36	SR	0	8918	1/1	0.11	-0.76	85,85,85,85	0
32	MG	0	8071	1/1	0.12	-0.77	60,60,60,60	0
36	SR	0	8984	1/1	0.09	-0.79	119,119,119,119	0
36	SR	0	8954	1/1	0.11	-0.80	108,108,108,108	0
36	SR	0	8937	1/1	0.15	-0.82	113,113,113,113	0
36	SR	0	8979	1/1	0.11	-0.88	196,196,196,196	0
34	NA	0	8520	1/1	0.09	-0.88	56,56,56,56	0
36	SR	0	8948	1/1	0.10	-0.91	115,115,115,115	0
36	SR	0	8934	1/1	0.12	-0.95	133,133,133,133	0
34	NA	9	8543	1/1	0.18	-0.96	61,61,61,61	0
34	NA	0	8504	1/1	0.12	-1.06	40,40,40,40	0
36	SR	0	8977	1/1	0.06	-1.07	200,200,200,200	0
34	NA	0	8515	1/1	0.13	-1.09	32,32,32,32	0
34	NA	0	8563	1/1	0.13	-1.11	117,117,117,117	0
35	CL	J	8821	1/1	0.10	-1.13	77,77,77,77	0
36	SR	0	8915	1/1	0.10	-1.13	126,126,126,126	0
36	SR	0	9001	1/1	0.11	-1.14	177,177,177,177	0
36	SR	3	8932	1/1	0.33	-1.14	178,178,178,178	0
32	MG	0	8058	1/1	0.05	-1.15	18,18,18,18	0
36	SR	0	8990	1/1	0.14	-1.18	137,137,137,137	0
32	MG	0	8026	1/1	0.08	-1.19	50,50,50,50	0
32	MG	B	8042	1/1	0.07	-1.29	69,69,69,69	0
36	SR	0	8902	1/1	0.13	-1.35	68,68,68,68	0
36	SR	0	8958	1/1	0.08	-1.36	116,116,116,116	0
35	CL	0	8813	1/1	0.08	-1.36	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8060	1/1	0.06	-1.38	53,53,53,53	0
37	CD	O	8705	1/1	0.08	-1.44	100,100,100,100	0
36	SR	F	9005	1/1	0.07	-1.45	147,147,147,147	0
32	MG	0	8068	1/1	0.10	-1.45	56,56,56,56	0
34	NA	0	8534	1/1	0.12	-1.50	50,50,50,50	0
36	SR	0	8908	1/1	0.10	-1.51	85,85,85,85	0
36	SR	0	8923	1/1	0.10	-1.54	109,109,109,109	0
34	NA	0	8557	1/1	0.07	-1.57	65,65,65,65	0
36	SR	0	8985	1/1	0.06	-1.60	164,164,164,164	0
36	SR	0	8933	1/1	0.04	-1.61	135,135,135,135	0
36	SR	9	9003	1/1	0.09	-1.61	187,187,187,187	0
34	NA	0	8533	1/1	0.09	-1.65	70,70,70,70	0
35	CL	0	8803	1/1	0.09	-1.67	60,60,60,60	0
36	SR	0	8938	1/1	0.08	-1.70	183,183,183,183	0
36	SR	0	9008	1/1	0.14	-1.75	92,92,92,92	0
36	SR	0	8968	1/1	0.07	-1.84	177,177,177,177	0
37	CD	1	8702	1/1	0.09	-1.86	61,61,61,61	0
32	MG	0	8053	1/1	0.06	-1.87	63,63,63,63	0
35	CL	J	8802	1/1	0.05	-1.88	67,67,67,67	0
36	SR	0	8940	1/1	0.10	-1.89	93,93,93,93	0
35	CL	B	8819	1/1	0.14	-1.90	69,69,69,69	0
34	NA	0	8570	1/1	0.08	-1.92	61,61,61,61	0
32	MG	0	8088	1/1	0.12	-2.06	35,35,35,35	0
32	MG	0	8017	1/1	0.11	-2.15	40,40,40,40	0
32	MG	0	8044	1/1	0.07	-2.21	58,58,58,58	0
36	SR	0	8991	1/1	0.07	-2.21	180,180,180,180	0
36	SR	0	8910	1/1	0.08	-2.26	108,108,108,108	0
32	MG	T	8057	1/1	0.08	-2.28	65,65,65,65	0
36	SR	0	8919	1/1	0.10	-2.29	168,168,168,168	0
32	MG	0	8073	1/1	0.07	-2.34	72,72,72,72	0
32	MG	0	8025	1/1	0.09	-2.35	37,37,37,37	0
36	SR	0	8960	1/1	0.03	-2.37	151,151,151,151	0
32	MG	0	8004	1/1	0.12	-2.49	29,29,29,29	0
35	CL	0	8812	1/1	0.06	-2.74	61,61,61,61	0
32	MG	0	8033	1/1	0.07	-2.74	63,63,63,63	0
