



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:16 PM GMT

PDB ID : 3CCL
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 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>

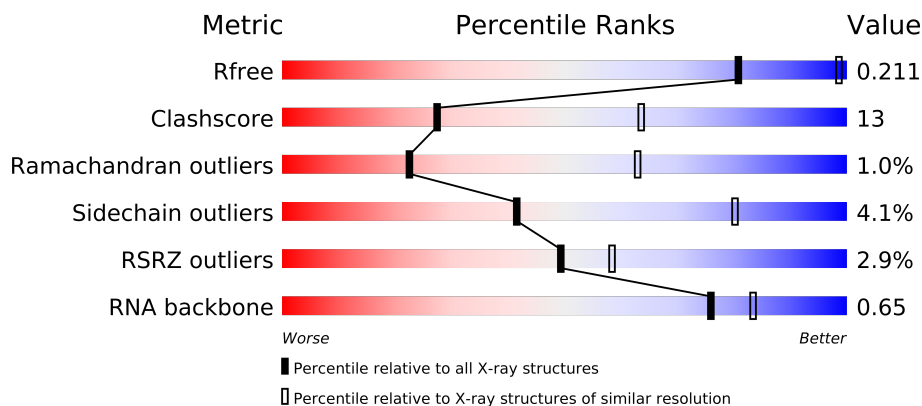
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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	8008	-	X
32	MG	0	8009	-	X
32	MG	0	8014	-	X
32	MG	0	8015	-	X
32	MG	0	8016	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8037	-	X
32	MG	0	8041	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8055	-	X
32	MG	0	8061	-	X
32	MG	0	8063	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8067	-	X
32	MG	0	8071	-	X
32	MG	0	8078	-	X
32	MG	0	8080	-	X
32	MG	0	8081	-	X
32	MG	0	8082	-	X
32	MG	0	8090	-	X
32	MG	0	8092	-	X
32	MG	A	8051	-	X
34	NA	0	8501	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8509	-	X
34	NA	0	8512	-	X
34	NA	0	8514	-	X
34	NA	0	8517	-	X
34	NA	0	8518	-	X
34	NA	0	8522	-	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	8534	-	X
34	NA	0	8535	-	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	8552	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8568	-	X
34	NA	0	8569	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	9	8572	-	X
35	CL	0	8816	-	X
35	CL	0	8822	-	X
35	CL	Y	8820	-	X
36	SR	0	8903	-	X
36	SR	0	8904	-	X
36	SR	0	8905	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8922	-	X
36	SR	0	8924	-	X
36	SR	0	8925	-	X
36	SR	0	8926	-	X
36	SR	0	8937	-	X
36	SR	0	8938	-	X
36	SR	0	8946	-	X
36	SR	0	8947	-	X
36	SR	0	8959	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	9004	-	X
36	SR	0	9007	-	X
36	SR	B	8987	-	X
36	SR	S	8961	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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
			59020	26349	10874	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	87	Total	Mg	0	0
			87	87		
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	1	Total	Mg	0	0
			1	1		
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	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	67	Total Na 67 67	0	0
34	J	1	Total Na 1 1	0	0
34	Q	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
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	93	Total 93	Sr 93	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	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
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	5929	Total 5929	O 5929	0	0
38	9	147	Total 147	O 147	0	0
38	A	116	Total 116	O 116	0	0
38	B	141	Total 141	O 141	0	0
38	C	170	Total 170	O 170	0	0
38	D	44	Total 44	O 44	0	0
38	E	45	Total 45	O 45	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	63	Total 63	O 63	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	85	Total 85	O 85	0	0
38	M	123	Total 123	O 123	0	0
38	N	55	Total 55	O 55	0	0
38	O	43	Total 43	O 43	0	0
38	P	67	Total 67	O 67	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	33	Total 33	O 33	0	0
38	T	34	Total 34	O 34	0	0

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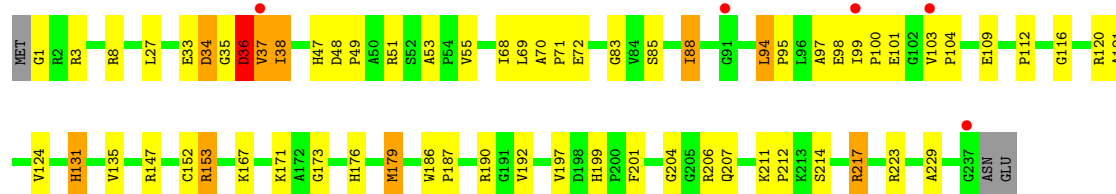
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	27	Total 27	O 27	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	25	Total 25	O 25	0	0
38	Y	95	Total 95	O 95	0	0
38	Z	26	Total 26	O 26	0	0
38	1	63	Total 63	O 63	0	0
38	2	50	Total 50	O 50	0	0
38	3	62	Total 62	O 62	0	0

3 Residue-property plots

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

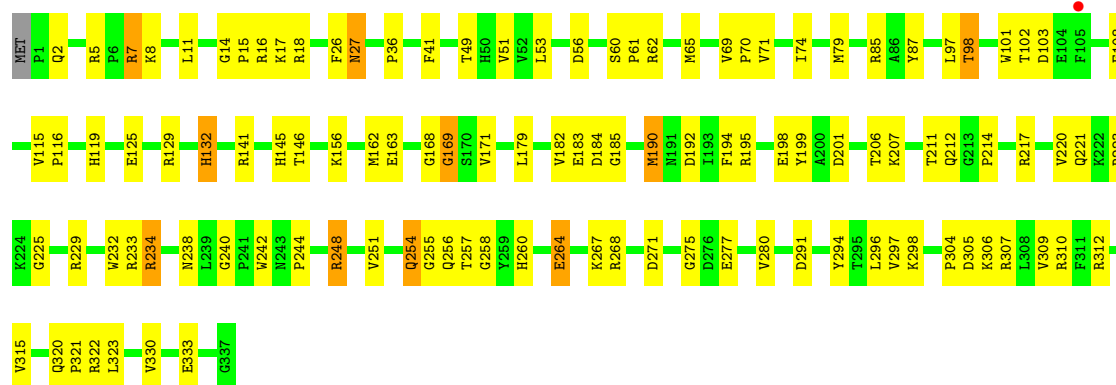
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



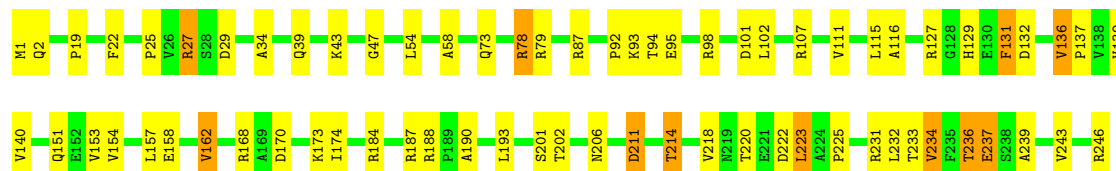
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



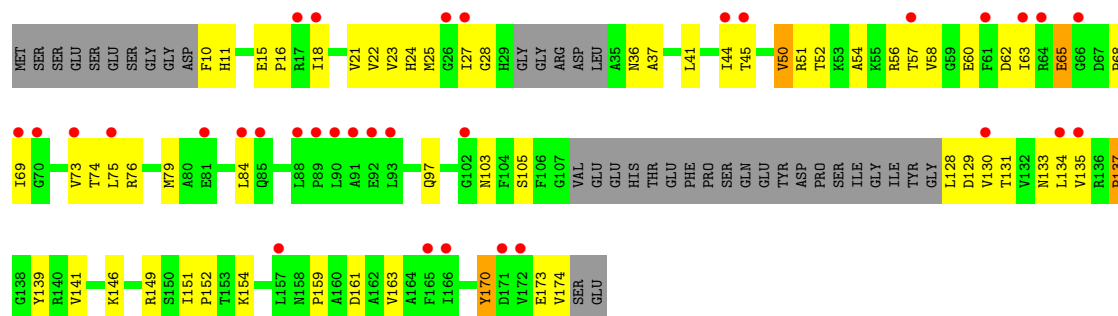
- Molecule 3: 50S ribosomal protein L4P

Chain C: 



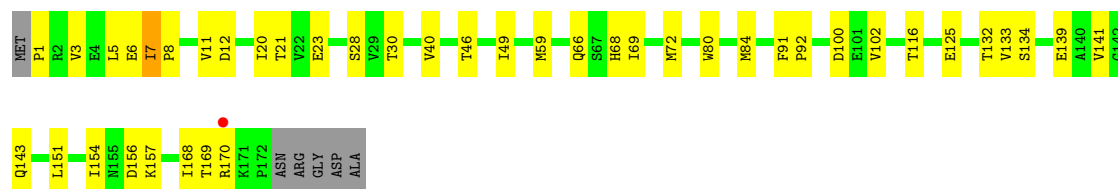
- Molecule 4: 50S ribosomal protein L5P

Chain D: 



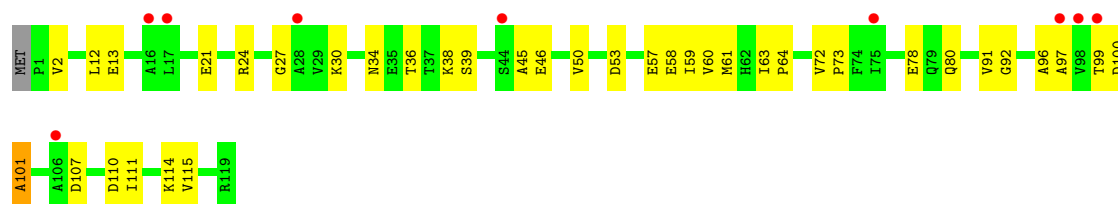
- Molecule 5: 50S ribosomal protein L6P

Chain E: 



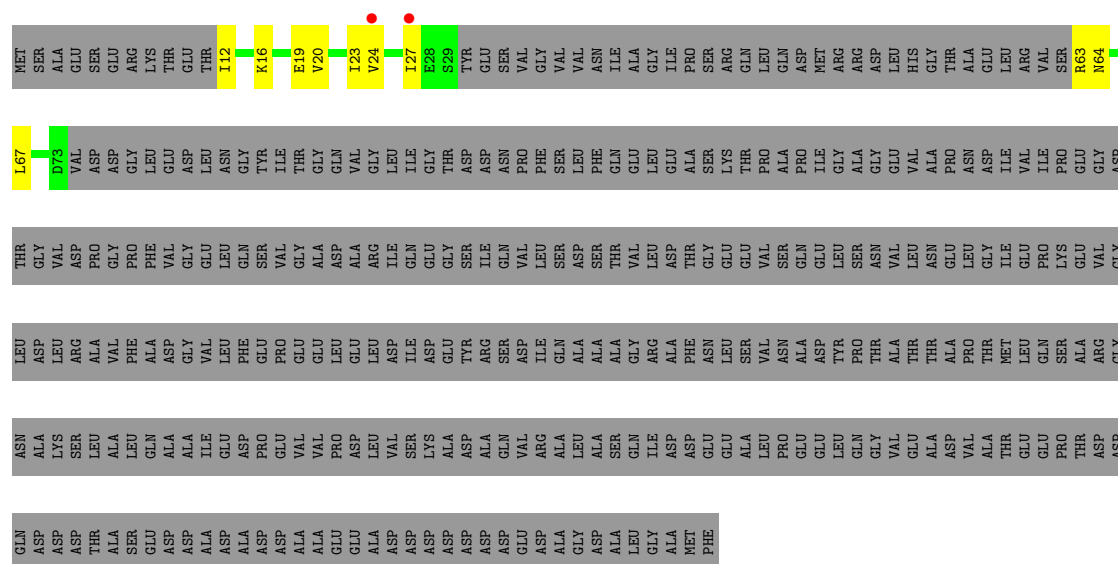
- Molecule 6: 50S ribosomal protein L7Ae

Chain F: 



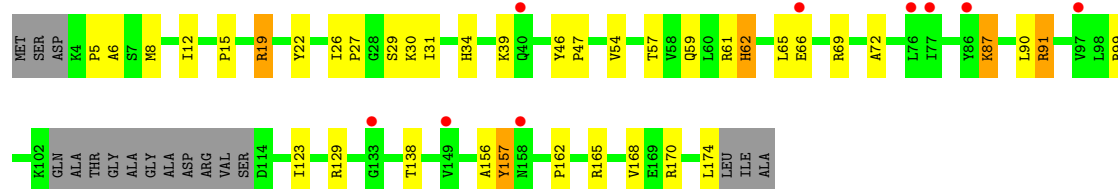
- Molecule 7: 50S ribosomal protein L10E

Chain G: 



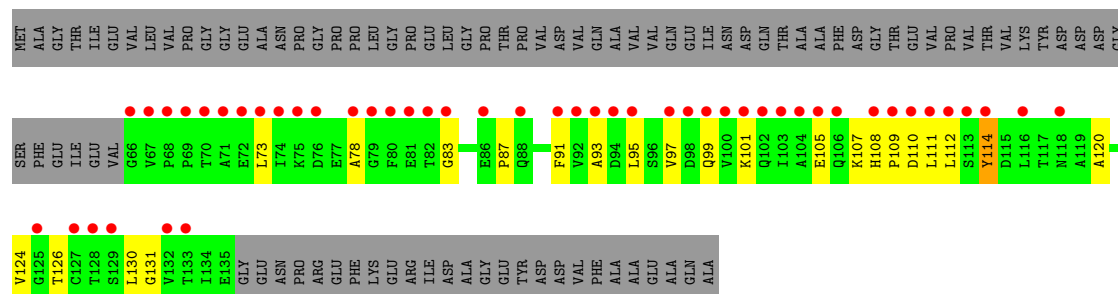
- Molecule 8: 50S ribosomal protein L10e

Chain H:



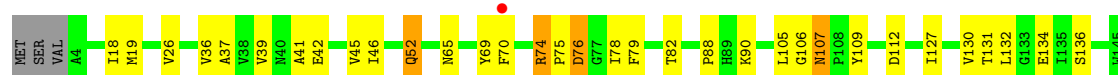
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

Chain J:



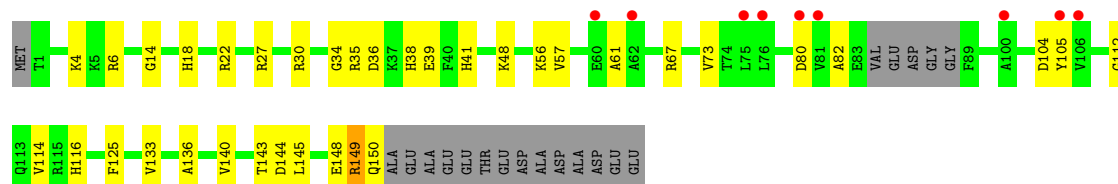
- Molecule 11: 50S ribosomal protein L14P

Chain K:



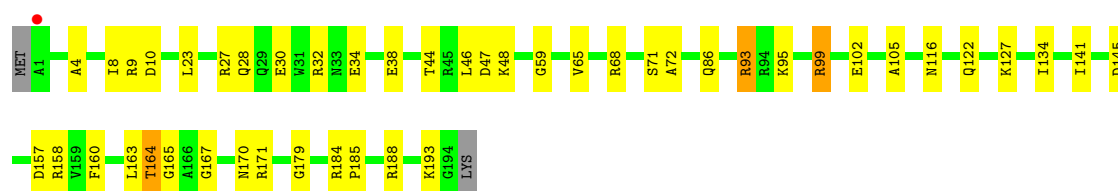
- Molecule 12: 50S ribosomal protein L15P

Chain L:



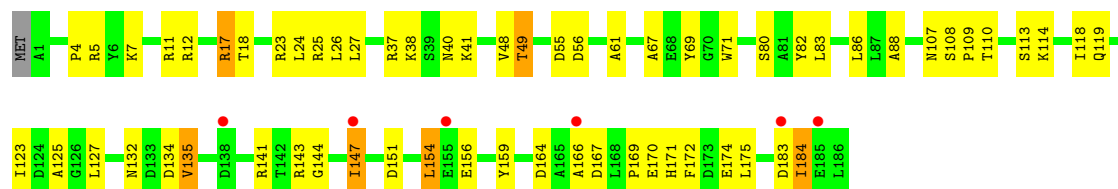
- Molecule 13: 50S ribosomal protein L15e

Chain M:



- Molecule 14: 50S ribosomal protein L18P

Chain N:



- Molecule 15: 50S ribosomal protein L18e

Chain O:



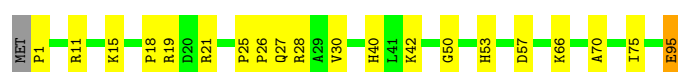
- Molecule 16: 50S ribosomal protein L19e

Chain P:



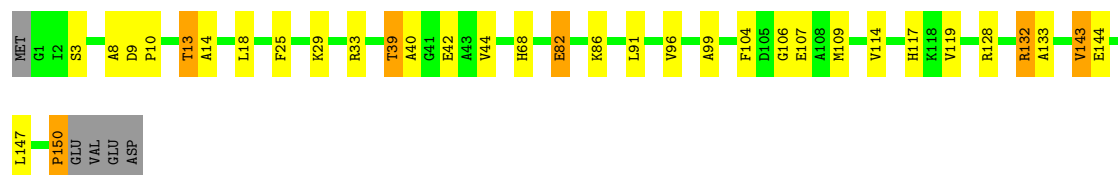
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:

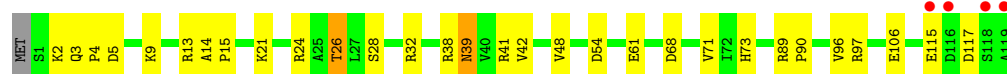


- Molecule 19: 50S ribosomal protein L23P

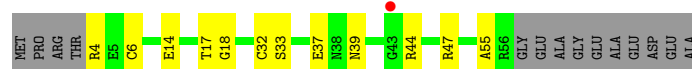
Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T: 

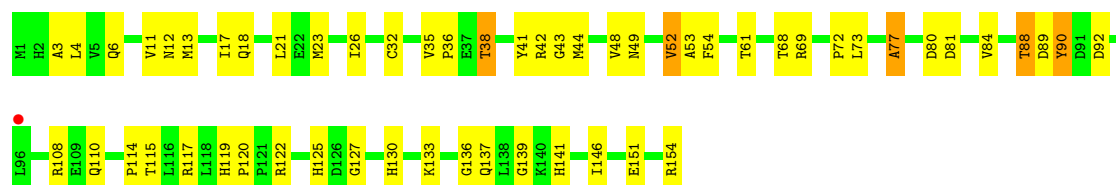
- Molecule 21: 50S ribosomal protein L24e

Chain U: 

- Molecule 22: 50S ribosomal protein L29P

Chain V: 

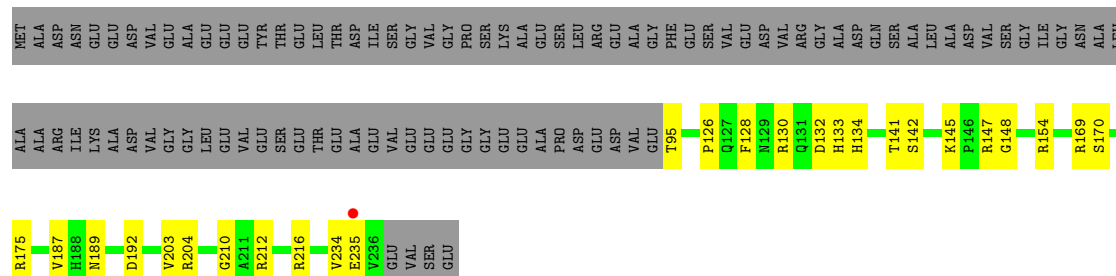
- Molecule 23: 50S ribosomal protein L30P

Chain W: 

- Molecule 24: 50S ribosomal protein L31e

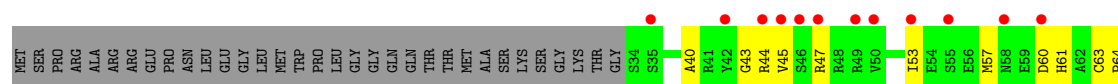
Chain X: 

- Molecule 25: 50S ribosomal protein L32e

Chain Y: 

- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 



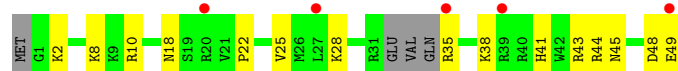
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



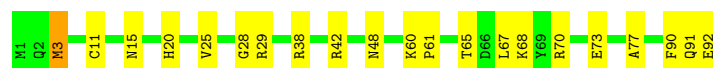
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



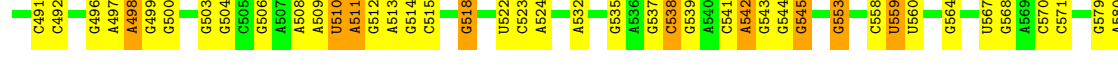
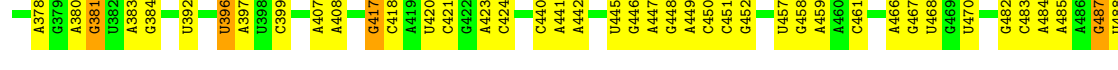
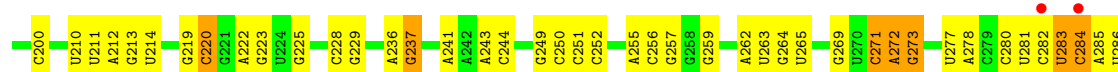
• Molecule 29: 50S ribosomal protein L44E

Chain 3:

