



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2020 – 03:04 AM EDT

PDB ID : 6NSH  
Title : Modified ASL proline bound to Thermus thermophilus 70S (near-cognate)  
Authors : Hoffer, E.D.; Maehigashi, T.; Subaramanian, S.; Hong, S.; Dunham, C.M.  
Deposited on : 2019-01-24  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

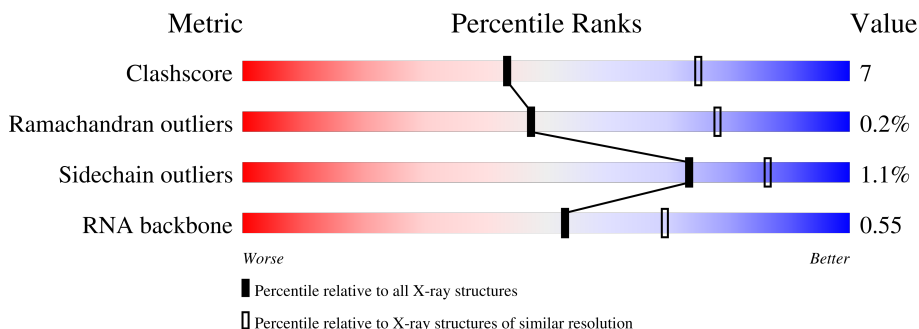
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)












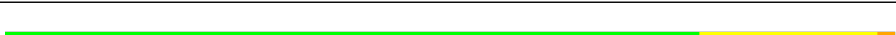

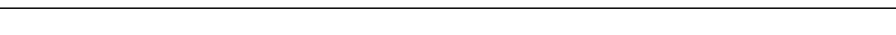
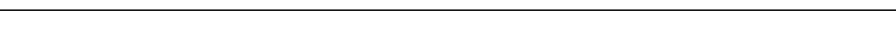
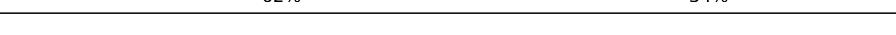

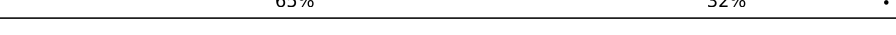







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	
3	RD	276	
3	YD	276	


























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Mol	Chain	Length	Quality of chain
4	RE	206	 78% 20% ..
4	YE	206	 76% 23% .
5	RF	210	 76% 20% .
5	YF	210	 72% 23% .
6	RG	182	 65% 30% ..
6	YG	182	 70% 27% ..
7	RH	180	 69% 24% . .
7	YH	180	 82% 13% . .
8	RI	148	 65% 28% 5% ..
8	YI	148	 66% 30% ..
9	RN	140	 76% 21% ..
9	YN	140	 78% 20% .
10	RO	122	 76% 23% .
10	YO	122	 83% 16% .
11	RP	150	 62% 34% ..
11	YP	150	 71% 25% . .
12	RQ	141	 65% 32% .
12	YQ	141	 82% 16% ..
13	RR	118	 83% 14% ..
13	YR	118	 82% 16% ..
14	RS	112	 75% 21% . .
14	YS	112	 87% 12% .
15	RT	146	 75% 18% . 6%
15	YT	146	 82% 12% 6%
16	RU	118	 79% 18% . .


























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Mol	Chain	Length	Quality of chain
16	YU	118	 82% 15% ..
17	RV	101	 77% 23%
17	YV	101	 83% 16% .
18	RW	113	 80% 18% .
18	YW	113	 82% 16% .
19	RX	96	 77% 19% .
19	YX	96	 76% 22% .
20	RY	110	 82% 15% ..
20	YY	110	 81% 15% ..
21	RZ	206	 67% 29% ..
21	YZ	206	 82% 15% .
22	R0	85	 75% 14% 11%
22	Y0	85	 69% 18% . 12%
23	R1	98	 81% 16% ..
23	Y1	98	 77% 18% 5%
24	R2	72	 74% 18% . .
24	Y2	72	 88% 13%
25	R3	60	 72% 25% ..
25	Y3	60	 72% 25% ..
26	R4	71	 61% 34% . .
26	Y4	71	 58% 34% 6% .
27	R5	60	 80% 18% .
27	Y5	60	 78% 20% .
28	R6	54	 93% 6% .
28	Y6	54	 85% 13% .









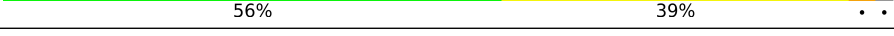

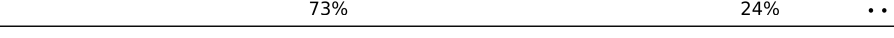
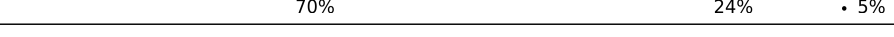

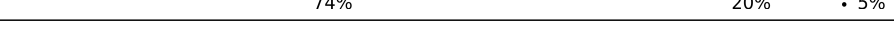


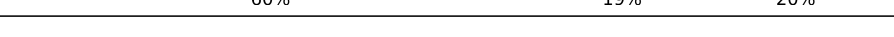

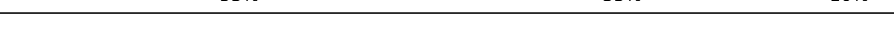




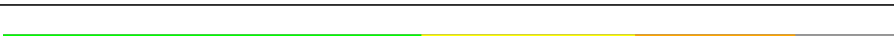

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Mol	Chain	Length	Quality of chain
29	R7	49	
29	Y7	49	
30	R8	65	
30	Y8	65	
31	R9	37	
31	Y9	37	
32	QA	1521	
32	XA	1521	
33	QB	256	
33	XB	256	
34	QC	239	
34	XC	239	
35	QD	209	
35	XD	209	
36	QE	162	
36	XE	162	
37	QF	101	
37	XF	101	
38	QG	156	
38	XG	156	
39	QH	138	
39	XH	138	
40	QI	128	
40	XI	128	
41	QJ	105	


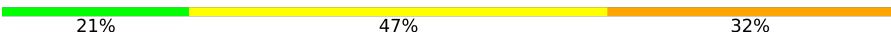
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Mol	Chain	Length	Quality of chain
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	
53	QV	17	
53	XV	17	

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Mol	Chain	Length	Quality of chain
54	QX	19	
54	XX	19	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	SF4	XD	301	-	-	X	-

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 290035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
1	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	YD	273	Total	C	N	O	S	0	0	0
			2126	1341	424	358	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	RE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
4	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
5	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
6	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
7	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
8	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
9	YN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RP	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			
11	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	YR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	YS	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
15	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	RX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				
19	YX	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
20	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
21	YZ	201	Total	C	N	O	S	0	0	0
			1587	1012	281	291	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
22	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
24	Y2	72	Total	C	N	O	S	0	0	0
			606	375	122	107	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
29	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R9	36	Total	C	N	O	S	0	0	0
			302	186	67	45	4			
31	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
32	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
33	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
34	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
35	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
36	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
37	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
38	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
39	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	QI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
40	XI	126	Total	C	N	O	0	0	0
			998	633	193	172			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
41	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
43	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
44	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
46	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
47	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
48	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	QR	70	Total	C	N	O		0	0	0
			574	367	112	95				
49	XR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
50	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
51	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
52	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 53 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	QV	17	Total	C	N	O	P	0	0	0
			365	163	65	120	17			
53	XV	15	Total	C	N	O	P	0	0	0
			322	144	57	106	15			

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	18	Total	C	N	O	P	0	0	0
			389	174	76	121	18			
54	XX	19	Total	C	N	O	P	0	0	0
			412	184	81	128	19			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	66	Total	Mg	0	0
			66	66		
55	RP	2	Total	Mg	0	0
			2	2		
55	YA	510	Total	Mg	0	0
			510	510		
55	Y5	1	Total	Mg	0	0
			1	1		
55	YR	1	Total	Mg	0	0
			1	1		
55	RT	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	1	Total	Mg	0	0
			1	1		
55	XS	1	Total	Mg	0	0
			1	1		
55	Y1	1	Total	Mg	0	0
			1	1		
55	YD	1	Total	Mg	0	0
			1	1		
55	RX	1	Total	Mg	0	0
			1	1		
55	Y8	1	Total	Mg	0	0
			1	1		
55	YO	1	Total	Mg	0	0
			1	1		

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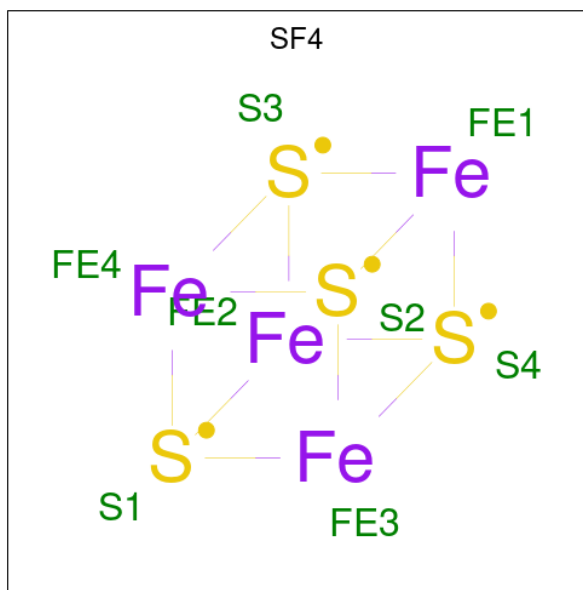
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XA	87	Total 87	Mg 87	0	0
55	RQ	2	Total 2	Mg 2	0	0
55	R0	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	R8	1	Total 1	Mg 1	0	0
55	R1	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0
55	R5	1	Total 1	Mg 1	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	RA	485	Total 485	Mg 485	0	0
55	YP	2	Total 2	Mg 2	0	0
55	RE	2	Total 2	Mg 2	0	0
55	XL	1	Total 1	Mg 1	0	0
55	YB	7	Total 7	Mg 7	0	0
55	RB	8	Total 8	Mg 8	0	0
55	RF	1	Total 1	Mg 1	0	0
55	YE	4	Total 4	Mg 4	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	Y9	1	Total Zn 1 1	0	0
56	YY	1	Total Zn 1 1	0	0
56	Y6	1	Total Zn 1 1	0	0
56	QN	1	Total Zn 1 1	0	0
56	XN	1	Total Zn 1 1	0	0
56	RY	1	Total Zn 1 1	0	0
56	Y4	1	Total Zn 1 1	0	0
56	R6	1	Total Zn 1 1	0	0
56	Y5	1	Total Zn 1 1	0	0
56	R5	1	Total Zn 1 1	0	0
56	R4	1	Total Zn 1 1	0	0
56	R9	1	Total Zn 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



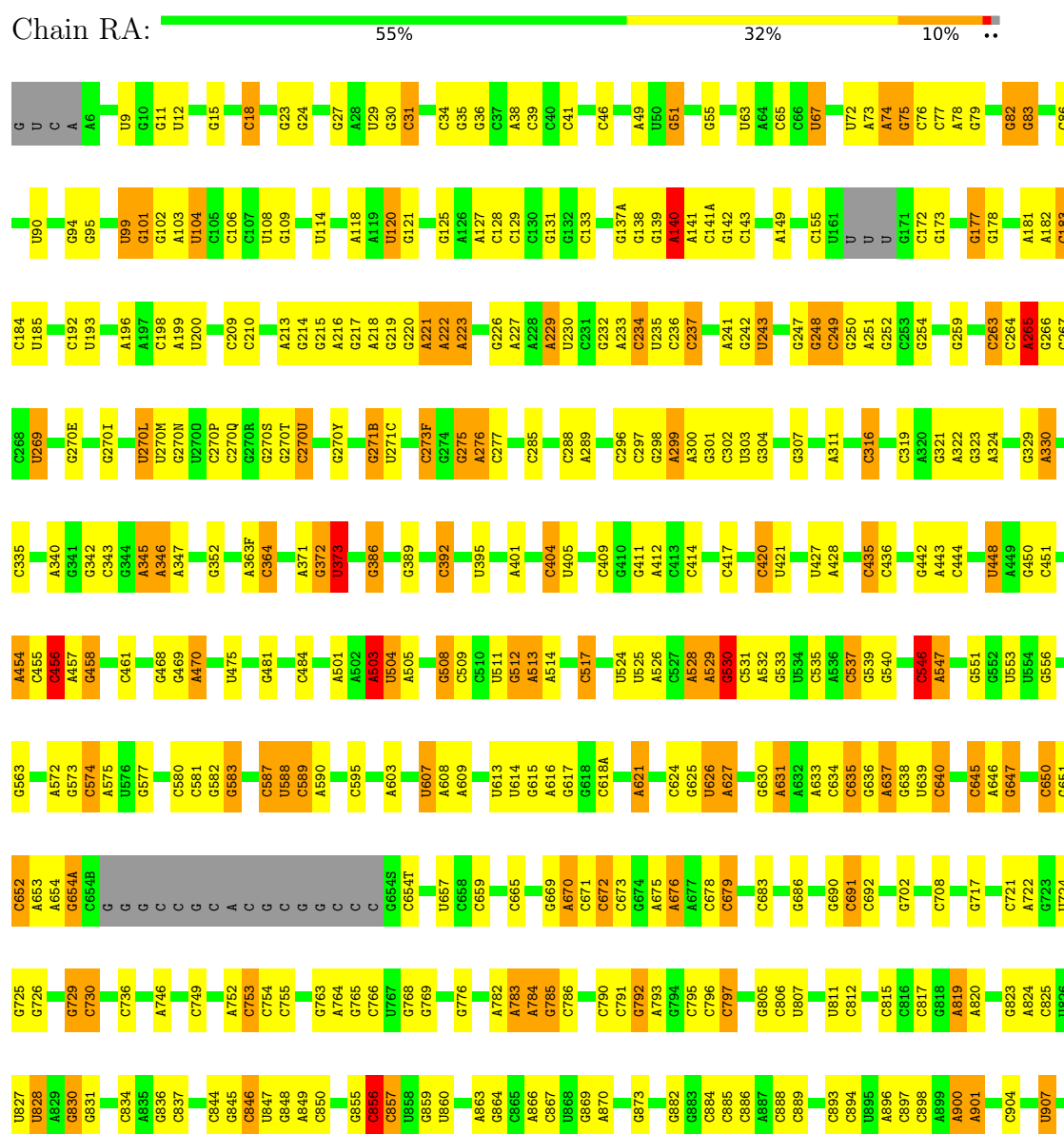
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	QD	1	Total 8	Fe 4	S 4	0	0
57	XD	1	Total 8	Fe 4	S 4	0	0

### 3 Residue-property plots [i](#)

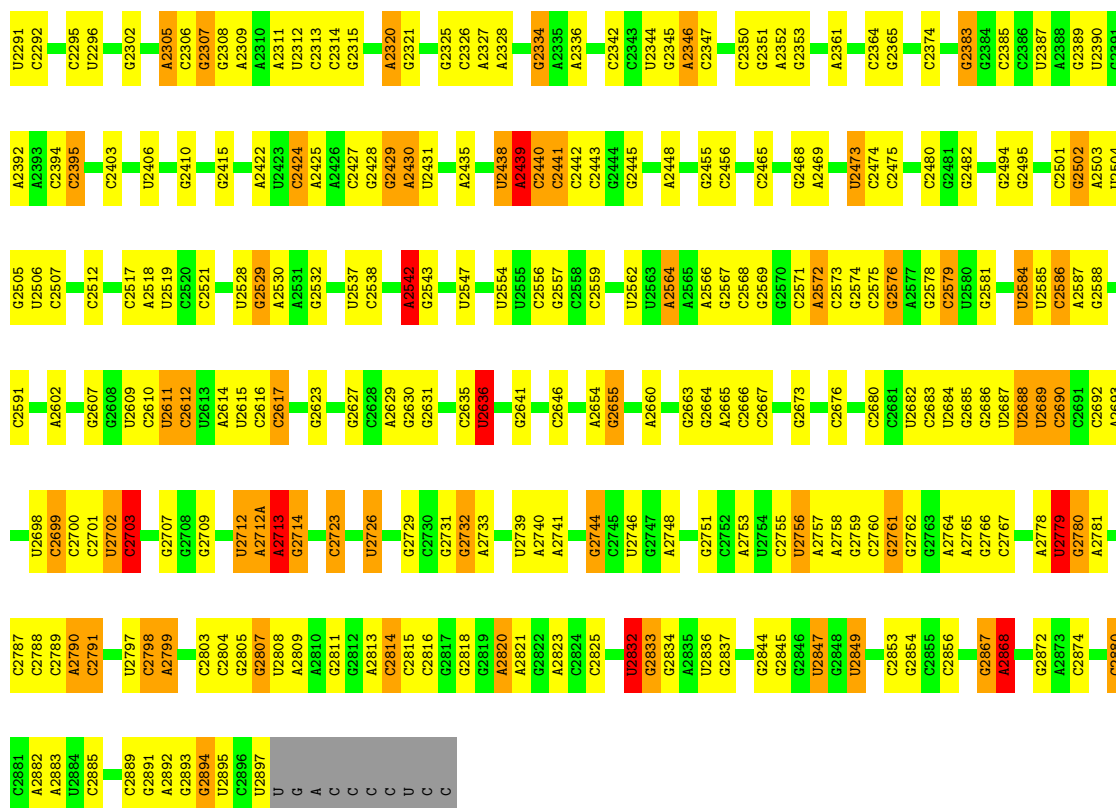
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

#### • Molecule 1: 23S rRNA

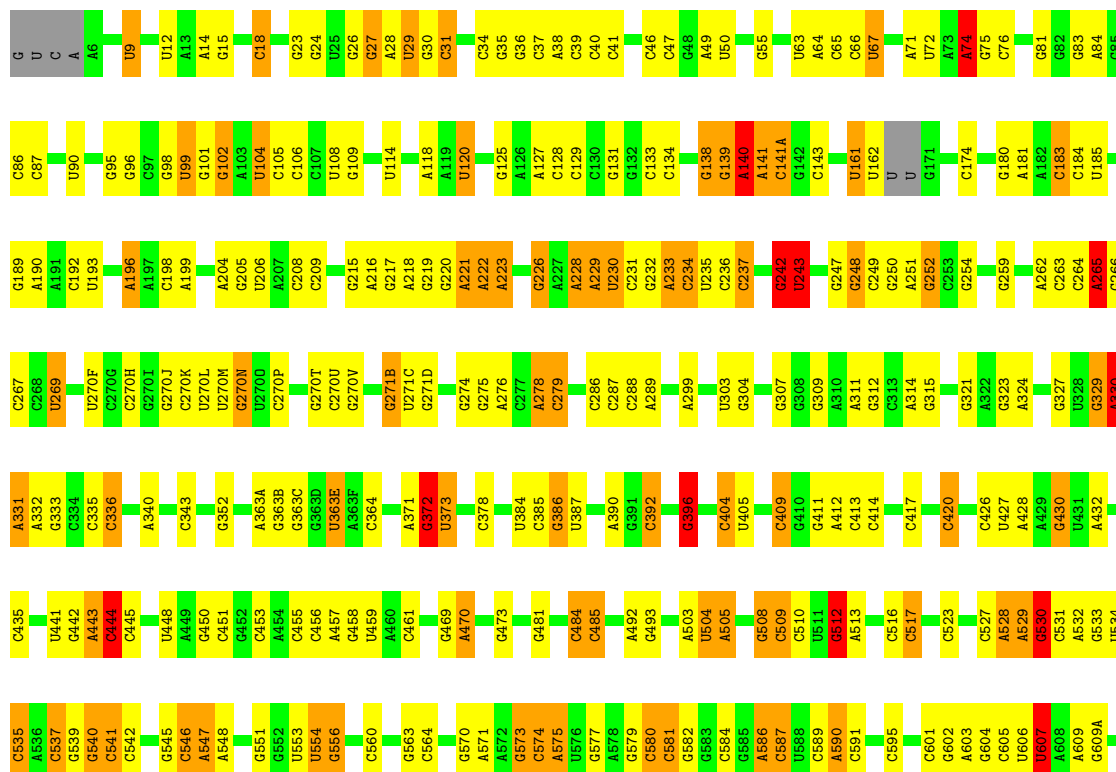


G2191	A2117	A1815	A1918	A1608	G1524	G1441	A1349	U1249	G1157	G1074	A1000	A910
G2192	U2118	G1816	A1919	A1609	G1525	G1442	U1352	G1250	C1158	C1075	A1001	A911
G2193		G1817	C1920	A1610	G1526		U1353	G1251	U1159	A1076	G1002	C912
		U1818		C1611	G1527	A1444A	A1353	G1252		A1077	G1003	U913
U2197	G2123	A1819	G1929		A1528	C1445	A1354	A1253	U1165	U1078	C1004	C914
A2198	G2124	U1820	G1930	A1616	A1529			A1254	U1166	C1079	C1005	C915
A2199	G2125		U1931	A1617		G1448	A1359	U1255	G1171		C1006	G916
C2205	G2127	G1823		A1618	C1533	A1449		G1256	U1082		G1007	A917
	C2128	G1824	C1934	G1619	G1534	A1449A	A1365	C1257	U1083	U1088	C1008	A918
U2208	G2129	C1827	G1935	G1622	U1535				U1084	A1085	A1009	C919
C2209	U2130	A2051	A1936		A1536	G1455	G1368	A1262	U1085	A1086	A1010	
G2210	G2131	G1828	A1937	A1634	C1537	A1460	G1369	U1263	G1177	C1087	G1011	U922
G2211	U2132	A1829	A1938	G1635	G1538	A1461	C1370	G1264	U1178		U1012	C923
A2212	G2133	C1830	U1939	G1636	G1539	G1462	G1371	A1265	C1179	A1088	C1013	C924
	A2134			A1637	G1540	C1463	U1372	U1267	C1180			
U2213	G2135	U1833	C1947	C1638	U1541	C1464	C1375		U1090			
G2215	A2136	U1834		U1639	G1542	C1464		A1272	G1181	U1091	U1019	C932
	C2137	G1835	G1950	C1640	A1543		A1379	U1273	G1182	C1092	A1020	
G2224	U2138	C1836	U1951		C1544	C1468		A1274	U1189	U1093	A1021	A941
A2225	G2139		A1952	C1644	A1545	A1471	G1385	A1275	U1187	A1094	U1023	G944
C2226		C1844				C1474	G1386	A1276	U1188	A1095	G1024	A945
		A1847	U1955	C1648	C1547			G1281	U1096	U1096	G1025	G946
C2229	G2141	A1848	U1956		C1549		C1387	U1282	U1097		U1026	
				G1653	C1550	G1478	U1390	G1283	C1100		A1027	A953
U2233	C2145	A1883	C1961	A1654		G1479	U1391		U1101		G1031	C955
	G2146		G1962		C1557	G1480		A1286	C1102		A1032	G956
C2236	G2147	G1858	U1963	C1656	A1558	U1482	U1394	U1288	A1103		G1033	A957
G2237	G2148	A1859		C1657	G1559	G1483	U1395			C1041		U958
C2238		C1967	G1968	C1658	G1560	G1484	U1396	U1294	C1109	G1110	G1042	A959
G2239	G2151	U1869	A1969	U1659		G1485	U1397	G1296	G1111			A960
U2243	G2153	C1870	A1970	C1660	A1666	A1486			A1112		A1045	C961
U2244	G2154	A1871	A1971			G1487		C1300	U1113		A1046	
U2245	G2155	A1872	A1972	G1667	A1569	C1493	C1403	U1300	U1114		G1047	C965
G2246	G2156	G1878	A1973	A1668	C1577	A1494	U1405	A1301	G1115		A1048	U969
A2247	G2157	C1881		C1670	U1578	A1495	U1406					
C2248	A2158	G1882	C1983	G1674	A1579	A1496	C1407	G1304	G1122		C1049	C970
U2249	G2159	C1883		C1675	A1580	C1498	C1408	C1306	C1123		G1052	A973
G2250	G2160		C1988		A1583	C1502	C1411		C1124		C1053	G974
	C2161	G1888			C1585	U1503	G1416	G1310			A1054	C974A
C2254	C2163	A1889	U1991	G1678	A1586	C1504	C1417	U1219	A1129		G1055	G975
	G2164	C1892	G1992	U1679	A1587	C1505	G1418	C1221	U1130		G1056	C976
A2286	G2165	C1899	U1993	G1681	U1590	C1506	G1419	C1222		C1135	G1057	
	G2166	A1900		G1682	G1591	A1507	U1420	G1224	U1136		G1058	
A2269	U2167	G1903	C1996		G1592	C1509	G1421		G1137		U1060	A983
	C2168	G1906		G1686	G1593	A1510		A1321	G1138		U	A984
C2275	A2170		G2002		G1594	G1511	G1426	U1323	G1139		G1062	C985
			C2006	A1689	G1595	G1512	A1427		U1140		C1063	C986
A2278	G2181	G1906		A1690		U1513	C1428	U1329	U1141		C1064	G987
G2279	G2182	C1909		C1691	G1598	U1514	G1429	C1330	U1142		U1065	
	C2183	G1909	G2010	U1692	C1599	C1515	C1430	A142A			A1066	C991
C2284	G2184		G2012	U1694	C1603	C1515	U1431	C1233	G1149		A1067	C992
C2285		A1913		G1695	C1604	G1519	C1432	G1235	G1150		G1068	C993
A2286	G2187	C1914	A2019		C1605		U1433	G1332			A1069	C994
A2287	C2188	U1915	A2020	G1698	G1606			G1333			G1070	C995
C2288	U2189	A1916				G1522	C1437	U1341	C1154		G1071	A996
	G2190	U1917	U2022	A1698	C1607	U1523		G1348			G1072	C997
											A1073	



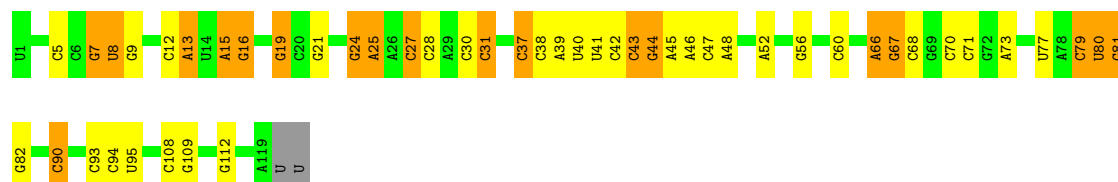
• Molecule 1: 23S rRNA

Chain YA: 54% 33% 11% ..

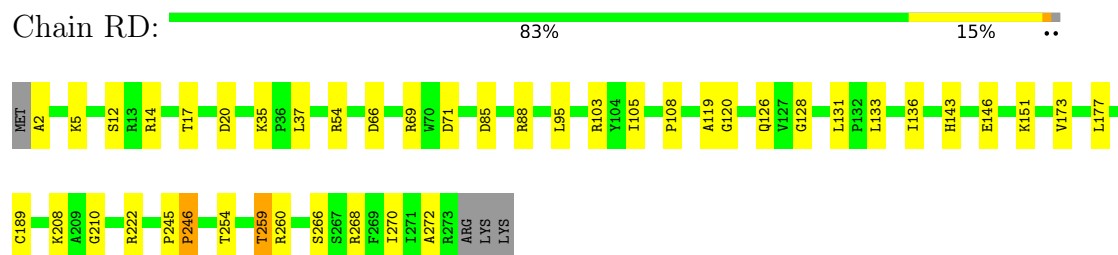




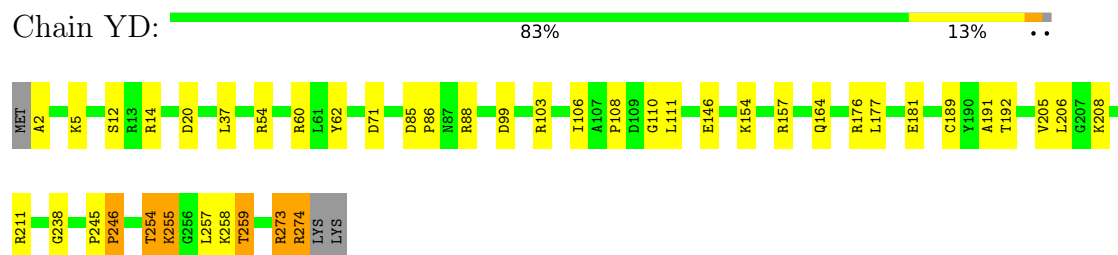




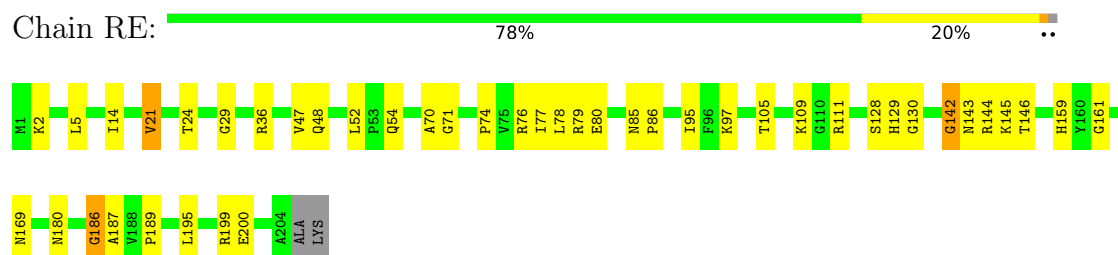
• Molecule 3: 50S ribosomal protein L2



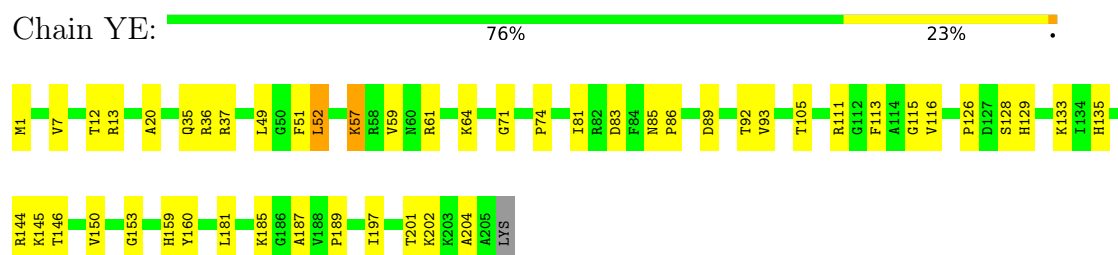
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3

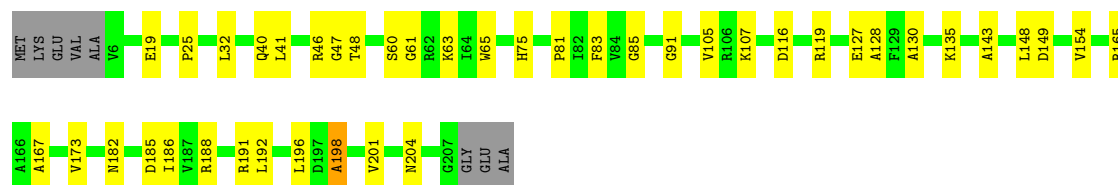


• Molecule 4: 50S ribosomal protein L3



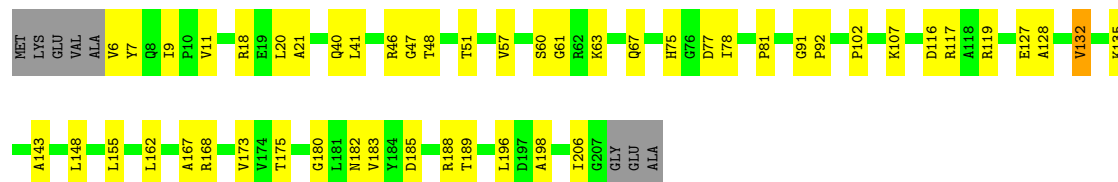
• Molecule 5: 50S ribosomal protein L4





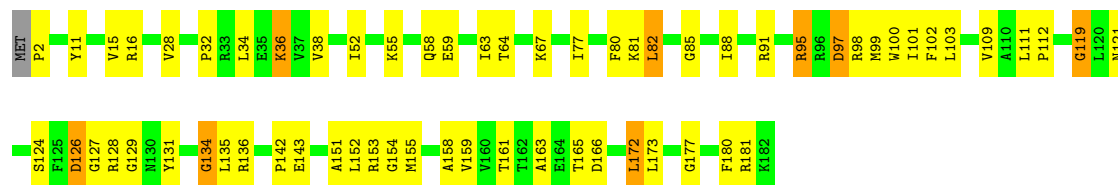
- Molecule 5: 50S ribosomal protein L4

Chain YF: 72% 23% .



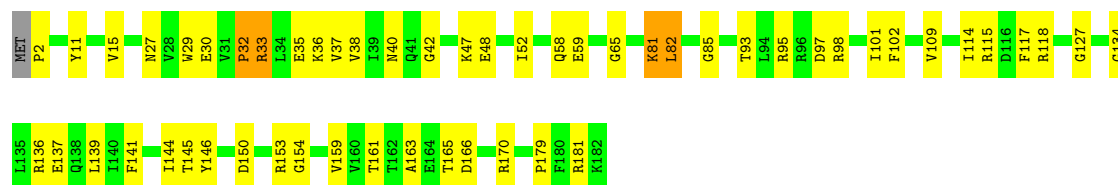
- Molecule 6: 50S ribosomal protein L5

Chain RG: 65% 30% . .



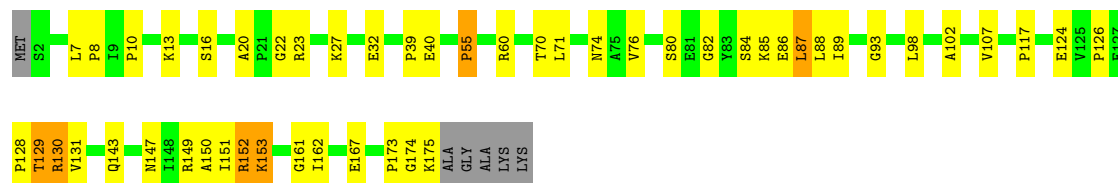
- Molecule 6: 50S ribosomal protein L5

Chain YG: 70% 27% . .



- Molecule 7: 50S ribosomal protein L6

Chain RH: 69% 24% . .



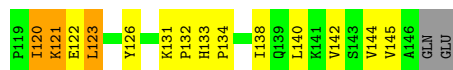
- Molecule 7: 50S ribosomal protein L6

Chain YH: 82% 13% . .



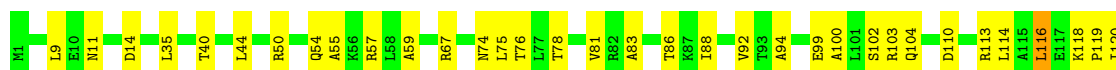
- Molecule 8: 50S ribosomal protein L9

Chain RI: 65% 28% 5% ..



- Molecule 8: 50S ribosomal protein L9

Chain YI: 66% 30% ..



- Molecule 9: 50S ribosomal protein L13

Chain RN: 76% 21% ..



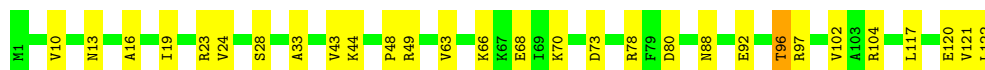
- Molecule 9: 50S ribosomal protein L13

Chain YN: 78% 20% .



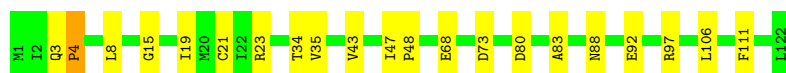
- Molecule 10: 50S ribosomal protein L14

Chain RO: 76% 23% .



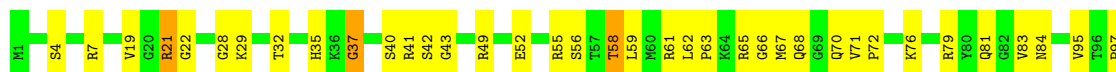
- Molecule 10: 50S ribosomal protein L14

Chain YO: 83% 16% .



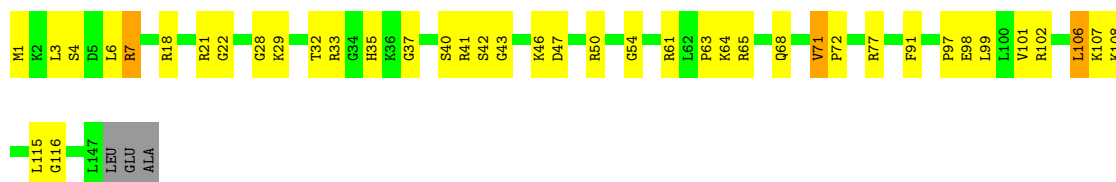
- Molecule 11: 50S ribosomal protein L15

Chain RP: 62% 34% ..



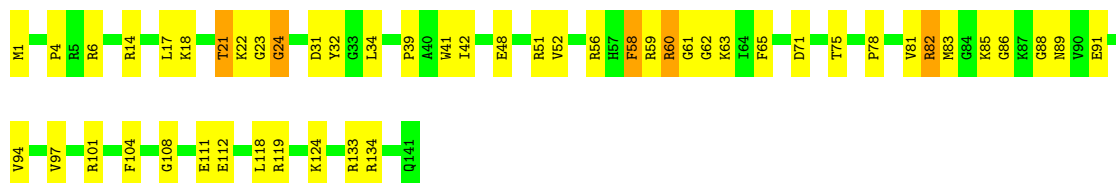
- Molecule 11: 50S ribosomal protein L15

Chain YP: 71% 25% ..



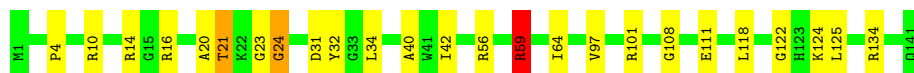
- Molecule 12: 50S ribosomal protein L16

Chain RQ: 65% 32% .



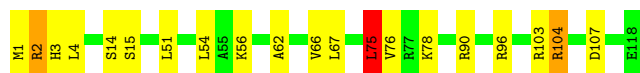
- Molecule 12: 50S ribosomal protein L16

Chain YQ: 82% 16% ..




- Molecule 13: 50S ribosomal protein L17

Chain RR: 83% 14% ..




- Molecule 13: 50S ribosomal protein L17

Chain YR:  82% 16% ..




- Molecule 14: 50S ribosomal protein L18

Chain RS:  75% 21% ..




- Molecule 14: 50S ribosomal protein L18

Chain YS:  87% 12% .



- Molecule 15: 50S ribosomal protein L19

Chain RT:  75% 18% • 6%




- Molecule 15: 50S ribosomal protein L19

Chain YT:  82% 12% 6%




- Molecule 16: 50S ribosomal protein L20

Chain RU:  79% 18% ..




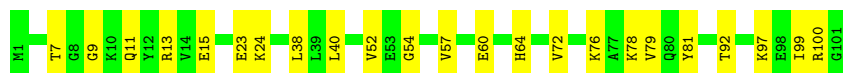
- Molecule 16: 50S ribosomal protein L20

Chain YU:  82% 15% ..




- Molecule 17: 50S ribosomal protein L21

Chain RV:  77% 23%




- Molecule 17: 50S ribosomal protein L21

Chain YV:  83% 16%




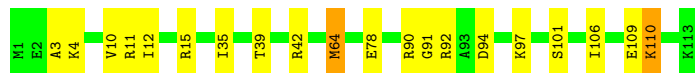
- Molecule 18: 50S ribosomal protein L22

Chain RW:  80% 18%




- Molecule 18: 50S ribosomal protein L22

Chain YW:  82% 16%




- Molecule 19: 50S ribosomal protein L23

Chain RX:  77% 19%




- Molecule 19: 50S ribosomal protein L23

Chain YX:  76% 22%




- Molecule 20: 50S ribosomal protein L24

Chain RY:  82% 15%



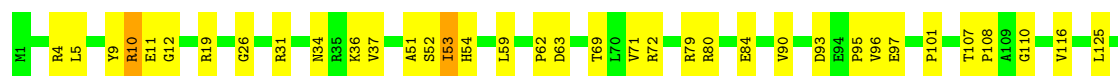
- Molecule 20: 50S ribosomal protein L24

Chain YY:  81% 15% ..




- Molecule 21: 50S ribosomal protein L25

Chain RZ:  67% 29% ..




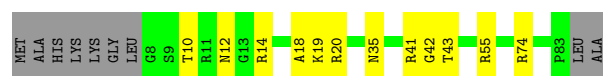
- Molecule 21: 50S ribosomal protein L25

Chain YZ:  82% 15% .



- Molecule 22: 50S ribosomal protein L27

Chain R0:  75% 14% 11%




- Molecule 22: 50S ribosomal protein L27

Chain Y0:  69% 18% 12%




- Molecule 23: 50S ribosomal protein L28

Chain R1:  81% 16% ..

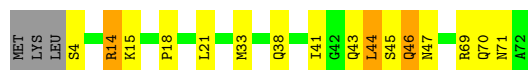
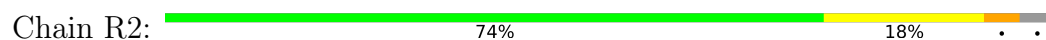


- Molecule 23: 50S ribosomal protein L28

Chain Y1:  77% 18% 5%



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



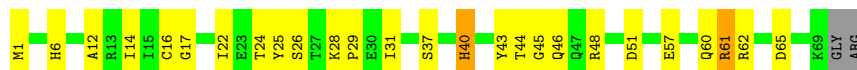
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



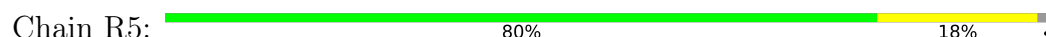
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32





- Molecule 27: 50S ribosomal protein L32

Chain Y5: 78% 20% .



- Molecule 28: 50S ribosomal protein L33

Chain R6: 93% 6% .



- Molecule 28: 50S ribosomal protein L33

Chain Y6: 85% 13% .



- Molecule 29: 50S ribosomal protein L34

Chain R7: 80% 14% . .



- Molecule 29: 50S ribosomal protein L34

Chain Y7: 82% 16% .



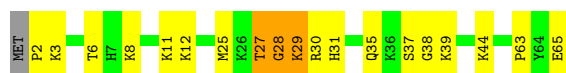
- Molecule 30: 50S ribosomal protein L35

Chain R8: 74% 18% 6% .

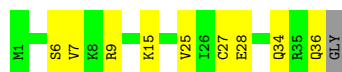


- Molecule 30: 50S ribosomal protein L35

Chain Y8: 69% 25% 5% .



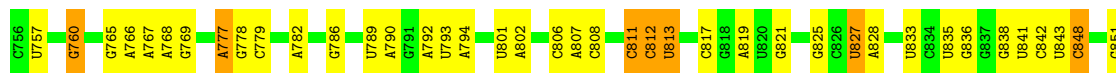
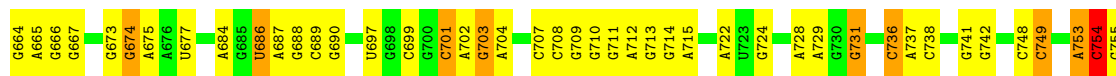
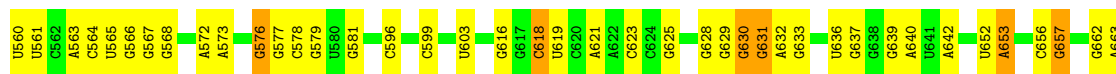
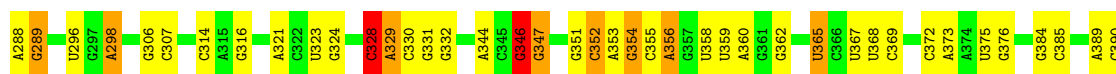
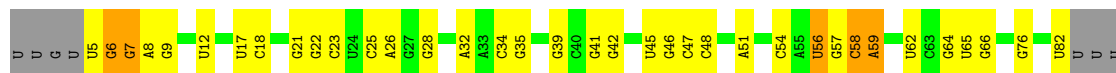
- Molecule 31: 50S ribosomal protein L36

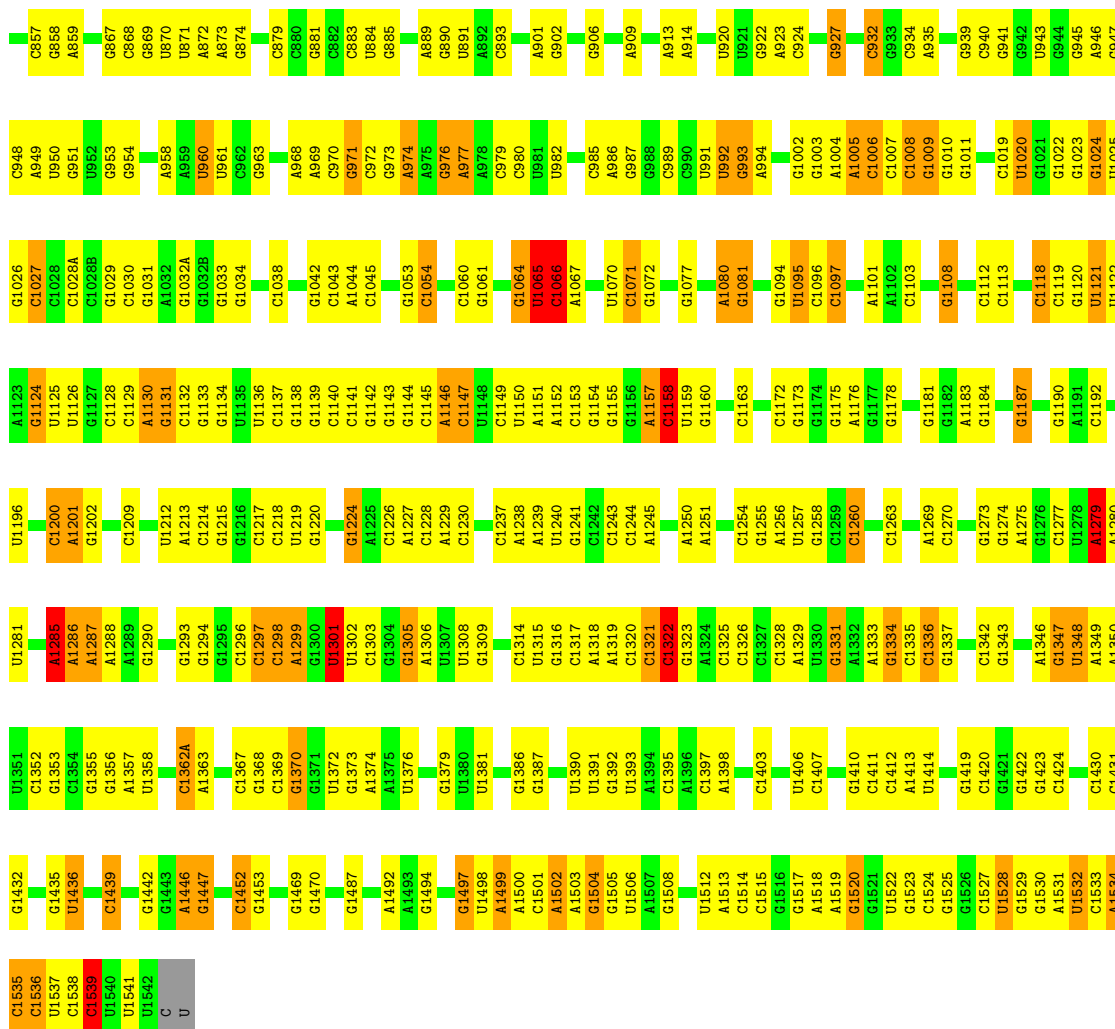


- Molecule 31: 50S ribosomal protein L36



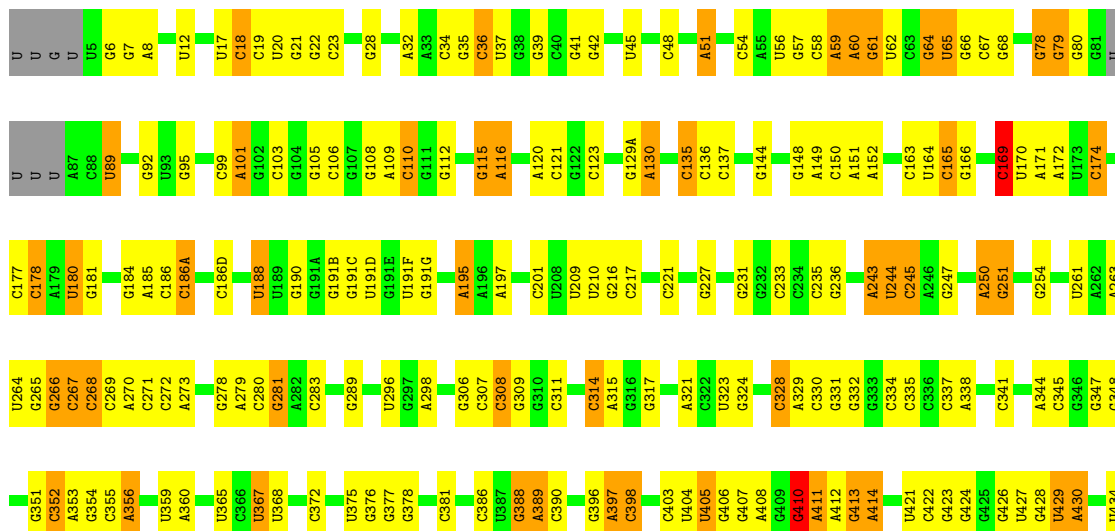
- Molecule 32: 16S rRNA

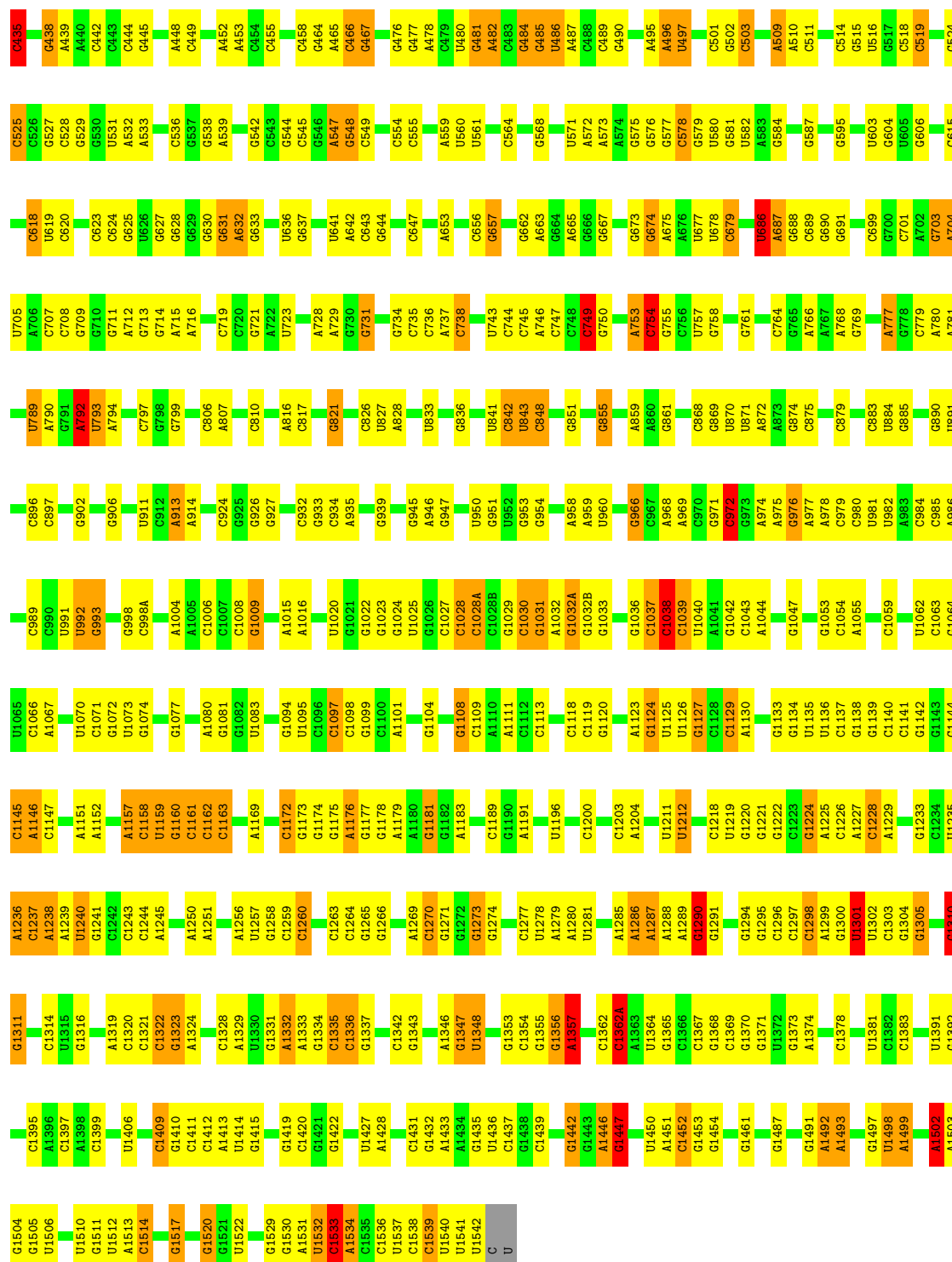




- Molecule 32: 16S rRNA

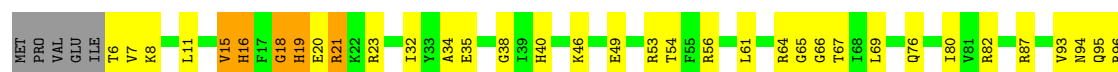
Chain XA:  51% 37% 10% 2%

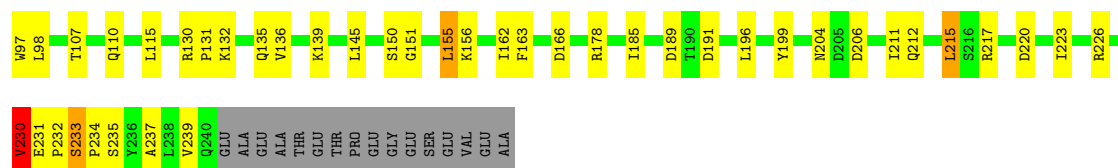




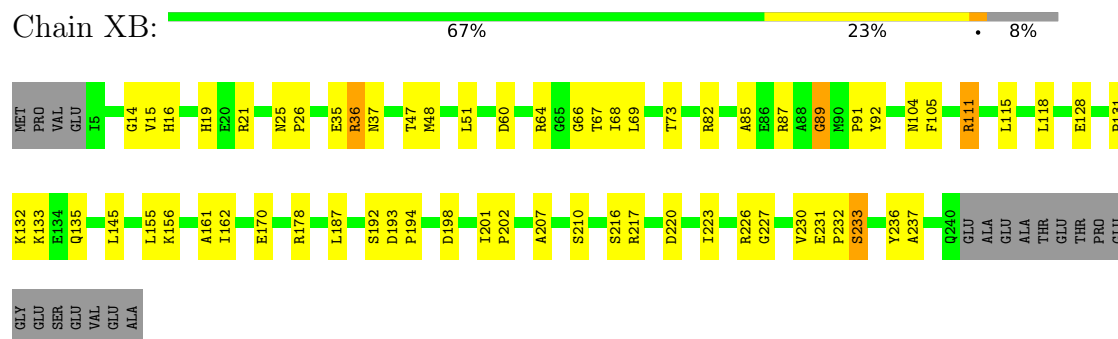
### • Molecule 33: 30S ribosomal protein S2

Chain QB:

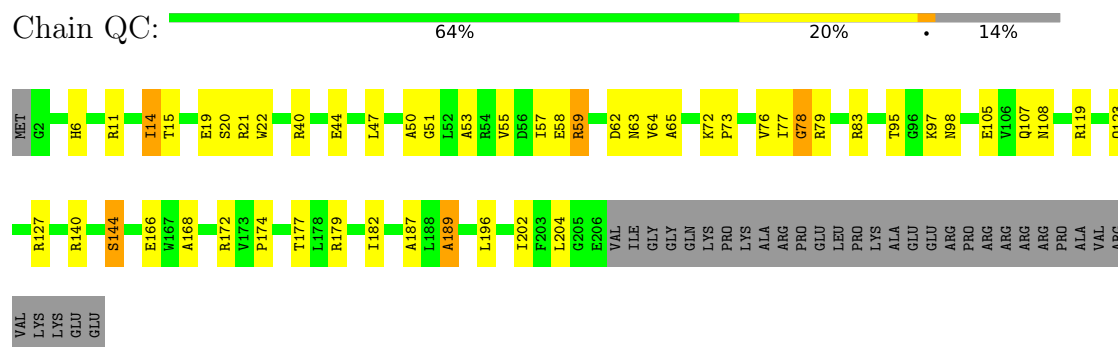




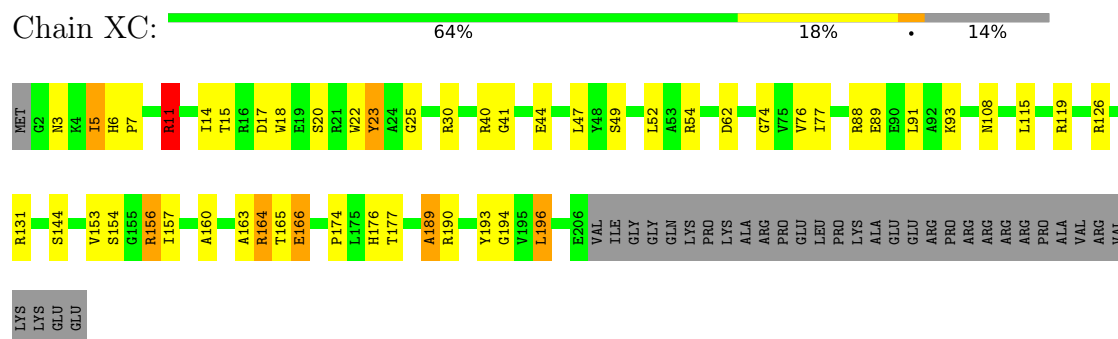
• Molecule 33: 30S ribosomal protein S2



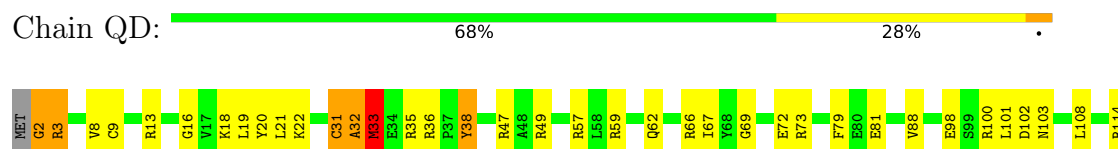
• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3



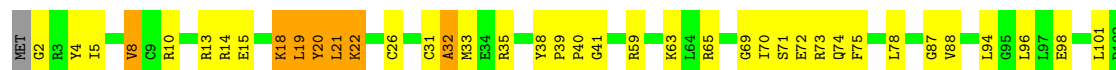
• Molecule 35: 30S ribosomal protein S4





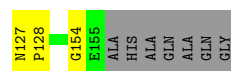
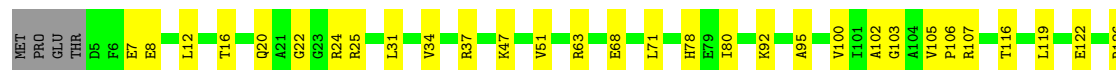
- Molecule 35: 30S ribosomal protein S4

Chain XD: 65% 31% .



- Molecule 36: 30S ribosomal protein S5

Chain QE: 73% 20% 7%



- Molecule 36: 30S ribosomal protein S5

Chain XE: 77% 16% 7%



GLY

- Molecule 37: 30S ribosomal protein S6

Chain QF: 75% 25%




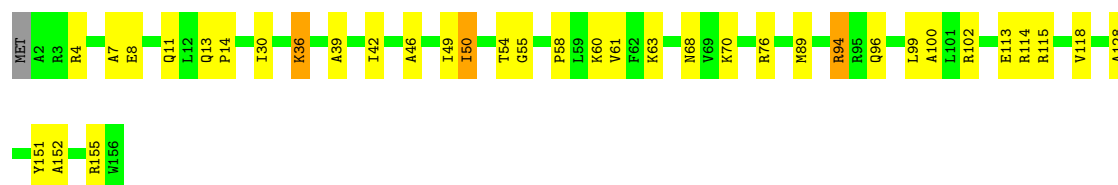
- Molecule 37: 30S ribosomal protein S6

Chain XF: 89% 11%



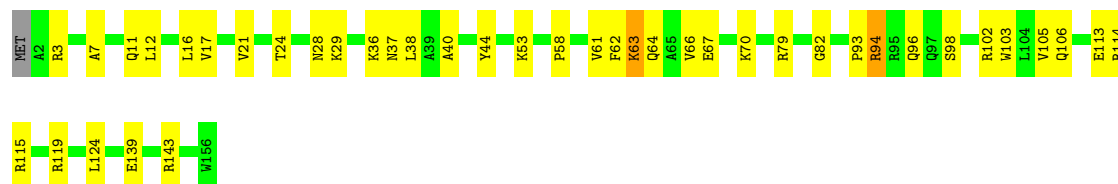
- Molecule 38: 30S ribosomal protein S7

Chain QG:  76% 21% ..




- Molecule 38: 30S ribosomal protein S7

Chain XG:  73% 25% ..




- Molecule 39: 30S ribosomal protein S8

Chain QH:  75% 24% .



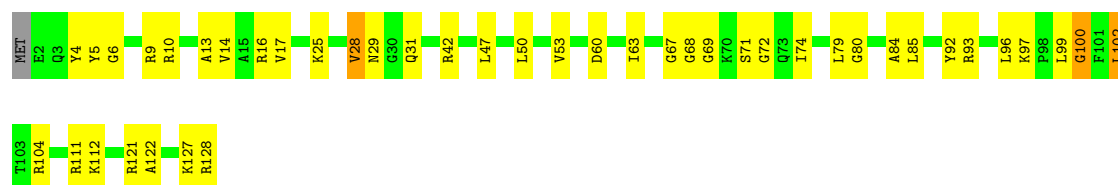
- Molecule 39: 30S ribosomal protein S8

Chain XH:  83% 17% .



- Molecule 40: 30S ribosomal protein S9

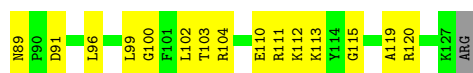
Chain QI:  66% 31% ..



- Molecule 40: 30S ribosomal protein S9

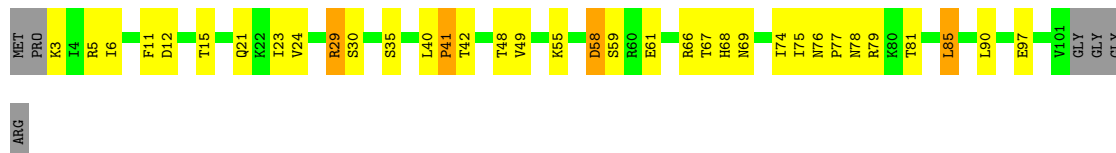
Chain XI:  59% 34% 6% .





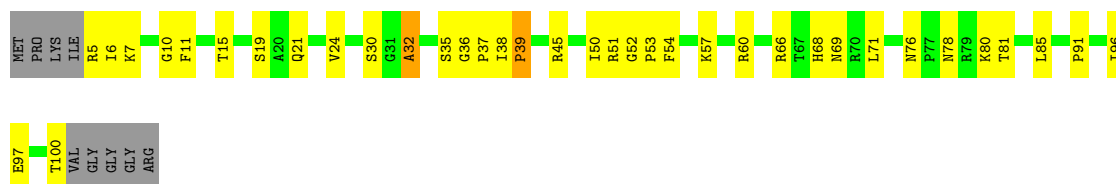
- Molecule 41: 30S ribosomal protein S10

Chain QJ: 61% 30% 6%



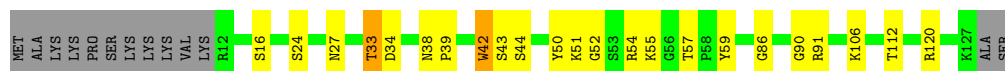
- Molecule 41: 30S ribosomal protein S10

Chain XJ: 56% 33% 9%



- Molecule 42: 30S ribosomal protein S11

Chain QK: 72% 16% 10%



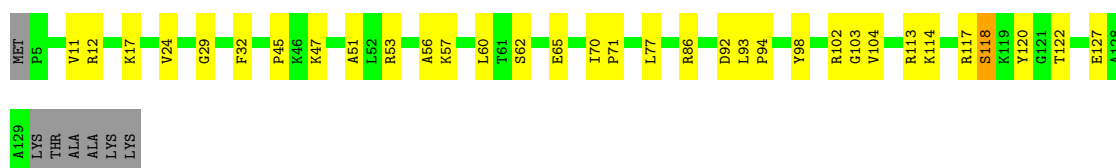
- Molecule 42: 30S ribosomal protein S11

Chain XK: 73% 17% 10%



- Molecule 43: 30S ribosomal protein S12

Chain QL: 70% 24% 5%



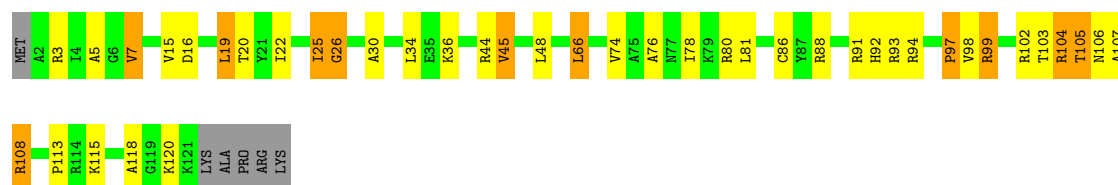
- Molecule 43: 30S ribosomal protein S12

Chain XL: 66% 25% 8%



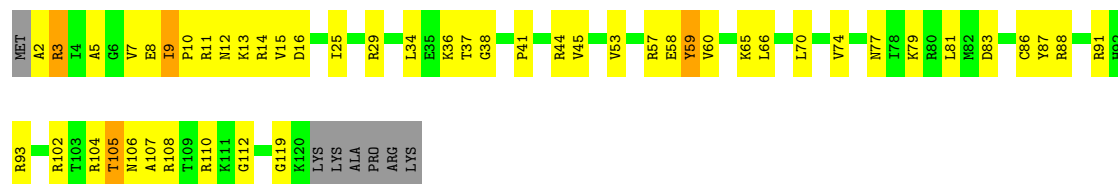
- Molecule 44: 30S ribosomal protein S13

Chain QM: 62% 25% 9% 5%



- Molecule 44: 30S ribosomal protein S13

Chain XM: 56% 36% 6%



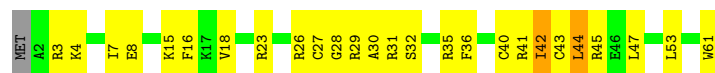
- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN: 72% 26%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN: 56% 39% 5%




- Molecule 46: 30S ribosomal protein S15

Chain QO: 83% 16%



- Molecule 46: 30S ribosomal protein S15

Chain XO:  73% 24% ..