32	MG	0	8059	1/1	0.09	-2.80	51,51,51,51	0
32	MG	0	8093	1/1	0.09	-2.85	36,36,36,36	0
36	SR	0	8988	1/1	0.06	-2.88	173,173,173,173	0
32	MG	0	8002	1/1	0.11	-2.96	40,40,40,40	0
32	MG	0	8052	1/1	0.06	-2.97	44,44,44,44	0
32	MG	Y	8086	1/1	0.07	-2.99	50,50,50,50	0
32	MG	0	8076	1/1	0.07	-3.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8067	1/1	0.09	-3.20	35,35,35,35	0
35	CL	L	8810	1/1	0.05	-3.31	64,64,64,64	0
32	MG	0	8046	1/1	0.11	-3.32	45,45,45,45	0
36	SR	0	8941	1/1	0.09	-3.42	114,114,114,114	0
32	MG	0	8021	1/1	0.08	-3.42	33,33,33,33	0
36	SR	9	8978	1/1	0.05	-3.51	157,157,157,157	0
36	SR	0	8962	1/1	0.12	-3.55	172,172,172,172	0
32	MG	0	8038	1/1	0.08	-3.55	74,74,74,74	0
32	MG	0	8001	1/1	0.12	-3.64	36,36,36,36	0
36	SR	1	8913	1/1	0.09	-3.64	95,95,95,95	0
36	SR	0	8939	1/1	0.05	-3.67	144,144,144,144	0
32	MG	0	8032	1/1	0.04	-3.73	52,52,52,52	0
35	CL	M	8818	1/1	0.05	-3.83	49,49,49,49	0
32	MG	0	8077	1/1	0.07	-3.89	48,48,48,48	0
36	SR	S	8961	1/1	0.08	-3.93	128,128,128,128	0
36	SR	0	8928	1/1	0.03	-3.98	137,137,137,137	0
36	SR	0	8916	1/1	0.04	-3.98	105,105,105,105	0
32	MG	0	8087	1/1	0.10	-4.08	38,38,38,38	0
32	MG	0	8069	1/1	0.10	-4.09	102,102,102,102	0
32	MG	0	8034	1/1	0.06	-4.14	50,50,50,50	0
36	SR	0	8945	1/1	0.08	-4.24	105,105,105,105	0
34	NA	S	8510	1/1	0.03	-4.41	44,44,44,44	0
32	MG	0	8075	1/1	0.05	-4.42	55,55,55,55	0
34	NA	M	8539	1/1	0.08	-4.48	42,42,42,42	0
36	SR	0	8965	1/1	0.05	-4.58	134,134,134,134	0
32	MG	0	8072	1/1	0.10	-4.71	59,59,59,59	0
32	MG	0	8055	1/1	0.06	-4.88	62,62,62,62	0
36	SR	0	8944	1/1	0.07	-5.01	172,172,172,172	0
32	MG	0	8035	1/1	0.07	-5.16	66,66,66,66	0
34	NA	0	8531	1/1	0.06	-5.25	39,39,39,39	0
36	SR	0	8970	1/1	0.05	-5.31	125,125,125,125	0
36	SR	0	8920	1/1	0.04	-5.36	127,127,127,127	0
32	MG	0	8065	1/1	0.05	-5.49	42,42,42,42	0
32	MG	9	8074	1/1	0.06	-5.77	87,87,87,87	0
32	MG	0	8013	1/1	0.05	-5.98	28,28,28,28	0
32	MG	A	8050	1/1	0.03	-6.11	64,64,64,64	0
36	SR	B	8950	1/1	0.15	-6.14	130,130,130,130	0
32	MG	0	8056	1/1	0.05	-6.29	57,57,57,57	0
34	NA	0	8517	1/1	0.07	-6.30	38,38,38,38	0
36	SR	0	9000	1/1	0.06	-6.48	183,183,183,183	0
35	CL	Y	8820	1/1	0.07	-6.81	52,52,52,52	0
36	SR	0	8967	1/1	0.05	-7.04	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CL	3	8804	1/1	0.19	-8.70	128,128,128,128	0
36	SR	0	8966	1/1	0.08	-9.90	105,105,105,105	0
36	SR	0	8927	1/1	0.08	-10.10	181,181,181,181	0
36	SR	0	8974	1/1	0.08	-11.82	166,166,166,166	0
36	SR	0	8942	1/1	0.07	-19.05	124,124,124,124	0
36	SR	0	8971	1/1	0.05	-63.00	192,192,192,192	0
36	SR	0	8955	1/1	0.07	-64.35	200,200,200,200	0
36	SR	0	8963	1/1	0.08	-	133,133,133,133	0

6.5 Other polymers ⓘ

There are no such residues in this entry.