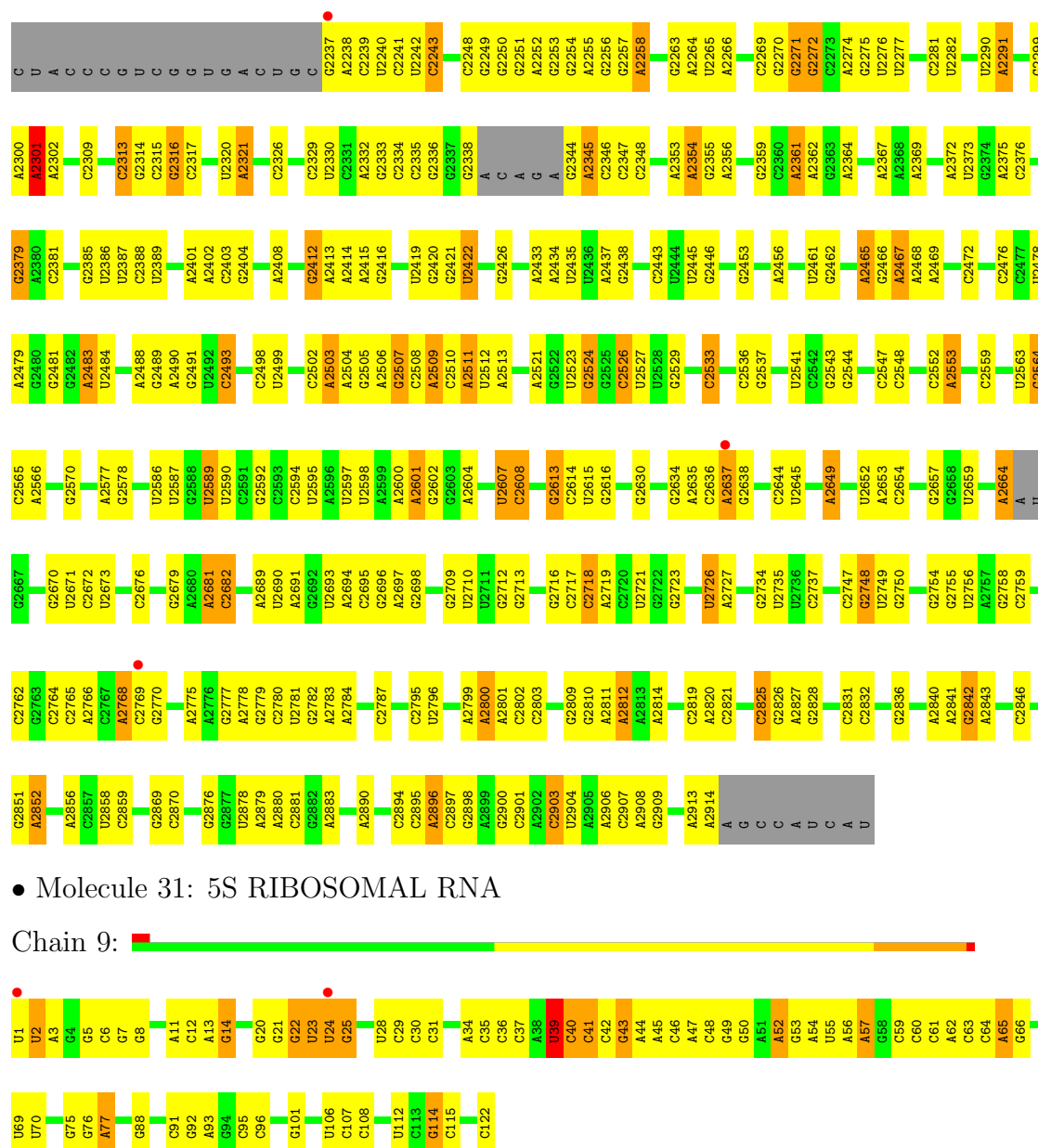


• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



G2073	C1853	G1743	C1652	G1546	A1434	C1343	A1242	C1168	C1068	C880	A790	G884
A2074	C1854	C1760	A1653	G1552	C1436	G1344	A1243	U1169	C1069	C	A791	C885
A2081	C1855	C1751	U1654	C1553	C1435	U1350	U1244	A1171	G1071	C	G792	C886
G2082	C1856	G1752	A1655	C1554	G1441	G1351	C1245	A1172	G1072	A	U800	G887
A2083	A1857	A1759	A1656	C1555	A1442	C1352	A1246	A1173	A1078	G	G801	G888
G2088	A1858	C1760	A1657	C1556	U1446	C1353	U1249	A1174	A1079	A	A807	G889
A2089	G1863	U1761	A1658	U	U1447	A1358	U1250	G1176	A1080	G	A808	G890
G2090	C1868	C1762	G1665	C1561	U1450	U1359	C1268	A1177	A1081	A	G809	C895
C2091	A1969	C1763	A1666	U1562	C1451	C1360	G1269	U1180	A1088	G	U903	C896
G2092	G1871	U1766	A1667	A1573	C1451	C1366	G1273	U1181	U1088	U	A812	G897
A2096	C1872	A1767	U1668	U1573	U1461	A1372	C1273	C1182	A1097	C	C905	A898
A2101	G1873	C1768	U1677	G1586	C1462	G1372	A1278	C1183	A1098	G	G912	C899
G2102	G1877	U1770	A1678	U1587	C1462	C1374	A1279	U1185	A1099	C	U920	A904
A2103	G1878	U1771	C1679	G1588	C1474	A1375	U1280	U1186	G1104	A	C921	A912
G2104	G1879	G1772	A1682	G1589	C1474	G1376	A1281	U1187	C1104	C	G820	G702
A2105	U1883	C1773	A1683	C1592	C1477	C1377	A1287	U1188	U1109	A	A922	G703
C2106	G1884	G1774	A1684	C1593	U1478	G1378	U1288	A1189	G1110	C999	U821	C705
G2110	A1885	A1778	A1685	C1594	C1482	U1380	C1289	G1190	G1111	C1000	C822	G709
A2111	A1886	A1779	G1686	G1595	A1483	G1381	G1290	A1191	U1115	U1001	U823	G710
G2112	A1887	U1795	C1687	U1596	G1484	G1382	A1291	A1192	U1116	G1002	G824	G711
C2113	G1892	C1787	C1688	A1597	A1485	U1383	A1294	A1193	A1117	A1005	U826	C712
C2114	U1897	U1788	G1697	A1598	A1486	C1384	G1295	A1194	U1113	A1006	A827	U713
G2115	G1903	G1789	C1699	A1603	A1487	G1385	A1296	G1195	G1119	A1007	C834	U714
U2116	A1904	U1791	C1700	G1604	U1488	C1386	U1297	U1120	U1120	C1008	U835	U
G2121	U1905	U1795	A1701	G1605	U1488	G1387	U1298	U1198	G1121	U1009	G836	G716
C2122	G1909	A1796	U1702	A1606	C1495	C1396	G1299	A1199	G1127	C1010	G944	C717
G2128	A1919	C1797	G1706	A1615	U1503	G1397	G1300	U1200	U1128	U1014	U840	C718
G2134	G1920	G1805	A1710	C1617	A1504	C1398	U1304	A1201	U1129	C1015	A841	G724
A2135	A1921	G1806	U1710	C1617	U1505	A1399	G1311	A1207	G1136	U1026	G848	C725
C2136	A1922	G1806	U1710	C1617	U1506	C1400	G1312	C1208	G1137	G1027	U849	U734
A	G1925	C1818	C1714	G1622	C1513	G1401	U1314	U1205	G1138	U1028	C853	C735
C	G1926	G1819	U1715	C1623	C1514	G1401	G1312	U1206	U1139	U1029	U854	A736
A	A1927	G1820	A1717	A1624	U1516	G1401	G1313	U1207	C1140	C1044	A857	A737
C	C1940	U1825	U1722	U1625	G1520	A1407	U1314	C1211	U1149	G1045	U858	G738
G	A1941	C1826	G1723	G1627	C1521	U1408	A1321	G1212	A1150	G1052	A861	C741
C	C1942	A1829	U1724	G1627	A1522	G1409	G1322	G1216	G1151	G1053	C959	G744
A	C1943	C1830	C1725	A1630	U1524	G1413	G1325	G1221	A1154	G1054	G960	G745
C	G1947	G1834	G1730	A1631	A1525	A1414	A1328	C1229	G1155	G1055	A867	G748
A	G1948	U1835	A1731	C1633	A1527	G1415	U1331	A1230	U1159	U1056	G868	C749
C	G1949	U1836	A1732	G1634	A1528	U1419	C1332	A1231	G1160	G1057	G869	A750
A	G1950	U1838	A1733	U1635	G1535	U1422	U1333	A1232	A1161	U	C870	C759
G	G1951	U1839	C1735	A1637	C1536	A1423	C1334	U1234	G1162	U	U872	C764
U	U	A1840	A1736	A1641	C1537	A1424	G1339	G1235	G1163	C1060	A875	G765
G	A	A1845	G1739	A1642	C1538	G1425	G1340	A1236	U1164	C	A876	G775
A	C	U1846	U1740	C1643	U1539	C1426	A1341	U1237	G1165	G	G877	A776
G	U	A1847	U1741	C1644	U1540	G1430	C1342	G1238	A1166	U1066	C878	U777
C	U	G1848	A1742	U1645	C1545	G1430	C1342	G1239	G1167	A1067	C879	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	213.16Å 300.03Å 576.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.90 85.91 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.90) 92.3 (85.91-2.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.220 0.167 , 0.211	Depositor DCC
R_{free} test set	3626 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 667133 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.31	0/241	0.49	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.33	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.32	0/648	0.55	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.59	0/562
22	V	0.33	0/502	0.52	0/675
23	W	0.34	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.37	0/584	0.60	0/781
27	1	0.39	0/438	0.59	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.55	0/1024
30	0	0.37	0/65957	0.68	13/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	20/147586 (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	28
31	9	0	1
All	All	1	30

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.29	2.86	1.50
18	R	150	PRO	CA-C	-18.25	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47
18	R	150	PRO	N-CD	10.73	1.62	1.47
18	R	150	PRO	CA-CB	7.62	1.68	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.40	61.65	112.10
18	R	150	PRO	CA-N-CD	12.30	128.92	111.70
18	R	150	PRO	N-CA-CB	10.97	116.46	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20
30	0	1120	U	C5'-C4'-C3'	-6.39	105.78	116.00
30	0	1942	A	C5'-C4'-C3'	6.16	125.85	116.00
18	R	150	PRO	CA-CB-CG	-6.09	92.42	104.00
30	0	1592	G	N9-C1'-C2'	5.90	121.67	114.00
30	0	1504	A	C1'-O4'-C4'	-5.90	105.18	109.90
31	9	39	U	N1-C1'-C2'	5.83	121.57	114.00
30	0	871	G	C5'-C4'-O4'	-5.67	102.30	109.10
30	0	2316	G	C5'-C4'-C3'	-5.59	107.06	116.00
30	0	1504	A	N9-C1'-C2'	5.50	121.15	114.00
30	0	841	A	C1'-O4'-C4'	-5.46	105.53	109.90
30	0	2313	C	C5'-C4'-O4'	5.29	115.45	109.10
30	0	2726	U	N1-C1'-C2'	5.25	120.83	114.00
30	0	1165	G	C1'-O4'-C4'	-5.21	105.73	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2291	A	N9-C1'-C2'	5.20	120.75	114.00
30	0	2301	A	N9-C1'-C2'	5.11	120.65	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	131	A	Sidechain
30	0	1430	G	Sidechain
30	0	1592	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	220	C	Sidechain
30	0	2301	A	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2524	G	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	333	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	888	U	Sidechain
31	9	39	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	63	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	59	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	29	0
6	F	890	0	843	26	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	32	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	51	0
15	O	865	0	873	18	0
16	P	1136	0	1123	24	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	10	0
20	T	950	0	924	21	0
21	U	410	0	364	8	0
22	V	499	0	511	17	0
23	W	1196	0	1137	56	0
24	X	654	0	653	18	0
25	Y	1130	0	1133	23	0
26	Z	573	0	532	15	0
27	1	431	0	426	23	0
28	2	396	0	413	15	0
29	3	755	0	728	18	0
30	0	59020	0	29811	1159	0
31	9	2599	0	1325	100	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	67	0	0	0	0
34	9	2	0	0	0	0
34	C	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	4	0
35	3	1	0	0	0	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	1	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	93	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	3	0	0	0	0
36	B	2	0	0	0	0
36	F	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	5929	0	0	185	0
38	1	63	0	0	4	0
38	2	50	0	0	1	0
38	3	62	0	0	3	0
38	9	147	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	116	0	0	5	0
38	B	141	0	0	13	0
38	C	170	0	0	13	0
38	D	44	0	0	3	0
38	E	45	0	0	2	0
38	F	27	0	0	2	0
38	G	19	0	0	1	0
38	H	63	0	0	7	0
38	I	8	0	0	3	0
38	J	53	0	0	1	0
38	K	56	0	0	5	0
38	L	85	0	0	6	0
38	M	123	0	0	2	0
38	N	55	0	0	5	0
38	O	43	0	0	3	0
38	P	67	0	0	2	0
38	Q	50	0	0	3	0
38	R	85	0	0	1	0
38	S	33	0	0	2	0
38	T	34	0	0	2	0
38	U	27	0	0	2	0
38	V	13	0	0	2	0
38	W	69	0	0	4	0
38	X	25	0	0	2	0
38	Y	95	0	0	5	0
38	Z	26	0	0	3	0
All	All	99122	0	59913	1941	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 13.