- Molecule 47: 30S ribosomal protein S16

Chain QP:  70% 24% • 5%




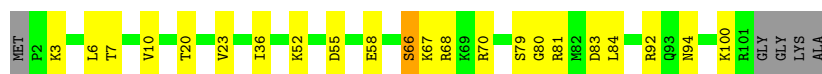
- Molecule 47: 30S ribosomal protein S16

Chain XP:  70% 23% • 5%



- Molecule 48: 30S ribosomal protein S17

Chain QQ:  74% 20% • 5%



- Molecule 48: 30S ribosomal protein S17

Chain XQ:  71% 23% • 5%



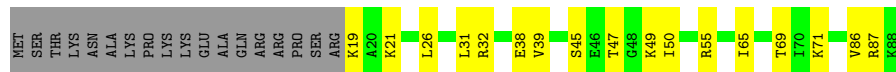
- Molecule 49: 30S ribosomal protein S18

Chain QR:  61% 18% 20%



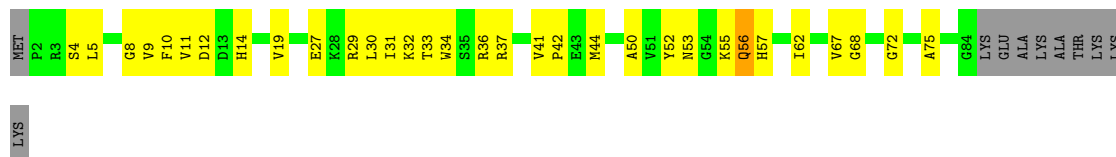
- Molecule 49: 30S ribosomal protein S18

Chain XR:  60% 19% 20%



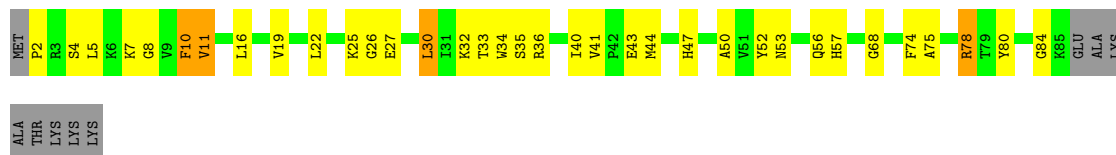
- Molecule 50: 30S ribosomal protein S19

Chain QS:  55% 33% 11%



- Molecule 50: 30S ribosomal protein S19

Chain XS:  53% 33% 10%



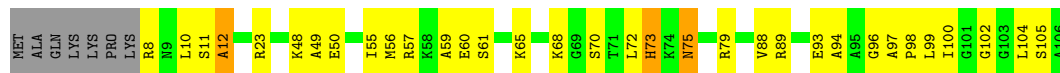
- Molecule 51: 30S ribosomal protein S20

Chain QT:  68% 23% 7%



- Molecule 51: 30S ribosomal protein S20

Chain XT:  62% 28% 7%



- Molecule 52: 30S ribosomal protein Thx

Chain QU:  56% 22% 11% 7%



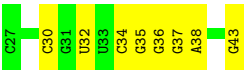
- Molecule 52: 30S ribosomal protein Thx

Chain XU:  41% 44% 7% 7%



- Molecule 53: P-site ASLPro

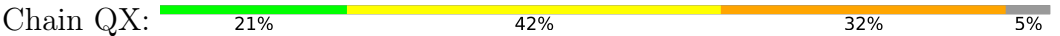
Chain QV:  53% 47%



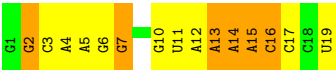
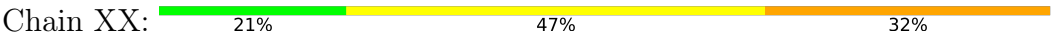
● Molecule 53: P-site ASLPro



● Molecule 54: mRNA



● Molecule 54: mRNA



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.12Å 451.80Å 622.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.68 – 3.40	Depositor
% Data completeness (in resolution range)	98.8 (188.68-3.40)	Depositor
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.198 , 0.237	Depositor
Wilson B-factor (Å <sup>2</sup> )	79.0	Xtriage
Anisotropy	0.210	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	290035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 1MG, SF4

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	RA	1.16	19/69498 (0.0%)	1.25	634/108491 (0.6%)
1	YA	1.43	115/69543 (0.2%)	1.33	828/108563 (0.8%)
2	RB	0.85	0/2878	1.24	33/4490 (0.7%)
2	YB	1.23	0/2878	1.34	43/4490 (1.0%)
3	RD	0.68	0/2165	0.60	0/2919
3	YD	0.80	0/2176	0.63	0/2933
4	RE	0.66	0/1596	0.60	0/2153
4	YE	0.77	0/1601	0.68	0/2160
5	RF	0.64	0/1620	0.59	0/2194
5	YF	0.79	1/1620 (0.1%)	0.63	0/2194
6	RG	0.36	0/1499	0.64	1/2016 (0.0%)
6	YG	0.45	0/1499	0.60	0/2016
7	RH	0.44	0/1362	0.59	0/1841
7	YH	0.63	0/1362	0.56	0/1841
8	RI	0.48	0/1151	0.68	0/1558
8	YI	0.47	0/1151	0.66	0/1558
9	RN	0.59	0/1131	0.58	0/1525
9	YN	0.73	1/1148 (0.1%)	0.61	0/1547
10	RO	0.67	0/943	0.60	0/1269
10	YO	0.77	0/943	0.63	0/1269
11	RP	0.56	0/1147	0.68	1/1525 (0.1%)
11	YP	0.70	0/1139	0.70	1/1514 (0.1%)
12	RQ	0.59	1/1143 (0.1%)	0.65	0/1527
12	YQ	0.75	0/1143	0.60	0/1527
13	RR	0.58	0/982	0.65	1/1312 (0.1%)
13	YR	0.70	0/974	0.69	0/1302
14	RS	0.43	0/892	0.68	1/1187 (0.1%)
14	YS	0.61	0/887	0.57	0/1180
15	RT	0.58	0/1155	0.64	2/1542 (0.1%)
15	YT	0.65	0/1155	0.55	0/1542
16	RU	0.61	0/982	0.57	0/1306
16	YU	0.83	0/982	0.63	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	RV	0.54	0/790	0.58	0/1057
17	YV	0.77	0/790	0.66	0/1057
18	RW	0.66	0/911	0.56	0/1220
18	YW	0.80	0/911	0.60	0/1220
19	RX	0.60	0/739	0.60	0/993
19	YX	0.76	0/756	0.64	0/1014
20	RY	0.55	0/831	0.52	0/1108
20	YY	0.72	1/831 (0.1%)	0.56	0/1108
21	RZ	0.45	0/1634	0.65	1/2216 (0.0%)
21	YZ	0.57	0/1620	0.55	0/2197
22	R0	0.56	0/611	0.58	0/814
22	Y0	0.76	0/607	0.60	0/809
23	R1	0.58	0/770	0.61	0/1022
23	Y1	0.70	0/736	0.57	0/978
24	R2	0.41	0/583	0.49	0/771
24	Y2	0.57	0/608	0.52	0/803
25	R3	0.52	0/474	0.54	0/635
25	Y3	0.66	0/474	0.62	0/635
26	R4	0.35	0/578	0.59	0/776
26	Y4	0.38	0/578	0.67	0/776
27	R5	0.70	0/473	0.57	0/639
27	Y5	0.80	0/473	0.62	1/639 (0.2%)
28	R6	0.57	0/460	0.56	0/613
28	Y6	0.71	0/460	0.63	0/613
29	R7	0.69	0/417	0.52	0/550
29	Y7	0.85	1/426 (0.2%)	0.58	0/561
30	R8	0.57	0/525	0.62	0/691
30	Y8	0.71	0/525	0.65	0/691
31	R9	0.54	0/305	0.48	0/402
31	Y9	0.71	0/310	0.52	0/407
32	QA	0.87	1/36343 (0.0%)	1.17	200/56720 (0.4%)
32	XA	0.88	0/36346	1.17	213/56725 (0.4%)
33	QB	0.39	0/1942	0.62	1/2619 (0.0%)
33	XB	0.39	0/1950	0.58	0/2630
34	QC	0.35	0/1629	0.62	0/2195
34	XC	0.35	0/1629	0.57	0/2195
35	QD	0.51	0/1733	0.55	0/2318
35	XD	0.47	0/1733	0.56	0/2318
36	QE	0.45	0/1171	0.58	0/1576
36	XE	0.46	0/1171	0.54	0/1576
37	QF	0.48	0/856	0.56	0/1154
37	XF	0.46	0/856	0.52	0/1154
38	QG	0.33	0/1276	0.56	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	XG	0.34	0/1276	0.53	0/1709
39	QH	0.51	0/1128	0.56	0/1517
39	XH	0.48	0/1128	0.57	0/1517
40	QI	0.32	0/1029	0.63	2/1379 (0.1%)
40	XI	0.34	0/1017	0.63	1/1365 (0.1%)
41	QJ	0.35	0/814	0.61	0/1095
41	XJ	0.32	0/790	0.53	0/1063
42	QK	0.44	0/879	0.54	0/1187
42	XK	0.44	0/879	0.53	0/1187
43	QL	0.56	0/991	0.59	0/1327
43	XL	0.51	0/972	0.62	0/1301
44	QM	0.36	0/965	0.64	1/1292 (0.1%)
44	XM	0.37	0/956	0.67	0/1281
45	QN	0.41	0/501	0.68	1/664 (0.2%)
45	XN	0.40	0/501	0.61	1/664 (0.2%)
46	QO	0.42	0/745	0.55	0/992
46	XO	0.44	0/740	0.47	0/987
47	QP	0.49	0/721	0.56	0/970
47	XP	0.44	0/721	0.57	0/970
48	QQ	0.51	0/847	0.55	0/1131
48	XQ	0.49	0/847	0.58	0/1131
49	QR	0.45	0/579	0.62	0/768
49	XR	0.44	0/579	0.60	0/768
50	QS	0.30	0/680	0.56	0/915
50	XS	0.31	0/689	0.65	2/926 (0.2%)
51	QT	0.39	0/765	0.52	0/1007
51	XT	0.35	0/765	0.52	0/1007
52	QU	0.34	0/221	0.66	0/288
52	XU	0.36	0/221	0.62	0/288
53	QV	0.55	0/380	1.09	2/590 (0.3%)
53	XV	0.56	0/332	1.15	5/515 (1.0%)
54	QX	0.61	0/436	1.06	1/678 (0.1%)
54	XX	0.52	0/462	1.17	5/719 (0.7%)
All	All	1.02	140/313742 (0.0%)	1.11	1982/468899 (0.4%)

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
3	RD	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	YD	0	10
4	RE	0	10
4	YE	0	13
5	RF	0	13
5	YF	0	9
6	RG	0	17
6	YG	0	18
7	RH	0	24
7	YH	0	5
8	RI	0	13
8	YI	0	18
9	RN	0	10
9	YN	0	6
10	RO	0	2
10	YO	0	2
11	RP	0	19
11	YP	0	18
12	RQ	0	11
12	YQ	0	8
13	RR	0	6
13	YR	0	5
14	RS	0	8
14	YS	0	2
15	RT	0	6
15	YT	0	4
16	RU	0	3
16	YU	0	5
17	RV	0	8
17	YV	0	4
18	RW	0	5
18	YW	0	5
19	RX	0	5
19	YX	0	4
20	RY	0	5
20	YY	0	2
21	RZ	0	22
21	YZ	0	9
22	R0	0	2
22	Y0	0	3
23	R1	0	6
23	Y1	0	2
24	R2	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	R3	0	3
25	Y3	0	1
26	R4	0	10
26	Y4	0	12
27	R5	0	1
27	Y5	0	2
29	R7	0	2
30	R8	0	7
30	Y8	0	4
31	Y9	0	1
33	QB	0	21
33	XB	0	18
34	QC	0	14
34	XC	0	17
35	QD	0	13
35	XD	0	13
36	QE	0	5
36	XE	0	5
37	QF	0	2
37	XF	0	1
38	QG	0	9
38	XG	0	6
39	QH	0	4
39	XH	0	8
40	QI	0	11
40	XI	0	19
41	QJ	0	6
41	XJ	0	9
42	QK	0	4
42	XK	0	5
43	QL	0	8
43	XL	0	12
44	QM	0	17
44	XM	0	14
45	QN	0	6
45	XN	0	5
46	QO	0	2
46	XO	0	3
47	QP	0	6
47	XP	0	7
48	QQ	0	2
48	XQ	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	QR	0	4
49	XR	0	4
50	QS	0	11
50	XS	0	14
51	QT	0	13
51	XT	0	13
52	QU	0	3
52	XU	0	5
All	All	0	749

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	528	A	N9-C4	-9.09	1.32	1.37
1	YA	1021	A	N9-C4	-8.37	1.32	1.37
1	YA	1142(A)	A	N9-C4	-8.06	1.33	1.37
1	YA	676	A	N9-C4	-7.65	1.33	1.37
1	YA	1783	A	N9-C4	-6.76	1.33	1.37
1	YA	71	A	N9-C4	-6.73	1.33	1.37
1	YA	676	A	N7-C5	-6.61	1.35	1.39
1	YA	139	G	N3-C4	-6.50	1.30	1.35
1	YA	587	C	N1-C6	-6.49	1.33	1.37
1	YA	2868	A	N7-C5	-6.48	1.35	1.39
1	YA	31	C	N1-C6	-6.43	1.33	1.37
1	YA	2542	A	N9-C4	-6.40	1.34	1.37
1	YA	198	C	C4-C5	-6.33	1.37	1.43
1	YA	1210	A	N7-C5	-6.31	1.35	1.39
1	YA	1803	A	N3-C4	-6.28	1.31	1.34
1	YA	141	A	N9-C4	-6.26	1.34	1.37
1	RA	676	A	N9-C4	-6.26	1.34	1.37
1	YA	2061	G	N7-C5	-6.26	1.35	1.39
1	YA	528	A	N7-C5	-6.20	1.35	1.39
1	YA	74	A	N9-C4	-6.17	1.34	1.37
1	YA	676	A	N3-C4	-6.14	1.31	1.34
1	YA	2060	A	N9-C4	-6.10	1.34	1.37
1	YA	141	A	N7-C5	-6.05	1.35	1.39
1	YA	729	G	C2-N3	-6.01	1.27	1.32
1	YA	2015	A	N7-C5	-6.01	1.35	1.39
1	YA	2287	A	N9-C4	-6.01	1.34	1.37
1	YA	2712(A)	A	N9-C8	-5.99	1.32	1.37
1	YA	782	A	N7-C5	-5.98	1.35	1.39
1	RA	676	A	N3-C4	-5.96	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	1320	C	N1-C6	-5.96	1.33	1.37
1	YA	2285	C	N1-C6	-5.94	1.33	1.37
1	YA	513	A	N7-C5	-5.92	1.35	1.39
1	YA	1787	A	N7-C5	-5.90	1.35	1.39
12	RQ	124	LYS	C-N	-5.89	1.20	1.34
29	Y7	23	ARG	C-N	-5.83	1.20	1.34
1	YA	2455	G	N7-C5	-5.78	1.35	1.39
9	YN	106	MET	C-N	-5.77	1.20	1.34
1	YA	564	C	C4-C5	-5.75	1.38	1.43
1	YA	1142(A)	A	N3-C4	-5.72	1.31	1.34
1	RA	729	G	C2-N3	-5.69	1.28	1.32
1	YA	1698	A	N9-C4	-5.69	1.34	1.37
1	YA	2006	C	C4-C5	-5.67	1.38	1.43
20	YY	64	GLU	C-N	-5.65	1.21	1.34
1	YA	1803	A	N9-C4	-5.63	1.34	1.37
1	YA	1202	C	N1-C6	-5.63	1.33	1.37
1	RA	1787	A	N7-C5	-5.59	1.35	1.39
1	YA	1286	A	N9-C4	-5.59	1.34	1.37
1	YA	1656	C	C4-C5	-5.57	1.38	1.43
1	YA	141	A	C5-C6	-5.55	1.36	1.41
1	YA	1596	A	N9-C4	-5.54	1.34	1.37
1	YA	1668	A	N3-C4	-5.54	1.31	1.34
1	YA	1021	A	N3-C4	-5.53	1.31	1.34
1	RA	2061	G	N7-C5	-5.51	1.35	1.39
1	YA	2443	C	N1-C6	-5.51	1.33	1.37
1	YA	528	A	N3-C4	-5.51	1.31	1.34
1	RA	1804	C	C4-C5	-5.49	1.38	1.43
1	RA	2713	A	N9-C4	-5.46	1.34	1.37
1	RA	783	A	N9-C4	-5.45	1.34	1.37
1	RA	1142(A)	A	N9-C4	-5.44	1.34	1.37
1	YA	537	C	C4-C5	-5.43	1.38	1.43
1	YA	581	C	N1-C6	-5.43	1.33	1.37
1	YA	1131	G	N7-C5	-5.43	1.35	1.39
1	YA	751	A	N9-C4	-5.42	1.34	1.37
1	YA	782	A	N9-C4	-5.42	1.34	1.37
1	RA	1783	A	N9-C4	-5.42	1.34	1.37
32	QA	1502	A	N7-C5	-5.41	1.36	1.39
1	YA	1783	A	N3-C4	-5.40	1.31	1.34
1	YA	1021	A	N7-C5	-5.39	1.36	1.39
1	YA	1020	A	N9-C4	-5.38	1.34	1.37
1	YA	1830	C	C4-C5	-5.37	1.38	1.43
1	YA	1202	C	C4-C5	-5.37	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	683	C	C4-C5	-5.37	1.38	1.43
1	RA	1286	A	N9-C4	-5.37	1.34	1.37
1	YA	753	C	C4-C5	-5.36	1.38	1.43
1	YA	783	A	N7-C5	-5.34	1.36	1.39
1	YA	1376	C	N1-C6	-5.33	1.33	1.37
1	RA	676	A	N7-C5	-5.33	1.36	1.39
1	YA	856	C	C4-C5	-5.32	1.38	1.43
1	YA	1314	C	C4-C5	-5.31	1.38	1.43
1	YA	1668	A	C5-C4	-5.31	1.35	1.38
1	YA	2509	G	N7-C5	-5.31	1.36	1.39
1	YA	2712(A)	A	N7-C5	-5.30	1.36	1.39
1	RA	528	A	N9-C4	-5.30	1.34	1.37
1	YA	2518	A	N9-C4	-5.29	1.34	1.37
1	YA	2052	G	N7-C5	-5.29	1.36	1.39
1	YA	736	C	C4-C5	-5.28	1.38	1.43
1	RA	31	C	N1-C6	-5.27	1.33	1.37
1	YA	2267	A	C6-N1	-5.27	1.31	1.35
1	YA	752	A	N7-C5	-5.27	1.36	1.39
1	YA	461	C	C4-C5	-5.27	1.38	1.43
1	YA	516	C	C4-C5	-5.26	1.38	1.43
1	YA	396	G	N7-C5	-5.25	1.36	1.39
1	YA	1804	C	C4-C5	-5.25	1.38	1.43
1	YA	672	C	C4-C5	-5.25	1.38	1.43
1	YA	445	C	N1-C6	-5.24	1.34	1.37
1	YA	556	G	N9-C8	-5.23	1.34	1.37
1	YA	2681	C	N1-C6	-5.23	1.34	1.37
1	YA	981	A	N7-C5	-5.23	1.36	1.39
1	YA	330	A	N9-C4	-5.23	1.34	1.37
1	YA	675	A	N7-C5	-5.22	1.36	1.39
1	YA	1571	A	N9-C4	-5.22	1.34	1.37
1	YA	1126	A	N9-C4	-5.21	1.34	1.37
1	YA	798	G	N9-C8	-5.21	1.34	1.37
1	YA	1658	C	N1-C6	-5.21	1.34	1.37
1	YA	1257	C	C4-C5	-5.19	1.38	1.43
1	YA	590	A	N7-C5	-5.18	1.36	1.39
1	YA	581	C	C4-C5	-5.18	1.38	1.43
1	YA	640	C	C4-C5	-5.17	1.38	1.43
1	YA	1187	G	N7-C5	-5.16	1.36	1.39
1	YA	686	G	C6-N1	-5.16	1.35	1.39
1	YA	2725	A	N9-C4	-5.16	1.34	1.37
1	RA	1330	C	N1-C6	-5.15	1.34	1.37
1	YA	754	C	C4-C5	-5.15	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2453	A	C5-C4	-5.13	1.35	1.38
1	YA	571	A	C5-C4	-5.13	1.35	1.38
1	YA	923	C	N1-C6	-5.12	1.34	1.37
1	YA	2711	A	N9-C4	-5.12	1.34	1.37
1	RA	736	C	C4-C5	-5.11	1.38	1.43
1	YA	390	A	N9-C4	-5.10	1.34	1.37
1	YA	140	A	N7-C5	-5.10	1.36	1.39
1	RA	213	A	N9-C4	-5.09	1.34	1.37
1	YA	801	G	C5-C4	-5.09	1.34	1.38
1	YA	74	A	N3-C4	-5.09	1.31	1.34
1	RA	2542	A	N9-C4	-5.08	1.34	1.37
1	YA	575	A	N7-C5	-5.07	1.36	1.39
1	YA	1659	U	C2-N3	-5.07	1.34	1.37
1	YA	114	U	C4-C5	-5.07	1.39	1.43
1	YA	453	C	N1-C6	-5.05	1.34	1.37
1	YA	2521	C	N1-C6	-5.05	1.34	1.37
1	YA	621	A	N7-C5	-5.04	1.36	1.39
1	YA	1324	G	C5-C4	-5.04	1.34	1.38
1	RA	1605	C	N1-C6	-5.04	1.34	1.37
1	YA	570	G	N7-C5	-5.03	1.36	1.39
1	YA	2407	G	N7-C5	-5.03	1.36	1.39
5	YF	57	VAL	CB-CG1	-5.03	1.42	1.52
1	YA	2450	A	N7-C5	-5.02	1.36	1.39
1	YA	1354	A	N7-C5	-5.02	1.36	1.39
1	YA	586	A	N7-C5	-5.02	1.36	1.39
1	YA	31	C	C4-C5	-5.01	1.39	1.43
1	YA	2510	C	N1-C6	-5.01	1.34	1.37