All (1941) 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	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.77	1.12
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.09	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.31	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.63	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.09
13:M:171:ARG:HD3	30:0:156:C:H5''	1.33	1.09
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.06
30:0:545:G:H8	30:0:545:G:H5'	1.19	1.06
30:0:1205:U:H2'	30:0:1206:U:H5''	1.32	1.04
30:0:1160:G:H5'	30:0:1161:A:H5'	1.03	1.02
30:0:1701:A:H4'	30:0:1702:U:H5''	1.42	1.01
15:O:3:THR:HG22	30:0:656:G:H5'	1.41	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
30:0:1979:G:H2'	38:0:3301:HOH:O	1.61	0.98
31:9:29:C:H2'	31:9:30:C:H5'	1.44	0.98
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.46	0.97
11:K:10:GLN:H	11:K:10:GLN:HE21	0.95	0.95
30:0:182:G:H5'	38:0:5168:HOH:O	1.67	0.95
30:0:1666:C:O2'	30:0:1667:A:H5''	1.67	0.94
30:0:1118:A:H3'	30:0:1118:A:H8	1.30	0.94
30:0:2717:C:H2'	30:0:2718:C:H5''	1.50	0.94
30:0:381:G:H5''	38:0:4330:HOH:O	1.67	0.93
30:0:1187:U:HO2'	30:0:1189:A:H2	1.01	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
30:0:1118:A:H3'	30:0:1118:A:C8	2.03	0.93
30:0:1603:A:H5'	30:0:1605:G:O4'	1.67	0.92
30:0:1634:G:H3'	38:0:3907:HOH:O	1.70	0.91
30:0:282:C:H1'	30:0:368:C:N4	1.84	0.91
16:P:115:SER:H	16:P:118:GLN:HE21	1.03	0.91
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.91
30:0:271:C:H41	30:0:378:A:H2	1.17	0.90
2:B:162:MET:SD	2:B:310:ARG:HD3	2.11	0.90
30:0:559:U:H5'	30:0:559:U:H6	1.35	0.90
30:0:545:G:C8	30:0:545:G:H5'	2.05	0.90
30:0:871:G:H8	30:0:871:G:C5'	1.85	0.90
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.20	0.90
30:0:542:A:H5'	30:0:542:A:H8	1.36	0.90
31:9:14:G:H5'	31:9:14:G:H8	1.37	0.90
31:9:56:A:C2'	31:9:57:A:H5''	2.03	0.89
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.55	0.89
30:0:1119:G:H22	30:0:1246:A:H2	1.20	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.88
30:0:1632:A:H2'	30:0:1633:C:H5'	1.56	0.88
30:0:2508:C:H2'	38:0:6764:HOH:O	1.73	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.87
30:0:558:C:C2'	30:0:559:U:H5''	2.05	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1205:U:C2'	30:0:1206:U:H5''	2.05	0.86
30:0:506:G:H22	30:0:509:A:H5'	1.40	0.86
30:0:1184:C:H1'	38:0:7480:HOH:O	1.74	0.86
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.73	0.86
30:0:2507:G:H2'	30:0:2510:C:H42	1.41	0.86
30:0:541:C:C2'	30:0:542:A:H5''	2.06	0.86
30:0:2908:A:H2'	30:0:2909:G:O4'	1.76	0.86
30:0:1189:A:H1'	30:0:1209:C:O4'	1.76	0.85
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.58	0.85
30:0:1183:C:H2'	38:0:6249:HOH:O	1.76	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.75	0.85
30:0:2717:C:O2'	30:0:2718:C:H5''	1.77	0.85
30:0:541:C:H2'	30:0:542:A:H5''	1.58	0.85
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.84
30:0:2291:A:C8	30:0:2309:C:H5'	2.12	0.84
2:B:238:ASN:HD22	2:B:240:GLY:H	1.24	0.84
38:O:7674:HOH:O	30:0:653:U:H5''	1.77	0.84
30:0:1206:U:H6	30:0:1206:U:H5'	1.41	0.84
30:0:2710:U:H1'	38:0:7632:HOH:O	1.77	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	1.21	0.84
31:9:2:U:OP2	31:9:3:A:H5'	1.78	0.84
30:0:1474:C:H6	30:0:1474:C:H5'	1.43	0.83
30:0:558:C:O2'	30:0:559:U:H5''	1.78	0.83
30:0:1474:C:C6	30:0:1474:C:H5'	2.13	0.83
18:R:29:LYS:HE2	30:0:524:A:C5'	2.08	0.83
4:D:154:LYS:HD2	4:D:154:LYS:H	1.43	0.83
30:0:506:G:H22	30:0:509:A:C5'	1.92	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.82
30:0:1116:U:O2'	30:0:1118:A:H2	1.62	0.82
14:N:37:ARG:HH12	31:9:6:C:H5''	1.43	0.82
18:R:29:LYS:HE2	30:0:524:A:H5''	1.59	0.82
30:0:1116:U:H3	30:0:1246:A:H62	1.24	0.82
30:0:283:U:H5	30:0:284:C:N3	1.78	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.27	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.15	0.81
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.62	0.81
30:0:1878:G:H1'	38:0:6126:HOH:O	1.77	0.81
30:0:2852:A:H5''	38:0:5244:HOH:O	1.80	0.81
15:O:3:THR:CG2	30:0:656:G:H5'	2.10	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.63	0.81
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.81
30:0:2529:G:H3'	38:0:7197:HOH:O	1.80	0.80
30:0:2506:A:O2'	30:0:2507:G:H8	1.64	0.79
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.62	0.79
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.63	0.79
30:0:2502:C:C2'	30:0:2503:A:H5'	2.13	0.78
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.65	0.78
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.64	0.78
11:K:39:GLY:HA2	38:0:5232:HOH:O	1.83	0.78
30:0:2578:G:H5'	30:0:2578:G:H8	1.48	0.78
30:0:1632:A:C2'	30:0:1633:C:H5'	2.13	0.78
30:0:2256:G:O2'	30:0:2257:G:H5'	1.82	0.78
3:C:236:THR:HG22	3:C:239:ALA:H	1.46	0.78
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.66	0.78
30:0:282:C:O2'	30:0:283:U:H5'	1.84	0.78
14:N:113:SER:HB2	38:N:8849:HOH:O	1.84	0.77
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.67	0.77
30:0:2526:C:H5'	30:0:2526:C:C6	2.19	0.77
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.65	0.77
30:0:1300:G:H1'	38:0:4694:HOH:O	1.83	0.77
30:0:2635:A:O2'	30:0:2636:C:H5'	1.84	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
30:0:272:A:H3'	38:0:7542:HOH:O	1.84	0.77
31:9:14:G:H5'	31:9:14:G:C8	2.19	0.77
30:0:2502:C:H2'	30:0:2503:A:H5'	1.65	0.77
30:0:2608:C:H3'	38:0:7824:HOH:O	1.85	0.77
30:0:396:U:H1'	38:0:7640:HOH:O	1.85	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.50	0.76
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.76
30:0:1701:A:H5'	38:0:6290:HOH:O	1.83	0.76
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.76
30:0:2783:A:H3'	38:0:5242:HOH:O	1.83	0.76
30:0:2812:A:H2	30:0:2814:A:H62	1.31	0.76
30:0:2679:G:H2'	30:0:2681:A:OP2	1.86	0.76
31:9:54:A:O2'	31:9:55:U:H5'	1.85	0.76
30:0:1372:A:H3'	38:0:7202:HOH:O	1.86	0.76
30:0:2403:C:H5'	38:0:6033:HOH:O	1.84	0.76
22:V:1:THR:HB	30:0:93:C:H5''	1.68	0.76
30:0:192:A:H5'	38:0:7655:HOH:O	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.75
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.69	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.52	0.75
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.51	0.75
30:0:1172:G:H5''	38:0:7271:HOH:O	1.85	0.75
30:0:1116:U:HO2'	30:0:1118:A:H2	0.79	0.74
30:0:558:C:H2'	30:0:559:U:C5'	2.17	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.15	0.74
3:C:1:MET:HG2	3:C:2:GLN:H	1.51	0.74
30:0:2748:G:H5'	38:0:7554:HOH:O	1.87	0.74
30:0:2768:A:O2'	30:0:2769:C:H5'	1.87	0.74
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.70	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
30:0:2404:G:H5''	38:0:5222:HOH:O	1.88	0.74
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.23	0.73
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.73
35:0:8812:CL:CL	38:0:5135:HOH:O	2.41	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.53	0.73
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.54	0.73
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.73
1:A:211:LYS:HB2	38:A:9082:HOH:O	1.87	0.73
30:0:2004:U:H4'	38:0:5316:HOH:O	1.88	0.73
30:0:138:U:H5''	30:0:139:C:OP2	1.88	0.73
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.87	0.73
30:0:2896:A:H5''	38:0:6105:HOH:O	1.87	0.73
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.53	0.73
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.89	0.73
3:C:139:VAL:HG13	38:C:8644:HOH:O	1.88	0.73
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.71	0.73
30:0:1666:C:C2'	30:0:1667:A:H5''	2.19	0.72
30:0:1641:A:H2'	30:0:1642:A:H5'	1.71	0.72
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.88	0.72
30:0:2765:C:H4'	38:0:5531:HOH:O	1.88	0.72
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.72
22:V:50:ARG:NH1	30:0:56:G:H5''	2.04	0.72
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.72
30:0:2256:G:C2'	30:0:2257:G:H5'	2.18	0.72
28:2:41:HIS:H	28:2:45:ASN:HD22	1.35	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:827:A:H1'	38:0:6220:HOH:O	1.88	0.72
30:0:468:U:H3'	38:0:7580:HOH:O	1.89	0.72
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.72
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.72
30:0:2769:C:C2'	30:0:2770:G:H5'	2.20	0.72
22:V:50:ARG:HH12	30:0:56:G:H5''	1.55	0.72
30:0:1201:C:H5''	38:0:6238:HOH:O	1.89	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.24	0.72
20:T:9:LYS:HE2	20:T:13:ARG:NH1	2.04	0.72
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.04	0.71
35:0:8813:CL:CL	38:0:4694:HOH:O	2.45	0.71
30:0:1183:C:N4	30:0:1184:C:H41	1.87	0.71
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.55	0.71
31:9:29:C:C2'	31:9:30:C:H5'	2.18	0.71
30:0:1525:G:H5'	30:0:1526:A:OP2	1.91	0.71
30:0:2491:G:H1'	38:0:6878:HOH:O	1.89	0.71
30:0:1189:A:H3'	38:0:7693:HOH:O	1.90	0.71
30:0:1741:U:H5'	30:0:1742:A:OP1	1.90	0.71
30:0:2372:A:H2'	30:0:2373:U:H6	1.56	0.70
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.21	0.70
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.92	0.70
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.57	0.70
2:B:206:THR:HG21	30:0:2716:G:H5''	1.73	0.70
31:9:20:G:O2'	31:9:21:G:H5'	1.91	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
30:0:2659:U:H5''	38:0:4138:HOH:O	1.92	0.70
30:0:2637:A:H5'	38:0:9281:HOH:O	1.92	0.70
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.70
30:0:567:U:H5''	38:0:5297:HOH:O	1.92	0.70
30:0:1973:A:H5'	30:0:1973:A:H8	1.57	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
30:0:1750:C:H5''	38:0:3676:HOH:O	1.91	0.69
30:0:544:G:H2'	30:0:545:G:H5''	1.74	0.69
30:0:380:A:H2'	38:0:7240:HOH:O	1.92	0.69
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.75	0.69
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.91	0.69
30:0:2010:A:H2'	38:0:5965:HOH:O	1.91	0.69
7:G:12:ILE:HG23	38:0:5468:HOH:O	1.93	0.69
30:0:281:U:O2'	30:0:282:C:H5'	1.93	0.69
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.23	0.69
16:P:115:SER:H	16:P:118:GLN:NE2	1.85	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.91	0.69
1:A:51:ARG:HB2	38:A:9066:HOH:O	1.91	0.69
30:0:2251:G:H2'	30:0:2252:A:C8	2.28	0.69
30:0:1377:C:H6	30:0:1377:C:H5'	1.58	0.69
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.68
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.68
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.91	0.68
30:0:2111:G:H1'	38:0:9053:HOH:O	1.92	0.68
30:0:2768:A:H2'	30:0:2769:C:O4'	1.93	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.94	0.68
30:0:1183:C:H42	30:0:1184:C:H41	1.42	0.68
13:M:23:LEU:HD13	13:M:27:ARG:HH21	1.57	0.68
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.75	0.68
3:C:174:ILE:HD11	30:0:338:C:H4'	1.75	0.68
12:L:133:VAL:HA	38:L:8874:HOH:O	1.92	0.68
30:0:1603:A:C5'	30:0:1605:G:H5'	2.23	0.68
6:F:91:VAL:HG12	6:F:92:GLY:N	2.09	0.68
14:N:141:ARG:HH21	31:9:48:C:H4'	1.58	0.68
30:0:2453:G:H3'	38:0:5927:HOH:O	1.94	0.68
14:N:80:SER:HB2	38:N:8830:HOH:O	1.93	0.68
30:0:558:C:H2'	30:0:559:U:H5''	1.72	0.67
30:0:2256:G:H2'	30:0:2257:G:C5'	2.23	0.67
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.76	0.67
31:9:39:U:H1'	31:9:44:A:H61	1.59	0.67
31:9:23:U:O2'	31:9:24:U:H4'	1.94	0.67
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.67
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.60	0.67
18:R:150:PRO:O	18:R:150:PRO:CG	2.41	0.67
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.67
30:0:1730:G:H5'	30:0:1731:C:C5	2.30	0.67
30:0:285:A:H2'	30:0:286:U:O4'	1.95	0.67
30:0:1834:C:H2'	30:0:1840:A:N6	2.09	0.66
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.77	0.66
23:W:88:THR:HG22	23:W:89:ASP:H	1.60	0.66
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.76	0.66
30:0:2509:A:OP2	30:0:2510:C:H5	1.78	0.66
30:0:2237:G:H1'	38:0:4866:HOH:O	1.94	0.66
30:0:853:C:H3'	38:0:4563:HOH:O	1.95	0.66
30:0:125:U:H2'	38:0:3776:HOH:O	1.94	0.66
30:0:2256:G:H2'	30:0:2257:G:H5'	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2372:A:H2'	30:0:2373:U:C6	2.30	0.66
30:0:1524:U:OP1	30:0:1524:U:H4'	1.95	0.66
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.76	0.66
30:0:1120:U:H5'	30:0:1121:G:OP2	1.95	0.66
21:U:14:GLU:O	21:U:17:THR:HB	1.95	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
31:9:22:G:H5'	31:9:23:U:OP1	1.94	0.66
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.66
30:0:31:C:H2'	38:0:7702:HOH:O	1.95	0.66
30:0:2836:G:H1'	38:0:6850:HOH:O	1.95	0.66
30:0:2498:C:O2'	30:0:2499:U:H5'	1.94	0.66
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.76	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.66
23:W:26:ILE:HB	38:W:5420:HOH:O	1.95	0.66
30:0:2320:U:H4'	30:0:2321:A:O4'	1.95	0.66
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.31	0.66
8:H:29:SER:HA	8:H:62:HIS:HD2	1.60	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.26	0.66
30:0:283:U:C5	30:0:284:C:N3	2.63	0.66
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.66
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.66
30:0:1562:C:O2	30:0:1562:C:H2'	1.95	0.66
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.66
30:0:2748:G:H1'	38:0:7914:HOH:O	1.95	0.65
30:0:485:A:N3	30:0:487:G:H5''	2.10	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.96	0.65
13:M:171:ARG:CD	30:0:156:C:H5''	2.18	0.65
1:A:35:GLY:O	1:A:36:ASP:HB3	1.96	0.65
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.65
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.78	0.65
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.96	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.26	0.65
30:0:1666:C:C2'	30:0:1667:A:C5'	2.74	0.65
30:0:2766:A:H5'	38:0:9565:HOH:O	1.97	0.65
30:0:836:G:H5''	38:0:9288:HOH:O	1.95	0.65
10:J:74:ARG:O	10:J:78:ILE:HG12	1.97	0.65
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.65
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:960:G:H3'	30:0:960:G:N3	2.12	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
30:0:1183:C:O2	30:0:1183:C:H2'	1.95	0.64
30:0:1279:U:O2	30:0:1279:U:H2'	1.95	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:281:U:H2'	30:0:282:C:O4'	1.96	0.64
31:9:31:C:H1'	38:9:9014:HOH:O	1.96	0.64
18:R:29:LYS:HE2	30:0:524:A:H5'	1.79	0.64
19:S:43:GLU:HB3	38:S:8991:HOH:O	1.97	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.10	0.64
10:J:107:ASN:ND2	10:J:109:TYR:H	1.96	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.80	0.64
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.63	0.64
30:0:814:G:H4'	38:0:3141:HOH:O	1.98	0.64
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.79	0.64
30:0:564:G:H1'	38:0:6317:HOH:O	1.97	0.64
29:3:73:GLU:HB3	38:3:9049:HOH:O	1.97	0.64
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.80	0.64
30:0:2481:G:H5''	38:0:4558:HOH:O	1.97	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.80	0.64
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
18:R:9:ASP:O	18:R:13:THR:HB	1.98	0.63
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.27	0.63
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.63
14:N:11:ARG:HD3	31:9:114:G:O6	1.99	0.63
30:0:12:U:H2'	30:0:13:G:H5'	1.80	0.63
3:C:184:ARG:NH2	30:0:450:C:OP1	2.32	0.63
12:L:41:HIS:HD2	30:0:926:A:O2'	1.80	0.63
38:I:1549:HOH:O	30:0:1180:U:H1'	1.97	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.63
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.28	0.63
3:C:140:VAL:HB	38:C:8647:HOH:O	1.99	0.63
30:0:2768:A:H5''	38:0:4438:HOH:O	1.98	0.63
30:0:1243:C:H3'	38:0:4848:HOH:O	1.99	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.62
30:0:1166:A:OP1	30:0:1174:A:H4'	1.99	0.62
30:0:671:A:O2'	30:0:672:G:H2'	1.99	0.62
30:0:1185:U:H5'	38:0:7480:HOH:O	1.99	0.62
30:0:2426:G:H1'	38:0:6098:HOH:O	1.99	0.62
30:0:2781:U:H2'	30:0:2782:G:H5'	1.79	0.62
31:9:114:G:H2'	31:9:115:C:C6	2.35	0.62
30:0:848:C:H5'	38:0:7283:HOH:O	1.99	0.62
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.97	0.62
31:9:49:G:O2'	31:9:50:G:H5'	1.99	0.62
30:0:1527:A:H1'	30:0:1528:A:C8	2.34	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.80	0.62
30:0:559:U:H5'	30:0:559:U:C6	2.26	0.62
12:L:136:ALA:HB3	38:L:8874:HOH:O	2.00	0.62
31:9:39:U:H3'	31:9:40:C:H5''	1.82	0.62
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.82	0.62
30:0:2316:G:H4'	38:0:6098:HOH:O	2.00	0.62
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.39	0.62
30:0:1398:G:O2'	30:0:1399:A:H5'	2.00	0.62
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.81	0.62
27:1:28:HIS:HE1	30:0:776:A:OP1	1.83	0.62
30:0:378:A:H1'	38:0:3510:HOH:O	1.98	0.62
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.62
30:0:2748:G:H2'	38:0:7554:HOH:O	1.98	0.62
30:0:1278:A:H4'	30:0:1279:U:C4	2.34	0.62
30:0:681:G:N3	30:0:681:G:H5'	2.15	0.62
30:0:1603:A:H5'	30:0:1605:G:C4'	2.30	0.61
30:0:2597:U:H2'	30:0:2598:U:H5'	1.81	0.61
38:B:9095:HOH:O	30:0:2672:C:H1'	2.00	0.61
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.81	0.61
30:0:1185:U:H2'	30:0:1186:C:C6	2.35	0.61
30:0:2781:U:C2'	30:0:2782:G:H5'	2.30	0.61
30:0:128:A:O2'	30:0:129:A:H5'	2.00	0.61
30:0:2300:A:H4'	30:0:2301:A:O5'	2.01	0.61
30:0:2851:G:O2'	30:0:2852:A:H5'	2.00	0.61
30:0:2769:C:H2'	30:0:2770:G:H5'	1.82	0.61
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.65	0.61
30:0:2252:A:C5	30:0:2253:G:H1'	2.34	0.61
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.61
9:I:110:ASP:O	30:0:1163:G:H5'	2.01	0.61
30:0:138:U:OP2	30:0:139:C:H5	1.83	0.61
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.61
23:W:81:ASP:OD1	23:W:92:ASP:HB2	1.99	0.61
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
30:0:308:U:H5'	30:0:309:C:OP1	1.99	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.12	0.61
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.83	0.61
30:0:255:A:H2'	30:0:256:C:H6	1.64	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.00	0.61
30:0:2894:C:O2'	30:0:2895:C:H5'	2.01	0.61
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.83	0.61
13:M:164:THR:HG22	13:M:167:GLY:N	2.15	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:1:U:O3'	31:9:3:A:H5''	2.01	0.61
30:0:1171:A:H2'	30:0:1172:G:H5'	1.81	0.61
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.61
30:0:1878:G:O2'	30:0:1879:U:C6	2.52	0.60
28:2:41:HIS:HD2	28:2:44:ARG:H	1.49	0.60
30:0:2718:C:H6	30:0:2718:C:H5'	1.66	0.60
13:M:145:ASP:HB2	38:M:8862:HOH:O	1.99	0.60
2:B:294:TYR:HE2	38:B:9111:HOH:O	1.84	0.60
30:0:2344:G:H2'	30:0:2344:G:N3	2.16	0.60
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.81	0.60
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.83	0.60
31:9:49:G:H2'	31:9:50:G:O4'	2.01	0.60
18:R:128:ARG:NH2	30:0:2054:A:N3	2.49	0.60
30:0:2616:G:H1'	38:0:9433:HOH:O	2.00	0.60
30:0:1174:A:C5	30:0:1201:C:H4'	2.36	0.60
30:0:1192:A:H3'	30:0:1193:A:H5'	1.83	0.60
30:0:1080:C:H4'	30:0:1081:A:OP1	2.01	0.60
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.83	0.60
30:0:1972:U:H2'	30:0:1973:A:C5'	2.31	0.60
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	1.99	0.60
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.83	0.60
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.19	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.01	0.60
30:0:2900:G:H2'	30:0:2901:C:O4'	2.01	0.60
2:B:62:ARG:HA	2:B:65:MET:CE	2.32	0.60
30:0:1182:C:H1'	30:0:1192:A:H8	1.67	0.60
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.01	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
30:0:1119:G:N2	30:0:1246:A:H2	1.92	0.60
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.42	0.60
1:A:48:ASP:HB3	38:A:9066:HOH:O	2.02	0.60
30:0:1730:G:H5''	30:0:1731:C:C6	2.37	0.60
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.83	0.60
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.59
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.59
30:0:515:C:H5''	38:0:5654:HOH:O	2.01	0.59
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.50	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:64:C:C2'	31:9:65:A:H5'	2.32	0.59
30:0:2505:G:H2'	30:0:2506:A:H5'	1.84	0.59
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.02	0.59
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
30:0:659:A:H5''	38:0:7111:HOH:O	2.03	0.59
30:0:2637:A:H4'	38:0:6071:HOH:O	2.02	0.59
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.59
30:0:1189:A:O2'	30:0:1208:C:H2'	2.03	0.59
31:9:49:G:H5''	38:9:9092:HOH:O	2.02	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
30:0:1189:A:H1'	30:0:1209:C:C1'	2.32	0.59
31:9:54:A:C2'	31:9:55:U:H5'	2.32	0.59
1:A:36:ASP:CB	1:A:85:SER:H	2.16	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
30:0:2613:G:O2'	30:0:2614:C:H5'	2.03	0.59
22:V:39:ALA:N	22:V:40:PRO:HD2	2.17	0.59
24:X:43:VAL:HG12	24:X:44:ASP:H	1.66	0.59
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.18	0.59
27:1:9:GLY:HA2	30:0:1687:C:O2	2.03	0.59
5:E:84:MET:HG2	5:E:168:ILE:HA	1.85	0.59
5:E:143:GLN:NE2	30:0:2779:G:H21	2.00	0.59
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.59
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.59
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.84	0.59
30:0:583:C:H2'	30:0:584:U:H6	1.68	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.59
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.84	0.59
30:0:1200:A:H3'	38:0:5763:HOH:O	2.03	0.58
31:9:76:G:C3'	31:9:77:A:H5''	2.24	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.86	0.58
23:W:13:MET:HE1	23:W:18:GLN:HA	1.83	0.58
31:9:1:U:H4'	31:9:3:A:OP1	2.03	0.58
30:0:2526:C:H5'	30:0:2526:C:H6	1.64	0.58
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.38	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
31:9:2:U:H4'	38:9:9104:HOH:O	2.02	0.58
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.02	0.58
30:0:1183:C:N3	30:0:1184:C:C5	2.72	0.58
30:0:2421:G:H1'	38:0:7033:HOH:O	2.03	0.58
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.58
8:H:168:VAL:HG13	38:H:210:HOH:O	2.03	0.58
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.85	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.68	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.58
30:0:90:A:H2'	30:0:91:G:O4'	2.02	0.58
30:0:1187:U:H2'	38:0:6907:HOH:O	2.04	0.58
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.58
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.85	0.58
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.04	0.58
30:0:644:G:N3	30:0:644:G:H5'	2.19	0.58
14:N:37:ARG:HH11	31:9:6:C:H5''	1.65	0.58
3:C:174:ILE:CD1	30:0:338:C:H4'	2.33	0.58
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.84	0.58
30:0:1174:A:C6	30:0:1201:C:H4'	2.39	0.58
21:U:17:THR:HG22	21:U:18:GLY:N	2.19	0.58
8:H:174:LEU:HA	38:H:220:HOH:O	2.02	0.58
9:I:126:THR:O	9:I:130:LEU:HG	2.03	0.58
2:B:258:GLY:H	2:B:260:HIS:CE1	2.21	0.58
31:9:107:C:O2'	31:9:108:C:H5'	2.04	0.57
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.57
30:0:2712:G:H5'	38:0:5232:HOH:O	2.03	0.57
30:0:2769:C:O2'	30:0:2770:G:H5'	2.04	0.57
2:B:98:THR:HG22	30:0:2820:A:OP1	2.04	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.39	0.57
30:0:952:G:N3	30:0:2302:A:H2'	2.19	0.57
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.20	0.57
31:9:29:C:H2'	31:9:30:C:C5'	2.28	0.57
30:0:2756:U:H3	30:0:2896:A:H2	1.48	0.57
30:0:420:U:H2'	30:0:421:C:C6	2.39	0.57
30:0:272:A:H5'	30:0:273:G:OP2	2.03	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.86	0.57
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.19	0.57
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.57
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.68	0.57
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.04	0.57
4:D:52:THR:HG21	30:0:2346:C:O2'	2.04	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.05	0.57
30:0:280:C:H2'	30:0:281:U:O4'	2.04	0.57
30:0:559:U:H6	30:0:559:U:C5'	2.12	0.57
17:Q:27:GLN:HE21	31:9:8:G:H4'	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.04	0.57
30:0:2135:A:O2'	30:0:2136:G:H5'	2.04	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.57
30:0:2787:C:H5	38:0:4643:HOH:O	1.86	0.57
30:0:2604:A:H5'	38:0:5798:HOH:O	2.04	0.57
13:M:28:GLN:O	13:M:32:ARG:HG3	2.04	0.57
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.57
30:0:1171:A:C2'	30:0:1172:G:H5'	2.35	0.57
30:0:1377:C:H5'	30:0:1377:C:C6	2.40	0.57
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.57
30:0:1942:A:H3'	38:0:7360:HOH:O	2.03	0.57
12:L:4:LYS:HE2	30:0:645:U:OP2	2.05	0.57
31:9:75:G:H1	31:9:106:U:H3	1.53	0.57
30:0:1016:U:H1'	38:0:3667:HOH:O	2.04	0.57
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.86	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.19	0.57
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.87	0.57
3:C:188:ARG:HD3	38:C:8559:HOH:O	2.04	0.57
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.35	0.57
30:0:960:G:H2'	30:0:960:G:N3	2.20	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:2559:C:H4'	38:0:7268:HOH:O	2.05	0.57
30:0:2488:A:H1'	38:0:9096:HOH:O	2.03	0.57
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.42	0.57
30:0:2005:G:OP2	30:0:2005:G:H3'	2.05	0.57
3:C:1:MET:HG2	3:C:2:GLN:N	2.19	0.56
1:A:99:ILE:O	1:A:131:HIS:HE1	1.88	0.56
30:0:941:G:C5	30:0:942:U:C4	2.93	0.56
30:0:1304:U:H2'	30:0:1305:C:C6	2.40	0.56
30:0:711:G:H1'	38:0:7108:HOH:O	2.04	0.56
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.35	0.56
30:0:2578:G:C8	30:0:2578:G:H5'	2.36	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
30:0:1632:A:C3'	30:0:1633:C:H5'	2.35	0.56
29:3:70:ARG:HB3	38:3:9059:HOH:O	2.04	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.20	0.56
30:0:734:U:O2'	30:0:736:A:N7	2.39	0.56
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.05	0.56
30:0:1474:C:C5'	30:0:1474:C:H6	2.15	0.56
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.86	0.56
30:0:1947:G:N2	30:0:1966:U:C2	2.73	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:66:ARG:HH22	30:0:1994:A:P	2.29	0.56
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.56
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.69	0.56
20:T:2:LYS:HG2	30:0:447:A:OP1	2.05	0.56
30:0:506:G:N2	30:0:509:A:H5'	2.18	0.56
30:0:31:C:H4'	38:0:7437:HOH:O	2.06	0.56
27:1:42:SER:HB2	38:1:8956:HOH:O	2.05	0.56
16:P:143:ALA:HA	38:P:192:HOH:O	2.04	0.56
30:0:1209:C:H2'	30:0:1210:G:H8	1.70	0.56
31:9:13:A:O2'	31:9:14:G:H5''	2.06	0.56
30:0:2032:U:H2'	30:0:2033:G:C5'	2.36	0.56
30:0:368:C:H2'	30:0:369:G:H5'	1.88	0.56
30:0:363:C:O2'	30:0:364:U:H5'	2.06	0.56
30:0:876:A:N3	30:0:876:A:H2'	2.21	0.56
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.71	0.56
1:A:199:HIS:HD2	1:A:201:PHE:H	1.54	0.56
27:1:16:HIS:HD2	30:0:470:U:O2'	1.88	0.56
30:0:1972:U:H2'	30:0:1973:A:H5''	1.87	0.55
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.55
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.70	0.55
9:I:120:ALA:O	9:I:124:VAL:HG23	2.06	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.55
10:J:107:ASN:C	10:J:107:ASN:HD22	2.09	0.55
10:J:107:ASN:HD22	10:J:109:TYR:H	1.54	0.55
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.55
30:0:2064:U:H5'	30:0:2652:U:H4'	1.88	0.55
25:Y:212:ARG:HD2	38:Y:8900:HOH:O	2.07	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.55
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.89	0.55
30:0:821:U:H3'	38:0:3780:HOH:O	2.07	0.55
30:0:2781:U:H2'	30:0:2782:G:C5'	2.36	0.55
4:D:159:PRO:O	4:D:163:VAL:HG23	2.05	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.07	0.55
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.72	0.55
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.87	0.55
30:0:2254:G:H1'	38:0:5546:HOH:O	2.07	0.55
30:0:407:A:H5'	38:0:6032:HOH:O	2.06	0.55
30:0:2840:A:H3'	38:0:7659:HOH:O	2.05	0.55
30:0:168:C:O5'	30:0:168:C:H6	1.89	0.55
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.55
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.06	0.55
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.89	0.55
30:0:711:G:C2	30:0:718:C:C2	2.95	0.55
30:0:660:A:H4'	30:0:661:G:O5'	2.07	0.55
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.88	0.55
29:3:15:ASN:O	30:0:2408:A:H4'	2.06	0.55
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.89	0.55
30:0:1596:U:H2'	30:0:1598:A:OP2	2.07	0.55
30:0:1132:A:N6	30:0:1229:C:H2'	2.22	0.55
3:C:132:ASP:HB3	38:C:8560:HOH:O	2.06	0.55
31:9:55:U:H4'	31:9:56:A:C8	2.42	0.55
30:0:2510:C:H5'	30:0:2511:A:OP2	2.07	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.37	0.55
27:1:1:THR:HA	38:1:8958:HOH:O	2.06	0.55
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.89	0.55
4:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.55
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.89	0.55
7:G:64:ASN:N	7:G:64:ASN:HD22	2.04	0.55
30:0:1538:C:O2'	30:0:1539:U:H5'	2.06	0.55
2:B:145:HIS:HD2	2:B:146:THR:O	1.90	0.55
7:G:23:ILE:O	7:G:27:ILE:HG13	2.06	0.55
13:M:95:LYS:HE2	30:0:157:G:H4'	1.89	0.55
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.90	0.54
12:L:150:GLN:HB3	38:L:8869:HOH:O	2.06	0.54
1:A:121:ALA:O	1:A:124:VAL:HG22	2.07	0.54
30:0:2577:A:H8	38:0:9602:HOH:O	1.89	0.54
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.38	0.54
30:0:2083:A:H3'	38:0:7590:HOH:O	2.07	0.54
30:0:1523:G:C5	30:0:1524:U:C4	2.96	0.54
30:0:2878:U:H2'	30:0:2879:A:O4'	2.06	0.54
30:0:1154:A:H2'	30:0:1155:G:C8	2.42	0.54
30:0:1291:A:H2	38:0:5300:HOH:O	1.89	0.54
31:9:59:C:H6	31:9:59:C:O5'	1.90	0.54
2:B:27:ASN:H	2:B:27:ASN:HD22	1.56	0.54
30:0:2256:G:C2'	30:0:2257:G:C5'	2.84	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.07	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.42	0.54
30:0:292:G:H2'	30:0:358:G:N2	2.23	0.54
30:0:812:A:H1'	38:0:3969:HOH:O	2.06	0.54
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.38	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:52:A:O2'	31:9:53:G:H5'	2.08	0.54
30:0:241:A:C2	30:0:378:A:H4'	2.42	0.54
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.22	0.54
30:0:1477:C:H5'	30:0:1868:G:H5'	1.89	0.54
3:C:154:VAL:O	3:C:158:GLU:HG3	2.07	0.54
30:0:282:C:H1'	30:0:368:C:H41	1.72	0.54
17:Q:27:GLN:HE21	31:9:8:G:C5'	2.20	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54
30:0:441:A:H1'	30:0:442:A:N7	2.23	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.08	0.54
12:L:73:VAL:HG21	12:L:116:HIS:CE1	2.42	0.54
25:Y:204:ARG:HH22	30:0:553:G:P	2.31	0.54
3:C:218:VAL:HG12	38:C:8620:HOH:O	2.07	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.08	0.54
18:R:68:HIS:O	30:0:2842:G:H5'	2.08	0.54
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.88	0.54
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.54
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.48	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.07	0.54
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.90	0.54
18:R:132:ARG:HG2	18:R:133:ALA:N	2.23	0.53
4:D:105:SER:OG	30:0:2338:G:H1'	2.07	0.53
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.53
3:C:236:THR:HA	38:C:8647:HOH:O	2.08	0.53
10:J:39:VAL:HG13	10:J:106:GLY:O	2.08	0.53
15:O:73:ASP:HA	15:O:92:VAL:O	2.08	0.53
13:M:30:GLU:O	13:M:34:GLU:HG3	2.09	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.90	0.53
30:0:2670:G:O2'	30:0:2671:U:H5'	2.07	0.53
30:0:1819:G:H2'	30:0:1820:G:C4'	2.39	0.53
30:0:1586:G:O2'	30:0:1587:U:H5'	2.08	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.23	0.53
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.53
30:0:2842:G:H2'	30:0:2843:A:H5'	1.90	0.53
30:0:488:U:H2'	38:0:4019:HOH:O	2.08	0.53
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.53
30:0:1919:A:H4'	38:0:4862:HOH:O	2.07	0.53
30:0:1373:G:H1'	38:0:6143:HOH:O	2.08	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.72	0.53
30:0:1339:G:C6	30:0:1340:G:N1	2.77	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1205:U:C2'	30:0:1206:U:C5'	2.76	0.53
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.53
14:N:144:GLY:O	14:N:147:ILE:HG23	2.08	0.53
30:0:1451:C:H5'	30:0:1505:U:C5	2.43	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.53
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.43	0.53
30:0:544:G:C3'	30:0:545:G:H5''	2.39	0.53
4:D:154:LYS:HD2	4:D:154:LYS:N	2.16	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.39	0.53
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.44	0.53
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.91	0.53
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.53
30:0:920:C:H5''	30:0:921:G:O5'	2.09	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:1135:G:H5'	38:0:5935:HOH:O	2.07	0.53
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.74	0.53
30:0:635:A:H2'	30:0:636:G:H5''	1.90	0.53
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.91	0.53
30:0:510:U:H6	38:0:7450:HOH:O	1.92	0.53
30:0:299:U:H5'	38:0:7349:HOH:O	2.08	0.53
30:0:282:C:O2'	30:0:283:U:C5'	2.56	0.53
30:0:1166:A:P	30:0:1174:A:H4'	2.49	0.53
9:I:108:HIS:H	9:I:109:PRO:HD2	1.74	0.53
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.57	0.53
30:0:820:G:H3'	38:0:3058:HOH:O	2.08	0.53
30:0:513:A:N3	38:0:3668:HOH:O	2.34	0.53
30:0:1066:U:H2'	30:0:1067:A:C8	2.42	0.53
23:W:154:ARG:NH1	30:0:588:G:O6	2.42	0.53
30:0:284:C:C6	30:0:284:C:OP2	2.62	0.52
27:1:16:HIS:HE1	30:0:775:G:OP1	1.92	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:958:G:H2'	30:0:959:C:C6	2.43	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.39	0.52
5:E:11:VAL:HG12	5:E:12:ASP:N	2.24	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
2:B:254:GLN:HG2	2:B:255:GLY:N	2.24	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.09	0.52
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.91	0.52
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1787:C:H4'	30:0:2883:A:O4'	2.09	0.52
30:0:2356:A:H5'	38:0:5644:HOH:O	2.09	0.52
25:Y:216:ARG:HD2	38:Y:8870:HOH:O	2.08	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.44	0.52
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.92	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
30:0:1268:C:O2'	30:0:1269:G:H5'	2.08	0.52
14:N:5:ARG:NH1	30:0:1010:C:OP1	2.42	0.52
30:0:2291:A:N9	30:0:2309:C:H5'	2.25	0.52
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.52
30:0:1181:A:N1	30:0:1192:A:O2'	2.43	0.52
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.91	0.52
30:0:2263:G:H1'	38:0:6631:HOH:O	2.09	0.52
30:0:1515:A:H2'	30:0:1516:U:C6	2.44	0.52
30:0:1624:A:H5'	30:0:1626:A:O4'	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.09	0.52
15:O:32:ARG:HD3	15:O:32:ARG:O	2.09	0.52
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.44	0.52
30:0:120:A:H2'	30:0:120:A:N3	2.25	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.91	0.52
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.52
30:0:1314:U:H2'	38:0:5880:HOH:O	2.09	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.92	0.52
30:0:2445:U:H2'	30:0:2446:G:H8	1.75	0.52
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.92	0.52
30:0:2103:A:H2'	30:0:2104:C:H5'	1.92	0.52
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
30:0:1972:U:C2'	30:0:1973:A:H5''	2.39	0.52
30:0:1679:C:H5'	38:0:9331:HOH:O	2.10	0.52
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.52
31:9:45:A:H2'	31:9:46:C:H6	1.75	0.52
30:0:2359:G:H3'	38:0:5698:HOH:O	2.10	0.52
30:0:1170:U:H2'	30:0:1172:G:OP2	2.09	0.52
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.52
30:0:2756:U:N3	30:0:2896:A:C2	2.74	0.52
30:0:1730:G:C5'	30:0:1731:C:C5	2.93	0.52
30:0:2326:C:H4'	30:0:2412:G:H4'	1.92	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.09	0.52
6:F:21:GLU:O	6:F:24:ARG:HG2	2.09	0.52
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
30:0:2764:C:O2'	30:0:2765:C:H5'	2.09	0.52
30:0:567:U:H5''	38:0:6408:HOH:O	2.08	0.52
2:B:79:MET:HE1	38:B:9089:HOH:O	2.09	0.52
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.91	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
3:C:43:LYS:HG2	30:0:449:A:N7	2.25	0.52
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.47	0.51
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.10	0.51
30:0:613:C:H2'	30:0:614:U:H6	1.74	0.51
30:0:2524:G:H21	30:0:2526:C:N4	2.08	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.40	0.51
13:M:188:ARG:NH1	30:0:154:C:H3'	2.24	0.51
30:0:619:U:H3'	38:0:3289:HOH:O	2.09	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51
16:P:115:SER:OG	16:P:118:GLN:HG3	2.10	0.51
31:9:2:U:C4'	38:9:9104:HOH:O	2.57	0.51
30:0:2768:A:N3	30:0:2768:A:H3'	2.25	0.51
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.40	0.51
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.51
30:0:65:C:O2'	30:0:66:G:H5'	2.10	0.51
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.51
30:0:506:G:H22	30:0:509:A:H5''	1.73	0.51
30:0:1592:G:H2'	30:0:1593:C:C6	2.45	0.51
30:0:1878:G:C1'	38:0:6126:HOH:O	2.44	0.51
30:0:812:A:H2'	30:0:813:C:C6	2.45	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.91	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
12:L:61:ALA:HB2	12:L:105:TYR:CE2	2.45	0.51
26:Z:57:MET:HE3	38:0:6288:HOH:O	2.09	0.51
30:0:447:A:O2'	30:0:448:G:H5'	2.11	0.51
19:S:11:THR:H	19:S:14:ALA:HB3	1.75	0.51
30:0:1447:U:H3'	30:0:1506:U:O2	2.11	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.10	0.51
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.51
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.26	0.51
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.51
30:0:1730:G:H5'	30:0:1731:C:H5	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:256:C:H2'	30:0:257:G:O4'	2.10	0.51
30:0:1080:C:O5'	30:0:1080:C:H6	1.94	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.92	0.51
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.11	0.51
30:0:445:U:H2'	30:0:446:G:H8	1.75	0.51
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.51
23:W:125:HIS:CD2	23:W:127:GLY:H	2.29	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
12:L:149:ARG:O	12:L:150:GLN:HB2	2.10	0.51
30:0:690:G:H4'	30:0:741:C:O2	2.11	0.51
30:0:318:U:H5'	30:0:339:A:C2	2.46	0.51
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.93	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.10	0.51
30:0:1535:G:H2'	30:0:1536:C:C6	2.46	0.51
30:0:545:G:H8	30:0:545:G:C5'	2.06	0.51
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.51
4:D:25:MET:HE2	4:D:41:LEU:HG	1.92	0.51
30:0:1973:A:H2'	30:0:1974:G:O4'	2.10	0.51
30:0:1015:C:H2'	30:0:1016:U:H6	1.75	0.51
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.91	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51
30:0:2401:A:H2'	30:0:2402:A:C8	2.46	0.51
31:9:1:U:O3'	31:9:3:A:C5'	2.58	0.51
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.11	0.51
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.09	0.51
6:F:101:ALA:HA	38:F:5413:HOH:O	2.10	0.51
30:0:968:G:C2	30:0:1001:U:O2	2.63	0.51
30:0:1160:G:H5''	30:0:1161:A:H5'	1.84	0.51
30:0:1183:C:C2	30:0:1184:C:C5	2.99	0.51
30:0:483:C:C4	30:0:484:A:C6	2.99	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.23	0.51
2:B:85:ARG:NH1	38:B:9095:HOH:O	2.44	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.11	0.51
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.93	0.51
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.45	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.91	0.51
30:0:2326:C:H4'	30:0:2412:G:C4'	2.41	0.51
30:0:407:A:H3'	38:0:4473:HOH:O	2.10	0.50
30:0:1268:C:H2'	30:0:1269:G:H8	1.76	0.50
30:0:101:C:H2'	30:0:102:A:H8	1.76	0.50
30:0:1139:U:H2'	30:0:1140:C:C6	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:95:GLU:HG3	38:C:8672:HOH:O	2.12	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
30:0:2754:G:H2'	30:0:2755:G:O4'	2.11	0.50
14:N:4:PRO:HG3	31:9:69:U:OP1	2.11	0.50
3:C:236:THR:HG22	3:C:239:ALA:N	2.20	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.79	0.50
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.50
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.58	0.50
30:0:951:A:C2'	30:0:952:G:H5'	2.41	0.50
9:I:95:LEU:HD22	9:I:99:GLN:HB3	1.93	0.50
8:H:69:ARG:HD3	38:H:229:HOH:O	2.11	0.50
30:0:1739:G:O2'	30:0:1740:U:H5'	2.11	0.50
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.50
31:9:76:G:H3'	31:9:77:A:C5'	2.24	0.50
30:0:1878:G:O2'	30:0:1879:U:H6	1.95	0.50
2:B:62:ARG:HA	2:B:65:MET:HE2	1.93	0.50
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.08	0.50
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.50
2:B:214:PRO:HD2	38:B:8990:HOH:O	2.11	0.50
27:1:2:GLY:O	27:1:6:PRO:HG2	2.11	0.50
30:0:899:C:H5'	38:0:3209:HOH:O	2.12	0.50
30:0:1183:C:O2	30:0:1183:C:C2'	2.60	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.75	0.50
30:0:271:C:C2	30:0:273:G:O4'	2.64	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.70	0.50
30:0:960:G:C3'	30:0:960:G:N3	2.74	0.50
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.50
12:L:143:THR:HG21	38:L:8838:HOH:O	2.10	0.50
30:0:737:A:H2'	30:0:738:G:O4'	2.10	0.50
30:0:2269:C:H2'	30:0:2270:G:H5'	1.93	0.50
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.50
30:0:700:A:H5''	30:0:701:U:H5'	1.93	0.50
29:3:29:ARG:NH2	30:0:1925:G:H5'	2.26	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
2:B:310:ARG:HB3	38:B:9109:HOH:O	2.11	0.50
2:B:217:ARG:CG	2:B:257:THR:HG22	2.38	0.50
30:0:661:G:C5	30:0:686:A:C2	3.00	0.50
3:C:214:THR:HG23	38:C:8633:HOH:O	2.11	0.50
20:T:54:ASP:OD2	30:0:316:A:H5'	2.11	0.50
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.77	0.50
8:H:170:ARG:HD2	38:H:190:HOH:O	2.11	0.50
30:0:1289:C:O2'	30:0:1290:G:H5'	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:5:G:O2'	31:9:6:C:H5'	2.11	0.50
30:0:1244:U:H4'	30:0:1246:A:O4'	2.11	0.50
30:0:1181:A:H2'	30:0:1182:C:H5'	1.94	0.50
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.50
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.93	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.47	0.50
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.50
30:0:947:U:H2'	30:0:948:G:C8	2.47	0.50
19:S:77:VAL:O	19:S:80:ARG:HG2	2.12	0.50
30:0:2276:U:H2'	30:0:2277:U:C6	2.46	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.42	0.50
30:0:137:U:OP1	30:0:259:G:O2'	2.30	0.50
18:R:33:ARG:NH1	38:R:8950:HOH:O	2.45	0.50
20:T:28:SER:O	20:T:32:ARG:HG3	2.11	0.50
30:0:2511:A:H4'	38:0:5478:HOH:O	2.12	0.50
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.50
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.92	0.50
30:0:1056:U:H2'	30:0:1057:A:O4'	2.12	0.50
2:B:275:GLY:O	2:B:291:ASP:HA	2.12	0.50
30:0:1185:U:H2'	30:0:1186:C:H6	1.77	0.50
15:O:37:ARG:HD2	30:0:656:G:OP2	2.12	0.50
30:0:182:G:H5''	38:0:3733:HOH:O	2.12	0.50
30:0:541:C:C2'	30:0:542:A:C5'	2.78	0.50
30:0:877:G:C5'	30:0:878:G:OP1	2.57	0.50
30:0:2010:A:C2'	38:0:5965:HOH:O	2.55	0.50
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.77	0.50
23:W:80:ASP:O	23:W:84:VAL:HG23	2.10	0.50
30:0:816:G:C6	30:0:817:G:N1	2.80	0.50
14:N:110:THR:HB	14:N:113:SER:OG	2.12	0.49
30:0:1743:G:N7	38:0:9265:HOH:O	2.35	0.49
30:0:1211:G:H2'	30:0:1212:C:H6	1.77	0.49
30:0:1588:G:C6	30:0:1589:G:N1	2.81	0.49
30:0:509:A:H2'	38:0:7099:HOH:O	2.11	0.49
2:B:212:GLN:HA	30:0:1733:A:H4'	1.93	0.49
30:0:1972:U:H2'	30:0:1973:A:H5'	1.93	0.49
30:0:2414:A:H2'	30:0:2415:A:C8	2.47	0.49
30:0:364:U:H2'	30:0:365:G:O4'	2.12	0.49
30:0:1657:A:H2'	30:0:1658:A:C8	2.47	0.49
30:0:2851:G:C2'	30:0:2852:A:H5'	2.43	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.40	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:59:C:H2'	31:9:60:C:C6	2.47	0.49
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.11	0.49
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.12	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.93	0.49
20:T:5:ASP:O	20:T:9:LYS:HB2	2.13	0.49
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.93	0.49
30:0:1903:U:O2'	30:0:1904:A:N7	2.42	0.49
30:0:1856:C:H5'	30:0:1858:A:O4'	2.12	0.49
14:N:154:LEU:C	14:N:156:GLU:H	2.14	0.49
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.93	0.49
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.94	0.49
30:0:1625:U:H3'	30:0:1625:U:H6	1.75	0.49
30:0:669:G:O2'	30:0:670:G:H5'	2.12	0.49
30:0:1838:U:H3'	38:0:5533:HOH:O	2.12	0.49
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.11	0.49
30:0:1762:C:H2'	30:0:1763:C:H6	1.77	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.45	0.49
30:0:1790:C:H2'	30:0:1791:U:H6	1.76	0.49
18:R:40:ALA:O	18:R:44:VAL:HG23	2.12	0.49
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.11	0.49
30:0:2709:G:N2	38:0:7632:HOH:O	2.46	0.49
30:0:1545:C:H2'	30:0:1546:G:O4'	2.12	0.49
30:0:1940:C:H4'	38:0:7360:HOH:O	2.12	0.49
30:0:407:A:H2'	30:0:408:A:C8	2.48	0.49
30:0:1503:U:H2'	30:0:1504:A:O4'	2.11	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.95	0.49
30:0:2493:C:O2	30:0:2493:C:H2'	2.11	0.49
2:B:238:ASN:HD22	2:B:240:GLY:N	2.02	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.47	0.49
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.49
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.49
30:0:2435:U:H1'	38:0:5440:HOH:O	2.13	0.49
1:A:33:GLU:CD	1:A:33:GLU:H	2.15	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.27	0.49
31:9:3:A:C2	31:9:21:G:N3	2.81	0.49
31:9:3:A:N6	31:9:22:G:H1'	2.28	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.27	0.49
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.49
30:0:702:G:O2'	30:0:703:G:H5'	2.13	0.49
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.78	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2880:A:H2'	30:0:2881:C:H5'	1.95	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.49
30:0:1149:U:H5''	30:0:1151:G:O4'	2.13	0.49
1:A:186:TRP:CG	1:A:187:PRO:HA	2.48	0.49
15:O:25:VAL:HG12	30:0:709:G:O2'	2.11	0.49
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.94	0.49
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.49
30:0:2908:A:O5'	30:0:2908:A:H8	1.94	0.49
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.23	0.49
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.49
30:0:2802:C:H2'	30:0:2803:C:C6	2.46	0.49
30:0:815:U:O2'	30:0:1598:A:H4'	2.12	0.49
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.95	0.49
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.12	0.49
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.94	0.49
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.49
30:0:297:U:H2'	30:0:298:C:C6	2.48	0.49
31:9:56:A:C3'	31:9:57:A:H5''	2.43	0.48
30:0:1118:A:C8	30:0:1119:G:H5''	2.47	0.48
24:X:85:VAL:HG12	24:X:86:GLU:N	2.28	0.48
31:9:63:C:O2'	31:9:64:C:H5'	2.13	0.48
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
31:9:2:U:P	31:9:3:A:H5'	2.53	0.48
30:0:2420:G:H2'	30:0:2421:G:C8	2.48	0.48
4:D:62:ASP:HA	38:D:4233:HOH:O	2.14	0.48
30:0:2697:A:H2'	30:0:2698:G:O4'	2.13	0.48
30:0:2335:C:H2'	30:0:2336:G:C8	2.48	0.48
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.95	0.48
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.95	0.48
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.94	0.48
30:0:2781:U:O2'	30:0:2782:G:H5'	2.13	0.48
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.28	0.48
23:W:38:THR:O	23:W:42:ARG:HB2	2.13	0.48
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.95	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
22:V:12:THR:HG22	22:V:15:GLU:CG	2.39	0.48
17:Q:50:GLY:HA2	38:0:6033:HOH:O	2.12	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.48	0.48
30:0:947:U:H2'	30:0:948:G:H8	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:1:PRO:HA	30:0:2299:G:O6	2.13	0.48
30:0:2419:U:H5''	30:0:2420:G:C5'	2.42	0.48
23:W:90:TYR:N	23:W:90:TYR:CD1	2.80	0.48
30:0:1523:G:H2'	30:0:1524:U:C6	2.48	0.48
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.48
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.13	0.48
30:0:2842:G:C2'	30:0:2843:A:H5'	2.43	0.48
8:H:34:HIS:HD2	8:H:90:LEU:O	1.96	0.48
30:0:1221:G:C8	38:0:5995:HOH:O	2.55	0.48
10:J:130:VAL:HG12	10:J:131:THR:N	2.28	0.48
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.11	0.48
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.48
4:D:170:TYR:CD1	4:D:170:TYR:N	2.81	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:1206:U:C5'	30:0:1206:U:H6	2.18	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.39	0.48
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.48
3:C:87:ARG:HD3	38:0:3517:HOH:O	2.14	0.48
30:0:1513:C:O2'	30:0:1514:C:H5'	2.13	0.48
30:0:482:G:H4'	30:0:508:A:N1	2.29	0.48
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.95	0.48
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
30:0:2896:A:N3	30:0:2896:A:H2'	2.29	0.48
30:0:2335:C:H2'	30:0:2336:G:H8	1.77	0.48
20:T:68:ASP:HB2	38:0:5667:HOH:O	2.12	0.48
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.48
10:J:74:ARG:CB	10:J:74:ARG:HH11	2.25	0.48
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.96	0.48
30:0:2598:U:O2	30:0:2600:A:H8	1.97	0.48
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.78	0.48
30:0:535:G:C6	30:0:2064:U:C5	3.01	0.48
7:G:19:GLU:O	7:G:23:ILE:HG13	2.14	0.48
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.96	0.48
30:0:2001:G:O2'	30:0:2002:C:H5'	2.13	0.48
13:M:164:THR:HG23	13:M:165:GLY:N	2.29	0.48
30:0:2506:A:N6	30:0:2511:A:O2'	2.46	0.48
6:F:91:VAL:CG1	6:F:92:GLY:H	2.25	0.48
30:0:130:C:H2'	38:0:3167:HOH:O	2.14	0.48
30:0:2587:OMU:H5	38:0:7497:HOH:O	2.12	0.48
30:0:2415:A:H2'	30:0:2416:G:H5'	1.96	0.48
30:0:2649:A:H5'	30:0:2649:A:C8	2.49	0.48
29:3:91:GLN:O	29:3:92:GLU:HB2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1562:C:O2	30:0:1562:C:C2'	2.62	0.48
13:M:163:LEU:HD21	30:0:188:C:H5''	1.96	0.48
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.95	0.48
14:N:119:GLN:O	14:N:123:ILE:HG13	2.14	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.14	0.48
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.96	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.78	0.48
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.73	0.48
14:N:11:ARG:NH1	31:9:8:G:O6	2.47	0.47
1:A:212:PRO:HA	30:0:1943:C:O4'	2.14	0.47
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.95	0.47
12:L:22:ARG:HG2	38:0:9996:HOH:O	2.14	0.47
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.95	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.95	0.47
30:0:1209:C:O2'	30:0:1210:G:H5'	2.13	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.44	0.47
30:0:1947:G:N2	30:0:1966:U:N3	2.61	0.47
30:0:821:U:H2'	30:0:822:C:H6	1.79	0.47
30:0:1130:U:H2'	30:0:1131:G:O4'	2.13	0.47
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.96	0.47
25:Y:210:GLY:N	30:0:1313:A:H5''	2.29	0.47
30:0:1161:A:O5'	30:0:1161:A:H8	1.96	0.47
30:0:523:C:H2'	30:0:524:A:C8	2.50	0.47
23:W:119:HIS:HE1	38:0:9557:HOH:O	1.97	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.95	0.47
30:0:407:A:H8	38:0:4473:HOH:O	1.98	0.47
3:C:246:ARG:NE	38:C:8620:HOH:O	2.40	0.47
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.30	0.47
30:0:2334:C:O2'	30:0:2335:C:H5'	2.14	0.47
18:R:114:VAL:HA	18:R:144:GLU:O	2.14	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.14	0.47
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.49	0.47
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.39	0.47
30:0:567:U:C5'	38:0:6408:HOH:O	2.63	0.47
31:9:47:A:C2	31:9:48:C:C2	3.02	0.47
30:0:2589:U:H2'	30:0:2590:U:H6	1.77	0.47
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.47
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.11	0.47
30:0:1762:C:H2'	30:0:1763:C:C6	2.50	0.47
1:A:33:GLU:O	1:A:34:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:22:PHE:HA	3:C:116:ALA:HA	1.96	0.47
30:0:1768:C:H2'	30:0:1769:C:O4'	2.14	0.47
5:E:21:THR:HG23	5:E:30:THR:OG1	2.14	0.47
3:C:233:THR:HG22	3:C:234:VAL:N	2.29	0.47
30:0:2112:A:H2'	30:0:2113:G:C8	2.49	0.47
30:0:823:U:H3'	38:0:4459:HOH:O	2.14	0.47
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.47
31:9:114:G:H2'	31:9:115:C:H6	1.78	0.47
30:0:1343:C:H2'	30:0:1344:G:O5'	2.15	0.47
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.48	0.47
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.97	0.47
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.47
30:0:523:C:H2'	30:0:524:A:H8	1.80	0.47
23:W:115:THR:HG23	38:W:5420:HOH:O	2.15	0.47
23:W:52:VAL:HG22	23:W:53:ALA:H	1.80	0.47
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.14	0.47
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.15	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.50	0.47
8:H:66:GLU:HA	38:H:229:HOH:O	2.13	0.47
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.49	0.47
30:0:1615:A:H5'	38:0:4194:HOH:O	2.14	0.47
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.52	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.80	0.47
30:0:1450:C:H5''	38:0:9621:HOH:O	2.15	0.47
23:W:125:HIS:HD2	23:W:127:GLY:H	1.62	0.47
30:0:2526:C:C6	30:0:2526:C:C5'	2.95	0.47
30:0:2637:A:C5'	38:0:4941:HOH:O	2.62	0.47
30:0:308:U:C4	30:0:342:C:H1'	2.49	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.50	0.47
10:J:131:THR:HB	10:J:134:GLU:HG3	1.96	0.47
30:0:2691:A:H5'	30:0:2693:U:H1'	1.96	0.47
30:0:312:U:C2	30:0:320:G:N2	2.83	0.47
1:A:8:ARG:HG2	38:A:9016:HOH:O	2.14	0.47
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.47
29:3:3:MET:O	29:3:90:PHE:HA	2.15	0.47
30:0:2506:A:O2'	30:0:2507:G:C8	2.50	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.47
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.80	0.47
30:0:2269:C:H2'	30:0:2270:G:C5'	2.45	0.47
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1682:A:H5''	38:0:9463:HOH:O	2.14	0.47
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.97	0.47
30:0:251:C:H2'	30:0:252:C:H6	1.80	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:545:G:C8	30:0:545:G:C5'	2.88	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.50	0.47
30:0:1632:A:H2'	30:0:1633:C:C5'	2.39	0.47
30:0:1165:G:H4'	30:0:1174:A:O2'	2.15	0.47
31:9:42:C:H5'	31:9:43:G:OP2	2.15	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
30:0:685:C:O2	30:0:748:C:H4'	2.15	0.47
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.28	0.47
30:0:629:A:C2	30:0:2074:A:C2	3.03	0.47
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.47
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.30	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.15	0.47
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.30	0.47
10:J:36:VAL:HG12	10:J:37:ALA:N	2.30	0.47
10:J:42:GLU:O	10:J:131:THR:HG23	2.15	0.47
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.96	0.47
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.47
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.47
30:0:638:C:H2'	30:0:639:A:C8	2.50	0.47
30:0:2073:G:OP2	30:0:2490:A:H5'	2.15	0.47
4:D:141:VAL:HG21	31:9:57:A:H8	1.80	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.47	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.14	0.46
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.97	0.46
30:0:1321:A:H2'	30:0:1322:G:C8	2.50	0.46
31:9:7:G:H5'	38:9:9100:HOH:O	2.16	0.46
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.46
2:B:298:LYS:HG2	38:0:5531:HOH:O	2.15	0.46
30:0:1180:U:O2'	30:0:1181:A:H5'	2.15	0.46
23:W:119:HIS:HD2	23:W:120:PRO:O	1.98	0.46
1:A:53:ALA:HB3	38:A:9066:HOH:O	2.15	0.46
30:0:853:C:H2'	30:0:854:G:O4'	2.15	0.46
30:0:1477:C:C5'	30:0:1868:G:H5''	2.45	0.46
30:0:1805:G:H2'	30:0:1806:G:H8	1.79	0.46
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.51	0.46
31:9:45:A:C5	31:9:46:C:C5	3.02	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:210:GLY:H	30:0:1313:A:H5''	1.80	0.46
17:Q:75:ILE:HB	38:Q:6286:HOH:O	2.15	0.46
30:0:2566:A:C2	30:0:2696:G:O4'	2.68	0.46
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.46
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.81	0.46
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.95	0.46
30:0:319:A:H4'	30:0:338:C:C4	2.50	0.46
30:0:255:A:C5	30:0:256:C:C5	3.02	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.97	0.46
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.46
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.80	0.46
30:0:2249:G:C2	30:0:2253:G:C6	3.04	0.46
30:0:2250:G:C2	30:0:2251:G:H1'	2.51	0.46
17:Q:27:GLN:HE21	31:9:8:G:H5''	1.80	0.46
20:T:26:THR:HA	20:T:39:ASN:HB3	1.97	0.46
31:9:65:A:N6	31:9:112:U:C6	2.83	0.46
1:A:204:GLY:N	30:0:2634:G:OP2	2.47	0.46
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.97	0.46
30:0:1139:U:H2'	30:0:1140:C:H6	1.80	0.46
29:3:29:ARG:NH2	30:0:1925:G:C5'	2.79	0.46
30:0:1925:G:O2'	30:0:1926:G:H5'	2.16	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.46
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.47	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.97	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.80	0.46
30:0:369:G:H2'	30:0:370:G:H8	1.81	0.46
8:H:31:ILE:HG23	38:H:229:HOH:O	2.15	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.46
12:L:6:ARG:HD3	30:0:1299:G:O6	2.15	0.46
30:0:2869:G:H2'	30:0:2870:C:C6	2.50	0.46
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.46
13:M:27:ARG:HH12	13:M:44:THR:CG2	2.28	0.46
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.15	0.46
30:0:255:A:C4	30:0:256:C:C6	3.04	0.46
30:0:1942:A:H4'	38:0:9046:HOH:O	2.16	0.46
30:0:736:A:H2'	30:0:737:A:O4'	2.16	0.46
30:0:365:G:C6	30:0:366:U:C4	3.04	0.46
30:0:1211:G:H2'	30:0:1212:C:C6	2.50	0.46
30:0:2826:G:C6	30:0:2913:A:N6	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.75	0.46
16:P:120:ARG:NH1	30:0:1594:C:C5	2.84	0.46
6:F:96:ALA:HA	38:F:3111:HOH:O	2.15	0.46
30:0:158:A:H3'	38:0:7573:HOH:O	2.15	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.15	0.46
30:0:2895:C:H2'	38:0:9573:HOH:O	2.15	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.64	0.46
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.98	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
30:0:2433:A:H2'	30:0:2434:A:C8	2.50	0.46
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.98	0.46
12:L:18:HIS:HB2	30:0:903:U:O4	2.16	0.46
30:0:451:C:O2'	30:0:452:G:H5'	2.16	0.46
30:0:1603:A:H5''	30:0:1604:G:H3'	1.98	0.46
13:M:27:ARG:NH1	13:M:44:THR:CG2	2.78	0.46
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.96	0.46
30:0:1825:U:O2'	30:0:1826:C:H5'	2.15	0.46
30:0:1015:C:O5'	30:0:1015:C:H6	1.98	0.46
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.46
31:9:45:A:H2'	31:9:46:C:C6	2.51	0.46
30:0:1506:U:H6	30:0:1506:U:H5'	1.81	0.46
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.46
30:0:466:A:H2'	30:0:467:G:O4'	2.15	0.46
23:W:21:LEU:O	23:W:26:ILE:HG23	2.16	0.46
30:0:1180:U:H2'	30:0:1181:A:O4'	2.16	0.46
30:0:1684:A:O2'	30:0:1685:A:H5''	2.16	0.46
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.16	0.46
4:D:103:ASN:HD22	4:D:134:LEU:H	1.60	0.46
30:0:1774:G:H1'	38:0:4551:HOH:O	2.14	0.46
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.46
30:0:958:G:O2'	30:0:959:C:H5'	2.15	0.46
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.83	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.46
8:H:165:ARG:HD2	38:H:231:HOH:O	2.16	0.46
30:0:1714:C:O2'	30:0:1715:C:H5'	2.16	0.46
30:0:1622:G:H2'	30:0:1623:C:H5'	1.98	0.46
15:O:24:ALA:HB3	30:0:710:G:OP1	2.16	0.46
30:0:1165:G:H1'	30:0:1174:A:H1'	1.97	0.45
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.45
30:0:1523:G:C6	30:0:1524:U:C4	3.04	0.45
30:0:1278:A:H2'	30:0:1280:A:C8	2.51	0.45
15:O:63:LYS:NZ	30:0:659:A:N7	2.53	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.16	0.45
30:0:735:C:C5	30:0:736:A:N3	2.84	0.45
30:0:2355:G:H5'	30:0:2356:A:OP2	2.16	0.45
30:0:2869:G:H2'	30:0:2870:C:H6	1.81	0.45
16:P:40:VAL:O	16:P:44:VAL:HG23	2.17	0.45
30:0:417:G:P	38:0:7432:HOH:O	2.74	0.45
30:0:271:C:N4	30:0:378:A:C2	2.71	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.51	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.30	0.45
31:9:106:U:O2'	31:9:107:C:H5'	2.15	0.45
30:0:711:G:O2'	30:0:712:C:H5'	2.17	0.45
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.49	0.45
30:0:64:G:H2'	30:0:65:C:O4'	2.16	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
3:C:79:ARG:O	3:C:87:ARG:HG2	2.16	0.45
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.31	0.45
30:0:496:G:H3'	38:0:7681:HOH:O	2.15	0.45
30:0:236:A:H4'	30:0:237:G:OP1	2.15	0.45
20:T:38:ARG:NH1	38:0:6693:HOH:O	2.42	0.45
9:I:114:TYR:N	9:I:114:TYR:CD1	2.84	0.45
2:B:26:PHE:HE1	38:B:9109:HOH:O	1.99	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.98	0.45
21:U:17:THR:CG2	21:U:18:GLY:N	2.79	0.45
30:0:2467:A:O2'	30:0:2468:A:H2'	2.17	0.45
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.99	0.45
30:0:2092:G:H2'	30:0:2613:G:OP1	2.16	0.45
15:O:25:VAL:HG23	15:O:26:TRP:N	2.31	0.45
4:D:170:TYR:HD1	4:D:170:TYR:N	2.14	0.45
3:C:233:THR:HG22	3:C:234:VAL:H	1.81	0.45
30:0:105:G:O2'	30:0:106:A:H5'	2.16	0.45
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.50	0.45
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.56	0.45