All (1982) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	856	C	C6-N1-C2	-13.93	114.73	120.30
1	YA	856	C	C5-C6-N1	13.46	127.73	121.00
1	YA	1535	U	N1-C2-O2	13.33	132.13	122.80
1	RA	856	C	C6-N1-C2	-13.11	115.06	120.30
1	YA	2868	A	N7-C8-N9	12.59	120.10	113.80
32	XA	328	C	N1-C2-O2	12.52	126.41	118.90
1	YA	1535	U	N3-C2-O2	-12.05	113.77	122.20
32	QA	328	C	N1-C2-O2	11.43	125.76	118.90
1	YA	2868	A	C8-N9-C4	-11.24	101.30	105.80
32	QA	1158	C	N1-C2-O2	11.19	125.62	118.90
1	YA	141	A	C5-N7-C8	-11.13	98.34	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	328	C	N3-C2-O2	-11.09	114.14	121.90
1	RA	1931	U	N3-C2-O2	-10.97	114.52	122.20
1	YA	120	U	N3-C2-O2	-10.96	114.53	122.20
1	YA	1313	U	N3-C2-O2	-10.96	114.53	122.20
1	RA	2474	C	N1-C2-O2	10.95	125.47	118.90
1	YA	141	A	N7-C8-N9	10.73	119.17	113.80
1	YA	860	U	N3-C2-O2	-10.69	114.72	122.20
1	RA	546	C	N1-C2-O2	10.56	125.24	118.90
1	YA	2712(A)	A	N7-C8-N9	10.51	119.05	113.80
1	YA	1313	U	N1-C2-O2	10.43	130.10	122.80
1	YA	1407	C	C6-N1-C2	-10.38	116.15	120.30
1	RA	2137	C	N1-C2-O2	10.37	125.12	118.90
1	RA	856	C	C5-C6-N1	10.35	126.17	121.00
32	QA	1066	C	N1-C2-O2	10.28	125.07	118.90
1	RA	1804	C	C5-C6-N1	10.26	126.13	121.00
1	RA	1931	U	N1-C2-O2	10.11	129.87	122.80
1	YA	1411	C	C5-C6-N1	10.09	126.05	121.00
1	YA	198	C	C5-C6-N1	10.01	126.00	121.00
1	RA	828	U	N1-C2-O2	9.98	129.78	122.80
1	YA	2815	C	C6-N1-C2	-9.92	116.33	120.30
1	RA	1313	U	N3-C2-O2	-9.90	115.27	122.20
1	RA	828	U	C2-N1-C1'	9.73	129.38	117.70
1	RA	1313	U	N1-C2-O2	9.73	129.61	122.80
2	RB	31	C	N1-C2-O2	9.70	124.72	118.90
1	YA	537	C	C5-C6-N1	9.69	125.84	121.00
32	XA	979	C	N1-C2-O2	9.67	124.70	118.90
1	YA	120	U	N1-C2-O2	9.66	129.56	122.80
2	RB	31	C	C2-N1-C1'	9.65	129.41	118.80
32	QA	1158	C	C2-N1-C1'	9.61	129.37	118.80
2	YB	31	C	N1-C2-O2	9.59	124.66	118.90
32	QA	1158	C	N3-C2-O2	-9.59	115.19	121.90
1	YA	1914	C	N1-C2-O2	9.54	124.62	118.90
1	YA	2688	U	N3-C2-O2	-9.46	115.58	122.20
1	YA	1920	C	C5-C6-N1	9.46	125.73	121.00
1	YA	2726	U	N3-C2-O2	-9.46	115.58	122.20
1	YA	2712	U	N3-C2-O2	-9.43	115.60	122.20
1	RA	1109	C	N1-C2-O2	9.42	124.55	118.90
1	RA	676	A	N7-C8-N9	9.38	118.49	113.80
1	RA	1092	C	N1-C2-O2	9.34	124.50	118.90
1	RA	1097	U	N1-C2-O2	9.33	129.33	122.80
32	QA	1301	U	N1-C2-O2	9.27	129.29	122.80
1	RA	828	U	N3-C2-O2	-9.23	115.74	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	753	C	C5-C6-N1	9.22	125.61	121.00
1	RA	2473	U	N1-C2-O2	9.12	129.18	122.80
1	RA	1804	C	C6-N1-C2	-9.01	116.70	120.30
1	RA	2137	C	N3-C2-O2	-9.01	115.59	121.90
1	RA	2473	U	N3-C2-O2	-9.01	115.89	122.20
1	RA	2584	U	C2-N1-C1'	9.00	128.50	117.70
1	RA	1396	U	N1-C2-O2	8.96	129.07	122.80
1	YA	867	C	N1-C2-O2	8.96	124.27	118.90
1	RA	537	C	C5-C6-N1	8.95	125.47	121.00
32	XA	328	C	C6-N1-C2	-8.92	116.73	120.30
32	XA	307	C	N1-C2-O2	8.86	124.22	118.90
1	RA	676	A	C5-N7-C8	-8.86	99.47	103.90
1	YA	1882	C	C5-C6-N1	8.85	125.43	121.00
32	QA	1322	C	N1-C2-O2	8.85	124.21	118.90
32	QA	328	C	N3-C2-O2	-8.80	115.74	121.90
1	YA	41	C	C5-C6-N1	8.80	125.40	121.00
1	YA	1407	C	C5-C6-N1	8.77	125.39	121.00
1	RA	1097	U	N3-C2-O2	-8.77	116.06	122.20
32	XA	435	C	C5-C6-N1	8.76	125.38	121.00
1	YA	12	U	N3-C2-O2	-8.76	116.07	122.20
32	XA	178	C	N1-C2-O2	8.73	124.14	118.90
32	XA	1028	C	C6-N1-C2	-8.71	116.81	120.30
1	YA	2584	U	C2-N1-C1'	8.71	128.15	117.70
32	XA	979	C	N3-C2-O2	-8.70	115.81	121.90
1	YA	1881	C	C6-N1-C2	-8.69	116.82	120.30
1	YA	1882	C	C6-N1-C2	-8.66	116.83	120.30
1	YA	1411	C	C6-N1-C2	-8.64	116.84	120.30
1	RA	588	U	C5-C6-N1	8.63	127.02	122.70
54	XX	17	C	N1-C2-O2	8.62	124.07	118.90
1	YA	2043	C	C5-C6-N1	8.62	125.31	121.00
1	RA	2474	C	N3-C2-O2	-8.61	115.87	121.90
1	YA	1076	C	N1-C2-O2	8.57	124.04	118.90
1	RA	1065	U	O4'-C1'-N1	8.52	115.02	108.20
1	YA	893	C	N1-C2-O2	8.52	124.01	118.90
32	QA	674	G	N7-C8-N9	8.49	117.35	113.10
32	QA	328	C	C6-N1-C2	-8.46	116.92	120.30
1	YA	1506	C	N1-C2-O2	8.44	123.97	118.90
2	RB	30	C	C6-N1-C2	-8.44	116.92	120.30
1	YA	2161	C	N1-C2-O2	8.44	123.97	118.90
1	YA	2701	C	C6-N1-C2	-8.44	116.92	120.30
1	YA	860	U	N1-C2-O2	8.42	128.69	122.80
1	RA	607	U	N3-C2-O2	-8.41	116.31	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	2779	U	N3-C2-O2	-8.39	116.33	122.20
1	YA	650	C	C5-C6-N1	8.37	125.19	121.00
1	RA	1640	C	N1-C2-O2	8.35	123.91	118.90
2	YB	31	C	C6-N1-C2	-8.35	116.96	120.30
1	RA	373	U	N3-C2-O2	-8.34	116.36	122.20
1	YA	676	A	C5-N7-C8	-8.34	99.73	103.90
32	QA	307	C	N1-C2-O2	8.34	123.90	118.90
1	RA	659	C	C5-C6-N1	8.33	125.17	121.00
32	QA	1263	C	N1-C2-O2	8.30	123.88	118.90
1	RA	2243	U	N3-C2-O2	-8.29	116.40	122.20
1	YA	2712	U	C2-N1-C1'	8.28	127.64	117.70
1	RA	2137	C	C6-N1-C2	-8.28	116.99	120.30
1	RA	837	C	C6-N1-C2	-8.27	116.99	120.30
1	RA	1109	C	N3-C2-O2	-8.27	116.11	121.90
1	RA	1934	C	C5-C6-N1	8.25	125.13	121.00
32	QA	346	G	N3-C4-N9	8.25	130.95	126.00
1	RA	1934	C	C6-N1-C2	-8.25	117.00	120.30
54	XX	16	C	N1-C2-O2	8.24	123.85	118.90
1	RA	2043	C	C5-C6-N1	8.22	125.11	121.00
32	QA	1237	C	C5-C6-N1	8.21	125.10	121.00
32	XA	1439	C	C6-N1-C2	-8.20	117.02	120.30
1	RA	2688	U	N3-C2-O2	-8.20	116.46	122.20
1	YA	2688	U	C2-N1-C1'	8.19	127.53	117.70
1	RA	373	U	N1-C2-O2	8.18	128.53	122.80
1	YA	265	A	O4'-C1'-N9	8.18	114.75	108.20
1	RA	613	U	N1-C2-O2	8.18	128.52	122.80
1	RA	2726	U	N3-C2-O2	-8.17	116.48	122.20
32	QA	328	C	C2-N1-C1'	8.17	127.78	118.80
2	YB	30	C	C6-N1-C2	-8.15	117.04	120.30
32	QA	110	C	N1-C2-O2	8.14	123.78	118.90
1	YA	18	C	C6-N1-C2	-8.13	117.05	120.30
32	QA	525	C	C5-C6-N1	8.13	125.07	121.00
1	YA	1513	C	C5-C6-N1	8.12	125.06	121.00
32	QA	58	C	C5-C6-N1	8.11	125.06	121.00
1	RA	659	C	C6-N1-C2	-8.11	117.06	120.30
1	YA	613	U	C2-N1-C1'	8.10	127.42	117.70
1	RA	546	C	N3-C2-O2	-8.09	116.24	121.90
1	YA	1881	C	C5-C6-N1	8.08	125.04	121.00
32	QA	1066	C	N3-C2-O2	-8.08	116.25	121.90
1	YA	417	C	C6-N1-C2	-8.08	117.07	120.30
1	YA	537	C	C6-N1-C2	-8.06	117.08	120.30
32	XA	435	C	C6-N1-C2	-8.06	117.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	41	C	C6-N1-C2	-8.05	117.08	120.30
1	YA	2584	U	N3-C2-O2	-8.04	116.57	122.20
1	RA	1396	U	N3-C2-O2	-8.04	116.57	122.20
1	YA	528	A	C2-N3-C4	-8.04	106.58	110.60
1	RA	1578	U	N3-C2-O2	-8.04	116.57	122.20
1	YA	1956	U	N3-C2-O2	-8.02	116.58	122.20
1	RA	2138	C	N1-C2-O2	8.01	123.70	118.90
1	RA	1914	C	N1-C2-O2	8.00	123.70	118.90
1	YA	2868	A	C5-N7-C8	-7.98	99.91	103.90
1	RA	456	C	N1-C2-O2	7.97	123.68	118.90
32	XA	307	C	N3-C2-O2	-7.97	116.32	121.90
1	YA	12	U	N1-C2-O2	7.97	128.38	122.80
1	RA	546	C	C5-C6-N1	7.96	124.98	121.00
1	YA	1314	C	C6-N1-C2	-7.96	117.12	120.30
32	QA	1301	U	C2-N1-C1'	7.95	127.24	117.70
1	RA	1064	C	N1-C2-O2	7.95	123.67	118.90
32	XA	827	U	C6-N1-C2	-7.95	116.23	121.00
32	XA	110	C	N1-C2-O2	7.93	123.66	118.90
1	RA	1779	U	C2-N1-C1'	7.93	127.22	117.70
1	YA	837	C	C6-N1-C2	-7.93	117.13	120.30
1	RA	2868	A	C8-N9-C4	-7.93	102.63	105.80
1	RA	1882	C	C5-C6-N1	7.92	124.96	121.00
32	XA	1533	C	C2-N1-C1'	7.91	127.50	118.80
1	YA	2808	U	N1-C2-O2	7.91	128.33	122.80
1	YA	650	C	C6-N1-C2	-7.90	117.14	120.30
1	RA	1947	C	C6-N1-C2	-7.89	117.14	120.30
1	YA	114	U	C5-C6-N1	7.88	126.64	122.70
1	YA	814	C	C5-C6-N1	7.87	124.94	121.00
1	YA	795	C	C6-N1-C2	-7.87	117.15	120.30
1	YA	1430	C	C5-C6-N1	7.86	124.93	121.00
1	RA	1049	C	N1-C2-O2	7.83	123.60	118.90
1	RA	1314	C	C6-N1-C2	-7.83	117.17	120.30
1	YA	1658	C	C5-C6-N1	7.83	124.92	121.00
32	QA	618	C	N1-C2-O2	7.83	123.60	118.90
1	RA	1332	G	N7-C8-N9	7.83	117.01	113.10
1	YA	828	U	C2-N1-C1'	7.82	127.09	117.70
1	YA	676	A	N7-C8-N9	7.82	117.71	113.80
1	RA	1407	C	C5-C6-N1	7.82	124.91	121.00
1	RA	1644	C	C6-N1-C2	-7.80	117.18	120.30
1	YA	2787	C	C6-N1-C2	-7.80	117.18	120.30
32	QA	1301	U	N3-C2-O2	-7.79	116.75	122.20
1	RA	546	C	C6-N1-C2	-7.79	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2868	A	N7-C8-N9	7.79	117.69	113.80
1	RA	1407	C	C6-N1-C2	-7.79	117.19	120.30
1	RA	634	C	C6-N1-C2	-7.78	117.19	120.30
1	RA	1599	C	C6-N1-C2	-7.77	117.19	120.30
1	YA	1314	C	C5-C6-N1	7.77	124.89	121.00
32	XA	307	C	C6-N1-C2	-7.77	117.19	120.30
2	YB	31	C	N3-C2-O2	-7.77	116.46	121.90
1	RA	797	C	C5-C6-N1	7.75	124.88	121.00
32	QA	1158	C	C6-N1-C2	-7.75	117.20	120.30
1	YA	1660	C	C6-N1-C2	-7.74	117.20	120.30
1	RA	1264	G	C8-N9-C4	-7.74	103.30	106.40
1	YA	1404	C	C6-N1-C2	-7.74	117.21	120.30
1	YA	2089	U	C5-C6-N1	7.74	126.57	122.70
32	QA	1066	C	C5-C6-N1	7.72	124.86	121.00
1	RA	2063	C	N3-C2-O2	-7.72	116.50	121.90
1	YA	269	U	N3-C2-O2	-7.72	116.80	122.20
1	RA	1092	C	C5-C6-N1	7.71	124.86	121.00
1	RA	1313	U	C2-N1-C1'	7.71	126.96	117.70
1	RA	2723	C	C6-N1-C2	-7.70	117.22	120.30
1	RA	269	U	N3-C2-O2	-7.70	116.81	122.20
1	YA	683	C	C5-C6-N1	7.69	124.84	121.00
1	YA	1882	C	C2-N1-C1'	7.69	127.26	118.80
32	QA	1502	A	C5-N7-C8	-7.69	100.06	103.90
1	YA	1506	C	C6-N1-C2	-7.68	117.23	120.30
1	RA	691	C	C6-N1-C2	-7.67	117.23	120.30
1	YA	2712(A)	A	C8-N9-C4	-7.67	102.73	105.80
32	QA	789	U	N3-C2-O2	-7.66	116.84	122.20
32	QA	1502	A	N7-C8-N9	7.66	117.63	113.80
32	QA	1066	C	C6-N1-C2	-7.64	117.24	120.30
1	YA	2248	C	C6-N1-C2	-7.64	117.24	120.30
1	RA	2559	C	C5-C6-N1	7.64	124.82	121.00
1	YA	1407	C	N1-C2-O2	7.64	123.48	118.90
32	QA	405	U	N3-C2-O2	-7.63	116.86	122.20
1	YA	1021	A	C5-N7-C8	-7.62	100.09	103.90
1	YA	1207	C	C5-C6-N1	7.62	124.81	121.00
1	YA	1830	C	C5-C6-N1	7.61	124.80	121.00
1	YA	1678	G	N7-C8-N9	7.60	116.90	113.10
1	RA	1578	U	N1-C2-O2	7.60	128.12	122.80
1	RA	613	U	N3-C2-O2	-7.59	116.89	122.20
32	QA	1028(A)	C	N1-C2-O2	7.58	123.45	118.90
32	QA	330	C	N1-C2-O2	7.58	123.44	118.90
1	YA	1535	U	C2-N1-C1'	7.57	126.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	837	C	C5-C6-N1	7.57	124.79	121.00
1	YA	2723	C	C6-N1-C2	-7.57	117.27	120.30
1	YA	749	C	N1-C2-O2	7.57	123.44	118.90
1	RA	537	C	C6-N1-C2	-7.56	117.28	120.30
1	YA	1157	G	C6-C5-N7	-7.55	125.87	130.40
1	YA	2559	C	C6-N1-C2	-7.55	117.28	120.30
1	RA	537	C	N1-C2-O2	7.55	123.43	118.90
32	XA	178	C	N3-C2-O2	-7.55	116.62	121.90
1	RA	192	C	C6-N1-C2	-7.54	117.28	120.30
1	YA	2779	U	N1-C2-O2	7.54	128.08	122.80
32	XA	328	C	C2-N1-C1'	7.54	127.09	118.80
32	XA	405	U	N3-C2-O2	-7.54	116.92	122.20
32	QA	58	C	C6-N1-C2	-7.54	117.28	120.30
1	YA	1207	C	C6-N1-C2	-7.54	117.28	120.30
1	RA	1660	C	C6-N1-C2	-7.54	117.28	120.30
1	YA	141	A	C4-C5-N7	7.54	114.47	110.70
1	YA	1915	U	N1-C2-O2	7.52	128.07	122.80
1	YA	198	C	C6-N1-C2	-7.52	117.29	120.30
1	YA	528	A	C5-N7-C8	-7.52	100.14	103.90
32	XA	1037	C	C6-N1-C2	-7.52	117.29	120.30
1	RA	1049	C	C6-N1-C2	-7.52	117.29	120.30
1	RA	1956	U	N1-C2-O2	7.52	128.06	122.80
1	YA	1578	U	N3-C2-O2	-7.51	116.94	122.20
1	RA	373	U	C5-C6-N1	7.50	126.45	122.70
1	RA	1956	U	N3-C2-O2	-7.50	116.95	122.20
1	YA	635	C	C6-N1-C2	-7.50	117.30	120.30
32	QA	328	C	C5-C6-N1	7.50	124.75	121.00
1	RA	2063	C	C6-N1-C2	-7.49	117.30	120.30
1	YA	1430	C	C6-N1-C2	-7.49	117.30	120.30
1	RA	1504	C	N1-C2-O2	7.49	123.39	118.90
1	YA	417	C	C5-C6-N1	7.49	124.74	121.00
1	RA	2726	U	C2-N1-C1'	7.49	126.68	117.70
1	YA	2726	U	N1-C2-O2	7.48	128.04	122.80
1	YA	461	C	C5-C6-N1	7.48	124.74	121.00
1	YA	1157	G	C4-C5-N7	7.48	113.79	110.80
32	XA	738	C	C5-C6-N1	7.47	124.73	121.00
32	XA	405	U	N1-C2-O2	7.46	128.02	122.80
1	RA	273(F)	C	C6-N1-C2	-7.46	117.32	120.30
1	YA	2008	C	C6-N1-C2	-7.46	117.32	120.30
32	XA	1439	C	N1-C2-O2	7.45	123.37	118.90
1	RA	2559	C	N1-C2-O2	7.44	123.37	118.90
1	YA	2787	C	C5-C6-N1	7.44	124.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1604	C	C6-N1-C2	-7.44	117.32	120.30
1	RA	120	U	N3-C2-O2	-7.44	116.99	122.20
1	YA	1313	U	C2-N1-C1'	7.43	126.62	117.70
1	YA	1332	G	N7-C8-N9	7.43	116.82	113.10
1	RA	1159	U	N3-C2-O2	-7.43	117.00	122.20
32	XA	749	C	C6-N1-C2	-7.42	117.33	120.30
1	YA	512	G	C4-N9-C1'	-7.42	116.85	126.50
32	QA	1066	C	C2-N1-C1'	7.42	126.96	118.80
1	RA	1049	C	N3-C2-O2	-7.41	116.71	121.90
1	RA	1332	G	C6-C5-N7	-7.41	125.96	130.40
1	YA	2006	C	C6-N1-C2	-7.41	117.34	120.30
32	XA	980	C	N1-C2-O2	7.40	123.34	118.90
1	RA	1474	C	N1-C2-O2	7.40	123.34	118.90
54	XX	17	C	N3-C2-O2	-7.39	116.73	121.90
1	RA	1097	U	C2-N1-C1'	7.39	126.57	117.70
1	YA	595	C	C6-N1-C2	-7.39	117.34	120.30
32	QA	1038	C	N1-C2-O2	7.38	123.33	118.90
1	RA	2616	C	C6-N1-C2	-7.37	117.35	120.30
1	YA	2808	U	N3-C2-O2	-7.37	117.04	122.20
1	YA	529	A	N7-C8-N9	7.36	117.48	113.80
2	YB	27	C	C6-N1-C2	-7.36	117.36	120.30
32	QA	405	U	N1-C2-O2	7.36	127.95	122.80
1	YA	2739	U	N3-C2-O2	-7.35	117.05	122.20
2	RB	31	C	N3-C2-O2	-7.35	116.76	121.90
32	QA	618	C	N3-C2-O2	-7.34	116.76	121.90
1	YA	731	C	C5-C6-N1	7.34	124.67	121.00
32	QA	110	C	N3-C2-O2	-7.33	116.77	121.90
1	RA	607	U	N1-C2-O2	7.33	127.93	122.80
1	YA	1406	U	C5-C6-N1	7.33	126.36	122.70
1	RA	1774	C	N1-C2-O2	7.32	123.29	118.90
32	XA	186	C	N1-C2-O2	7.32	123.29	118.90
1	YA	860	U	C2-N1-C1'	7.31	126.48	117.70
1	RA	2394	C	N1-C2-O2	7.31	123.29	118.90
1	RA	1920	C	C5-C6-N1	7.30	124.65	121.00
1	YA	838	C	C6-N1-C2	-7.29	117.38	120.30
32	XA	525	C	C5-C6-N1	7.29	124.65	121.00
1	YA	1804	C	C5-C6-N1	7.29	124.64	121.00
1	RA	691	C	C5-C6-N1	7.29	124.64	121.00
32	QA	169	C	N1-C2-O2	7.29	123.27	118.90
1	RA	183	C	N1-C2-O2	7.29	123.27	118.90
1	YA	2712	U	N1-C2-O2	7.28	127.89	122.80
2	YB	79	C	C6-N1-C2	-7.28	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	365	U	C2-N1-C1'	7.27	126.43	117.70
1	YA	672	C	C5-C6-N1	7.27	124.64	121.00
1	RA	2103	C	C5-C6-N1	7.27	124.64	121.00
32	XA	1260	C	N3-C2-O2	-7.27	116.81	121.90
1	RA	2043	C	C6-N1-C2	-7.26	117.40	120.30
1	YA	1774	C	C5-C6-N1	7.25	124.63	121.00
1	YA	2841	C	C6-N1-C2	-7.25	117.40	120.30
1	YA	797	C	C5-C6-N1	7.25	124.62	121.00
1	RA	898	C	N1-C2-O2	7.24	123.24	118.90
1	YA	2359	C	C5-C6-N1	7.24	124.62	121.00
1	YA	2465	C	C6-N1-C2	-7.24	117.41	120.30
32	QA	1502	A	C4-C5-N7	7.23	114.32	110.70
1	YA	2043	C	C6-N1-C2	-7.23	117.41	120.30
32	XA	169	C	N1-C2-O2	7.23	123.24	118.90
32	QA	1407	C	C6-N1-C2	-7.22	117.41	120.30
1	YA	529	A	C8-N9-C4	-7.22	102.91	105.80
1	RA	1502	C	C5-C6-N1	7.22	124.61	121.00
1	RA	2559	C	C6-N1-C2	-7.21	117.42	120.30
1	YA	754	C	C5-C6-N1	7.21	124.61	121.00
1	RA	1788	C	C5-C6-N1	7.21	124.61	121.00
1	YA	1956	U	N1-C2-O2	7.20	127.84	122.80
1	YA	2559	C	C5-C6-N1	7.20	124.60	121.00
1	YA	640	C	C5-C6-N1	7.20	124.60	121.00
1	RA	120	U	N1-C2-O2	7.20	127.84	122.80
1	RA	1502	C	C6-N1-C2	-7.20	117.42	120.30
32	XA	135	C	C6-N1-C2	-7.20	117.42	120.30
32	XA	58	C	C5-C6-N1	7.20	124.60	121.00
1	YA	1781	C	N1-C2-O2	7.19	123.22	118.90
1	YA	753	C	C6-N1-C2	-7.18	117.43	120.30
32	QA	960	U	N1-C2-O2	7.17	127.82	122.80
1	RA	1947	C	C5-C6-N1	7.17	124.59	121.00
1	RA	1304	C	C5-C6-N1	7.17	124.58	121.00
32	XA	1533	C	C6-N1-C1'	-7.17	112.20	120.80
1	YA	2588	G	C4-C5-N7	7.16	113.67	110.80
1	YA	985	C	N1-C2-O2	7.16	123.20	118.90
1	YA	2584	U	N1-C2-O2	7.16	127.81	122.80
32	XA	1439	C	C5-C6-N1	7.16	124.58	121.00
1	YA	867	C	N3-C2-O2	-7.15	116.89	121.90
1	YA	2841	C	C5-C6-N1	7.15	124.58	121.00
1	RA	546	C	C2-N1-C1'	7.15	126.67	118.80
40	QI	102	LEU	CA-CB-CG	7.15	131.74	115.30
1	RA	2726	U	N1-C2-O2	7.14	127.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	749	C	N1-C2-O2	7.14	123.18	118.90
1	RA	2591	C	C6-N1-C2	-7.14	117.44	120.30
32	XA	699	C	C6-N1-C2	-7.14	117.44	120.30
1	YA	1021	A	C8-N9-C4	-7.13	102.95	105.80
32	XA	58	C	N1-C2-O2	7.13	123.18	118.90
1	RA	1375	C	C6-N1-C2	-7.12	117.45	120.30
1	YA	1914	C	N3-C2-O2	-7.12	116.91	121.90
32	XA	1028	C	N1-C2-O2	7.12	123.17	118.90
1	RA	2063	C	N1-C2-O2	7.12	123.17	118.90
1	RA	1064	C	C6-N1-C2	-7.12	117.45	120.30
1	YA	208	C	C5-C6-N1	7.12	124.56	121.00
32	QA	1502	A	C6-C5-N7	-7.11	127.32	132.30
1	YA	965	C	C5-C6-N1	7.10	124.55	121.00
1	RA	1437	C	C6-N1-C2	-7.10	117.46	120.30
1	YA	783	A	C8-N9-C4	-7.10	102.96	105.80
1	RA	1914	C	N3-C2-O2	-7.10	116.93	121.90
1	YA	512	G	C8-N9-C1'	7.09	136.22	127.00
32	XA	330	C	N1-C2-O2	7.09	123.15	118.90
1	YA	783	A	N7-C8-N9	7.08	117.34	113.80
1	YA	1431	U	C5-C6-N1	7.08	126.24	122.70
1	YA	269	U	N1-C2-O2	7.08	127.75	122.80
1	YA	1021	A	C2-N3-C4	-7.07	107.06	110.60
1	YA	183	C	N1-C2-O2	7.07	123.14	118.90
1	YA	1920	C	C6-N1-C2	-7.07	117.47	120.30
1	YA	1407	C	C2-N1-C1'	7.06	126.56	118.80
1	RA	417	C	C5-C6-N1	7.05	124.53	121.00
1	YA	528	A	N3-C4-N9	-7.05	121.76	127.40
32	QA	1420	C	C6-N1-C2	-7.04	117.48	120.30
2	RB	68	C	C6-N1-C2	-7.04	117.48	120.30
1	YA	1437	C	C5-C6-N1	7.04	124.52	121.00
1	RA	1882	C	C6-N1-C2	-7.04	117.48	120.30
1	YA	2512	C	C5-C6-N1	7.04	124.52	121.00
1	YA	580	C	C5-C6-N1	7.03	124.51	121.00
32	XA	792	A	O4'-C1'-N9	7.02	113.82	108.20
1	RA	1109	C	C6-N1-C2	-7.02	117.49	120.30
32	QA	1118	C	N1-C2-O2	7.02	123.11	118.90
1	RA	1407	C	C2-N1-C1'	7.01	126.51	118.80
1	RA	417	C	C6-N1-C2	-7.01	117.50	120.30
1	RA	2137	C	C2-N1-C1'	7.00	126.50	118.80
2	RB	31	C	C6-N1-C1'	-7.00	112.40	120.80
1	YA	1306	C	C5-C6-N1	7.00	124.50	121.00
32	XA	23	C	C5-C6-N1	6.99	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	571	U	C5-C6-N1	6.99	126.19	122.70
1	YA	976	C	C6-N1-C2	-6.99	117.50	120.30
32	QA	674	G	C8-N9-C4	-6.99	103.61	106.40
32	XA	789	U	N3-C2-O2	-6.98	117.31	122.20
1	YA	335	C	C6-N1-C2	-6.98	117.51	120.30
1	YA	1788	C	C5-C6-N1	6.98	124.49	121.00
1	RA	837	C	N3-C2-O2	-6.98	117.02	121.90
32	XA	738	C	C6-N1-C2	-6.97	117.51	120.30
2	RB	60	C	C5-C6-N1	6.97	124.49	121.00
32	XA	827	U	N3-C2-O2	-6.97	117.32	122.20
1	RA	1947	C	N1-C2-O2	6.96	123.08	118.90
32	XA	23	C	C6-N1-C2	-6.96	117.52	120.30
1	YA	772	C	C5-C6-N1	6.96	124.48	121.00
1	YA	2307	G	C4-N9-C1'	6.96	135.55	126.50
1	RA	806	C	C6-N1-C2	-6.96	117.52	120.30
1	RA	1774	C	N3-C2-O2	-6.96	117.03	121.90
2	YB	60	C	C5-C6-N1	6.95	124.47	121.00
1	YA	537	C	N1-C2-O2	6.95	123.07	118.90
1	YA	1306	C	C6-N1-C2	-6.95	117.52	120.30
2	RB	27	C	N1-C2-O2	6.94	123.07	118.90
1	YA	683	C	C6-N1-C2	-6.94	117.52	120.30
1	YA	2827	C	C5-C6-N1	6.94	124.47	121.00
1	YA	2063	C	N1-C2-O2	6.93	123.06	118.90
1	RA	2880	C	C6-N1-C2	-6.93	117.53	120.30
1	YA	930	U	N3-C2-O2	-6.93	117.35	122.20
32	XA	186	C	N3-C2-O2	-6.92	117.06	121.90
1	YA	2616	C	C6-N1-C2	-6.92	117.53	120.30
32	XA	1158	C	C2-N1-C1'	6.91	126.40	118.80
1	RA	273(F)	C	C5-C6-N1	6.91	124.45	121.00
1	YA	1640	C	N1-C2-O2	6.90	123.04	118.90
32	QA	1237	C	C6-N1-C2	-6.89	117.54	120.30
1	YA	1021	A	N7-C8-N9	6.89	117.25	113.80
32	XA	1028	C	C5-C6-N1	6.89	124.44	121.00
1	RA	708	C	N1-C2-O2	6.89	123.03	118.90
32	QA	346	G	N3-C4-C5	-6.88	125.16	128.60
1	YA	621	A	N7-C8-N9	6.88	117.24	113.80
32	XA	749	C	C5-C6-N1	6.88	124.44	121.00
1	YA	1774	C	C6-N1-C2	-6.88	117.55	120.30
32	QA	1322	C	C6-N1-C2	-6.88	117.55	120.30
2	YB	27	C	N1-C2-O2	6.88	123.03	118.90
32	QA	623	C	C5-C6-N1	6.87	124.44	121.00
1	YA	1411	C	N1-C2-O2	6.87	123.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1437	C	C6-N1-C2	-6.87	117.55	120.30
1	RA	2439	A	C8-N9-C4	-6.87	103.05	105.80
1	RA	198	C	C5-C6-N1	6.86	124.43	121.00
1	YA	1678	G	C8-N9-C4	-6.86	103.66	106.40
1	YA	2006	C	C5-C6-N1	6.86	124.43	121.00
1	RA	2205	C	C6-N1-C2	-6.85	117.56	120.30
1	YA	1474	C	C5-C6-N1	6.85	124.43	121.00
1	YA	2474	C	N1-C2-O2	6.85	123.01	118.90
1	YA	1332	G	C6-C5-N7	-6.84	126.29	130.40
1	YA	2063	C	N3-C2-O2	-6.84	117.11	121.90
32	XA	449	C	C2-N1-C1'	6.84	126.33	118.80
32	QA	1322	C	C5-C6-N1	6.84	124.42	121.00
1	RA	1640	C	N3-C2-O2	-6.83	117.12	121.90
1	YA	1915	U	N3-C2-O2	-6.83	117.42	122.20
1	YA	243	U	C5-C6-N1	6.83	126.11	122.70
1	YA	530	G	N1-C6-O6	-6.82	115.81	119.90
32	QA	1322	C	N3-C2-O2	-6.81	117.14	121.90
1	RA	1109	C	C2-N1-C1'	6.80	126.28	118.80
32	XA	797	C	C6-N1-C2	-6.79	117.58	120.30
32	XA	754	C	C2-N1-C1'	6.79	126.27	118.80
32	QA	449	C	C2-N1-C1'	6.78	126.26	118.80
1	YA	1640	C	C6-N1-C2	-6.78	117.59	120.30
1	YA	2655	G	C4-N9-C1'	-6.77	117.70	126.50
32	XA	135	C	N1-C2-O2	6.77	122.96	118.90
1	YA	1961	C	N1-C2-O2	6.77	122.96	118.90
1	YA	1013	C	C6-N1-C2	-6.76	117.59	120.30
1	RA	2584	U	N3-C2-O2	-6.76	117.47	122.20
1	YA	2416	C	C5-C6-N1	6.76	124.38	121.00
1	YA	817	C	C5-C6-N1	6.75	124.38	121.00
1	RA	140	A	N7-C8-N9	6.75	117.17	113.80
1	YA	1930	G	C8-N9-C1'	6.75	135.78	127.00
1	RA	1514	U	N1-C2-O2	6.75	127.52	122.80
1	RA	837	C	N1-C2-O2	6.74	122.94	118.90
1	RA	753	C	C5-C6-N1	6.73	124.37	121.00
32	QA	307	C	N3-C2-O2	-6.73	117.19	121.90
32	XA	455	C	N1-C2-O2	6.73	122.94	118.90
1	RA	2065	C	C6-N1-C2	-6.73	117.61	120.30
1	RA	2394	C	N3-C2-O2	-6.73	117.19	121.90
32	XA	58	C	C6-N1-C2	-6.73	117.61	120.30
1	RA	672	C	C5-C6-N1	6.72	124.36	121.00
1	RA	2321	G	N3-C4-C5	-6.72	125.24	128.60
1	YA	2473	U	N1-C2-O2	6.72	127.50	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1187	G	C8-N9-C4	-6.72	103.71	106.40
32	XA	528	C	N1-C2-O2	6.71	122.93	118.90
1	YA	1332	G	C4-N9-C1'	6.71	135.22	126.50
1	YA	409	C	C5-C6-N1	6.71	124.36	121.00
1	YA	541	C	C6-N1-C2	-6.71	117.62	120.30
1	YA	510	C	C5-C6-N1	6.71	124.35	121.00
32	QA	754	C	C2-N1-C1'	6.71	126.18	118.80
1	RA	2138	C	C6-N1-C2	-6.70	117.62	120.30
1	YA	517	C	C5-C6-N1	6.70	124.35	121.00
1	YA	2726	U	C2-N1-C1'	6.70	125.74	117.70
1	YA	2712(A)	A	C5-N7-C8	-6.69	100.55	103.90
1	RA	1774	C	C6-N1-C2	-6.69	117.62	120.30
1	YA	1892	C	C6-N1-C2	-6.69	117.62	120.30
1	YA	435	C	N1-C2-O2	6.69	122.91	118.90
54	XX	16	C	N3-C2-O2	-6.69	117.22	121.90
1	RA	1407	C	N1-C2-O2	6.68	122.91	118.90
1	RA	2688	U	C2-N1-C1'	6.68	125.72	117.70
1	YA	31	C	C5-C6-N1	6.68	124.34	121.00
1	YA	535	C	C5-C6-N1	6.68	124.34	121.00
1	YA	1805	U	C6-N1-C2	-6.68	116.99	121.00
1	RA	1314	C	C5-C6-N1	6.67	124.34	121.00
1	YA	1385	G	O4'-C1'-N9	6.67	113.54	108.20
1	RA	31	C	C5-C6-N1	6.67	124.33	121.00
1	YA	731	C	C6-N1-C2	-6.67	117.63	120.30
1	YA	1506	C	N3-C2-O2	-6.67	117.23	121.90
1	YA	856	C	C2-N3-C4	6.67	123.23	119.90
1	YA	2870	C	C6-N1-C2	-6.67	117.63	120.30
1	YA	893	C	N3-C2-O2	-6.66	117.23	121.90
1	RA	595	C	C5-C6-N1	6.66	124.33	121.00
1	RA	1437	C	C5-C6-N1	6.66	124.33	121.00
2	YB	27	C	N3-C2-O2	-6.66	117.24	121.90
1	YA	783	A	C5-N7-C8	-6.66	100.57	103.90
1	YA	1462	C	N1-C2-O2	6.66	122.89	118.90
1	YA	1513	C	C6-N1-C2	-6.66	117.64	120.30
1	RA	2161	C	N1-C2-O2	6.65	122.89	118.90
1	YA	2229	C	C6-N1-C2	-6.65	117.64	120.30
1	RA	2006	C	C5-C6-N1	6.65	124.33	121.00
32	XA	1113	C	C6-N1-C2	-6.65	117.64	120.30
1	YA	613	U	N3-C2-O2	-6.64	117.55	122.20
2	YB	28	C	C6-N1-C2	-6.63	117.65	120.30
1	YA	1407	C	N3-C2-O2	-6.63	117.26	121.90
32	XA	810	C	C6-N1-C2	-6.63	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	442	C	C6-N1-C2	-6.63	117.65	120.30
1	YA	772	C	C6-N1-C2	-6.63	117.65	120.30
2	YB	37	C	N3-C2-O2	-6.63	117.26	121.90
1	YA	2243	U	N3-C2-O2	-6.62	117.56	122.20
32	XA	1158	C	C6-N1-C2	-6.62	117.65	120.30
1	RA	1306	C	C5-C6-N1	6.61	124.31	121.00
32	XA	1028	C	N3-C2-O2	-6.60	117.28	121.90
1	RA	834	C	C6-N1-C2	-6.60	117.66	120.30
1	RA	860	U	N3-C2-O2	-6.60	117.58	122.20
1	RA	2229	C	C6-N1-C2	-6.59	117.67	120.30
1	YA	825	C	C5-C6-N1	6.59	124.29	121.00
1	YA	528	A	C8-N9-C4	-6.58	103.17	105.80
1	YA	1402	C	C6-N1-C2	-6.58	117.67	120.30
1	YA	1375	C	C5-C6-N1	6.58	124.29	121.00
1	RA	1983	C	C6-N1-C2	-6.58	117.67	120.30
32	QA	1539	C	N3-C2-O2	-6.58	117.30	121.90
1	YA	1076	C	N3-C2-O2	-6.58	117.30	121.90
1	YA	1294	U	N3-C2-O2	-6.58	117.60	122.20
32	XA	980	C	N3-C2-O2	-6.57	117.30	121.90
2	YB	31	C	C5-C6-N1	6.57	124.28	121.00
1	YA	2506	U	N3-C2-O2	-6.57	117.60	122.20
1	YA	1892	C	C5-C6-N1	6.56	124.28	121.00
1	YA	2006	C	N1-C2-O2	6.56	122.83	118.90
53	XV	34	C	N1-C2-O2	6.56	122.83	118.90
32	XA	1097	C	C6-N1-C2	-6.55	117.68	120.30
1	YA	1506	C	C5-C6-N1	6.54	124.27	121.00
32	QA	699	C	C6-N1-C2	-6.54	117.68	120.30
1	YA	2034	U	C5-C6-N1	6.54	125.97	122.70
1	YA	1830	C	C6-N1-C2	-6.54	117.68	120.30
1	YA	1411	C	C2-N1-C1'	6.54	125.99	118.80
1	YA	1218	C	C5-C6-N1	6.54	124.27	121.00
1	YA	1958	C	C5-C6-N1	6.54	124.27	121.00
1	RA	269	U	N1-C2-O2	6.54	127.38	122.80
1	YA	385	C	C6-N1-C2	-6.53	117.69	120.30
1	YA	1535	U	C5-C6-N1	6.53	125.96	122.70
1	YA	2516	G	C2-N3-C4	6.53	115.16	111.90
2	RB	27	C	C6-N1-C2	-6.52	117.69	120.30
32	QA	1536	C	N3-C2-O2	-6.52	117.34	121.90
1	YA	2616	C	C5-C6-N1	6.52	124.26	121.00
1	RA	986	C	C6-N1-C2	-6.51	117.69	120.30
1	RA	2107	C	C6-N1-C2	-6.51	117.69	120.30
1	RA	2210	G	N3-C4-N9	6.51	129.91	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	1113	C	C6-N1-C2	-6.51	117.69	120.30
1	YA	1204	A	O4'-C1'-N9	6.51	113.41	108.20
32	XA	283	C	C5-C6-N1	6.51	124.25	121.00
1	RA	1691	C	C5-C6-N1	6.51	124.25	121.00
1	YA	2456	C	C6-N1-C2	-6.50	117.70	120.30
1	RA	912	C	C6-N1-C2	-6.50	117.70	120.30
1	YA	1930	G	C4-N9-C1'	-6.50	118.05	126.50
1	RA	659	C	N1-C2-O2	6.50	122.80	118.90
1	RA	1836	C	C6-N1-C2	-6.50	117.70	120.30
1	YA	992	C	C5-C6-N1	6.50	124.25	121.00
1	RA	1660	C	C5-C6-N1	6.49	124.25	121.00
1	RA	1920	C	C6-N1-C2	-6.49	117.70	120.30
1	RA	2885	C	C6-N1-C2	-6.49	117.70	120.30
1	YA	2460	U	C5-C6-N1	6.49	125.94	122.70
1	RA	1092	C	N3-C2-O2	-6.48	117.36	121.90
1	YA	2617	C	N1-C2-O2	6.48	122.79	118.90
1	YA	564	C	C5-C6-N1	6.48	124.24	121.00
1	RA	1264	G	N7-C8-N9	6.48	116.34	113.10
1	YA	556	G	N7-C8-N9	6.48	116.34	113.10
1	RA	1430	C	C5-C6-N1	6.48	124.24	121.00
1	YA	18	C	C5-C6-N1	6.47	124.23	121.00
1	RA	456	C	C2-N1-C1'	6.47	125.92	118.80
1	RA	1882	C	C2-N1-C1'	6.47	125.92	118.80
2	YB	31	C	C2-N1-C1'	6.47	125.92	118.80
1	YA	672	C	C6-N1-C2	-6.46	117.71	120.30
1	YA	1187	G	N7-C8-N9	6.46	116.33	113.10
1	RA	1514	U	N3-C2-O2	-6.46	117.68	122.20
32	QA	91	C	C5-C6-N1	6.46	124.23	121.00
1	RA	104	U	N3-C2-O2	-6.46	117.68	122.20
1	RA	2512	C	C5-C6-N1	6.46	124.23	121.00
1	YA	856	C	N1-C2-O2	6.46	122.78	118.90
1	YA	766	C	C5-C6-N1	6.46	124.23	121.00
1	YA	857	C	N1-C2-O2	6.45	122.77	118.90
1	YA	373	U	N3-C2-O2	-6.45	117.69	122.20
1	YA	2772	C	C5-C6-N1	6.45	124.22	121.00
1	RA	2576	G	C4-N9-C1'	6.44	134.88	126.50
1	YA	1683	C	C5-C6-N1	6.44	124.22	121.00
1	RA	140	A	C5-N7-C8	-6.44	100.68	103.90
32	XA	36	C	C6-N1-C2	-6.44	117.72	120.30
54	XX	17	C	C6-N1-C2	-6.44	117.72	120.30
1	RA	1064	C	N3-C2-O2	-6.43	117.40	121.90
1	YA	528	A	N7-C8-N9	6.43	117.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1013	C	C5-C6-N1	6.43	124.22	121.00
1	RA	183	C	C5-C6-N1	6.43	124.22	121.00
1	YA	2559	C	N1-C2-O2	6.43	122.76	118.90
1	RA	392	C	C5-C6-N1	6.43	124.21	121.00
1	RA	1314	C	C2-N1-C1'	6.43	125.87	118.80
1	YA	1793	C	C6-N1-C2	-6.42	117.73	120.30
1	RA	828	U	C5-C6-N1	6.42	125.91	122.70
1	RA	155	C	C6-N1-C2	-6.42	117.73	120.30
32	XA	690	G	C4-N9-C1'	6.42	134.84	126.50
1	RA	343	C	C6-N1-C2	-6.42	117.73	120.30
1	RA	1375	C	C5-C6-N1	6.42	124.21	121.00
1	RA	364	C	C6-N1-C2	-6.42	117.73	120.30
32	QA	1163	C	C6-N1-C2	-6.41	117.73	120.30
1	YA	1257	C	C5-C6-N1	6.41	124.21	121.00
1	RA	2507	C	C5-C6-N1	6.41	124.20	121.00
1	YA	528	A	N3-C4-C5	6.41	131.29	126.80
32	QA	1279	A	N7-C8-N9	6.41	117.00	113.80
1	YA	2205	C	C6-N1-C2	-6.41	117.74	120.30
1	RA	683	C	N1-C2-O2	6.40	122.74	118.90
1	YA	392	C	C5-C6-N1	6.40	124.20	121.00
1	YA	2676	C	C5-C6-N1	6.40	124.20	121.00
1	RA	1678	G	N7-C8-N9	6.40	116.30	113.10
1	RA	976	C	C6-N1-C2	-6.39	117.74	120.30
1	RA	1523	U	C5-C6-N1	6.39	125.90	122.70
1	YA	198	C	N1-C2-O2	6.39	122.73	118.90
1	RA	1961	C	N1-C2-O2	6.39	122.73	118.90
32	QA	749	C	C6-N1-C2	-6.39	117.75	120.30
1	RA	456	C	C5-C6-N1	6.39	124.19	121.00
1	RA	708	C	C5-C6-N1	6.39	124.19	121.00
32	XA	827	U	N1-C2-N3	6.39	118.73	114.90
32	QA	1028(A)	C	N3-C2-O2	-6.38	117.43	121.90
1	RA	392	C	C6-N1-C2	-6.38	117.75	120.30
1	RA	18	C	C6-N1-C2	-6.38	117.75	120.30
1	RA	243	U	C5-C6-N1	6.38	125.89	122.70
32	QA	972	C	C6-N1-C2	-6.38	117.75	120.30
1	RA	1830	C	C5-C6-N1	6.38	124.19	121.00
45	QN	44	LEU	CA-CB-CG	6.38	129.96	115.30
1	RA	461	C	C5-C6-N1	6.37	124.19	121.00
1	RA	1656	C	C5-C6-N1	6.37	124.19	121.00
32	QA	497	U	N1-C2-O2	6.37	127.26	122.80
32	QA	1263	C	N3-C2-O2	-6.37	117.44	121.90
1	YA	2161	C	N3-C2-O2	-6.37	117.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2138	C	N3-C2-O2	-6.37	117.44	121.90
32	QA	1381	U	N1-C2-O2	6.37	127.26	122.80
1	YA	1683	C	C6-N1-C2	-6.37	117.75	120.30
1	YA	2342	C	C6-N1-C2	-6.37	117.75	120.30
1	RA	1502	C	N1-C2-O2	6.36	122.72	118.90
1	YA	834	C	C6-N1-C2	-6.36	117.75	120.30
1	YA	2229	C	C5-C6-N1	6.36	124.18	121.00
1	YA	2248	C	C5-C6-N1	6.36	124.18	121.00
1	YA	267	C	C6-N1-C2	-6.36	117.76	120.30
1	YA	2506	U	N1-C2-O2	6.36	127.25	122.80
1	RA	2616	C	C5-C6-N1	6.36	124.18	121.00
1	YA	445	C	C6-N1-C2	-6.36	117.76	120.30
32	XA	497	U	N1-C2-O2	6.36	127.25	122.80
32	QA	442	C	C2-N1-C1'	6.36	125.79	118.80
1	YA	1402	C	C5-C6-N1	6.36	124.18	121.00
1	YA	140	A	C5-N7-C8	-6.35	100.72	103.90
32	QA	266	G	C5-C6-O6	-6.35	124.79	128.60
2	YB	44	G	C4-N9-C1'	-6.35	118.24	126.50
1	RA	373	U	C2-N1-C1'	6.35	125.32	117.70
1	YA	1598	C	C5-C6-N1	6.34	124.17	121.00
1	YA	1660	C	C5-C6-N1	6.34	124.17	121.00
1	RA	721	C	N1-C2-O2	6.34	122.70	118.90
1	YA	517	C	C6-N1-C2	-6.34	117.76	120.30
1	YA	1130	U	P-O3'-C3'	6.34	127.31	119.70
1	RA	1914	C	C2-N1-C1'	6.34	125.77	118.80
1	YA	2646	C	C5-C6-N1	6.34	124.17	121.00
32	QA	266	G	C6-C5-N7	-6.34	126.60	130.40
1	RA	912	C	C2-N1-C1'	6.34	125.77	118.80
1	RA	373	U	C6-N1-C2	-6.33	117.20	121.00
1	RA	2107	C	C5-C6-N1	6.33	124.17	121.00
1	RA	1267	U	N1-C2-O2	6.33	127.23	122.80
1	YA	2516	G	N3-C4-C5	-6.33	125.44	128.60
32	XA	690	G	O4'-C1'-N9	6.33	113.26	108.20
1	RA	2073	C	C6-N1-C2	-6.33	117.77	120.30
1	RA	1092	C	C2-N1-C1'	6.32	125.76	118.80
2	YB	19	G	C6-C5-N7	-6.32	126.61	130.40
1	YA	1578	U	N1-C2-O2	6.32	127.22	122.80
1	YA	2840	C	C5-C6-N1	6.32	124.16	121.00
1	YA	2044	C	C5-C6-N1	6.31	124.16	121.00
1	YA	2856	C	C6-N1-C2	-6.31	117.78	120.30
1	RA	2617	C	N1-C2-O2	6.31	122.69	118.90
1	RA	708	C	C6-N1-C2	-6.31	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	828	U	C6-N1-C1'	-6.31	112.37	121.20
1	RA	1844	C	C6-N1-C2	-6.30	117.78	120.30
1	RA	265	A	O4'-C1'-N9	6.30	113.24	108.20
32	QA	1502	A	N9-C4-C5	-6.30	103.28	105.80
1	YA	2420	C	C5-C6-N1	6.30	124.15	121.00
1	YA	2342	C	C5-C6-N1	6.29	124.15	121.00
1	YA	106	C	C6-N1-C2	-6.29	117.78	120.30
1	YA	816	C	C5-C6-N1	6.29	124.14	121.00
1	RA	1445	C	C6-N1-C2	-6.29	117.78	120.30
1	RA	1644	C	C5-C6-N1	6.29	124.14	121.00
1	RA	2442	C	C6-N1-C2	-6.29	117.78	120.30
1	RA	650	C	C6-N1-C2	-6.28	117.79	120.30
1	RA	1950	G	C4-N9-C1'	6.28	134.67	126.50
1	YA	1496	A	N7-C8-N9	6.28	116.94	113.80
1	RA	530	G	N1-C6-O6	-6.28	116.13	119.90
1	RA	1788	C	C6-N1-C2	-6.28	117.79	120.30
1	YA	976	C	C5-C6-N1	6.28	124.14	121.00
1	YA	1404	C	C5-C6-N1	6.28	124.14	121.00
1	YA	1598	C	N1-C2-O2	6.28	122.67	118.90
1	RA	755	C	C5-C6-N1	6.28	124.14	121.00
1	RA	2666	C	N1-C2-O2	6.28	122.67	118.90
32	XA	1260	C	C6-N1-C2	-6.28	117.79	120.30
32	XA	1395	C	C6-N1-C2	-6.28	117.79	120.30
1	RA	12	U	N3-C2-O2	-6.28	117.81	122.20
1	RA	1468	C	C6-N1-C2	-6.28	117.79	120.30
1	YA	2739	U	N1-C2-O2	6.28	127.19	122.80
1	YA	2667	C	C6-N1-C2	-6.27	117.79	120.30
1	YA	484	C	C6-N1-C2	-6.27	117.79	120.30
32	XA	135	C	N3-C2-O2	-6.27	117.51	121.90
1	RA	2439	A	N7-C8-N9	6.27	116.93	113.80
1	YA	1836	C	N1-C2-O2	6.27	122.66	118.90
1	RA	2043	C	N1-C2-O2	6.26	122.66	118.90
32	QA	1395	C	C5-C6-N1	6.26	124.13	121.00
2	RB	44	G	C4-N9-C1'	-6.26	118.36	126.50
1	YA	2785	C	C6-N1-C2	-6.26	117.80	120.30
32	QA	435	C	C5-C6-N1	6.26	124.13	121.00
1	RA	2395	C	C5-C6-N1	6.26	124.13	121.00
32	QA	54	C	C6-N1-C2	-6.26	117.80	120.30
32	QA	789	U	C2-N1-C1'	6.26	125.21	117.70
11	RP	59	LEU	CA-CB-CG	6.25	129.68	115.30
1	YA	67	U	C5-C6-N1	6.25	125.83	122.70
1	YA	1533	C	C5-C6-N1	6.25	124.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1833	U	N3-C2-O2	-6.25	117.82	122.20
1	RA	965	C	C6-N1-C2	-6.25	117.80	120.30
1	RA	1406	U	N1-C2-O2	6.25	127.17	122.80
1	YA	1779	U	C2-N1-C1'	6.25	125.20	117.70
1	YA	595	C	C5-C6-N1	6.25	124.12	121.00
1	RA	2814	C	N1-C2-O2	6.25	122.65	118.90
1	RA	1257	C	C6-N1-C2	-6.24	117.81	120.30
32	XA	826	C	C6-N1-C2	-6.24	117.81	120.30
1	YA	2039	C	C5-C6-N1	6.23	124.12	121.00
1	YA	1899	G	N1-C2-N2	-6.23	110.59	116.20
1	RA	915	C	C6-N1-C2	-6.23	117.81	120.30
1	YA	591	C	C6-N1-C2	-6.23	117.81	120.30
32	XA	458	C	C6-N1-C2	-6.23	117.81	120.30
1	YA	802	A	N1-C6-N6	6.23	122.34	118.60
1	RA	1306	C	C6-N1-C2	-6.22	117.81	120.30
1	YA	2856	C	C5-C6-N1	6.22	124.11	121.00
1	YA	580	C	C6-N1-C2	-6.21	117.81	120.30
1	YA	2407	G	C6-C5-N7	-6.21	126.67	130.40
32	QA	1158	C	C6-N1-C1'	-6.21	113.34	120.80
32	QA	1536	C	N1-C2-O2	6.21	122.63	118.90
32	QA	252	U	N3-C2-O2	-6.21	117.85	122.20
1	YA	1894	C	C6-N1-C2	-6.21	117.82	120.30
2	RB	60	C	C6-N1-C2	-6.21	117.82	120.30
1	RA	1092	C	C6-N1-C2	-6.21	117.82	120.30
1	YA	944	G	C4-N9-C1'	6.21	134.57	126.50
1	RA	2584	U	C6-N1-C1'	-6.20	112.52	121.20
1	YA	691	C	C5-C6-N1	6.20	124.10	121.00
32	XA	1362(A)	C	N3-C2-O2	-6.20	117.56	121.90
32	XA	932	C	C6-N1-C2	-6.19	117.82	120.30
1	RA	595	C	C6-N1-C2	-6.19	117.82	120.30
2	YB	70	C	C5-C6-N1	6.19	124.09	121.00
1	YA	537	C	C2-N1-C1'	6.18	125.60	118.80
1	YA	1958	C	C6-N1-C2	-6.18	117.83	120.30
32	XA	497	U	N3-C2-O2	-6.18	117.87	122.20
1	RA	2688	U	N1-C2-O2	6.18	127.13	122.80
1	RA	420	C	C6-N1-C2	-6.18	117.83	120.30
1	YA	1166	C	N1-C2-O2	6.18	122.61	118.90
32	QA	623	C	C6-N1-C2	-6.18	117.83	120.30
1	RA	1406	U	N3-C2-O2	-6.17	117.88	122.20
1	YA	1804	C	C6-N1-C2	-6.17	117.83	120.30
1	YA	1314	C	C2-N1-C1'	6.17	125.59	118.80
1	YA	1678	G	C5-N7-C8	-6.17	101.22	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1691	C	C5-C6-N1	6.17	124.08	121.00
32	XA	449	C	N1-C2-O2	6.17	122.60	118.90
1	RA	343	C	C5-C6-N1	6.17	124.08	121.00
1	YA	877	U	N3-C2-O2	-6.17	117.89	122.20
1	YA	795	C	C5-C6-N1	6.16	124.08	121.00
1	YA	1644	C	C6-N1-C2	-6.16	117.84	120.30
45	XN	44	LEU	CA-CB-CG	6.16	129.46	115.30
1	RA	1505	C	C6-N1-C2	-6.15	117.84	120.30
32	QA	525	C	C6-N1-C2	-6.15	117.84	120.30
1	YA	1781	C	N3-C2-O2	-6.15	117.59	121.90
1	YA	2308	G	N3-C4-N9	6.15	129.69	126.00
1	RA	2205	C	C5-C6-N1	6.15	124.07	121.00
1	YA	2041	U	C5-C6-N1	6.15	125.77	122.70
2	RB	30	C	N1-C2-O2	6.15	122.59	118.90
1	YA	2584	U	C6-N1-C1'	-6.15	112.60	121.20
1	YA	2655	G	C8-N9-C1'	6.15	134.99	127.00
1	RA	1899	G	N3-C4-N9	6.14	129.69	126.00
1	YA	104	U	N3-C2-O2	-6.14	117.90	122.20
1	YA	140	A	N7-C8-N9	6.14	116.87	113.80
32	QA	1395	C	C6-N1-C2	-6.14	117.84	120.30
1	YA	964	C	C6-N1-C2	-6.14	117.84	120.30
32	QA	266	G	C4-C5-N7	6.14	113.25	110.80
1	YA	992	C	C6-N1-C2	-6.14	117.84	120.30
1	RA	1833	U	N3-C2-O2	-6.14	117.90	122.20
1	YA	141	A	C8-N9-C4	-6.14	103.35	105.80
1	YA	2008	C	C5-C6-N1	6.14	124.07	121.00
1	RA	1352	U	N3-C2-O2	-6.13	117.91	122.20
2	RB	30	C	N3-C2-O2	-6.13	117.61	121.90
1	YA	766	C	C6-N1-C2	-6.13	117.85	120.30
1	YA	1496	A	C8-N9-C4	-6.13	103.35	105.80
1	RA	1513	C	N1-C2-O2	6.12	122.58	118.90
1	RA	1333	C	C5-C6-N1	6.12	124.06	121.00
32	XA	528	C	C6-N1-C2	-6.12	117.85	120.30
1	YA	409	C	C6-N1-C2	-6.12	117.85	120.30
1	YA	2065	C	C5-C6-N1	6.12	124.06	121.00
32	XA	555	C	C6-N1-C2	-6.12	117.85	120.30
1	RA	1899	G	N3-C4-C5	-6.12	125.54	128.60
1	RA	1332	G	C4-C5-N7	6.11	113.25	110.80
1	YA	461	C	C6-N1-C2	-6.11	117.86	120.30
1	YA	838	C	C5-C6-N1	6.11	124.05	121.00
1	YA	806	C	C6-N1-C2	-6.11	117.86	120.30
1	YA	2335	A	O4'-C1'-N9	6.11	113.08	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	503	C	C6-N1-C2	-6.11	117.86	120.30
32	QA	1301	U	C5-C6-N1	6.10	125.75	122.70
1	YA	1947	C	C6-N1-C2	-6.10	117.86	120.30
1	YA	2456	C	C5-C6-N1	6.10	124.05	121.00
32	XA	1420	C	C6-N1-C2	-6.10	117.86	120.30
2	RB	27	C	N3-C2-O2	-6.10	117.63	121.90
32	XA	1158	C	N3-C2-O2	-6.10	117.63	121.90
1	YA	243	U	N1-C2-O2	6.10	127.07	122.80
1	RA	1683	C	C5-C6-N1	6.09	124.05	121.00
1	YA	1549	C	C6-N1-C2	-6.09	117.86	120.30
1	YA	1549	C	C5-C6-N1	6.09	124.04	121.00
1	YA	1433	U	C5-C6-N1	6.08	125.74	122.70
1	RA	1432	C	C5-C6-N1	6.08	124.04	121.00
32	XA	1228	C	N1-C2-O2	6.08	122.55	118.90
32	XA	1420	C	C5-C6-N1	6.08	124.04	121.00
2	YB	68	C	C6-N1-C2	-6.08	117.87	120.30
32	XA	1383	C	N1-C2-O2	6.08	122.55	118.90
32	QA	960	U	N3-C2-O2	-6.08	117.95	122.20
1	YA	1314	C	N1-C2-O2	6.08	122.55	118.90
1	YA	2308	G	N3-C4-C5	-6.08	125.56	128.60
1	YA	2416	C	C6-N1-C2	-6.08	117.87	120.30
1	RA	1332	G	C5-N7-C8	-6.07	101.26	104.30
1	RA	1686	C	C6-N1-C2	-6.07	117.87	120.30
32	QA	690	G	O4'-C1'-N9	6.07	113.06	108.20
1	YA	2465	C	C5-C6-N1	6.07	124.04	121.00
1	RA	786	C	C5-C6-N1	6.07	124.03	121.00
1	RA	1619	G	C4-C5-N7	6.07	113.23	110.80
1	YA	1619	G	C4-C5-N7	6.07	113.23	110.80
1	YA	2576	G	C4-N9-C1'	6.07	134.39	126.50
2	YB	28	C	C5-C6-N1	6.07	124.03	121.00
1	YA	857	C	C6-N1-C2	-6.07	117.87	120.30
1	YA	1640	C	C5-C6-N1	6.07	124.03	121.00
1	YA	1544	C	N1-C2-O2	6.06	122.54	118.90
1	YA	825	C	C6-N1-C2	-6.06	117.88	120.30
32	XA	1439	C	C2-N1-C1'	6.06	125.47	118.80
1	YA	66	C	C5-C6-N1	6.06	124.03	121.00
1	RA	634	C	C5-C6-N1	6.06	124.03	121.00
1	YA	840	C	C5-C6-N1	6.06	124.03	121.00
1	RA	2739	U	N3-C2-O2	-6.06	117.96	122.20
1	YA	837	C	N1-C2-O2	6.06	122.53	118.90
1	YA	1599	C	C5-C6-N1	6.06	124.03	121.00
1	RA	1332	G	C4-N9-C1'	6.05	134.37	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	174	C	C5-C6-N1	6.05	124.03	121.00
1	YA	1830	C	N1-C2-O2	6.05	122.53	118.90
1	RA	1598	C	C6-N1-C2	-6.05	117.88	120.30
32	QA	497	U	N3-C2-O2	-6.05	117.97	122.20
32	QA	1028(A)	C	C6-N1-C2	-6.04	117.88	120.30
1	YA	2463	C	C5-C6-N1	6.04	124.02	121.00
2	RB	37	C	N1-C2-O2	6.04	122.53	118.90
1	RA	2295	C	C6-N1-C2	-6.04	117.88	120.30
1	YA	2794	C	N1-C2-O2	6.04	122.52	118.90
1	RA	1462	C	N3-C2-O2	-6.03	117.68	121.90
32	QA	1158	C	C5-C6-N1	6.03	124.02	121.00
1	YA	435	C	C6-N1-C2	-6.03	117.89	120.30
1	YA	535	C	C6-N1-C2	-6.03	117.89	120.30
1	YA	1398	C	C5-C6-N1	6.03	124.01	121.00
1	RA	1504	C	C6-N1-C2	-6.03	117.89	120.30
1	YA	1432	C	C5-C6-N1	6.03	124.01	121.00
1	YA	2044	C	C6-N1-C2	-6.03	117.89	120.30
1	RA	2089	U	C5-C6-N1	6.02	125.71	122.70
1	YA	945	A	O4'-C1'-N9	6.02	113.02	108.20
1	RA	1640	C	C6-N1-C2	-6.02	117.89	120.30
1	YA	1021	A	N3-C4-N9	-6.02	122.59	127.40
32	QA	1038	C	N3-C2-O2	-6.01	117.69	121.90
1	RA	923	C	C6-N1-C2	-6.01	117.90	120.30
1	RA	1691	C	C6-N1-C2	-6.01	117.90	120.30
32	QA	690	G	C4-N9-C1'	6.01	134.31	126.50
32	XA	891	U	N3-C2-O2	-6.01	117.99	122.20
32	QA	556	C	C5-C6-N1	6.01	124.00	121.00
32	QA	330	C	N3-C2-O2	-6.01	117.70	121.90
1	YA	1644	C	N3-C2-O2	-6.01	117.70	121.90
32	XA	18	C	C5-C6-N1	6.01	124.00	121.00
1	RA	461	C	C6-N1-C2	-6.00	117.90	120.30
1	YA	621	A	C5-N7-C8	-6.00	100.90	103.90
32	XA	1362	C	C6-N1-C2	-6.00	117.90	120.30
1	RA	672	C	C6-N1-C2	-6.00	117.90	120.30
1	YA	2205	C	C5-C6-N1	6.00	124.00	121.00
2	YB	37	C	C6-N1-C2	-6.00	117.90	120.30
1	YA	1836	C	C5-C6-N1	6.00	124.00	121.00
1	YA	2874	C	C6-N1-C2	-6.00	117.90	120.30
32	XA	1260	C	N1-C2-O2	6.00	122.50	118.90
1	RA	1159	U	N1-C2-O2	6.00	127.00	122.80
1	RA	1208	C	C6-N1-C2	-6.00	117.90	120.30
1	RA	1506	C	N1-C2-O2	6.00	122.50	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	1279	A	C8-N9-C4	-6.00	103.40	105.80
53	QV	32	U	N1-C2-O2	5.99	127.00	122.80
1	RA	1658	C	C5-C6-N1	5.99	124.00	121.00
2	YB	95	U	C6-N1-C2	-5.99	117.41	121.00
1	YA	1686	C	N1-C2-O2	5.99	122.49	118.90
32	QA	514	C	C5-C6-N1	5.99	123.99	121.00
1	YA	736	C	C5-C6-N1	5.99	123.99	121.00
1	YA	817	C	C6-N1-C2	-5.99	117.91	120.30
32	XA	54	C	C6-N1-C2	-5.98	117.91	120.30
1	YA	2558	C	C5-C6-N1	5.98	123.99	121.00
1	YA	828	U	N3-C2-O2	-5.98	118.01	122.20
1	RA	624	C	C6-N1-C2	-5.98	117.91	120.30
1	RA	1417	C	C5-C6-N1	5.98	123.99	121.00
2	YB	44	G	C8-N9-C1'	5.98	134.77	127.00
32	XA	110	C	N3-C2-O2	-5.98	117.72	121.90
2	RB	44	G	C8-N9-C1'	5.97	134.77	127.00
1	YA	2419	U	C5-C6-N1	5.97	125.69	122.70
1	YA	2281	C	C5-C6-N1	5.97	123.99	121.00
1	YA	2073	C	C6-N1-C2	-5.97	117.91	120.30
1	RA	1830	C	N1-C2-O2	5.97	122.48	118.90
1	YA	12	U	C6-N1-C2	-5.97	117.42	121.00
1	YA	335	C	C5-C6-N1	5.97	123.98	121.00
1	RA	1294	U	N3-C2-O2	-5.96	118.03	122.20
2	RB	37	C	N3-C2-O2	-5.96	117.72	121.90
1	YA	1221	C	C6-N1-C2	-5.96	117.91	120.30
1	YA	2683	C	C6-N1-C2	-5.96	117.92	120.30
2	YB	77	U	N1-C2-O2	5.96	126.97	122.80
1	YA	413	C	C5-C6-N1	5.96	123.98	121.00
1	YA	912	C	C6-N1-C2	-5.96	117.92	120.30
32	XA	891	U	N1-C2-O2	5.96	126.97	122.80
1	YA	231	C	N1-C2-O2	5.96	122.47	118.90
1	YA	2682	U	N1-C2-O2	5.96	126.97	122.80
1	RA	736	C	C5-C6-N1	5.95	123.98	121.00
32	XA	1301	U	N1-C2-O2	5.95	126.97	122.80
32	QA	1097	C	C6-N1-C2	-5.95	117.92	120.30
1	RA	837	C	C5-C6-N1	5.95	123.97	121.00
1	RA	1396	U	C2-N1-C1'	5.95	124.84	117.70
1	YA	1188	U	N1-C2-O2	5.95	126.96	122.80
32	XA	1290	G	N3-C4-N9	5.95	129.57	126.00
1	RA	1463	C	C6-N1-C2	-5.94	117.92	120.30
1	RA	2295	C	C5-C6-N1	5.94	123.97	121.00
1	YA	1879	C	C6-N1-C2	-5.94	117.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	1414	U	N3-C2-O2	-5.94	118.04	122.20
1	YA	139	G	N9-C4-C5	5.94	107.78	105.40
1	YA	1549	C	N1-C2-O2	5.94	122.46	118.90
50	XS	5	LEU	CA-CB-CG	5.94	128.96	115.30
1	YA	2295	C	C5-C6-N1	5.94	123.97	121.00
32	QA	674	G	C5-N7-C8	-5.94	101.33	104.30
1	RA	2006	C	C6-N1-C2	-5.93	117.93	120.30
32	QA	1381	U	N3-C2-O2	-5.93	118.05	122.20
32	XA	797	C	C5-C6-N1	5.93	123.97	121.00
1	YA	683	C	N1-C2-O2	5.93	122.46	118.90
1	YA	755	C	C6-N1-C2	-5.93	117.93	120.30
32	XA	1290	G	N3-C4-C5	-5.93	125.64	128.60
1	RA	1063	G	N3-C4-C5	-5.92	125.64	128.60
32	XA	1109	C	C6-N1-C2	-5.92	117.93	120.30
1	RA	1882	C	N1-C2-O2	5.92	122.45	118.90
1	YA	2506	U	C5-C6-N1	5.91	125.66	122.70
1	YA	2894	G	N3-C2-N2	-5.91	115.76	119.90
32	XA	449	C	N3-C2-O2	-5.91	117.76	121.90
1	RA	1267	U	N3-C2-O2	-5.91	118.06	122.20
54	QX	17	C	N1-C2-O2	5.91	122.45	118.90
1	RA	580	C	C6-N1-C2	-5.91	117.94	120.30
1	RA	1992	G	P-O3'-C3'	5.91	126.79	119.70
1	RA	2321	G	C4-N9-C1'	5.91	134.18	126.50
1	RA	589	C	C6-N1-C2	-5.91	117.94	120.30
1	RA	923	C	C5-C6-N1	5.91	123.95	121.00
1	YA	856	C	N3-C4-N4	5.91	122.13	118.00
32	XA	679	C	C5-C6-N1	5.91	123.95	121.00
1	YA	2295	C	C6-N1-C2	-5.90	117.94	120.30
1	YA	2688	U	N1-C2-N3	5.90	118.44	114.90
32	QA	1362(A)	C	N3-C2-O2	-5.90	117.77	121.90
1	YA	955	C	C6-N1-C2	-5.90	117.94	120.30
1	RA	420	C	C5-C6-N1	5.89	123.95	121.00
1	RA	1323	U	C5-C6-N1	5.89	125.65	122.70
1	RA	1742	C	C6-N1-C2	-5.89	117.94	120.30
1	YA	120	U	C2-N1-C1'	5.89	124.77	117.70
1	YA	2874	C	C5-C6-N1	5.89	123.94	121.00
1	RA	285	C	N1-C2-O2	5.89	122.43	118.90
1	RA	1257	C	C5-C6-N1	5.89	123.94	121.00
1	YA	2586	C	C6-N1-C2	-5.89	117.94	120.30
1	YA	1961	C	N3-C2-O2	-5.89	117.78	121.90
32	QA	1260	C	C6-N1-C2	-5.88	117.95	120.30
1	YA	837	C	N3-C2-O2	-5.88	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1604	C	C5-C6-N1	5.88	123.94	121.00
1	YA	1788	C	N1-C2-O2	5.88	122.43	118.90
1	RA	985	C	N1-C2-O2	5.88	122.43	118.90
1	RA	1097	U	C5-C6-N1	5.88	125.64	122.70
53	QV	32	U	N3-C2-O2	-5.88	118.09	122.20
1	YA	2889	C	N1-C2-O2	5.87	122.42	118.90
32	QA	1452	C	N3-C2-O2	-5.87	117.79	121.90
1	YA	1528	A	O4'-C1'-N9	5.87	112.89	108.20
1	YA	2463	C	C6-N1-C2	-5.87	117.95	120.30
1	YA	560	C	C6-N1-C2	-5.86	117.95	120.30
1	RA	856	C	N1-C2-O2	5.86	122.42	118.90
32	QA	435	C	N1-C2-O2	5.86	122.42	118.90
2	RB	79	C	C6-N1-C2	-5.86	117.96	120.30
1	RA	1462	C	N1-C2-O2	5.86	122.41	118.90
1	YA	2591	C	C6-N1-C2	-5.86	117.96	120.30
1	RA	1314	C	N1-C2-O2	5.86	122.41	118.90
32	QA	618	C	C6-N1-C2	-5.86	117.96	120.30
1	RA	1752	C	C6-N1-C2	-5.85	117.96	120.30
1	RA	2576	G	C8-N9-C1'	-5.85	119.39	127.00
32	QA	1118	C	N3-C2-O2	-5.85	117.80	121.90
1	RA	1983	C	C5-C6-N1	5.85	123.92	121.00
1	YA	1375	C	C6-N1-C2	-5.85	117.96	120.30
1	YA	2474	C	N3-C2-O2	-5.85	117.81	121.90
32	XA	410	G	C8-N9-C4	-5.85	104.06	106.40
1	RA	155	C	N1-C2-O2	5.85	122.41	118.90
1	RA	1988	C	C5-C6-N1	5.85	123.92	121.00
32	XA	390	C	C6-N1-C2	-5.85	117.96	120.30
32	XA	780	A	C8-N9-C4	-5.85	103.46	105.80
32	XA	1037	C	N3-C2-O2	-5.85	117.81	121.90
32	QA	697	U	N3-C2-O2	-5.85	118.11	122.20
1	YA	2248	C	N1-C2-O2	5.85	122.41	118.90
1	RA	364	C	C5-C6-N1	5.84	123.92	121.00
1	RA	976	C	C5-C6-N1	5.84	123.92	121.00
2	RB	91	C	C6-N1-C2	-5.84	117.96	120.30
15	RT	105	LEU	CA-CB-CG	5.84	128.74	115.30
1	YA	1914	C	C2-N1-C1'	5.84	125.23	118.80
33	QB	215	LEU	CA-CB-CG	5.84	128.73	115.30
32	QA	479	C	N1-C2-O2	5.84	122.40	118.90
1	RA	1742	C	C5-C6-N1	5.84	123.92	121.00
1	YA	1390	U	N1-C2-O2	5.84	126.89	122.80
1	YA	2043	C	N1-C2-O2	5.83	122.40	118.90
32	QA	1045	C	N1-C2-O2	5.83	122.40	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	485	C	C6-N1-C2	-5.83	117.97	120.30
1	YA	1931	U	N3-C2-O2	-5.83	118.12	122.20
1	RA	2066	C	N1-C2-O2	5.83	122.40	118.90
32	QA	1260	C	N1-C2-O2	5.83	122.40	118.90
1	YA	1805	U	N3-C2-O2	-5.83	118.12	122.20
1	YA	2579	C	C5-C6-N1	5.83	123.92	121.00
1	YA	1899	G	N3-C2-N2	5.83	123.98	119.90
1	YA	2179	C	C6-N1-C2	-5.83	117.97	120.30
1	YA	1406	U	N1-C2-O2	5.82	126.88	122.80
1	RA	517	C	C5-C6-N1	5.82	123.91	121.00
1	RA	676	A	O4'-C1'-N9	5.82	112.85	108.20
1	RA	1892	C	C5-C6-N1	5.82	123.91	121.00
32	QA	528	C	N1-C2-O2	5.82	122.39	118.90
32	QA	812	C	P-O3'-C3'	5.82	126.68	119.70
32	XA	341	C	C5-C6-N1	5.82	123.91	121.00
1	YA	2825	C	N3-C2-O2	-5.81	117.83	121.90
1	YA	1076	C	C6-N1-C2	-5.81	117.98	120.30
1	YA	850	C	C5-C6-N1	5.81	123.90	121.00
1	YA	1218	C	C6-N1-C2	-5.81	117.98	120.30
1	YA	242	G	P-O3'-C3'	5.80	126.66	119.70
1	RA	234	C	N3-C2-O2	-5.80	117.84	121.90
2	YB	68	C	C5-C6-N1	5.80	123.90	121.00
1	YA	2827	C	C6-N1-C2	-5.80	117.98	120.30
1	RA	1658	C	C6-N1-C2	-5.80	117.98	120.30
1	YA	484	C	C5-C6-N1	5.80	123.90	121.00
1	RA	192	C	N3-C2-O2	-5.80	117.84	121.90
1	RA	1052	C	N3-C2-O2	-5.80	117.84	121.90
1	YA	435	C	N3-C2-O2	-5.80	117.84	121.90
1	YA	877	U	C5-C6-N1	5.80	125.60	122.70
1	YA	1333	C	C6-N1-C2	-5.80	117.98	120.30
1	YA	2746	U	C5-C6-N1	5.79	125.60	122.70
1	YA	1893	C	C6-N1-C2	-5.79	117.98	120.30
1	YA	2794	C	C5-C6-N1	5.79	123.90	121.00
1	RA	456	C	C6-N1-C2	-5.79	117.98	120.30
1	RA	1779	U	C6-N1-C1'	-5.79	113.10	121.20
1	YA	2701	C	C5-C6-N1	5.79	123.89	121.00
1	YA	2704	C	N1-C2-O2	5.78	122.37	118.90
53	XV	39	C	C6-N1-C2	-5.78	117.99	120.30
1	YA	2064	C	C6-N1-C2	-5.78	117.99	120.30
1	YA	2785	C	C5-C6-N1	5.78	123.89	121.00
1	YA	2888	C	C6-N1-C2	-5.78	117.99	120.30
1	RA	1505	C	N1-C2-O2	5.78	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2683	C	N1-C2-O2	5.77	122.36	118.90
1	YA	2683	C	N3-C2-O2	-5.77	117.86	121.90
1	YA	2512	C	C6-N1-C2	-5.77	117.99	120.30
1	RA	1599	C	C5-C6-N1	5.77	123.89	121.00
32	QA	1336	C	C6-N1-C2	-5.77	117.99	120.30
1	YA	2471	C	C5-C6-N1	5.77	123.89	121.00
1	RA	2507	C	C6-N1-C2	-5.77	117.99	120.30
32	QA	314	C	C5-C6-N1	5.77	123.88	121.00
32	QA	736	C	C6-N1-C2	-5.77	117.99	120.30
1	YA	930	U	N1-C2-O2	5.77	126.84	122.80
1	YA	2473	U	N3-C2-O2	-5.76	118.17	122.20
1	YA	2611	U	C5-C6-N1	5.76	125.58	122.70
1	RA	1535	U	N3-C2-O2	-5.76	118.17	122.20
1	YA	2586	C	C5-C6-N1	5.76	123.88	121.00
1	RA	676	A	C8-N9-C4	-5.76	103.50	105.80
1	YA	161	U	N3-C2-O2	-5.76	118.17	122.20
32	XA	979	C	C6-N1-C2	-5.76	118.00	120.30
32	XA	1395	C	C5-C6-N1	5.76	123.88	121.00
1	YA	676	A	C8-N9-C4	-5.76	103.50	105.80
1	YA	1934	C	C5-C6-N1	5.76	123.88	121.00
1	RA	898	C	C6-N1-C2	-5.76	118.00	120.30
32	QA	932	C	C6-N1-C2	-5.76	118.00	120.30
1	YA	1882	C	N1-C2-O2	5.76	122.35	118.90
1	YA	105	C	C5-C6-N1	5.75	123.88	121.00
1	YA	1332	G	C8-N9-C4	-5.75	104.10	106.40
1	YA	2226	C	N1-C2-O2	5.75	122.35	118.90
1	RA	621	A	C5-N7-C8	-5.75	101.03	103.90
1	RA	198	C	C6-N1-C2	-5.75	118.00	120.30
1	RA	1915	U	N3-C2-O2	-5.74	118.18	122.20
1	YA	2686	G	N3-C4-N9	5.74	129.44	126.00
1	RA	364	C	N1-C2-O2	5.74	122.34	118.90
32	QA	369	C	C6-N1-C2	-5.74	118.00	120.30
32	XA	779	C	N1-C2-O2	5.74	122.34	118.90
1	RA	1100	C	C6-N1-C2	-5.74	118.00	120.30
1	YA	2248	C	N3-C2-O2	-5.74	117.88	121.90
1	YA	512	G	O4'-C1'-N9	5.74	112.79	108.20
32	XA	1028(A)	C	C6-N1-C2	-5.74	118.01	120.30
1	RA	1656	C	C6-N1-C2	-5.73	118.01	120.30
32	XA	1113	C	C5-C6-N1	5.73	123.87	121.00
1	RA	1295	C	C6-N1-C2	-5.73	118.01	120.30
1	RA	2703	C	N1-C2-O2	5.73	122.34	118.90
1	RA	2682	U	N3-C2-O2	-5.73	118.19	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	RB	31	C	C6-N1-C2	-5.73	118.01	120.30
1	RA	183	C	C6-N1-C2	-5.73	118.01	120.30
1	YA	877	U	N1-C2-O2	5.72	126.81	122.80
1	YA	1679	U	N3-C2-O2	-5.72	118.19	122.20
1	RA	2591	C	C5-C6-N1	5.72	123.86	121.00
1	RA	1304	C	C6-N1-C2	-5.72	118.01	120.30
1	RA	104	U	N1-C2-O2	5.72	126.80	122.80
32	QA	827	U	N1-C2-N3	5.72	118.33	114.90
32	QA	1019	C	C6-N1-C2	-5.72	118.01	120.30
1	YA	925	C	C5-C6-N1	5.72	123.86	121.00
1	YA	1264	G	C8-N9-C4	-5.72	104.11	106.40
32	XA	1038	C	C5-C6-N1	5.72	123.86	121.00
1	RA	1103	A	N7-C8-N9	5.71	116.66	113.80
1	YA	1180	C	N1-C2-O2	5.71	122.33	118.90
1	YA	963	U	C5-C6-N1	5.71	125.56	122.70
1	YA	1658	C	C6-N1-C2	-5.71	118.02	120.30
1	YA	2297	C	C6-N1-C2	-5.71	118.02	120.30
2	YB	80	U	N3-C2-O2	-5.71	118.20	122.20
1	YA	2885	C	C6-N1-C2	-5.71	118.02	120.30
1	RA	2210	G	N3-C4-C5	-5.71	125.75	128.60
53	XV	39	C	C5-C6-N1	5.71	123.85	121.00
1	RA	155	C	C5-C6-N1	5.71	123.85	121.00
32	QA	365	U	C2-N1-C1'	5.70	124.54	117.70
1	YA	1474	C	C6-N1-C2	-5.70	118.02	120.30
32	XA	221	C	C6-N1-C2	-5.70	118.02	120.30
1	RA	912	C	C5-C6-N1	5.70	123.85	121.00
32	XA	1502	A	N7-C8-N9	5.70	116.65	113.80
1	RA	2815	C	C6-N1-C2	-5.70	118.02	120.30
32	QA	1452	C	N1-C2-O2	5.70	122.32	118.90
1	RA	1844	C	C5-C6-N1	5.70	123.85	121.00
1	YA	877	U	C6-N1-C2	-5.70	117.58	121.00
1	YA	1390	U	N3-C2-O2	-5.70	118.21	122.20
1	YA	1463	C	C5-C6-N1	5.70	123.85	121.00
1	YA	2179	C	N1-C2-O2	5.70	122.32	118.90
1	YA	2424	C	C5-C4-N4	-5.70	116.21	120.20
1	YA	2558	C	C6-N1-C2	-5.70	118.02	120.30
32	XA	1109	C	N3-C2-O2	-5.70	117.91	121.90
32	XA	1228	C	N3-C2-O2	-5.70	117.91	121.90
2	YB	38	C	C6-N1-C2	-5.69	118.02	120.30
32	QA	514	C	C6-N1-C2	-5.69	118.02	120.30
1	RA	2137	C	C5-C6-N1	5.69	123.85	121.00
40	QI	85	LEU	CA-CB-CG	5.69	128.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	814	C	C6-N1-C2	-5.69	118.02	120.30
1	RA	2226	C	C6-N1-C2	-5.69	118.03	120.30
1	YA	1992	G	P-O3'-C3'	5.69	126.52	119.70
1	RA	114	U	C5-C6-N1	5.68	125.54	122.70
1	YA	1619	G	C6-C5-N7	-5.68	126.99	130.40
1	RA	1187	G	C8-N9-C4	-5.68	104.13	106.40
1	YA	2712	U	P-O3'-C3'	5.68	126.52	119.70
1	RA	1504	C	N3-C2-O2	-5.68	117.92	121.90
1	RA	806	C	C5-C6-N1	5.68	123.84	121.00
1	RA	1417	C	C6-N1-C2	-5.68	118.03	120.30
1	YA	1544	C	C2-N1-C1'	5.68	125.04	118.80
1	RA	2211	G	N3-C4-N9	5.67	129.40	126.00
32	XA	686	U	N3-C2-O2	-5.67	118.23	122.20
1	YA	658	C	C6-N1-C2	-5.67	118.03	120.30
1	YA	1793	C	C5-C6-N1	5.67	123.83	121.00
1	YA	2047	U	C5-C6-N1	5.67	125.53	122.70
32	XA	169	C	C6-N1-C2	-5.67	118.03	120.30
1	RA	1961	C	N3-C2-O2	-5.66	117.94	121.90
1	RA	2825	C	N3-C2-O2	-5.66	117.94	121.90
1	YA	2210	G	N3-C4-N9	5.66	129.40	126.00
1	RA	1934	C	N1-C2-O2	5.66	122.30	118.90
1	YA	2847	U	C5-C6-N1	5.66	125.53	122.70
1	YA	413	C	C6-N1-C2	-5.66	118.04	120.30
32	QA	1395	C	N1-C2-O2	5.66	122.29	118.90
1	YA	1533	C	N1-C2-O2	5.66	122.29	118.90
32	XA	764	C	C5-C6-N1	5.66	123.83	121.00
1	YA	828	U	C5-C6-N1	5.65	125.53	122.70
1	YA	1332	G	C4-C5-N7	5.65	113.06	110.80
1	YA	2307	G	C8-N9-C1'	-5.65	119.65	127.00
32	QA	779	C	N1-C2-O2	5.65	122.29	118.90
32	XA	1381	U	N1-C2-O2	5.65	126.76	122.80
1	RA	904	C	N1-C2-O2	5.65	122.29	118.90
1	YA	2756	U	C5-C4-O4	-5.65	122.51	125.90
32	XA	178	C	C6-N1-C2	-5.65	118.04	120.30
1	RA	106	C	C6-N1-C2	-5.64	118.04	120.30
32	QA	1403	C	C6-N1-C2	-5.64	118.04	120.30
1	RA	1836	C	C5-C6-N1	5.64	123.82	121.00
1	YA	923	C	C5-C6-N1	5.64	123.82	121.00
1	YA	1404	C	N1-C2-O2	5.64	122.28	118.90
1	RA	2320	A	C2-N3-C4	5.64	113.42	110.60
1	YA	209	C	C5-C6-N1	5.64	123.82	121.00
1	YA	231	C	C6-N1-C2	-5.64	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	QM	19	LEU	CA-CB-CG	5.64	128.26	115.30
2	YB	77	U	N3-C2-O2	-5.64	118.25	122.20
1	RA	2064	C	C6-N1-C2	-5.63	118.05	120.30
1	YA	607	U	N3-C2-O2	-5.63	118.26	122.20
1	YA	1157	G	N1-C6-O6	5.63	123.28	119.90
32	XA	779	C	N3-C2-O2	-5.63	117.96	121.90
1	RA	529	A	N7-C8-N9	5.63	116.62	113.80
1	YA	2692	C	N1-C2-O2	5.63	122.28	118.90
1	YA	1105	U	N3-C2-O2	-5.63	118.26	122.20
1	RA	766	C	C6-N1-C2	-5.63	118.05	120.30
1	YA	1158	C	C6-N1-C2	-5.63	118.05	120.30
1	RA	898	C	N3-C2-O2	-5.63	117.96	121.90
1	RA	2712	U	C2-N1-C1'	5.63	124.45	117.70
1	YA	1656	C	C5-C6-N1	5.63	123.81	121.00
32	XA	896	C	C5-C6-N1	5.62	123.81	121.00
1	RA	797	C	C6-N1-C2	-5.62	118.05	120.30
32	QA	980	C	N1-C2-O2	5.62	122.27	118.90
1	YA	2574	G	C4-C5-N7	5.62	113.05	110.80
32	XA	341	C	N1-C2-O2	5.62	122.27	118.90
1	RA	2006	C	N1-C2-O2	5.62	122.27	118.90
32	QA	1071	C	C6-N1-C2	-5.62	118.05	120.30
1	RA	1881	C	C5-C6-N1	5.62	123.81	121.00
32	XA	1038	C	C6-N1-C2	-5.61	118.06	120.30
1	RA	1233	C	C6-N1-C2	-5.61	118.06	120.30
32	XA	690	G	C8-N9-C1'	-5.61	119.70	127.00
32	QA	169	C	N3-C2-O2	-5.61	117.97	121.90
1	RA	2096	U	N3-C2-O2	-5.60	118.28	122.20
1	YA	944	G	C8-N9-C1'	-5.60	119.72	127.00
1	YA	1258	C	C5-C6-N1	5.60	123.80	121.00
1	YA	1528	A	C5-N7-C8	-5.60	101.10	103.90
32	QA	528	C	C6-N1-C2	-5.60	118.06	120.30
32	XA	620	C	N1-C2-O2	5.60	122.26	118.90
27	Y5	6	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	RA	1611	C	C6-N1-C2	-5.60	118.06	120.30
2	YB	43	C	C6-N1-C2	-5.60	118.06	120.30
32	QA	943	U	N3-C2-O2	-5.60	118.28	122.20
2	YB	37	C	N1-C2-O2	5.60	122.26	118.90
32	XA	897	C	C6-N1-C2	-5.60	118.06	120.30
1	RA	650	C	C5-C6-N1	5.59	123.80	121.00
1	RA	1187	G	N7-C8-N9	5.59	115.90	113.10
1	RA	1513	C	C6-N1-C2	-5.59	118.06	120.30
1	RA	1313	U	C5-C6-N1	5.59	125.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2755	C	C5-C6-N1	5.59	123.79	121.00
2	RB	81	G	C4-N9-C1'	5.59	133.77	126.50
1	YA	2779	U	C2-N1-C1'	5.59	124.41	117.70
1	RA	2584	U	N1-C2-O2	5.59	126.71	122.80
1	YA	2579	C	N1-C2-O2	5.59	122.25	118.90
1	RA	234	C	N1-C2-O2	5.58	122.25	118.90
1	YA	9	U	N1-C2-O2	5.58	126.71	122.80
1	RA	965	C	C5-C6-N1	5.58	123.79	121.00
1	YA	965	C	C6-N1-C2	-5.58	118.07	120.30
1	YA	1188	U	C5-C6-N1	5.58	125.49	122.70
1	RA	1180	C	C5-C6-N1	5.58	123.79	121.00
1	YA	1012	U	P-O3'-C3'	5.58	126.39	119.70
1	YA	2260	C	C6-N1-C2	-5.58	118.07	120.30
1	RA	795	C	C6-N1-C2	-5.58	118.07	120.30
1	RA	817	C	C5-C6-N1	5.57	123.78	121.00
32	QA	328	C	C2-N3-C4	5.57	122.69	119.90
1	YA	2359	C	C6-N1-C2	-5.57	118.07	120.30
1	RA	679	C	C5-C6-N1	5.57	123.78	121.00
1	YA	692	C	N1-C2-O2	5.57	122.24	118.90
32	QA	91	C	C6-N1-C2	-5.56	118.08	120.30
32	QA	1038	C	C6-N1-C2	-5.56	118.08	120.30
32	QA	1439	C	N1-C2-O2	5.56	122.24	118.90
1	YA	802	A	C4-C5-N7	5.56	113.48	110.70
1	YA	1332	G	C5-N7-C8	-5.56	101.52	104.30
1	YA	1535	U	C6-N1-C2	-5.56	117.66	121.00
1	RA	850	C	C5-C6-N1	5.56	123.78	121.00
1	YA	581	C	C5-C6-N1	5.56	123.78	121.00
32	XA	747	C	C5-C6-N1	5.56	123.78	121.00
1	RA	1333	C	C6-N1-C2	-5.55	118.08	120.30
1	RA	1333	C	N1-C2-O2	5.55	122.23	118.90
1	RA	517	C	C6-N1-C2	-5.55	118.08	120.30
1	YA	420	C	N1-C2-O2	5.55	122.23	118.90
1	RA	692	C	N1-C2-O2	5.55	122.23	118.90
1	YA	1267	U	N1-C2-O2	5.55	126.68	122.80
1	YA	2825	C	C6-N1-C2	-5.55	118.08	120.30
32	QA	266	G	N1-C6-O6	5.54	123.23	119.90
1	YA	445	C	N3-C4-C5	-5.54	119.68	121.90
1	YA	12	U	C5-C6-N1	5.54	125.47	122.70
1	RA	456	C	N3-C2-O2	-5.54	118.02	121.90
1	YA	237	C	N1-C2-O2	5.54	122.22	118.90
1	YA	915	C	N1-C2-O2	5.54	122.22	118.90
1	YA	2847	U	N3-C2-O2	-5.54	118.32	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	363(E)	U	N1-C2-O2	5.54	126.68	122.80
1	RA	1386	C	C6-N1-C2	-5.54	118.09	120.30
1	RA	1543	A	O4'-C1'-N9	5.54	112.63	108.20
1	YA	2392	A	N7-C8-N9	5.53	116.57	113.80
1	YA	2395	C	C5-C6-N1	5.53	123.77	121.00
53	XV	34	C	N3-C2-O2	-5.53	118.03	121.90
1	RA	2814	C	N3-C2-O2	-5.53	118.03	121.90
2	YB	60	C	C6-N1-C2	-5.53	118.09	120.30
1	YA	828	U	N1-C2-O2	5.53	126.67	122.80
1	RA	912	C	N1-C2-O2	5.53	122.22	118.90
2	RB	77	U	N1-C2-O2	5.52	126.67	122.80
1	YA	1210	A	N7-C8-N9	5.52	116.56	113.80
1	RA	1915	U	N1-C2-O2	5.52	126.66	122.80
1	YA	384	U	N1-C2-O2	5.52	126.66	122.80
1	YA	1157	G	N9-C4-C5	-5.52	103.19	105.40
1	YA	510	C	C6-N1-C2	-5.52	118.09	120.30
1	YA	1446	C	C6-N1-C2	-5.52	118.09	120.30
1	RA	1708	C	C6-N1-C2	-5.52	118.09	120.30
32	XA	169	C	N3-C2-O2	-5.52	118.04	121.90
1	RA	753	C	C6-N1-C2	-5.51	118.09	120.30
1	YA	426	C	N1-C2-O2	5.51	122.21	118.90
32	XA	1140	C	C6-N1-C2	-5.51	118.09	120.30
1	YA	691	C	C6-N1-C2	-5.51	118.09	120.30
32	QA	328	C	P-O3'-C3'	5.51	126.31	119.70
1	YA	1640	C	N3-C2-O2	-5.51	118.04	121.90
1	RA	1502	C	C2-N1-C1'	5.51	124.86	118.80
1	RA	624	C	C5-C6-N1	5.50	123.75	121.00
1	RA	2849	U	C2-N1-C1'	-5.50	111.09	117.70
32	QA	789	U	N1-C2-O2	5.50	126.65	122.80
1	RA	2260	C	C6-N1-C2	-5.50	118.10	120.30
1	YA	140	A	C8-N9-C4	-5.50	103.60	105.80
1	RA	1064	C	C2-N1-C1'	5.50	124.85	118.80
32	QA	603	U	C5-C6-N1	5.50	125.45	122.70
40	XI	56	LEU	CA-CB-CG	5.50	127.95	115.30
1	RA	1387	C	C5-C6-N1	5.50	123.75	121.00
1	RA	1774	C	C5-C6-N1	5.50	123.75	121.00
2	RB	91	C	C5-C6-N1	5.50	123.75	121.00
1	YA	2320	A	C2-N3-C4	5.50	113.35	110.60
32	XA	674	G	N7-C8-N9	5.50	115.85	113.10
32	XA	623	C	C6-N1-C2	-5.49	118.10	120.30
2	RB	77	U	N3-C2-O2	-5.49	118.36	122.20
1	YA	2031	A	C2-N3-C4	5.49	113.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	1180	C	N1-C2-O2	5.49	122.19	118.90
1	RA	1779	U	N3-C2-O2	-5.49	118.36	122.20
1	YA	1504	C	C5-C6-N1	5.49	123.75	121.00
2	YB	27	C	C5-C6-N1	5.49	123.75	121.00
1	RA	856	C	N3-C2-O2	-5.49	118.06	121.90
21	RZ	5	LEU	CA-CB-CG	5.49	127.92	115.30
1	RA	1779	U	N1-C2-O2	5.49	126.64	122.80
2	YB	71	C	N1-C2-O2	5.49	122.19	118.90
1	RA	1506	C	C6-N1-C2	-5.48	118.11	120.30
1	YA	1644	C	N1-C2-O2	5.48	122.19	118.90
2	YB	43	C	N1-C2-O2	5.48	122.19	118.90
1	RA	1678	G	C8-N9-C4	-5.48	104.21	106.40
1	RA	2868	A	C5-N7-C8	-5.48	101.16	103.90
1	YA	673	C	N1-C2-O2	5.48	122.19	118.90
1	YA	1064	C	C6-N1-C2	-5.48	118.11	120.30
1	YA	2655	G	O4'-C1'-N9	5.48	112.58	108.20
1	YA	1394	U	C6-N1-C1'	5.48	128.87	121.20
1	YA	1686	C	C6-N1-C2	-5.48	118.11	120.30
1	RA	647	G	C6-C5-N7	-5.47	127.11	130.40
1	RA	786	C	C6-N1-C2	-5.47	118.11	120.30
1	YA	47	C	C5-C6-N1	5.47	123.74	121.00
1	YA	2549	G	C8-N9-C4	-5.47	104.21	106.40
1	RA	635	C	C6-N1-C2	-5.47	118.11	120.30
1	YA	635	C	C5-C6-N1	5.47	123.74	121.00
1	YA	1695	G	C4-N9-C1'	5.47	133.61	126.50
1	YA	2836	U	C5-C6-N1	5.47	125.44	122.70
1	RA	2787	C	N1-C2-O2	5.47	122.18	118.90
1	RA	234	C	C6-N1-C2	-5.47	118.11	120.30
2	YB	43	C	N3-C2-O2	-5.47	118.07	121.90
1	RA	1534	G	N3-C4-N9	5.46	129.28	126.00
1	RA	2667	C	C6-N1-C2	-5.46	118.11	120.30
32	QA	283	C	C5-C6-N1	5.46	123.73	121.00
1	YA	183	C	C5-C6-N1	5.46	123.73	121.00
1	YA	904	C	N1-C2-O2	5.46	122.18	118.90
1	YA	1691	C	C6-N1-C2	-5.46	118.12	120.30
32	XA	328	C	P-O3'-C3'	5.46	126.25	119.70
1	YA	1404	C	C2-N1-C1'	5.46	124.81	118.80
32	XA	528	C	C5-C6-N1	5.46	123.73	121.00
32	QA	449	C	N1-C2-O2	5.46	122.17	118.90
32	QA	355	C	C6-N1-C2	-5.45	118.12	120.30
1	YA	392	C	C6-N1-C2	-5.45	118.12	120.30
1	YA	1142(A)	A	N3-C4-N9	-5.45	123.04	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2676	C	N1-C2-O2	5.45	122.17	118.90
1	YA	1021	A	N3-C4-C5	5.45	130.61	126.80
1	YA	1504	C	N1-C2-O2	5.45	122.17	118.90
1	YA	2771	C	C6-N1-C2	-5.45	118.12	120.30
32	XA	307	C	C5-C6-N1	5.45	123.72	121.00
32	XA	1357	A	N7-C8-N9	5.45	116.52	113.80
1	RA	1686	C	C5-C6-N1	5.45	123.72	121.00
1	YA	779	U	C5-C6-N1	5.45	125.42	122.70
1	RA	754	C	C5-C6-N1	5.45	123.72	121.00
1	YA	161	U	N1-C2-O2	5.45	126.61	122.80
1	YA	1612	C	C5-C6-N1	5.45	123.72	121.00
1	YA	2576	G	C8-N9-C1'	-5.45	119.92	127.00
32	XA	1158	C	N1-C2-O2	5.45	122.17	118.90
1	YA	1463	C	C6-N1-C2	-5.44	118.12	120.30
32	XA	615	C	C6-N1-C2	-5.44	118.12	120.30
1	RA	2103	C	C6-N1-C2	-5.44	118.12	120.30
1	YA	1417	C	C5-C6-N1	5.44	123.72	121.00
1	RA	1881	C	C6-N1-C2	-5.44	118.12	120.30
1	RA	2506	U	N1-C2-O2	5.44	126.61	122.80
32	QA	283	C	C6-N1-C2	-5.44	118.12	120.30
1	RA	537	C	C2-N1-C1'	5.43	124.78	118.80
1	YA	1210	A	C5-N7-C8	-5.43	101.18	103.90
1	YA	2568	C	C5-C6-N1	5.43	123.72	121.00
1	YA	27	G	N3-C4-N9	-5.43	122.74	126.00
32	QA	1065	U	P-O3'-C3'	5.43	126.22	119.70
1	YA	1506	C	C2-N1-C1'	5.43	124.77	118.80
2	RB	27	C	C5-C6-N1	5.43	123.72	121.00
32	QA	90	C	N1-C2-O2	5.43	122.16	118.90
1	YA	665	C	C6-N1-C2	-5.43	118.13	120.30
1	YA	1333	C	C5-C6-N1	5.43	123.71	121.00
32	XA	1362	C	N3-C2-O2	-5.43	118.10	121.90
1	YA	2638	G	C8-N9-C4	-5.43	104.23	106.40
32	XA	810	C	C5-C6-N1	5.43	123.71	121.00
32	XA	1381	U	N3-C2-O2	-5.43	118.40	122.20
32	QA	1163	C	C5-C6-N1	5.42	123.71	121.00
1	YA	654(T)	C	N1-C2-O2	5.42	122.16	118.90
1	YA	2063	C	C6-N1-C2	-5.42	118.13	120.30
1	RA	915	C	N1-C2-O2	5.42	122.15	118.90
1	YA	1947	C	C5-C6-N1	5.42	123.71	121.00
32	QA	528	C	C5-C6-N1	5.42	123.71	121.00
1	YA	441	U	C5-C6-N1	5.42	125.41	122.70
1	RA	846	C	N3-C2-O2	-5.42	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	2832	U	P-O3'-C3'	5.42	126.20	119.70
2	YB	77	U	C5-C6-N1	5.42	125.41	122.70
32	XA	699	C	C5-C6-N1	5.42	123.71	121.00
1	YA	40	C	C5-C6-N1	5.42	123.71	121.00
1	YA	1686	C	C5-C6-N1	5.42	123.71	121.00
1	RA	1504	C	C5-C6-N1	5.41	123.71	121.00
1	YA	754	C	C6-N1-C2	-5.41	118.14	120.30
1	YA	584	C	C5-C6-N1	5.41	123.70	121.00
32	QA	1113	C	C5-C6-N1	5.41	123.70	121.00
1	YA	1233	C	C5-C6-N1	5.41	123.70	121.00
1	YA	2210	G	C4-N9-C1'	5.41	133.53	126.50
1	YA	417	C	N1-C2-O2	5.41	122.14	118.90
1	RA	1385	G	O4'-C1'-N9	5.41	112.52	108.20
1	RA	1678	G	C5-N7-C8	-5.41	101.60	104.30
1	YA	815	C	C6-N1-C2	-5.41	118.14	120.30
1	YA	2164	C	N1-C2-O2	5.41	122.14	118.90
1	YA	2065	C	C6-N1-C2	-5.40	118.14	120.30
1	RA	2188	C	C6-N1-C2	-5.40	118.14	120.30
32	QA	252	U	N1-C2-O2	5.40	126.58	122.80
1	YA	1135	C	N1-C2-O2	5.39	122.14	118.90
1	RA	749	C	N3-C2-O2	-5.39	118.12	121.90
1	YA	430	G	C5-C6-O6	5.39	131.84	128.60
1	YA	1161	C	C6-N1-C2	-5.39	118.14	120.30
2	YB	47	C	N1-C2-O2	5.39	122.14	118.90
1	RA	1150	C	C5-C6-N1	5.39	123.69	121.00
1	RA	1950	G	O4'-C1'-N9	5.39	112.51	108.20
1	YA	41	C	N1-C2-O2	5.39	122.13	118.90
1	YA	1589	C	C5-C6-N1	5.39	123.69	121.00
1	RA	1063	G	C2-N3-C4	5.39	114.59	111.90
1	RA	2254	C	C6-N1-C2	-5.39	118.14	120.30
1	YA	1022	G	P-O3'-C3'	5.39	126.17	119.70
1	YA	29	U	C5-C6-N1	5.39	125.39	122.70
1	RA	1267	U	C2-N1-C1'	5.38	124.16	117.70
1	RA	1052	C	N1-C2-O2	5.38	122.13	118.90
1	RA	1135	C	N1-C2-O2	5.38	122.13	118.90
1	RA	786	C	C6-N1-C1'	5.38	127.25	120.80
1	RA	1534	G	N3-C4-C5	-5.38	125.91	128.60
1	RA	2456	C	C6-N1-C2	-5.38	118.15	120.30
32	XA	180	U	N3-C2-O2	-5.38	118.44	122.20
1	YA	105	C	C6-N1-C2	-5.38	118.15	120.30
1	YA	749	C	N3-C2-O2	-5.38	118.14	121.90
1	YA	1076	C	C5-C6-N1	5.38	123.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1534	G	N3-C4-N9	5.38	129.23	126.00
1	RA	193	U	N1-C2-O2	5.37	126.56	122.80
1	RA	229	A	P-O3'-C3'	5.37	126.15	119.70
1	YA	2739	U	C6-N1-C2	-5.37	117.78	121.00
1	RA	1065	U	C5-C6-N1	5.37	125.39	122.70
1	YA	2681	C	P-O3'-C3'	5.37	126.14	119.70
1	RA	129	C	N1-C2-O2	5.37	122.12	118.90
1	YA	1406	U	C2-N1-C1'	5.37	124.14	117.70
1	YA	2504	U	N1-C2-O2	5.37	126.56	122.80
2	YB	94	C	C6-N1-C2	-5.37	118.15	120.30
1	RA	1065	U	C6-N1-C2	-5.37	117.78	121.00
32	XA	186(A)	C	N1-C2-O2	5.37	122.12	118.90
1	RA	1430	C	C6-N1-C2	-5.37	118.15	120.30
1	RA	1830	C	C6-N1-C2	-5.37	118.15	120.30
32	QA	960	U	C2-N1-C1'	5.37	124.14	117.70
32	XA	1008	C	N1-C2-O2	5.36	122.12	118.90
1	RA	618(A)	C	C5-C6-N1	5.36	123.68	121.00
1	YA	1558	A	P-O3'-C3'	5.36	126.13	119.70
1	YA	2145	C	C2-N3-C4	5.36	122.58	119.90
32	XA	314	C	C6-N1-C2	-5.36	118.16	120.30
32	QA	674	G	C6-C5-N7	-5.36	127.19	130.40
1	YA	2667	C	C5-C6-N1	5.36	123.68	121.00
32	QA	307	C	C6-N1-C2	-5.36	118.16	120.30
1	YA	444	C	C6-N1-C2	-5.36	118.16	120.30
32	XA	449	C	C6-N1-C2	-5.36	118.16	120.30
1	RA	1686	C	C2-N1-C1'	5.36	124.69	118.80
1	RA	2229	C	C5-C6-N1	5.36	123.68	121.00
1	YA	12	U	C2-N1-C1'	5.35	124.12	117.70
1	YA	815	C	C5-C6-N1	5.35	123.68	121.00
32	XA	18	C	C6-N1-C2	-5.35	118.16	120.30
2	RB	81	G	C4-C5-N7	5.35	112.94	110.80
1	YA	554	U	C2-N1-C1'	-5.35	111.28	117.70
1	YA	1653	G	P-O3'-C3'	5.35	126.12	119.70
1	RA	2501	C	C2-N1-C1'	-5.35	112.91	118.80
1	YA	1629	U	C6-N1-C2	-5.35	117.79	121.00
32	XA	1452	C	N1-C2-O2	5.35	122.11	118.90
32	XA	135	C	C5-C6-N1	5.35	123.67	121.00
32	XA	554	C	C6-N1-C2	-5.35	118.16	120.30
32	QA	833	U	N3-C2-O2	-5.34	118.46	122.20
1	YA	206	U	N1-C2-O2	5.34	126.54	122.80
1	RA	1022	G	P-O3'-C3'	5.34	126.11	119.70
32	QA	891	U	N1-C2-O2	5.34	126.54	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	989	C	N1-C2-O2	5.34	122.11	118.90
1	YA	192	C	N3-C2-O2	-5.34	118.16	121.90
1	RA	67	U	C5-C6-N1	5.34	125.37	122.70
1	YA	802	A	C5-C6-N6	-5.34	119.43	123.70
1	YA	1930	G	N3-C4-N9	-5.34	122.80	126.00
32	XA	826	C	N3-C2-O2	-5.34	118.16	121.90
1	YA	2676	C	N1-C2-O2	5.34	122.10	118.90
32	QA	827	U	C6-N1-C2	-5.34	117.80	121.00
1	RA	1795	C	C5-C6-N1	5.34	123.67	121.00
1	RA	1992	G	O4'-C1'-N9	-5.34	103.93	108.20
32	QA	1147	C	N1-C2-O2	5.34	122.10	118.90
2	YB	95	U	C5-C6-N1	5.34	125.37	122.70
6	RG	152	LEU	CA-CB-CG	5.33	127.57	115.30
32	QA	217	C	N1-C2-O2	5.33	122.10	118.90
1	YA	2794	C	C6-N1-C2	-5.33	118.17	120.30
1	RA	640	C	C5-C6-N1	5.33	123.67	121.00
1	YA	198	C	C2-N3-C4	5.33	122.57	119.90
1	YA	637	A	P-O3'-C3'	5.33	126.10	119.70
1	YA	196	A	O4'-C1'-N9	5.33	112.46	108.20
1	YA	1041	C	C6-N1-C2	-5.33	118.17	120.30
1	YA	1398	C	N1-C2-O2	5.33	122.10	118.90
32	XA	1109	C	N1-C2-O2	5.33	122.10	118.90
32	XA	1140	C	N1-C2-O2	5.33	122.09	118.90
2	RB	68	C	C5-C6-N1	5.32	123.66	121.00
1	YA	862	G	N3-C4-C5	-5.32	125.94	128.60
1	YA	1795	C	N1-C2-O2	5.32	122.09	118.90
2	YB	70	C	C6-N1-C2	-5.32	118.17	120.30
1	RA	269	U	C2-N1-C1'	5.32	124.08	117.70
1	RA	316	C	C6-N1-C2	-5.32	118.17	120.30
1	YA	923	C	C6-N1-C2	-5.32	118.17	120.30
32	XA	308	C	N1-C2-O2	5.31	122.09	118.90
1	YA	2350	C	C5-C6-N1	5.31	123.66	121.00
1	RA	1505	C	C5-C6-N1	5.31	123.65	121.00
1	RA	1619	G	N9-C4-C5	-5.31	103.28	105.40
1	RA	2586	C	C5-C6-N1	5.31	123.66	121.00
32	QA	1502	A	N1-C6-N6	5.31	121.78	118.60
1	RA	1021	A	C8-N9-C4	-5.30	103.68	105.80
1	YA	2493	U	C5-C6-N1	5.30	125.35	122.70
1	RA	237	C	N1-C2-O2	5.30	122.08	118.90
1	RA	914	C	C6-N1-C2	-5.30	118.18	120.30
1	YA	1290	C	C5-C6-N1	5.30	123.65	121.00
1	YA	2096	U	N3-C2-O2	-5.30	118.49	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	209	C	C5-C6-N1	5.30	123.65	121.00
1	RA	1644	C	N3-C2-O2	-5.30	118.19	121.90
32	XA	314	C	C5-C6-N1	5.30	123.65	121.00
50	XS	30	LEU	CA-CB-CG	5.30	127.49	115.30
1	YA	1835	G	N3-C4-C5	-5.30	125.95	128.60
1	YA	208	C	C6-N1-C2	-5.30	118.18	120.30
1	YA	834	C	C5-C6-N1	5.30	123.65	121.00
32	XA	334	C	C6-N1-C2	-5.30	118.18	120.30
32	XA	442	C	C6-N1-C2	-5.30	118.18	120.30
32	XA	1437	C	C5-C6-N1	5.30	123.65	121.00
32	XA	455	C	C5-C6-N1	5.29	123.65	121.00
1	YA	542	C	C6-N1-C2	-5.29	118.18	120.30
1	YA	658	C	C5-C6-N1	5.29	123.65	121.00
1	RA	2759	G	N3-C4-N9	5.29	129.18	126.00
2	YB	30	C	C5-C6-N1	5.29	123.65	121.00
32	QA	169	C	C6-N1-C2	-5.29	118.18	120.30
1	YA	860	U	C5-C4-O4	5.29	129.07	125.90
1	YA	2787	C	N1-C2-O2	5.28	122.07	118.90
1	YA	2874	C	N1-C2-O2	5.28	122.07	118.90
32	XA	509	A	C8-N9-C4	-5.28	103.69	105.80
1	RA	846	C	P-O3'-C3'	5.28	126.04	119.70
1	YA	2394	C	N1-C2-O2	5.28	122.07	118.90
32	XA	1452	C	N3-C2-O2	-5.28	118.20	121.90
1	YA	2702	U	C5-C6-N1	5.28	125.34	122.70
1	YA	2651	C	C6-N1-C2	-5.28	118.19	120.30
2	YB	81	G	C6-C5-N7	-5.28	127.23	130.40
32	QA	554	C	C5-C6-N1	5.28	123.64	121.00
1	YA	1852	C	C6-N1-C2	-5.28	118.19	120.30
1	YA	1595	G	N1-C6-O6	-5.27	116.74	119.90
1	RA	1549	C	C6-N1-C2	-5.27	118.19	120.30
1	RA	1683	C	C6-N1-C2	-5.27	118.19	120.30
1	YA	1445	C	C6-N1-C2	-5.27	118.19	120.30
1	YA	2392	A	C5-N7-C8	-5.27	101.27	103.90
1	YA	2615	U	C5-C6-N1	5.27	125.33	122.70
1	YA	396	G	C6-C5-N7	-5.27	127.24	130.40
1	YA	2406	U	O4'-C1'-N1	-5.27	103.99	108.20
1	YA	2815	C	C5-C6-N1	5.27	123.63	121.00
32	XA	536	C	C5-C6-N1	5.27	123.63	121.00
32	QA	736	C	C5-C6-N1	5.26	123.63	121.00
32	QA	891	U	N3-C2-O2	-5.26	118.52	122.20
1	YA	76	C	N1-C2-O2	5.26	122.06	118.90
32	XA	328	C	C5-C6-N1	5.26	123.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	192	C	C6-N1-C2	-5.26	118.19	120.30
1	YA	373	U	N1-C2-O2	5.26	126.48	122.80
1	RA	665	C	C6-N1-C2	-5.26	118.20	120.30
32	QA	811	C	N1-C2-O2	5.26	122.06	118.90
2	RB	77	U	C5-C6-N1	5.26	125.33	122.70
32	QA	1406	U	N3-C2-O2	-5.26	118.52	122.20
1	RA	2044	C	C5-C6-N1	5.25	123.63	121.00
1	RA	2699	C	C5-C6-N1	5.25	123.63	121.00
1	RA	76	C	N1-C2-O2	5.25	122.05	118.90
32	QA	501	C	C6-N1-C2	-5.25	118.20	120.30
1	YA	183	C	C6-N1-C2	-5.25	118.20	120.30
1	YA	985	C	C5-C6-N1	5.25	123.63	121.00
1	YA	1053	C	C6-N1-C2	-5.25	118.20	120.30
1	RA	657	U	N3-C2-O2	-5.25	118.53	122.20
1	YA	2089	U	C6-N1-C2	-5.25	117.85	121.00
1	RA	589	C	C5-C6-N1	5.25	123.62	121.00
1	RA	120	U	C2-N1-C1'	5.25	124.00	117.70
1	RA	817	C	C6-N1-C2	-5.25	118.20	120.30
1	RA	2065	C	C5-C6-N1	5.25	123.62	121.00
32	XA	528	C	N3-C2-O2	-5.25	118.23	121.90
1	RA	867	C	N1-C2-O2	5.24	122.05	118.90
32	QA	449	C	N3-C2-O2	-5.24	118.23	121.90
1	YA	2196	C	N1-C2-O2	5.24	122.05	118.90
1	YA	2784	C	C5-C6-N1	5.24	123.62	121.00
1	RA	1218	C	C6-N1-C2	-5.24	118.20	120.30
1	YA	2336	A	C5-C6-N6	-5.24	119.51	123.70
1	RA	613	U	C2-N1-C1'	5.24	123.99	117.70
1	RA	721	C	C5-C6-N1	5.24	123.62	121.00
1	YA	231	C	C2-N1-C1'	5.24	124.56	118.80
1	YA	444	C	C5-C6-N1	5.24	123.62	121.00
1	YA	1326	U	N1-C2-O2	5.24	126.47	122.80
32	XA	647	C	C6-N1-C2	-5.24	118.20	120.30
1	RA	1510	A	C2-N3-C4	5.24	113.22	110.60
1	YA	104	U	N1-C2-O2	5.24	126.46	122.80
1	YA	1411	C	C5-C4-N4	-5.24	116.53	120.20
1	YA	1934	C	C6-N1-C2	-5.24	118.21	120.30
32	XA	381	C	N1-C2-O2	5.24	122.04	118.90
1	YA	1180	C	C2-N1-C1'	5.23	124.56	118.80
1	RA	766	C	C5-C6-N1	5.23	123.62	121.00
1	YA	1306	C	N1-C2-O2	5.23	122.04	118.90
1	YA	1362	C	C6-N1-C2	-5.23	118.21	120.30
1	RA	404	C	P-O3'-C3'	5.23	125.98	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2321	G	C8-N9-C4	-5.23	104.31	106.40
1	RA	2438	U	C5-C6-N1	5.23	125.32	122.70
1	YA	404	C	P-O3'-C3'	5.23	125.98	119.70
1	RA	435	C	N1-C2-O2	5.23	122.04	118.90
32	QA	56	U	C5-C6-N1	5.23	125.31	122.70
1	RA	1157	G	C4-C5-N7	5.23	112.89	110.80
1	RA	1462	C	C6-N1-C2	-5.23	118.21	120.30
1	YA	2312	U	C5-C6-N1	5.23	125.31	122.70
32	QA	1539	C	N1-C2-O2	5.23	122.04	118.90
1	YA	1386	C	C6-N1-C2	-5.23	118.21	120.30
1	RA	730	C	C6-N1-C2	-5.22	118.21	120.30
1	RA	815	C	C6-N1-C2	-5.22	118.21	120.30
1	RA	1097	U	C6-N1-C2	-5.22	117.87	121.00
32	QA	435	C	C6-N1-C2	-5.22	118.21	120.30
32	QA	1439	C	C6-N1-C2	-5.22	118.21	120.30
1	YA	676	A	C4-C5-N7	5.22	113.31	110.70
1	YA	1026	U	O4'-C1'-N1	5.22	112.38	108.20
1	YA	2683	C	N1-C2-O2	5.22	122.03	118.90
32	XA	705	U	C5-C6-N1	5.22	125.31	122.70
32	XA	1514	C	C6-N1-C2	-5.22	118.21	120.30
1	RA	2756	U	C5-C4-O4	-5.22	122.77	125.90
1	RA	2874	C	N1-C2-O2	5.22	122.03	118.90
1	YA	1788	C	C6-N1-C2	-5.22	118.21	120.30
1	YA	2039	C	C6-N1-C2	-5.22	118.21	120.30
32	XA	174	C	C6-N1-C2	-5.22	118.21	120.30
1	RA	2746	U	N3-C2-O2	-5.22	118.55	122.20
1	RA	825	C	C6-N1-C2	-5.22	118.21	120.30
1	RA	420	C	N1-C2-O2	5.21	122.03	118.90
1	RA	508	G	N3-C4-C5	-5.21	125.99	128.60
1	YA	537	C	C2-N3-C4	5.21	122.51	119.90
1	YA	613	U	C6-N1-C1'	-5.21	113.90	121.20
1	YA	1635	G	C6-C5-N7	-5.21	127.27	130.40
1	YA	2588	G	C6-C5-N7	-5.21	127.27	130.40
32	XA	1310	G	C6-C5-N7	-5.21	127.27	130.40
1	YA	396	G	C4-C5-N7	5.21	112.89	110.80
1	YA	1668	A	C2-N3-C4	5.21	113.21	110.60
1	RA	637	A	P-O3'-C3'	5.21	125.95	119.70
1	RA	1396	U	C5-C6-N1	5.21	125.30	122.70
1	RA	2759	G	C4-C5-N7	5.21	112.88	110.80
32	QA	401	C	C6-N1-C2	-5.21	118.22	120.30
32	QA	1121	U	C5-C6-N1	5.21	125.30	122.70
1	YA	134	C	C6-N1-C2	-5.21	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	846	C	P-O3'-C3'	5.21	125.95	119.70
1	YA	1630(A)	C	C5-C6-N1	5.21	123.61	121.00
2	YB	90	C	C5-C6-N1	5.21	123.60	121.00
1	RA	209	C	C6-N1-C2	-5.21	118.22	120.30
1	YA	2075	U	N3-C4-O4	5.21	123.05	119.40
1	YA	2723	C	C5-C6-N1	5.20	123.60	121.00
1	YA	1992	G	O4'-C1'-N9	-5.20	104.04	108.20
32	XA	548	G	N3-C4-N9	5.20	129.12	126.00
1	YA	2682	U	N3-C2-O2	-5.20	118.56	122.20
32	XA	1033	G	N3-C2-N2	5.20	123.54	119.90
1	RA	106	C	N1-C2-O2	5.20	122.02	118.90
1	YA	1504	C	C6-N1-C2	-5.20	118.22	120.30
1	RA	229	A	OP2-P-O3'	5.20	116.63	105.20
32	QA	1420	C	C5-C6-N1	5.20	123.60	121.00
32	XA	1409	C	C6-N1-C2	-5.20	118.22	120.30
1	RA	1411	C	C6-N1-C2	-5.19	118.22	120.30
1	YA	183	C	N3-C2-O2	-5.19	118.26	121.90
32	XA	674	G	C8-N9-C4	-5.19	104.32	106.40
32	XA	1237	C	C6-N1-C2	-5.19	118.22	120.30
1	RA	1679	U	N3-C2-O2	-5.19	118.57	122.20
1	YA	1416	G	C8-N9-C1'	5.19	133.75	127.00
32	QA	442	C	C5-C6-N1	5.19	123.59	121.00
1	YA	1516	U	C5-C6-N1	5.19	125.30	122.70
1	RA	1063	G	N1-C6-O6	-5.19	116.79	119.90
32	QA	453	A	C8-N9-C4	-5.19	103.72	105.80
1	YA	384	U	N3-C2-O2	-5.19	118.57	122.20
1	YA	2699	C	C5-C6-N1	5.19	123.59	121.00
1	YA	1294	U	N1-C2-O2	5.19	126.43	122.80
1	RA	580	C	C5-C6-N1	5.18	123.59	121.00
1	RA	898	C	C5-C6-N1	5.18	123.59	121.00
1	RA	1404	C	N1-C2-O2	5.18	122.01	118.90
1	RA	2686	G	N3-C4-N9	5.18	129.11	126.00
1	YA	138	G	O4'-C1'-N9	5.18	112.35	108.20
1	RA	783	A	C8-N9-C4	-5.18	103.73	105.80
1	RA	860	U	C2-N1-C1'	5.18	123.92	117.70
1	RA	2568	C	C5-C6-N1	5.18	123.59	121.00
1	YA	676	A	O4'-C1'-N9	5.18	112.34	108.20
32	XA	217	C	N1-C2-O2	5.18	122.01	118.90
1	RA	1063	G	C8-N9-C4	-5.18	104.33	106.40
32	QA	174	C	C6-N1-C2	-5.18	118.23	120.30
1	RA	41	C	C6-N1-C2	-5.18	118.23	120.30
1	RA	1474	C	N3-C2-O2	-5.18	118.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	753	C	N1-C2-O2	5.18	122.00	118.90
1	RA	1827	C	N3-C2-O2	-5.18	118.28	121.90
1	RA	2575	C	C5-C6-N1	5.18	123.59	121.00
1	RA	846	C	C6-N1-C2	-5.17	118.23	120.30
1	YA	925	C	C6-N1-C2	-5.17	118.23	120.30
1	RA	914	C	N1-C2-O2	5.17	122.00	118.90
1	RA	343	C	N1-C2-O2	5.17	122.00	118.90
1	RA	2248	C	C6-N1-C2	-5.17	118.23	120.30
1	RA	2889	C	C5-C6-N1	5.17	123.58	121.00
32	QA	1301	U	C6-N1-C1'	-5.17	113.96	121.20
1	YA	2889	C	C5-C6-N1	5.17	123.58	121.00
32	XA	623	C	C5-C6-N1	5.17	123.58	121.00
32	QA	23	C	C5-C6-N1	5.17	123.58	121.00
1	YA	846	C	C2-N1-C1'	5.17	124.49	118.80
1	YA	1983	C	C6-N1-C2	-5.17	118.23	120.30
1	RA	1071	G	C8-N9-C4	-5.17	104.33	106.40
32	QA	455	C	N1-C2-O2	5.17	122.00	118.90
1	RA	1230	C	C6-N1-C2	-5.17	118.23	120.30
1	RA	1899	G	C4-N9-C1'	5.17	133.21	126.50
32	QA	1071	C	C5-C6-N1	5.17	123.58	121.00
1	YA	378	C	C5-C6-N1	5.17	123.58	121.00
1	YA	857	C	C5-C6-N1	5.17	123.58	121.00
1	YA	1053	C	C5-C6-N1	5.17	123.58	121.00
1	RA	503	A	P-O3'-C3'	5.16	125.89	119.70
1	RA	2581	G	C4-N9-C1'	5.16	133.21	126.50
1	YA	2816	C	C5-C6-N1	5.16	123.58	121.00
1	RA	263	C	C6-N1-C1'	5.16	126.99	120.80
32	QA	754	C	C6-N1-C1'	-5.16	114.61	120.80
1	RA	2767	C	C6-N1-C2	-5.16	118.24	120.30
1	YA	2828	C	C5-C6-N1	5.16	123.58	121.00
1	RA	1686	C	N1-C2-O2	5.16	122.00	118.90
1	RA	2636	U	N1-C2-O2	5.16	126.41	122.80
1	YA	1291	C	C6-N1-C2	-5.16	118.24	120.30
1	YA	87	C	C6-N1-C2	-5.16	118.24	120.30
1	RA	535	C	C6-N1-C1'	5.16	126.99	120.80
1	YA	2471	C	C6-N1-C2	-5.16	118.24	120.30
2	YB	94	C	C5-C6-N1	5.16	123.58	121.00
32	XA	1383	C	N3-C2-O2	-5.16	118.29	121.90
32	XA	1439	C	N3-C2-O2	-5.16	118.29	121.90
1	YA	2676	C	C6-N1-C2	-5.15	118.24	120.30
1	YA	1390	U	C5-C6-N1	5.15	125.28	122.70
1	RA	1514	U	C2-N1-C1'	5.15	123.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	2455	G	C8-N9-C4	-5.15	104.34	106.40
1	YA	1795	C	C5-C6-N1	5.15	123.57	121.00
1	RA	316	C	C5-C6-N1	5.15	123.57	121.00
1	YA	267	C	C5-C6-N1	5.15	123.57	121.00
32	QA	697	U	N1-C2-O2	5.14	126.40	122.80
1	YA	234	C	N3-C2-O2	-5.14	118.30	121.90
1	YA	721	C	C5-C6-N1	5.14	123.57	121.00
32	XA	620	C	N3-C2-O2	-5.14	118.30	121.90
1	RA	1407	C	N3-C2-O2	-5.14	118.30	121.90
1	YA	1839	G	N3-C4-N9	5.14	129.09	126.00
1	YA	2267	A	N1-C2-N3	-5.14	126.73	129.30
1	RA	1892	C	C6-N1-C2	-5.14	118.24	120.30
32	QA	980	C	N3-C2-O2	-5.14	118.30	121.90
1	YA	2606	C	C5-C6-N1	5.14	123.57	121.00
1	RA	270(Y)	G	C8-N9-C4	-5.14	104.34	106.40
32	XA	268	C	C6-N1-C2	-5.13	118.25	120.30
1	RA	270(U)	C	N3-C2-O2	-5.13	118.31	121.90
1	YA	2506	U	C6-N1-C2	-5.13	117.92	121.00
32	XA	103	C	N1-C2-O2	5.13	121.98	118.90
32	XA	1172	C	C6-N1-C2	-5.13	118.25	120.30
1	RA	508	G	N3-C4-N9	5.13	129.08	126.00
32	QA	1290	G	N3-C4-C5	-5.13	126.03	128.60
1	YA	459	U	C5-C6-N1	5.13	125.27	122.70
1	YA	2044	C	N1-C2-O2	5.13	121.98	118.90
1	YA	2321	G	C4-N9-C1'	5.13	133.17	126.50
1	RA	676	A	C4-N9-C1'	5.13	135.53	126.30
32	QA	346	G	C2-N3-C4	5.13	114.47	111.90
32	QA	398	C	N3-C2-O2	-5.13	118.31	121.90
32	QA	442	C	N1-C2-O2	5.13	121.98	118.90
1	YA	1161	C	C5-C6-N1	5.13	123.56	121.00
1	YA	2755	C	C5-C6-N1	5.13	123.56	121.00
32	QA	1436	U	C5-C6-N1	5.13	125.26	122.70
1	RA	2832	U	P-O3'-C3'	5.12	125.85	119.70
32	QA	1285	A	P-O3'-C3'	5.12	125.85	119.70
1	YA	2881	C	C6-N1-C2	-5.12	118.25	120.30
1	RA	140	A	C8-N9-C4	-5.12	103.75	105.80
1	RA	537	C	C2-N3-C4	5.12	122.46	119.90
2	RB	30	C	C5-C6-N1	5.12	123.56	121.00
1	YA	523	C	C5-C6-N1	5.12	123.56	121.00
1	YA	931	G	C8-N9-C4	-5.12	104.35	106.40
1	YA	1313	U	C6-N1-C2	-5.12	117.93	121.00
1	YA	2096	U	N1-C2-O2	5.12	126.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	975	G	C8-N9-C4	-5.12	104.35	106.40
1	RA	1833	U	C6-N1-C2	-5.12	117.93	121.00
1	YA	141	A	C6-C5-N7	-5.12	128.72	132.30
1	YA	951	C	C5-C6-N1	5.12	123.56	121.00
1	YA	2465	C	C2-N1-C1'	5.12	124.43	118.80
1	RA	2342	C	N1-C2-O2	5.12	121.97	118.90
1	RA	2506	U	N3-C2-O2	-5.12	118.62	122.20
32	XA	1502	A	C5-N7-C8	-5.12	101.34	103.90
2	RB	22	U	N1-C2-O2	5.11	126.38	122.80
1	YA	237	C	C6-N1-C2	-5.11	118.25	120.30
32	XA	1161	C	N1-C2-O2	5.11	121.97	118.90
32	XA	1163	C	N1-C2-O2	5.11	121.97	118.90
1	RA	2579	C	C5-C6-N1	5.11	123.56	121.00
32	QA	1297	C	P-O3'-C3'	5.11	125.83	119.70
1	RA	1881	C	N1-C2-O2	5.11	121.97	118.90
1	YA	2032	G	N3-C4-C5	5.11	131.16	128.60
1	YA	2772	C	C6-N1-C2	-5.11	118.25	120.30
1	RA	1379	A	C4-C5-N7	5.11	113.25	110.70
1	YA	133	C	C5-C6-N1	5.11	123.55	121.00
1	YA	372	G	C4-N9-C1'	-5.11	119.86	126.50
1	YA	730	C	N1-C2-O2	5.11	121.97	118.90
1	YA	2307	G	O4'-C1'-N9	5.11	112.29	108.20
1	RA	267	C	C6-N1-C2	-5.11	118.26	120.30
1	RA	1598	C	N1-C2-O2	5.11	121.96	118.90
1	YA	1881	C	C2-N1-C1'	5.11	124.42	118.80
1	RA	133	C	C6-N1-C2	-5.10	118.26	120.30
1	YA	336	C	C5-C6-N1	5.10	123.55	121.00
1	RA	1198	U	C6-N1-C2	-5.10	117.94	121.00
1	RA	1432	C	C6-N1-C2	-5.10	118.26	120.30
1	RA	2213	U	N1-C2-O2	5.10	126.37	122.80
1	YA	236	C	C6-N1-C2	-5.10	118.26	120.30
1	YA	721	C	N1-C2-O2	5.10	121.96	118.90
1	YA	1437	C	N1-C2-O2	5.10	121.96	118.90
1	RA	1535	U	N1-C2-O2	5.10	126.37	122.80
1	RA	2439	A	P-O3'-C3'	5.10	125.82	119.70
1	YA	2419	U	C6-N1-C2	-5.10	117.94	121.00
1	YA	2787	C	C2-N1-C1'	5.10	124.41	118.80
32	XA	1140	C	N3-C2-O2	-5.10	118.33	121.90
32	XA	1437	C	N1-C2-O2	5.10	121.96	118.90
53	XV	34	C	C6-N1-C2	-5.10	118.26	120.30
1	RA	475	U	C6-N1-C2	-5.10	117.94	121.00
1	RA	755	C	C6-N1-C2	-5.10	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	1778	U	C5-C4-O4	-5.09	122.84	125.90
32	QA	314	C	C6-N1-C2	-5.09	118.26	120.30
1	YA	343	C	C6-N1-C2	-5.09	118.26	120.30
1	YA	2873	A	O4'-C1'-N9	5.09	112.28	108.20
1	YA	1208	C	C5-C6-N1	5.09	123.55	121.00
1	RA	1233	C	C5-C6-N1	5.09	123.55	121.00
1	YA	271(B)	G	P-O3'-C3'	5.09	125.81	119.70
1	RA	1598	C	C5-C6-N1	5.09	123.54	121.00
32	QA	488	C	C5-C6-N1	5.09	123.54	121.00
1	YA	1417	C	N1-C2-O2	5.09	121.95	118.90
1	RA	1332	G	C8-N9-C4	-5.09	104.37	106.40
1	RA	1406	U	C5-C6-N1	5.09	125.24	122.70
1	RA	2161	C	C2-N1-C1'	5.09	124.40	118.80
1	YA	943	U	C2-N1-C1'	-5.09	111.60	117.70
1	YA	986	C	C5-C6-N1	5.09	123.54	121.00
1	YA	1917	U	N3-C2-O2	-5.09	118.64	122.20
32	QA	6	G	C4-N9-C1'	5.08	133.11	126.50
1	YA	806	C	C5-C6-N1	5.08	123.54	121.00
1	YA	1694	C	C2-N1-C1'	5.08	124.39	118.80
1	YA	2830	G	C8-N9-C4	-5.08	104.37	106.40
32	XA	341	C	C6-N1-C2	-5.08	118.27	120.30
1	RA	1445	C	C5-C6-N1	5.08	123.54	121.00
1	YA	270(H)	C	C6-N1-C2	-5.08	118.27	120.30
1	YA	1437	C	C2-N1-C1'	5.08	124.39	118.80
32	XA	555	C	C5-C6-N1	5.08	123.54	121.00
32	XA	833	U	N3-C2-O2	-5.08	118.64	122.20
32	XA	1037	C	C5-C6-N1	5.08	123.54	121.00
1	YA	822	U	C5-C6-N1	5.08	125.24	122.70
32	XA	365	U	C6-N1-C1'	-5.08	114.09	121.20
1	RA	1640	C	C5-C6-N1	5.08	123.54	121.00
32	QA	1149	C	N1-C2-O2	5.08	121.95	118.90
2	RB	31	C	C5-C6-N1	5.08	123.54	121.00
1	RA	1313	U	C6-N1-C2	-5.08	117.95	121.00
1	RA	2703	C	C5-C6-N1	5.08	123.54	121.00
1	YA	607	U	N1-C2-O2	5.08	126.35	122.80
1	YA	2538	C	N1-C2-O2	5.08	121.94	118.90
1	RA	475	U	C5-C6-N1	5.07	125.24	122.70
1	RA	846	C	C2-N1-C1'	5.07	124.38	118.80
1	YA	1629	U	N3-C2-O2	-5.07	118.65	122.20
1	RA	1513	C	N3-C2-O2	-5.07	118.35	121.90
32	QA	1430	C	N1-C2-O2	5.07	121.94	118.90
1	YA	76	C	C6-N1-C2	-5.07	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	99	U	OP2-P-O3'	5.07	116.36	105.20
1	YA	120	U	C6-N1-C2	-5.07	117.96	121.00
1	YA	193	U	N1-C2-O2	5.07	126.35	122.80
1	YA	2073	C	N1-C2-O2	5.07	121.94	118.90
1	RA	1742	C	N1-C2-O2	5.07	121.94	118.90
2	RB	71	C	N1-C2-O2	5.07	121.94	118.90
1	RA	183	C	N3-C2-O2	-5.07	118.35	121.90
1	RA	2832	U	N1-C2-O2	5.07	126.35	122.80
1	YA	2174	C	C5-C6-N1	5.07	123.53	121.00
32	XA	525	C	C6-N1-C2	-5.07	118.27	120.30
1	YA	2244	U	N3-C4-O4	5.07	122.95	119.40
1	RA	484	C	C5-C6-N1	5.06	123.53	121.00
1	YA	1370	C	N1-C2-O2	5.06	121.94	118.90
1	RA	1506	C	C5-C6-N1	5.06	123.53	121.00
1	YA	2594	C	C6-N1-C2	-5.06	118.28	120.30
32	XA	1070	U	N3-C2-O2	-5.06	118.66	122.20
1	RA	1158	C	N1-C2-O2	5.06	121.94	118.90
1	RA	1218	C	C5-C6-N1	5.06	123.53	121.00
1	RA	1558	A	P-O3'-C3'	5.06	125.77	119.70
1	YA	1416	G	C4-N9-C1'	-5.06	119.92	126.50
1	RA	106	C	C5-C6-N1	5.06	123.53	121.00
1	RA	1544	C	N1-C2-O2	5.06	121.94	118.90
1	RA	2779	U	O4'-C1'-N1	5.06	112.25	108.20
1	RA	2787	C	C6-N1-C2	-5.06	118.28	120.30
1	RA	2395	C	C6-N1-C2	-5.06	118.28	120.30
1	RA	2723	C	C5-C6-N1	5.06	123.53	121.00
1	YA	2385	C	C6-N1-C2	-5.06	118.28	120.30
1	RA	2504	U	N1-C2-O2	5.05	126.34	122.80
15	RT	99	LEU	CA-CB-CG	5.05	126.92	115.30
32	QA	1414	U	N1-C2-O2	5.05	126.34	122.80
1	YA	752	A	P-O3'-C3'	5.05	125.77	119.70
1	YA	949	C	C5-C6-N1	5.05	123.53	121.00
2	YB	93	C	C5-C6-N1	5.05	123.53	121.00
1	RA	1519	G	N3-C4-N9	5.05	129.03	126.00
1	RA	2101	G	N7-C8-N9	5.05	115.63	113.10
32	QA	330	C	C6-N1-C2	-5.05	118.28	120.30
1	YA	138	G	C4-N9-C1'	5.05	133.07	126.50
1	YA	1362	C	C5-C6-N1	5.05	123.53	121.00
1	YA	2179	C	C5-C6-N1	5.05	123.53	121.00
1	RA	141(A)	C	C6-N1-C2	-5.05	118.28	120.30
1	RA	645	C	N1-C2-O2	5.05	121.93	118.90
1	YA	143	C	C5-C6-N1	5.05	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	YP	99	LEU	CA-CB-CG	5.05	126.91	115.30
1	RA	2729	G	N3-C4-N9	5.05	129.03	126.00
1	YA	2688	U	C6-N1-C1'	-5.05	114.14	121.20
32	XA	989	C	C6-N1-C2	-5.05	118.28	120.30
1	YA	31	C	C6-N1-C2	-5.04	118.28	120.30
1	YA	230	U	C5-C6-N1	5.04	125.22	122.70
1	YA	1528	A	N7-C8-N9	5.04	116.32	113.80
1	YA	2455	G	C8-N9-C4	-5.04	104.38	106.40
1	YA	2712	U	C6-N1-C1'	-5.04	114.14	121.20
1	RA	783	A	C5-N7-C8	-5.04	101.38	103.90
1	RA	1741	C	C5-C6-N1	5.04	123.52	121.00
32	XA	1059	C	C6-N1-C2	-5.04	118.28	120.30
32	XA	1356	G	N7-C8-N9	5.04	115.62	113.10
1	RA	2856	C	C6-N1-C2	-5.04	118.28	120.30
32	QA	1260	C	N3-C2-O2	-5.04	118.37	121.90
1	YA	1476	C	C6-N1-C2	-5.04	118.28	120.30
1	RA	2759	G	C6-C5-N7	-5.04	127.38	130.40
1	YA	1901	A	C2-N3-C4	5.04	113.12	110.60
32	XA	536	C	C6-N1-C2	-5.04	118.28	120.30
32	XA	1447	G	C6-C5-N7	-5.04	127.38	130.40
1	YA	2336	A	C4-C5-N7	5.04	113.22	110.70
1	RA	138	G	O4'-C1'-N9	5.04	112.23	108.20
1	YA	141(A)	C	C5-C6-N1	5.04	123.52	121.00
32	XA	578	C	C6-N1-C2	-5.03	118.29	120.30
1	YA	2712	U	C6-N1-C2	-5.03	117.98	121.00
1	RA	1947	C	N3-C2-O2	-5.03	118.38	121.90
1	YA	1669	A	C2-N3-C4	5.03	113.12	110.60
1	YA	1799	G	P-O3'-C3'	5.03	125.74	119.70
1	YA	2468	G	C4-N9-C1'	5.03	133.04	126.50
1	YA	2756	U	N3-C4-O4	5.03	122.92	119.40
1	RA	335	C	C5-C6-N1	5.03	123.51	121.00
1	RA	647	G	N3-C4-N9	5.03	129.02	126.00
1	YA	2261	C	C6-N1-C2	-5.03	118.29	120.30
1	RA	2295	C	N1-C2-O2	5.03	121.92	118.90
1	YA	976	C	N1-C2-O2	5.03	121.92	118.90
32	XA	165	C	C5-C6-N1	5.03	123.51	121.00
32	XA	1259	C	C6-N1-C2	-5.03	118.29	120.30
32	XA	1397	C	C2-N1-C1'	5.03	124.33	118.80
1	RA	985	C	C5-C6-N1	5.03	123.51	121.00
1	YA	1433	U	C6-N1-C2	-5.03	117.98	121.00
1	YA	2254	C	C5-C6-N1	5.03	123.51	121.00
1	YA	564	C	C6-N1-C2	-5.02	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1063	G	N1-C2-N2	-5.02	111.68	116.20
2	RB	81	G	C8-N9-C1'	-5.02	120.47	127.00
1	YA	857	C	C2-N1-C1'	5.02	124.32	118.80
32	XA	705	U	C6-N1-C2	-5.02	117.99	121.00
32	XA	233	C	C6-N1-C2	-5.02	118.29	120.30
1	RA	436	C	N1-C2-O2	5.02	121.91	118.90
1	YA	2461	C	N1-C2-O2	5.02	121.91	118.90
1	YA	2686	G	C6-C5-N7	-5.02	127.39	130.40
32	XA	435	C	N1-C2-O2	5.02	121.91	118.90
32	XA	754	C	C6-N1-C1'	-5.02	114.78	120.80
1	RA	834	C	C5-C6-N1	5.02	123.51	121.00
1	RA	2699	C	C6-N1-C2	-5.02	118.29	120.30
1	YA	231	C	C5-C6-N1	5.02	123.51	121.00
1	YA	665	C	C5-C6-N1	5.02	123.51	121.00
1	YA	974(A)	C	N1-C2-O2	5.02	121.91	118.90
1	YA	1476	C	C5-C6-N1	5.02	123.51	121.00
1	YA	621	A	C8-N9-C4	-5.01	103.79	105.80
1	RA	991	C	C5-C6-N1	5.01	123.51	121.00
1	RA	1644	C	N1-C2-O2	5.01	121.91	118.90
1	RA	2114	A	C2-N3-C4	5.01	113.11	110.60
1	RA	2248	C	C5-C6-N1	5.01	123.51	121.00
14	RS	56	LEU	CA-CB-CG	5.01	126.83	115.30
1	YA	74	A	C5-N7-C8	-5.01	101.39	103.90
32	XA	1447	G	N3-C4-N9	5.01	129.01	126.00
1	RA	198	C	N1-C2-O2	5.01	121.91	118.90
1	RA	1065	U	P-O3'-C3'	5.01	125.71	119.70
1	YA	2846	G	C8-N9-C4	-5.01	104.40	106.40
1	RA	2210	G	C4-N9-C1'	5.01	133.01	126.50
32	QA	1132	C	N1-C2-O2	5.01	121.90	118.90
32	XA	137	C	C5-C6-N1	5.01	123.50	121.00
1	YA	1899	G	C6-C5-N7	-5.00	127.40	130.40
32	XA	972	C	N1-C2-O2	5.00	121.90	118.90
1	RA	621	A	C4-C5-N7	5.00	113.20	110.70
1	RA	2439	A	C5-N7-C8	-5.00	101.40	103.90
13	RR	75	LEU	CA-CB-CG	5.00	126.81	115.30
32	QA	23	C	C6-N1-C2	-5.00	118.30	120.30
32	XA	1362(A)	C	N1-C2-O2	5.00	121.90	118.90
1	RA	1675	C	N1-C2-O2	5.00	121.90	118.90
1	YA	556	G	C6-C5-N7	-5.00	127.40	130.40