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.30	0.45
30:0:1909:A:N1	30:0:2128:G:H1'	2.31	0.45
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.80	0.45
31:9:2:U:OP2	31:9:2:U:H4'	2.16	0.45
30:0:1942:A:HO2'	30:0:1943:C:H5'	1.80	0.45
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
30:0:1015:C:H2'	30:0:1016:U:C6	2.51	0.45
30:0:210:U:H2'	30:0:211:U:C6	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1834:C:H2'	30:0:1840:A:H62	1.82	0.45
3:C:236:THR:CG2	3:C:239:ALA:H	2.21	0.45
30:0:2895:C:O2'	30:0:2896:A:H5''	2.16	0.45
27:1:25:LYS:O	27:1:25:LYS:HG2	2.17	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.52	0.45
30:0:1001:U:O2'	30:0:1002:G:H5'	2.17	0.45
30:0:1855:G:H4'	30:0:1856:C:O5'	2.16	0.45
30:0:843:A:C2	30:0:846:A:C8	3.04	0.45
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.98	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
4:D:141:VAL:HG21	31:9:57:A:C8	2.51	0.45
30:0:1634:G:C3'	38:0:3907:HOH:O	2.46	0.45
28:2:48:ASP:O	28:2:49:GLU:HB2	2.17	0.45
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.82	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.81	0.45
30:0:945:U:H2'	30:0:946:C:C6	2.52	0.45
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.52	0.45
30:0:682:A:H2'	30:0:683:G:O4'	2.16	0.45
30:0:2456:A:H5'	38:0:5702:HOH:O	2.17	0.45
30:0:423:A:C5	30:0:424:C:C5	3.05	0.45
25:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.98	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
30:0:1183:C:H42	30:0:1184:C:N4	2.10	0.45
30:0:2506:A:C4	38:0:6063:HOH:O	2.67	0.45
30:0:2681:A:H4'	30:0:2682:C:OP1	2.16	0.45
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.45
23:W:13:MET:CE	23:W:17:ILE:HG22	2.47	0.45
30:0:1624:A:H4'	30:0:1626:A:H5''	1.99	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.69	0.45
30:0:73:U:O2'	30:0:74:G:H5'	2.17	0.45
30:0:1386:G:O2'	30:0:1387:G:H5'	2.17	0.45
30:0:1379:A:H1'	38:0:9695:HOH:O	2.16	0.45
14:N:40:ASN:ND2	31:9:28:U:H5''	2.31	0.45
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.99	0.45
30:0:670:G:H2'	30:0:671:A:C8	2.51	0.45
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.49	0.45
30:0:1014:A:H2'	30:0:1015:C:H5'	1.99	0.45
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.52	0.45
30:0:1484:G:H2'	38:0:9106:HOH:O	2.17	0.45
2:B:223:ARG:HG3	2:B:232:TRP:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2727:A:C6	30:0:2756:U:C2	3.05	0.45
30:0:2248:C:C4	30:0:2249:G:N7	2.85	0.45
30:0:1221:G:H8	38:0:5995:HOH:O	1.95	0.45
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.47	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
30:0:1400:C:O2'	30:0:1401:G:H5'	2.17	0.45
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.16	0.45
5:E:154:ILE:HD11	5:E:157:LYS:NZ	2.32	0.45
30:0:1191:A:C2	30:0:1207:A:C2	3.05	0.45
30:0:1279:U:O2	30:0:1279:U:C2'	2.64	0.45
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.47	0.45
30:0:2819:C:H2'	30:0:2820:A:C8	2.51	0.45
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.45
30:0:2002:C:H2'	30:0:2003:U:H5'	1.99	0.45
11:K:34:VAL:HB	38:K:7169:HOH:O	2.17	0.45
30:0:861:A:H4'	30:0:1697:G:H4'	1.99	0.45
30:0:1425:G:O2'	30:0:1426:C:H5'	2.17	0.45
30:0:1537:C:H1'	38:0:6597:HOH:O	2.16	0.45
27:1:20:ARG:HG2	30:0:111:C:O2'	2.17	0.45
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.44
30:0:2812:A:H1'	38:0:5796:HOH:O	2.17	0.44
31:9:39:U:HO2'	31:9:42:C:H5	1.65	0.44
30:0:128:A:H3'	30:0:128:A:C8	2.52	0.44
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.18	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.50	0.44
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.82	0.44
30:0:107:U:H2'	30:0:108:U:H5'	1.99	0.44
31:9:36:C:C5	31:9:37:C:C5	3.05	0.44
30:0:2072:G:C6	30:0:2533:C:H1'	2.52	0.44
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.17	0.44
30:0:1333:U:H2'	30:0:1334:C:C6	2.52	0.44
30:0:2483:A:H4'	30:0:2484:U:OP2	2.17	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.47	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.72	0.44
23:W:4:LEU:O	23:W:32:CYS:HA	2.17	0.44
20:T:9:LYS:HD2	38:0:3766:HOH:O	2.16	0.44
30:0:2689:A:H2'	30:0:2690:U:H5'	1.99	0.44
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.44
30:0:213:G:N2	30:0:225:G:H2'	2.32	0.44
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.99	0.44
30:0:2543:G:H2'	30:0:2544:G:O4'	2.17	0.44
30:0:790:A:H1'	30:0:1710:A:H2'	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:905:C:H3'	38:0:5198:HOH:O	2.17	0.44
30:0:1759:A:N3	30:0:1818:C:H2'	2.33	0.44
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.44
13:M:164:THR:CG2	13:M:167:GLY:H	2.27	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.31	0.44
30:0:1545:C:H1'	30:0:1641:A:N6	2.33	0.44
20:T:9:LYS:HG3	38:0:7437:HOH:O	2.16	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.44
30:0:579:G:H2'	30:0:580:A:C8	2.52	0.44
30:0:1522:A:C2	30:0:1665:G:C6	3.05	0.44
30:0:343:C:O2'	30:0:344:C:H5'	2.17	0.44
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.32	0.44
21:U:33:SER:O	21:U:37:GLU:HG3	2.16	0.44
30:0:281:U:H5	38:0:7606:HOH:O	2.01	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
30:0:1175:G:H8	30:0:1193:A:HO2'	1.64	0.44
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.29	0.44
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.17	0.44
17:Q:95:GLU:HA	30:0:949:U:H4'	1.99	0.44
30:0:1622:G:C2'	30:0:1623:C:H5'	2.47	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.06	0.44
30:0:2239:C:H2'	30:0:2240:U:C6	2.53	0.44
30:0:2375:A:H2'	30:0:2376:C:C6	2.53	0.44
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
1:A:109:GLU:HG2	1:A:116:GLY:N	2.33	0.44
5:E:169:THR:HG22	5:E:170:ARG:HG3	2.00	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.18	0.44
14:N:141:ARG:NH2	31:9:48:C:H4'	2.27	0.44
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.44
14:N:143:ARG:HE	14:N:143:ARG:HB3	1.61	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.44
2:B:211:THR:HG21	38:0:7469:HOH:O	2.17	0.44
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.44
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.01	0.44
19:S:57:THR:HG22	19:S:58:MET:N	2.32	0.44
38:C:8546:HOH:O	30:0:457:U:H4'	2.17	0.44
30:0:2858:U:H2'	30:0:2859:C:O4'	2.16	0.44
31:9:1:U:H5''	31:9:3:A:OP1	2.18	0.44
30:0:2812:A:N7	38:0:7529:HOH:O	2.36	0.44
30:0:1973:A:H5'	30:0:1973:A:C8	2.44	0.44
11:K:87:ARG:NE	38:0:5721:HOH:O	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.44
30:0:2800:A:H5'	30:0:2801:A:OP2	2.18	0.44
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.98	0.44
30:0:277:U:O2'	30:0:278:A:H5'	2.18	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.18	0.44
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.64	0.44
30:0:1593:C:H1'	38:0:6112:HOH:O	2.17	0.44
30:0:1592:G:O2'	30:0:1593:C:O4'	2.33	0.44
23:W:122:ARG:NH2	38:0:5297:HOH:O	2.49	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.48	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.53	0.44
30:0:636:G:H1'	30:0:2058:G:C4	2.53	0.44
30:0:302:A:O2'	30:0:303:C:H5'	2.17	0.44
30:0:1950:G:H2'	30:0:1951:G:C8	2.53	0.44
4:D:57:THR:HG23	4:D:63:ILE:HA	2.00	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.44
23:W:133:LYS:HG3	38:W:5904:HOH:O	2.18	0.44
7:G:63:ARG:N	38:G:2569:HOH:O	2.50	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44
30:0:2718:C:H5'	30:0:2718:C:C6	2.50	0.44
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.44
4:D:76:ARG:NE	31:9:44:A:O4'	2.51	0.44
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.98	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.18	0.44
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.32	0.44
30:0:1067:A:H3'	38:0:4304:HOH:O	2.17	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.17	0.44
7:G:63:ARG:O	7:G:67:LEU:HG	2.17	0.44
30:0:289:G:O2'	30:0:290:C:H5'	2.17	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.95	0.44
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.43	0.44
30:0:1181:A:H2'	30:0:1182:C:C5'	2.48	0.44
30:0:1202:A:C2'	30:0:1203:G:H5'	2.48	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.82	0.44
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.99	0.44
30:0:1044:C:H5''	38:0:9029:HOH:O	2.18	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.32	0.44
30:0:699:C:H6	30:0:744:G:O4'	2.01	0.44
30:0:2264:A:H2'	30:0:2265:U:C6	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.18	0.44
30:0:705:C:H2'	30:0:705:C:O2	2.17	0.44
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.33	0.43
30:0:2598:U:O2	30:0:2600:A:C8	2.71	0.43
30:0:129:A:H4'	30:0:130:C:OP1	2.18	0.43
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.43
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.33	0.43
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.18	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
30:0:47:G:N3	30:0:114:A:C2	2.86	0.43
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.43
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.43
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.45	0.43
30:0:1552:G:N2	30:0:1634:G:H1'	2.33	0.43
4:D:154:LYS:H	4:D:154:LYS:CD	2.24	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.43
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.01	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.86	0.43
30:0:2488:A:H2'	30:0:2489:G:O4'	2.19	0.43
30:0:1947:G:H2'	30:0:1948:G:H8	1.82	0.43
30:0:2379:G:H5'	30:0:2381:C:O4'	2.18	0.43
30:0:677:C:P	38:0:7147:HOH:O	2.75	0.43
30:0:2566:A:H2	30:0:2695:C:O2	2.01	0.43
31:9:35:C:H5''	38:9:9080:HOH:O	2.17	0.43
30:0:134:U:C2	30:0:145:A:C2	3.07	0.43
14:N:114:LYS:O	14:N:118:ILE:HG13	2.18	0.43
30:0:1115:U:O2'	30:0:1116:U:H5'	2.18	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.83	0.43
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.83	0.43
30:0:1762:C:O2'	30:0:1763:C:H5'	2.17	0.43
22:V:44:GLY:HA3	30:0:92:G:H4'	1.99	0.43
30:0:2607:U:H4'	38:0:9448:HOH:O	2.18	0.43
12:L:48:LYS:HE2	30:0:220:C:C2	2.53	0.43
5:E:80:TRP:O	5:E:134:SER:HA	2.18	0.43
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.45	0.43
30:0:1700:C:H5''	30:0:1701:A:OP2	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:O5'	2.17	0.43
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1395:C:H2'	30:0:1396:C:C6	2.53	0.43
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.43
30:0:17:G:H2'	30:0:18:C:H6	1.82	0.43
35:0:8814:CL:CL	38:0:7753:HOH:O	2.59	0.43
14:N:41:LYS:HD3	38:9:9063:HOH:O	2.19	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.01	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:2504:A:H2'	30:0:2505:G:H5'	2.00	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
8:H:61:ARG:HG3	38:0:4984:HOH:O	2.17	0.43
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.52	0.43
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.83	0.43
1:A:95:PRO:HA	1:A:153:ARG:HA	1.99	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
4:D:50:VAL:HG13	31:9:41:C:O4'	2.18	0.43
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.84	0.43
3:C:93:LYS:O	3:C:98:ARG:NH2	2.51	0.43
30:0:1896:G:C6	30:0:1897:U:C4	3.07	0.43
30:0:522:U:O2'	30:0:1366:C:H5'	2.18	0.43
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.18	0.43
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.99	0.43
2:B:198:GLU:HA	38:B:9119:HOH:O	2.19	0.43
1:A:55:VAL:HG23	1:A:68:ILE:O	2.19	0.43
30:0:1964:U:H2'	30:0:1964:U:O2	2.17	0.43
30:0:1187:U:C2	30:0:1189:A:OP2	2.72	0.43
30:0:1702:U:H5'	38:0:3432:HOH:O	2.18	0.43
31:9:28:U:H2'	31:9:29:C:C6	2.54	0.43
23:W:125:HIS:HB2	23:W:137:GLN:HG2	2.00	0.43
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.43
4:D:25:MET:CE	4:D:41:LEU:HG	2.47	0.43
12:L:39:GLU:HG2	30:0:926:A:C4'	2.48	0.43
25:Y:216:ARG:NH1	38:Y:8833:HOH:O	2.51	0.43
30:0:2070:G:H2'	30:0:2072:G:OP1	2.19	0.43
30:0:570:C:H2'	30:0:571:C:H5'	2.01	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	1.99	0.43
30:0:2437:A:H2'	30:0:2438:G:C8	2.54	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.43
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.19	0.43
30:0:1063:G:H8	38:0:9865:HOH:O	2.01	0.43
30:0:1198:U:C6	30:0:1200:A:OP2	2.72	0.43
30:0:2587:OMU:H2'	30:0:2589:U:H5''	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.00	0.43
30:0:969:G:H1	30:0:999:C:H42	1.66	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.54	0.43
2:B:87:TYR:HD1	38:B:9041:HOH:O	2.01	0.43
30:0:243:A:H61	30:0:269:G:H1'	1.83	0.43
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.43
3:C:25:PRO:HG2	38:C:8523:HOH:O	2.18	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.54	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.16	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.07	0.43
2:B:297:VAL:HB	38:B:9070:HOH:O	2.19	0.43
23:W:13:MET:HE3	23:W:17:ILE:HG22	2.00	0.43
30:0:734:U:H2'	30:0:736:A:OP2	2.19	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
30:0:947:U:O2'	30:0:948:G:H5'	2.19	0.43
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.43
30:0:886:A:OP2	30:0:2113:G:H5'	2.19	0.43
28:2:28:LYS:O	30:0:87:C:H2'	2.18	0.43
3:C:173:LYS:HE3	30:0:1311:G:O6	2.18	0.43
30:0:652:G:H8	38:0:3020:HOH:O	2.00	0.43
2:B:248:ARG:NH1	38:B:9080:HOH:O	2.50	0.43
16:P:133:SER:HA	38:0:3512:HOH:O	2.18	0.43
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.85	0.43
4:D:10:PHE:CG	4:D:11:HIS:N	2.87	0.43
30:0:1553:C:H2'	30:0:1554:C:H6	1.84	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
30:0:1186:C:N4	30:0:1187:U:C4	2.87	0.43
31:9:1:U:O3'	31:9:3:A:OP1	2.36	0.43
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.43
30:0:1942:A:H2'	30:0:1943:C:H6	1.83	0.43
31:9:106:U:O5'	31:9:106:U:H6	2.01	0.43
30:0:735:C:C5	30:0:736:A:C2	3.06	0.43
30:0:297:U:H1'	38:0:3947:HOH:O	2.18	0.43
30:0:792:G:H4'	38:0:3424:HOH:O	2.19	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.59	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.51	0.43
30:0:2712:G:O2'	30:0:2713:G:H5'	2.19	0.43
30:0:2820:A:H2'	30:0:2821:C:C6	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2842:G:H2'	30:0:2843:A:C5'	2.48	0.43
30:0:1883:U:O2'	30:0:1884:G:H5'	2.19	0.43
19:S:57:THR:C	19:S:59:ASP:H	2.22	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.54	0.43
30:0:282:C:O2'	30:0:283:U:C4'	2.67	0.42
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.46	0.42
3:C:236:THR:HG22	3:C:239:ALA:HB2	2.01	0.42
30:0:2783:A:H2'	30:0:2784:A:C8	2.54	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.37	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.66	0.42
5:E:69:ILE:HA	5:E:72:MET:CE	2.48	0.42
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.34	0.42
26:Z:47:ARG:NH1	38:Z:8704:HOH:O	2.50	0.42
30:0:305:A:C5	30:0:329:A:C2	3.07	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
15:O:81:PHE:HB2	15:O:86:GLU:HB2	2.01	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
14:N:171:HIS:CE1	38:N:8855:HOH:O	2.72	0.42
14:N:23:ARG:O	14:N:27:LEU:HG	2.18	0.42
13:M:47:ASP:CG	13:M:48:LYS:N	2.72	0.42
21:U:4:ARG:N	38:U:5334:HOH:O	2.52	0.42
30:0:1965:C:O5'	30:0:1965:C:H6	2.02	0.42
30:0:1052:G:H2'	30:0:1052:G:N3	2.33	0.42
3:C:184:ARG:NH1	30:0:1306:U:OP1	2.51	0.42
30:0:128:A:O2'	30:0:129:A:C5'	2.67	0.42
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.53	0.42
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.42
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.33	0.42
30:0:1921:A:C6	30:0:1922:A:C2	3.08	0.42
30:0:2332:A:H3'	30:0:2333:G:H8	1.84	0.42
30:0:867:A:H2	30:0:880:C:O2	2.02	0.42
3:C:237:GLU:HA	38:C:8626:HOH:O	2.18	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.07	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.02	0.42
2:B:238:ASN:ND2	2:B:240:GLY:H	2.04	0.42
2:B:74:ILE:HG13	38:B:9070:HOH:O	2.17	0.42
30:0:31:C:C4'	38:0:7437:HOH:O	2.66	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.02	0.42
19:S:57:THR:HG23	38:S:8979:HOH:O	2.19	0.42
14:N:164:ASP:CG	14:N:167:ASP:HA	2.39	0.42
30:0:2347:C:H2'	30:0:2348:C:H6	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:69:TYR:CE2	14:N:184:ILE:HD11	2.55	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
30:0:932:U:H1'	30:0:1296:A:H1'	2.00	0.42
30:0:1350:U:H4'	38:0:5134:HOH:O	2.18	0.42
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
18:R:104:PHE:CB	18:R:109:MET:HE1	2.49	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.07	0.42
30:0:699:C:C2	30:0:744:G:C2	3.07	0.42
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.42
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.85	0.42
15:O:105:ASN:HD21	15:O:109:SER:N	2.17	0.42
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.42
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:40:C:H6	30:0:40:C:O5'	2.02	0.42
23:W:4:LEU:HD23	23:W:4:LEU:HA	1.83	0.42
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.42
30:0:2032:U:O2'	30:0:2033:G:H5''	2.20	0.42
14:N:71:TRP:HB2	38:N:8833:HOH:O	2.19	0.42
18:R:3:SER:HB2	30:0:20:G:O3'	2.19	0.42
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.42
30:0:74:G:H2'	30:0:75:U:C6	2.54	0.42
30:0:2801:A:H2'	30:0:2801:A:N3	2.34	0.42
30:0:1020:A:H1'	38:0:7242:HOH:O	2.19	0.42
16:P:87:ARG:HG2	38:P:188:HOH:O	2.18	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:1081:A:H5''	38:0:3159:HOH:O	2.19	0.42
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.55	0.42
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.42
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
30:0:316:A:N3	30:0:336:G:O2'	2.46	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1760:G:H5'	30:0:1818:C:O2'	2.20	0.42
30:0:1495:C:H1'	30:0:1573:A:H1'	2.02	0.42
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.19	0.42
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.19	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.85	0.42
30:0:2523:U:O2'	30:0:2524:G:H5'	2.20	0.42
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1735:C:O2'	30:0:1736:A:H5'	2.19	0.42
2:B:56:ASP:HB2	2:B:322:ARG:HE	1.85	0.42
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.01	0.42
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.42
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.84	0.42
28:2:41:HIS:HB3	28:2:44:ARG:HB2	2.02	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.42
30:0:2600:A:H2'	30:0:2601:A:O4'	2.19	0.42
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.42
30:0:445:U:H2'	30:0:446:G:C8	2.54	0.42
11:K:29:LEU:HD22	11:K:55:VAL:HG11	2.02	0.42
30:0:2265:U:H2'	30:0:2266:A:C8	2.55	0.42
30:0:113:A:OP2	30:0:114:A:H2'	2.19	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.19	0.42
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.50	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
14:N:37:ARG:NH2	38:N:8828:HOH:O	2.51	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.49	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.42
30:0:2255:A:O2'	30:0:2256:G:H5'	2.20	0.42
30:0:1562:C:N4	38:0:5872:HOH:O	2.52	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
19:S:37:VAL:O	19:S:41:VAL:HG23	2.20	0.42
16:P:13:VAL:HG13	16:P:14:LEU:N	2.35	0.42
9:I:114:TYR:N	9:I:114:TYR:HD1	2.17	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
28:2:2:LYS:HG3	30:0:1486:A:C5	2.55	0.42
1:A:206:ARG:NH2	30:0:2630:G:O6	2.53	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.42
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42
30:0:1644:C:O2'	30:0:1645:U:H5'	2.19	0.42
30:0:2032:U:C2'	30:0:2033:G:C5'	2.98	0.42
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.42
20:T:97:ARG:NH2	30:0:308:U:H5'	2.35	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.88	0.42
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.53	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.01	0.42
3:C:111:VAL:HB	38:C:8522:HOH:O	2.20	0.42
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2461:U:O2	30:0:2466:G:H1'	2.19	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.07	0.42
30:0:634:G:O2'	30:0:1358:A:OP1	2.35	0.42
30:0:2758:G:H2'	30:0:2759:C:C6	2.55	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.34	0.42
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.90	0.41
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.41
30:0:1942:A:C4'	38:0:9046:HOH:O	2.67	0.41
30:0:1845:A:O2'	30:0:1846:U:H5'	2.19	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.20	0.41
4:D:131:THR:HG21	30:0:2348:C:H1'	2.01	0.41
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.20	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.20	0.41
6:F:38:LYS:HE3	30:0:244:C:OP2	2.20	0.41
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.41
30:0:2290:U:H2'	38:0:7148:HOH:O	2.19	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.49	0.41
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.56	0.41
22:V:1:THR:HG23	22:V:2:VAL:HG23	2.02	0.41
29:3:70:ARG:HD3	38:3:9059:HOH:O	2.19	0.41
30:0:1598:A:N6	35:0:8815:CL:CL	2.90	0.41
30:0:488:U:C2'	38:0:4019:HOH:O	2.67	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.19	0.41
30:0:297:U:H2'	30:0:298:C:H6	1.83	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.41
30:0:351:A:O2'	30:0:352:A:H5'	2.20	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.92	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.02	0.41
26:Z:63:CYS:HA	26:Z:64:PRO:HD3	1.91	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
24:X:22:ASN:HA	24:X:25:ARG:HG3	2.02	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.19	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.35	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.03	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.20	0.41
13:M:59:GLY:HA3	13:M:141:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.33	0.41
30:0:1625:U:H3'	30:0:1625:U:C6	2.54	0.41
30:0:1706:G:C6	30:0:1707:G:C6	3.09	0.41
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	2.02	0.41
1:A:214:SER:HB2	38:0:4377:HOH:O	2.20	0.41
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.20	0.41
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.85	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:69:A:H2'	30:0:70:A:OP2	2.20	0.41
30:0:2635:A:C2'	30:0:2636:C:H5'	2.50	0.41
12:L:114:VAL:HG11	38:L:8874:HOH:O	2.20	0.41
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.50	0.41
30:0:920:C:H4'	30:0:921:G:N2	2.35	0.41
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.20	0.41
11:K:37:TYR:HB3	38:K:7169:HOH:O	2.20	0.41
23:W:43:GLY:HA3	30:0:945:U:O2'	2.20	0.41
30:0:423:A:C4	30:0:424:C:C6	3.09	0.41
30:0:2274:A:O2'	30:0:2275:G:H5'	2.20	0.41
15:O:21:SER:OG	15:O:106:PRO:HB2	2.20	0.41
30:0:1069:C:H2'	30:0:1070:A:O4'	2.21	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41
30:0:724:G:O2'	30:0:725:C:H5'	2.21	0.41
27:1:12:ASN:O	30:0:1415:G:H5'	2.20	0.41
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:1193:A:H2	30:0:1194:A:N6	2.16	0.41
10:J:19:MET:CE	10:J:132:LEU:HD11	2.51	0.41
30:0:1787:C:O2'	30:0:1788:U:H5'	2.20	0.41
30:0:1594:C:O2'	30:0:1607:A:H4'	2.20	0.41
30:0:307:G:H3'	38:0:6693:HOH:O	2.21	0.41
30:0:1483:C:O2'	30:0:1484:G:H5'	2.21	0.41
3:C:107:ARG:O	3:C:111:VAL:HG23	2.21	0.41
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.03	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.50	0.41
30:0:2032:U:H2'	30:0:2033:G:H5'	2.03	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.85	0.41
30:0:309:C:O2	30:0:309:C:H2'	2.20	0.41
30:0:736:A:H8	38:0:7219:HOH:O	2.03	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:571:C:H6	30:0:571:C:O5'	2.04	0.41
3:C:101:ASP:HB2	30:0:750:A:O3'	2.21	0.41
30:0:2903:C:O2'	30:0:2904:U:H5'	2.21	0.41
30:0:1381:A:N3	30:0:1382:G:H1'	2.36	0.41
4:D:128:LEU:N	38:D:6007:HOH:O	2.53	0.41
30:0:459:A:H4'	38:0:9460:HOH:O	2.20	0.41
2:B:233:ARG:NH1	2:B:233:ARG:HG2	2.35	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.20	0.41
30:0:764:C:H2'	30:0:765:G:O4'	2.20	0.41
30:0:1829:A:H2'	30:0:1830:C:H5'	2.03	0.41
30:0:962:C:H2'	30:0:963:C:H5'	2.03	0.41
30:0:1159:G:H2'	30:0:1160:G:O4'	2.21	0.41
30:0:1634:G:H2'	30:0:1635:U:C6	2.56	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.39	0.41
30:0:653:U:H2'	30:0:654:A:C8	2.55	0.41
29:3:38:ARG:NH1	30:0:396:U:C2	2.89	0.41
23:W:119:HIS:CG	38:0:5297:HOH:O	2.74	0.41
30:0:2316:G:H8	38:0:5663:HOH:O	2.03	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.48	0.41
5:E:7:ILE:HG13	5:E:11:VAL:HB	2.03	0.41
30:0:2354:A:C2	30:0:2367:A:C8	3.09	0.41
30:0:535:G:O6	30:0:2064:U:C6	2.74	0.41
5:E:68:HIS:CE1	38:E:5919:HOH:O	2.74	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.41
30:0:1625:U:C3'	30:0:1625:U:C6	3.04	0.41
30:0:1298:U:H2'	30:0:1299:G:C8	2.56	0.41
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.41
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.41
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.08	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:1520:G:C6	30:0:1521:C:C4	3.08	0.41
5:E:125:GLU:HB2	5:E:132:THR:HG23	2.03	0.41
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.41
14:N:82:TYR:CD2	14:N:82:TYR:C	2.93	0.41
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.41
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.56	0.41
31:9:61:C:H2'	31:9:62:A:H8	1.85	0.41
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.72	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:694:A:C2'	30:0:695:C:H5'	2.51	0.41
18:R:18:LEU:HG	18:R:91:LEU:HD13	2.03	0.41
30:0:2754:G:O2'	30:0:2755:G:H5'	2.20	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.90	0.41
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.56	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
2:B:225:GLY:HA3	38:B:9027:HOH:O	2.21	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.74	0.41
30:0:1795:G:H2'	30:0:1796:A:O4'	2.21	0.41
30:0:615:G:H2'	30:0:616:U:C6	2.56	0.41
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.21	0.41
30:0:1205:U:H2'	30:0:1206:U:H5'	1.94	0.40
30:0:1116:U:C2	30:0:1246:A:N6	2.89	0.40
30:0:2491:G:C1'	38:0:6878:HOH:O	2.58	0.40
9:I:112:LEU:HG	30:0:1162:G:O2'	2.21	0.40
22:V:39:ALA:N	22:V:40:PRO:CD	2.84	0.40
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
1:A:109:GLU:HG2	1:A:116:GLY:H	1.85	0.40
30:0:1375:A:H2'	30:0:1376:G:H5'	2.04	0.40
23:W:130:HIS:NE2	31:9:88:G:OP1	2.50	0.40
23:W:130:HIS:O	23:W:136:GLY:HA3	2.21	0.40
30:0:626:U:C4	30:0:627:G:C6	3.09	0.40
30:0:1555:G:H4'	30:0:1630:A:H2	1.86	0.40
3:C:131:PHE:CD2	3:C:131:PHE:N	2.89	0.40
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.40
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.53	0.40
20:T:9:LYS:HE2	20:T:13:ARG:HH12	1.84	0.40
30:0:2564:G:OP2	30:0:2565:C:H5''	2.21	0.40
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.88	0.40
1:A:88:ILE:HG22	1:A:88:ILE:O	2.21	0.40
30:0:1992:U:H2'	30:0:1994:A:OP2	2.20	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.40
30:0:423:A:H2'	30:0:424:C:H6	1.87	0.40
30:0:499:G:O2'	30:0:500:G:H5'	2.21	0.40
14:N:170:GLU:O	14:N:174:GLU:HG3	2.20	0.40
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.21	0.40
30:0:2614:C:O2'	30:0:2615:U:H5'	2.21	0.40
30:0:1947:G:H2'	30:0:1948:G:C8	2.56	0.40
30:0:821:U:H2'	30:0:822:C:C6	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:553:G:O4'	30:0:1325:G:H5'	2.22	0.40
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.40
30:0:570:C:H6	30:0:570:C:O5'	2.04	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.04	0.40
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.21	0.40
3:C:193:LEU:HD12	3:C:211:ASP:O	2.21	0.40
3:C:102:LEU:HD12	3:C:102:LEU:HA	1.91	0.40
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.21	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.70	0.40
30:0:2032:U:H2'	30:0:2033:G:H5''	2.03	0.40
4:D:22:VAL:HA	4:D:73:VAL:O	2.21	0.40
9:I:130:LEU:HA	38:I:6825:HOH:O	2.22	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.54	0.40
30:0:1014:A:H5''	31:9:101:G:O2'	2.22	0.40
5:E:68:HIS:O	5:E:72:MET:HG3	2.22	0.40
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.03	0.40
4:D:23:VAL:HG12	4:D:130:VAL:HG22	2.03	0.40
18:R:114:VAL:HG13	18:R:114:VAL:O	2.22	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.62	0.40
30:0:1311:G:C2	30:0:1312:G:C8	3.09	0.40
30:0:939:A:N1	30:0:1027:G:O2'	2.50	0.40
2:B:229:ARG:HD2	38:0:9111:HOH:O	2.20	0.40
30:0:503:G:H2'	30:0:504:G:H8	1.87	0.40
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.40
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.22	0.40
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.21	0.40
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.85	0.40
30:0:2509:A:C2	30:0:2510:C:H1'	2.56	0.40
2:B:267:LYS:HD3	38:0:9565:HOH:O	2.22	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.90	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.40
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.86	0.40
30:0:695:C:H2'	30:0:696:C:C6	2.57	0.40
13:M:188:ARG:HH11	30:0:154:C:H3'	1.86	0.40
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.57	0.40
30:0:214:U:H5'	38:0:6146:HOH:O	2.22	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.40
30:0:2897:C:O2'	30:0:2898:G:H5'	2.22	0.40
30:0:1236:A:H2'	30:0:1237:U:O4'	2.22	0.40
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.85	0.40
30:0:2734:G:O2'	30:0:2735:U:H5'	2.22	0.40
27:1:53:LYS:HA	27:1:53:LYS:HD3	1.91	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%)	211 (90%)	18 (8%)	6 (3%)	8	32
2	B	335/338 (99%)	306 (91%)	25 (8%)	4 (1%)	19	57
3	C	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	43	82
4	D	134/177 (76%)	113 (84%)	16 (12%)	5 (4%)	5	20
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	8	32
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	147 (94%)	8 (5%)	1 (1%)	33	76
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	15	50
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	30	72
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	27	68
12	L	141/165 (86%)	125 (89%)	14 (10%)	2 (1%)	16	52
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	38	79
14	N	184/187 (98%)	169 (92%)	12 (6%)	3 (2%)	14	47
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
21	U	51/67 (76%)	45 (88%)	5 (10%)	1 (2%)	11	40
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	14	47
23	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	18	54
24	X	80/92 (87%)	75 (94%)	4 (5%)	1 (1%)	18	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	7 (10%)	2 (3%)	8	29
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3447 (93%)	222 (6%)	36 (1%)	22	63