There are no chirality outliers.

All (749) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	15	VAL	Peptide
33	QB	155	LEU	Peptide
33	QB	156	LYS	Peptide
33	QB	16	HIS	Peptide
33	QB	166	ASP	Peptide
33	QB	18	GLY	Peptide
33	QB	19	HIS	Peptide
33	QB	21	ARG	Peptide
33	QB	230	VAL	Peptide
33	QB	232	PRO	Peptide
33	QB	233	SER	Peptide
33	QB	234	PRO	Peptide
33	QB	237	ALA	Peptide
33	QB	239	VAL	Peptide
33	QB	34	ALA	Peptide
33	QB	35	GLU	Peptide
33	QB	38	GLY	Peptide
33	QB	64	ARG	Peptide
33	QB	66	GLY	Peptide
33	QB	95	GLN	Peptide
33	QB	96	ARG	Peptide
34	QC	11	ARG	Peptide
34	QC	14	ILE	Peptide
34	QC	144	SER	Peptide
34	QC	166	GLU	Peptide
34	QC	168	ALA	Peptide
34	QC	187	ALA	Peptide
34	QC	189	ALA	Peptide
34	QC	204	LEU	Peptide
34	QC	44	GLU	Peptide
34	QC	51	GLY	Peptide
34	QC	53	ALA	Peptide
34	QC	59	ARG	Peptide
34	QC	62	ASP	Peptide
34	QC	78	GLY	Peptide
35	QD	146	ILE	Peptide
35	QD	154	ASN	Peptide
35	QD	155	LEU	Peptide
35	QD	175	SER	Peptide
35	QD	198	VAL	Peptide
35	QD	2	GLY	Peptide
35	QD	208	SER	Peptide
35	QD	3	ARG	Peptide

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Mol	Chain	Res	Type	Group
35	QD	38	TYR	Peptide
35	QD	47	ARG	Peptide
35	QD	49	ARG	Peptide
35	QD	69	GLY	Peptide
35	QD	88	VAL	Peptide
36	QE	103	GLY	Peptide
36	QE	154	GLY	Peptide
36	QE	22	GLY	Peptide
36	QE	68	GLU	Peptide
36	QE	95	ALA	Peptide
37	QF	58	GLY	Peptide
37	QF	71	ARG	Peptide
38	QG	11	GLN	Peptide
38	QG	113	GLU	Peptide
38	QG	152	ALA	Peptide
38	QG	30	ILE	Peptide
38	QG	50	ILE	Peptide
38	QG	54	THR	Peptide
38	QG	55	GLY	Peptide
38	QG	7	ALA	Peptide
38	QG	8	GLU	Peptide
39	QH	101	PRO	Peptide
39	QH	137	VAL	Peptide
39	QH	55	GLY	Peptide
39	QH	96	GLY	Peptide
40	QI	100	GLY	Peptide
40	QI	102	LEU	Peptide
40	QI	127	LYS	Peptide
40	QI	28	VAL	Peptide
40	QI	29	ASN	Peptide
40	QI	4	TYR	Peptide
40	QI	42	ARG	Peptide
40	QI	6	GLY	Peptide
40	QI	69	GLY	Peptide
40	QI	92	TYR	Peptide
40	QI	99	LEU	Peptide
41	QJ	35	SER	Peptide
41	QJ	41	PRO	Peptide
41	QJ	5	ARG	Peptide
41	QJ	76	ASN	Peptide
41	QJ	85	LEU	Peptide
41	QJ	90	LEU	Peptide

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Mol	Chain	Res	Type	Group
42	QK	38	ASN	Peptide
42	QK	42	TRP	Peptide
42	QK	90	GLY	Peptide
42	QK	91	ARG	Peptide
43	QL	103	GLY	Peptide
43	QL	104	VAL	Peptide
43	QL	118	SER	Peptide
43	QL	120	TYR	Peptide
43	QL	127	GLU	Peptide
43	QL	17	LYS	Peptide
43	QL	29	GLY	Peptide
43	QL	47	LYS	Peptide
44	QM	104	ARG	Peptide
44	QM	105	THR	Peptide
44	QM	107	ALA	Peptide
44	QM	108	ARG	Peptide
44	QM	113	PRO	Peptide
44	QM	118	ALA	Peptide
44	QM	120	LYS	Peptide
44	QM	25	ILE	Peptide
44	QM	26	GLY	Peptide
44	QM	3	ARG	Peptide
44	QM	36	LYS	Peptide
44	QM	48	LEU	Peptide
44	QM	5	ALA	Peptide
44	QM	66	LEU	Peptide
44	QM	7	VAL	Peptide
44	QM	97	PRO	Peptide
44	QM	99	ARG	Peptide
45	QN	14	PRO	Peptide
45	QN	15	LYS	Peptide
45	QN	16	PHE	Peptide
45	QN	42	ILE	Peptide
45	QN	53	LEU	Peptide
45	QN	54	PRO	Peptide
46	QO	3	ILE	Peptide
46	QO	88	ARG	Peptide
47	QP	2	VAL	Peptide
47	QP	36	ILE	Peptide
47	QP	62	VAL	Peptide
47	QP	77	ALA	Peptide
47	QP	82	GLN	Peptide

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Mol	Chain	Res	Type	Group
47	QP	83	GLU	Peptide
48	QQ	100	LYS	Peptide
48	QQ	66	SER	Peptide
49	QR	21	LYS	Peptide
49	QR	26	LEU	Peptide
49	QR	54	ARG	Peptide
49	QR	87	ARG	Peptide
50	QS	10	PHE	Peptide
50	QS	11	VAL	Peptide
50	QS	27	GLU	Peptide
50	QS	41	VAL	Peptide
50	QS	5	LEU	Peptide
50	QS	56	GLN	Peptide
50	QS	62	ILE	Peptide
50	QS	67	VAL	Peptide
50	QS	68	GLY	Peptide
50	QS	8	GLY	Peptide
50	QS	9	VAL	Peptide
51	QT	101	GLY	Peptide
51	QT	11	SER	Peptide
51	QT	12	ALA	Peptide
51	QT	13	LEU	Peptide
51	QT	48	LYS	Peptide
51	QT	49	ALA	Peptide
51	QT	72	LEU	Peptide
51	QT	73	HIS	Peptide
51	QT	94	ALA	Peptide
51	QT	95	ALA	Peptide
51	QT	96	GLY	Peptide
51	QT	97	ALA	Peptide
51	QT	98	PRO	Peptide
52	QU	21	TYR	Peptide
52	QU	23	PRO	Peptide
52	QU	8	THR	Peptide
22	R0	42	GLY	Peptide
22	R0	43	THR	Peptide
23	R1	53	VAL	Peptide
23	R1	54	ALA	Peptide
23	R1	80	LEU	Peptide
23	R1	85	LEU	Peptide
23	R1	87	PRO	Peptide
23	R1	96	LYS	Peptide

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Mol	Chain	Res	Type	Group
24	R2	14	ARG	Peptide
24	R2	15	LYS	Peptide
24	R2	4	SER	Peptide
24	R2	43	GLN	Peptide
24	R2	44	LEU	Peptide
24	R2	46	GLN	Peptide
24	R2	69	ARG	Peptide
24	R2	70	GLN	Peptide
24	R2	71	ASN	Peptide
25	R3	2	PRO	Peptide
25	R3	36	VAL	Peptide
25	R3	48	GLU	Peptide
26	R4	43	TYR	Peptide
26	R4	44	THR	Peptide
26	R4	45	GLY	Peptide
26	R4	46	GLN	Peptide
26	R4	48	ARG	Peptide
26	R4	57	GLU	Peptide
26	R4	60	GLN	Peptide
26	R4	61	ARG	Peptide
26	R4	62	ARG	Peptide
26	R4	65	ASP	Peptide
27	R5	5	PRO	Peptide
29	R7	46	VAL	Peptide
29	R7	6	GLN	Peptide
30	R8	27	THR	Peptide
30	R8	28	GLY	Peptide
30	R8	29	LYS	Peptide
30	R8	51	ALA	Peptide
30	R8	52	LYS	Peptide
30	R8	62	LEU	Peptide
30	R8	64	TYR	Peptide
3	RD	119	ALA	Peptide
3	RD	120	GLY	Peptide
3	RD	126	GLN	Peptide
3	RD	2	ALA	Peptide
3	RD	246	PRO	Peptide
3	RD	259	THR	Peptide
3	RD	272	ALA	Peptide
4	RE	130	GLY	Peptide
4	RE	142	GLY	Peptide
4	RE	161	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	RE	180	ASN	Peptide
4	RE	186	GLY	Peptide
4	RE	187	ALA	Peptide
4	RE	29	GLY	Peptide
4	RE	70	ALA	Peptide
4	RE	71	GLY	Peptide
4	RE	74	PRO	Peptide
5	RF	127	GLU	Peptide
5	RF	128	ALA	Peptide
5	RF	130	ALA	Peptide
5	RF	135	LYS	Peptide
5	RF	19	GLU	Peptide
5	RF	196	LEU	Peptide
5	RF	198	ALA	Peptide
5	RF	25	PRO	Peptide
5	RF	47	GLY	Peptide
5	RF	65	TRP	Peptide
5	RF	83	PHE	Peptide
5	RF	85	GLY	Peptide
5	RF	91	GLY	Peptide
6	RG	111	LEU	Peptide
6	RG	112	PRO	Peptide
6	RG	119	GLY	Peptide
6	RG	126	ASP	Peptide
6	RG	127	GLY	Peptide
6	RG	128	ARG	Peptide
6	RG	134	GLY	Peptide
6	RG	136	ARG	Peptide
6	RG	159	VAL	Peptide
6	RG	180	PHE	Peptide
6	RG	2	PRO	Peptide
6	RG	36	LYS	Peptide
6	RG	52	ILE	Peptide
6	RG	82	LEU	Peptide
6	RG	85	GLY	Peptide
6	RG	95	ARG	Peptide
6	RG	97	ASP	Peptide
7	RH	10	PRO	Peptide
7	RH	124	GLU	Peptide
7	RH	126	PRO	Peptide
7	RH	128	PRO	Peptide
7	RH	129	THR	Peptide

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Mol	Chain	Res	Type	Group
7	RH	13	LYS	Peptide
7	RH	130	ARG	Peptide
7	RH	150	ALA	Peptide
7	RH	151	ILE	Peptide
7	RH	152	ARG	Peptide
7	RH	153	LYS	Peptide
7	RH	16	SER	Peptide
7	RH	161	GLY	Peptide
7	RH	173	PRO	Peptide
7	RH	174	GLY	Peptide
7	RH	22	GLY	Peptide
7	RH	39	PRO	Peptide
7	RH	55	PRO	Peptide
7	RH	7	LEU	Peptide
7	RH	8	PRO	Peptide
7	RH	82	GLY	Peptide
7	RH	87	LEU	Peptide
7	RH	93	GLY	Peptide
7	RH	98	LEU	Peptide
8	RI	10	GLU	Peptide
8	RI	11	ASN	Peptide
8	RI	122	GLU	Mainchain
8	RI	131	LYS	Peptide
8	RI	132	PRO	Peptide
8	RI	133	HIS	Peptide
8	RI	134	PRO	Peptide
8	RI	14	ASP	Peptide
8	RI	142	VAL	Peptide
8	RI	144	VAL	Peptide
8	RI	145	VAL	Peptide
8	RI	16	GLY	Peptide
8	RI	9	LEU	Peptide
9	RN	113	GLY	Peptide
9	RN	114	ARG	Peptide
9	RN	127	ASP	Peptide
9	RN	130	HIS	Peptide
9	RN	132	ALA	Peptide
9	RN	134	ARG	Peptide
9	RN	17	ASP	Peptide
9	RN	21	LYS	Peptide
9	RN	22	THR	Peptide
9	RN	34	LEU	Peptide

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Mol	Chain	Res	Type	Group
10	RO	28	SER	Peptide
10	RO	96	THR	Peptide
11	RP	106	LEU	Peptide
11	RP	107	LYS	Peptide
11	RP	115	LEU	Peptide
11	RP	117	GLU	Peptide
11	RP	118	GLY	Peptide
11	RP	144	GLU	Peptide
11	RP	147	LEU	Peptide
11	RP	21	ARG	Peptide
11	RP	22	GLY	Peptide
11	RP	28	GLY	Peptide
11	RP	35	HIS	Peptide
11	RP	37	GLY	Peptide
11	RP	43	GLY	Peptide
11	RP	58	THR	Peptide
11	RP	63	PRO	Peptide
11	RP	66	GLY	Peptide
11	RP	67	MET	Peptide
11	RP	72	PRO	Peptide
11	RP	97	PRO	Peptide
12	RQ	1	MET	Peptide
12	RQ	104	PHE	Peptide
12	RQ	108	GLY	Peptide
12	RQ	112	GLU	Peptide
12	RQ	23	GLY	Peptide
12	RQ	24	GLY	Peptide
12	RQ	4	PRO	Peptide
12	RQ	82	ARG	Peptide
12	RQ	88	GLY	Peptide
12	RQ	89	ASN	Peptide
12	RQ	91	GLU	Peptide
13	RR	1	MET	Peptide
13	RR	103	ARG	Peptide
13	RR	104	ARG	Peptide
13	RR	2	ARG	Peptide
13	RR	3	HIS	Peptide
13	RR	75	LEU	Peptide
14	RS	105	ALA	Peptide
14	RS	106	ARG	Peptide
14	RS	109	GLY	Peptide
14	RS	42	ASP	Peptide

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Mol	Chain	Res	Type	Group
14	RS	5	THR	Peptide
14	RS	56	LEU	Peptide
14	RS	61	ASN	Peptide
14	RS	81	GLY	Peptide
15	RT	111	ARG	Peptide
15	RT	135	ALA	Peptide
15	RT	136	GLN	Peptide
15	RT	17	THR	Peptide
15	RT	58	ASN	Peptide
15	RT	93	ARG	Peptide
16	RU	91	ASP	Peptide
16	RU	95	LEU	Peptide
16	RU	96	ALA	Peptide
17	RV	100	ARG	Peptide
17	RV	15	GLU	Peptide
17	RV	23	GLU	Peptide
17	RV	40	LEU	Peptide
17	RV	52	VAL	Peptide
17	RV	54	GLY	Peptide
17	RV	72	VAL	Peptide
17	RV	9	GLY	Peptide
18	RW	110	LYS	Peptide
18	RW	64	MET	Peptide
18	RW	90	ARG	Peptide
18	RW	91	GLY	Peptide
18	RW	92	ARG	Peptide
19	RX	22	ALA	Peptide
19	RX	28	PHE	Peptide
19	RX	70	LEU	Peptide
19	RX	84	ALA	Peptide
19	RX	93	GLU	Peptide
20	RY	39	VAL	Peptide
20	RY	51	VAL	Peptide
20	RY	52	SER	Peptide
20	RY	62	GLU	Peptide
20	RY	9	LYS	Peptide
21	RZ	10	ARG	Peptide
21	RZ	11	GLU	Peptide
21	RZ	12	GLY	Peptide
21	RZ	125	LEU	Peptide
21	RZ	131	ARG	Peptide
21	RZ	136	PHE	Peptide

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Mol	Chain	Res	Type	Group
21	RZ	148	ASP	Peptide
21	RZ	155	LEU	Peptide
21	RZ	160	GLY	Peptide
21	RZ	162	GLU	Peptide
21	RZ	165	VAL	Peptide
21	RZ	167	PRO	Peptide
21	RZ	168	GLU	Peptide
21	RZ	191	VAL	Peptide
21	RZ	37	VAL	Peptide
21	RZ	51	ALA	Peptide
21	RZ	52	SER	Peptide
21	RZ	62	PRO	Peptide
21	RZ	63	ASP	Peptide
21	RZ	95	PRO	Peptide
21	RZ	96	VAL	Peptide
21	RZ	97	GLU	Peptide
33	XB	111	ARG	Peptide
33	XB	128	GLU	Peptide
33	XB	15	VAL	Peptide
33	XB	19	HIS	Peptide
33	XB	194	PRO	Peptide
33	XB	21	ARG	Peptide
33	XB	227	GLY	Peptide
33	XB	230	VAL	Peptide
33	XB	232	PRO	Peptide
33	XB	233	SER	Peptide
33	XB	236	TYR	Peptide
33	XB	237	ALA	Peptide
33	XB	35	GLU	Peptide
33	XB	36	ARG	Peptide
33	XB	60	ASP	Peptide
33	XB	64	ARG	Peptide
33	XB	66	GLY	Peptide
33	XB	89	GLY	Peptide
34	XC	11	ARG	Peptide
34	XC	156	ARG	Peptide
34	XC	163	ALA	Peptide
34	XC	164	ARG	Peptide
34	XC	166	GLU	Peptide
34	XC	189	ALA	Peptide
34	XC	193	TYR	Peptide
34	XC	194	GLY	Peptide

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Mol	Chain	Res	Type	Group
34	XC	196	LEU	Peptide
34	XC	23	TYR	Peptide
34	XC	25	GLY	Peptide
34	XC	41	GLY	Peptide
34	XC	47	LEU	Peptide
34	XC	49	SER	Peptide
34	XC	5	ILE	Peptide
34	XC	62	ASP	Peptide
34	XC	76	VAL	Peptide
35	XD	124	GLY	Peptide
35	XD	130	GLY	Peptide
35	XD	153	ARG	Peptide
35	XD	154	ASN	Peptide
35	XD	157	LEU	Peptide
35	XD	167	GLY	Peptide
35	XD	168	ARG	Peptide
35	XD	170	VAL	Peptide
35	XD	188	LEU	Peptide
35	XD	194	LEU	Peptide
35	XD	69	GLY	Peptide
35	XD	87	GLY	Peptide
35	XD	88	VAL	Peptide
36	XE	153	LYS	Peptide
36	XE	154	GLY	Peptide
36	XE	22	GLY	Peptide
36	XE	68	GLU	Peptide
36	XE	72	GLN	Peptide
37	XF	99	ALA	Peptide
38	XG	113	GLU	Peptide
38	XG	44	TYR	Peptide
38	XG	53	LYS	Peptide
38	XG	63	LYS	Peptide
38	XG	64	GLN	Peptide
38	XG	7	ALA	Peptide
39	XH	101	PRO	Peptide
39	XH	108	GLY	Peptide
39	XH	137	VAL	Peptide
39	XH	28	ALA	Peptide
39	XH	69	ARG	Peptide
39	XH	70	GLN	Peptide
39	XH	71	GLY	Peptide
39	XH	96	GLY	Peptide

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Mol	Chain	Res	Type	Group
40	XI	13	ALA	Peptide
40	XI	15	ALA	Peptide
40	XI	21	PRO	Peptide
40	XI	23	ASN	Peptide
40	XI	24	GLY	Peptide
40	XI	25	LYS	Peptide
40	XI	39	GLY	Peptide
40	XI	40	LEU	Peptide
40	XI	42	ARG	Peptide
40	XI	54	ASP	Peptide
40	XI	56	LEU	Peptide
40	XI	58	HIS	Peptide
40	XI	63	ILE	Peptide
40	XI	66	ARG	Peptide
40	XI	68	GLY	Peptide
40	XI	69	GLY	Peptide
40	XI	89	ASN	Peptide
40	XI	91	ASP	Peptide
40	XI	99	LEU	Peptide
41	XJ	30	SER	Peptide
41	XJ	32	ALA	Peptide
41	XJ	35	SER	Peptide
41	XJ	39	PRO	Peptide
41	XJ	52	GLY	Peptide
41	XJ	54	PHE	Peptide
41	XJ	80	LYS	Peptide
41	XJ	85	LEU	Peptide
41	XJ	91	PRO	Peptide
42	XK	100	ALA	Peptide
42	XK	102	GLY	Peptide
42	XK	13	GLN	Peptide
42	XK	14	VAL	Peptide
42	XK	67	ASP	Peptide
43	XL	102	ARG	Peptide
43	XL	103	GLY	Peptide
43	XL	104	VAL	Peptide
43	XL	118	SER	Peptide
43	XL	120	TYR	Peptide
43	XL	17	LYS	Peptide
43	XL	26	ALA	Peptide
43	XL	27	LEU	Peptide
43	XL	28	LYS	Peptide

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Mol	Chain	Res	Type	Group
43	XL	29	GLY	Peptide
43	XL	37	CYS	Peptide
43	XL	61	THR	Peptide
44	XM	10	PRO	Peptide
44	XM	105	THR	Peptide
44	XM	107	ALA	Peptide
44	XM	11	ARG	Peptide
44	XM	110	ARG	Peptide
44	XM	112	GLY	Peptide
44	XM	119	GLY	Peptide
44	XM	12	ASN	Peptide
44	XM	25	ILE	Peptide
44	XM	37	THR	Peptide
44	XM	38	GLY	Peptide
44	XM	58	GLU	Peptide
44	XM	59	TYR	Peptide
44	XM	66	LEU	Peptide
45	XN	15	LYS	Peptide
45	XN	16	PHE	Peptide
45	XN	3	ARG	Peptide
45	XN	42	ILE	Peptide
45	XN	8	GLU	Peptide
46	XO	19	PRO	Peptide
46	XO	20	GLY	Peptide
46	XO	87	ILE	Peptide
47	XP	15	PRO	Peptide
47	XP	19	ILE	Peptide
47	XP	37	GLY	Peptide
47	XP	46	PRO	Peptide
47	XP	62	VAL	Peptide
47	XP	82	GLN	Peptide
47	XP	83	GLU	Peptide
48	XQ	44	ALA	Peptide
48	XQ	66	SER	Peptide
48	XQ	7	THR	Peptide
48	XQ	79	SER	Peptide
49	XR	21	LYS	Peptide
49	XR	31	LEU	Peptide
49	XR	38	GLU	Peptide
49	XR	55	ARG	Peptide
50	XS	10	PHE	Peptide
50	XS	11	VAL	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
50	XS	22	LEU	Peptide
50	XS	25	LYS	Peptide
50	XS	26	GLY	Peptide
50	XS	27	GLU	Peptide
50	XS	34	TRP	Peptide
50	XS	4	SER	Peptide
50	XS	40	ILE	Peptide
50	XS	47	HIS	Peptide
50	XS	68	GLY	Peptide
50	XS	74	PHE	Peptide
50	XS	8	GLY	Peptide
50	XS	84	GLY	Peptide
51	XT	11	SER	Peptide
51	XT	12	ALA	Peptide
51	XT	48	LYS	Peptide
51	XT	49	ALA	Peptide
51	XT	60	GLU	Peptide
51	XT	72	LEU	Peptide
51	XT	73	HIS	Peptide
51	XT	75	ASN	Peptide
51	XT	8	ARG	Peptide
51	XT	94	ALA	Peptide
51	XT	96	GLY	Peptide
51	XT	97	ALA	Peptide
51	XT	98	PRO	Peptide
52	XU	11	GLY	Peptide
52	XU	19	GLY	Peptide
52	XU	21	TYR	Peptide
52	XU	23	PRO	Peptide
52	XU	25	LYS	Peptide
22	Y0	28	GLY	Peptide
22	Y0	42	GLY	Peptide
22	Y0	43	THR	Peptide
23	Y1	30	VAL	Peptide
23	Y1	84	GLY	Peptide
25	Y3	2	PRO	Peptide
26	Y4	42	PHE	Peptide
26	Y4	43	TYR	Peptide
26	Y4	44	THR	Peptide
26	Y4	45	GLY	Peptide
26	Y4	46	GLN	Peptide
26	Y4	47	GLN	Peptide

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Mol	Chain	Res	Type	Group
26	Y4	48	ARG	Peptide
26	Y4	53	GLU	Peptide
26	Y4	55	ARG	Peptide
26	Y4	56	VAL	Peptide
26	Y4	57	GLU	Peptide
26	Y4	62	ARG	Peptide
27	Y5	5	PRO	Peptide
27	Y5	59	GLU	Peptide
30	Y8	27	THR	Peptide
30	Y8	28	GLY	Peptide
30	Y8	29	LYS	Peptide
30	Y8	35	GLN	Peptide
31	Y9	5	ALA	Peptide
3	YD	106	ILE	Peptide
3	YD	110	GLY	Peptide
3	YD	191	ALA	Peptide
3	YD	192	THR	Peptide
3	YD	2	ALA	Peptide
3	YD	238	GLY	Peptide
3	YD	246	PRO	Peptide
3	YD	254	THR	Peptide
3	YD	255	LYS	Peptide
3	YD	259	THR	Peptide
4	YE	115	GLY	Peptide
4	YE	146	THR	Peptide
4	YE	153	GLY	Peptide
4	YE	185	LYS	Peptide
4	YE	20	ALA	Peptide
4	YE	202	LYS	Peptide
4	YE	204	ALA	Peptide
4	YE	52	LEU	Peptide
4	YE	57	LYS	Peptide
4	YE	71	GLY	Peptide
4	YE	74	PRO	Peptide
4	YE	81	ILE	Peptide
4	YE	89	ASP	Peptide
5	YF	127	GLU	Peptide
5	YF	128	ALA	Peptide
5	YF	132	VAL	Peptide
5	YF	196	LEU	Peptide
5	YF	198	ALA	Peptide
5	YF	47	GLY	Peptide

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Mol	Chain	Res	Type	Group
5	YF	6	VAL	Peptide
5	YF	67	GLN	Peptide
5	YF	91	GLY	Peptide
6	YG	109	VAL	Peptide
6	YG	118	ARG	Peptide
6	YG	127	GLY	Peptide
6	YG	134	GLY	Peptide
6	YG	136	ARG	Peptide
6	YG	145	THR	Peptide
6	YG	150	ASP	Peptide
6	YG	181	ARG	Peptide
6	YG	2	PRO	Peptide
6	YG	32	PRO	Peptide
6	YG	35	GLU	Peptide
6	YG	48	GLU	Peptide
6	YG	52	ILE	Peptide
6	YG	58	GLN	Peptide
6	YG	82	LEU	Peptide
6	YG	85	GLY	Peptide
6	YG	95	ARG	Peptide
6	YG	97	ASP	Peptide
7	YH	12	PRO	Peptide
7	YH	174	GLY	Peptide
7	YH	33	LEU	Peptide
7	YH	58	GLU	Peptide
7	YH	85	LYS	Peptide
8	YI	11	ASN	Peptide
8	YI	116	LEU	Peptide
8	YI	119	PRO	Peptide
8	YI	121	LYS	Peptide
8	YI	122	GLU	Peptide
8	YI	123	LEU	Peptide
8	YI	131	LYS	Peptide
8	YI	133	HIS	Peptide
8	YI	134	PRO	Peptide
8	YI	14	ASP	Peptide
8	YI	142	VAL	Peptide
8	YI	144	VAL	Peptide
8	YI	145	VAL	Peptide
8	YI	35	LEU	Peptide
8	YI	55	ALA	Peptide
8	YI	59	ALA	Peptide

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Mol	Chain	Res	Type	Group
8	YI	75	LEU	Peptide
8	YI	9	LEU	Peptide
9	YN	113	GLY	Peptide
9	YN	114	ARG	Peptide
9	YN	17	ASP	Peptide
9	YN	21	LYS	Peptide
9	YN	22	THR	Peptide
9	YN	95	PRO	Peptide
10	YO	4	PRO	Peptide
10	YO	83	ALA	Peptide
11	YP	102	ARG	Peptide
11	YP	106	LEU	Peptide
11	YP	107	LYS	Peptide
11	YP	108	LYS	Peptide
11	YP	115	LEU	Peptide
11	YP	116	GLY	Peptide
11	YP	18	ARG	Peptide
11	YP	21	ARG	Peptide
11	YP	22	GLY	Peptide
11	YP	28	GLY	Peptide
11	YP	29	LYS	Peptide
11	YP	35	HIS	Peptide
11	YP	37	GLY	Peptide
11	YP	43	GLY	Peptide
11	YP	54	GLY	Peptide
11	YP	91	PHE	Peptide
11	YP	97	PRO	Peptide
11	YP	98	GLU	Peptide
12	YQ	108	GLY	Peptide
12	YQ	20	ALA	Peptide
12	YQ	21	THR	Peptide
12	YQ	23	GLY	Peptide
12	YQ	24	GLY	Peptide
12	YQ	4	PRO	Peptide
12	YQ	40	ALA	Peptide
12	YQ	59	ARG	Peptide
13	YR	102	GLU	Peptide
13	YR	103	ARG	Peptide
13	YR	3	HIS	Peptide
13	YR	73	VAL	Peptide
13	YR	75	LEU	Peptide
14	YS	111	GLU	Peptide

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Mol	Chain	Res	Type	Group
14	YS	84	GLN	Peptide
15	YT	110	ILE	Peptide
15	YT	111	ARG	Peptide
15	YT	27	THR	Peptide
15	YT	38	ASN	Peptide
16	YU	115	ALA	Peptide
16	YU	117	GLN	Peptide
16	YU	91	ASP	Peptide
16	YU	95	LEU	Peptide
16	YU	96	ALA	Peptide
17	YV	42	GLY	Peptide
17	YV	43	GLU	Peptide
17	YV	44	LYS	Peptide
17	YV	54	GLY	Peptide
18	YW	110	LYS	Peptide
18	YW	3	ALA	Peptide
18	YW	64	MET	Peptide
18	YW	90	ARG	Peptide
18	YW	91	GLY	Peptide
19	YX	48	LYS	Peptide
19	YX	68	ARG	Peptide
19	YX	84	ALA	Peptide
19	YX	93	GLU	Peptide
20	YY	106	LEU	Peptide
20	YY	52	SER	Peptide
21	YZ	106	GLY	Peptide
21	YZ	11	GLU	Peptide
21	YZ	136	PHE	Peptide
21	YZ	159	PRO	Peptide
21	YZ	160	GLY	Peptide
21	YZ	188	ALA	Peptide
21	YZ	37	VAL	Peptide
21	YZ	50	GLN	Peptide
21	YZ	51	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	62051	0	31279	531	1
1	YA	62091	0	31300	497	0
2	RB	2573	0	1306	25	0
2	YB	2573	0	1306	16	0
3	RD	2115	0	2195	31	0
3	YD	2126	0	2208	39	0
4	RE	1563	0	1629	28	0
4	YE	1568	0	1633	30	0
5	RF	1585	0	1632	21	0
5	YF	1585	0	1632	28	0
6	RG	1474	0	1535	38	0
6	YG	1474	0	1535	26	0
7	RH	1336	0	1418	21	0
7	YH	1336	0	1418	23	1
8	RI	1136	0	1223	35	2
8	YI	1136	0	1223	21	0
9	RN	1104	0	1179	14	0
9	YN	1121	0	1194	16	0
10	RO	933	0	996	22	0
10	YO	933	0	995	14	0
11	RP	1130	0	1217	26	0
11	YP	1122	0	1206	23	0
12	RQ	1122	0	1178	48	0
12	YQ	1122	0	1179	16	0
13	RR	968	0	1033	10	0
13	YR	960	0	1021	10	0
14	RS	882	0	943	13	0
14	YS	877	0	938	9	0
15	RT	1141	0	1202	15	0
15	YT	1141	0	1202	11	0
16	RU	964	0	1022	21	0
16	YU	964	0	1022	19	0
17	RV	779	0	852	12	0
17	YV	779	0	852	17	0
18	RW	900	0	964	16	1
18	YW	900	0	964	12	0
19	RX	725	0	778	7	0
19	YX	742	0	803	9	0
20	RY	818	0	909	11	0
20	YY	818	0	909	9	2
21	RZ	1601	0	1630	43	0
21	YZ	1587	0	1622	16	0
22	R0	603	0	619	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y0	599	0	617	9	0
23	R1	763	0	848	10	0
23	Y1	729	0	802	12	0
24	R2	581	0	629	9	0
24	Y2	606	0	665	5	1
25	R3	469	0	518	7	0
25	Y3	469	0	518	12	0
26	R4	565	0	557	11	0
26	Y4	565	0	557	16	0
27	R5	459	0	476	10	0
27	Y5	459	0	476	9	0
28	R6	453	0	473	3	0
28	Y6	453	0	473	3	0
29	R7	409	0	454	6	0
29	Y7	418	0	466	4	0
30	R8	517	0	582	12	0
30	Y8	517	0	582	15	0
31	R9	302	0	332	7	0
31	Y9	307	0	335	9	0
32	QA	32469	0	16393	418	0
32	XA	32471	0	16393	441	2
33	QB	1907	0	1958	36	0
33	XB	1915	0	1969	28	0
34	QC	1605	0	1668	27	0
34	XC	1605	0	1668	28	0
35	QD	1703	0	1763	63	0
35	XD	1703	0	1764	50	0
36	QE	1155	0	1213	18	0
36	XE	1155	0	1213	11	0
37	QF	843	0	857	16	0
37	XF	843	0	857	13	0
38	QG	1257	0	1296	20	0
38	XG	1257	0	1296	24	0
39	QH	1108	0	1165	17	0
39	XH	1108	0	1165	11	0
40	QI	1010	0	1037	25	0
40	XI	998	0	1024	28	0
41	QJ	801	0	849	21	0
41	XJ	777	0	816	24	0
42	QK	864	0	881	15	0
42	XK	864	0	881	12	0
43	QL	975	0	1062	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	XL	956	0	1046	18	0
44	QM	955	0	1021	25	0
44	XM	946	0	1008	32	0
45	QN	492	0	529	10	0
45	XN	492	0	529	17	0
46	QO	734	0	771	11	0
46	XO	729	0	768	14	0
47	QP	705	0	725	12	0
47	XP	705	0	725	11	0
48	QQ	834	0	904	16	0
48	XQ	834	0	904	15	0
49	QR	574	0	644	9	0
49	XR	574	0	644	9	0
50	QS	665	0	686	16	0
50	XS	674	0	699	16	0
51	QT	763	0	861	12	0
51	XT	763	0	861	16	0
52	QU	217	0	234	9	0
52	XU	217	0	234	10	0
53	QV	365	0	186	5	0
53	XV	322	0	164	6	0
54	QX	389	0	197	27	0
54	XX	412	0	208	12	0
55	QA	66	0	0	0	0
55	QF	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	1	0	0	0	0
55	R5	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	485	0	0	0	0
55	RB	8	0	0	0	0
55	RE	2	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	2	0	0	0	0
55	RQ	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	XA	87	0	0	0	0
55	XE	1	0	0	0	0
55	XL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	510	0	0	0	0
55	YB	7	0	0	0	0
55	YD	1	0	0	0	0
55	YE	4	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	1	0	0	0	0
56	QN	1	0	0	0	0
56	R4	1	0	0	0	0
56	R5	1	0	0	0	0
56	R6	1	0	0	0	0
56	R9	1	0	0	0	0
56	RY	1	0	0	0	0
56	XN	1	0	0	0	0
56	Y4	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	3	0
All	All	290035	0	196997	3129	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (3129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1535:C:N4	54:QX:9:G:C2	1.91	1.37
32:QA:1535:C:N4	54:QX:9:G:N2	1.78	1.30
17:YV:49:THR:OG1	17:YV:50:PRO:HD2	1.30	1.25
21:RZ:182:LYS:O	21:RZ:186:GLU:HG2	1.39	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1535:C:C4	54:QX:9:G:N2	2.07	1.22
17:YV:49:THR:OG1	17:YV:50:PRO:CD	1.88	1.18
32:QA:1534:A:H1'	54:QX:10:G:H22	1.15	1.07
8:RI:120:ILE:HD11	8:RI:126:TYR:CE2	1.89	1.06
32:XA:356:A:H2	32:XA:368:U:O2	1.37	1.05
1:RA:2135:A:H62	1:RA:2156:G:N2	1.55	1.04
1:RA:2135:A:N6	1:RA:2156:G:H21	1.56	1.03
35:XD:20:TYR:HE1	35:XD:106:TYR:OH	1.41	1.02
44:XM:2:ALA:O	44:XM:9:ILE:HD12	1.61	1.01
12:RQ:56:ARG:HD2	21:RZ:180:VAL:HG11	1.37	1.01
32:XA:452:A:N6	32:XA:480:U:H3	1.59	1.00
17:YV:49:THR:CB	17:YV:50:PRO:CD	2.39	1.00
17:YV:49:THR:CB	17:YV:50:PRO:HD3	1.92	1.00
1:YA:1359:A:N6	1:YA:1372:U:H3	1.60	0.99
17:YV:49:THR:HB	17:YV:50:PRO:HD3	1.44	0.97
32:XA:438:G:H21	32:XA:496:A:H62	1.02	0.96
7:YH:3:ARG:HE	7:YH:54:ARG:NH1	1.62	0.96
12:RQ:56:ARG:HD2	21:RZ:180:VAL:CG1	1.97	0.94
8:RI:77:LEU:HD11	8:RI:79:ILE:HD11	1.46	0.93
1:YA:2701:C:H3'	1:YA:2702:U:H5''	1.50	0.93
32:XA:992:U:H3	32:XA:1044:A:H62	0.97	0.92
3:YD:258:LYS:HE2	3:YD:273:ARG:HH12	1.31	0.92
35:QD:31:CYS:SG	35:QD:31:CYS:O	2.28	0.91
12:RQ:60:ARG:HH11	21:RZ:177:PRO:HG3	1.34	0.91
32:XA:356:A:C2	32:XA:368:U:O2	2.22	0.91
8:RI:120:ILE:HD11	8:RI:126:TYR:CD2	2.06	0.91
1:YA:2099:U:H3	1:YA:2190:G:H1	0.98	0.91
25:Y3:10:LYS:NZ	25:Y3:15:TYR:OH	2.05	0.90
12:RQ:56:ARG:CD	21:RZ:180:VAL:CG1	2.50	0.89
32:QA:1535:C:C5	54:QX:9:G:N2	2.38	0.89
35:XD:20:TYR:CE1	35:XD:106:TYR:OH	2.26	0.88
12:RQ:60:ARG:NH1	21:RZ:177:PRO:HG3	1.88	0.88
1:YA:1607:C:N4	1:YA:1622:G:OP2	2.07	0.88
32:QA:1534:A:C1'	54:QX:10:G:H22	1.86	0.88
32:QA:429:U:O3'	35:QD:22:LYS:NZ	2.06	0.88
1:RA:2788:C:O2'	1:RA:2809:A:N3	2.07	0.88
1:RA:2245:U:H5'	1:RA:2246:G:H5'	1.55	0.87
35:XD:31:CYS:SG	35:XD:31:CYS:O	2.33	0.87
32:XA:992:U:H3	32:XA:1044:A:N6	1.72	0.86
3:YD:274:ARG:HG3	3:YD:274:ARG:HH11	1.39	0.86
32:XA:438:G:H21	32:XA:496:A:N6	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:XD:20:TYR:HE1	35:XD:106:TYR:HH	0.92	0.86
35:XD:21:LEU:HD12	57:XD:301:SF4:S1	2.16	0.85
32:XA:438:G:N2	32:XA:496:A:H62	1.74	0.85
1:RA:2096:U:H3	1:RA:2193:G:H1	1.25	0.84
35:QD:19:LEU:HD22	35:QD:67:ILE:CG1	2.08	0.84
32:QA:410:G:H21	32:QA:432:A:H62	1.23	0.84
32:XA:180:U:H3	32:XA:195:A:H62	1.26	0.84
32:XA:56:U:H2'	32:XA:57:G:H8	1.44	0.82
32:QA:1532:U:C6	54:QX:10:G:O6	2.33	0.81
1:RA:1433:U:H3	1:RA:1560:G:H1	1.27	0.81
32:XA:62:U:H3	32:XA:105:G:H1	1.29	0.81
7:YH:3:ARG:HD2	7:YH:54:ARG:HH12	1.45	0.80
17:YV:49:THR:HG1	17:YV:50:PRO:HD2	1.43	0.80
12:RQ:56:ARG:HD3	21:RZ:180:VAL:HG12	1.62	0.80
7:YH:3:ARG:CD	7:YH:54:ARG:HH12	1.95	0.80
32:QA:150:C:H42	32:QA:171:A:H62	1.28	0.80
32:QA:1539:C:H42	54:QX:5:A:H61	1.30	0.80
1:RA:1069:A:H5'	1:RA:1096:A:H5'	1.63	0.80
32:QA:1534:A:H1'	54:QX:10:G:N2	1.96	0.79
12:RQ:56:ARG:CD	21:RZ:180:VAL:HG11	2.13	0.79
8:RI:77:LEU:HD23	8:RI:140:LEU:CB	2.11	0.79
1:RA:1264:G:OP1	27:R5:19:ARG:NH2	2.15	0.79
1:YA:996:A:OP2	16:YU:92:ARG:NH2	2.16	0.79
7:YH:3:ARG:NE	7:YH:54:ARG:NH1	2.31	0.78
54:QX:10:G:H2'	54:QX:11:U:H5	1.48	0.78
1:RA:676:A:H8	1:RA:2069:G:H21	1.31	0.78
1:YA:2096:U:H3	1:YA:2193:G:H1	1.30	0.78
35:QD:19:LEU:HD22	35:QD:67:ILE:HG13	1.66	0.77
1:RA:517:C:OP1	27:R5:16:ARG:NH2	2.16	0.77
1:RA:1607:C:N4	1:RA:1622:G:OP2	2.18	0.77
35:XD:32:ALA:HB3	57:XD:301:SF4:S3	2.25	0.77
1:RA:1479:G:OP2	1:RA:1510:A:N6	2.18	0.77
1:RA:2701:C:H3'	1:RA:2702:U:H5''	1.65	0.76
2:YB:8:U:H3	2:YB:112:G:H1	1.32	0.76
32:XA:686:U:H1'	42:XK:42:TRP:HE1	1.50	0.76
1:RA:1102:C:H2'	1:RA:1103:A:H8	1.49	0.76
1:RA:1094:U:OP1	1:RA:1096:A:N6	2.19	0.76
3:YD:258:LYS:CE	3:YD:273:ARG:HH12	1.98	0.76
32:XA:978:A:OP2	32:XA:1362(A):C:N4	2.20	0.75
32:XA:261:U:OP2	51:XT:79:ARG:NH2	2.19	0.75
32:QA:1372:U:H5''	40:QI:71:SER:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:139:G:N2	1:RA:141:A:C6	2.53	0.75
35:QD:20:TYR:CE2	37:XF:15:ASP:CB	2.70	0.74
12:RQ:62:GLY:HA2	21:RZ:116:VAL:HG21	1.67	0.74
3:YD:274:ARG:NH1	3:YD:274:ARG:HG3	1.97	0.74
1:RA:2135:A:H62	1:RA:2156:G:H21	0.81	0.74
1:RA:31:C:O2'	1:RA:1238:G:OP1	2.05	0.74
1:RA:2882:A:OP1	13:RR:96:ARG:NH1	2.19	0.74
32:QA:1536:C:H42	54:QX:8:A:H61	1.35	0.74
12:RQ:60:ARG:NH1	21:RZ:177:PRO:CG	2.50	0.74
32:XA:180:U:H3	32:XA:195:A:N6	1.85	0.74
35:XD:26:CYS:HA	57:XD:301:SF4:S2	2.27	0.74
32:QA:1373:G:H5'	38:QG:36:LYS:HG2	1.70	0.74
1:YA:1693:U:O2'	3:YD:14:ARG:NH2	2.21	0.74
32:XA:544:G:OP1	35:XD:59:ARG:NH2	2.21	0.73
1:RA:27:G:N2	1:RA:513:A:OP2	2.20	0.73
32:XA:12:U:H3	32:XA:22:G:H1	1.36	0.73
1:RA:299:A:N3	1:RA:319:C:O2'	2.21	0.73
1:YA:265:A:N6	1:YA:427:U:O2'	2.22	0.73
1:RA:2392:A:OP2	1:RA:2422:A:N6	2.22	0.73
1:YA:517:C:OP1	27:Y5:16:ARG:NH2	2.22	0.73
1:YA:1264:G:OP1	27:Y5:19:ARG:NH2	2.18	0.73
32:QA:316:G:OP2	32:QA:351:G:O2'	2.06	0.72
39:XH:7:ALA:HB2	39:XH:85:ARG:HD3	1.71	0.72
1:RA:1165:U:H3	1:RA:1184:G:H1	1.36	0.72
25:Y3:15:TYR:CE2	25:Y3:53:LEU:HD21	2.23	0.72
35:QD:8:VAL:HG11	35:QD:21:LEU:HB2	1.72	0.72
32:XA:388:G:O2'	32:XA:389:A:OP2	2.06	0.72
1:YA:1359:A:N7	1:YA:1372:U:O4	2.23	0.72
33:QB:185:ILE:HG22	33:QB:199:TYR:HB2	1.72	0.72
1:RA:301:G:OP2	20:RY:84:ARG:NH2	2.23	0.72
1:YA:2304:G:H22	1:YA:2312:U:H3	1.36	0.72
1:YA:2808:U:C2	1:YA:2892:A:N6	2.56	0.71
35:XD:8:VAL:HG12	35:XD:21:LEU:HD13	1.70	0.71
1:YA:993:G:OP1	16:YU:50:ARG:NH2	2.24	0.71
1:YA:2621:A:HO2'	4:YE:159:HIS:HD1	1.38	0.71
1:YA:819:A:OP2	1:YA:1187:G:N2	2.23	0.71
1:YA:2712:U:HO2'	1:YA:2712(A):A:H8	1.38	0.71
54:QX:10:G:H2'	54:QX:11:U:C5	2.26	0.71
7:YH:3:ARG:NE	7:YH:54:ARG:HH12	1.87	0.71
51:QT:54:LYS:HD2	51:QT:57:ARG:HH22	1.56	0.71
32:QA:346:G:H1'	32:QA:347:G:H5'	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:790:A:OP1	53:XV:38:A:O2'	2.09	0.71
1:YA:24:G:O2'	18:YW:78:GLU:O	2.09	0.71
32:QA:1009:G:H1	32:QA:1020:U:H3	0.77	0.70
32:QA:1306:A:N6	32:QA:1331:G:O2'	2.24	0.70
1:YA:1823:G:OP1	3:YD:54:ARG:NH1	2.24	0.70
32:QA:954:G:H21	32:QA:1227:A:H62	1.38	0.70
1:RA:572:A:OP2	17:RV:78:LYS:NZ	2.23	0.70
8:RI:120:ILE:CD1	8:RI:126:TYR:CD2	2.73	0.70
40:XI:53:VAL:HG23	40:XI:55:ALA:H	1.55	0.70
1:RA:139:G:N2	1:RA:141:A:N6	2.40	0.70
32:QA:410:G:N2	32:QA:432:A:H62	1.89	0.70
1:RA:993:G:OP1	16:RU:50:ARG:NH2	2.24	0.70
42:QK:86:GLY:H	42:QK:112:THR:HG22	1.57	0.70
32:XA:152:A:H62	32:XA:169:C:N4	1.90	0.70
35:QD:19:LEU:CD2	35:QD:67:ILE:CG1	2.70	0.70
8:RI:77:LEU:CD2	8:RI:140:LEU:HB2	2.22	0.70
32:XA:201:C:H42	32:XA:216:G:H1	1.40	0.70
32:QA:514:C:H2'	32:QA:515:G:H8	1.58	0.69
32:XA:56:U:H2'	32:XA:57:G:C8	2.26	0.69
32:QA:1141:C:H2'	32:QA:1142:G:H8	1.58	0.69
1:RA:1980:G:O2'	1:RA:1982:C:OP2	2.10	0.69
1:YA:2680:C:H5'	4:YE:189:PRO:HA	1.74	0.69
1:RA:259:G:H21	1:RA:621:A:H8	1.39	0.69
1:RA:819:A:OP2	1:RA:1187:G:N2	2.26	0.69
32:XA:1157:A:N7	32:XA:1178:G:N2	2.41	0.69
1:RA:300:A:OP1	20:RY:86:ARG:NH2	2.26	0.69
32:QA:490:G:OP2	35:QD:132:ARG:NH2	2.26	0.68
1:YA:676:A:H8	1:YA:2069:G:H21	1.41	0.68
1:YA:2788:C:OP1	4:YE:61:ARG:NH2	2.26	0.68
35:QD:32:ALA:O	35:QD:35:ARG:N	2.27	0.68
35:QD:19:LEU:HD22	35:QD:67:ILE:HG12	1.76	0.68
32:XA:1269:A:OP1	52:XU:24:ARG:NH1	2.27	0.68
32:XA:972:C:OP2	41:XJ:57:LYS:NZ	2.26	0.68
32:QA:12:U:H3	32:QA:22:G:H1	1.40	0.68
43:XL:60:LEU:HD12	43:XL:62:SER:H	1.59	0.68
1:RA:141:A:H8	1:RA:1595:G:H21	1.39	0.68
1:YA:2521:C:O2'	1:YA:2564:A:N3	2.26	0.68
1:YA:1566:A:OP1	3:YD:211:ARG:NH1	2.27	0.68
32:QA:62:U:H3	32:QA:105:G:H1	1.41	0.67
41:QJ:6:ILE:HA	41:QJ:97:GLU:O	1.93	0.67
8:RI:77:LEU:HD23	8:RI:140:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:XB:69:LEU:HB3	33:XB:162:ILE:HG22	1.76	0.67
31:Y9:27:CYS:SG	31:Y9:28:GLU:N	2.67	0.67
1:YA:270(F):U:H3	1:YA:270(T):G:H1	1.43	0.67
1:YA:2777:G:OP2	1:YA:2781:A:O2'	2.11	0.67
32:QA:1251:A:N3	32:QA:1369:C:O2'	2.28	0.67
48:QQ:66:SER:O	48:QQ:70:ARG:NH1	2.27	0.67
1:YA:2296:U:OP2	14:YS:9:ARG:NH2	2.26	0.67
32:QA:827:U:O2	32:QA:874:G:N2	2.28	0.67
35:QD:3:ARG:HH21	35:QD:118:ARG:HD3	1.60	0.67
44:QM:91:ARG:HG2	44:QM:98:VAL:HA	1.77	0.67
1:YA:2392:A:H2	1:YA:2424:C:H42	1.43	0.67
2:RB:80:U:H2'	2:RB:81:G:H21	1.60	0.67
8:RI:77:LEU:HD23	8:RI:140:LEU:HB3	1.77	0.67
5:RF:143:ALA:HB1	5:RF:148:LEU:HB2	1.77	0.67
44:XM:3:ARG:NE	44:XM:3:ARG:H	1.93	0.67
41:XJ:6:ILE:HD11	41:XJ:96:ILE:HB	1.76	0.67
8:RI:120:ILE:CD1	8:RI:126:TYR:CE2	2.76	0.67
32:XA:1316:G:N2	32:XA:1319:A:OP2	2.26	0.66
33:QB:230:VAL:HG12	33:QB:231:GLU:HG3	1.78	0.66
1:YA:226:G:O2'	1:YA:228:A:N6	2.28	0.66
32:QA:1118:C:OP1	40:QI:104:ARG:NH1	2.28	0.66
1:YA:141:A:H8	1:YA:1595:G:H21	1.41	0.66
32:QA:547:A:OP1	35:QD:73:ARG:NH1	2.29	0.66
32:QA:1119:C:OP2	40:QI:9:ARG:NH2	2.29	0.66
8:RI:77:LEU:CD1	8:RI:79:ILE:HD11	2.23	0.66
32:XA:674:G:H2'	32:XA:675:A:H8	1.59	0.66
32:XA:1251:A:N3	32:XA:1369:C:O2'	2.28	0.66
1:YA:987:G:O2'	1:YA:1000:A:N3	2.28	0.66
15:YT:16:ARG:NH2	15:YT:83:ILE:O	2.28	0.66
32:XA:403:C:OP2	35:XD:74:GLN:NE2	2.28	0.66
32:XA:547:A:OP1	35:XD:73:ARG:NH2	2.29	0.66
3:YD:273:ARG:O	3:YD:273:ARG:HG3	1.95	0.66
1:RA:994:C:OP1	16:RU:53:ARG:NH2	2.29	0.66
32:XA:1347:G:N2	32:XA:1374:A:OP2	2.29	0.66
26:Y4:16:CYS:SG	26:Y4:17:GLY:N	2.68	0.66
6:YG:27:ASN:HB3	6:YG:30:GLU:HG3	1.77	0.66
32:QA:1023:G:H3'	32:QA:1024:G:H5''	1.78	0.66
1:RA:2502:G:H5''	1:RA:2503:A:H5''	1.76	0.66
20:RY:102:CYS:SG	20:RY:103:GLY:N	2.69	0.66
1:RA:372:G:N2	1:RA:401:A:OP2	2.28	0.66
1:RA:137(A):G:O6	1:RA:139:G:O2'	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2023:G:H5'	1:RA:2617:C:H4'	1.78	0.65
1:YA:220:G:O2'	1:YA:233:A:N3	2.27	0.65
32:QA:673:G:H2'	32:QA:674:G:C8	2.31	0.65
2:RB:74:U:H1'	21:RZ:34:ASN:HD21	1.59	0.65
1:YA:994:C:OP1	16:YU:53:ARG:NH2	2.29	0.65
38:QG:46:ALA:HA	38:QG:49:ILE:HD12	1.78	0.65
8:RI:77:LEU:CD2	8:RI:140:LEU:CB	2.74	0.65
32:XA:1373:G:H5''	38:XG:36:LYS:HE3	1.78	0.65
32:QA:152:A:H62	32:QA:169:C:H42	1.44	0.65
34:QC:172:ARG:HG2	34:QC:174:PRO:HD3	1.80	0.64
1:YA:573:G:O2'	1:YA:574:C:H3'	1.97	0.64
1:RA:2660:A:N7	7:RH:175:LYS:NZ	2.46	0.64
32:XA:514:C:H2'	32:XA:515:G:H8	1.62	0.64
32:XA:618:C:H5'	32:XA:619:U:H5''	1.78	0.64
48:XQ:66:SER:O	48:XQ:70:ARG:NH1	2.29	0.64
1:YA:1062:G:H2'	1:YA:1063:G:H8	1.62	0.64
1:YA:2133:G:O2'	1:YA:2158:A:N1	2.29	0.64
1:RA:219:G:N3	1:RA:234:C:O2'	2.30	0.64
32:XA:1304:G:H21	32:XA:1333:A:H62	1.45	0.64
1:YA:1228:G:OP2	16:YU:16:LYS:NZ	2.30	0.64
1:RA:1509:C:H3'	1:RA:1510:A:H5''	1.78	0.64
32:QA:1349:A:H62	32:QA:1373:G:H21	1.43	0.64
12:RQ:63:LYS:HD3	12:RQ:65:PHE:CE2	2.33	0.64
1:YA:1645:G:H5''	1:YA:1646:C:H5'	1.79	0.64
1:YA:1980:G:O2'	1:YA:1982:C:OP2	2.14	0.64
1:RA:302:C:OP2	20:RY:73:ARG:NH1	2.31	0.64
4:RE:128:SER:OG	4:RE:129:HIS:N	2.31	0.64
41:XJ:57:LYS:HE2	41:XJ:60:ARG:HH12	1.62	0.64
25:Y3:13:ILE:HD13	25:Y3:13:ILE:N	2.12	0.64
1:RA:1403:C:H5''	1:RA:1471:A:H1'	1.79	0.64
1:RA:2578:G:OP1	1:RA:2614:A:N6	2.31	0.64
15:RT:51:ARG:HG3	15:RT:98:LYS:HE3	1.80	0.64
32:QA:1318:A:H1'	50:QS:37:ARG:HH21	1.62	0.64
5:RF:40:GLN:HE22	5:RF:182:ASN:HB2	1.63	0.64
53:XV:36:G:H1	54:XX:16:C:H42	1.45	0.64
1:YA:2022:U:O2'	1:YA:2617:C:H5'	1.97	0.64
1:YA:458:G:N2	1:YA:470:A:OP2	2.23	0.64
5:YF:63:LYS:NZ	5:YF:75:HIS:O	2.30	0.64
7:YH:3:ARG:HE	7:YH:54:ARG:HH11	1.46	0.64
16:YU:92:ARG:NH1	17:YV:11:GLN:O	2.31	0.64
34:QC:119:ARG:HD3	34:QC:140:ARG:HH22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1310:G:OP2	29:R7:9:ARG:NE	2.30	0.63
1:RA:2285:C:OP2	28:R6:6:ARG:NH1	2.30	0.63
32:QA:838:G:H1	32:QA:848:C:H42	1.44	0.63
32:XA:1239:A:N3	38:XG:115:ARG:NH2	2.45	0.63
1:YA:2655:G:N2	1:YA:2665:A:OP2	2.31	0.63
32:QA:674:G:H2'	32:QA:675:A:H8	1.62	0.63
34:QC:119:ARG:HE	34:QC:140:ARG:HH12	1.45	0.63
40:QI:9:ARG:H	40:QI:79:LEU:HD23	1.63	0.63
35:XD:104:VAL:HA	35:XD:107:ARG:HB2	1.81	0.63
14:YS:27:SER:HA	14:YS:88:ASP:HB3	1.80	0.63
1:YA:2010:G:H5''	18:YW:42:ARG:HB2	1.80	0.63
11:YP:63:PRO:HB2	30:Y8:30:ARG:HH21	1.62	0.63
1:RA:94:G:N3	24:R2:47:ASN:ND2	2.47	0.63
32:XA:992:U:O4	32:XA:1044:A:N7	2.32	0.63
40:XI:111:ARG:NH1	40:XI:112:LYS:O	2.31	0.63
26:R4:61:ARG:HH21	50:QS:42:PRO:HD3	1.63	0.63
1:YA:1995:U:O2	10:YO:3:GLN:NE2	2.31	0.63
51:XT:56:MET:HE1	51:XT:88:VAL:HG21	1.80	0.63
1:RA:1078:U:H4'	1:RA:1079:C:H5''	1.81	0.63
16:RU:92:ARG:HD2	17:RV:11:GLN:HB2	1.81	0.63
1:YA:2483:C:N3	12:YQ:124:LYS:NZ	2.45	0.63
32:QA:686:U:H1'	42:QK:42:TRP:HE1	1.64	0.63
1:RA:2022:U:O2'	1:RA:2617:C:H5'	1.98	0.63
1:RA:2684:U:O2'	10:RO:68:GLU:OE1	2.16	0.63
32:XA:1009:G:H1	32:XA:1020:U:H3	1.47	0.63
1:YA:1109:C:O2'	1:YA:1110:G:OP1	2.16	0.63
1:YA:1939:U:H3'	1:YA:1940:U:H5'	1.81	0.63
3:YD:258:LYS:NZ	3:YD:273:ARG:NH1	2.47	0.63
35:QD:98:GLU:OE2	35:QD:103:ASN:ND2	2.32	0.62
1:YA:2213:U:H1'	23:Y1:52:ARG:HH22	1.64	0.62
7:YH:3:ARG:HH11	7:YH:3:ARG:CG	2.12	0.62
9:RN:133:GLN:HG2	9:RN:135:PRO:HD3	1.80	0.62
21:RZ:182:LYS:C	21:RZ:186:GLU:HG2	2.18	0.62
32:XA:689:C:OP1	42:XK:27:ASN:ND2	2.31	0.62
32:XA:1540:U:O2	54:XX:2:G:N2	2.32	0.62
20:YY:102:CYS:SG	20:YY:103:GLY:N	2.71	0.62
48:QQ:7:THR:HG22	48:QQ:58:GLU:HG2	1.81	0.62
32:QA:278:G:N7	48:QQ:92:ARG:NH1	2.47	0.62
49:QR:53:ARG:HH21	49:QR:59:SER:HA	1.64	0.62
1:RA:2353:G:O2'	22:R0:35:ASN:ND2	2.33	0.62
6:RG:16:ARG:HH21	6:RG:28:VAL:HG22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2315:G:OP1	6:YG:36:LYS:NZ	2.31	0.62
32:QA:412:A:N7	35:QD:35:ARG:NH1	2.48	0.62
1:RA:300:A:OP2	20:RY:84:ARG:NH1	2.32	0.62
12:RQ:56:ARG:HD3	21:RZ:180:VAL:CG1	2.20	0.62
16:YU:50:ARG:O	16:YU:54:LYS:NZ	2.31	0.62
41:XJ:57:LYS:O	41:XJ:60:ARG:NH1	2.32	0.62
1:RA:830:G:N2	1:RA:2445:G:O2'	2.32	0.62
32:XA:789:U:H4'	54:XX:14:A:H2	1.63	0.62
16:RU:92:ARG:NH1	17:RV:11:GLN:O	2.32	0.62
6:YG:101:ILE:HD11	26:Y4:25:TYR:H	1.63	0.62
31:R9:27:CYS:SG	31:R9:28:GLU:N	2.73	0.62
1:YA:602:G:HO2'	1:YA:604:G:HO2'	1.35	0.62
3:YD:274:ARG:CG	3:YD:274:ARG:HH11	2.13	0.62
5:YF:167:ALA:HB1	5:YF:173:VAL:HG11	1.81	0.62
1:RA:1011:G:OP1	16:RU:66:ASN:ND2	2.33	0.62
6:RG:161:THR:HG22	6:RG:163:ALA:H	1.65	0.62
43:XL:27:LEU:O	43:XL:33:ARG:NH2	2.33	0.62
32:QA:1112:C:H42	34:QC:177:THR:HA	1.65	0.61
32:XA:152:A:H62	32:XA:169:C:H42	1.47	0.61
34:XC:189:ALA:HB3	34:XC:196:LEU:HB2	1.82	0.61
1:YA:2312:U:O2	6:YG:40:ASN:ND2	2.33	0.61
32:QA:765:G:N2	32:QA:813:U:OP2	2.26	0.61
33:QB:53:ARG:HA	33:QB:56:ARG:HH21	1.64	0.61
1:RA:270(L):U:H2'	8:RI:50:ARG:HH12	1.63	0.61
8:RI:86:THR:O	8:RI:87:LYS:HG2	2.00	0.61
1:YA:259:G:H21	1:YA:621:A:H8	1.46	0.61
13:YR:75:LEU:HA	13:YR:78:LYS:HB3	1.81	0.61
32:QA:1147:C:O2	40:QI:16:ARG:NH2	2.33	0.61
1:RA:1693:U:O2'	3:RD:14:ARG:NH2	2.34	0.61
5:RF:167:ALA:HB1	5:RF:173:VAL:HG11	1.82	0.61
9:RN:97:ARG:HA	9:RN:100:GLU:HB2	1.82	0.61
14:RS:25:ARG:NH1	14:RS:42:ASP:OD2	2.32	0.61
1:YA:620:G:H4'	1:YA:621:A:H5'	1.83	0.61
1:YA:793:A:OP2	1:YA:2071:A:O2'	2.18	0.61
1:RA:39:C:O2	5:RF:46:ARG:NH2	2.33	0.61
6:RG:38:VAL:HB	6:RG:158:ALA:HB3	1.82	0.61
32:XA:51:A:N1	32:XA:314:C:O2'	2.32	0.61
32:XA:1073:U:O2'	33:XB:104:ASN:OD1	2.17	0.61
6:YG:146:TYR:HE2	44:XM:8:GLU:HB3	1.64	0.61
40:QI:71:SER:HA	40:QI:74:ILE:HD12	1.81	0.61
32:XA:1289:A:OP1	52:XU:9:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:64:G:H5''	32:XA:65:U:H5'	1.81	0.61
32:XA:954:G:H21	32:XA:1227:A:H62	1.48	0.61
1:YA:2107:C:O2	1:YA:2182:G:N2	2.33	0.61
1:YA:2168:G:N2	1:YA:2170:A:N7	2.48	0.61
51:QT:51:GLU:HA	51:QT:54:LYS:HG2	1.80	0.61
15:RT:108:ARG:N	32:QA:1432:G:OP1	2.32	0.61
40:XI:21:PRO:HA	40:XI:59:PHE:HA	1.80	0.61
4:YE:128:SER:OG	4:YE:129:HIS:N	2.33	0.61
32:QA:1446:A:O2'	32:QA:1447:G:O5'	2.18	0.61
32:QA:427:U:OP1	35:QD:13:ARG:NH1	2.34	0.61
32:XA:1071:C:H2'	32:XA:1072:G:H8	1.66	0.61
32:XA:707:C:OP1	42:XK:85:ARG:NH1	2.33	0.61
1:YA:1689:A:H62	1:YA:1698:A:H2	1.47	0.61
32:QA:664:G:H22	32:QA:741:G:H1	1.49	0.61
1:RA:1728:G:H3'	1:RA:1729:A:H5''	1.83	0.61
1:RA:517:C:O2'	18:RW:18:ARG:NH2	2.34	0.61
1:RA:2052:G:H4'	4:RE:143:ASN:H	1.65	0.61
32:XA:1286:A:H2'	32:XA:1287:A:H4'	1.83	0.61
35:XD:18:LYS:O	35:XD:18:LYS:HG3	1.99	0.61
32:QA:642:A:N3	39:QH:113:SER:OG	2.34	0.61
6:RG:82:LEU:HD21	6:RG:88:ILE:HG21	1.83	0.61
1:YA:2019:A:N7	27:Y5:9:LYS:NZ	2.44	0.61
32:QA:1124:G:H3'	32:QA:1145:C:N4	2.15	0.61
33:QB:67:THR:HG21	33:QB:155:LEU:HG	1.82	0.61
32:QA:1147:C:HO2'	40:QI:5:TYR:HH	1.48	0.61
1:RA:2118:U:O2	1:RA:2148:G:O2'	2.18	0.61
32:XA:1356:G:H2'	32:XA:1357:A:C8	2.36	0.61
1:YA:577:G:O2'	1:YA:1254:A:OP1	2.19	0.61
39:QH:12:ARG:HD2	39:QH:26:VAL:HG12	1.83	0.60
21:RZ:10:ARG:NH1	21:RZ:26:GLY:O	2.34	0.60
32:XA:243:A:H4'	32:XA:244:U:O5'	1.99	0.60
37:QF:3:ARG:NH1	37:QF:38:GLU:OE2	2.33	0.60
1:RA:1689:A:H62	1:RA:1698:A:H2	1.47	0.60
7:YH:3:ARG:NH1	7:YH:3:ARG:HG2	2.16	0.60
1:YA:958:U:OP2	12:YQ:14:ARG:NH1	2.34	0.60
32:QA:262:A:H5'	51:QT:74:LYS:HG3	1.84	0.60
1:RA:2079:U:OP1	23:R1:21:ARG:NH1	2.30	0.60
1:RA:2468:G:OP1	12:RQ:119:ARG:NH2	2.35	0.60
7:RH:143:GLN:O	7:RH:147:ASN:ND2	2.33	0.60
1:YA:574:C:N3	4:YE:145:LYS:NZ	2.42	0.60
2:RB:22:U:H3	2:RB:61:G:H1	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1356:G:H2'	32:XA:1357:A:H8	1.66	0.60
32:XA:352:C:O2	32:XA:355:C:N4	2.32	0.60
2:YB:37:C:O2	14:YS:95:HIS:NE2	2.33	0.60
1:RA:1066:U:O2'	1:RA:1068:G:OP2	2.19	0.60
1:RA:1667:G:O2'	1:RA:1991:U:O4	2.19	0.60
32:XA:662:G:O2'	32:XA:836:G:OP1	2.19	0.60
34:XC:11:ARG:NH2	34:XC:177:THR:O	2.34	0.60
35:QD:20:TYR:CE2	37:XF:15:ASP:HB3	2.35	0.60
8:RI:107:VAL:O	8:RI:107:VAL:HG12	2.01	0.60
32:XA:150:C:H42	32:XA:171:A:H62	1.49	0.60
32:XA:933:G:O6	38:XG:3:ARG:NH2	2.34	0.60
26:Y4:27:THR:HG23	26:Y4:28:LYS:HG3	1.84	0.60
1:YA:1496:A:H8	1:YA:1577:C:HO2'	1.48	0.60
32:QA:1393:U:HO2'	32:QA:1501:C:HO2'	1.48	0.60
1:RA:2612:C:OP2	27:R5:2:ALA:N	2.34	0.60
32:XA:503:C:OP1	43:XL:119:LYS:NZ	2.34	0.60
33:XB:231:GLU:HG3	33:XB:233:SER:H	1.66	0.60
5:YF:116:ASP:OD2	11:YP:1:MET:N	2.35	0.60
26:R4:16:CYS:SG	26:R4:17:GLY:N	2.75	0.60
1:RA:2588:G:O6	1:RA:2607:G:C6	2.54	0.60
1:YA:1728:G:N2	1:YA:1730:U:OP1	2.35	0.60
1:YA:84:A:OP2	20:YY:8:LYS:NZ	2.34	0.60
1:RA:2438:U:O3'	1:RA:2439:A:H3'	2.02	0.60
32:XA:152:A:N6	32:XA:169:C:H42	2.00	0.60
44:XM:86:CYS:SG	44:XM:87:TYR:N	2.75	0.60
1:YA:1403:C:H5''	1:YA:1471:A:H1'	1.82	0.60
1:RA:1348:G:H2'	1:RA:1349:A:H5''	1.84	0.60
11:RP:58:THR:O	11:RP:61:ARG:NH2	2.29	0.60
32:XA:1305:G:N2	32:XA:1332:A:OP2	2.24	0.60
40:XI:45:ALA:HA	40:XI:48:GLU:HG2	1.84	0.60
1:RA:1426:G:OP2	1:RA:1427:A:O2'	2.18	0.59
1:RA:223:A:O2'	1:RA:420:C:O2	2.19	0.59
1:RA:2392:A:H2	1:RA:2424:C:H42	1.50	0.59
2:RB:8:U:H3	2:RB:112:G:H1	1.50	0.59
1:RA:1262:A:OP2	18:RW:97:LYS:NZ	2.35	0.59
30:Y8:6:THR:OG1	30:Y8:8:LYS:NZ	2.35	0.59
1:YA:249:C:O2	30:Y8:12:LYS:NZ	2.31	0.59
1:YA:2808:U:O2	1:YA:2892:A:C6	2.54	0.59
32:QA:1532:U:C5	54:QX:10:G:O6	2.54	0.59
1:RA:1815:A:OP2	3:RD:54:ARG:NH2	2.35	0.59
32:XA:587:G:N2	32:XA:754:C:OP2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1203:G:H3'	1:YA:1204:A:H5''	1.83	0.59
1:YA:1454:U:H5'	13:YR:63:ARG:NH2	2.16	0.59
32:QA:1002:G:H2'	32:QA:1003:G:H8	1.67	0.59
32:QA:150:C:N4	32:QA:171:A:H62	2.00	0.59
2:RB:37:C:O2	14:RS:95:HIS:NE2	2.35	0.59
41:XJ:78:ASN:HB2	41:XJ:81:THR:HG23	1.83	0.59
1:YA:140:A:H8	1:YA:1408:C:HO2'	1.50	0.59
1:YA:675:A:N3	1:YA:2443:C:O2'	2.29	0.59
32:QA:448:A:H62	32:QA:486:U:H3	1.51	0.59
54:QX:2:G:N7	54:QX:3:C:N4	2.50	0.59
1:RA:675:A:N3	1:RA:2443:C:O2'	2.34	0.59
32:XA:266:G:O2'	32:XA:267:C:OP2	2.18	0.59
32:XA:486:U:H2'	32:XA:487:A:H8	1.67	0.59
32:XA:542:G:H5'	35:XD:41:GLY:HA3	1.83	0.59
1:YA:2334:G:O6	22:Y0:74:ARG:NH2	2.35	0.59
1:YA:442:G:H1'	5:YF:48:THR:HG21	1.84	0.59
1:RA:2588:G:O6	1:RA:2607:G:N1	2.36	0.59
32:QA:662:G:O2'	32:QA:836:G:OP1	2.21	0.59
31:R9:25:VAL:HB	31:R9:34:GLN:HB2	1.83	0.59
1:RA:65:C:H1'	1:RA:456:C:H42	1.67	0.59
1:RA:956:G:OP2	12:RQ:14:ARG:NH2	2.35	0.59
32:XA:59:A:H3'	32:XA:331:G:H22	1.68	0.59
1:YA:2245:U:H5'	1:YA:2246:G:H5'	1.84	0.59
1:YA:848:G:H2'	1:YA:849:A:C8	2.37	0.59
6:YG:161:THR:HG22	6:YG:163:ALA:H	1.67	0.59
41:QJ:3:LYS:N	41:QJ:74:ILE:O	2.36	0.59
54:QX:2:G:C8	54:QX:3:C:H5	2.20	0.59
1:RA:1586:A:H3'	1:RA:1587:A:H8	1.67	0.59
1:RA:996:A:OP2	16:RU:92:ARG:NH2	2.36	0.59
15:RT:16:ARG:NH2	15:RT:83:ILE:O	2.36	0.59
1:YA:504:U:H5''	1:YA:505:A:H5'	1.85	0.59
9:YN:14:VAL:HG13	9:YN:138:LEU:HB2	1.85	0.59
32:QA:1230:C:H5'	53:QV:30:C:H5''	1.84	0.59
11:RP:4:SER:O	11:RP:7:ARG:NH2	2.36	0.59
32:XA:643:C:H2'	32:XA:644:G:H8	1.68	0.59
1:YA:890:A:H2'	1:YA:892:G:H8	1.68	0.59
21:YZ:180:VAL:O	21:YZ:183:LEU:HB2	2.03	0.59
32:QA:1286:A:H2'	32:QA:1287:A:H4'	1.84	0.59
32:QA:1502:A:H2	32:QA:1505:G:H1	1.50	0.59
33:QB:69:LEU:HB3	33:QB:162:ILE:HG22	1.83	0.59
33:QB:54:THR:HG22	33:QB:199:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:QJ:77:PRO:O	41:QJ:79:ARG:NH1	2.35	0.59
1:RA:139:G:N3	1:RA:141:A:N1	2.50	0.59
1:RA:1816:G:O6	3:RD:35:LYS:NZ	2.35	0.59
12:RQ:75:THR:HG21	12:RQ:85:LYS:HE3	1.85	0.59
3:YD:85:ASP:OD2	3:YD:88:ARG:NH1	2.35	0.59
19:YX:72:LYS:NZ	19:YX:75:ASP:OD1	2.35	0.59
48:QQ:83:ASP:OD1	48:QQ:83:ASP:N	2.35	0.59
32:QA:1535:C:H41	54:QX:9:G:N2	1.68	0.59
4:YE:7:VAL:HG13	4:YE:51:PHE:HE2	1.67	0.59
8:YI:94:ALA:HB1	8:YI:114:LEU:HD23	1.84	0.59
1:RA:1171:G:N7	1:RA:1174:A:N6	2.50	0.58
1:RA:2126:A:N6	1:RA:2163:C:O2'	2.36	0.58
32:XA:1047:G:H5''	45:XN:4:LYS:HD3	1.85	0.58
41:QJ:29:ARG:NH1	32:XA:1163:C:OP1	2.35	0.58
32:XA:191(F):U:H2'	32:XA:191(G):G:H8	1.68	0.58
47:XP:45:THR:HG22	47:XP:47:ASP:H	1.68	0.58
32:QA:28:G:O2'	32:QA:296:U:OP1	2.19	0.58
34:QC:182:ILE:HA	34:QC:202:ILE:O	2.03	0.58
1:RA:856:C:O2'	1:RA:857:C:OP1	2.20	0.58
33:XB:82:ARG:NH1	33:XB:92:TYR:OH	2.36	0.58
32:XA:430:A:OP2	35:XD:8:VAL:HG23	2.02	0.58
1:YA:2701:C:H3'	1:YA:2702:U:C5'	2.29	0.58
1:YA:2867:G:O2'	1:YA:2868:A:H8	1.86	0.58
1:YA:1815:A:OP2	3:YD:54:ARG:NH2	2.36	0.58
39:QH:10:LEU:HD22	39:QH:83:ILE:HD11	1.85	0.58
40:QI:96:LEU:O	40:QI:100:GLY:N	2.36	0.58
26:R4:28:LYS:HB2	26:R4:31:ILE:HD11	1.84	0.58
1:RA:546:C:H3'	1:RA:547:A:H8	1.69	0.58
1:RA:627:A:N7	11:RP:84:ASN:ND2	2.46	0.58
32:XA:642:A:N3	39:XH:113:SER:OG	2.34	0.58
1:YA:2621:A:O2'	4:YE:159:HIS:ND1	2.33	0.58
34:QC:14:ILE:HG13	34:QC:15:THR:HB	1.85	0.58
32:QA:656:C:O2'	46:QO:28:GLN:OE1	2.18	0.58
32:XA:1229:A:O2'	53:XV:30:C:OP1	2.20	0.58
32:XA:388:G:HO2'	32:XA:389:A:P	2.24	0.58
1:YA:2791:C:H5	1:YA:2893:G:H3'	1.68	0.58
32:QA:684:A:O2'	42:QK:39:PRO:O	2.20	0.58
37:QF:100:ASN:ND2	49:QR:23:LYS:O	2.33	0.58
12:RQ:59:ARG:HG3	21:RZ:180:VAL:HG23	1.84	0.58
32:XA:1191:A:OP2	34:XC:3:ASN:ND2	2.36	0.58
32:XA:1227:A:OP1	50:XS:80:TYR:OH	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:219:G:N3	1:YA:234:C:O2'	2.34	0.58
6:YG:47:LYS:HD3	6:YG:81:LYS:HD3	1.86	0.58
32:QA:1080:A:H5'	36:QE:16:THR:HG21	1.86	0.58
39:QH:7:ALA:HB2	39:QH:85:ARG:HD3	1.86	0.58
32:QA:970:C:N4	40:QI:128:ARG:O	2.37	0.58
11:RP:49:ARG:HH11	30:R8:58:ILE:HG22	1.68	0.58
1:RA:1059:G:OP2	1:RA:1060:U:H3'	2.03	0.58
1:RA:1286:A:HO2'	1:RA:1288:U:P	2.26	0.58
1:RA:1496:A:H8	1:RA:1577:C:HO2'	1.52	0.58
1:RA:2779:U:O2'	1:RA:2781:A:N7	2.35	0.58
32:XA:376:G:H5''	47:XP:5:ARG:HB2	1.86	0.58
33:QB:19:HIS:HB3	33:QB:20:GLU:HG2	1.85	0.58
33:QB:223:ILE:HA	33:QB:226:ARG:HB3	1.86	0.58
1:RA:1019:U:H3	1:RA:1142(A):A:H62	1.51	0.58
32:XA:946:A:O2'	32:XA:1333:A:N3	2.32	0.58
1:YA:2791:C:OP1	1:YA:2893:G:N2	2.37	0.58
32:QA:742:G:OP2	46:QO:35:ARG:NH2	2.37	0.58
32:QA:835:U:H3	32:QA:851:G:H1	1.52	0.58
1:RA:1969:A:O2'	1:RA:1972:A:N3	2.29	0.58
40:XI:112:LYS:NZ	40:XI:113:LYS:O	2.37	0.58
34:QC:77:ILE:HG23	34:QC:79:ARG:H	1.69	0.58
1:RA:2588:G:C6	1:RA:2607:G:C2	2.92	0.58
32:XA:1095:U:OP1	32:XA:1108:G:N2	2.27	0.58
32:XA:673:G:H2'	32:XA:674:G:C8	2.38	0.58
1:YA:2680:C:OP2	4:YE:111:ARG:NH2	2.33	0.58
10:RO:48:PRO:HB3	32:QA:1422:G:H5''	1.85	0.58
32:QA:401:C:O2'	32:QA:621:A:N3	2.33	0.58
2:RB:13:A:N1	2:RB:69:G:O2'	2.34	0.58
10:RO:80:ASP:OD2	15:RT:64:ARG:NH2	2.37	0.58
1:RA:24:G:O2'	18:RW:78:GLU:O	2.20	0.58
32:XA:359:U:H2'	32:XA:360:A:H8	1.69	0.58
32:XA:842:C:O2'	32:XA:848:C:N4	2.37	0.58
32:XA:1298:C:H2'	38:XG:114:ARG:HH12	1.69	0.58
1:YA:919:G:N2	1:YA:2269:A:OP2	2.34	0.58
1:YA:1824:G:N3	3:YD:254:THR:OG1	2.37	0.58
32:QA:1009:G:O6	32:QA:1020:U:O4	2.22	0.57
32:QA:1119:C:H2'	32:QA:1120:G:H8	1.69	0.57
32:QA:1321:C:O2	50:QS:36:ARG:NH1	2.37	0.57
1:RA:503:A:H4'	1:RA:504:U:H5'	1.85	0.57
32:XA:250:A:H4'	32:XA:251:G:O5'	2.03	0.57
34:XC:20:SER:OG	34:XC:22:TRP:NE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:XI:10:ARG:NH2	40:XI:103:THR:O	2.37	0.57
49:XR:32:ARG:HA	49:XR:69:THR:HG21	1.86	0.57
11:YP:65:ARG:NH1	30:Y8:25:MET:SD	2.77	0.57
1:YA:2711:A:H5''	1:YA:2712:U:H5'	1.86	0.57
35:QD:108:LEU:HD23	35:QD:170:VAL:HG21	1.85	0.57
32:QA:191(G):G:O2'	51:QT:101:GLY:O	2.22	0.57
32:XA:1236:A:OP1	52:XU:3:LYS:NZ	2.36	0.57
9:YN:39:ARG:NH2	9:YN:41:ASP:OD2	2.37	0.57
10:YO:88:ASN:HD21	10:YO:92:GLU:HB2	1.69	0.57
21:YZ:157:LEU:HD23	21:YZ:161:VAL:HG12	1.86	0.57
21:YZ:10:ARG:HH21	21:YZ:26:GLY:H	1.52	0.57
32:QA:769:G:H4'	32:QA:1513:A:H4'	1.85	0.57
32:QA:152:A:H62	32:QA:169:C:N4	2.02	0.57
27:R5:16:ARG:NH1	27:R5:17:ASP:OD1	2.35	0.57
1:RA:1047:G:N3	1:RA:1111:A:N6	2.52	0.57
1:RA:200:U:O2	1:RA:386:G:N2	2.38	0.57
1:RA:65:C:O2'	1:RA:456:C:N3	2.32	0.57
32:XA:1273:G:H3'	32:XA:1274:G:H8	1.70	0.57
32:XA:405:U:O4	35:XD:2:GLY:N	2.37	0.57
38:XG:139:GLU:O	38:XG:143:ARG:N	2.37	0.57
1:YA:2808:U:C2	1:YA:2892:A:C6	2.93	0.57
16:YU:92:ARG:HD2	17:YV:11:GLN:HB2	1.85	0.57
36:QE:100:VAL:O	36:QE:107:ARG:NH2	2.35	0.57
50:QS:19:VAL:HG21	50:QS:44:MET:HG3	1.86	0.57
54:QX:2:G:C8	54:QX:3:C:C5	2.93	0.57
4:RE:77:ILE:HD13	4:RE:195:LEU:HD13	1.85	0.57
5:RF:198:ALA:HA	5:RF:201:VAL:H	1.69	0.57
12:RQ:62:GLY:HA2	21:RZ:116:VAL:CG2	2.33	0.57
21:RZ:19:ARG:NH1	21:RZ:84:GLU:O	2.36	0.57
32:XA:407:G:H5''	35:XD:115:ARG:HB3	1.86	0.57
5:YF:143:ALA:HB1	5:YF:148:LEU:HB2	1.86	0.57
1:RA:221:A:H4'	1:RA:222:A:O5'	2.04	0.57
12:RQ:71:ASP:N	12:RQ:71:ASP:OD1	2.38	0.57
32:XA:1499:A:H1'	32:XA:1520:G:H5'	1.86	0.57
32:XA:1111:A:N6	34:XC:176:HIS:O	2.37	0.57
34:XC:20:SER:HG	34:XC:22:TRP:HE1	1.52	0.57
44:XM:83:ASP:OD1	44:XM:93:ARG:NH2	2.38	0.57
32:XA:1243:C:OP2	52:XU:10:ARG:NH2	2.38	0.57
1:YA:2776:A:OP1	1:YA:2776:A:H3'	2.05	0.57
6:YG:29:TRP:O	6:YG:33:ARG:NH1	2.37	0.57
7:YH:164:TYR:HB2	7:YH:167:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1275:A:N1	1:RA:1295:C:O2'	2.32	0.57
1:RA:918:A:N3	2:RB:80:U:O2'	2.35	0.57
32:XA:1498:U:OP2	54:XX:16:C:O2'	2.22	0.57
1:YA:2701:C:C3'	1:YA:2702:U:H5''	2.30	0.57
1:YA:2832:U:H4'	1:YA:2833:G:H5''	1.87	0.57
2:YB:48:A:H4'	14:YS:95:HIS:HD2	1.70	0.57
12:YQ:34:LEU:HB2	12:YQ:118:LEU:HD22	1.85	0.57
18:YW:92:ARG:NH1	18:YW:94:ASP:OD1	2.38	0.57
1:RA:392:C:H5''	1:RA:409:C:H5''	1.87	0.57
32:XA:769:G:H4'	32:XA:1513:A:H4'	1.85	0.57
9:YN:58:ASP:OD1	9:YN:58:ASP:N	2.35	0.57
15:YT:18:ASP:OD1	15:YT:18:ASP:N	2.37	0.57
35:QD:57:ARG:NH2	35:QD:205:GLU:OE1	2.38	0.57
32:QA:430:A:OP1	35:QD:9:CYS:HB2	2.05	0.57
1:RA:1889:A:N3	1:RA:2086:U:O2'	2.38	0.57
1:RA:2006:C:O2'	1:RA:2823:A:N3	2.36	0.57
12:RQ:59:ARG:HA	21:RZ:180:VAL:CG2	2.35	0.57
32:XA:1266:G:N2	32:XA:1269:A:OP2	2.33	0.57
31:Y9:6:SER:O	31:Y9:6:SER:OG	2.22	0.57
3:YD:258:LYS:CE	3:YD:273:ARG:NH1	2.67	0.57
8:YI:92:VAL:HB	8:YI:120:ILE:HG22	1.87	0.57
32:QA:130:A:O2'	32:QA:263:A:O2'	2.22	0.57
35:QD:120:LEU:HB3	35:QD:126:ILE:HD11	1.86	0.57
35:QD:18:LYS:HE2	35:QD:20:TYR:HE1	1.67	0.57
1:RA:140:A:H8	1:RA:1408:C:HO2'	1.52	0.57
6:RG:151:ALA:HB3	6:RG:153:ARG:HH21	1.70	0.57
32:XA:272:C:H2'	32:XA:273:A:H8	1.68	0.57
44:XM:8:GLU:O	44:XM:9:ILE:C	2.43	0.57
50:XS:41:VAL:HG23	50:XS:43:GLU:H	1.70	0.57
5:YF:116:ASP:OD1	5:YF:119:ARG:NH2	2.38	0.57
12:YQ:31:ASP:OD1	12:YQ:134:ARG:NH1	2.38	0.57
20:YY:17:SER:OG	20:YY:71:LYS:NZ	2.35	0.57
32:QA:1071:C:H2'	32:QA:1072:G:H8	1.70	0.57
44:QM:16:ASP:N	44:QM:16:ASP:OD1	2.37	0.57
49:XR:45:SER:HG	49:XR:47:THR:HG1	1.53	0.57
1:YA:138:G:N2	19:YX:44:GLU:OE1	2.37	0.57
48:QQ:66:SER:OG	48:QQ:67:LYS:O	2.22	0.56
1:RA:18:C:O2'	1:RA:553:U:OP1	2.23	0.56
13:RR:56:LYS:NZ	13:RR:90:ARG:O	2.37	0.56
32:XA:1124:G:H1'	41:XJ:38:ILE:HD13	1.87	0.56
1:YA:1086:A:O2'	1:YA:1103:A:N6	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:QJ:11:PHE:HE2	41:QJ:67:THR:HG22	1.70	0.56
42:QK:52:GLY:H	42:QK:55:LYS:HE2	1.69	0.56
1:RA:2055:C:OP1	27:R5:8:LYS:NZ	2.38	0.56
3:RD:12:SER:HB3	3:RD:208:LYS:HB3	1.85	0.56
1:RA:2547:U:O2	10:RO:23:ARG:NH2	2.37	0.56
1:YA:2788:C:O2'	1:YA:2809:A:N3	2.35	0.56
1:YA:2867:G:O2'	1:YA:2868:A:O5'	2.23	0.56
41:QJ:66:ARG:HB3	41:QJ:68:HIS:CE1	2.39	0.56
48:QQ:79:SER:OG	48:QQ:80:GLY:N	2.38	0.56
26:R4:12:ALA:HA	26:R4:29:PRO:HA	1.87	0.56
9:RN:17:ASP:OD1	9:RN:56:ASN:ND2	2.38	0.56
32:XA:529:G:O6	43:XL:49:ASN:ND2	2.37	0.56
1:YA:1127:A:N7	1:YA:2488:A:O2'	2.34	0.56
1:YA:67:U:H3	1:YA:74:A:H2	1.54	0.56
8:YI:102:SER:OG	8:YI:103:ARG:N	2.38	0.56
32:XA:516:U:O2'	32:XA:519:C:N3	2.36	0.56
33:XB:192:SER:OG	33:XB:193:ASP:N	2.39	0.56
1:YA:2729:G:H1'	4:YE:187:ALA:HB2	1.87	0.56
32:QA:501:C:H2'	32:QA:502:G:H8	1.70	0.56
48:QQ:81:ARG:HE	48:QQ:84:LEU:HD11	1.71	0.56
32:XA:1238:A:H62	32:XA:1301:U:H3	1.53	0.56
32:XA:768:A:N3	32:XA:1512:U:O2'	2.37	0.56
40:XI:53:VAL:HG11	40:XI:85:LEU:HD11	1.86	0.56
46:XO:24:SER:OG	46:XO:25:THR:N	2.39	0.56
31:Y9:25:VAL:HB	31:Y9:34:GLN:HB2	1.88	0.56
1:YA:83:G:H1	1:YA:102:G:HO2'	1.53	0.56
1:YA:2306:C:N4	6:YG:42:GLY:O	2.38	0.56
42:QK:43:SER:OG	42:QK:44:SER:N	2.38	0.56
1:RA:1812:A:H2'	1:RA:1813:G:H8	1.70	0.56
1:RA:2114:A:N7	1:RA:2168:G:N2	2.52	0.56
32:XA:959:A:HO2'	32:XA:984:C:HO2'	1.49	0.56
1:YA:2099:U:O4	1:YA:2190:G:O6	2.22	0.56
1:YA:2335:A:O2'	1:YA:2336:A:H2'	2.06	0.56
1:YA:336:C:O2'	20:YY:35:TYR:OH	2.23	0.56
2:YB:7:G:H3'	2:YB:8:U:H5''	1.88	0.56
8:YI:99:GLU:OE2	8:YI:103:ARG:NH2	2.38	0.56
32:QA:1412:C:H2'	32:QA:1413:A:C8	2.41	0.56
1:RA:1542:G:O6	1:RA:1543:A:N6	2.38	0.56
32:QA:1367:C:H4'	41:QJ:48:THR:HG21	1.87	0.56
1:RA:1041:C:O2	1:RA:1115:G:N2	2.38	0.56
1:RA:873:G:H4'	12:RQ:63:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:RP:118:GLY:O	11:RP:137:LYS:NZ	2.38	0.56
21:RZ:158:PRO:HG2	21:RZ:161:VAL:HG21	1.87	0.56
32:XA:452:A:N7	32:XA:480:U:O4	2.39	0.56
40:XI:9:ARG:HB3	40:XI:104:ARG:HH21	1.70	0.56
43:XL:76:ASN:HD21	43:XL:108:ALA:H	1.54	0.56
25:Y3:12:PRO:HA	25:Y3:15:TYR:HD2	1.70	0.56
7:YH:3:ARG:HH11	7:YH:3:ARG:HG2	1.69	0.56
32:QA:1096:C:H2'	32:QA:1097:C:H6	1.71	0.56
1:RA:458:G:N2	1:RA:470:A:OP2	2.31	0.56
32:XA:1224:G:N3	44:XM:102:ARG:NH1	2.45	0.56
32:XA:123:C:OP1	32:XA:311:C:O2'	2.21	0.56
32:XA:235:C:H2'	32:XA:236:G:H8	1.71	0.56
36:XE:102:ALA:HB1	36:XE:106:PRO:HG2	1.88	0.56
44:XM:105:THR:OG1	44:XM:106:ASN:N	2.39	0.56
1:YA:1062:G:H2'	1:YA:1063:G:C8	2.40	0.56
1:YA:247:G:O6	30:Y8:12:LYS:NZ	2.33	0.56
5:YF:117:ARG:NH2	5:YF:189:THR:O	2.39	0.56
32:QA:56:U:H2'	32:QA:57:G:C8	2.41	0.56
43:QL:71:PRO:O	43:QL:102:ARG:NH1	2.39	0.56
7:RH:70:THR:O	7:RH:74:ASN:N	2.36	0.56
32:XA:1189:C:H5''	34:XC:5:ILE:HG21	1.88	0.56
32:XA:1354:C:H2'	32:XA:1355:G:H8	1.70	0.56
32:XA:1355:G:H2'	32:XA:1356:G:H8	1.71	0.56
32:XA:1450:U:O2'	32:XA:1451:A:N7	2.39	0.56
32:XA:1533:C:H2'	32:XA:1534:A:H5'	1.86	0.56
48:XQ:6:LEU:HD13	48:XQ:23:VAL:HG11	1.87	0.56
32:QA:501:C:H2'	32:QA:502:G:C8	2.41	0.56
32:QA:953:G:N7	44:QM:104:ARG:NH2	2.54	0.56
39:QH:41:ARG:NH2	39:QH:123:GLU:OE1	2.38	0.56
34:XC:74:GLY:HA2	34:XC:77:ILE:HD12	1.88	0.56
1:YA:2134:A:N6	1:YA:2156:G:O2'	2.39	0.56
1:YA:363(B):G:H2'	1:YA:363(C):G:H8	1.70	0.56
8:YI:88:ILE:O	8:YI:121:LYS:NZ	2.38	0.56
12:YQ:10:ARG:HD2	21:YZ:196:VAL:HG21	1.87	0.56
1:RA:2576:G:O2'	1:RA:2579:C:OP2	2.19	0.55
12:RQ:59:ARG:HG3	21:RZ:180:VAL:CG2	2.36	0.55
27:Y5:16:ARG:NH1	27:Y5:17:ASP:OD1	2.35	0.55
6:YG:37:VAL:HG22	6:YG:159:VAL:HG12	1.88	0.55
8:YI:110:ASP:OD2	8:YI:113:ARG:NH2	2.39	0.55
11:RP:52:GLU:OE1	11:RP:55:ARG:NH1	2.40	0.55
12:RQ:58:PHE:CD2	12:RQ:61:GLY:HA3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:29:U:H5''	16:YU:7:GLY:HA2	1.87	0.55
32:QA:1061:G:OP1	41:QJ:59:SER:OG	2.23	0.55
1:RA:2224:G:OP1	3:RD:268:ARG:NH1	2.39	0.55
32:XA:745:C:OP1	32:XA:851:G:O2'	2.23	0.55
1:YA:2784:C:O2'	4:YE:37:ARG:NH1	2.39	0.55
1:YA:1163:G:OP1	17:YV:24:LYS:NZ	2.39	0.55
17:YV:62:LEU:HD12	17:YV:93:GLU:HG2	1.87	0.55
34:QC:59:ARG:HD3	34:QC:64:VAL:HG12	1.87	0.55
32:QA:1243:C:H5''	52:QU:8:THR:HG21	1.88	0.55
1:RA:987:G:O2'	1:RA:1000:A:N3	2.37	0.55
1:RA:2517:C:N3	1:RA:2542:A:N6	2.54	0.55
1:RA:1788:C:OP1	3:RD:222:ARG:NH2	2.40	0.55
1:RA:907:U:O2'	12:RQ:101:ARG:NH2	2.39	0.55
32:XA:1354:C:H2'	32:XA:1355:G:C8	2.41	0.55
32:XA:135:C:H2'	32:XA:136:C:H5'	1.88	0.55
32:XA:1446:A:O2'	32:XA:1447:G:O5'	2.23	0.55
1:YA:1190:G:H5'	11:YP:32:THR:HA	1.88	0.55
21:YZ:183:LEU:O	21:YZ:186:GLU:N	2.39	0.55
32:QA:266:G:O2'	32:QA:267:C:OP2	2.23	0.55
32:QA:689:C:OP2	42:QK:55:LYS:NZ	2.40	0.55
32:QA:522:C:H41	43:QL:53:ARG:HH22	1.55	0.55
1:RA:2814:C:O2'	27:R5:29:THR:OG1	2.17	0.55
4:RE:54:GLN:HB2	4:RE:76:ARG:HG3	1.87	0.55
1:YA:620:G:H4'	1:YA:621:A:C5'	2.36	0.55
1:RA:2395:C:O2'	23:R1:30:VAL:O	2.24	0.55
1:RA:793:A:OP2	1:RA:2071:A:O2'	2.24	0.55
32:XA:1342:C:H2'	32:XA:1343:G:H8	1.72	0.55
32:XA:1431:C:H2'	32:XA:1432:G:O4'	2.07	0.55
39:XH:106:GLY:O	39:XH:122:ARG:NH2	2.40	0.55
41:XJ:5:ARG:HE	41:XJ:100:THR:HA	1.71	0.55
48:XQ:18:THR:OG1	48:XQ:69:LYS:NZ	2.39	0.55
22:Y0:27:GLU:HG3	22:Y0:68:GLU:HA	1.87	0.55
32:QA:1296:C:OP1	44:QM:44:ARG:NH2	2.39	0.55
1:RA:23:G:OP1	1:RA:504:U:N3	2.36	0.55
21:RZ:31:ARG:NH2	21:RZ:93:ASP:OD2	2.35	0.55
32:XA:80:G:H1	32:XA:89:U:H3	1.54	0.55
50:XS:32:LYS:HA	50:XS:50:ALA:HB3	1.89	0.55
1:YA:1509:C:H3'	1:YA:1510:A:H5''	1.88	0.55
1:YA:2068:U:H3	1:YA:2430:A:H2	1.55	0.55
1:YA:270(N):G:N3	8:YI:50:ARG:NH1	2.54	0.55
21:YZ:92:SER:OG	21:YZ:94:GLU:OE1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1347:G:N2	32:QA:1374:A:OP2	2.24	0.55
41:QJ:58:ASP:N	41:QJ:58:ASP:OD2	2.36	0.55
32:XA:624:C:H2'	32:XA:625:G:H8	1.70	0.55
34:XC:17:ASP:O	34:XC:54:ARG:NH2	2.39	0.55
35:XD:65:ARG:NH1	35:XD:70:ILE:O	2.39	0.55
38:XG:62:PHE:HA	38:XG:124:LEU:HD11	1.88	0.55
40:XI:13:ALA:HB2	40:XI:68:GLY:HA3	1.89	0.55
1:YA:2151:G:H2'	1:YA:2152:G:H8	1.72	0.55
18:YW:12:ILE:O	18:YW:101:SER:OG	2.25	0.55
33:QB:87:ARG:NH2	33:QB:220:ASP:OD2	2.39	0.55
1:RA:247:G:H4'	1:RA:386:G:C5	2.41	0.55
1:RA:807:U:O2'	1:RA:2060:A:N1	2.40	0.55
18:RW:88:ARG:NH1	18:RW:94:ASP:OD2	2.40	0.55
32:XA:170:U:H2'	32:XA:171:A:H8	1.72	0.55
32:XA:657:G:N2	46:XO:22:THR:OG1	2.37	0.55
1:YA:527:C:N4	1:YA:2779:U:OP2	2.40	0.55
1:YA:666:G:N2	30:Y8:2:PRO:O	2.39	0.55
32:QA:1250:A:OP1	40:QI:67:GLY:N	2.40	0.55
33:QB:178:ARG:NH2	33:QB:196:LEU:O	2.40	0.55
34:QC:20:SER:OG	34:QC:22:TRP:NE1	2.40	0.55
30:R8:26:LYS:HD3	30:R8:47:LYS:HB3	1.89	0.55
1:RA:1022:G:N2	1:RA:1023:U:O4	2.38	0.55
40:XI:20:ARG:NH2	40:XI:60:ASP:OD1	2.40	0.55
32:XA:264:U:O2'	48:XQ:64:PRO:O	2.23	0.55
25:Y3:18:ASP:OD1	25:Y3:18:ASP:N	2.36	0.55
1:YA:617:G:OP1	5:YF:40:GLN:NE2	2.39	0.55
32:QA:811:C:O2'	32:QA:901:A:N1	2.41	0.54
1:RA:265:A:N6	1:RA:427:U:O2'	2.40	0.54
1:YA:508:G:HO2'	1:YA:509:C:P	2.30	0.54
4:YE:105:THR:HB	4:YE:197:ILE:HG23	1.89	0.54
11:YP:4:SER:O	11:YP:7:ARG:NH2	2.39	0.54
37:QF:30:LEU:HD23	37:QF:75:LEU:HD11	1.89	0.54
1:RA:1359:A:H62	1:RA:1372:U:H3	1.55	0.54
8:RI:77:LEU:CD2	8:RI:140:LEU:HB3	2.38	0.54
32:XA:1123:A:H4'	41:XJ:36:GLY:HA3	1.89	0.54
35:XD:4:TYR:OH	35:XD:10:ARG:NH2	2.40	0.54
38:XG:11:GLN:NE2	38:XG:12:LEU:O	2.40	0.54
42:XK:33:THR:HA	42:XK:39:PRO:HA	1.87	0.54
32:XA:1329:A:H5'	44:XM:29:ARG:HE	1.73	0.54
3:YD:71:ASP:HB2	3:YD:103:ARG:HH12	1.73	0.54
50:QS:72:GLY:HA2	50:QS:75:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1992:G:N2	1:RA:1996:C:O2'	2.40	0.54
1:RA:2680:C:H5'	4:RE:189:PRO:HA	1.88	0.54
32:XA:1147:C:HO2'	40:XI:5:TYR:HH	1.53	0.54
33:XB:47:THR:HG23	33:XB:202:PRO:HG2	1.88	0.54
38:XG:94:ARG:NH1	38:XG:98:SER:OG	2.40	0.54
48:XQ:81:ARG:NH2	48:XQ:83:ASP:OD2	2.39	0.54
1:YA:1196:C:HO2'	1:YA:1228:G:HO2'	1.54	0.54
2:YB:90:C:OP2	12:YQ:16:ARG:NH2	2.40	0.54
8:RI:88:ILE:HG13	8:RI:121:LYS:HA	1.89	0.54
16:RU:85:LYS:HG3	16:RU:117:GLN:HG3	1.88	0.54
32:XA:1342:C:H2'	32:XA:1343:G:C8	2.42	0.54
33:QB:23:ARG:NH2	33:QB:191:ASP:OD1	2.40	0.54
1:RA:2133:G:O2'	1:RA:2158:A:N1	2.41	0.54
1:RA:2183:C:H2'	1:RA:2184:G:C8	2.42	0.54
1:RA:2805:G:H2'	1:RA:2807:G:C8	2.42	0.54
1:YA:1427:A:H4'	1:YA:1428:C:O5'	2.07	0.54
32:QA:673:G:H2'	32:QA:674:G:H8	1.72	0.54
32:QA:1350:A:OP1	40:QI:121:ARG:NH1	2.40	0.54
54:QX:12:A:O2'	54:QX:13:A:N7	2.39	0.54
1:RA:177:G:H5'	1:RA:178:G:C8	2.42	0.54
1:RA:2811:G:C6	1:RA:2891:G:N2	2.75	0.54
1:RA:873:G:H4'	12:RQ:63:LYS:HZ3	1.73	0.54
2:RB:52:A:HO2'	2:RB:53:A:H8	1.53	0.54
4:RE:105:THR:OG1	4:RE:199:ARG:NH2	2.40	0.54
9:RN:30:ILE:HG23	9:RN:52:VAL:HG11	1.89	0.54
21:RZ:163:LEU:HD13	21:RZ:167:PRO:HD3	1.88	0.54
32:XA:45:U:H3	32:XA:396:G:H1	1.54	0.54
35:XD:32:ALA:O	35:XD:35:ARG:N	2.38	0.54
1:YA:2741:A:H5'	31:Y9:22:ARG:HH12	1.73	0.54
1:YA:2030:A:H4'	1:YA:2031:A:H8	1.73	0.54
32:QA:1502:A:H5'	32:QA:1504:G:N7	2.23	0.54
42:QK:16:SER:OG	42:QK:106:LYS:NZ	2.41	0.54
50:QS:32:LYS:HA	50:QS:50:ALA:HB3	1.88	0.54
1:RA:1731:G:H2'	1:RA:1732:A:H8	1.73	0.54
32:XA:269:C:H2'	32:XA:270:A:C8	2.43	0.54
35:XD:20:TYR:O	35:XD:20:TYR:CD1	2.61	0.54
32:XA:1290:G:H5'	38:XG:38:LEU:HD11	1.89	0.54
52:XU:6:ARG:HE	52:XU:15:ARG:HH21	1.55	0.54
31:Y9:2:LYS:NZ	31:Y9:31:LYS:O	2.39	0.54
9:YN:63:THR:OG1	9:YN:64:GLY:N	2.40	0.54
43:QL:60:LEU:HD12	43:QL:62:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:468:G:OP2	29:R7:37:LYS:NZ	2.40	0.54
16:RU:91:ASP:HA	16:RU:95:LEU:HB2	1.88	0.54
32:XA:426:G:OP1	35:XD:38:TYR:OH	2.19	0.54
32:XA:753:A:H4'	32:XA:754:C:O5'	2.08	0.54
32:XA:789:U:H4'	54:XX:14:A:C2	2.42	0.54
36:XE:137:GLU:OE1	36:XE:140:ARG:NH1	2.40	0.54
45:XN:23:ARG:HH21	45:XN:30:ALA:HB2	1.73	0.54
1:YA:96:G:OP1	24:Y2:46:GLN:NE2	2.40	0.54
1:YA:2335:A:O2'	1:YA:2336:A:O5'	2.26	0.54
4:YE:92:THR:OG1	4:YE:93:VAL:N	2.40	0.54
6:YG:38:VAL:HG22	6:YG:93:THR:HG22	1.90	0.54
1:YA:2684:U:O2'	10:YO:68:GLU:OE1	2.18	0.54
32:QA:736:C:H2'	32:QA:737:A:C8	2.43	0.54
34:QC:108:ASN:HD21	34:QC:144:SER:HB3	1.73	0.54
35:QD:2:GLY:N	35:QD:3:ARG:O	2.41	0.54
23:R1:87:PRO:HA	23:R1:90:ILE:HG22	1.89	0.54
1:RA:1800:C:H42	1:RA:1817:G:N2	2.05	0.54
1:RA:2305:A:N6	6:RG:154:GLY:O	2.41	0.54
32:XA:129(A):G:N2	32:XA:188:U:O2'	2.41	0.54
1:YA:1964:G:O2'	1:YA:1967:C:OP2	2.17	0.54
1:YA:2712:U:O2'	1:YA:2712(A):A:H8	1.89	0.54
1:YA:312:G:H5'	1:YA:331:A:O2'	2.08	0.54
41:QJ:23:ILE:HG23	41:QJ:85:LEU:HD21	1.90	0.54
1:RA:2364:C:OP1	22:R0:55:ARG:NH1	2.39	0.54
1:RA:322:A:H5'	1:RA:340:A:H1'	1.89	0.54
6:RG:124:SER:HB2	6:RG:131:TYR:HE1	1.73	0.54
32:XA:1291:G:H4'	40:XI:39:GLY:HA3	1.88	0.54
1:YA:1097:U:H3'	1:YA:1098:A:H8	1.74	0.54
1:YA:1019:U:H3	1:YA:1142(A):A:H62	1.56	0.54
18:YW:4:LYS:HB2	18:YW:106:ILE:HG12	1.90	0.54
32:QA:760:G:N2	48:QQ:94:ASN:OD1	2.41	0.53
33:QB:107:THR:HA	33:QB:110:GLN:HG3	1.89	0.53
45:QN:27:CYS:SG	45:QN:28:GLY:N	2.81	0.53
23:R1:46:LEU:O	23:R1:47:GLN:NE2	2.40	0.53
1:RA:137(A):G:H21	19:RX:41:ASN:HD21	1.55	0.53
3:RD:71:ASP:OD2	3:RD:103:ARG:NH2	2.35	0.53
32:XA:1264:C:H2'	32:XA:1265:G:H8	1.73	0.53
10:YO:48:PRO:HB3	32:XA:1422:G:H5''	1.90	0.53
32:XA:958:A:N3	32:XA:985:C:O2'	2.35	0.53
33:XB:178:ARG:NH2	33:XB:198:ASP:OD1	2.36	0.53
32:QA:768:A:N3	32:QA:1512:U:O2'	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:QB:8:LYS:H	33:QB:11:LEU:HD12	1.71	0.53
6:RG:101:ILE:HD11	26:R4:25:TYR:H	1.74	0.53
2:RB:14:U:OP2	2:RB:70:C:O2'	2.22	0.53
10:RO:88:ASN:HD21	10:RO:92:GLU:HB2	1.73	0.53
21:RZ:110:GLY:HA3	21:RZ:174:VAL:HG11	1.90	0.53
32:XA:1277:C:O2'	32:XA:1279:A:H1'	2.09	0.53
1:YA:1364:G:OP2	23:Y1:2:SER:N	2.41	0.53
1:YA:1061:U:H3'	1:YA:1062:G:H5''	1.90	0.53
1:YA:2352:A:N6	1:YA:2365:G:O2'	2.42	0.53
32:QA:278:G:OP2	48:QQ:92:ARG:NH2	2.41	0.53
32:XA:1492:A:H1'	32:XA:1493:A:H8	1.72	0.53
34:XC:18:TRP:O	34:XC:54:ARG:NH2	2.40	0.53
36:XE:78:HIS:HB2	39:XH:104:ARG:HG2	1.90	0.53
5:YF:185:ASP:OD1	5:YF:188:ARG:NH1	2.38	0.53
7:YH:90:LYS:HD3	7:YH:159:GLU:HG2	1.90	0.53
32:QA:359:U:H2'	32:QA:360:A:C8	2.43	0.53
32:QA:56:U:H2'	32:QA:57:G:H8	1.73	0.53
35:QD:100:ARG:NH2	35:QD:136:PRO:O	2.42	0.53
39:QH:49:GLU:OE2	39:QH:62:TYR:OH	2.26	0.53
32:QA:552:U:O2'	43:QL:86:ARG:O	2.26	0.53
1:RA:526:A:O2'	1:RA:2043:C:O2	2.21	0.53
1:RA:2893:G:H5''	1:RA:2894:G:H5'	1.90	0.53
1:RA:74:A:H4'	1:RA:75:G:O5'	2.09	0.53
41:XJ:51:ARG:HB2	41:XJ:60:ARG:HA	1.91	0.53
1:YA:2031:A:N3	1:YA:2455:G:O2'	2.35	0.53
1:YA:2429:G:O6	11:YP:61:ARG:NH2	2.34	0.53
32:QA:1002:G:H2'	32:QA:1003:G:C8	2.44	0.53
32:QA:1142:G:H3'	32:QA:1143:G:H8	1.73	0.53
1:RA:1138:G:O2'	9:RN:102:ALA:O	2.26	0.53
1:RA:2115:G:N2	1:RA:2165:G:N7	2.52	0.53
1:RA:2068:U:H3	1:RA:2430:A:H2	1.55	0.53
7:RH:71:LEU:HA	7:RH:74:ASN:HB2	1.90	0.53
32:XA:1296:C:OP1	44:XM:44:ARG:NH2	2.42	0.53
32:XA:28:G:O2'	32:XA:296:U:OP1	2.24	0.53
37:XF:14:LEU:HD22	37:XF:18:GLN:HB2	1.90	0.53
42:XK:34:ASP:OD1	42:XK:38:ASN:N	2.40	0.53
48:XQ:66:SER:OG	48:XQ:67:LYS:N	2.42	0.53
1:YA:1869:G:H5'	1:YA:1870:C:OP2	2.08	0.53
5:YF:60:SER:OG	5:YF:61:GLY:N	2.38	0.53
7:YH:101:ARG:HB3	7:YH:117:PRO:HG2	1.91	0.53
3:RD:146:GLU:HB2	3:RD:189:CYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1795:C:O2	3:YD:255:LYS:NZ	2.39	0.53
32:QA:1386:G:H2'	32:QA:1387:G:H8	1.74	0.53
52:QU:22:ARG:HE	52:QU:23:PRO:HD2	1.74	0.53
32:XA:152:A:N6	32:XA:169:C:N4	2.56	0.53
46:XO:7:GLU:OE2	46:XO:38:ARG:NH2	2.42	0.53
4:YE:36:ARG:NH1	4:YE:85:ASN:OD1	2.42	0.53
5:YF:107:LYS:HD2	5:YF:206:ILE:HA	1.91	0.53
12:YQ:56:ARG:HE	21:YZ:180:VAL:HG13	1.74	0.53
52:QU:24:ARG:HH12	52:QU:26:LYS:H	1.57	0.53
1:RA:848:G:H2'	1:RA:849:A:C8	2.43	0.53
17:RV:60:GLU:OE2	17:RV:97:LYS:NZ	2.40	0.53
32:XA:992:U:O2'	32:XA:993:G:OP2	2.22	0.53
35:XD:108:LEU:HD23	35:XD:174:LEU:HD13	1.91	0.53
40:XI:25:LYS:N	40:XI:60:ASP:OD2	2.42	0.53
3:YD:206:LEU:HA	3:YD:211:ARG:HE	1.73	0.53
32:QA:12:U:O4	32:QA:22:G:O6	2.27	0.53
32:QA:34:C:H2'	32:QA:35:G:H8	1.73	0.53
32:QA:359:U:H2'	32:QA:360:A:H8	1.74	0.53
40:QI:17:VAL:HG22	40:QI:63:ILE:HD12	1.91	0.53
54:QX:7:G:N1	54:QX:8:A:N6	2.56	0.53
25:R3:12:PRO:O	25:R3:20:LYS:NZ	2.42	0.53
1:RA:1056:G:H5''	1:RA:1057:A:H5'	1.90	0.53
1:RA:626:U:H5''	1:RA:627:A:H5'	1.91	0.53
1:YA:31:C:O2'	1:YA:1238:G:H5'	2.08	0.53
1:YA:2125:G:O2'	1:YA:2173:A:N6	2.41	0.53
7:YH:43:VAL:HG22	7:YH:52:VAL:HG22	1.90	0.53
11:YP:65:ARG:O	11:YP:68:GLN:NE2	2.42	0.53
36:QE:122:GLU:O	36:QE:126:ARG:NH2	2.39	0.53
49:QR:31:LEU:HD12	49:QR:66:LEU:HB2	1.91	0.53
1:RA:1149:G:H2'	1:RA:1150:C:C6	2.44	0.53
1:RA:2364:C:H2'	1:RA:2365:G:O4'	2.09	0.53
1:RA:2790:A:H2'	1:RA:2791:C:H5''	1.92	0.53
3:RD:69:ARG:NH2	3:RD:128:GLY:O	2.42	0.53
32:XA:1233:G:O2'	32:XA:1365:G:OP1	2.26	0.53
32:XA:691:G:O6	42:XK:55:LYS:NZ	2.42	0.53
1:YA:1340:U:OP2	19:YX:78:LYS:NZ	2.42	0.53
1:YA:2145:C:O2	1:YA:2147:G:N2	2.43	0.53
1:YA:2306:C:H3'	1:YA:2307:G:H5''	1.89	0.53
32:QA:209:U:H2'	32:QA:210:U:H4'	1.91	0.52
22:R0:18:ALA:O	22:R0:20:ARG:NH1	2.38	0.52
1:RA:1441:G:H2'	1:RA:1442:G:H8	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:764:A:H5''	3:RD:210:GLY:HA3	1.90	0.52
9:RN:39:ARG:HH11	9:RN:48:MET:HE2	1.74	0.52
9:RN:58:ASP:OD1	9:RN:58:ASP:N	2.40	0.52
32:XA:595:G:H1	32:XA:641:U:HO2'	1.56	0.52
32:XA:701:C:O2	32:XA:703:G:N1	2.42	0.52
32:XA:890:G:O2'	32:XA:906:G:O6	2.26	0.52
35:XD:191:ARG:NH2	35:XD:200:GLU:OE1	2.38	0.52
32:XA:953:G:N7	44:XM:104:ARG:NH2	2.57	0.52
54:XX:3:C:H2'	54:XX:4:A:H8	1.74	0.52
33:QB:76:GLN:NE2	33:QB:206:ASP:OD1	2.41	0.52
37:QF:79:LEU:HB3	37:QF:88:VAL:HG21	1.91	0.52
1:RA:511:U:H4'	1:RA:1235:G:H4'	1.91	0.52
1:RA:2134:A:N7	1:RA:2157:G:O2'	2.42	0.52
1:RA:2867:G:OP2	15:RT:119:LYS:NZ	2.34	0.52
1:RA:995:C:O2	9:RN:3:THR:OG1	2.26	0.52
32:XA:1310:G:O2'	32:XA:1311:G:OP1	2.26	0.52
43:XL:71:PRO:O	43:XL:102:ARG:NH1	2.42	0.52
45:XN:27:CYS:SG	45:XN:28:GLY:N	2.82	0.52
1:YA:1000:A:H2'	1:YA:1001:A:C8	2.44	0.52
1:YA:554:U:HO2'	1:YA:556:G:H8	1.56	0.52
32:QA:1151:A:H2'	32:QA:1152:A:C8	2.44	0.52
32:QA:1200:C:O2'	32:QA:1201:A:OP2	2.21	0.52
32:QA:1435:G:H2'	32:QA:1436:U:C6	2.44	0.52
1:RA:220:G:O2'	1:RA:233:A:N3	2.41	0.52
1:RA:2344:U:OP1	28:R6:37:ARG:NH1	2.38	0.52
1:RA:77:C:O3'	24:R2:14:ARG:NH2	2.40	0.52
17:RV:24:LYS:HA	17:RV:92:THR:HG23	1.90	0.52
32:XA:1368:G:OP1	40:XI:111:ARG:NH1	2.34	0.52
34:XC:23:TYR:HB2	41:XJ:10:GLY:HA2	1.92	0.52
50:XS:33:THR:HG23	50:XS:35:SER:H	1.73	0.52
1:YA:30:G:O2'	1:YA:1214:A:N3	2.34	0.52
1:YA:2114:A:H2'	1:YA:2168:G:H1'	1.92	0.52
9:YN:12:ARG:NH2	9:YN:50:ASP:OD2	2.42	0.52
20:YY:15:VAL:HG21	20:YY:42:VAL:HG11	1.91	0.52
32:QA:1269:A:O2'	32:QA:1325:C:O2'	2.20	0.52
32:QA:130:A:N6	32:QA:233:C:O2	2.41	0.52
35:QD:3:ARG:HD3	35:QD:118:ARG:HD3	1.91	0.52
38:QG:99:LEU:HD22	38:QG:102:ARG:HH12	1.75	0.52
1:RA:1482:U:H5'	1:RA:1483:G:OP2	2.09	0.52
18:RW:68:ARG:NE	18:RW:110:LYS:O	2.42	0.52
32:XA:1235:U:H5''	52:XU:3:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:XO:82:ILE:HB	46:XO:87:ILE:HB	1.91	0.52
22:Y0:26:TYR:N	22:Y0:29:GLN:OE1	2.41	0.52
27:Y5:41:PRO:O	27:Y5:44:THR:OG1	2.28	0.52
1:YA:1020:A:N6	1:YA:1141:U:O2'	2.42	0.52
1:YA:2808:U:N3	1:YA:2892:A:C6	2.77	0.52
3:YD:164:GLN:OE1	3:YD:176:ARG:NH2	2.43	0.52
33:QB:18:GLY:O	33:QB:204:ASN:ND2	2.43	0.52
40:QI:28:VAL:O	40:QI:31:GLN:N	2.42	0.52
1:RA:1786:A:C8	1:RA:1938:A:N6	2.77	0.52
1:RA:2529:G:H5''	1:RA:2530:A:H5''	1.92	0.52
11:RP:62:LEU:HD12	30:R8:30:ARG:HH21	1.74	0.52
16:RU:29:SER:OG	16:RU:30:LYS:NZ	2.40	0.52
32:XA:17:U:H2'	32:XA:18:C:C6	2.45	0.52
40:XI:26:VAL:HA	40:XI:61:ALA:HB3	1.91	0.52
26:Y4:2:LYS:HB2	26:Y4:5:ILE:HD13	1.92	0.52
1:YA:263:C:H2'	1:YA:264:C:O4'	2.10	0.52
32:QA:1026:G:H5''	32:QA:1027:C:H5	1.73	0.52
32:QA:1060:C:H2'	32:QA:1061:G:H8	1.75	0.52
1:RA:1869:G:H5'	1:RA:1870:C:OP2	2.09	0.52
1:RA:2351:G:HO2'	1:RA:2352:A:H8	1.57	0.52
1:YA:2845:G:H2'	1:YA:2846:G:C8	2.44	0.52
9:YN:97:ARG:HA	9:YN:100:GLU:HB2	1.90	0.52
32:QA:1112:C:O2	34:QC:179:ARG:NH1	2.43	0.52
40:QI:9:ARG:HG2	40:QI:14:VAL:HG12	1.91	0.52
42:QK:57:THR:HG22	42:QK:59:TYR:H	1.74	0.52
26:R4:26:SER:OG	26:R4:28:LYS:O	2.27	0.52
1:RA:1681:G:HO2'	1:RA:1762:A:HO2'	1.56	0.52
36:XE:81:GLU:HG2	36:XE:90:VAL:HG23	1.92	0.52
33:QB:61:LEU:O	33:QB:65:GLY:N	2.36	0.52
1:RA:577:G:O2'	1:RA:1254:A:OP1	2.24	0.52
1:RA:2011:U:OP2	18:RW:16:LYS:NZ	2.30	0.52
1:RA:2314:C:H2'	1:RA:2315:G:H8	1.74	0.52
1:RA:654(A):G:H1	1:RA:654(T):C:H42	1.58	0.52
7:RH:40:GLU:OE2	7:RH:60:ARG:NH2	2.43	0.52
32:XA:1412:C:H2'	32:XA:1413:A:C8	2.45	0.52
32:XA:719:C:H1'	49:XR:49:LYS:HB3	1.91	0.52
34:XC:156:ARG:NE	34:XC:160:ALA:O	2.39	0.52
1:YA:2154:G:H2'	1:YA:2155:G:H8	1.75	0.52
1:YA:996:A:H4'	16:YU:92:ARG:NE	2.24	0.52
1:YA:1695:G:N7	3:YD:14:ARG:NH2	2.57	0.52
3:YD:12:SER:HB3	3:YD:208:LYS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:RO:49:ARG:NH1	32:QA:1422:G:O3'	2.42	0.52
1:RA:551:G:H5'	1:RA:1220:A:H1'	1.92	0.52
32:XA:946:A:H2'	32:XA:947:G:C8	2.45	0.52
34:XC:88:ARG:HA	34:XC:91:LEU:HD12	1.91	0.52
1:YA:988:A:C6	25:Y3:13:ILE:HG21	2.45	0.52
9:YN:95:PRO:O	9:YN:97:ARG:N	2.41	0.52
32:QA:1356:G:H2'	32:QA:1357:A:C8	2.45	0.52
35:QD:19:LEU:CD2	35:QD:67:ILE:HG13	2.36	0.52
1:RA:1638:C:O3'	1:RA:2709:G:N2	2.43	0.52
1:RA:1952:A:OP1	10:RO:44:LYS:NZ	2.37	0.52
1:RA:288:C:H2'	1:RA:289:A:H8	1.75	0.52
3:RD:259:THR:O	3:RD:259:THR:OG1	2.26	0.52
7:RH:84:SER:OG	7:RH:85:LYS:N	2.43	0.52
14:RS:58:LEU:HD12	14:RS:59:LYS:H	1.75	0.52
32:XA:99:C:H2'	32:XA:101:A:C8	2.45	0.52
32:XA:1287:A:H2	32:XA:1353:G:H1'	1.74	0.52
32:XA:667:G:H4'	46:XO:51:HIS:CE1	2.44	0.52
32:XA:656:C:O2'	46:XO:28:GLN:OE1	2.20	0.52
26:Y4:15:ILE:HB	26:Y4:32:TYR:HA	1.92	0.52
1:YA:1021:A:H3'	1:YA:1022:G:H5''	1.92	0.52
1:YA:414:C:O2	1:YA:1864:U:O2'	2.27	0.52
4:YE:59:VAL:O	4:YE:64:LYS:NZ	2.36	0.52
12:YQ:122:GLY:HA2	12:YQ:125:LEU:HD12	1.92	0.52
32:QA:1129:C:H4'	32:QA:1130:A:H8	1.76	0.51
36:QE:12:LEU:HB3	36:QE:31:LEU:HB3	1.90	0.51
44:QM:15:VAL:O	44:QM:19:LEU:HB3	2.10	0.51
1:RA:1266:G:O2'	1:RA:2012:G:O6	2.22	0.51
10:RO:19:ILE:HG22	10:RO:43:VAL:HA	1.92	0.51
32:XA:1240:U:OP1	38:XG:119:ARG:NH2	2.42	0.51
32:XA:581:G:N2	32:XA:582:U:O4	2.44	0.51
23:Y1:49:VAL:HG21	23:Y1:70:VAL:HG21	1.91	0.51
1:YA:1266:G:O2'	1:YA:2012:G:O6	2.25	0.51
1:YA:252:G:OP2	11:YP:50:ARG:NH1	2.43	0.51
1:YA:820:A:H4'	1:YA:836:G:N2	2.25	0.51
8:YI:141:LYS:HG3	8:YI:143:SER:HB3	1.91	0.51
32:QA:243:A:H4'	32:QA:244:U:O5'	2.10	0.51
32:QA:244:U:O4	32:QA:893:C:N3	2.42	0.51
35:QD:19:LEU:CD2	35:QD:67:ILE:HG12	2.37	0.51
1:RA:2816:C:O2	1:RA:2883:A:O2'	2.24	0.51
32:XA:606:G:H1	32:XA:631:G:H5''	1.75	0.51
25:Y3:15:TYR:CD2	25:Y3:53:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1022:G:N2	1:YA:1023:U:O4	2.42	0.51
32:QA:1192:C:O2	36:QE:25:ARG:NH2	2.44	0.51
32:QA:946:A:H2'	32:QA:947:G:H8	1.75	0.51
35:QD:62:GLN:O	35:QD:66:ARG:HB2	2.11	0.51
38:QG:50:ILE:HG21	38:QG:61:VAL:HG11	1.92	0.51
1:RA:2126:A:H4'	1:RA:2127:G:O5'	2.11	0.51
1:RA:2584:U:H2'	1:RA:2585:U:H2'	1.93	0.51
2:RB:8:U:O4	2:RB:112:G:O6	2.28	0.51
32:XA:152:A:N6	32:XA:169:C:C4	2.78	0.51
32:XA:375:U:O2	47:XP:28:ARG:NH1	2.44	0.51
32:XA:41:G:H2'	32:XA:42:G:H8	1.75	0.51
32:XA:745:C:H2'	32:XA:746:A:H8	1.73	0.51
32:XA:254:G:O2'	48:XQ:16:GLN:O	2.27	0.51
32:XA:966:G:C2	53:XV:34:C:H5'	2.45	0.51
28:Y6:23:THR:OG1	28:Y6:24:GLU:N	2.43	0.51
1:YA:758:C:O2'	1:YA:1981:A:N3	2.34	0.51
1:YA:2006:C:O2'	1:YA:2823:A:N3	2.43	0.51
1:YA:229:A:OP1	1:YA:229:A:H4'	2.08	0.51
1:YA:247:G:H4'	1:YA:386:G:C5	2.46	0.51
1:YA:2679:A:OP2	4:YE:160:TYR:OH	2.28	0.51
1:YA:2809:A:H2'	1:YA:2810:A:C8	2.45	0.51
32:QA:1349:A:H62	32:QA:1373:G:N2	2.08	0.51
32:QA:430:A:P	35:QD:22:LYS:NZ	2.82	0.51
32:QA:426:G:OP1	35:QD:36:ARG:NH1	2.43	0.51
23:R1:83:GLU:HG2	23:R1:85:LEU:H	1.75	0.51
1:RA:1786:A:C8	1:RA:1938:A:C6	2.98	0.51
1:RA:820:A:H4'	1:RA:836:G:H22	1.76	0.51
7:RH:89:ILE:HG22	7:RH:162:ILE:HG23	1.92	0.51
14:RS:35:ILE:HD11	14:RS:101:LEU:HD12	1.92	0.51
32:XA:180:U:H2'	32:XA:181:G:C8	2.45	0.51
32:XA:545:C:O2'	32:XA:549:C:OP1	2.25	0.51
34:XC:131:ARG:NH1	34:XC:166:GLU:OE1	2.37	0.51
52:XU:4:GLY:HA2	52:XU:15:ARG:HH12	1.76	0.51
1:YA:2074:U:HO2'	1:YA:2597:G:HO2'	1.59	0.51
1:YA:995:C:O2	9:YN:3:THR:OG1	2.23	0.51
32:QA:1103:C:H5''	33:QB:98:LEU:HD13	1.92	0.51
32:QA:1287:A:H2'	32:QA:1288:A:C8	2.45	0.51
32:QA:1392:G:H21	32:QA:1502:A:H8	1.57	0.51
35:QD:20:TYR:CE2	37:XF:15:ASP:HB2	2.44	0.51
41:QJ:78:ASN:HB2	41:QJ:81:THR:HG23	1.92	0.51
51:QT:72:LEU:O	51:QT:74:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1323:U:OP1	18:RW:98:LYS:NZ	2.40	0.51
1:RA:321:G:O2'	1:RA:340:A:N3	2.44	0.51
1:RA:372:G:HO2'	1:RA:373:U:P	2.33	0.51
2:RB:48:A:OP2	14:RS:30:ARG:NH2	2.44	0.51
1:RA:870:A:OP1	12:RQ:6:ARG:NH1	2.44	0.51
32:XA:1038:C:H2'	32:XA:1039:C:C6	2.45	0.51
1:YA:1056:G:H5''	1:YA:1057:A:H5'	1.92	0.51
1:YA:1063:G:H22	1:YA:1076:C:H1'	1.75	0.51
1:YA:547:A:H2'	1:YA:548:A:C8	2.45	0.51
44:QM:102:ARG:HH21	44:QM:105:THR:H	1.57	0.51
32:QA:376:G:H5''	47:QP:5:ARG:HB2	1.92	0.51
50:QS:36:ARG:HH21	50:QS:53:ASN:HA	1.75	0.51
6:RG:67:LYS:H	26:R4:6:HIS:CE1	2.28	0.51
1:RA:1433:U:O4	1:RA:1560:G:O6	2.28	0.51
17:RV:76:LYS:HB2	17:RV:81:TYR:HB3	1.93	0.51
32:XA:1172:C:H2'	32:XA:1173:G:H8	1.76	0.51
32:XA:1211:U:H5'	32:XA:1212:U:H5'	1.91	0.51
32:XA:1435:G:H2'	32:XA:1436:U:C6	2.45	0.51
32:XA:736:C:H2'	32:XA:737:A:H8	1.76	0.51
32:XA:978:A:N6	32:XA:1316:G:O2'	2.44	0.51
1:YA:2346:A:H5''	1:YA:2383:G:H1'	1.92	0.51
1:YA:606:U:H4'	1:YA:658:C:H4'	1.92	0.51
4:YE:126:PRO:O	4:YE:135:HIS:ND1	2.39	0.51
36:QE:105:VAL:HG21	36:QE:128:PRO:HB3	1.91	0.51
27:R5:41:PRO:O	27:R5:44:THR:OG1	2.28	0.51
1:RA:1817:G:OP1	3:RD:88:ARG:NH2	2.42	0.51
1:RA:270(S):G:H2'	1:RA:270(T):G:H8	1.75	0.51
1:RA:2712(A):A:H5''	1:RA:2713:A:OP2	2.11	0.51
2:RB:28:C:H2'	2:RB:29:A:C8	2.46	0.51
8:RI:75:LEU:HD13	8:RI:105:HIS:NE2	2.26	0.51
44:XM:2:ALA:O	44:XM:9:ILE:CD1	2.49	0.51
1:YA:2743:C:OP1	31:Y9:33:LYS:NZ	2.38	0.51
1:YA:551:G:H5'	1:YA:1220:A:H1'	1.93	0.51
20:YY:83:THR:OG1	20:YY:84:ARG:O	2.27	0.51
32:QA:449:C:H5	47:QP:42:ARG:HH21	1.59	0.51
51:QT:85:MET:HB2	51:QT:104:LEU:HD21	1.93	0.51
1:RA:514:A:N3	1:RA:581:C:O2'	2.37	0.51
1:RA:636:G:N7	11:RP:113:LYS:NZ	2.50	0.51
21:RZ:183:LEU:HA	21:RZ:186:GLU:HB2	1.92	0.51
34:XC:115:LEU:O	34:XC:119:ARG:N	2.42	0.51
40:XI:71:SER:HA	40:XI:74:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2577:A:H5'	27:Y5:3:LYS:HD2	1.93	0.51
1:YA:2618:G:H21	4:YE:150:VAL:HG21	1.76	0.51
34:QC:123:GLN:O	34:QC:127:ARG:N	2.44	0.51
1:RA:210:C:OP2	29:R7:29:LYS:NZ	2.43	0.51
1:RA:2291:U:O2'	1:RA:2374:C:O2	2.28	0.51
20:RY:11:ASP:OD1	20:RY:11:ASP:N	2.38	0.51
46:XO:26:GLU:HG3	46:XO:70:LEU:HD11	1.93	0.51
1:YA:1178:C:H2'	1:YA:1179:C:C6	2.46	0.51
1:YA:127:A:H5''	1:YA:128:C:C6	2.46	0.51
1:YA:1889:A:N3	1:YA:2086:U:O2'	2.42	0.51
32:QA:1226:C:OP2	44:QM:103:THR:OG1	2.22	0.51
32:QA:1368:G:H5''	40:QI:112:LYS:HB3	1.93	0.51
32:QA:1499:A:H1'	32:QA:1520:G:H5'	1.92	0.51
32:QA:946:A:H2'	32:QA:947:G:C8	2.46	0.51
35:QD:103:ASN:OD1	35:QD:114:ARG:NE	2.35	0.51
36:QE:7:GLU:OE1	36:QE:37:ARG:NE	2.36	0.51
40:QI:93:ARG:HD3	40:QI:97:LYS:HE2	1.92	0.51
43:QL:114:LYS:O	43:QL:117:ARG:NH1	2.44	0.51
1:RA:2849:U:OP2	15:RT:95:ARG:NH1	2.44	0.51
10:RO:104:ARG:HH11	10:RO:121:VAL:HG12	1.76	0.51
32:XA:736:C:H2'	32:XA:737:A:C8	2.46	0.51
44:XM:34:LEU:HB3	44:XM:41:PRO:HG3	1.92	0.51
1:YA:1405:U:H2'	1:YA:1406:U:H6	1.76	0.51
1:YA:321:G:OP2	5:YF:135:LYS:HD3	2.10	0.51
13:YR:56:LYS:NZ	13:YR:90:ARG:O	2.43	0.51
32:QA:119:A:H4'	32:QA:120:A:O5'	2.10	0.50
35:QD:72:GLU:OE2	35:QD:207:TYR:OH	2.27	0.50
54:QX:2:G:C5	54:QX:3:C:N4	2.79	0.50
16:RU:90:VAL:HG22	17:RV:38:LEU:HB3	1.93	0.50
32:XA:452:A:H62	32:XA:480:U:H3	0.74	0.50
32:XA:713:G:H2'	32:XA:714:G:C8	2.45	0.50
1:YA:2186:G:H2'	1:YA:2187:G:C8	2.46	0.50
11:YP:47:ASP:OD2	11:YP:50:ARG:NH2	2.44	0.50
32:QA:985:C:H2'	32:QA:986:A:H8	1.76	0.50
1:RA:630:G:N2	1:RA:633:A:OP2	2.38	0.50
1:RA:83:G:H1	1:RA:102:G:HO2'	1.58	0.50
8:RI:81:VAL:HG21	8:RI:88:ILE:HD12	1.93	0.50
32:XA:1127:G:O6	32:XA:1144:G:N1	2.40	0.50
32:XA:1336:C:O2	32:XA:1337:G:N1	2.44	0.50
36:XE:110:LEU:HD13	36:XE:118:ILE:HD13	1.92	0.50
44:XM:81:LEU:HD12	44:XM:88:ARG:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:XN:44:LEU:HA	45:XN:47:LEU:HB2	1.94	0.50
8:YI:81:VAL:HG21	8:YI:88:ILE:HD12	1.92	0.50
32:QA:673:G:O3'	37:QF:87:ARG:NH2	2.44	0.50
40:QI:13:ALA:HB2	40:QI:68:GLY:HA3	1.91	0.50
24:R2:45:SER:O	24:R2:46:GLN:NE2	2.44	0.50
1:RA:2199:A:OP1	23:R1:50:ARG:NH2	2.45	0.50
6:RG:121:ASN:ND2	6:RG:124:SER:OG	2.44	0.50
12:RQ:52:VAL:HG22	21:RZ:183:LEU:HD22	1.94	0.50
32:XA:745:C:H2'	32:XA:746:A:C8	2.47	0.50
32:XA:619:U:N3	35:XD:134:ASP:OD1	2.40	0.50
38:XG:24:THR:O	38:XG:28:ASN:ND2	2.42	0.50
1:YA:2539:C:H4'	31:Y9:3:VAL:HG21	1.94	0.50
1:YA:2355:C:H1'	22:Y0:39:ARG:HH21	1.76	0.50
1:YA:2404:C:O3'	11:YP:77:ARG:NH2	2.44	0.50
32:QA:1342:C:H2'	32:QA:1343:G:C8	2.47	0.50
32:QA:45:U:H2'	32:QA:46:G:C8	2.47	0.50
32:QA:516:U:O2'	32:QA:519:C:N3	2.44	0.50
34:QC:19:GLU:O	34:QC:40:ARG:NH2	2.45	0.50
44:QM:92:HIS:CE1	44:QM:98:VAL:HG21	2.46	0.50
1:RA:226:G:H2'	1:RA:227:A:C8	2.46	0.50
8:RI:104:GLN:HG2	8:RI:105:HIS:CD2	2.46	0.50
32:XA:1055:A:H62	32:XA:1200:C:H42	1.59	0.50
32:XA:584:G:H1	32:XA:757:U:H3	1.58	0.50
32:XA:757:U:H2'	32:XA:758:G:O4'	2.12	0.50
34:XC:153:VAL:O	34:XC:166:GLU:N	2.43	0.50
35:XD:160:GLN:HA	35:XD:163:GLU:HG2	1.93	0.50
48:XQ:83:ASP:N	48:XQ:83:ASP:OD1	2.44	0.50
1:YA:1500:G:N2	3:YD:99:ASP:O	2.38	0.50
44:QM:93:ARG:O	44:QM:94:ARG:NH1	2.44	0.50
51:QT:75:ASN:N	51:QT:75:ASN:OD1	2.42	0.50
1:RA:1728:G:H8	1:RA:1732:A:H62	1.59	0.50
1:RA:1800:C:N3	1:RA:1817:G:N1	2.60	0.50
3:RD:254:THR:O	3:RD:254:THR:OG1	2.27	0.50
3:RD:260:ARG:HH22	3:RD:270:ILE:HD12	1.76	0.50
5:RF:149:ASP:N	5:RF:149:ASP:OD1	2.43	0.50
7:RH:149:ARG:NH2	7:RH:167:GLU:OE2	2.38	0.50
15:RT:62:THR:HB	15:RT:75:ILE:HG12	1.93	0.50
32:XA:1203:C:H2'	32:XA:1204:A:H8	1.76	0.50
32:XA:1264:C:H2'	32:XA:1265:G:C8	2.46	0.50
32:XA:1355:G:H2'	32:XA:1356:G:C8	2.47	0.50
54:XX:5:A:H2'	54:XX:6:G:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2469:A:H2	1:YA:2481:G:H21	1.58	0.50
1:YA:2522:U:O2'	1:YA:2647:U:OP1	2.22	0.50
32:QA:1064:G:H1'	32:QA:1066:C:C6	2.46	0.50
32:QA:1224:G:O2'	32:QA:1322:C:OP2	2.21	0.50
32:QA:481:G:O2'	32:QA:482:A:O5'	2.29	0.50
35:QD:187:ARG:NH2	35:QD:193:ASP:OD2	2.33	0.50
37:QF:9:VAL:HB	37:QF:87:ARG:HB2	1.94	0.50
1:RA:1042:G:O6	1:RA:1113:U:O2	2.29	0.50
1:RA:955:C:OP1	12:RQ:85:LYS:NZ	2.42	0.50
32:XA:1151:A:H2'	32:XA:1152:A:H8	1.76	0.50
32:XA:992:U:C2	32:XA:1044:A:N6	2.79	0.50
1:YA:2475:C:H42	1:YA:2529:G:H22	1.58	0.50
32:QA:909:A:N3	32:QA:1413:A:O2'	2.33	0.50
1:RA:2123:G:H2'	1:RA:2124:G:H8	1.77	0.50
3:RD:85:ASP:OD2	3:RD:88:ARG:NH1	2.38	0.50
6:RG:11:TYR:HA	6:RG:15:VAL:HB	1.94	0.50
40:XI:20:ARG:O	40:XI:60:ASP:N	2.44	0.50
41:XJ:38:ILE:HG23	41:XJ:71:LEU:HB3	1.92	0.50
1:YA:1265:A:H8	1:YA:1265:A:OP1	1.94	0.50
1:YA:2246:G:H2'	1:YA:2247:A:H8	1.75	0.50
7:YH:3:ARG:CD	7:YH:54:ARG:NH1	2.70	0.50
17:YV:38:LEU:HD13	17:YV:50:PRO:O	2.11	0.50
44:QM:15:VAL:O	44:QM:19:LEU:CB	2.60	0.50
1:RA:2168:G:N2	1:RA:2170:A:N7	2.59	0.50
1:RA:232:G:H8	1:RA:232:G:OP2	1.95	0.50
1:RA:2571:C:O2'	4:RE:146:THR:O	2.26	0.50
32:XA:1296:C:O3'	44:XM:13:LYS:NZ	2.40	0.50
32:XA:1414:U:H2'	32:XA:1415:G:H8	1.76	0.50
32:XA:875:C:H1'	39:XH:15:ASN:HD21	1.75	0.50
41:XJ:24:VAL:HG11	41:XJ:37:PRO:HD3	1.93	0.50
41:XJ:50:ILE:HA	41:XJ:60:ARG:HG2	1.94	0.50
1:YA:1012:U:OP1	16:YU:75:ASN:ND2	2.44	0.50
1:YA:2096:U:O4	1:YA:2193:G:O6	2.29	0.50
1:YA:2547:U:O2	10:YO:23:ARG:NH2	2.45	0.50
32:QA:1022:G:H2'	32:QA:1023:G:C8	2.47	0.50
32:QA:1244:C:H2'	32:QA:1245:A:C8	2.46	0.50
32:QA:1274:G:N2	32:QA:1275:A:N7	2.59	0.50
32:QA:1329:A:N7	52:QU:7:ARG:NH2	2.53	0.50
32:QA:1500:A:H5''	32:QA:1508:G:H5''	1.93	0.50
1:RA:1993:U:H4'	4:RE:128:SER:HB3	1.93	0.50
12:RQ:48:GLU:HA	12:RQ:51:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2101:G:H2'	1:YA:2102:U:C6	2.47	0.50
1:YA:243:U:OP2	1:YA:254:G:N1	2.43	0.50
1:YA:996:A:H4'	16:YU:92:ARG:HE	1.76	0.50
35:QD:19:LEU:HD23	35:QD:67:ILE:HD11	1.94	0.49
36:QE:8:GLU:HA	36:QE:34:VAL:HG12	1.93	0.49
1:RA:1509:C:N3	1:RA:1511:A:N6	2.60	0.49
1:RA:2074:U:H2'	1:RA:2075:U:C6	2.47	0.49
1:RA:2867:G:O2'	1:RA:2868:A:H8	1.93	0.49
21:RZ:140:ASP:OD1	21:RZ:142:SER:OG	2.28	0.49
3:YD:37:LEU:HD13	3:YD:62:TYR:HB2	1.94	0.49
9:YN:16:ILE:HG22	9:YN:18:ALA:HB2	1.94	0.49
36:QE:102:ALA:HB1	36:QE:106:PRO:HG2	1.94	0.49
1:RA:2296:U:OP2	14:RS:9:ARG:NH1	2.40	0.49
5:RF:185:ASP:HA	5:RF:188:ARG:HD3	1.93	0.49
32:XA:404:U:H2'	32:XA:405:U:H6	1.77	0.49
34:XC:14:ILE:HG12	34:XC:15:THR:HB	1.94	0.49
40:XI:112:LYS:HA	40:XI:119:ALA:HB2	1.95	0.49
1:YA:2074:U:H2'	1:YA:2075:U:C6	2.47	0.49
1:YA:1797:C:H4'	3:YD:257:LEU:O	2.12	0.49
32:QA:1446:A:HO2'	32:QA:1447:G:P	2.35	0.49
32:QA:152:A:N6	32:QA:169:C:H42	2.08	0.49
34:QC:78:GLY:HA3	34:QC:83:ARG:H	1.78	0.49
37:QF:11:ASN:HB3	37:QF:14:LEU:HD13	1.94	0.49
25:R3:51:ALA:HA	25:R3:54:VAL:HG12	1.93	0.49
7:RH:153:LYS:HB2	7:RH:162:ILE:H	1.77	0.49
32:XA:1022:G:H2'	32:XA:1023:G:C8	2.48	0.49
32:XA:1294:G:H2'	32:XA:1295:G:H8	1.76	0.49
32:XA:411:A:N3	32:XA:413:G:O2'	2.43	0.49
32:XA:662:G:H2'	32:XA:663:A:C8	2.47	0.49
33:XB:68:ILE:HG12	33:XB:161:ALA:HB3	1.94	0.49
33:XB:73:THR:OG1	33:XB:170:GLU:OE2	2.30	0.49
1:YA:2100:G:H2'	1:YA:2101:G:H8	1.78	0.49
1:YA:248:G:H5'	1:YA:250:G:N7	2.27	0.49
1:YA:2867:G:HO2'	1:YA:2868:A:P	2.34	0.49
10:YO:80:ASP:OD2	15:YT:64:ARG:NH2	2.45	0.49
32:QA:45:U:H2'	32:QA:46:G:H8	1.77	0.49
35:QD:9:CYS:O	35:QD:13:ARG:HB2	2.13	0.49
1:RA:1427:A:H4'	1:RA:1428:C:O5'	2.11	0.49
1:RA:389:G:H1	11:RP:71:VAL:HG12	1.77	0.49
32:XA:323:U:H5'	51:XT:23:ARG:HB3	1.93	0.49
34:XC:89:GLU:O	34:XC:93:LYS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:XG:66:VAL:HG13	38:XG:67:GLU:HG2	1.93	0.49
1:YA:714:U:OP2	46:XO:88:ARG:NH1	2.44	0.49
30:Y8:6:THR:HG22	30:Y8:63:PRO:HD2	1.92	0.49
8:YI:86:THR:H	8:YI:123:LEU:HD12	1.77	0.49
10:YO:4:PRO:HA	10:YO:21:CYS:HB3	1.95	0.49
32:QA:1209:C:O2'	32:QA:1214:C:N4	2.40	0.49
47:QP:43:LYS:HG2	47:QP:48:TRP:CD2	2.48	0.49
1:RA:1464:C:O2'	1:RA:1528:A:H8	1.94	0.49
1:RA:1782:C:C4	1:RA:2587:A:C2	3.00	0.49
5:RF:60:SER:OG	5:RF:61:GLY:N	2.46	0.49
32:XA:1409:C:H2'	32:XA:1410:G:H8	1.77	0.49
10:YO:97:ARG:NH2	32:XA:338:A:OP2	2.44	0.49
35:XD:19:LEU:O	35:XD:19:LEU:HD12	2.12	0.49
24:Y2:12:GLU:HA	24:Y2:15:LYS:HE2	1.95	0.49
1:YA:190:A:N3	1:YA:679:C:O2'	2.42	0.49
1:YA:813:U:H2'	1:YA:814:C:C6	2.47	0.49
32:QA:130:A:HO2'	32:QA:263:A:HO2'	1.53	0.49
33:QB:46:LYS:NZ	33:QB:49:GLU:OE1	2.38	0.49
32:QA:1298:C:OP2	38:QG:114:ARG:NH1	2.45	0.49
39:QH:23:SER:OG	39:QH:24:THR:N	2.46	0.49
42:QK:24:SER:OG	42:QK:27:ASN:N	2.38	0.49
1:RA:11:G:H22	1:RA:2627:G:H5''	1.78	0.49
1:RA:2327:A:H2'	1:RA:2328:A:C8	2.46	0.49
4:RE:78:LEU:O	4:RE:79:ARG:NH1	2.37	0.49
1:RA:2250:G:C4	12:RQ:82:ARG:HG3	2.48	0.49
18:RW:82:LEU:HB2	18:RW:98:LYS:HB2	1.94	0.49
20:RY:39:VAL:HG13	20:RY:42:VAL:HB	1.95	0.49
32:XA:1129:C:N4	32:XA:1135:U:O4	2.46	0.49
32:XA:708:C:H2'	32:XA:709:G:H8	1.77	0.49
32:XA:711:G:H2'	32:XA:712:A:H8	1.78	0.49
34:XC:157:ILE:HD12	34:XC:164:ARG:HB2	1.94	0.49
40:XI:96:LEU:O	40:XI:100:GLY:N	2.45	0.49
32:XA:1228:C:OP1	44:XM:108:ARG:NH1	2.45	0.49
44:XM:65:LYS:HE2	44:XM:70:LEU:HD23	1.94	0.49
1:YA:1021:A:H8	1:YA:1022:G:H5''	1.78	0.49
6:YG:98:ARG:HA	6:YG:101:ILE:HG22	1.94	0.49
32:QA:922:G:H4'	36:QE:20:GLN:HA	1.95	0.49
35:QD:18:LYS:HE2	35:QD:20:TYR:CE1	2.47	0.49
1:RA:1543:A:O2'	1:RA:1544:C:H3'	2.13	0.49
5:RF:63:LYS:NZ	5:RF:75:HIS:O	2.37	0.49
10:RO:13:ASN:ND2	10:RO:96:THR:OG1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:RP:95:VAL:HB	11:RP:125:VAL:HG23	1.94	0.49
16:RU:8:VAL:HG22	16:RU:12:ARG:HD2	1.94	0.49
39:XH:91:ARG:NE	48:XQ:32:TYR:O	2.46	0.49
30:Y8:11:LYS:NZ	30:Y8:65:GLU:OE1	2.42	0.49
39:QH:84:ARG:NH2	39:QH:136:GLU:OE2	2.44	0.49
1:RA:1639:U:H2'	1:RA:1640:C:H5''	1.95	0.49
1:RA:2521:C:O2'	1:RA:2564:A:N3	2.37	0.49
1:RA:2655:G:HO2'	1:RA:2664:G:H1	1.55	0.49
8:RI:86:THR:O	8:RI:87:LYS:CG	2.60	0.49
32:XA:1036:G:N7	32:XA:1037:C:N4	2.60	0.49
32:XA:184:G:H2'	32:XA:185:A:H8	1.76	0.49
32:XA:578:C:O2'	32:XA:728:A:N3	2.33	0.49
32:XA:79:G:H2'	32:XA:80:G:C8	2.47	0.49
37:XF:22:GLU:OE2	37:XF:84:ASN:ND2	2.38	0.49
1:YA:1210:A:H8	1:YA:1210:A:H5'	1.78	0.49
1:YA:183:C:O2'	1:YA:432:A:N3	2.40	0.49
32:QA:1065:U:O2'	32:QA:1066:C:OP2	2.26	0.49
32:QA:946:A:O2'	32:QA:1333:A:N3	2.42	0.49
32:QA:1347:G:O2'	32:QA:1348:U:OP2	2.27	0.49
32:QA:728:A:H2'	32:QA:729:A:H8	1.77	0.49
33:QB:150:SER:OG	33:QB:151:GLY:N	2.46	0.49
1:RA:1000:A:H2'	1:RA:1001:A:C8	2.47	0.49
1:RA:1165:U:O4	1:RA:1184:G:O6	2.30	0.49
1:RA:1171:G:H5''	1:RA:1173:G:H5''	1.94	0.49
1:RA:30:G:O2'	1:RA:1214:A:N3	2.38	0.49
6:RG:63:ILE:HG13	6:RG:64:THR:HG23	1.95	0.49
8:RI:93:THR:O	8:RI:97:ILE:HG13	2.12	0.49
32:XA:1287:A:H2'	32:XA:1288:A:C8	2.48	0.49
32:XA:1328:C:OP1	52:XU:21:TYR:OH	2.29	0.49
32:XA:985:C:H2'	32:XA:986:A:C8	2.47	0.49
1:YA:587:C:O2	11:YP:33:ARG:NH2	2.45	0.49
5:YF:168:ARG:HG3	5:YF:175:THR:HG21	1.95	0.49
7:YH:3:ARG:NH2	7:YH:62:LYS:O	2.46	0.49
32:QA:576:G:N2	32:QA:760:G:OP2	2.46	0.49
1:RA:1525:G:H2'	1:RA:1526:G:H8	1.78	0.49
1:RA:1728:G:H3'	1:RA:1729:A:C5'	2.43	0.49
1:RA:2246:G:H2'	1:RA:2247:A:H8	1.78	0.49
1:RA:2692:C:H2'	1:RA:2693:A:C8	2.48	0.49
19:RX:29:TRP:HZ3	19:RX:59:VAL:HG11	1.77	0.49
32:XA:60:A:H4'	32:XA:61:G:O5'	2.12	0.49
34:XC:20:SER:HB2	34:XC:40:ARG:HH22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:XI:110:GLU:OE1	40:XI:120:ARG:NH2	2.44	0.49
41:XJ:21:GLN:HA	41:XJ:24:VAL:HG22	1.95	0.49
44:XM:79:LYS:NZ	44:XM:79:LYS:O	2.41	0.49
30:Y8:37:SER:OG	30:Y8:38:GLY:N	2.46	0.49
1:YA:1031:G:H4'	31:Y9:6:SER:HB2	1.95	0.49
1:YA:242:G:O2'	1:YA:254:G:O6	2.21	0.49
32:QA:677:U:O2	32:QA:777:A:O2'	2.30	0.48
38:QG:39:ALA:HA	38:QG:42:ILE:HD12	1.94	0.48
1:RA:1057:A:O2'	1:RA:1058:G:OP1	2.26	0.48
1:RA:30:G:H2'	1:RA:31:C:C6	2.48	0.48
4:RE:36:ARG:NH1	4:RE:85:ASN:OD1	2.47	0.48
32:XA:1032(A):G:H2'	32:XA:1032(B):G:C8	2.48	0.48
32:XA:78:G:O2'	32:XA:79:G:OP1	2.25	0.48
32:XA:971:G:H5''	32:XA:972:C:H5''	1.94	0.48
32:QA:439:A:OP2	32:QA:493:G:N1	2.34	0.48
34:QC:105:GLU:OE1	34:QC:107:GLN:NE2	2.47	0.48
2:RB:15:A:H5'	2:RB:16:G:C8	2.48	0.48
9:RN:96:GLU:HB2	9:RN:122:VAL:HG12	1.95	0.48
32:XA:1118:C:H1'	32:XA:1179:A:C5	2.48	0.48
32:XA:1175:G:H2'	32:XA:1176:A:C8	2.48	0.48
1:YA:1055:G:H1	1:YA:1104:C:H42	1.61	0.48
1:YA:237:C:O2	1:YA:609:A:O2'	2.27	0.48
1:YA:1453:A:O2'	1:YA:2702:U:O4	2.31	0.48
1:YA:27:G:HO2'	1:YA:28:A:H8	1.57	0.48
9:YN:47:ALA:HB2	9:YN:112:LEU:HD11	1.95	0.48
19:YX:64:LYS:HZ2	19:YX:73:ARG:HE	1.60	0.48
32:QA:1316:G:N2	32:QA:1319:A:OP2	2.45	0.48
32:QA:950:U:H2'	32:QA:951:G:C8	2.48	0.48
32:QA:958:A:N3	32:QA:985:C:O2'	2.43	0.48
35:QD:79:PHE:HE1	35:QD:204:ILE:HD13	1.78	0.48
40:QI:25:LYS:N	40:QI:60:ASP:OD1	2.46	0.48
1:RA:121:G:H4'	1:RA:149:A:H5'	1.95	0.48
1:RA:78:A:H2'	1:RA:79:G:H8	1.78	0.48
32:XA:41:G:H2'	32:XA:42:G:C8	2.48	0.48
44:XM:53:VAL:HG23	44:XM:57:ARG:HH22	1.78	0.48
26:Y4:53:GLU:HG2	26:Y4:56:VAL:HG13	1.95	0.48
1:YA:2185:C:H2'	1:YA:2186:G:H8	1.78	0.48
1:YA:2774:C:H2'	1:YA:2775:A:O4'	2.13	0.48
1:YA:309:G:N3	1:YA:329:G:O2'	2.44	0.48
1:YA:589:C:H2'	1:YA:590:A:C8	2.48	0.48
3:YD:254:THR:O	3:YD:254:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:YD:181:GLU:HB2	3:YD:274:ARG:H	1.78	0.48
6:YG:11:TYR:OH	6:YG:32:PRO:O	2.28	0.48
32:QA:1228:C:OP1	44:QM:115:LYS:N	2.40	0.48
32:QA:235:C:H2'	32:QA:236:G:H8	1.78	0.48
32:QA:438:G:H4'	35:QD:123:HIS:CD2	2.48	0.48
1:RA:1417:C:H2'	1:RA:1418:G:O4'	2.13	0.48
1:RA:2010:G:H5''	18:RW:42:ARG:HB2	1.95	0.48
1:RA:86:C:H4'	1:RA:104:U:H1'	1.94	0.48
16:RU:17:ILE:HG13	16:RU:32:PHE:HE1	1.78	0.48
32:XA:924:C:O2'	32:XA:1502:A:N6	2.46	0.48
35:XD:15:GLU:HB3	35:XD:63:LYS:HE2	1.95	0.48
35:QD:20:TYR:CE2	37:XF:15:ASP:HA	2.47	0.48
34:XC:30:ARG:NH2	45:XN:35:ARG:O	2.42	0.48
30:Y8:37:SER:OG	30:Y8:39:LYS:N	2.45	0.48
1:YA:288:C:H2'	1:YA:289:A:H8	1.79	0.48
1:YA:443:A:H5''	1:YA:444:C:OP1	2.14	0.48
12:YQ:59:ARG:HA	21:YZ:180:VAL:HG23	1.94	0.48
33:QB:80:ILE:HD13	33:QB:211:ILE:HG22	1.94	0.48
25:R3:39:ASP:OD1	25:R3:44:ARG:NH2	2.46	0.48
1:RA:1638:C:O2	1:RA:2698:U:O2'	2.30	0.48
1:RA:2210:G:H3'	1:RA:2211:G:C8	2.49	0.48
1:RA:270(I):G:H1	1:RA:270(Q):C:H42	1.60	0.48
1:RA:67:U:H3	1:RA:74:A:H2	1.62	0.48
1:RA:792:G:O2'	1:RA:2440:C:N3	2.47	0.48
3:RD:131:LEU:HD12	3:RD:136:ILE:HG12	1.95	0.48
11:RP:68:GLN:HG2	30:R8:12:LYS:HG2	1.95	0.48
21:RZ:79:ARG:HB3	21:RZ:80:ARG:HG3	1.95	0.48
35:XD:78:LEU:HD12	35:XD:96:LEU:HB3	1.94	0.48
45:XN:27:CYS:SG	45:XN:29:ARG:N	2.87	0.48
51:XT:55:ILE:O	51:XT:59:ALA:N	2.44	0.48
1:YA:1429:G:H2'	1:YA:1430:C:C6	2.49	0.48
1:YA:1478:G:HO2'	1:YA:1558:A:H2	1.60	0.48
1:YA:1637:A:H4'	1:YA:2711:A:O2'	2.14	0.48
1:YA:2364:C:H2'	1:YA:2365:G:O4'	2.14	0.48
1:YA:2629:A:O2'	1:YA:2630:G:H5''	2.14	0.48
1:YA:956:G:OP2	12:YQ:14:ARG:NH2	2.47	0.48
5:YF:132:VAL:HG13	5:YF:162:LEU:HD12	1.95	0.48
5:YF:77:ASP:OD1	5:YF:77:ASP:N	2.42	0.48
21:YZ:140:ASP:OD1	21:YZ:142:SER:OG	2.31	0.48
35:QD:201:GLN:NE2	36:QE:116:THR:O	2.45	0.48
32:QA:375:U:O2	47:QP:28:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:QS:55:LYS:HG3	50:QS:56:GLN:HB3	1.95	0.48
24:R2:41:ILE:HD11	24:R2:44:LEU:HG	1.96	0.48
26:R4:12:ALA:HB3	26:R4:24:THR:HG23	1.95	0.48
1:RA:2131:G:H4'	1:RA:2132:U:H4'	1.95	0.48
1:RA:184:C:O2'	1:RA:217:G:N3	2.42	0.48
1:RA:2701:C:H3'	1:RA:2702:U:C5'	2.40	0.48
1:RA:922:U:H2'	1:RA:923:C:C6	2.48	0.48
1:RA:958:U:OP2	12:RQ:14:ARG:NH1	2.46	0.48
4:RE:36:ARG:HG2	4:RE:47:VAL:HG22	1.95	0.48
32:XA:414:A:OP2	32:XA:428:G:N2	2.33	0.48
36:XE:20:GLN:O	36:XE:23:GLY:N	2.43	0.48
41:XJ:53:PRO:HB3	45:XN:42:ILE:HG12	1.94	0.48
1:YA:1239:G:H2'	1:YA:1240:U:O4'	2.13	0.48
2:YB:5:C:O2'	2:YB:27:C:O2	2.31	0.48
32:QA:1326:C:OP1	52:QU:17:THR:OG1	2.30	0.48
32:QA:262:A:H2'	32:QA:263:A:C8	2.47	0.48
1:RA:1031:G:O2'	31:R9:7:VAL:O	2.26	0.48
1:RA:140:A:H8	1:RA:1408:C:O2'	1.96	0.48
1:RA:855:G:H1	1:RA:922:U:H3	1.61	0.48
18:RW:58:ALA:HB1	18:RW:64:MET:HB2	1.96	0.48
32:XA:1174:G:H2'	32:XA:1175:G:H8	1.79	0.48
32:XA:714:G:H2'	32:XA:715:A:C8	2.48	0.48
35:XD:98:GLU:HA	35:XD:103:ASN:HD22	1.78	0.48
32:XA:186(A):C:N3	51:XT:105:SER:OG	2.47	0.48
29:Y7:10:ARG:HE	29:Y7:14:LYS:HD2	1.79	0.48
1:YA:2740:A:H2'	1:YA:2741:A:C8	2.49	0.48
1:YA:321:G:O2'	1:YA:340:A:N3	2.40	0.48
1:YA:540:G:H5'	1:YA:541:C:OP2	2.14	0.48
2:YB:8:U:O2	2:YB:112:G:N2	2.42	0.48
13:YR:28:LEU:HD23	13:YR:48:VAL:HG21	1.96	0.48
32:QA:272:C:H2'	32:QA:273:A:H8	1.79	0.48
32:QA:452:A:H62	32:QA:480:U:H3	1.62	0.48
34:QC:95:THR:HG23	34:QC:97:LYS:HE2	1.95	0.48
38:QG:76:ARG:NH1	38:QG:89:MET:SD	2.87	0.48
31:R9:6:SER:OG	31:R9:6:SER:O	2.28	0.48
1:RA:1557:C:OP2	1:RA:1558:A:O2'	2.26	0.48
2:RB:50:G:OP1	14:RS:63:THR:HG23	2.12	0.48
21:RZ:108:PRO:HG3	21:RZ:141:VAL:HG23	1.96	0.48
32:XA:1161:C:O2'	32:XA:1162:C:H5'	2.14	0.48