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	27	LEU
8	H	19	ARG
1	A	34	ASP
10	J	65	ASN
23	W	49	ASN
23	W	77	ALA
26	Z	44	ARG
1	A	36	ASP
2	B	2	GLN
2	B	185	GLY
4	D	65	GLU
11	K	127	ALA
12	L	149	ARG
13	M	71	SER
24	X	70	ILE
26	Z	65	ASN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	82	ALA
21	U	55	ALA
22	V	43	PRO
1	A	69	LEU
3	C	201	SER

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Mol	Chain	Res	Type
4	D	27	ILE
4	D	97	GLN
9	I	83	GLY
1	A	88	ILE
2	B	169	GLY
6	F	27	GLY

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%)	170 (95%)	9 (5%)	34	73
2	B	282/283 (100%)	263 (93%)	19 (7%)	23	56
3	C	193/193 (100%)	176 (91%)	17 (9%)	14	40
4	D	117/148 (79%)	110 (94%)	7 (6%)	27	63
5	E	152/156 (97%)	149 (98%)	3 (2%)	68	92
6	F	93/94 (99%)	91 (98%)	2 (2%)	64	92
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	45	84
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	94
10	J	118/121 (98%)	110 (93%)	8 (7%)	22	55
11	K	106/106 (100%)	104 (98%)	2 (2%)	69	93
12	L	113/127 (89%)	110 (97%)	3 (3%)	57	90
13	M	158/160 (99%)	151 (96%)	7 (4%)	39	77
14	N	149/150 (99%)	142 (95%)	7 (5%)	36	75
15	O	93/94 (99%)	92 (99%)	1 (1%)	84	97
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	94
17	Q	79/80 (99%)	76 (96%)	3 (4%)	44	83
18	R	117/122 (96%)	111 (95%)	6 (5%)	33	72
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	96
20	T	105/106 (99%)	97 (92%)	8 (8%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	92
22	V	51/57 (90%)	50 (98%)	1 (2%)	68	92
23	W	130/130 (100%)	126 (97%)	4 (3%)	52	88
24	X	66/74 (89%)	62 (94%)	4 (6%)	26	62
25	Y	120/196 (61%)	116 (97%)	4 (3%)	50	87
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	91
29	3	79/79 (100%)	78 (99%)	1 (1%)	80	96
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	41	80

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	37	VAL
1	A	38	ILE
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	103	ASP
2	B	108	GLU
2	B	132	HIS
2	B	190	MET
2	B	192	ASP
2	B	234	ARG
2	B	248	ARG
2	B	251	VAL

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Mol	Chain	Res	Type
2	B	254	GLN
2	B	264	GLU
2	B	277	GLU
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	131	PHE
3	C	136	VAL
3	C	151	GLN
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	211	ASP
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN
4	D	50	VAL
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP
4	D	170	TYR
5	E	7	ILE
5	E	102	VAL
5	E	156	ASP
6	F	12	LEU
6	F	46	GLU
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG

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Mol	Chain	Res	Type
10	J	76	ASP
10	J	79	PHE
10	J	107	ASN
10	J	112	ASP
11	K	10	GLN
11	K	119	GLN
12	L	35	ARG
12	L	80	ASP
12	L	104	ASP
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
14	N	134	ASP
14	N	135	VAL
14	N	147	ILE
15	O	38	ARG
16	P	21	VAL
16	P	98	ILE
17	Q	11	ARG
17	Q	57	ASP
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
19	S	10	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	73	HIS
20	T	89	ARG
20	T	96	VAL

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Mol	Chain	Res	Type
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
22	V	22	ASP
23	W	38	THR
23	W	52	VAL
23	W	88	THR
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	79	GLU
24	X	82	GLU
25	Y	95	THR
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	3	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	103	ASN
5	E	119	HIS
5	E	143	GLN
5	E	150	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS

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Mol	Chain	Res	Type
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
10	J	142	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	118	GLN
17	Q	27	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
22	V	4	HIS
22	V	60	GLN
23	W	2	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS

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Mol	Chain	Res	Type
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	27 (0%)
31	9	121/122 (99%)	15 (12%)	1 (0%)
All	All	2866/3045 (94%)	257 (8%)	28 (0%)

All (257) 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	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	187	A

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Mol	Chain	Res	Type
30	0	191	A
30	0	192	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	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
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	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U

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Mol	Chain	Res	Type
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
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

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Mol	Chain	Res	Type
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	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
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
30	0	1409	G
30	0	1474	C
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	1562	C
30	0	1592	G
30	0	1617	C
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

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Mol	Chain	Res	Type
30	0	1722	U
30	0	1723	G
30	0	1725	C
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
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
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	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G

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Mol	Chain	Res	Type
30	0	2272	G
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
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	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2747	C

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Mol	Chain	Res	Type
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
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 (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	604	G
30	0	644	G
30	0	681	G
30	0	699	C
30	0	834	G
30	0	857	A