32:XA:22:G:H4'	32:XA:885:G:C8	2.48	0.48
32:XA:911:U:OP2	43:XL:97:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y0:11:ARG:O	22:Y0:14:ARG:NH2	2.47	0.48
1:YA:2131:G:H4'	1:YA:2132:U:H4'	1.96	0.48
1:YA:2155:G:H3'	1:YA:2156:G:C8	2.48	0.48
3:YD:20:ASP:OD1	3:YD:20:ASP:N	2.47	0.48
7:YH:58:GLU:OE2	7:YH:60:ARG:NH2	2.47	0.48
32:QA:1151:A:H2'	32:QA:1152:A:H8	1.79	0.48
32:QA:1172:C:H2'	32:QA:1173:G:H8	1.79	0.48
32:QA:1250:A:H2	32:QA:1370:G:H1'	1.79	0.48
32:QA:1316:G:H4'	45:QN:18:VAL:HG21	1.96	0.48
1:RA:1174:A:O2'	1:RA:1178:C:N4	2.46	0.48
1:RA:1525:G:H2'	1:RA:1526:G:C8	2.48	0.48
1:RA:1593:G:H2'	1:RA:1594:G:C8	2.49	0.48
1:RA:784:A:O2'	1:RA:785:G:H5''	2.13	0.48
18:RW:92:ARG:NH1	18:RW:94:ASP:OD1	2.37	0.48
37:XF:30:LEU:HB3	37:XF:35:ALA:HB3	1.94	0.48
1:YA:303:U:H2'	1:YA:304:G:H8	1.79	0.48
1:YA:673:C:H5''	5:YF:81:PRO:HD2	1.94	0.48
5:YF:40:GLN:HE22	5:YF:182:ASN:HD22	1.62	0.48
32:QA:1150:U:H4'	41:QJ:41:PRO:HB3	1.95	0.48
32:QA:1376:U:OP1	38:QG:94:ARG:NH1	2.44	0.48
1:RA:729:G:O2'	1:RA:763:G:H4'	2.14	0.48
7:RH:27:LYS:HD3	7:RH:32:GLU:HB3	1.95	0.48
11:RP:83:VAL:HB	11:RP:114:ILE:HG22	1.96	0.48
15:RT:24:PRO:HA	15:RT:49:VAL:HG13	1.95	0.48
32:XA:945:G:N2	32:XA:1334:G:O2'	2.46	0.48
32:XA:1406:U:O2	32:XA:1517:G:N2	2.40	0.48
32:XA:269:C:H2'	32:XA:270:A:H8	1.79	0.48
41:XJ:50:ILE:HD13	41:XJ:60:ARG:HD3	1.95	0.48
1:YA:1799:G:H5'	1:YA:1819:A:N6	2.29	0.48
1:YA:2246:G:H2'	1:YA:2247:A:C8	2.48	0.48
1:YA:2328:A:H2'	1:YA:2329:G:C8	2.49	0.48
1:YA:2853:C:H2'	1:YA:2854:G:H8	1.79	0.48
3:YD:273:ARG:HE	3:YD:274:ARG:HB2	1.79	0.48
16:YU:90:VAL:HG22	17:YV:38:LEU:HD12	1.94	0.48
32:QA:1005:A:OP2	32:QA:1006:C:N4	2.47	0.47
32:QA:483:C:OP2	32:QA:484:G:O2'	2.17	0.47
32:QA:539:A:H2'	32:QA:540:G:C8	2.49	0.47
32:QA:581:G:OP1	46:QO:65:ARG:NH1	2.46	0.47
32:QA:713:G:H2'	32:QA:714:G:C8	2.49	0.47
35:QD:101:LEU:HB2	35:QD:138:TYR:HB3	1.96	0.47
40:QI:80:GLY:O	40:QI:84:ALA:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:QJ:40:LEU:HB2	41:QJ:69:ASN:HB2	1.96	0.47
44:QM:25:ILE:HG12	44:QM:66:LEU:HD11	1.96	0.47
1:RA:589:C:H2'	1:RA:590:A:C8	2.49	0.47
10:RO:66:LYS:NZ	10:RO:80:ASP:O	2.43	0.47
38:XG:21:VAL:O	38:XG:24:THR:OG1	2.29	0.47
48:XQ:4:LYS:H	48:XQ:61:GLU:HB3	1.78	0.47
1:YA:2361:A:O5'	30:Y8:27:THR:OG1	2.32	0.47
1:YA:1968:G:O2'	1:YA:1969:A:O4'	2.26	0.47
1:YA:2529:G:H5''	1:YA:2530:A:H5''	1.96	0.47
1:YA:827:U:H5'	1:YA:828:U:O5'	2.14	0.47
4:YE:1:MET:N	4:YE:83:ASP:O	2.46	0.47
8:YI:40:THR:O	8:YI:44:LEU:N	2.44	0.47
32:QA:524:G:H2'	32:QA:525:C:C6	2.49	0.47
49:QR:74:ARG:HD3	49:QR:81:PHE:HA	1.96	0.47
1:RA:1109:C:H3'	1:RA:1110:G:C8	2.50	0.47
1:RA:2387:U:O2'	22:R0:41:ARG:NH2	2.46	0.47
1:RA:345:A:H2'	1:RA:347:A:H62	1.79	0.47
6:RG:129:GLY:HA2	6:RG:166:ASP:HB3	1.96	0.47
11:RP:100:LEU:O	11:RP:104:GLY:N	2.47	0.47
33:XB:87:ARG:NH1	33:XB:220:ASP:OD1	2.47	0.47
34:XC:174:PRO:O	34:XC:177:THR:OG1	2.32	0.47
52:XU:8:THR:OG1	52:XU:9:ARG:N	2.47	0.47
1:YA:1262:A:N3	27:Y5:10:LYS:NZ	2.50	0.47
32:QA:1228:C:H2'	32:QA:1229:A:H8	1.79	0.47
32:QA:579:G:H5'	32:QA:728:A:H1'	1.96	0.47
41:QJ:49:VAL:HG23	45:QN:41:ARG:HB2	1.97	0.47
7:RH:76:VAL:O	7:RH:80:SER:OG	2.32	0.47
21:RZ:157:LEU:HD23	21:RZ:161:VAL:HG12	1.96	0.47
1:RA:2327:A:H5'	21:RZ:201:LYS:HD2	1.96	0.47
32:XA:986:A:N3	50:XS:52:TYR:OH	2.42	0.47
34:XC:154:SER:HA	34:XC:165:THR:HA	1.97	0.47
43:XL:70:ILE:HG13	43:XL:100:ILE:HD12	1.95	0.47
7:YH:3:ARG:NH2	7:YH:65:HIS:HB3	2.28	0.47
32:QA:150:C:H42	32:QA:171:A:N6	2.06	0.47
32:QA:122:G:H1	32:QA:239:U:H3	1.62	0.47
33:QB:93:VAL:HG21	33:QB:97:TRP:HD1	1.80	0.47
32:QA:1070:U:O5'	36:QE:25:ARG:NH1	2.47	0.47
37:QF:76:ALA:HB1	37:QF:80:ARG:HH12	1.78	0.47
1:RA:1076:C:H4'	1:RA:1077:A:OP1	2.15	0.47
1:RA:1539:G:H2'	1:RA:1540:G:C8	2.50	0.47
32:XA:1178:G:N1	32:XA:1181:G:N7	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:670:A:H5''	11:YP:42:SER:O	2.13	0.47
5:YF:155:LEU:HB2	5:YF:189:THR:HG21	1.96	0.47
12:YQ:42:ILE:HD12	12:YQ:97:VAL:HG21	1.95	0.47
32:QA:411:A:H62	32:QA:413:G:H21	1.62	0.47
32:QA:426:G:OP1	35:QD:38:TYR:OH	2.24	0.47
32:QA:41:G:H2'	32:QA:42:G:H8	1.79	0.47
32:QA:662:G:H2'	32:QA:663:A:C8	2.49	0.47
1:RA:1405:U:H2'	1:RA:1406:U:H6	1.79	0.47
1:RA:2137:C:H42	1:RA:2154:G:H22	1.62	0.47
1:RA:51:G:H8	1:RA:51:G:OP2	1.97	0.47
2:RB:28:C:H2'	2:RB:29:A:H8	1.78	0.47
2:RB:42:C:N4	6:RG:91:ARG:HH12	2.12	0.47
1:RA:443:A:N6	5:RF:41:LEU:O	2.43	0.47
10:RO:10:VAL:HG11	10:RO:16:ALA:HB3	1.95	0.47
32:XA:985:C:H2'	32:XA:986:A:H8	1.80	0.47
35:QD:20:TYR:HE2	37:XF:15:ASP:CB	2.23	0.47
40:X1:83:ARG:HG2	40:X1:102:LEU:HD11	1.96	0.47
45:XN:7:ILE:HG22	45:XN:23:ARG:HH11	1.79	0.47
54:XX:5:A:H2'	54:XX:6:G:C8	2.50	0.47
23:Y1:49:VAL:HG23	23:Y1:60:PHE:HB2	1.97	0.47
1:YA:330:A:O2'	1:YA:331:A:H8	1.98	0.47
11:YP:6:LEU:HA	11:YP:6:LEU:HD23	1.81	0.47
13:YR:86:ARG:NH2	13:YR:118:GLU:OXT	2.39	0.47
15:YT:54:ARG:HA	15:YT:59:THR:HG23	1.96	0.47
32:QA:731:G:OP1	32:QA:766:A:H1'	2.14	0.47
37:QF:97:PHE:HB3	49:QR:32:ARG:HG3	1.96	0.47
38:QG:70:LYS:HG2	38:QG:100:ALA:HB2	1.95	0.47
1:RA:1419:A:H61	1:RA:1494:A:H61	1.61	0.47
1:RA:1782:C:C4	1:RA:2587:A:N1	2.82	0.47
13:RR:51:LEU:HD22	13:RR:66:VAL:HG13	1.97	0.47
32:XA:1305:G:H21	32:XA:1332:A:H8	1.63	0.47
32:XA:711:G:H2'	32:XA:712:A:C8	2.50	0.47
42:XK:24:SER:HG	42:XK:27:ASN:H	1.63	0.47
1:YA:1801:G:OP2	3:YD:154:LYS:NZ	2.47	0.47
1:YA:2734:A:H5'	1:YA:2735:G:OP2	2.15	0.47
1:YA:624:C:H1'	1:YA:657:U:H5'	1.97	0.47
32:QA:985:C:H2'	32:QA:986:A:C8	2.50	0.47
38:QG:70:LYS:HB3	38:QG:96:GLN:HB3	1.97	0.47
32:QA:1187:G:O2'	40:QI:111:ARG:NH1	2.48	0.47
14:RS:69:VAL:O	14:RS:73:LEU:N	2.46	0.47
16:RU:102:GLU:OE2	17:RV:13:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:RV:57:VAL:HG22	17:RV:99:ILE:HG23	1.96	0.47
21:RZ:153:SER:OG	21:RZ:154:ASP:OD2	2.29	0.47
32:XA:177:C:H2'	32:XA:178:C:H6	1.80	0.47
32:XA:464:G:N2	32:XA:467:G:N7	2.63	0.47
32:XA:7:G:O2'	36:XE:120:THR:O	2.32	0.47
37:XF:70:ASP:OD1	37:XF:70:ASP:N	2.40	0.47
45:XN:47:LEU:HB3	45:XN:53:LEU:HD13	1.96	0.47
38:XG:82:GLY:HA3	54:XX:13:A:H5''	1.96	0.47
26:Y4:68:ARG:H	50:XS:16:LEU:HD21	1.78	0.47
1:YA:2313:C:O4'	6:YG:40:ASN:ND2	2.47	0.47
1:YA:2576:G:O2'	1:YA:2579:C:OP2	2.23	0.47
10:YO:34:THR:OG1	10:YO:35:VAL:N	2.47	0.47
32:QA:1060:C:H2'	32:QA:1061:G:C8	2.50	0.47
32:QA:768:A:H5'	32:QA:1524:C:H1'	1.97	0.47
32:QA:801:U:H2'	32:QA:802:A:H8	1.79	0.47
32:QA:806:C:H2'	32:QA:807:A:H8	1.79	0.47
39:QH:21:LYS:O	39:QH:65:TYR:OH	2.24	0.47
1:RA:1800:C:H42	1:RA:1817:G:H22	1.61	0.47
14:RS:10:ARG:NH1	14:RS:91:PRO:O	2.47	0.47
32:XA:1250:A:H2	32:XA:1370:G:H1'	1.80	0.47
32:XA:130:A:N3	32:XA:263:A:O2'	2.42	0.47
32:XA:636:U:H2'	32:XA:637:G:H8	1.79	0.47
33:XB:69:LEU:HD13	33:XB:91:PRO:HB2	1.97	0.47
41:XJ:32:ALA:HB3	41:XJ:76:ASN:HB2	1.97	0.47
41:XJ:51:ARG:HG2	45:XN:45:ARG:HH21	1.80	0.47
1:YA:1756:G:H4'	1:YA:1758:G:O4'	2.15	0.47
1:YA:2789:C:O3'	1:YA:2790:A:H4'	2.15	0.47
1:YA:392:C:H5''	1:YA:409:C:H5''	1.96	0.47
34:QC:47:LEU:HB3	34:QC:50:ALA:HB3	1.95	0.47
32:QA:429:U:OP2	35:QD:13:ARG:NH2	2.47	0.47
1:RA:1021:A:H8	1:RA:1022:G:H5''	1.79	0.47
1:RA:1824:G:N3	3:RD:254:THR:OG1	2.48	0.47
1:RA:2302:G:H21	6:RG:126:ASP:HB2	1.79	0.47
2:RB:44:G:H5''	2:RB:45:A:OP1	2.14	0.47
32:XA:434:U:H2'	32:XA:435:C:C6	2.50	0.47
32:XA:883:C:N4	32:XA:884:U:O4	2.48	0.47
32:XA:719:C:O2'	49:XR:50:ILE:O	2.25	0.47
50:XS:53:ASN:HD21	50:XS:56:GLN:HE22	1.63	0.47
1:YA:2262:U:H5	22:Y0:16:SER:HB3	1.80	0.47
1:YA:1062:G:H22	1:YA:1078:U:H1'	1.80	0.47
1:YA:1266:G:O5'	18:YW:15:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2105:C:H2'	1:YA:2106:G:H8	1.78	0.47
1:YA:2287:A:H62	1:YA:2344:U:H3	1.62	0.47
1:YA:1759:A:H1'	1:YA:2711:A:C2	2.50	0.47
1:YA:2845:G:H2'	1:YA:2846:G:H8	1.79	0.47
17:YV:8:GLY:O	17:YV:10:LYS:NZ	2.48	0.47
32:QA:1321:C:H3'	32:QA:1322:C:H5''	1.96	0.47
32:QA:825:G:O2'	39:QH:12:ARG:NH2	2.47	0.47
35:QD:59:ARG:HD3	35:QD:59:ARG:HA	1.71	0.47
1:RA:1478:G:H2'	1:RA:1479:G:H8	1.78	0.47
1:RA:2646:C:OP2	1:RA:2732:G:O2'	2.25	0.47
5:RF:185:ASP:OD1	5:RF:188:ARG:NH1	2.40	0.47
12:RQ:31:ASP:OD1	12:RQ:134:ARG:NH2	2.48	0.47
32:XA:115:G:H4'	32:XA:116:A:O5'	2.13	0.47
32:XA:484:G:H4'	32:XA:485:G:O5'	2.15	0.47
32:XA:643:C:H2'	32:XA:644:G:C8	2.49	0.47
32:XA:806:C:H2'	32:XA:807:A:H8	1.79	0.47
1:YA:249:C:O2'	11:YP:64:LYS:NZ	2.28	0.47
1:YA:862:G:H2'	1:YA:863:A:O4'	2.15	0.47
2:YB:24:G:H5''	2:YB:25:A:OP1	2.14	0.47
1:YA:340:A:O2'	5:YF:168:ARG:NH2	2.47	0.47
32:QA:1010:G:H2'	32:QA:1011:G:H8	1.78	0.47
32:QA:920:U:HO2'	32:QA:1081:G:HO2'	1.59	0.47
32:QA:429:U:C3'	35:QD:22:LYS:HZ1	2.26	0.47
43:QL:11:VAL:HG11	48:QQ:36:ILE:HG21	1.96	0.47
50:QS:12:ASP:HB3	50:QS:14:HIS:H	1.80	0.47
30:R8:29:LYS:HG2	30:R8:44:LYS:HG3	1.96	0.47
1:RA:1790:C:H5''	1:RA:1791:A:OP1	2.15	0.47
1:RA:1800:C:O2	1:RA:1817:G:O6	2.32	0.47
1:RA:49:A:H61	1:RA:177:G:H2'	1.78	0.47
6:RG:36:LYS:HE3	6:RG:95:ARG:HH22	1.78	0.47
8:RI:75:LEU:HD13	8:RI:105:HIS:CE1	2.50	0.47
32:XA:1147:C:O2'	40:XI:5:TYR:OH	2.27	0.47
54:XX:6:G:H2'	54:XX:7:G:C8	2.50	0.47
22:Y0:68:GLU:HG3	22:Y0:80:HIS:HB2	1.97	0.47
25:Y3:26:LEU:O	25:Y3:35:ARG:NE	2.48	0.47
1:YA:2211:G:H21	1:YA:2212:A:H2	1.63	0.47
1:YA:579:G:H2'	1:YA:580:C:C6	2.50	0.47
4:YE:57:LYS:HA	4:YE:59:VAL:H	1.80	0.47
32:QA:1175:G:H2'	32:QA:1176:A:H8	1.81	0.46
32:QA:1527:C:O2'	32:QA:1528:U:H5'	2.15	0.46
32:QA:493:G:N2	32:QA:494:U:O4	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:59:A:H3'	32:QA:331:G:H22	1.79	0.46
32:QA:1229:A:O2'	53:QV:30:C:OP1	2.33	0.46
24:R2:18:PRO:HA	24:R2:21:LEU:HB2	1.97	0.46
1:RA:1550:C:OP1	1:RA:1727:U:O2'	2.27	0.46
1:RA:631:A:N3	1:RA:2415:G:O2'	2.41	0.46
32:XA:1219:U:H2'	32:XA:1220:G:C8	2.50	0.46
32:XA:1321:C:H5''	32:XA:1322:C:H2'	1.96	0.46
32:XA:1412:C:H2'	32:XA:1413:A:H8	1.80	0.46
32:XA:1427:U:H2'	32:XA:1428:A:C8	2.50	0.46
40:XI:48:GLU:HA	40:XI:51:ARG:HB3	1.96	0.46
40:XI:8:GLY:HA3	40:XI:15:ALA:HB3	1.97	0.46
1:YA:372:G:HO2'	1:YA:373:U:H5	1.62	0.46
1:YA:528:A:C2	1:YA:2042:A:H2'	2.50	0.46
1:YA:528:A:O2'	1:YA:529:A:H5'	2.15	0.46
1:YA:813:U:H2'	1:YA:814:C:H6	1.79	0.46
6:YG:179:PRO:HB3	26:Y4:43:TYR:HE2	1.79	0.46
12:YQ:32:TYR:OH	12:YQ:111:GLU:OE1	2.26	0.46
13:YR:67:LEU:HD13	13:YR:76:VAL:HG21	1.97	0.46
32:QA:867:G:O2'	32:QA:873:A:N1	2.43	0.46
35:QD:173:TRP:CD1	35:QD:174:LEU:HG	2.50	0.46
32:QA:625:G:OP1	47:QP:9:PHE:HB3	2.16	0.46
51:QT:29:LYS:O	51:QT:33:ILE:HG12	2.15	0.46
1:RA:1800:C:N4	1:RA:1817:G:H22	2.13	0.46
7:RH:88:LEU:HA	7:RH:130:ARG:HA	1.96	0.46
32:XA:359:U:H2'	32:XA:360:A:C8	2.48	0.46
1:YA:1353:A:H2'	1:YA:1354:A:C8	2.49	0.46
16:YU:85:LYS:HA	16:YU:85:LYS:HD3	1.65	0.46
32:QA:1244:C:H2'	32:QA:1245:A:H8	1.79	0.46
33:QB:80:ILE:HG12	33:QB:215:LEU:HD12	1.96	0.46
32:QA:711:G:P	37:QF:54:LYS:HZ1	2.38	0.46
1:RA:1590:U:H2'	1:RA:1591:G:H8	1.80	0.46
1:RA:2346:A:H5''	1:RA:2383:G:H1'	1.97	0.46
1:RA:2844:G:H3'	1:RA:2845:G:H8	1.81	0.46
1:RA:724:U:H2'	1:RA:725:G:O4'	2.15	0.46
1:RA:823:G:H2'	1:RA:824:A:H8	1.81	0.46
8:RI:94:ALA:HA	8:RI:97:ILE:HG13	1.97	0.46
35:XD:134:ASP:OD1	35:XD:134:ASP:N	2.44	0.46
1:YA:860:U:H1'	1:YA:2268:A:H5'	1.97	0.46
18:YW:35:ILE:O	18:YW:39:THR:OG1	2.27	0.46
32:QA:1129:C:H4'	32:QA:1130:A:C8	2.50	0.46
32:QA:1329:A:H5''	44:QM:26:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1469:G:H2'	32:QA:1470:G:H8	1.80	0.46
32:QA:410:G:H2'	32:QA:429:U:C5	2.49	0.46
32:QA:616:G:OP2	35:QD:141:ARG:NH2	2.46	0.46
32:QA:1539:C:N4	54:QX:5:A:H61	2.06	0.46
1:RA:1341:U:OP1	1:RA:1397:U:N3	2.36	0.46
1:RA:1461:G:OP2	1:RA:1461:G:H8	1.98	0.46
1:RA:1991:U:H2'	1:RA:1992:G:H5''	1.98	0.46
1:RA:823:G:H2'	1:RA:824:A:C8	2.50	0.46
8:RI:5:LEU:HD11	8:RI:19:VAL:HG22	1.96	0.46
11:RP:37:GLY:O	11:RP:40:SER:OG	2.27	0.46
33:XB:36:ARG:HG3	33:XB:37:ASN:HB2	1.97	0.46
42:XK:58:PRO:O	42:XK:62:GLN:N	2.45	0.46
23:Y1:17:SER:HB2	23:Y1:40:ARG:HD2	1.96	0.46
1:YA:2115:G:N2	1:YA:2164:C:OP2	2.49	0.46
1:YA:2591:C:H2'	1:YA:2592:G:C8	2.50	0.46
1:YA:270(J):G:H2'	1:YA:270(K):C:O4'	2.16	0.46
1:YA:534:U:H2'	1:YA:535:C:C6	2.50	0.46
4:YE:12:THR:OG1	4:YE:13:ARG:N	2.48	0.46
13:YR:59:ASP:OD1	13:YR:59:ASP:N	2.35	0.46
32:QA:356:A:N3	32:QA:368:U:O2'	2.34	0.46
32:QA:736:C:H2'	32:QA:737:A:H8	1.81	0.46
33:QB:132:LYS:HA	33:QB:135:GLN:HB2	1.97	0.46
38:QG:89:MET:HA	38:QG:155:ARG:HH22	1.81	0.46
40:QI:10:ARG:O	40:QI:13:ALA:HB3	2.14	0.46
54:QX:11:U:H2'	54:QX:12:A:C8	2.51	0.46
1:RA:1668:A:N3	1:RA:1670:C:N4	2.63	0.46
1:RA:182:A:H2'	1:RA:183:C:H6	1.80	0.46
1:RA:270(E):G:H1	1:RA:270(U):C:H42	1.64	0.46
3:RD:260:ARG:NH2	3:RD:266:SER:OG	2.49	0.46
9:RN:27:ALA:HB1	9:RN:103:VAL:HG22	1.98	0.46
32:XA:749:C:H2'	32:XA:750:G:H8	1.81	0.46
32:XA:757:U:O2'	32:XA:879:C:O2	2.30	0.46
32:XA:946:A:H2'	32:XA:947:G:H8	1.80	0.46
1:YA:1593:G:H2'	1:YA:1594:G:C8	2.50	0.46
1:YA:2327:A:H2'	1:YA:2328:A:C8	2.51	0.46
32:QA:114:U:O2'	32:QA:115:G:H5'	2.16	0.46
32:QA:1285:A:H1'	32:QA:1286:A:OP2	2.16	0.46
32:QA:376:G:O3'	47:QP:5:ARG:NH1	2.47	0.46
32:QA:971:G:H22	32:QA:1363:A:P	2.39	0.46
41:QJ:21:GLN:HA	41:QJ:24:VAL:HG12	1.97	0.46
46:QO:84:LYS:HD3	46:QO:84:LYS:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:QX:13:A:H4'	54:QX:14:A:OP2	2.14	0.46
53:QV:36:G:H1	54:QX:17:C:H42	1.64	0.46
10:RO:63:VAL:HB	10:RO:102:VAL:HG12	1.96	0.46
1:RA:2428:G:O2'	11:RP:56:SER:OG	2.33	0.46
12:RQ:32:TYR:CZ	12:RQ:111:GLU:HB3	2.50	0.46
32:XA:1250:A:C2	32:XA:1370:G:H1'	2.50	0.46
32:XA:1539:C:H2'	32:XA:1540:U:C6	2.51	0.46
32:XA:280:C:H3'	32:XA:281:G:H5'	1.98	0.46
32:XA:538:G:H2'	32:XA:539:A:H8	1.81	0.46
22:Y0:18:ALA:O	22:Y0:20:ARG:NH1	2.41	0.46
3:YD:146:GLU:HB2	3:YD:189:CYS:HB3	1.97	0.46
1:YA:952:G:OP1	12:YQ:16:ARG:NH1	2.49	0.46
1:YA:1278:A:OP1	13:YR:36:THR:HG22	2.15	0.46
32:QA:1009:G:N2	32:QA:1020:U:O2	2.39	0.46
32:QA:1060:C:OP1	45:QN:45:ARG:NH2	2.43	0.46
32:QA:767:A:O2'	32:QA:1524:C:O2	2.29	0.46
33:QB:163:PHE:HE2	33:QB:215:LEU:HD22	1.79	0.46
34:QC:63:ASN:OD1	34:QC:63:ASN:N	2.49	0.46
35:QD:175:SER:HB3	35:QD:186:LEU:HD11	1.98	0.46
44:QM:20:THR:HA	44:QM:26:GLY:HA2	1.98	0.46
1:RA:2692:C:O2	1:RA:2847:U:O2'	2.33	0.46
13:RR:54:LEU:HB3	13:RR:62:ALA:HB1	1.98	0.46
15:RT:19:LEU:HD22	15:RT:86:ILE:HG22	1.98	0.46
32:XA:1221:G:OP1	50:XS:36:ARG:NH1	2.48	0.46
32:XA:1323:G:H2'	32:XA:1324:A:C8	2.50	0.46
32:XA:335:C:O2'	32:XA:1433:A:N3	2.37	0.46
32:XA:1505:G:H2'	54:XX:15:A:OP2	2.15	0.46
32:XA:737:A:H2'	32:XA:738:C:C6	2.51	0.46
32:XA:959:A:O2'	32:XA:984:C:O2'	2.24	0.46
32:XA:1316:G:H4'	45:XN:18:VAL:HG11	1.96	0.46
3:YD:258:LYS:HE2	3:YD:273:ARG:NH1	2.13	0.46
32:QA:1157:A:OP1	32:QA:1158:C:N4	2.49	0.46
32:QA:254:G:OP1	48:QQ:68:ARG:HB3	2.16	0.46
32:QA:663:A:H61	32:QA:742:G:H1	1.64	0.46
32:QA:674:G:H2'	32:QA:675:A:C8	2.48	0.46
32:QA:757:U:O2'	32:QA:879:C:O2	2.32	0.46
33:QB:136:VAL:HA	33:QB:139:LYS:HG2	1.98	0.46
1:RA:652:C:H5'	1:RA:653:A:OP2	2.15	0.46
1:RA:863:A:H2'	1:RA:864:G:H8	1.80	0.46
1:RA:94:G:H21	24:R2:47:ASN:HD22	1.64	0.46
3:RD:5:LYS:HG2	3:RD:17:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1190:G:H5'	11:RP:32:THR:HA	1.98	0.46
32:XA:308:C:H2'	32:XA:309:G:H8	1.80	0.46
33:XB:67:THR:HG21	33:XB:155:LEU:HD22	1.96	0.46
33:XB:85:ALA:O	33:XB:89:GLY:N	2.48	0.46
1:YA:2823:A:OP1	4:YE:113:PHE:HB2	2.15	0.46
1:YA:631:A:N3	1:YA:2415:G:O2'	2.35	0.46
8:YI:116:LEU:HD13	8:YI:128:LEU:HD11	1.97	0.46
32:QA:1239:A:H62	32:QA:1299:A:H62	1.62	0.46
32:QA:945:G:N2	32:QA:1334:G:O2'	2.49	0.46
32:QA:1522:U:H2'	32:QA:1523:G:H8	1.80	0.46
35:QD:9:CYS:SG	35:QD:32:ALA:HB3	2.55	0.46
1:RA:1864:U:OP1	1:RA:2410:G:O2'	2.34	0.46
1:RA:38:A:H2'	1:RA:39:C:C6	2.51	0.46
1:RA:574:C:N3	4:RE:145:LYS:NZ	2.45	0.46
6:RG:63:ILE:HG22	6:RG:143:GLU:HB2	1.97	0.46
12:RQ:56:ARG:HA	21:RZ:180:VAL:HG13	1.97	0.46
18:RW:4:LYS:HB2	18:RW:106:ILE:HG12	1.98	0.46
32:XA:1141:C:H2'	32:XA:1142:G:C8	2.51	0.46
32:XA:1141:C:H2'	32:XA:1142:G:H8	1.81	0.46
32:XA:875:C:H1'	39:XH:15:ASN:ND2	2.31	0.46
38:XG:79:ARG:HH21	38:XG:82:GLY:HA2	1.81	0.46
1:YA:2306:C:H2'	1:YA:2307:G:H21	1.80	0.46
1:YA:922:U:H2'	1:YA:923:C:C6	2.51	0.46
32:QA:652:U:H1'	32:QA:653:A:H2	1.81	0.46
32:QA:974:A:N3	45:QN:31:ARG:NH1	2.64	0.46
4:RE:47:VAL:HG21	4:RE:86:PRO:HD2	1.98	0.46
6:RG:34:LEU:HB3	6:RG:99:MET:HE1	1.98	0.46
1:RA:2744:G:N2	7:RH:143:GLN:OE1	2.41	0.46
7:RH:152:ARG:HG2	7:RH:153:LYS:HD2	1.98	0.46
32:XA:1022:G:H2'	32:XA:1023:G:H8	1.80	0.46
32:XA:112:G:H4'	32:XA:389:A:H4'	1.97	0.46
32:XA:410:G:H2'	32:XA:429:U:C5	2.50	0.46
44:XM:3:ARG:NE	44:XM:3:ARG:N	2.62	0.46
45:YN:40:CYS:SG	45:YN:41:ARG:N	2.88	0.46
1:YA:1557:C:OP2	1:YA:1558:A:O2'	2.25	0.46
1:YA:1783:A:H5'	1:YA:2608:G:H4'	1.97	0.46
1:YA:2832:U:H4'	1:YA:2833:G:C5'	2.46	0.46
2:YB:40:U:O4	26:Y4:1:MET:N	2.39	0.46
1:YA:616:A:C4	5:YF:180:GLY:HA3	2.51	0.46
6:YG:137:GLU:HG3	6:YG:139:LEU:HB2	1.97	0.46
7:YH:11:VAL:HA	7:YH:12:PRO:HD3	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:997:G:OP1	16:YU:93:LYS:HE2	2.16	0.46
19:YX:88:LYS:NZ	19:YX:90:GLU:OE2	2.45	0.46
32:QA:1431:C:H2'	32:QA:1432:G:O4'	2.17	0.45
32:QA:979:C:H42	45:QN:18:VAL:HG12	1.81	0.45
35:QD:31:CYS:HA	57:QD:301:SF4:S4	2.56	0.45
29:R7:13:ALA:HB2	29:R7:46:VAL:HG11	1.98	0.45
1:RA:263:C:H2'	1:RA:264:C:O4'	2.16	0.45
1:RA:671:C:H2'	1:RA:672:C:C6	2.51	0.45
8:RI:113:ARG:HH22	8:RI:115:ALA:HB2	1.81	0.45
32:XA:1346:A:H1'	32:XA:1348:U:C2	2.51	0.45
32:XA:1442:G:H1	32:XA:1461:G:H21	1.64	0.45
32:XA:186(D):C:H42	32:XA:191(D):U:H3	1.64	0.45
35:XD:19:LEU:HD13	35:XD:21:LEU:HD21	1.98	0.45
32:XA:736:C:O2'	37:XF:90:VAL:O	2.31	0.45
47:XP:11:SER:HB2	47:XP:14:ASN:HB3	1.96	0.45
25:Y3:51:ALA:HA	25:Y3:54:VAL:HG12	1.98	0.45
1:YA:1598:C:O3'	19:YX:35:THR:OG1	2.34	0.45
1:YA:2183:C:N4	1:YA:2184:G:O6	2.49	0.45
1:YA:2392:A:H8	11:YP:61:ARG:HG2	1.82	0.45
32:QA:1150:U:H2'	32:QA:1151:A:C8	2.51	0.45
32:QA:115:G:H4'	32:QA:116:A:O5'	2.16	0.45
32:QA:578:C:O2'	32:QA:728:A:N3	2.33	0.45
33:QB:6:THR:O	33:QB:217:ARG:NE	2.49	0.45
49:QR:32:ARG:HA	49:QR:69:THR:HG21	1.96	0.45
23:R1:82:LEU:HA	23:R1:82:LEU:HD23	1.86	0.45
1:RA:820:A:H4'	1:RA:836:G:N2	2.31	0.45
10:RO:104:ARG:NH1	10:RO:121:VAL:O	2.49	0.45
10:RO:24:VAL:HG13	10:RO:33:ALA:HB2	1.97	0.45
15:RT:20:PRO:HD2	15:RT:86:ILE:HG23	1.97	0.45
32:XA:731:G:OP1	32:XA:766:A:H1'	2.16	0.45
32:XA:737:A:H2'	32:XA:738:C:H6	1.81	0.45
33:XB:132:LYS:HA	33:XB:135:GLN:HB2	1.98	0.45
41:XJ:7:LYS:HB2	41:XJ:97:GLU:HB2	1.98	0.45
47:XP:67:THR:O	47:XP:71:ARG:N	2.49	0.45
1:YA:1460:A:H4'	1:YA:1461:G:OP2	2.16	0.45
1:YA:1817:G:OP1	3:YD:88:ARG:NH2	2.47	0.45
1:YA:2756:U:H1'	1:YA:2757:A:H5''	1.97	0.45
32:QA:448:A:N7	32:QA:486:U:O4	2.49	0.45
34:QC:73:PRO:HA	34:QC:76:VAL:HG12	1.98	0.45
32:QA:406:G:N3	35:QD:119:GLN:NE2	2.64	0.45
35:QD:16:GLY:C	35:QD:33:MET:HE3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:QH:109:ILE:HD11	39:QH:120:THR:HB	1.98	0.45
39:QH:121:ASP:N	39:QH:121:ASP:OD1	2.49	0.45
39:QH:25:ASP:HB3	39:QH:58:TYR:HD2	1.80	0.45
32:QA:657:G:N2	46:QO:22:THR:OG1	2.45	0.45
46:QO:48:LYS:HB2	46:QO:48:LYS:HE2	1.84	0.45
1:RA:1203:G:O6	1:RA:1204:A:N6	2.48	0.45
1:RA:1539:G:H2'	1:RA:1540:G:H8	1.80	0.45
6:RG:32:PRO:HB2	6:RG:172:LEU:HD13	1.97	0.45
7:RH:129:THR:OG1	7:RH:129:THR:O	2.34	0.45
9:RN:1:MET:HE1	16:RU:95:LEU:HD21	1.99	0.45
11:RP:76:LYS:HD2	11:RP:79:ARG:HH22	1.81	0.45
15:RT:16:ARG:NH1	15:RT:18:ASP:OD2	2.48	0.45
32:XA:79:G:H2'	32:XA:80:G:H8	1.80	0.45
44:XM:57:ARG:HA	44:XM:60:VAL:HG12	1.98	0.45
1:YA:189:G:O6	1:YA:205:G:O2'	2.26	0.45
1:YA:1027:A:C2	1:YA:2488:A:H5'	2.52	0.45
1:YA:2023:G:H5'	1:YA:2617:C:H4'	1.97	0.45
1:YA:2836:U:H2'	1:YA:2837:G:C8	2.51	0.45
13:YR:19:ALA:O	13:YR:23:ASN:ND2	2.49	0.45
32:QA:1217:C:H2'	32:QA:1218:C:C6	2.51	0.45
32:QA:940:C:H2'	32:QA:941:G:C8	2.51	0.45
41:QJ:3:LYS:HG3	41:QJ:75:ILE:HA	1.99	0.45
32:QA:778:G:O2'	42:QK:120:ARG:O	2.29	0.45
42:QK:33:THR:OG1	42:QK:34:ASP:O	2.32	0.45
42:QK:50:TYR:HB3	42:QK:54:ARG:HG3	1.99	0.45
1:RA:1141:U:H1'	1:RA:1142(A):A:C6	2.51	0.45
1:RA:137(A):G:H2'	1:RA:139:G:N7	2.32	0.45
1:RA:1485:G:H1	1:RA:1504:C:H42	1.63	0.45
6:RG:109:VAL:HG11	6:RG:142:PRO:HG3	1.99	0.45
7:RH:20:ALA:HB3	7:RH:23:ARG:HG2	1.98	0.45
10:RO:120:GLU:OE2	15:RT:67:SER:OG	2.31	0.45
32:XA:1151:A:H2'	32:XA:1152:A:C8	2.52	0.45
32:XA:477:G:H2'	32:XA:478:A:H8	1.80	0.45
32:XA:673:G:O3'	37:XF:87:ARG:NH2	2.50	0.45
36:XE:105:VAL:HG21	36:XE:128:PRO:HB3	1.99	0.45
24:Y2:31:GLU:HB3	24:Y2:53:LEU:HD21	1.99	0.45
1:YA:363(B):G:H2'	1:YA:363(C):G:C8	2.49	0.45
6:YG:165:THR:OG1	6:YG:166:ASP:N	2.49	0.45
32:QA:560:U:H4'	32:QA:561:U:H5''	1.97	0.45
34:QC:40:ARG:HE	34:QC:55:VAL:HB	1.82	0.45
50:QS:32:LYS:HD3	50:QS:57:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1283:G:H1'	1:RA:1329:U:H3	1.80	0.45
1:RA:1365:A:O2'	23:R1:11:ARG:NH2	2.46	0.45
1:RA:844:C:H2'	1:RA:845:G:O4'	2.17	0.45
1:RA:900:A:H3'	1:RA:901:A:H8	1.81	0.45
6:RG:166:ASP:OD1	6:RG:166:ASP:N	2.49	0.45
1:RA:2313:C:H4'	6:RG:91:ARG:HD3	1.98	0.45
21:RZ:181:GLU:O	21:RZ:181:GLU:HG3	2.15	0.45
32:XA:1492:A:O2'	32:XA:1493:A:H5''	2.16	0.45
32:XA:164:U:H2'	32:XA:165:C:C6	2.52	0.45
42:XK:62:GLN:OE1	42:XK:93:GLN:NE2	2.42	0.45
32:XA:377:G:OP1	47:XP:3:LYS:HD2	2.16	0.45
48:XQ:95:TYR:HA	48:XQ:98:LEU:HD12	1.99	0.45
1:YA:1310:G:OP2	29:Y7:9:ARG:NE	2.42	0.45
1:YA:264:C:C2'	1:YA:265:A:H5''	2.46	0.45
1:YA:2776:A:H4'	1:YA:2777:G:O5'	2.17	0.45
1:YA:529:A:H8	1:YA:530:G:C6	2.35	0.45
7:YH:90:LYS:NZ	7:YH:159:GLU:OE1	2.41	0.45
8:YI:67:ARG:HE	8:YI:67:ARG:HB2	1.62	0.45
32:QA:1157:A:H62	32:QA:1178:G:N2	2.15	0.45
32:QA:261:U:OP2	51:QT:79:ARG:NH2	2.50	0.45
32:QA:410:G:H21	32:QA:432:A:N6	2.03	0.45
34:QC:63:ASN:HB3	34:QC:98:ASN:HB2	1.98	0.45
1:RA:1073:A:H2'	1:RA:1074:G:H8	1.81	0.45
1:RA:184:C:H2'	1:RA:185:U:H6	1.82	0.45
1:RA:2680:C:OP2	4:RE:111:ARG:NH2	2.50	0.45
1:RA:944:G:H5''	1:RA:945:A:O5'	2.17	0.45
5:RF:32:LEU:HD11	5:RF:105:VAL:HG13	1.98	0.45
10:RO:73:ASP:N	10:RO:73:ASP:OD1	2.42	0.45
13:RR:104:ARG:HG3	13:RR:107:ASP:HB3	1.98	0.45
18:RW:18:ARG:HG2	18:RW:76:VAL:HB	1.98	0.45
32:XA:1540:U:N3	54:XX:2:G:N1	2.64	0.45
1:YA:2151:G:H2'	1:YA:2152:G:C8	2.51	0.45
1:YA:2213:U:O2	23:Y1:52:ARG:NH2	2.44	0.45
1:YA:2298:A:H62	1:YA:2318:G:H8	1.65	0.45
1:YA:746:A:H2'	1:YA:2612:C:H5''	1.98	0.45
10:YO:8:LEU:HB2	10:YO:19:ILE:HG13	1.99	0.45
21:YZ:110:GLY:HA3	21:YZ:174:VAL:HG11	1.97	0.45
32:QA:1077:G:N2	32:QA:1080:A:OP2	2.47	0.45
32:QA:922:G:H2'	32:QA:923:A:C8	2.52	0.45
32:QA:987:G:H1'	50:QS:34:TRP:HH2	1.82	0.45
50:QS:31:ILE:HG22	50:QS:33:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:RX:46:ALA:HB1	24:R2:33:MET:HE1	1.99	0.45
30:R8:61:LEU:H	30:R8:61:LEU:HG	1.68	0.45
1:RA:2236:C:H2'	1:RA:2237:G:O4'	2.17	0.45
1:RA:249:C:O2	30:R8:12:LYS:NZ	2.38	0.45
19:RX:53:LYS:HB3	19:RX:82:GLN:HB3	1.98	0.45
32:XA:1237:C:H5''	32:XA:1238:A:C8	2.51	0.45
32:XA:1513:A:H2'	32:XA:1514:C:C6	2.52	0.45
32:XA:603:U:H2'	32:XA:604:G:H8	1.81	0.45
32:XA:627:G:H2'	32:XA:628:G:H8	1.82	0.45
32:XA:22:G:O2'	32:XA:913:A:N1	2.38	0.45
44:XM:3:ARG:HB3	44:XM:8:GLU:HA	1.99	0.45
1:YA:443:A:N6	5:YF:41:LEU:O	2.45	0.45
1:YA:81:G:N2	20:YY:1:MET:SD	2.90	0.45
32:QA:17:U:H2'	32:QA:18:C:H6	1.82	0.45
32:QA:8:A:N6	35:QD:205:GLU:O	2.48	0.45
1:RA:108:U:H2'	1:RA:109:G:H8	1.81	0.45
1:RA:1210:A:H4'	1:RA:1211:U:O5'	2.17	0.45
1:RA:2086:U:H2'	1:RA:2087:G:C8	2.52	0.45
1:RA:2116:G:H2'	1:RA:2117:A:C4	2.52	0.45
5:RF:116:ASP:OD1	5:RF:119:ARG:NH2	2.36	0.45
18:RW:12:ILE:O	18:RW:101:SER:OG	2.24	0.45
32:XA:1145:C:H4'	32:XA:1146:A:H5'	1.98	0.45
35:XD:22:LYS:N	35:XD:26:CYS:SG	2.88	0.45
26:Y4:50:VAL:HG11	44:XM:65:LYS:HG3	1.99	0.45
1:YA:278:A:H2'	1:YA:279:C:C6	2.52	0.45
1:YA:2791:C:C5	1:YA:2893:G:H3'	2.51	0.45
1:YA:18:C:O2'	1:YA:553:U:OP1	2.28	0.45
6:YG:65:GLY:HA3	26:Y4:9:LEU:HD21	1.97	0.45
10:YO:106:LEU:HB3	10:YO:111:PHE:HB2	1.98	0.45
32:QA:1067:A:N1	32:QA:1108:G:O2'	2.36	0.45
32:QA:1410:G:H2'	32:QA:1411:C:H6	1.82	0.45
32:QA:1497:G:H1'	32:QA:1518:A:H2	1.82	0.45
32:QA:17:U:H2'	32:QA:18:C:C6	2.52	0.45
32:QA:279:A:OP1	32:QA:280:C:O2'	2.30	0.45
34:QC:21:ARG:NH2	34:QC:58:GLU:OE2	2.49	0.45
43:QL:45:PRO:HB2	43:QL:92:ASP:HB3	1.98	0.45
1:RA:1009:A:N3	1:RA:1153:C:O2'	2.37	0.45
1:RA:2061:G:H5''	1:RA:2503:A:C2	2.52	0.45
1:RA:848:G:H2'	1:RA:849:A:H8	1.82	0.45
2:RB:70:C:H2'	2:RB:71:C:H6	1.82	0.45
1:RA:807:U:OP2	11:RP:41:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1238:A:OP1	32:XA:1335:C:O2'	2.29	0.45
32:XA:514:C:H2'	32:XA:515:G:C8	2.47	0.45
33:XB:187:LEU:HA	33:XB:201:ILE:HB	1.98	0.45
42:XK:21:ILE:HB	42:XK:84:VAL:HA	1.99	0.45
44:XM:36:LYS:HE3	44:XM:36:LYS:HB3	1.86	0.45
44:XM:74:VAL:HA	44:XM:77:ASN:HB2	1.99	0.45
45:XN:29:ARG:HG3	45:XN:31:ARG:H	1.82	0.45
1:YA:139:G:N2	1:YA:1596:A:H4'	2.32	0.45
1:YA:2030:A:H4'	1:YA:2031:A:C8	2.52	0.45
1:YA:888:C:OP1	44:XM:93:ARG:NH2	2.49	0.45
5:YF:182:ASN:N	5:YF:182:ASN:OD1	2.48	0.45
32:QA:1095:U:P	32:QA:1108:G:H1	2.39	0.45
32:QA:701:C:H1'	32:QA:703:G:C6	2.52	0.45
48:QQ:92:ARG:HD3	48:QQ:92:ARG:HA	1.82	0.45
23:R1:58:ILE:HD13	23:R1:87:PRO:HD3	1.99	0.45
1:RA:2532:G:N2	1:RA:2663:G:O2'	2.50	0.45
1:RA:2630:G:H2'	1:RA:2631:G:H8	1.83	0.45
43:XL:76:ASN:OD1	43:XL:76:ASN:N	2.50	0.45
51:XT:75:ASN:OD1	51:XT:75:ASN:N	2.43	0.45
23:Y1:75:GLU:OE2	23:Y1:78:LYS:NZ	2.49	0.45
1:YA:1639:U:H2'	1:YA:1640:C:H5''	1.98	0.45
1:YA:1363:C:O2'	1:YA:1809:A:N3	2.40	0.45
1:YA:2154:G:H2'	1:YA:2155:G:C8	2.51	0.45
1:YA:2808:U:N3	1:YA:2892:A:C5	2.85	0.45
44:QM:76:ALA:O	44:QM:80:ARG:HG2	2.18	0.44
22:R0:10:THR:HG22	22:R0:12:ASN:H	1.82	0.44
1:RA:2387:U:O2'	22:R0:19:LYS:NZ	2.50	0.44
1:RA:2811:G:C5	1:RA:2891:G:N2	2.85	0.44
1:RA:414:C:O2	1:RA:1864:U:O2'	2.34	0.44
1:RA:458:G:O2'	1:RA:469:G:O6	2.26	0.44
32:XA:444:C:H2'	32:XA:445:G:H8	1.82	0.44
32:XA:448:A:OP2	32:XA:485:G:N2	2.39	0.44
35:XD:129:ASN:HA	35:XD:145:GLU:HB2	1.98	0.44
2:YB:43:C:H5'	26:Y4:1:MET:H1	1.82	0.44
1:YA:1203:G:H5'	11:YP:3:LEU:HD12	2.00	0.44
1:YA:1417:C:H2'	1:YA:1418:G:O4'	2.17	0.44
1:YA:2540:C:O2'	1:YA:2740:A:N3	2.44	0.44
1:YA:508:G:O2'	1:YA:509:C:P	2.75	0.44
1:YA:84:A:N1	1:YA:98:G:O2'	2.37	0.44
9:YN:54:VAL:HB	9:YN:122:VAL:HG22	2.00	0.44
32:QA:1343:G:H4'	40:QI:122:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:714:G:H2'	32:QA:715:A:C8	2.51	0.44
32:QA:728:A:H2'	32:QA:729:A:C8	2.51	0.44
40:QI:47:LEU:HG	40:QI:50:LEU:HD12	1.98	0.44
2:RB:24:G:H5'	2:RB:25:A:OP1	2.17	0.44
35:XD:176:LEU:HG	35:XD:178:VAL:HG22	1.97	0.44
1:YA:1113:U:H2'	1:YA:1114:G:C8	2.52	0.44
1:YA:1913:A:O2'	1:YA:1914:C:OP1	2.27	0.44
1:YA:2577:A:O4'	27:Y5:3:LYS:HB2	2.17	0.44
1:YA:262:A:N3	1:YA:430:G:O2'	2.35	0.44
1:YA:455:C:N3	1:YA:473:G:H5'	2.32	0.44
1:YA:581:C:H2'	1:YA:582:G:H8	1.83	0.44
1:YA:589:C:H2'	1:YA:590:A:H8	1.83	0.44
1:YA:639:U:H2'	1:YA:640:C:C6	2.52	0.44
15:YT:73:GLU:OE2	15:YT:103:ARG:NH2	2.48	0.44
32:QA:1228:C:OP2	44:QM:108:ARG:NH2	2.26	0.44
32:QA:21:G:H2'	32:QA:22:G:C8	2.52	0.44
32:QA:932:C:OP1	38:QG:4:ARG:NH1	2.49	0.44
1:RA:1817:G:H2'	1:RA:1818:U:H5'	2.00	0.44
1:RA:2019:A:N7	27:R5:9:LYS:NZ	2.46	0.44
1:RA:30:G:H2'	1:RA:31:C:H6	1.81	0.44
12:RQ:32:TYR:CE1	12:RQ:133:ARG:HG3	2.53	0.44
32:XA:1037:C:H2'	32:XA:1038:C:C6	2.52	0.44
32:XA:1218:C:H2'	32:XA:1219:U:C6	2.52	0.44
32:XA:1244:C:H2'	32:XA:1245:A:C8	2.53	0.44
32:XA:1391:U:H2'	32:XA:1392:G:C8	2.52	0.44
32:XA:855:G:N2	32:XA:1539:C:OP1	2.47	0.44
43:XL:67:THR:OG1	43:XL:95:GLY:O	2.34	0.44
26:Y4:56:VAL:HG12	26:Y4:57:GLU:H	1.83	0.44
1:YA:1508:A:O2'	1:YA:1509:C:O4'	2.35	0.44
1:YA:223:A:O2'	1:YA:420:C:O2	2.29	0.44
1:YA:657:U:H2'	1:YA:658:C:C6	2.53	0.44
2:YB:15:A:H5'	2:YB:16:G:C8	2.52	0.44
32:QA:1145:C:H4'	32:QA:1146:A:H8	1.81	0.44
32:QA:890:G:O2'	32:QA:906:G:O6	2.26	0.44
32:QA:950:U:H2'	32:QA:951:G:H8	1.82	0.44
38:QG:151:TYR:OH	42:QK:54:ARG:NH2	2.51	0.44
46:QO:26:GLU:OE1	46:QO:77:ARG:NH1	2.51	0.44
46:QO:70:LEU:HD21	46:QO:77:ARG:HG3	1.99	0.44
1:RA:2314:C:H2'	1:RA:2315:G:C8	2.52	0.44
1:RA:2611:U:O4	27:R5:3:LYS:NZ	2.50	0.44
1:RA:2689:U:H4'	1:RA:2690:C:O5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:RE:144:ARG:HB3	4:RE:145:LYS:H	1.54	0.44
8:RI:118:LYS:HG2	8:RI:118:LYS:O	2.18	0.44
14:RS:28:VAL:HG11	14:RS:98:VAL:HG12	1.99	0.44
32:XA:165:C:H2'	32:XA:166:G:C8	2.53	0.44
32:XA:356:A:O2'	32:XA:367:U:O2'	2.30	0.44
32:XA:1314:C:N4	50:XS:2:PRO:O	2.50	0.44
53:XV:39:C:H2'	53:XV:40:G:H8	1.82	0.44
1:YA:1394:U:H4'	1:YA:1603:A:H4'	2.00	0.44
1:YA:38:A:H2'	1:YA:39:C:C6	2.52	0.44
1:YA:855:G:H1	1:YA:922:U:H3	1.65	0.44
3:YD:108:PRO:HG2	3:YD:111:LEU:HG	2.00	0.44
15:YT:24:PRO:HD3	15:YT:52:ILE:HD12	1.98	0.44
32:QA:565:U:H3'	32:QA:566:G:H2'	1.99	0.44
32:QA:782:A:O3'	32:QA:1515:C:H4'	2.18	0.44
1:RA:248:G:C2	1:RA:2431:U:H4'	2.53	0.44
1:RA:768:G:O2'	1:RA:1379:A:N6	2.50	0.44
1:RA:796:C:H2'	1:RA:797:C:C6	2.53	0.44
1:RA:99:U:H4'	1:RA:101:G:O5'	2.17	0.44
5:RF:107:LYS:HB3	5:RF:107:LYS:HE2	1.83	0.44
11:RP:98:GLU:O	11:RP:102:ARG:NE	2.51	0.44
32:XA:1174:G:H2'	32:XA:1175:G:C8	2.53	0.44
32:XA:753:A:OP1	46:XO:69:TYR:OH	2.20	0.44
35:XD:159:ARG:O	35:XD:163:GLU:N	2.46	0.44
41:XJ:38:ILE:HD12	41:XJ:39:PRO:HD2	1.98	0.44
49:XR:19:LYS:HB3	49:XR:19:LYS:HE2	1.74	0.44
1:YA:1930:G:N2	1:YA:1969:A:OP2	2.42	0.44
1:YA:2291:U:O2'	1:YA:2374:C:O2	2.33	0.44
4:YE:35:GLN:HG2	4:YE:37:ARG:HE	1.81	0.44
1:YA:1262:A:OP2	18:YW:97:LYS:NZ	2.50	0.44
32:QA:514:C:H2'	32:QA:515:G:C8	2.45	0.44
41:QJ:30:SER:O	41:QJ:30:SER:OG	2.36	0.44
26:R4:37:SER:HA	26:R4:40:HIS:HB2	1.99	0.44
1:RA:1583:A:H4'	1:RA:1586:A:C4	2.52	0.44
1:RA:785:G:O2'	1:RA:1779:U:H5''	2.18	0.44
1:RA:678:C:H2'	1:RA:679:C:C6	2.53	0.44
10:RO:120:GLU:HG2	10:RO:122:LEU:HG	1.99	0.44
33:XB:105:PHE:HZ	33:XB:156:LYS:HA	1.82	0.44
35:XD:13:ARG:HB3	35:XD:39:PRO:HA	1.99	0.44
38:XG:58:PRO:HA	38:XG:61:VAL:HG22	1.99	0.44
1:YA:2140:C:H2'	1:YA:2141:G:C8	2.53	0.44
1:YA:218:A:N1	1:YA:235:U:H4'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:65:C:O2	1:YA:456:C:N4	2.51	0.44
32:QA:1053:G:H5'	32:QA:1054:C:H5'	2.00	0.44
32:QA:1352:C:H2'	32:QA:1353:G:C8	2.53	0.44
32:QA:973:G:H3'	32:QA:974:A:H5''	1.98	0.44
33:QB:15:VAL:H	33:QB:16:HIS:CE1	2.35	0.44
39:QH:103:VAL:HG21	39:QH:110:ALA:HB2	1.99	0.44
44:QM:15:VAL:HG12	44:QM:45:VAL:HG13	1.99	0.44
1:RA:1073:A:HO2'	1:RA:1074:G:C5'	2.30	0.44
1:RA:1853:A:N3	1:RA:2233:U:O2'	2.43	0.44
32:XA:105:G:H2'	32:XA:106:C:C6	2.53	0.44
32:XA:781:A:O2'	32:XA:1522:U:O2	2.35	0.44
33:XB:131:PRO:HB2	33:XB:133:LYS:HG2	2.00	0.44
33:XB:207:ALA:O	33:XB:210:SER:N	2.44	0.44
34:XC:6:HIS:HD2	34:XC:7:PRO:HD2	1.83	0.44
43:XL:113:ARG:HB3	43:XL:122:THR:HG21	2.00	0.44
49:XR:65:ILE:O	49:XR:69:THR:OG1	2.28	0.44
26:Y4:26:SER:OG	26:Y4:27:THR:N	2.51	0.44
1:YA:2291:U:H2'	1:YA:2292:C:C6	2.52	0.44
43:QL:77:LEU:HD23	43:QL:77:LEU:HA	1.78	0.44
1:RA:1221:C:H2'	1:RA:1222:C:H6	1.82	0.44
1:RA:139:G:C2	1:RA:141:A:N6	2.86	0.44
1:RA:956:G:H2'	1:RA:957:A:H2'	2.00	0.44
3:RD:20:ASP:OD1	3:RD:20:ASP:N	2.37	0.44
20:RY:83:THR:OG1	20:RY:84:ARG:N	2.50	0.44
32:XA:1427:U:H2'	32:XA:1428:A:H8	1.83	0.44
32:XA:476:G:H2'	32:XA:477:G:H8	1.82	0.44
1:YA:1076:C:H2'	1:YA:1077:A:H5''	1.98	0.44
1:YA:1430:C:H2'	1:YA:1431:U:C6	2.53	0.44
5:YF:7:TYR:HD1	5:YF:21:ALA:HB1	1.81	0.44
1:YA:2311:A:H8	6:YG:82:LEU:HD11	1.83	0.44
20:YY:52:SER:N	20:YY:55:TYR:O	2.51	0.44
32:QA:1391:U:H2'	32:QA:1392:G:C8	2.52	0.44
32:QA:224:C:H2'	32:QA:225:C:H6	1.83	0.44
32:QA:630:G:H2'	32:QA:631:G:H4'	1.99	0.44
51:QT:10:LEU:HD23	51:QT:12:ALA:H	1.82	0.44
51:QT:22:ARG:O	51:QT:26:ASN:ND2	2.51	0.44
1:RA:1296:G:OP1	1:RA:2709:G:O2'	2.23	0.44
1:RA:184:C:H2'	1:RA:185:U:C6	2.52	0.44
32:XA:1015:A:H2'	32:XA:1016:A:C8	2.53	0.44
32:XA:191(G):G:C5	51:XT:105:SER:HB3	2.53	0.44
32:XA:636:U:H2'	32:XA:637:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:806:C:H2'	32:XA:807:A:C8	2.53	0.44
53:XV:37:1MG:HM11	53:XV:37:1MG:HN21	1.66	0.44
1:YA:1779:U:OP2	1:YA:1784:A:N6	2.42	0.44
1:YA:2591:C:H2'	1:YA:2592:G:H8	1.81	0.44
1:YA:2810:A:H61	1:YA:2891:G:H2'	1.83	0.44
1:YA:601:C:O2'	1:YA:605:C:OP1	2.35	0.44
3:YD:259:THR:OG1	3:YD:259:THR:O	2.26	0.44
1:YA:2032:G:H1'	4:YE:145:LYS:HD3	2.00	0.44
21:YZ:10:ARG:NH2	21:YZ:26:GLY:O	2.51	0.44
32:QA:1152:A:H2'	32:QA:1153:C:C6	2.53	0.43
32:QA:244:U:H4'	32:QA:245:C:O5'	2.16	0.43
32:QA:475:G:H2'	32:QA:476:G:H8	1.83	0.43
32:QA:711:G:H2'	32:QA:712:A:C8	2.53	0.43
1:RA:1273:U:O2	1:RA:2002:G:O2'	2.33	0.43
1:RA:639:U:H2'	1:RA:640:C:C6	2.52	0.43
8:RI:30:LEU:HB3	8:RI:36:ALA:HB3	1.99	0.43
32:XA:1098:C:H2'	32:XA:1099:G:H8	1.83	0.43
32:XA:266:G:H5'	32:XA:268:C:H41	1.83	0.43
32:XA:444:C:H2'	32:XA:445:G:C8	2.53	0.43
39:XH:112:LEU:HA	39:XH:134:ILE:HG12	1.99	0.43
50:XS:53:ASN:HD22	50:XS:75:ALA:HB1	1.83	0.43
1:YA:86:C:H4'	1:YA:104:U:H1'	1.99	0.43
1:YA:693:C:O2'	1:YA:1353:A:N3	2.43	0.43
1:YA:1729:A:O2'	1:YA:1730:U:H2'	2.18	0.43
1:YA:1790:C:H5''	1:YA:1791:A:OP1	2.18	0.43
1:YA:1792:G:H5'	3:YD:205:VAL:HG13	2.00	0.43
1:YA:546:C:H5''	1:YA:547:A:N7	2.33	0.43
1:YA:820:A:H4'	1:YA:836:G:H22	1.83	0.43
1:YA:607:U:OP1	5:YF:102:PRO:HA	2.18	0.43
32:QA:1172:C:H2'	32:QA:1173:G:C8	2.52	0.43
32:QA:1287:A:C2	32:QA:1353:G:H1'	2.53	0.43
32:QA:1534:A:C1'	54:QX:10:G:N2	2.68	0.43
32:QA:194:C:H2'	32:QA:195:A:H5''	2.00	0.43
39:QH:81:HIS:ND1	39:QH:138:TRP:O	2.38	0.43
32:QA:963:G:H21	41:QJ:55:LYS:HE3	1.83	0.43
26:R4:14:ILE:HB	26:R4:22:ILE:HB	1.99	0.43
1:RA:1403:C:C5'	1:RA:1471:A:H1'	2.46	0.43
1:RA:2126:A:H1'	1:RA:2127:G:OP2	2.19	0.43
1:RA:2140:C:O2	1:RA:2151:G:N1	2.43	0.43
1:RA:2115:G:N1	1:RA:2164:C:OP2	2.50	0.43
1:RA:2441:C:OP2	1:RA:2586:C:O2'	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:275:G:H3'	1:RA:276:A:H5''	2.00	0.43
1:RA:811:U:H2'	11:RP:21:ARG:HA	1.99	0.43
8:RI:92:VAL:HB	8:RI:120:ILE:CG2	2.48	0.43
10:RO:97:ARG:H	10:RO:117:LEU:HD22	1.82	0.43
32:XA:34:C:H2'	32:XA:35:G:H8	1.83	0.43
33:XB:48:MET:HA	33:XB:51:LEU:HB2	1.99	0.43
50:XS:50:ALA:HB1	50:XS:57:HIS:HB2	2.00	0.43
1:YA:492:A:H2'	1:YA:493:G:O4'	2.18	0.43
1:YA:49:A:H4'	1:YA:50:U:H5''	2.00	0.43
17:YV:76:LYS:HB2	17:YV:81:TYR:HB3	1.99	0.43
32:QA:1355:G:H2'	32:QA:1356:G:C8	2.54	0.43
47:QP:21:VAL:HG13	47:QP:34:GLU:H	1.83	0.43
1:RA:1823:G:OP1	3:RD:54:ARG:NH1	2.52	0.43
1:RA:2291:U:H2'	1:RA:2292:C:C6	2.53	0.43
1:RA:2572:A:OP1	1:RA:2574:G:H4'	2.18	0.43
1:RA:2051:A:H5'	1:RA:2578:G:O4'	2.18	0.43
1:RA:303:U:H2'	1:RA:304:G:H8	1.83	0.43
6:RG:77:ILE:HG22	6:RG:80:PHE:H	1.84	0.43
11:RP:65:ARG:HE	11:RP:65:ARG:HB3	1.58	0.43
16:RU:16:LYS:HE2	16:RU:16:LYS:HB2	1.85	0.43
32:XA:1030:C:H3'	32:XA:1031:G:C8	2.54	0.43
32:XA:1410:G:H2'	32:XA:1411:C:H6	1.84	0.43
32:XA:150:C:N4	32:XA:171:A:H62	2.14	0.43
32:XA:405:U:H3'	32:XA:406:G:H5'	2.00	0.43
33:XB:115:LEU:HD13	33:XB:145:LEU:HB3	2.00	0.43
33:XB:14:GLY:H	33:XB:16:HIS:HD1	1.66	0.43
35:XD:128:VAL:HG12	35:XD:129:ASN:HB2	1.98	0.43
43:XL:53:ARG:HB3	43:XL:69:TYR:HE1	1.84	0.43
50:XS:19:VAL:HG21	50:XS:44:MET:HG2	2.00	0.43
1:YA:396:G:O2'	23:Y1:43:TYR:O	2.36	0.43
1:YA:1359:A:H62	1:YA:1372:U:H3	0.74	0.43
1:YA:1678:G:N2	1:YA:1989:G:H22	2.16	0.43
1:YA:848:G:H2'	1:YA:849:A:H8	1.83	0.43
2:YB:39:A:O2'	2:YB:46:A:N1	2.41	0.43
9:YN:6:PRO:HG3	9:YN:41:ASP:HB2	2.00	0.43
32:QA:927:G:H1	32:QA:1390:U:H3	1.66	0.43
32:QA:25:C:H2'	32:QA:26:A:C8	2.52	0.43
32:QA:427:U:OP2	32:QA:428:G:O2'	2.31	0.43
32:QA:619:U:N3	35:QD:134:ASP:OD1	2.34	0.43
43:QL:32:PHE:HE1	43:QL:86:ARG:HG3	1.83	0.43
32:QA:667:G:H4'	46:QO:51:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QP:1:MET:N	47:QP:1:MET:SD	2.83	0.43
48:QQ:6:LEU:HD22	48:QQ:23:VAL:HG11	2.00	0.43
50:QS:29:ARG:HG2	50:QS:30:LEU:HD23	1.99	0.43
1:RA:1153:C:H2'	1:RA:1154:G:O4'	2.18	0.43
1:RA:2151:G:H2'	1:RA:2152:G:H8	1.82	0.43
1:RA:2779:U:H5'	1:RA:2780:G:OP1	2.18	0.43
1:RA:271(B):G:O2'	1:RA:421:U:OP2	2.32	0.43
1:RA:82:G:H5'	1:RA:296:C:H5'	2.01	0.43
1:RA:870:A:H5'	12:RQ:6:ARG:O	2.17	0.43
6:RG:165:THR:OG1	6:RG:166:ASP:N	2.51	0.43
12:RQ:60:ARG:HE	12:RQ:60:ARG:HB3	1.67	0.43
13:RR:14:SER:OG	13:RR:15:SER:N	2.51	0.43
32:XA:337:C:H2'	32:XA:338:A:C8	2.53	0.43
42:XK:66:LEU:O	42:XK:69:ALA:N	2.50	0.43
28:Y6:6:ARG:HD2	28:Y6:6:ARG:HA	1.67	0.43
1:YA:1059:G:OP2	1:YA:1060:U:H5''	2.18	0.43
1:YA:2502:G:H5''	1:YA:2503:A:H5''	2.00	0.43
1:YA:545:G:N2	1:YA:548:A:OP2	2.51	0.43
4:YE:144:ARG:HB3	4:YE:145:LYS:H	1.47	0.43
4:YE:49:LEU:HD12	4:YE:49:LEU:HA	1.79	0.43
1:YA:2305:A:N6	6:YG:154:GLY:O	2.52	0.43
6:YG:166:ASP:O	6:YG:170:ARG:N	2.49	0.43
28:R6:17:LYS:HE3	28:R6:17:LYS:HB3	1.79	0.43
30:R8:29:LYS:HE2	30:R8:44:LYS:HB2	2.00	0.43
1:RA:108:U:H2'	1:RA:109:G:C8	2.54	0.43
1:RA:1528:A:H2'	1:RA:1529:A:C8	2.53	0.43
1:RA:1917:U:H2'	1:RA:1918:A:C8	2.54	0.43
1:RA:2096:U:O4	1:RA:2193:G:O6	2.36	0.43
1:RA:635:C:O2'	1:RA:639:U:OP1	2.34	0.43
32:XA:17:U:H2'	32:XA:18:C:H6	1.81	0.43
1:YA:286:C:H2'	1:YA:287:C:H6	1.83	0.43
7:YH:66:GLY:O	7:YH:70:THR:OG1	2.30	0.43
16:YU:92:ARG:CZ	17:YV:11:GLN:H	2.32	0.43
18:YW:110:LYS:HA	18:YW:110:LYS:HD2	1.86	0.43
32:QA:1228:C:OP1	44:QM:108:ARG:NH1	2.45	0.43
32:QA:636:U:H2'	32:QA:637:G:H8	1.83	0.43
32:QA:883:C:O2'	32:QA:884:U:H5'	2.19	0.43
32:QA:986:A:H2'	32:QA:987:G:H8	1.83	0.43
37:QF:70:ASP:OD1	37:QF:70:ASP:N	2.49	0.43
32:QA:932:C:OP1	38:QG:4:ARG:HD2	2.19	0.43
1:RA:1033:U:OP1	31:R9:9:ARG:NH1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1073:A:H2'	1:RA:1074:G:C8	2.53	0.43
1:RA:2808:U:O2	1:RA:2808:U:H2'	2.19	0.43
2:RB:44:G:H1'	2:RB:47:C:N4	2.33	0.43
3:RD:66:ASP:OD2	3:RD:103:ARG:NH1	2.52	0.43
32:XA:1077:G:N2	32:XA:1080:A:OP2	2.41	0.43
32:XA:278:G:OP2	48:XQ:92:ARG:NH2	2.44	0.43
32:XA:67:C:H2'	32:XA:68:G:C8	2.54	0.43
32:XA:792:A:H4'	32:XA:793:U:O5'	2.18	0.43
35:XD:14:ARG:HD2	35:XD:40:PRO:HD2	1.99	0.43
1:YA:205:G:O6	23:Y1:39:LYS:NZ	2.34	0.43
2:YB:66:A:O2'	2:YB:67:G:P	2.76	0.43
3:YD:245:PRO:HA	3:YD:246:PRO:HD3	1.80	0.43
6:YG:139:LEU:HD13	6:YG:144:ILE:HG22	2.00	0.43
32:QA:1218:C:H2'	32:QA:1219:U:C6	2.54	0.43
38:QG:68:ASN:HD22	38:QG:128:ALA:HA	1.83	0.43
34:QC:6:HIS:HB3	45:QN:49:HIS:ND1	2.33	0.43
1:RA:1859:A:N6	1:RA:1883:G:O2'	2.50	0.43
1:RA:236:C:H2'	1:RA:237:C:H6	1.84	0.43
1:RA:512:G:H4'	1:RA:513:A:O5'	2.18	0.43
3:RD:245:PRO:HA	3:RD:246:PRO:HD3	1.90	0.43
9:RN:25:ARG:O	9:RN:29:LYS:NZ	2.52	0.43
11:RP:81:GLN:NE2	11:RP:105:LEU:O	2.52	0.43
32:XA:1062:U:H2'	32:XA:1063:C:C6	2.54	0.43
32:XA:165:C:H2'	32:XA:166:G:H8	1.84	0.43
35:XD:94:LEU:O	35:XD:98:GLU:N	2.49	0.43
38:XG:29:LYS:HB3	38:XG:105:VAL:HG21	2.00	0.43
32:XA:735:C:H5'	49:XR:71:LYS:HD3	2.01	0.43
26:Y4:28:LYS:HA	26:Y4:29:PRO:HD3	1.91	0.43
1:YA:1859:A:N6	1:YA:1883:G:O2'	2.51	0.43
10:YO:15:GLY:HA2	10:YO:47:ILE:HG22	2.00	0.43
32:QA:192:U:H2'	32:QA:193:C:C6	2.54	0.43
32:QA:986:A:H2'	32:QA:987:G:C8	2.53	0.43
35:QD:81:GLU:OE2	35:QD:139:ARG:NH1	2.52	0.43
48:QQ:10:VAL:HA	48:QQ:20:THR:O	2.19	0.43
25:R3:18:ASP:OD1	25:R3:18:ASP:N	2.52	0.43
1:RA:1636:C:H2'	1:RA:1637:A:C8	2.54	0.43
32:XA:1172:C:H2'	32:XA:1173:G:C8	2.54	0.43
32:XA:1304:G:N2	32:XA:1333:A:H62	2.14	0.43
32:XA:545:C:H5'	35:XD:72:GLU:HG3	2.00	0.43
46:XO:76:GLU:OE1	46:XO:79:ARG:NH1	2.52	0.43
47:XP:72:ARG:HA	47:XP:75:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:XT:100:ILE:HG23	51:XT:102:GLY:H	1.84	0.43
30:Y8:29:LYS:O	30:Y8:31:HIS:N	2.50	0.43
1:YA:2478:A:OP1	31:Y9:31:LYS:HD3	2.19	0.43
1:YA:2152:G:H2'	1:YA:2153:G:C8	2.54	0.43
10:YO:73:ASP:N	10:YO:73:ASP:OD1	2.41	0.43
18:YW:64:MET:HE3	18:YW:109:GLU:HG3	2.00	0.43
32:QA:280:C:H3'	32:QA:281:G:H5'	1.99	0.43
32:QA:362:G:N2	32:QA:365:U:OP2	2.52	0.43
32:QA:545:C:O2'	32:QA:549:C:OP1	2.36	0.43
32:QA:868:C:H2'	32:QA:869:G:O4'	2.19	0.43
35:QD:145:GLU:HG3	35:QD:184:LYS:HE3	2.01	0.43
37:QF:99:ALA:HB1	49:QR:23:LYS:HE3	2.00	0.43
43:QL:56:ALA:HB2	43:QL:70:ILE:HD11	2.01	0.43
32:QA:1308:U:H3'	44:QM:99:ARG:HH21	1.84	0.43
48:QQ:52:LYS:N	48:QQ:55:ASP:OD2	2.44	0.43
1:RA:1124:C:O2	31:R9:36:GLN:NE2	2.52	0.43
1:RA:1183:G:O3'	25:R3:29:ARG:NH1	2.51	0.43
1:RA:184:C:O3'	1:RA:217:G:N2	2.50	0.43
1:RA:2712:U:H2'	1:RA:2714:G:H5''	2.01	0.43
6:RG:119:GLY:O	6:RG:181:ARG:NE	2.49	0.43
7:RH:87:LEU:HB2	7:RH:131:VAL:HG22	2.01	0.43
1:RA:1142(A):A:H4'	9:RN:25:ARG:NH2	2.33	0.43
12:RQ:59:ARG:HA	21:RZ:180:VAL:HG22	2.00	0.43
19:RX:35:THR:OG1	19:RX:36:LYS:N	2.51	0.43
32:XA:1095:U:P	32:XA:1108:G:H1	2.42	0.43
32:XA:148:G:H2'	32:XA:149:A:H8	1.83	0.43
32:XA:21:G:H2'	32:XA:22:G:C8	2.54	0.43
32:XA:315:A:H5''	32:XA:317:G:OP2	2.19	0.43
32:XA:677:U:O2	32:XA:777:A:O2'	2.34	0.43
40:XI:37:PHE:HB3	40:XI:40:LEU:HD22	2.01	0.43
52:XU:22:ARG:HD2	52:XU:23:PRO:HD2	1.99	0.43
30:Y8:28:GLY:HA2	30:Y8:44:LYS:HE2	2.01	0.43
1:YA:251:A:C5	1:YA:252:G:H1'	2.54	0.43
1:YA:2074:U:O2'	1:YA:2597:G:O2'	2.28	0.43
1:YA:2646:C:OP2	1:YA:2732:G:O2'	2.23	0.43
1:YA:691:C:H2'	1:YA:692:C:H6	1.83	0.43
13:YR:18:LEU:HD12	13:YR:18:LEU:HA	1.90	0.43
21:YZ:183:LEU:HD23	21:YZ:183:LEU:HA	1.74	0.43
32:QA:1143:G:H2'	32:QA:1144:G:C8	2.54	0.43
32:QA:1298:C:H4'	32:QA:1299:A:C4	2.53	0.43
32:QA:1410:G:H2'	32:QA:1411:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1532:U:H2'	32:QA:1534:A:H2	1.84	0.43
32:QA:992:U:O2'	32:QA:993:G:OP2	2.34	0.43
36:QE:78:HIS:HE1	36:QE:80:ILE:HD13	1.84	0.43
32:QA:1320:C:N4	50:QS:36:ARG:O	2.49	0.43
1:RA:2070:G:H2'	1:RA:2071:A:C8	2.53	0.43
1:RA:2635:C:O2'	4:RE:48:GLN:NE2	2.52	0.43
6:RG:55:LYS:HA	6:RG:58:GLN:HG2	2.00	0.43
8:RI:86:THR:HA	8:RI:123:LEU:HD11	2.01	0.43
8:RI:86:THR:O	8:RI:87:LYS:HD3	2.19	0.43
32:XA:377:G:H2'	32:XA:378:G:C8	2.54	0.43
32:XA:427:U:OP1	35:XD:13:ARG:NH2	2.52	0.43
32:XA:667:G:H4'	46:XO:51:HIS:ND1	2.34	0.43
32:XA:950:U:H2'	32:XA:951:G:C8	2.53	0.43
35:XD:15:GLU:OE2	35:XD:59:ARG:NH1	2.52	0.43
41:XJ:45:ARG:HH21	45:XN:36:PHE:HB2	1.84	0.43
32:XA:501:C:P	43:XL:117:ARG:HH21	2.41	0.43
44:XM:15:VAL:HG22	44:XM:45:VAL:HB	2.00	0.43
1:YA:2064:C:H2'	1:YA:2065:C:C6	2.54	0.43
1:YA:2102:U:H2'	1:YA:2103:C:C6	2.54	0.43
1:YA:184:C:O2'	1:YA:217:G:N3	2.49	0.43
1:YA:2392:A:C8	11:YP:61:ARG:HG2	2.54	0.43
1:YA:2625:G:H2'	1:YA:2626:C:O4'	2.18	0.43
1:YA:2870:C:H2'	1:YA:2871:C:O4'	2.19	0.43
14:YS:32:LEU:O	14:YS:62:LYS:NZ	2.42	0.43
14:YS:62:LYS:HA	14:YS:65:VAL:HG22	2.01	0.43
32:QA:1077:G:O6	36:QE:47:LYS:NZ	2.52	0.42
32:QA:1254:C:H2'	32:QA:1255:G:C8	2.53	0.42
33:QB:130:ARG:HA	33:QB:131:PRO:HD3	1.90	0.42
33:QB:32:ILE:HD12	33:QB:40:HIS:HB3	2.01	0.42
54:QX:14:A:H2'	54:QX:15:A:C8	2.54	0.42
1:RA:127:A:H5''	1:RA:128:C:C6	2.54	0.42
1:RA:140:A:C8	1:RA:1408:C:O2'	2.72	0.42
1:RA:2562:U:H1'	10:RO:23:ARG:HE	1.83	0.42
12:RQ:34:LEU:HB2	12:RQ:118:LEU:HD22	2.01	0.42
21:RZ:107:THR:HA	21:RZ:108:PRO:HD3	1.78	0.42
32:XA:109:A:H5'	32:XA:110:C:H5	1.84	0.42
32:XA:1119:C:H2'	32:XA:1120:G:H8	1.84	0.42
32:XA:1097:C:O2'	32:XA:1169:A:N3	2.40	0.42
32:XA:686:U:H2'	32:XA:687:A:C8	2.53	0.42
32:XA:978:A:H2	32:XA:1316:G:H21	1.66	0.42
35:XD:119:GLN:HE21	35:XD:123:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:XH:10:LEU:HD22	39:XH:83:ILE:HD11	2.01	0.42
29:Y7:13:ALA:HB2	29:Y7:46:VAL:HG21	2.01	0.42
1:YA:1243:G:O2'	11:YP:7:ARG:NH2	2.49	0.42
1:YA:2123:G:H2'	1:YA:2124:G:H8	1.83	0.42
1:YA:218:A:C2	1:YA:235:U:H4'	2.54	0.42
9:YN:5:VAL:HA	9:YN:6:PRO:HD3	1.84	0.42
32:QA:1128:C:H1'	32:QA:1146:A:H61	1.84	0.42
32:QA:1391:U:H2'	32:QA:1392:G:H8	1.84	0.42
32:QA:436:C:H2'	32:QA:437:U:C6	2.54	0.42
32:QA:790:A:OP1	53:QV:38:A:O2'	2.22	0.42
33:QB:115:LEU:HD13	33:QB:145:LEU:HB3	2.00	0.42
38:QG:115:ARG:HB2	38:QG:118:VAL:HG22	2.02	0.42
1:RA:1478:G:H1'	1:RA:1557:C:O2'	2.19	0.42
1:RA:1583:A:H5'	1:RA:1586:A:H1'	2.01	0.42
1:RA:1833:U:O2'	1:RA:1969:A:N1	2.44	0.42
1:RA:2306:C:H3'	1:RA:2307:G:H5''	2.01	0.42
1:RA:639:U:H2'	1:RA:640:C:H6	1.83	0.42
6:RG:34:LEU:HD21	6:RG:172:LEU:HD21	2.01	0.42
32:XA:405:U:H5''	32:XA:495:A:H2	1.84	0.42
32:XA:501:C:H2'	32:XA:502:G:H8	1.83	0.42
32:XA:1104:G:H4'	33:XB:111:ARG:NH1	2.34	0.42
39:XH:121:ASP:N	39:XH:121:ASP:OD1	2.50	0.42
40:XI:27:THR:OG1	40:XI:61:ALA:O	2.29	0.42
49:XR:26:LEU:HD11	49:XR:39:VAL:HG13	2.00	0.42
24:Y2:25:VAL:HG13	24:Y2:57:ILE:HG23	2.02	0.42
1:YA:1061:U:H3'	1:YA:1062:G:C5'	2.48	0.42
1:YA:108:U:H2'	1:YA:109:G:H8	1.85	0.42
1:YA:1671:U:H2'	1:YA:1673:U:OP2	2.18	0.42
1:YA:858:U:O2	1:YA:2268:A:H2'	2.20	0.42
2:YB:79:C:H2'	2:YB:80:U:O4'	2.19	0.42
10:YO:19:ILE:HG22	10:YO:43:VAL:HA	2.00	0.42
17:YV:18:LEU:HD12	17:YV:18:LEU:HA	1.85	0.42
32:QA:808:C:OP1	46:QO:48:LYS:HD3	2.18	0.42
32:QA:939:G:H4'	38:QG:102:ARG:HH21	1.84	0.42
6:RG:98:ARG:NH1	26:R4:1:MET:SD	2.92	0.42
30:R8:54:GLU:O	30:R8:58:ILE:HG12	2.19	0.42
1:RA:1353:A:H2'	1:RA:1354:A:C8	2.54	0.42
1:RA:769:G:H4'	1:RA:1379:A:N1	2.34	0.42
1:RA:1448:G:H5'	1:RA:1449:A:OP1	2.19	0.42
1:RA:2611:U:C4	27:R5:3:LYS:HG2	2.54	0.42
1:RA:675:A:OP1	5:RF:63:LYS:NZ	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:RO:68:GLU:HG3	10:RO:78:ARG:HD3	2.01	0.42
32:XA:243:A:H5''	32:XA:244:U:H3'	2.02	0.42
32:XA:265:G:H2'	32:XA:266:G:H5''	2.01	0.42
30:Y8:2:PRO:HB2	30:Y8:3:LYS:H	1.72	0.42
1:YA:1217:C:OP1	16:YU:15:LYS:NZ	2.49	0.42
1:YA:1539:G:H2'	1:YA:1540:G:C8	2.54	0.42
1:YA:1796:U:H2'	1:YA:1797:C:H6	1.84	0.42
1:YA:639:U:H2'	1:YA:640:C:H6	1.84	0.42
8:YI:100:ALA:O	8:YI:104:GLN:N	2.52	0.42
32:QA:924:C:O2'	32:QA:1502:A:N6	2.52	0.42
32:QA:1513:A:H2'	32:QA:1514:C:C6	2.55	0.42
36:QE:80:ILE:HA	36:QE:80:ILE:HD12	1.91	0.42
37:QF:3:ARG:NH1	37:QF:66:GLU:OE1	2.52	0.42
32:QA:599:C:O2'	39:QH:129:VAL:O	2.23	0.42
32:QA:1228:C:P	44:QM:108:ARG:HH12	2.42	0.42
49:QR:73:ALA:HB3	49:QR:79:LEU:HD22	2.00	0.42
24:R2:38:GLN:HG2	24:R2:44:LEU:HD12	2.01	0.42
30:R8:54:GLU:HG3	30:R8:57:ARG:HH21	1.85	0.42
1:RA:1782:C:N4	1:RA:2587:A:C2	2.87	0.42
1:RA:2556:C:H2'	1:RA:2557:G:O4'	2.19	0.42
1:RA:448:U:C4	1:RA:583:G:H1'	2.55	0.42
35:XD:114:ARG:HA	35:XD:117:ALA:HB3	2.01	0.42
41:XJ:15:THR:O	41:XJ:19:SER:N	2.40	0.42
43:XL:46:LYS:HG2	43:XL:47:LYS:H	1.85	0.42
1:YA:1204:A:O2'	1:YA:1205:U:O5'	2.37	0.42
1:YA:1454:U:O2'	1:YA:1455:G:N7	2.52	0.42
1:YA:1678:G:H8	1:YA:1678:G:O5'	2.02	0.42
1:YA:1882:C:H5'	1:YA:1883:G:OP2	2.19	0.42
3:YD:177:LEU:HA	3:YD:177:LEU:HD23	1.79	0.42
8:YI:76:THR:OG1	8:YI:139:GLN:NE2	2.53	0.42
9:YN:35:ARG:HG2	9:YN:35:ARG:H	1.71	0.42
15:YT:113:LYS:HA	15:YT:113:LYS:HD3	1.82	0.42
1:YA:1322:A:OP1	18:YW:11:ARG:HG2	2.19	0.42
21:YZ:77:ASP:OD2	21:YZ:80:ARG:NH1	2.53	0.42
32:QA:476:G:H2'	32:QA:477:G:H8	1.85	0.42
32:QA:7:G:H5'	32:QA:298:A:O4'	2.19	0.42
33:QB:212:GLN:NE2	33:QB:235:SER:HB3	2.34	0.42
43:QL:117:ARG:HB2	43:QL:122:THR:HB	2.01	0.42
46:QO:26:GLU:HG2	46:QO:81:LEU:HD22	2.02	0.42
25:R3:4:LEU:N	25:R3:37:LEU:O	2.53	0.42
1:RA:2130:U:H2'	1:RA:2131:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2183:C:H2'	1:RA:2184:G:H8	1.84	0.42
1:RA:2832:U:O2'	1:RA:2833:G:P	2.77	0.42
1:RA:524:U:H2'	1:RA:525:U:C6	2.54	0.42
2:RB:75:G:H4'	21:RZ:36:LYS:HD3	2.01	0.42
3:RD:108:PRO:HG3	3:RD:143:HIS:CE1	2.55	0.42
8:RI:77:LEU:HD21	8:RI:140:LEU:HB2	1.98	0.42
17:RV:64:HIS:ND1	17:RV:92:THR:HG22	2.34	0.42
32:XA:1409:C:H2'	32:XA:1410:G:C8	2.53	0.42
32:XA:673:G:H2'	32:XA:674:G:H8	1.84	0.42
51:XT:89:ARG:O	51:XT:93:GLU:N	2.53	0.42
1:YA:2814:C:O2'	27:Y5:29:THR:OG1	2.27	0.42
1:YA:458:G:O2'	1:YA:469:G:O6	2.32	0.42
1:YA:826:U:H2'	1:YA:828:U:O4'	2.19	0.42
7:YH:121:ILE:HD13	7:YH:121:ILE:HA	1.89	0.42
8:YI:54:GLN:O	8:YI:57:ARG:N	2.51	0.42
15:YT:91:ARG:NE	15:YT:124:ASP:OD2	2.48	0.42
32:QA:452:A:H2'	32:QA:453:A:C8	2.55	0.42
32:QA:452:A:H2'	32:QA:453:A:H8	1.83	0.42
1:RA:142:G:H2'	1:RA:143:C:H6	1.85	0.42
1:RA:1441:G:H2'	1:RA:1442:G:C8	2.54	0.42
1:RA:2853:C:H2'	1:RA:2854:G:C8	2.55	0.42
1:RA:29:U:H2'	1:RA:30:G:C8	2.53	0.42
2:RB:66:A:O2'	2:RB:67:G:OP2	2.30	0.42
6:RG:97:ASP:HA	6:RG:100:TRP:HD1	1.85	0.42
8:RI:56:LYS:O	8:RI:60:GLU:N	2.44	0.42
11:RP:100:LEU:HD23	11:RP:105:LEU:HD22	2.01	0.42
13:RR:75:LEU:HA	13:RR:78:LYS:HB3	2.01	0.42
32:XA:1270:C:H2'	32:XA:1271:G:H8	1.85	0.42
32:XA:376:G:OP2	47:XP:67:THR:HG21	2.20	0.42
32:XA:452:A:H2'	32:XA:453:A:H8	1.85	0.42
1:YA:1019:U:O2'	1:YA:1021:A:H2	2.02	0.42
1:YA:30:G:H2'	1:YA:31:C:H6	1.84	0.42
7:YH:40:GLU:OE1	7:YH:60:ARG:NH1	2.52	0.42
12:YQ:24:GLY:H	12:YQ:101:ARG:HD2	1.82	0.42
32:QA:1121:U:H2'	32:QA:1122:U:C6	2.54	0.42
32:QA:1273:G:H3'	32:QA:1274:G:H8	1.84	0.42
32:QA:404:U:H2'	32:QA:405:U:H6	1.84	0.42
43:QL:57:LYS:NZ	43:QL:65:GLU:OE2	2.49	0.42
47:QP:8:ARG:HA	47:QP:17:TYR:HD1	1.84	0.42
1:RA:1882:C:H5'	1:RA:1883:G:OP2	2.19	0.42
1:RA:2102:U:H2'	1:RA:2103:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2151:G:H2'	1:RA:2152:G:C8	2.54	0.42
2:RB:104:A:OP1	21:RZ:72:ARG:NH1	2.52	0.42
32:XA:1145:C:H4'	32:XA:1146:A:H8	1.85	0.42
32:XA:1295:G:O3'	44:XM:14:ARG:NH1	2.53	0.42
32:XA:1299:A:N7	32:XA:1301:U:H1'	2.35	0.42
32:XA:1296:C:H5'	44:XM:14:ARG:HD2	2.02	0.42
46:XO:4:THR:OG1	46:XO:5:LYS:N	2.52	0.42
1:YA:530:G:C5	1:YA:2022:U:H5''	2.54	0.42
1:YA:2112:G:O6	1:YA:2169:A:N6	2.53	0.42
5:YF:11:VAL:HB	5:YF:18:ARG:HG3	2.01	0.42
32:QA:1298:C:H4'	32:QA:1299:A:C8	2.55	0.42
32:QA:1328:C:OP1	52:QU:21:TYR:OH	2.26	0.42
32:QA:737:A:H2'	32:QA:738:C:H6	1.85	0.42
35:QD:102:ASP:OD1	35:QD:102:ASP:N	2.49	0.42
37:QF:5:GLU:HG3	37:QF:93:SER:HB3	2.01	0.42
38:QG:58:PRO:HA	38:QG:61:VAL:HG12	2.01	0.42
32:QA:881:G:P	43:QL:12:ARG:HH22	2.42	0.42
44:QM:74:VAL:O	44:QM:78:ILE:HG12	2.19	0.42
53:QV:34:C:H2'	53:QV:35:G:H8	1.85	0.42
1:RA:218:A:N1	1:RA:235:U:H4'	2.35	0.42
1:RA:2023:G:H4'	1:RA:2617:C:O3'	2.20	0.42
1:RA:2630:G:H2'	1:RA:2631:G:C8	2.54	0.42
1:RA:321:G:C4	5:RF:165:ARG:HD3	2.53	0.42
6:RG:67:LYS:HE3	6:RG:67:LYS:HB2	1.88	0.42
12:RQ:60:ARG:NH1	21:RZ:177:PRO:HG2	2.31	0.42
32:XA:1219:U:H2'	32:XA:1220:G:H8	1.83	0.42
32:XA:244:U:H4'	32:XA:245:C:O5'	2.20	0.42
32:XA:271:C:H2'	32:XA:272:C:H6	1.84	0.42
32:XA:575:G:O2'	32:XA:821:G:H5'	2.20	0.42
32:XA:728:A:H2'	32:XA:729:A:C8	2.54	0.42
33:XB:25:ASN:HA	33:XB:26:PRO:HD3	1.88	0.42
38:XG:16:LEU:HD12	38:XG:17:VAL:HG23	2.02	0.42
1:YA:363(A):A:H2'	1:YA:363(B):G:H8	1.83	0.42
1:YA:535:C:O3'	16:YU:53:ARG:NH1	2.53	0.42
21:YZ:108:PRO:HG3	21:YZ:141:VAL:HG23	2.02	0.42
32:QA:976:G:H5''	32:QA:1358:U:O2'	2.19	0.42
38:QG:13:GLN:HA	38:QG:14:PRO:HD3	1.88	0.42
32:QA:1325:C:H4'	52:QU:17:THR:HG21	2.01	0.42
1:RA:2130:U:HO2'	1:RA:2133:G:HO2'	1.66	0.42
1:RA:670:A:H5''	11:RP:42:SER:O	2.20	0.42
3:RD:37:LEU:HD12	3:RD:37:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:RE:24:THR:OG1	4:RE:186:GLY:O	2.27	0.42
7:RH:89:ILE:O	7:RH:129:THR:OG1	2.36	0.42
15:RT:56:GLY:O	15:RT:59:THR:OG1	2.28	0.42
32:XA:1294:G:H2'	32:XA:1295:G:C8	2.53	0.42
32:XA:377:G:H2'	32:XA:378:G:H8	1.84	0.42
34:XC:108:ASN:HD21	34:XC:144:SER:HB2	1.85	0.42
36:XE:94:ALA:HB1	36:XE:98:THR:HG21	2.02	0.42
41:XJ:11:PHE:O	41:XJ:68:HIS:ND1	2.39	0.42
26:Y4:10:VAL:N	26:Y4:26:SER:O	2.45	0.42
1:YA:2533:A:H2'	1:YA:2534:A:O4'	2.20	0.42
1:YA:484:C:H2'	1:YA:485:C:H6	1.85	0.42
1:YA:635:C:O2'	1:YA:639:U:OP1	2.37	0.42
32:QA:1314:C:H2'	32:QA:1315:U:C6	2.55	0.42
32:QA:1423:G:H2'	32:QA:1424:C:C6	2.54	0.42
32:QA:328:C:H4'	32:QA:329:A:H5'	2.02	0.42
32:QA:410:G:H2'	32:QA:429:U:C4	2.55	0.42
32:QA:639:G:H2'	32:QA:640:A:H8	1.85	0.42
32:QA:974:A:P	45:QN:41:ARG:HH12	2.43	0.42
32:QA:429:U:C3'	35:QD:22:LYS:NZ	2.80	0.42
44:QM:30:ALA:O	44:QM:34:LEU:HG	2.20	0.42
47:QP:26:ARG:HA	47:QP:26:ARG:HD3	1.87	0.42
1:RA:1011:G:H4'	16:RU:75:ASN:ND2	2.35	0.42
1:RA:1084:A:H8	1:RA:1085:A:H4'	1.84	0.42
1:RA:1497:U:H5''	1:RA:1498:C:H5	1.85	0.42
1:RA:1394:U:H4'	1:RA:1603:A:H4'	2.01	0.42
1:RA:2103:C:N4	1:RA:2187:G:O6	2.53	0.42
1:RA:2528:U:H2'	1:RA:2530:A:O5'	2.20	0.42
1:RA:608:A:H2'	1:RA:609:A:C8	2.55	0.42
1:RA:997:G:OP1	16:RU:93:LYS:HB2	2.19	0.42
2:RB:3:C:H2'	2:RB:4:C:H6	1.85	0.42
4:RE:2:LYS:HG2	4:RE:200:GLU:HB2	2.01	0.42
12:RQ:85:LYS:HG2	12:RQ:86:GLY:H	1.85	0.42
14:RS:12:PHE:O	14:RS:16:ASN:ND2	2.53	0.42
1:RA:1218:C:P	16:RU:15:LYS:HZ1	2.43	0.42
20:RY:16:ALA:O	20:RY:21:LYS:HE3	2.18	0.42
21:RZ:69:THR:HG22	21:RZ:90:VAL:HG22	2.02	0.42
32:XA:1074:G:H1	32:XA:1083:U:H3	1.67	0.42
32:XA:36:C:H2'	32:XA:37:U:O4'	2.20	0.42
32:XA:580:U:H3	32:XA:761:G:H1	1.68	0.42
32:XA:715:A:H2'	32:XA:716:A:C8	2.55	0.42
34:XC:190:ARG:HD2	34:XC:190:ARG:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1368:G:H4'	45:XN:61:TRP:HZ2	1.84	0.42
1:YA:1286:A:H1'	1:YA:1288:U:OP2	2.20	0.42
1:YA:1394:U:O2	19:YX:16:LYS:NZ	2.50	0.42
1:YA:1411:C:H5'	1:YA:1412:A:OP2	2.19	0.42
1:YA:2086:U:H2'	1:YA:2087:G:C8	2.55	0.42
1:YA:2185:C:H2'	1:YA:2186:G:C8	2.55	0.42
1:YA:2389:G:H5''	1:YA:2390:U:O4'	2.19	0.42
1:YA:2853:C:H2'	1:YA:2854:G:C8	2.55	0.42
32:QA:1355:G:H2'	32:QA:1356:G:H8	1.85	0.41
32:QA:801:U:H2'	32:QA:802:A:C8	2.55	0.41
32:QA:857:C:H2'	32:QA:858:G:O4'	2.20	0.41
32:QA:948:C:H2'	32:QA:949:A:H8	1.83	0.41
49:QR:53:ARG:NE	49:QR:58:LEU:O	2.48	0.41
1:RA:1204:A:O2'	1:RA:1205:U:O5'	2.37	0.41
1:RA:2208:U:O2'	3:RD:151:LYS:HG2	2.19	0.41
1:RA:2740:A:H2'	1:RA:2741:A:C8	2.54	0.41
1:RA:746:A:O2'	1:RA:2611:U:O2'	2.31	0.41
3:RD:133:LEU:HB3	3:RD:173:VAL:HG21	2.02	0.41
6:RG:36:LYS:HG3	6:RG:95:ARG:NH1	2.35	0.41
8:RI:86:THR:C	8:RI:87:LYS:HG2	2.40	0.41
12:RQ:17:LEU:HD23	12:RQ:39:PRO:HB2	2.02	0.41
1:RA:2495:G:H5''	12:RQ:81:VAL:HG12	2.01	0.41
18:RW:110:LYS:HA	18:RW:110:LYS:HD3	1.78	0.41
38:XG:63:LYS:HE3	38:XG:63:LYS:HB3	1.89	0.41
48:XQ:89:LEU:O	48:XQ:93:GLN:N	2.52	0.41
23:Y1:82:LEU:HA	23:Y1:82:LEU:HD23	1.93	0.41
24:Y2:57:ILE:HG22	24:Y2:61:LEU:HD12	2.02	0.41
29:Y7:6:GLN:HA	29:Y7:7:PRO:HD3	1.90	0.41
1:YA:1149:G:H2'	1:YA:1150:C:C6	2.55	0.41
1:YA:1178:C:H2'	1:YA:1179:C:H6	1.84	0.41
1:YA:2111:C:C2	1:YA:2118:U:H4'	2.55	0.41
1:YA:2140:C:N4	1:YA:2141:G:O6	2.53	0.41
3:YD:60:ARG:NH1	3:YD:86:PRO:O	2.53	0.41
16:YU:29:SER:OG	16:YU:30:LYS:NZ	2.52	0.41
16:YU:17:ILE:HG13	16:YU:32:PHE:HE1	1.85	0.41
32:QA:1372:U:OP1	40:QL:72:GLY:N	2.54	0.41
32:QA:139:G:H2'	32:QA:140:A:H8	1.85	0.41
32:QA:628:G:H2'	32:QA:629:G:C8	2.55	0.41
32:QA:806:C:H2'	32:QA:807:A:C8	2.54	0.41
32:QA:537:G:H5''	43:QL:113:ARG:HH12	1.85	0.41
1:RA:769:G:H5'	1:RA:1379:A:N6	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1695:G:N7	3:RD:14:ARG:NH2	2.67	0.41
1:RA:2197:U:H1'	1:RA:2198:A:C8	2.54	0.41
1:RA:2315:G:OP1	6:RG:36:LYS:NZ	2.49	0.41
1:RA:2287:A:N6	1:RA:2344:U:H3	2.18	0.41
1:RA:250:G:H2'	1:RA:251:A:C8	2.55	0.41
1:RA:442:G:H1'	5:RF:48:THR:HG21	2.02	0.41
4:RE:5:LEU:HD11	4:RE:79:ARG:HB2	2.02	0.41
5:RF:182:ASN:N	5:RF:182:ASN:OD1	2.52	0.41
6:RG:102:PHE:HD1	6:RG:103:LEU:HD23	1.85	0.41
8:RI:86:THR:O	8:RI:87:LYS:CD	2.69	0.41
32:XA:1288:A:N1	32:XA:1371:G:H1'	2.35	0.41
32:XA:434:U:H2'	32:XA:435:C:H6	1.84	0.41
32:XA:481:G:O2'	32:XA:482:A:O5'	2.37	0.41
44:XM:106:ASN:N	44:XM:106:ASN:OD1	2.53	0.41
22:Y0:64:ASP:OD1	22:Y0:64:ASP:N	2.53	0.41
30:Y8:29:LYS:HG2	30:Y8:29:LYS:H	1.66	0.41
1:YA:1796:U:H2'	1:YA:1797:C:C6	2.56	0.41
1:YA:1871:A:H2'	1:YA:1872:A:C8	2.55	0.41
1:YA:307:G:H21	1:YA:330:A:N6	2.17	0.41
6:YG:59:GLU:OE2	6:YG:153:ARG:NH2	2.38	0.41
32:QA:1043:C:H2'	32:QA:1044:A:C8	2.55	0.41
32:QA:110:C:H2'	32:QA:111:G:O4'	2.20	0.41
32:QA:1308:U:H2'	32:QA:1309:G:C8	2.55	0.41
32:QA:224:C:H2'	32:QA:225:C:C6	2.55	0.41
32:QA:41:G:H2'	32:QA:42:G:C8	2.54	0.41
32:QA:466:C:H4'	32:QA:467:G:OP2	2.20	0.41
40:QI:93:ARG:HB2	40:QI:97:LYS:HE2	2.03	0.41
24:R2:38:GLN:HB3	24:R2:45:SER:HB2	2.01	0.41
1:RA:1608:A:H1'	1:RA:1610:A:OP2	2.20	0.41
1:RA:2537:U:H2'	1:RA:2538:C:C6	2.54	0.41
1:RA:2636:U:H5'	4:RE:80:GLU:HB2	2.02	0.41
1:RA:2832:U:HO2'	1:RA:2833:G:P	2.42	0.41
4:RE:97:LYS:HE3	4:RE:97:LYS:HB2	1.83	0.41
6:RG:135:LEU:HD23	6:RG:155:MET:HG2	2.02	0.41
12:RQ:58:PHE:HD2	12:RQ:61:GLY:HA3	1.83	0.41
12:RQ:41:TRP:HB3	12:RQ:94:VAL:HG21	2.03	0.41
20:RY:65:ALA:HA	20:RY:66:PRO:HD3	1.95	0.41
32:XA:1532:U:H1'	32:XA:1533:C:H5	1.86	0.41
38:XG:103:TRP:HA	38:XG:106:GLN:HB2	2.02	0.41
43:XL:77:LEU:HD23	43:XL:77:LEU:HA	1.83	0.41
32:XA:1222:G:H5''	50:XS:78:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:XT:68:LYS:O	51:XT:73:HIS:NE2	2.54	0.41
1:YA:1021:A:H2'	1:YA:1023:U:H5'	2.02	0.41
1:YA:1297:C:O2'	1:YA:1302:A:N1	2.47	0.41
1:YA:1657:C:H2'	1:YA:1658:C:C6	2.56	0.41
1:YA:2487:G:H2'	1:YA:2488:A:C8	2.55	0.41
1:YA:2632:A:O2'	1:YA:2811:G:O2'	2.31	0.41
1:YA:37:C:H4'	1:YA:451:C:OP1	2.21	0.41
8:YI:74:ASN:N	8:YI:74:ASN:OD1	2.50	0.41
32:QA:1269:A:HO2'	32:QA:1325:C:HO2'	1.56	0.41
32:QA:708:C:H2'	32:QA:709:G:H8	1.85	0.41
32:QA:753:A:H4'	32:QA:754:C:O5'	2.20	0.41
33:QB:7:VAL:HB	33:QB:217:ARG:HD2	2.03	0.41
33:QB:82:ARG:HB2	33:QB:94:ASN:HD21	1.86	0.41
35:QD:9:CYS:SG	35:QD:32:ALA:CB	3.08	0.41
25:R3:8:LEU:HD21	25:R3:23:LEU:HD21	2.02	0.41
1:RA:1064:C:H3'	1:RA:1065:U:H5'	2.02	0.41
1:RA:242:G:O2'	1:RA:254:G:O6	2.33	0.41
1:RA:29:U:H2'	1:RA:30:G:H8	1.85	0.41
1:RA:863:A:H2'	1:RA:864:G:C8	2.55	0.41
2:RB:15:A:H5'	2:RB:16:G:H8	1.85	0.41
1:RA:2305:A:H5''	6:RG:134:GLY:HA3	2.02	0.41
1:RA:2820:A:C5	13:RR:4:LEU:HD11	2.56	0.41
14:RS:101:LEU:O	14:RS:105:ALA:N	2.53	0.41
32:XA:1299:A:C8	32:XA:1301:U:H1'	2.55	0.41
32:XA:1346:A:O3'	32:XA:1347:G:H4'	2.20	0.41
32:XA:164:U:H2'	32:XA:165:C:H6	1.85	0.41
32:XA:397:A:H5'	32:XA:398:C:OP1	2.20	0.41
32:XA:452:A:H2'	32:XA:453:A:C8	2.56	0.41
32:XA:861:G:HO2'	32:XA:874:G:HO2'	1.64	0.41
33:XB:115:LEU:HA	33:XB:118:LEU:HB2	2.01	0.41
45:XN:26:ARG:HD3	45:XN:43:CYS:SG	2.61	0.41
1:YA:1225:C:O2'	17:YV:85:LYS:HA	2.20	0.41
1:YA:184:C:H2'	1:YA:185:U:H6	1.84	0.41
1:YA:2105:C:H2'	1:YA:2106:G:C8	2.55	0.41
1:YA:2543:G:H2'	1:YA:2544:G:C8	2.56	0.41
1:YA:314:A:N6	1:YA:315:G:O6	2.52	0.41
8:YI:78:THR:HG22	8:YI:141:LYS:HB3	2.02	0.41
32:QA:1133:G:H2'	32:QA:1134:G:C8	2.55	0.41
32:QA:323:U:H5'	51:QT:23:ARG:HB3	2.03	0.41
32:QA:563:A:H2'	32:QA:567:G:C8	2.55	0.41
34:QC:57:ILE:HA	34:QC:65:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:QC:72:LYS:HD2	34:QC:72:LYS:HA	1.86	0.41
36:QE:92:LYS:HB3	36:QE:119:LEU:HB2	2.03	0.41
32:QA:963:G:H21	41:QJ:55:LYS:HG2	1.85	0.41
41:QJ:61:GLU:OE2	45:QN:45:ARG:NE	2.53	0.41
42:QK:51:LYS:HE2	42:QK:51:LYS:HB2	1.82	0.41
23:R1:65:SER:OG	23:R1:66:HIS:ND1	2.48	0.41
1:RA:1756:G:H4'	1:RA:1758:G:O4'	2.20	0.41
1:RA:2136:C:H2'	1:RA:2137:C:H6	1.85	0.41
1:RA:969:U:H2'	1:RA:970:C:C6	2.55	0.41
5:RF:186:ILE:HD12	5:RF:192:LEU:HD11	2.02	0.41
9:RN:112:LEU:HD12	9:RN:112:LEU:HA	1.85	0.41
32:XA:627:G:H2'	32:XA:628:G:C8	2.55	0.41
35:XD:101:LEU:HB2	35:XD:138:TYR:HB3	2.03	0.41
32:XA:227:G:N2	47:XP:62:VAL:O	2.52	0.41
1:YA:1018:C:O3'	1:YA:1120:G:N2	2.53	0.41
1:YA:1657:C:H2'	1:YA:1658:C:H6	1.86	0.41
1:YA:1923:U:H2'	1:YA:1924:C:C6	2.55	0.41
1:YA:2137:C:H2'	1:YA:2138:C:C6	2.55	0.41
1:YA:36:G:N3	1:YA:450:G:O2'	2.52	0.41
1:YA:579:G:H2'	1:YA:580:C:H6	1.84	0.41
1:YA:867:C:N3	1:YA:912:C:O2'	2.36	0.41
3:YD:5:LYS:HB3	3:YD:5:LYS:HE3	1.80	0.41
1:YA:807:U:OP2	11:YP:41:ARG:NH1	2.54	0.41
32:QA:1130:A:N6	32:QA:1131:G:O6	2.53	0.41
32:QA:1314:C:OP2	50:QS:4:SER:OG	2.20	0.41
32:QA:35:G:N3	43:QL:118:SER:OG	2.49	0.41
34:QC:95:THR:HG22	34:QC:97:LYS:H	1.84	0.41
1:RA:1005:C:H2'	1:RA:1006:C:C6	2.55	0.41
1:RA:1063:G:OP1	1:RA:1065:U:O2'	2.39	0.41
1:RA:125:G:OP1	29:R7:14:LYS:NZ	2.54	0.41
1:RA:1536:A:H5''	1:RA:1537:C:C6	2.56	0.41
1:RA:1541:U:H2'	1:RA:1542:G:C8	2.56	0.41
1:RA:919:G:N2	1:RA:2269:A:OP2	2.53	0.41
1:RA:78:A:H2'	1:RA:79:G:C8	2.54	0.41
12:RQ:18:LYS:HE2	12:RQ:18:LYS:HB3	1.78	0.41
1:RA:960:A:H61	12:RQ:82:ARG:HH12	1.67	0.41
1:RA:302:C:P	20:RY:73:ARG:HH12	2.44	0.41
32:XA:148:G:H2'	32:XA:149:A:C8	2.55	0.41
32:XA:1531:A:H5'	32:XA:1532:U:OP1	2.20	0.41
32:XA:477:G:H2'	32:XA:478:A:C8	2.56	0.41
32:XA:678:U:H2'	32:XA:679:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:868:C:H2'	32:XA:869:G:O4'	2.21	0.41
35:XD:129:ASN:OD1	35:XD:145:GLU:N	2.53	0.41
38:XG:93:PRO:HA	38:XG:96:GLN:HB3	2.02	0.41
23:Y1:86:SER:OG	23:Y1:89:GLU:OE2	2.31	0.41
1:YA:2314:C:H2'	1:YA:2315:G:H8	1.86	0.41
1:YA:2611:U:OP2	1:YA:2611:U:H3'	2.20	0.41
1:YA:2626:C:H2'	1:YA:2627:G:C8	2.56	0.41
1:YA:2712:U:OP1	1:YA:2714:G:H4'	2.21	0.41
21:YZ:19:ARG:NH1	21:YZ:84:GLU:O	2.54	0.41
32:QA:977:A:N6	32:QA:1224:G:OP1	2.53	0.41
33:QB:223:ILE:HD12	33:QB:230:VAL:HG23	2.02	0.41
33:QB:233:SER:OG	33:QB:233:SER:O	2.29	0.41
36:QE:71:LEU:HD23	36:QE:71:LEU:HA	1.88	0.41
43:QL:51:ALA:HB3	43:QL:53:ARG:HE	1.86	0.41
44:QM:81:LEU:HD13	44:QM:88:ARG:HB3	2.03	0.41
1:RA:625:G:P	30:R8:64:TYR:HB3	2.59	0.41
6:RG:101:ILE:HD12	6:RG:101:ILE:HA	1.96	0.41
1:RA:2326:C:O3'	21:RZ:201:LYS:NZ	2.54	0.41
32:XA:1043:C:H2'	32:XA:1044:A:C8	2.56	0.41
32:XA:324:G:OP1	51:XT:70:SER:HB2	2.20	0.41
32:XA:378:G:N1	32:XA:386:C:N3	2.69	0.41
32:XA:80:G:H22	32:XA:89:U:H3	1.68	0.41
36:XE:69:VAL:HG21	36:XE:113:ALA:HB1	2.03	0.41
32:XA:1491:G:H5'	43:XL:47:LYS:HE2	2.01	0.41
47:XP:69:THR:OG1	47:XP:69:THR:O	2.38	0.41
50:XS:7:LYS:HE3	50:XS:7:LYS:HB3	1.77	0.41
51:XT:57:ARG:O	51:XT:61:SER:OG	2.35	0.41
23:Y1:50:ARG:HG2	23:Y1:59:THR:HG22	2.03	0.41
1:YA:141:A:H5''	1:YA:141(A):C:OP2	2.20	0.41
1:YA:2781:A:H5''	1:YA:2782:G:H5'	2.02	0.41
1:YA:27:G:N2	1:YA:512:G:O2'	2.54	0.41
1:YA:581:C:H2'	1:YA:582:G:C8	2.56	0.41
1:YA:932:G:H4'	1:YA:933:A:O5'	2.21	0.41
14:YS:15:ARG:NE	14:YS:88:ASP:OD2	2.53	0.41
14:YS:5:THR:OG1	14:YS:8:GLU:OE2	2.36	0.41
32:QA:1238:A:H62	32:QA:1301:U:H3	1.69	0.41
32:QA:1305:G:HO2'	32:QA:1306:A:H8	1.69	0.41
44:QM:19:LEU:HD12	44:QM:22:ILE:HD13	2.02	0.41
1:RA:1657:C:H2'	1:RA:1658:C:H6	1.85	0.41
1:RA:2424:C:O2	1:RA:2429:G:O2'	2.25	0.41
1:RA:2685:G:P	15:RT:51:ARG:HH22	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:29:U:H5''	16:RU:7:GLY:HA2	2.03	0.41
1:RA:673:C:H5''	5:RF:81:PRO:HD2	2.03	0.41
1:RA:2574:G:N2	4:RE:142:GLY:O	2.37	0.41
12:RQ:24:GLY:H	12:RQ:101:ARG:HD2	1.86	0.41
12:RQ:21:THR:HB	12:RQ:22:LYS:H	1.70	0.41
32:XA:19:C:H2'	32:XA:20:U:C6	2.56	0.41
32:XA:407:G:H2'	32:XA:408:A:H8	1.84	0.41
32:XA:464:G:C6	32:XA:466:C:H5'	2.56	0.41
32:XA:636:U:H5'	48:XQ:2:PRO:HG3	2.02	0.41
32:XA:707:C:H2'	32:XA:708:C:H6	1.84	0.41
32:XA:8:A:N6	35:XD:205:GLU:O	2.53	0.41
42:XK:31:THR:HA	42:XK:42:TRP:HA	2.03	0.41
44:XM:16:ASP:N	44:XM:16:ASP:OD1	2.53	0.41
46:XO:36:ILE:O	46:XO:40:SER:N	2.42	0.41
51:XT:10:LEU:HD23	51:XT:12:ALA:H	1.85	0.41
51:XT:50:GLU:HG2	51:XT:99:LEU:HD12	2.02	0.41
1:YA:1186:G:H2'	1:YA:1187:G:O4'	2.21	0.41
1:YA:2183:C:H2'	1:YA:2184:G:C8	2.56	0.41
1:YA:2845:G:OP1	15:YT:54:ARG:HB3	2.19	0.41
1:YA:307:G:H21	1:YA:330:A:H62	1.67	0.41
1:YA:805:G:N2	1:YA:829:A:OP1	2.52	0.41
5:YF:9:ILE:O	5:YF:20:LEU:N	2.51	0.41
8:YI:83:ALA:HB1	8:YI:123:LEU:HD11	2.03	0.41
2:YB:48:A:P	14:YS:30:ARG:HH12	2.44	0.41
32:QA:1071:C:H2'	32:QA:1072:G:C8	2.54	0.41
32:QA:1277:C:O2'	32:QA:1279:A:H8	2.04	0.41
32:QA:153:C:N3	32:QA:169:C:N4	2.69	0.41
35:QD:20:TYR:HE2	37:XF:15:ASP:HB2	1.85	0.41
37:QF:3:ARG:HA	37:QF:65:VAL:O	2.20	0.41
39:QH:73:ASP:OD2	39:QH:75:ARG:NH1	2.54	0.41
1:RA:1181:C:H2'	1:RA:1182:A:C8	2.56	0.41
1:RA:1300:U:H4'	1:RA:1301:A:H5''	2.01	0.41
1:RA:2053:G:OP1	4:RE:144:ARG:HG2	2.21	0.41
1:RA:237:C:O2	1:RA:609:A:O2'	2.37	0.41
1:RA:241:A:OP1	1:RA:243:U:H1'	2.21	0.41
1:RA:2687:U:H2'	1:RA:2688:U:O4'	2.21	0.41
1:RA:2753:A:N3	31:R9:15:LYS:NZ	2.68	0.41
1:RA:923:C:H2'	1:RA:924:C:C6	2.56	0.41
7:RH:102:ALA:HA	7:RH:117:PRO:HD3	2.01	0.41
32:XA:1446:A:HO2'	32:XA:1447:G:P	2.44	0.41
32:XA:243:A:H4'	32:XA:244:U:H3'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:406:G:H5''	35:XD:5:ILE:HG12	2.02	0.41
40:XI:21:PRO:HA	40:XI:59:PHE:HD1	1.86	0.41
41:XJ:69:ASN:HA	41:XJ:69:ASN:HD22	1.68	0.41
43:XL:77:LEU:HD21	43:XL:107:ALA:HB2	2.03	0.41
43:XL:53:ARG:HH12	43:XL:92:ASP:HB2	1.86	0.41
1:YA:1883:G:HO2'	1:YA:1884:A:H8	1.67	0.41
1:YA:2544:G:H1'	1:YA:2646:C:H4'	2.03	0.41
1:YA:776:G:N7	1:YA:793:A:O2'	2.53	0.41
2:YB:13:A:O2'	2:YB:15:A:O5'	2.39	0.41
6:YG:114:ILE:HG13	6:YG:115:ARG:H	1.85	0.41
1:YA:1006:C:O2'	9:YN:106:MET:O	2.25	0.41
9:YN:128:HIS:O	9:YN:131:GLN:NE2	2.53	0.41
11:YP:71:VAL:HG22	11:YP:72:PRO:HA	2.01	0.41
32:QA:1411:C:H2'	32:QA:1412:C:C6	2.56	0.41
32:QA:25:C:H2'	32:QA:26:A:H8	1.86	0.41
1:RA:2389:G:H5''	1:RA:2390:U:O4'	2.21	0.41
1:RA:2699:C:H2'	1:RA:2700:C:O4'	2.21	0.41
1:RA:2820:A:OP1	13:RR:2:ARG:NH2	2.54	0.41
1:RA:451:C:H41	1:RA:454:A:H5'	1.86	0.41
6:RG:59:GLU:OE2	6:RG:153:ARG:NH1	2.53	0.41
21:RZ:53:ILE:HG22	21:RZ:71:VAL:HG13	2.02	0.41
32:XA:1510:U:H2'	32:XA:1511:G:C8	2.56	0.41
32:XA:272:C:H2'	32:XA:273:A:C8	2.52	0.41
32:XA:279:A:OP1	32:XA:280:C:O2'	2.24	0.41
32:XA:631:G:O2'	32:XA:632:A:O4'	2.31	0.41
35:XD:71:SER:O	35:XD:75:PHE:N	2.50	0.41
44:XM:87:TYR:OH	44:XM:91:ARG:NH2	2.48	0.41
51:XT:89:ARG:HH21	51:XT:104:LEU:HD21	1.85	0.41
1:YA:2698:U:H2'	1:YA:2699:C:C6	2.55	0.41
1:YA:2699:C:H2'	1:YA:2700:C:O4'	2.21	0.41
4:YE:51:PHE:CD2	4:YE:52:LEU:HG	2.56	0.41
8:YI:88:ILE:HG12	8:YI:122:GLU:H	1.86	0.41
32:QA:352:C:O2'	32:QA:354:G:OP1	2.29	0.41
32:QA:358:U:H2'	32:QA:359:U:H6	1.86	0.41
32:QA:384:G:H2'	32:QA:385:C:C6	2.56	0.41
32:QA:709:G:H2'	32:QA:710:G:H8	1.86	0.41
34:QC:189:ALA:HB3	34:QC:196:LEU:HB2	2.03	0.41
35:QD:20:TYR:CE2	37:XF:15:ASP:CA	3.04	0.41
32:QA:1326:C:OP2	52:QU:6:ARG:NH1	2.54	0.41
1:RA:177:G:H3'	1:RA:178:G:H8	1.86	0.41
1:RA:2731:G:OP1	4:RE:169:ASN:ND2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2803:C:H2'	1:RA:2804:C:C6	2.56	0.41
19:RX:34:ALA:O	19:RX:77:LYS:NZ	2.46	0.41
32:XA:1067:A:N1	32:XA:1108:G:O2'	2.46	0.41
32:XA:1159:U:O2'	32:XA:1160:G:N7	2.51	0.41
32:XA:1367:C:OP1	40:XI:115:GLY:N	2.40	0.41
32:XA:1511:G:H2'	32:XA:1512:U:O4'	2.20	0.41
32:XA:842:C:H5'	32:XA:843:U:OP1	2.21	0.41
33:XB:216:SER:OG	33:XB:217:ARG:N	2.54	0.41
1:YA:1062:G:N2	1:YA:1077:A:N1	2.69	0.41
1:YA:1639:U:C2'	1:YA:1640:C:H5''	2.51	0.41
1:YA:2424:C:O2	1:YA:2429:G:O2'	2.31	0.41
1:YA:2867:G:O2'	1:YA:2868:A:P	2.79	0.41
32:QA:1154:G:H2'	32:QA:1155:G:H8	1.86	0.40
32:QA:1342:C:H2'	32:QA:1343:G:H8	1.87	0.40
32:QA:57:G:H2'	32:QA:58:C:C6	2.56	0.40
32:QA:636:U:H2'	32:QA:637:G:C8	2.55	0.40
36:QE:127:ASN:HA	36:QE:128:PRO:HD3	1.93	0.40
32:QA:1220:G:H1'	50:QS:52:TYR:HD2	1.86	0.40
1:RA:1224:G:N2	1:RA:1227:A:OP2	2.52	0.40
1:RA:1638:C:H2'	1:RA:1639:U:O4'	2.21	0.40
1:RA:1786:A:N3	1:RA:1786:A:H2'	2.35	0.40
1:RA:582:G:OP1	16:RU:14:HIS:ND1	2.49	0.40
1:RA:764:A:H5''	3:RD:210:GLY:CA	2.51	0.40
3:RD:177:LEU:HA	3:RD:177:LEU:HD23	1.83	0.40
7:RH:107:VAL:O	7:RH:153:LYS:NZ	2.49	0.40
14:RS:27:SER:HA	14:RS:88:ASP:HB3	2.02	0.40
1:RA:1188:U:H5'	17:RV:79:VAL:HG13	2.02	0.40
32:XA:1191:A:OP1	34:XC:3:ASN:HB3	2.21	0.40
32:XA:1348:U:N3	32:XA:1374:A:H2	2.20	0.40
32:XA:781:A:H4'	32:XA:1522:U:O2'	2.20	0.40
32:XA:538:G:H2'	32:XA:539:A:C8	2.56	0.40
32:XA:998:G:H2'	32:XA:998(A):C:C6	2.57	0.40
32:XA:939:G:H4'	38:XG:102:ARG:NH2	2.36	0.40
1:YA:1348:G:H2'	1:YA:1349:A:H5''	2.03	0.40
1:YA:1818:U:H2'	3:YD:157:ARG:HB2	2.02	0.40
1:YA:2287:A:O2'	1:YA:2288:A:O5'	2.38	0.40
1:YA:924:C:H2'	1:YA:925:C:H6	1.86	0.40
4:YE:36:ARG:HH12	4:YE:86:PRO:HD2	1.86	0.40
8:YI:130:TYR:HB3	8:YI:136:VAL:HG22	2.03	0.40
11:YP:33:ARG:HD3	11:YP:40:SER:HA	2.03	0.40
32:QA:1217:C:H2'	32:QA:1218:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:553:A:H2'	32:QA:554:C:C6	2.56	0.40
32:QA:616:G:OP1	35:QD:141:ARG:NH1	2.54	0.40
47:QP:14:ASN:OD1	47:QP:16:HIS:NE2	2.55	0.40
1:RA:1266:G:O5'	18:RW:15:ARG:NH2	2.54	0.40
1:RA:1542:G:H5''	1:RA:1543:A:OP2	2.21	0.40
1:RA:1593:G:H2'	1:RA:1594:G:H8	1.85	0.40
1:RA:2702:U:HO2'	1:RA:2703:C:H6	1.65	0.40
1:RA:36:G:N3	1:RA:450:G:O2'	2.52	0.40
3:RD:95:LEU:HD11	3:RD:105:ILE:HG12	2.04	0.40
4:RE:52:LEU:HD23	4:RE:52:LEU:HA	1.92	0.40
10:RO:70:LYS:HB3	10:RO:70:LYS:HE3	1.76	0.40
12:RQ:42:ILE:HD12	12:RQ:97:VAL:HG21	2.04	0.40
17:RV:97:LYS:HD3	17:RV:97:LYS:HA	1.81	0.40
32:XA:407:G:H2'	32:XA:408:A:C8	2.55	0.40
32:XA:743:U:H2'	32:XA:744:C:C6	2.56	0.40
36:XE:145:LYS:HA	36:XE:148:VAL:HG22	2.03	0.40
38:XG:36:LYS:O	38:XG:40:ALA:N	2.44	0.40
46:XO:85:LEU:HD23	46:XO:85:LEU:HA	1.89	0.40
48:XQ:45:HIS:NE2	48:XQ:47:PRO:HG3	2.37	0.40
51:XT:61:SER:O	51:XT:65:LYS:HG3	2.22	0.40
25:Y3:8:LEU:HD21	25:Y3:23:LEU:HD21	2.04	0.40
28:Y6:35:GLU:OE2	28:Y6:50:ARG:NH2	2.55	0.40
1:YA:129:C:OP1	1:YA:1599:C:O2'	2.39	0.40
1:YA:1429:G:H2'	1:YA:1430:C:H6	1.85	0.40
1:YA:184:C:H2'	1:YA:185:U:C6	2.56	0.40
1:YA:221:A:H4'	1:YA:222:A:O5'	2.20	0.40
1:YA:270(U):C:H2'	1:YA:270(V):G:H8	1.86	0.40
1:YA:2832:U:O2'	1:YA:2833:G:P	2.79	0.40
6:YG:102:PHE:HE1	6:YG:141:PHE:HE2	1.69	0.40
6:YG:11:TYR:HA	6:YG:15:VAL:HB	2.03	0.40
32:QA:128:G:O2'	48:QQ:3:LYS:NZ	2.54	0.40
32:QA:1305:G:O2'	32:QA:1306:A:O4'	2.40	0.40
32:QA:288:A:H2'	32:QA:289:G:H4'	2.02	0.40
32:QA:384:G:H2'	32:QA:385:C:H6	1.86	0.40
32:QA:478:A:H2'	32:QA:479:C:H6	1.86	0.40
32:QA:940:C:H2'	32:QA:941:G:H8	1.86	0.40
43:QL:24:VAL:HG13	43:QL:98:TYR:HE1	1.86	0.40
44:QM:91:ARG:HH21	44:QM:97:PRO:HD2	1.85	0.40
47:QP:1:MET:HG3	47:QP:65:GLN:HB2	2.03	0.40
32:QA:1505:G:H2'	54:QX:16:C:OP2	2.21	0.40
1:RA:2361:A:O5'	30:R8:27:THR:OG1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2334:G:O6	22:R0:74:ARG:NH2	2.51	0.40
1:RA:2723:C:P	4:RE:109:LYS:HZ3	2.44	0.40
1:RA:2760:C:H2'	1:RA:2761:G:H5''	2.03	0.40
1:RA:2847:U:H2'	1:RA:2847:U:O2	2.22	0.40
1:RA:297:C:H2'	1:RA:298:G:O4'	2.22	0.40
1:RA:587:C:O2'	11:RP:19:VAL:HG22	2.21	0.40
13:RR:67:LEU:HD13	13:RR:76:VAL:HG21	2.03	0.40
1:RA:1252:G:N2	16:RU:37:GLU:OE2	2.39	0.40
19:RX:8:ILE:HD11	19:RX:42:ALA:HB1	2.03	0.40
32:XA:1133:G:H2'	32:XA:1134:G:C8	2.56	0.40
32:XA:1134:G:H2'	32:XA:1135:U:O4'	2.20	0.40
32:XA:151:A:H62	32:XA:170:U:H3	1.68	0.40
32:XA:1532:U:H1'	32:XA:1533:C:C5	2.56	0.40
33:XB:223:ILE:HA	33:XB:226:ARG:HB2	2.03	0.40
32:XA:976:G:P	45:XN:32:SER:H	2.44	0.40
49:XR:86:VAL:HG12	49:XR:87:ARG:HG2	2.04	0.40
25:Y3:12:PRO:HB2	25:Y3:20:LYS:HG2	2.04	0.40
1:YA:724:U:H2'	1:YA:725:G:O4'	2.22	0.40
1:YA:676:A:H2	1:YA:802:A:H61	1.68	0.40
5:YF:51:THR:HG23	5:YF:92:PRO:HD2	2.04	0.40
12:YQ:64:ILE:HG13	21:YZ:178:GLU:HG3	2.01	0.40
32:QA:323:U:H2'	32:QA:324:G:O4'	2.21	0.40
38:QG:60:LYS:HA	38:QG:63:LYS:HG2	2.04	0.40
41:QJ:12:ASP:HB3	41:QJ:15:THR:HG22	2.02	0.40
43:QL:93:LEU:HA	43:QL:94:PRO:HD3	1.94	0.40
45:QN:2:ALA:HB1	45:QN:6:LEU:HD21	2.04	0.40
1:RA:2798:C:H2'	1:RA:2799:A:N7	2.37	0.40
1:RA:345:A:H5''	1:RA:346:A:OP1	2.22	0.40
1:RA:690:G:H2'	1:RA:691:C:C6	2.56	0.40
1:RA:893:C:H2'	1:RA:894:C:H6	1.87	0.40
4:RE:14:ILE:HG13	4:RE:21:VAL:HG13	2.03	0.40
6:RG:173:LEU:O	6:RG:177:GLY:N	2.53	0.40
15:RT:110:ILE:HG21	15:RT:110:ILE:HD13	1.92	0.40
21:RZ:4:ARG:HA	21:RZ:59:LEU:H	1.86	0.40
32:XA:1220:G:H2'	32:XA:1221:G:H8	1.86	0.40
32:XA:337:C:H2'	32:XA:338:A:H8	1.86	0.40
32:XA:489:C:H2'	32:XA:490:G:H8	1.86	0.40
32:XA:950:U:H2'	32:XA:951:G:H8	1.84	0.40
33:XB:217:ARG:HA	33:XB:220:ASP:HB2	2.02	0.40
47:XP:8:ARG:HA	47:XP:17:TYR:HD1	1.86	0.40
50:XS:10:PHE:HE2	50:XS:16:LEU:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1222:G:H5''	50:XS:78:ARG:HH11	1.87	0.40
25:Y3:30:ARG:HH21	25:Y3:33:GLN:NE2	2.20	0.40
1:YA:1657:C:H4'	4:YE:133:LYS:HB3	2.04	0.40
1:YA:180:G:N2	1:YA:215:G:O6	2.53	0.40
1:YA:2712:U:O2'	1:YA:2712(A):A:C8	2.64	0.40
4:YE:181:LEU:HD21	15:YT:6:LEU:HG	2.04	0.40
1:YA:2788:C:P	4:YE:61:ARG:HH21	2.45	0.40
5:YF:78:ILE:HG13	5:YF:78:ILE:H	1.71	0.40
7:YH:3:ARG:HD3	7:YH:6:ARG:HG2	2.02	0.40
15:YT:16:ARG:NH1	15:YT:18:ASP:OD2	2.54	0.40
19:YX:31:HIS:HA	19:YX:32:PRO:HD3	1.93	0.40
32:QA:1007:C:H2'	32:QA:1008:C:C6	2.57	0.40
32:QA:1293:G:H2'	32:QA:1294:G:H8	1.85	0.40
32:QA:1524:C:H2'	32:QA:1525:G:C8	2.56	0.40
32:QA:510:A:N3	32:QA:543:C:H1'	2.36	0.40
32:QA:707:C:H1'	42:QK:39:PRO:HG3	2.03	0.40
33:QB:189:ASP:OD1	33:QB:189:ASP:N	2.54	0.40
37:QF:82:ARG:HB2	37:QF:85:VAL:HG23	2.04	0.40
52:QU:6:ARG:HH21	52:QU:15:ARG:HE	1.69	0.40
1:RA:1368:G:OP1	29:R7:28:ARG:NH2	2.55	0.40
1:RA:172:C:H2'	1:RA:173:G:C8	2.56	0.40
1:RA:1796:U:H2'	1:RA:1797:C:H6	1.87	0.40
1:RA:1858:G:HO2'	1:RA:1859:A:H8	1.68	0.40
1:RA:530:G:C5	1:RA:2022:U:H5''	2.57	0.40
1:RA:2059:A:H5'	1:RA:2060:A:OP2	2.21	0.40
1:RA:2712:U:H1'	1:RA:2712(A):A:C8	2.57	0.40
1:RA:2836:U:H2'	1:RA:2837:G:C8	2.57	0.40
1:RA:307:G:H21	1:RA:330:A:H62	1.70	0.40
4:RE:2:LYS:HD3	4:RE:95:ILE:HB	2.03	0.40
5:RF:154:VAL:HG22	5:RF:191:ARG:HB3	2.03	0.40
7:RH:87:LEU:HD22	7:RH:162:ILE:HG22	2.04	0.40
8:RI:72:LEU:HD13	8:RI:107:VAL:HG11	2.03	0.40
11:RP:121:LYS:HB3	11:RP:123:LEU:HD22	2.03	0.40
21:RZ:54:HIS:ND1	21:RZ:101:PRO:HG3	2.37	0.40
32:XA:1410:G:H2'	32:XA:1411:C:C6	2.56	0.40
32:XA:191(B):G:H2'	32:XA:191(C):G:C8	2.57	0.40
32:XA:524:G:H2'	32:XA:525:C:C6	2.56	0.40
32:XA:704:A:H8	32:XA:704:A:OP2	2.04	0.40
34:XC:44:GLU:HB3	34:XC:52:LEU:HD11	2.03	0.40
38:XG:67:GLU:HA	38:XG:70:LYS:HB2	2.03	0.40
39:XH:109:ILE:HD11	39:XH:120:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1113:U:H2'	1:YA:1114:G:H8	1.86	0.40
1:YA:1590:U:H2'	1:YA:1591:G:H8	1.86	0.40
1:YA:1939:U:OP1	1:YA:2604:U:O2'	2.34	0.40
11:YP:101:VAL:HB	11:YP:106:LEU:HB3	2.04	0.40
11:YP:46:LYS:HD2	11:YP:46:LYS:HA	1.91	0.40
1:YA:2484:G:O2'	12:YQ:124:LYS:O	2.33	0.40
18:YW:10:VAL:HG12	18:YW:12:ILE:HG22	2.02	0.40
19:YX:43:VAL:HG13	19:YX:47:PHE:HD2	1.86	0.40
1:YA:336:C:HO2'	20:YY:35:TYR:HH	1.56	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:307:G:O6	24:Y2:71:ASN:O[3_555]	1.47	0.73
7:YH:46:GLU:CB	20:YY:22:GLY:O[4_445]	1.82	0.38
8:RI:82:ARG:NH1	32:XA:56:U:O2'[4_555]	2.05	0.15
8:RI:91:SER:OG	32:XA:368:U:OP1[4_555]	2.07	0.13
18:RW:63:ASP:OD1	20:YY:92:ASN:ND2[3_555]	2.08	0.12