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Mol	Chain	Res	Type
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
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	0.69	0	24,31,34	0.73	0
30	OMG	0	2588	30	24,26,27	0.79	1 (4%)	32,38,41	5.06	3 (9%)
30	UR3	0	2619	30	20,22,23	0.72	0	23,32,35	0.87	0
30	PSU	0	2621	30	19,21,22	1.19	3 (15%)	23,30,33	1.13	2 (8%)
30	1MA	0	628	30	23,25,26	0.83	0	32,37,40	0.92	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	-	1/8/25/26	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	2.91	1.43	1.37
30	0	2621	PSU	C6-N1	2.23	1.34	1.32
30	0	2621	PSU	P-OP1	2.19	1.49	1.46
30	0	2588	OMG	P-OP1	2.03	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	-28.02	130.37	134.14
30	0	628	1MA	C2-N3-C4	-3.20	110.76	116.23
30	0	2588	OMG	C6-N1-C2	3.20	125.11	119.51
30	0	2588	OMG	C2-N3-C4	-2.35	111.79	115.09
30	0	2621	PSU	C5-C1'-C2'	-2.28	111.59	115.61
30	0	2621	PSU	C5-C4-N3	-2.18	114.89	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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%)	-0.36	5 (2%) 60 69	35, 59, 97, 117	0
2	B	337/338 (99%)	-0.57	1 (0%) 91 95	36, 60, 90, 100	0
3	C	246/246 (100%)	-0.57	0 100 100	30, 51, 75, 89	0
4	D	140/177 (79%)	1.20	33 (23%) 1 2	73, 108, 135, 146	0
5	E	172/178 (96%)	-0.48	1 (0%) 86 91	51, 74, 96, 104	0
6	F	119/120 (99%)	0.22	9 (7%) 14 17	55, 78, 111, 125	0
7	G	29/348 (8%)	0.72	2 (6%) 17 20	83, 103, 109, 112	0
8	H	160/177 (90%)	0.15	9 (5%) 24 28	50, 73, 106, 113	0
9	I	70/162 (43%)	3.35	49 (70%) 0 0	137, 156, 173, 174	0
10	J	142/145 (97%)	-0.51	1 (0%) 84 90	41, 58, 78, 97	0
11	K	132/132 (100%)	-0.74	0 100 100	40, 55, 79, 82	0
12	L	145/165 (87%)	0.16	9 (6%) 20 23	34, 73, 123, 136	0
13	M	194/196 (98%)	-0.70	1 (0%) 88 93	35, 50, 66, 73	0
14	N	186/187 (99%)	0.02	6 (3%) 45 54	52, 75, 123, 135	0
15	O	115/116 (99%)	-0.51	0 100 100	45, 61, 78, 84	0
16	P	143/149 (95%)	-0.60	0 100 100	46, 61, 77, 84	0
17	Q	95/96 (98%)	-0.52	0 100 100	44, 55, 71, 86	0
18	R	150/155 (96%)	-0.72	0 100 100	39, 52, 71, 86	0
19	S	81/85 (95%)	-0.41	2 (2%) 54 64	49, 65, 86, 98	0
20	T	119/120 (99%)	-0.35	4 (3%) 43 51	47, 62, 89, 123	0
21	U	53/67 (79%)	-0.61	1 (1%) 64 72	48, 62, 79, 88	0
22	V	65/71 (91%)	0.89	10 (15%) 3 4	55, 80, 129, 134	0
23	W	154/154 (100%)	-0.45	1 (0%) 86 91	41, 57, 74, 88	0
24	X	82/92 (89%)	-0.11	5 (6%) 21 24	49, 67, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.72	1 (0%) 84 90	31, 50, 73, 94	0
26	Z	73/116 (62%)	0.92	14 (19%) 2 2	63, 87, 101, 106	0
27	1	56/57 (98%)	-0.69	0 100 100	32, 39, 45, 53	0
28	2	46/50 (92%)	-0.01	5 (10%) 6 8	41, 69, 104, 115	0
29	3	92/92 (100%)	-0.36	0 100 100	44, 68, 81, 91	0
30	0	2754/2923 (94%)	-0.49	22 (0%) 83 89	28, 53, 96, 172	0
31	9	122/122 (100%)	-0.67	2 (1%) 68 78	45, 74, 96, 153	0
All	All	6651/7517 (88%)	-0.34	193 (2%) 49 58	28, 58, 108, 174	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	11.1
9	I	74	ILE	9.9
9	I	66	GLY	9.0
22	V	1	THR	8.7
4	D	63	ILE	8.3
9	I	72	GLU	8.1
26	Z	46	SER	8.0
9	I	104	ALA	7.9
9	I	71	ALA	7.8
9	I	70	THR	7.7
22	V	43	PRO	7.7
22	V	40	PRO	7.2
9	I	106	GLN	7.2
14	N	166	ALA	7.0
9	I	100	VAL	7.0
4	D	57	THR	6.6
26	Z	44	ARG	6.0
9	I	128	THR	5.7
26	Z	35	SER	5.7
9	I	108	HIS	5.5
30	0	735	C	5.4
9	I	132	VAL	5.4
9	I	109	PRO	5.3
26	Z	45	VAL	5.3
4	D	85	GLN	5.3
9	I	80	PHE	5.2
9	I	113	SER	5.1
26	Z	58	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
9	I	105	GLU	4.8
4	D	134	LEU	4.8
9	I	97	VAL	4.8
12	L	60	GLU	4.8
9	I	102	GLN	4.8
9	I	79	GLY	4.8
9	I	112	LEU	4.7
31	9	1	U	4.6
26	Z	50	VAL	4.5
14	N	155	GLU	4.5
9	I	99	GLN	4.5
8	H	133	GLY	4.4
22	V	38	GLY	4.4
26	Z	60	ASP	4.3
4	D	90	LEU	4.3
1	A	237	GLY	4.2
9	I	111	LEU	4.2
4	D	64	ARG	4.2
9	I	93	ALA	4.2
4	D	18	ILE	4.1
9	I	110	ASP	4.1
6	F	106	ALA	4.0
20	T	116	ASP	3.9
12	L	81	VAL	3.9
19	S	81	ILE	3.8
24	X	71	ARG	3.8
26	Z	49	ARG	3.8
9	I	76	ASP	3.8
9	I	88	GLN	3.8
9	I	98	ASP	3.7
9	I	69	PRO	3.7
4	D	88	LEU	3.7
30	0	1198	U	3.7
12	L	75	LEU	3.6
22	V	41	GLU	3.6
4	D	69	ILE	3.5
22	V	37	GLY	3.5
28	2	49	GLU	3.5
30	0	1199	A	3.5
30	0	282	C	3.4
4	D	92	GLU	3.4
4	D	17	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
9	I	103	ILE	3.4
4	D	93	LEU	3.3
9	I	83	GLY	3.3
4	D	172	VAL	3.3
20	T	118	SER	3.3
25	Y	235	GLU	3.3
9	I	92	VAL	3.3
7	G	27	ILE	3.2
30	O	1172	G	3.2
4	D	81	GLU	3.2
9	I	116	LEU	3.2
6	F	99	THR	3.2
9	I	82	THR	3.2
9	I	86	GLU	3.2
8	H	86	TYR	3.2
1	A	37	VAL	3.1
9	I	114	TYR	3.1
4	D	91	ALA	3.1
1	A	91	GLY	3.1
28	2	35	ARG	3.1
9	I	67	VAL	3.0
9	I	118	ASN	3.0
4	D	75	LEU	3.0
8	H	40	GLN	2.9
26	Z	69	ASP	2.9
4	D	84	LEU	2.9
4	D	44	ILE	2.9
4	D	171	ASP	2.9
12	L	80	ASP	2.9
12	L	106	VAL	2.9
12	L	62	ALA	2.9
12	L	100	ALA	2.9
9	I	81	GLU	2.9
22	V	2	VAL	2.8
9	I	78	ALA	2.8
4	D	66	GLY	2.8
26	Z	55	SER	2.7
4	D	45	THR	2.7
4	D	166	ILE	2.7
4	D	102	GLY	2.7
20	T	119	ALA	2.7
4	D	165	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	98	VAL	2.7
4	D	89	PRO	2.6
30	0	1169	U	2.6
30	0	1200	A	2.6
6	F	28	ALA	2.6
28	2	39	ARG	2.6
9	I	73	LEU	2.6
24	X	85	VAL	2.6
10	J	70	PHE	2.6
24	X	10	VAL	2.6
9	I	127	CYS	2.6
14	N	183	ASP	2.6
31	9	24	U	2.6
2	B	105	PHE	2.5
4	D	27	ILE	2.5
23	W	96	LEU	2.5
30	0	497	A	2.5
9	I	95	LEU	2.5
26	Z	47	ARG	2.5
4	D	135	VAL	2.4
22	V	45	ARG	2.4
4	D	70	GLY	2.4
9	I	75	LYS	2.4
6	F	97	ALA	2.4
30	0	1202	A	2.4
12	L	105	TYR	2.4
24	X	7	GLU	2.4
14	N	138	ASP	2.4
9	I	91	PHE	2.4
14	N	147	ILE	2.4
6	F	75	ILE	2.4
30	0	2637	A	2.3
30	0	1177	A	2.3
30	0	1181	A	2.3
9	I	101	LYS	2.3
9	I	133	THR	2.3
26	Z	68	GLU	2.3
6	F	17	LEU	2.3
4	D	73	VAL	2.3
30	0	2237	G	2.3
9	I	94	ASP	2.3
30	0	970	U	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	103	VAL	2.3
14	N	185	GLU	2.3
26	Z	42	TYR	2.3
30	0	1951	G	2.3
24	X	80	GLU	2.2
8	H	158	ASN	2.2
30	0	1163	G	2.2
12	L	76	LEU	2.2
30	0	1196	C	2.2
4	D	130	VAL	2.2
4	D	157	LEU	2.2
30	0	284	C	2.2
6	F	16	ALA	2.2
8	H	77	ILE	2.2
6	F	44	SER	2.2
7	G	24	VAL	2.2
20	T	115	GLU	2.2
30	0	1170	U	2.2
9	I	125	GLY	2.2
4	D	61	PHE	2.1
28	2	20	ARG	2.1
8	H	97	VAL	2.1
26	Z	53	ILE	2.1
9	I	68	PRO	2.1
4	D	26	GLY	2.1
9	I	129	SER	2.1
1	A	99	ILE	2.1
13	M	1	ALA	2.1
5	E	170	ARG	2.1
28	2	27	LEU	2.1
22	V	31	ARG	2.1
8	H	149	VAL	2.1
30	0	2769	C	2.1
21	U	43	GLY	2.0
30	0	736	A	2.0
8	H	76	LEU	2.0
8	H	66	GLU	2.0
30	0	1180	U	2.0
19	S	20	PHE	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	UR3	0	2619	21/22	0.14	1.46	43,45,48,49	0
30	OMU	0	2587	21/22	0.12	0.40	40,43,46,49	0
30	1MA	0	628	23/24	0.14	-0.08	35,38,38,39	0
30	PSU	0	2621	20/21	0.13	-0.83	35,38,47,48	0
30	OMG	0	2588	24/25	0.12	-0.98	38,42,43,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
35	CL	0	8822	1/1	0.53	189.49	106,106,106,106	0
36	SR	0	9007	1/1	1.21	128.93	200,200,200,200	0
34	NA	0	8505	1/1	1.03	106.45	49,49,49,49	0
36	SR	0	8994	1/1	1.02	97.03	200,200,200,200	0
34	NA	0	8509	1/1	0.15	90.51	69,69,69,69	0
34	NA	0	8554	1/1	0.89	76.13	78,78,78,78	0
34	NA	0	8562	1/1	0.76	65.01	74,74,74,74	0
36	SR	0	8996	1/1	0.95	63.49	200,200,200,200	0
32	MG	0	8037	1/1	0.33	62.43	90,90,90,90	0
34	NA	0	8561	1/1	0.53	55.50	78,78,78,78	0
36	SR	0	8997	1/1	0.61	54.45	200,200,200,200	0
36	SR	0	8982	1/1	1.13	52.45	200,200,200,200	0
34	NA	0	8546	1/1	1.23	48.86	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8565	1/1	0.66	48.44	68,68,68,68	0
32	MG	0	8031	1/1	0.32	36.26	72,72,72,72	0
34	NA	0	8574	1/1	0.36	34.69	55,55,55,55	0
36	SR	0	8983	1/1	0.37	34.60	195,195,195,195	0
36	SR	0	9004	1/1	0.67	33.92	200,200,200,200	0
34	NA	0	8514	1/1	0.47	28.92	48,48,48,48	0
34	NA	0	8550	1/1	0.48	28.31	61,61,61,61	0
34	NA	0	8564	1/1	0.40	26.17	81,81,81,81	0
34	NA	0	8522	1/1	0.38	25.28	83,83,83,83	0
34	NA	0	8566	1/1	0.29	23.78	60,60,60,60	0
34	NA	0	8547	1/1	0.56	23.39	54,54,54,54	0
34	NA	0	8568	1/1	0.51	21.84	50,50,50,50	0
36	SR	0	8914	1/1	0.26	21.37	110,110,110,110	0
32	MG	0	8092	1/1	0.16	21.00	67,67,67,67	0
36	SR	0	8979	1/1	0.20	20.21	198,198,198,198	0
34	NA	0	8573	1/1	0.28	19.38	77,77,77,77	0
32	MG	0	8030	1/1	0.49	18.95	69,69,69,69	0
34	NA	0	8512	1/1	0.44	17.70	56,56,56,56	0
32	MG	0	8090	1/1	0.31	17.24	62,62,62,62	0
34	NA	0	8555	1/1	0.45	15.53	51,51,51,51	0
34	NA	0	8549	1/1	0.33	14.15	58,58,58,58	0
34	NA	0	8525	1/1	0.20	13.78	78,78,78,78	0
36	SR	0	8959	1/1	0.19	13.35	174,174,174,174	0
34	NA	0	8535	1/1	0.24	12.75	53,53,53,53	0
32	MG	0	8080	1/1	0.35	12.73	69,69,69,69	0
34	NA	0	8530	1/1	0.43	12.58	55,55,55,55	0
36	SR	B	8987	1/1	0.49	12.06	200,200,200,200	0
34	NA	0	8560	1/1	0.39	12.03	83,83,83,83	0
36	SR	0	8905	1/1	0.27	12.00	68,68,68,68	0
34	NA	0	8556	1/1	0.51	11.34	49,49,49,49	0
34	NA	0	8544	1/1	0.22	11.32	75,75,75,75	0
32	MG	0	8082	1/1	0.24	11.24	69,69,69,69	0
32	MG	0	8071	1/1	0.17	11.04	71,71,71,71	0
34	NA	0	8563	1/1	0.34	10.58	94,94,94,94	0
34	NA	0	8506	1/1	0.23	10.38	68,68,68,68	0
34	NA	0	8552	1/1	0.33	9.72	72,72,72,72	0
34	NA	0	8548	1/1	0.18	9.57	55,55,55,55	0
34	NA	0	8528	1/1	0.26	8.98	58,58,58,58	0
34	NA	0	8551	1/1	0.30	8.42	59,59,59,59	0
34	NA	0	8518	1/1	0.38	8.40	94,94,94,94	0
32	MG	0	8078	1/1	0.32	7.86	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8542	1/1	0.30	7.77	66,66,66,66	0
36	SR	0	8903	1/1	0.18	7.48	58,58,58,58	0
34	NA	9	8572	1/1	0.23	6.99	111,111,111,111	0
34	NA	0	8501	1/1	0.20	6.97	44,44,44,44	0
35	CL	Y	8820	1/1	0.24	6.67	51,51,51,51	0
32	MG	0	8063	1/1	0.17	6.27	71,71,71,71	0
34	NA	0	8541	1/1	0.26	6.18	69,69,69,69	0
32	MG	0	8081	1/1	0.16	5.96	74,74,74,74	0
36	SR	0	8976	1/1	0.26	5.80	200,200,200,200	0
32	MG	0	8047	1/1	0.29	5.79	65,65,65,65	0
36	SR	0	8938	1/1	0.13	5.77	192,192,192,192	0
34	NA	0	8545	1/1	0.20	5.74	41,41,41,41	0
36	SR	0	8922	1/1	0.24	5.35	170,170,170,170	0
34	NA	0	8569	1/1	0.24	5.19	54,54,54,54	0
34	NA	0	8534	1/1	0.26	5.15	42,42,42,42	0
34	NA	0	8559	1/1	0.14	4.94	76,76,76,76	0
35	CL	0	8816	1/1	0.27	4.91	85,85,85,85	0
34	NA	0	8517	1/1	0.18	4.75	36,36,36,36	0
32	MG	0	8029	1/1	0.17	4.73	48,48,48,48	0
34	NA	0	8527	1/1	0.23	4.67	71,71,71,71	0
32	MG	A	8051	1/1	0.45	4.66	72,72,72,72	0
36	SR	0	8925	1/1	0.12	4.63	91,91,91,91	0
36	SR	0	8924	1/1	0.15	4.45	135,135,135,135	0
36	SR	0	8947	1/1	0.26	4.44	200,200,200,200	0
32	MG	0	8017	1/1	0.20	4.36	25,25,25,25	0
32	MG	0	8041	1/1	0.20	4.19	31,31,31,31	0
32	MG	0	8015	1/1	0.15	4.12	36,36,36,36	0
36	SR	0	8926	1/1	0.11	3.93	127,127,127,127	0
34	NA	0	8567	1/1	0.19	3.86	80,80,80,80	0
32	MG	0	8016	1/1	0.20	3.76	60,60,60,60	0
32	MG	0	8014	1/1	0.17	3.67	35,35,35,35	0
32	MG	0	8048	1/1	0.19	3.63	26,26,26,26	0
36	SR	0	8946	1/1	0.21	3.54	122,122,122,122	0
32	MG	0	8009	1/1	0.20	3.46	29,29,29,29	0
32	MG	0	8008	1/1	0.15	3.37	27,27,27,27	0
32	MG	0	8018	1/1	0.18	3.29	46,46,46,46	0
36	SR	0	8909	1/1	0.15	3.20	85,85,85,85	0
32	MG	0	8067	1/1	0.22	2.98	34,34,34,34	0
34	NA	0	8524	1/1	0.16	2.89	58,58,58,58	0
34	NA	0	8558	1/1	0.23	2.86	50,50,50,50	0
36	SR	0	8904	1/1	0.18	2.85	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8055	1/1	0.19	2.78	46,46,46,46	0
36	SR	S	8961	1/1	0.09	2.67	122,122,122,122	0
36	SR	0	8937	1/1	0.21	2.51	115,115,115,115	0
36	SR	0	8986	1/1	0.15	2.37	200,200,200,200	0
32	MG	0	8061	1/1	0.21	2.01	30,30,30,30	0
32	MG	0	8040	1/1	0.16	1.97	96,96,96,96	0
34	NA	0	8511	1/1	0.14	1.95	59,59,59,59	0
36	SR	0	8918	1/1	0.13	1.93	85,85,85,85	0
32	MG	0	8028	1/1	0.16	1.90	27,27,27,27	0
32	MG	0	8084	1/1	0.14	1.81	37,37,37,37	0
32	MG	0	8003	1/1	0.17	1.76	34,34,34,34	0
34	NA	0	8553	1/1	0.17	1.61	68,68,68,68	0
36	SR	0	8906	1/1	0.20	1.56	60,60,60,60	0
32	MG	0	8066	1/1	0.15	1.46	76,76,76,76	0
32	MG	0	8019	1/1	0.19	1.45	27,27,27,27	0
36	SR	0	8944	1/1	0.12	1.43	182,182,182,182	0
34	NA	0	8570	1/1	0.12	1.42	60,60,60,60	0
36	SR	9	8980	1/1	0.12	1.40	200,200,200,200	0
34	NA	0	8502	1/1	0.13	1.37	65,65,65,65	0
32	MG	0	8007	1/1	0.18	1.33	38,38,38,38	0
32	MG	0	8062	1/1	0.18	1.25	50,50,50,50	0
36	SR	0	8948	1/1	0.12	1.16	102,102,102,102	0
35	CL	J	8801	1/1	0.19	1.14	79,79,79,79	0
34	NA	0	8533	1/1	0.14	1.11	67,67,67,67	0
32	MG	0	8004	1/1	0.17	1.06	30,30,30,30	0
36	SR	0	8958	1/1	0.11	1.05	123,123,123,123	0
36	SR	R	8912	1/1	0.15	0.97	86,86,86,86	0
32	MG	0	8022	1/1	0.12	0.93	32,32,32,32	0
36	SR	A	8929	1/1	0.16	0.90	137,137,137,137	0
36	SR	0	8921	1/1	0.12	0.87	92,92,92,92	0
32	MG	0	8023	1/1	0.14	0.82	32,32,32,32	0
34	NA	0	8575	1/1	0.15	0.76	86,86,86,86	0
36	SR	0	8915	1/1	0.12	0.71	131,131,131,131	0
34	NA	0	8531	1/1	0.11	0.67	44,44,44,44	0
36	SR	0	8995	1/1	0.17	0.64	140,140,140,140	0
34	NA	0	8537	1/1	0.12	0.61	41,41,41,41	0
36	SR	0	8955	1/1	0.11	0.57	200,200,200,200	0
32	MG	0	8036	1/1	0.10	0.57	50,50,50,50	0
35	CL	0	8815	1/1	0.10	0.56	78,78,78,78	0
32	MG	0	8020	1/1	0.10	0.56	43,43,43,43	0
36	SR	0	8989	1/1	0.13	0.54	185,185,185,185	0
34	NA	0	8507	1/1	0.14	0.48	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8508	1/1	0.12	0.42	39,39,39,39	0
36	SR	0	8981	1/1	0.14	0.28	153,153,153,153	0
32	MG	0	8070	1/1	0.13	0.10	45,45,45,45	0
32	MG	K	8054	1/1	0.14	0.08	50,50,50,50	0
36	SR	0	8907	1/1	0.12	0.06	56,56,56,56	0
37	CD	U	8701	1/1	0.11	0.03	72,72,72,72	0
36	SR	0	8933	1/1	0.14	-0.06	150,150,150,150	0
32	MG	0	8011	1/1	0.16	-0.12	33,33,33,33	0
32	MG	0	8043	1/1	0.11	-0.18	49,49,49,49	0
34	NA	0	8504	1/1	0.15	-0.18	37,37,37,37	0
34	NA	0	8513	1/1	0.16	-0.29	58,58,58,58	0
36	SR	0	8972	1/1	0.14	-0.30	141,141,141,141	0
32	MG	B	8042	1/1	0.09	-0.30	50,50,50,50	0
32	MG	0	8069	1/1	0.16	-0.32	72,72,72,72	0
32	MG	0	8045	1/1	0.10	-0.33	35,35,35,35	0
32	MG	0	8006	1/1	0.12	-0.36	30,30,30,30	0
34	NA	J	8538	1/1	0.15	-0.39	60,60,60,60	0
34	NA	0	8523	1/1	0.11	-0.39	45,45,45,45	0
32	MG	0	8064	1/1	0.13	-0.40	37,37,37,37	0
36	SR	0	9001	1/1	0.11	-0.42	173,173,173,173	0
35	CL	J	8821	1/1	0.13	-0.49	71,71,71,71	0
34	NA	9	8543	1/1	0.16	-0.53	49,49,49,49	0
35	CL	0	8817	1/1	0.11	-0.57	65,65,65,65	0
33	K	0	8401	1/1	0.12	-0.57	74,74,74,74	0
32	MG	0	8039	1/1	0.15	-0.60	77,77,77,77	0
32	MG	0	8021	1/1	0.10	-0.65	30,30,30,30	0
32	MG	0	8083	1/1	0.10	-0.66	73,73,73,73	0
36	SR	0	9008	1/1	0.14	-0.70	89,89,89,89	0
36	SR	3	8932	1/1	0.11	-0.71	79,79,79,79	0
34	NA	0	8520	1/1	0.09	-0.75	53,53,53,53	0
32	MG	0	8012	1/1	0.15	-0.78	25,25,25,25	0
36	SR	0	8957	1/1	0.10	-0.78	196,196,196,196	0
36	SR	0	8964	1/1	0.09	-0.83	139,139,139,139	0
36	SR	0	8993	1/1	0.08	-0.88	182,182,182,182	0
36	SR	0	8954	1/1	0.11	-0.90	112,112,112,112	0
36	SR	0	8936	1/1	0.10	-0.97	94,94,94,94	0
35	CL	J	8802	1/1	0.09	-0.99	76,76,76,76	0
34	NA	C	8503	1/1	0.11	-0.99	44,44,44,44	0
32	MG	0	8035	1/1	0.10	-1.02	68,68,68,68	0
36	SR	0	8935	1/1	0.09	-1.02	80,80,80,80	0
32	MG	0	8050	1/1	0.12	-1.04	37,37,37,37	0
36	SR	0	8956	1/1	0.08	-1.05	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8088	1/1	0.12	-1.09	42,42,42,42	0
34	NA	0	8571	1/1	0.07	-1.16	77,77,77,77	0
36	SR	0	8941	1/1	0.14	-1.17	116,116,116,116	0
36	SR	F	9005	1/1	0.07	-1.18	134,134,134,134	0
35	CL	M	8818	1/1	0.09	-1.19	47,47,47,47	0
35	CL	O	8808	1/1	0.10	-1.21	81,81,81,81	0
36	SR	0	8934	1/1	0.12	-1.22	130,130,130,130	0
34	NA	M	8539	1/1	0.09	-1.22	34,34,34,34	0
32	MG	0	8005	1/1	0.16	-1.24	33,33,33,33	0
36	SR	0	8992	1/1	0.11	-1.25	137,137,137,137	0
37	CD	Z	8703	1/1	0.09	-1.25	91,91,91,91	0
32	MG	0	8058	1/1	0.07	-1.28	23,23,23,23	0
36	SR	0	8991	1/1	0.09	-1.28	197,197,197,197	0
35	CL	L	8810	1/1	0.09	-1.33	61,61,61,61	0
32	MG	0	8010	1/1	0.12	-1.34	35,35,35,35	0
36	SR	0	8931	1/1	0.09	-1.35	117,117,117,117	0
36	SR	0	8911	1/1	0.06	-1.41	85,85,85,85	0
37	CD	1	8702	1/1	0.10	-1.51	65,65,65,65	0
36	SR	0	8988	1/1	0.10	-1.56	173,173,173,173	0
34	NA	0	8515	1/1	0.11	-1.59	37,37,37,37	0
36	SR	B	8950	1/1	0.15	-1.60	132,132,132,132	0
36	SR	0	9000	1/1	0.10	-1.61	177,177,177,177	0
34	NA	Q	8540	1/1	0.07	-1.61	60,60,60,60	0
35	CL	0	8811	1/1	0.09	-1.62	68,68,68,68	0
35	CL	N	8807	1/1	0.10	-1.62	71,71,71,71	0
36	SR	0	8969	1/1	0.10	-1.62	160,160,160,160	0
35	CL	R	8806	1/1	0.12	-1.63	52,52,52,52	0
32	MG	9	8074	1/1	0.11	-1.65	77,77,77,77	0
36	SR	0	8917	1/1	0.10	-1.65	111,111,111,111	0
36	SR	A	8977	1/1	0.07	-1.65	161,161,161,161	0
37	CD	3	8704	1/1	0.07	-1.68	81,81,81,81	0
36	SR	0	8975	1/1	0.07	-1.72	135,135,135,135	0
36	SR	0	9002	1/1	0.07	-1.72	184,184,184,184	0
32	MG	0	8046	1/1	0.10	-1.77	41,41,41,41	0
32	MG	T	8057	1/1	0.08	-1.78	65,65,65,65	0
34	NA	0	8516	1/1	0.12	-1.78	42,42,42,42	0
36	SR	0	8951	1/1	0.07	-1.86	142,142,142,142	0
32	MG	0	8001	1/1	0.10	-1.87	33,33,33,33	0
36	SR	A	8930	1/1	0.04	-1.87	104,104,104,104	0
35	CL	A	8809	1/1	0.10	-1.90	74,74,74,74	0
36	SR	1	8952	1/1	0.13	-1.92	91,91,91,91	0
34	NA	R	8532	1/1	0.06	-1.98	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8967	1/1	0.06	-1.98	132,132,132,132	0
33	K	0	8402	1/1	0.12	-2.02	87,87,87,87	0
36	SR	0	8949	1/1	0.09	-2.04	119,119,119,119	0
36	SR	0	8985	1/1	0.07	-2.05	143,143,143,143	0
32	MG	0	8079	1/1	0.09	-2.08	55,55,55,55	0
36	SR	0	8943	1/1	0.07	-2.13	117,117,117,117	0
35	CL	0	8813	1/1	0.06	-2.38	61,61,61,61	0
36	SR	0	8998	1/1	0.12	-2.45	175,175,175,175	0
32	MG	0	8073	1/1	0.07	-2.54	83,83,83,83	0
36	SR	0	8901	1/1	0.11	-2.68	85,85,85,85	0
32	MG	0	8068	1/1	0.07	-2.73	54,54,54,54	0
37	CD	O	8705	1/1	0.05	-2.74	94,94,94,94	0
36	SR	9	8978	1/1	0.06	-2.75	133,133,133,133	0
36	SR	0	8928	1/1	0.06	-2.76	135,135,135,135	0
36	SR	3	8999	1/1	0.04	-2.78	106,106,106,106	0
36	SR	0	8960	1/1	0.04	-2.79	150,150,150,150	0
34	NA	0	8519	1/1	0.13	-2.81	50,50,50,50	0
36	SR	0	8908	1/1	0.08	-2.86	110,110,110,110	0
36	SR	0	8940	1/1	0.07	-2.93	93,93,93,93	0
32	MG	0	8027	1/1	0.08	-3.03	49,49,49,49	0
36	SR	0	8923	1/1	0.08	-3.08	116,116,116,116	0
36	SR	0	8990	1/1	0.09	-3.13	137,137,137,137	0
34	NA	0	8557	1/1	0.06	-3.16	52,52,52,52	0
32	MG	0	8065	1/1	0.08	-3.17	49,49,49,49	0
34	NA	S	8510	1/1	0.10	-3.36	49,49,49,49	0
34	NA	0	8521	1/1	0.09	-3.39	65,65,65,65	0
35	CL	0	8805	1/1	0.05	-3.41	67,67,67,67	0
35	CL	3	8804	1/1	0.08	-3.43	67,67,67,67	0
32	MG	0	8053	1/1	0.03	-3.43	59,59,59,59	0
32	MG	0	8025	1/1	0.08	-3.46	35,35,35,35	0
36	SR	0	8910	1/1	0.06	-3.47	101,101,101,101	0
34	NA	0	8529	1/1	0.03	-3.52	45,45,45,45	0
36	SR	0	8902	1/1	0.11	-3.54	66,66,66,66	0
32	MG	0	8044	1/1	0.08	-3.55	53,53,53,53	0
36	SR	0	8945	1/1	0.07	-3.60	112,112,112,112	0
32	MG	0	8085	1/1	0.07	-3.61	73,73,73,73	0
35	CL	0	8812	1/1	0.06	-3.61	54,54,54,54	0
36	SR	0	8968	1/1	0.07	-3.73	165,165,165,165	0
32	MG	0	8026	1/1	0.07	-3.75	37,37,37,37	0
32	MG	0	8060	1/1	0.06	-3.81	61,61,61,61	0
34	NA	0	8536	1/1	0.06	-3.86	65,65,65,65	0
32	MG	0	8052	1/1	0.04	-3.86	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8939	1/1	0.04	-3.87	160,160,160,160	0
32	MG	0	8038	1/1	0.10	-3.88	75,75,75,75	0
32	MG	Y	8086	1/1	0.06	-3.90	46,46,46,46	0
32	MG	0	8032	1/1	0.05	-3.92	46,46,46,46	0
36	SR	0	8919	1/1	0.12	-4.02	192,192,192,192	0
32	MG	0	8056	1/1	0.10	-4.10	51,51,51,51	0
35	CL	0	8803	1/1	0.07	-4.16	62,62,62,62	0
32	MG	0	8002	1/1	0.09	-4.20	32,32,32,32	0
36	SR	0	8920	1/1	0.04	-4.23	134,134,134,134	0
32	MG	0	8077	1/1	0.07	-4.31	49,49,49,49	0
36	SR	0	8974	1/1	0.10	-4.34	149,149,149,149	0
36	SR	1	8913	1/1	0.08	-4.36	96,96,96,96	0
36	SR	0	8927	1/1	0.06	-4.42	151,151,151,151	0
32	MG	0	8076	1/1	0.07	-4.57	42,42,42,42	0
35	CL	0	8814	1/1	0.09	-4.67	60,60,60,60	0
32	MG	0	8093	1/1	0.07	-4.96	35,35,35,35	0
36	SR	0	8916	1/1	0.05	-5.21	113,113,113,113	0
32	MG	0	8072	1/1	0.10	-5.28	53,53,53,53	0
32	MG	0	8075	1/1	0.04	-5.34	46,46,46,46	0
32	MG	0	8033	1/1	0.06	-5.40	49,49,49,49	0
32	MG	0	8024	1/1	0.11	-5.46	55,55,55,55	0
35	CL	B	8819	1/1	0.07	-5.53	54,54,54,54	0
36	SR	0	8953	1/1	0.07	-5.68	157,157,157,157	0
36	SR	0	8966	1/1	0.07	-5.70	111,111,111,111	0
36	SR	0	8984	1/1	0.05	-5.76	123,123,123,123	0
36	SR	0	8970	1/1	0.03	-6.19	128,128,128,128	0
34	NA	0	8526	1/1	0.04	-6.46	57,57,57,57	0
36	SR	0	8965	1/1	0.04	-6.52	124,124,124,124	0
36	SR	0	8963	1/1	0.07	-8.27	134,134,134,134	0
32	MG	0	8087	1/1	0.09	-8.41	47,47,47,47	0
36	SR	9	9003	1/1	0.02	-9.21	170,170,170,170	0
36	SR	0	8962	1/1	0.05	-9.32	175,175,175,175	0
32	MG	0	8013	1/1	0.03	-9.50	30,30,30,30	0
32	MG	0	8034	1/1	0.04	-9.64	45,45,45,45	0
36	SR	0	8942	1/1	0.06	-10.05	133,133,133,133	0
32	MG	0	8089	1/1	0.10	-11.73	57,57,57,57	0
36	SR	0	8973	1/1	0.06	-17.80	137,137,137,137	0
36	SR	0	8971	1/1	0.06	-19.50	180,180,180,180	0
32	MG	0	8059	1/1	0.04	-19.52	59,59,59,59	0
32	MG	0	8091	1/1	0.04	-26.50	62,62,62,62	0
32	MG	0	8049	1/1	0.45	-	68,68,68,68	0
36	SR	0	9006	1/1	1.02	-	200,200,200,200	0

6.5 Other polymers ⓘ

There are no such residues in this entry.