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
3	YD	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
4	RE	202/206 (98%)	190 (94%)	12 (6%)	0	100	100
4	YE	203/206 (98%)	170 (84%)	32 (16%)	1 (0%)	29	61
5	RF	200/210 (95%)	191 (96%)	9 (4%)	0	100	100
5	YF	200/210 (95%)	182 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	RG	179/182 (98%)	153 (86%)	25 (14%)	1 (1%)	25	57
6	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	57
7	RH	172/180 (96%)	149 (87%)	21 (12%)	2 (1%)	13	41
7	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
8	RI	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	22	55
8	YI	144/148 (97%)	122 (85%)	22 (15%)	0	100	100
9	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
9	YN	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	22	55
10	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	RP	146/150 (97%)	122 (84%)	24 (16%)	0	100	100
11	YP	145/150 (97%)	129 (89%)	15 (10%)	1 (1%)	22	55
12	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	22	55
12	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	RR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
13	YR	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
14	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
14	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
15	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
15	YT	135/146 (92%)	127 (94%)	8 (6%)	0	100	100
16	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	49
16	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	49
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	46
18	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
18	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
19	YX	92/96 (96%)	84 (91%)	8 (9%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	RZ	201/206 (98%)	180 (90%)	20 (10%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	YZ	199/206 (97%)	188 (94%)	9 (4%)	2 (1%)	15	46
22	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
22	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100
23	Y1	91/98 (93%)	91 (100%)	0	0	100	100
24	R2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
24	Y2	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
25	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
26	Y4	67/71 (94%)	58 (87%)	9 (13%)	0	100	100
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	45/49 (92%)	45 (100%)	0	0	100	100
29	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	R8	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
30	Y8	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
31	R9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
31	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	QB	233/256 (91%)	201 (86%)	32 (14%)	0	100	100
33	XB	234/256 (91%)	205 (88%)	29 (12%)	0	100	100
34	QC	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
34	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
35	QD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	46
35	XD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	46
36	QE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	XE	149/162 (92%)	135 (91%)	14 (9%)	0	100	100
37	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
37	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	QG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	XG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
39	QH	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
40	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
41	QJ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
41	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
42	QK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
42	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
43	QL	123/132 (93%)	108 (88%)	15 (12%)	0	100	100
43	XL	120/132 (91%)	106 (88%)	14 (12%)	0	100	100
44	QM	118/126 (94%)	104 (88%)	13 (11%)	1 (1%)	19	51
44	XM	117/126 (93%)	105 (90%)	10 (8%)	2 (2%)	9	34
45	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
47	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	XP	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
48	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
48	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
49	QR	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
49	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
50	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	XS	82/93 (88%)	68 (83%)	13 (16%)	1 (1%)	13	41
51	QT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
51	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
52	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
52	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	11486/12128 (95%)	10518 (92%)	945 (8%)	23 (0%)	47	78

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	YV	49	THR
35	XD	32	ALA
21	YZ	52	SER
16	RU	93	LYS
35	QD	32	ALA
35	XD	20	TYR
44	XM	5	ALA
6	RG	81	LYS
21	RZ	53	ILE
44	QM	106	ASN
6	YG	81	LYS
16	YU	93	LYS
7	RH	86	GLU
8	RI	118	LYS
12	RQ	78	PRO
35	QD	33	MET
9	YN	22	THR
21	YZ	183	LEU
50	XS	30	LEU
7	RH	55	PRO
11	YP	7	ARG
4	YE	116	VAL
44	XM	9	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	214 (100%)	0	100	100
3	YD	215/218 (99%)	213 (99%)	2 (1%)	78	90
4	RE	165/166 (99%)	163 (99%)	2 (1%)	71	85
4	YE	165/166 (99%)	164 (99%)	1 (1%)	86	94
5	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
5	YF	161/166 (97%)	159 (99%)	2 (1%)	71	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
6	YG	155/156 (99%)	153 (99%)	2 (1%)	69	84
7	RH	145/148 (98%)	145 (100%)	0	100	100
7	YH	145/148 (98%)	143 (99%)	2 (1%)	67	83
8	RI	122/124 (98%)	109 (89%)	13 (11%)	6	24
8	YI	122/124 (98%)	121 (99%)	1 (1%)	81	91
9	RN	117/119 (98%)	116 (99%)	1 (1%)	78	90
9	YN	119/119 (100%)	118 (99%)	1 (1%)	81	91
10	RO	100/100 (100%)	100 (100%)	0	100	100
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	113 (98%)	2 (2%)	60	80
11	YP	114/116 (98%)	113 (99%)	1 (1%)	78	90
12	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	63
12	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	79
13	RR	101/101 (100%)	101 (100%)	0	100	100
13	YR	100/101 (99%)	100 (100%)	0	100	100
14	RS	87/88 (99%)	87 (100%)	0	100	100
14	YS	87/88 (99%)	87 (100%)	0	100	100
15	RT	120/127 (94%)	119 (99%)	1 (1%)	81	91
15	YT	120/127 (94%)	120 (100%)	0	100	100
16	RU	93/94 (99%)	93 (100%)	0	100	100
16	YU	93/94 (99%)	92 (99%)	1 (1%)	73	86
17	RV	82/82 (100%)	81 (99%)	1 (1%)	71	85
17	YV	82/82 (100%)	82 (100%)	0	100	100
18	RW	92/92 (100%)	92 (100%)	0	100	100
18	YW	92/92 (100%)	92 (100%)	0	100	100
19	RX	74/78 (95%)	73 (99%)	1 (1%)	67	83
19	YX	76/78 (97%)	73 (96%)	3 (4%)	32	61
20	RY	88/91 (97%)	88 (100%)	0	100	100
20	YY	88/91 (97%)	87 (99%)	1 (1%)	73	86
21	RZ	174/179 (97%)	169 (97%)	5 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	YZ	173/179 (97%)	171 (99%)	2 (1%)	71	85
22	R0	61/67 (91%)	60 (98%)	1 (2%)	62	81
22	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	81
23	R1	82/83 (99%)	82 (100%)	0	100	100
23	Y1	78/83 (94%)	78 (100%)	0	100	100
24	R2	64/67 (96%)	64 (100%)	0	100	100
24	Y2	67/67 (100%)	67 (100%)	0	100	100
25	R3	51/52 (98%)	49 (96%)	2 (4%)	32	61
25	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	77
26	R4	62/63 (98%)	60 (97%)	2 (3%)	39	67
26	Y4	62/63 (98%)	62 (100%)	0	100	100
27	R5	51/52 (98%)	51 (100%)	0	100	100
27	Y5	51/52 (98%)	51 (100%)	0	100	100
28	R6	51/52 (98%)	51 (100%)	0	100	100
28	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	61
29	R7	40/42 (95%)	40 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	53 (98%)	1 (2%)	57	78
30	Y8	54/55 (98%)	54 (100%)	0	100	100
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	203/220 (92%)	201 (99%)	2 (1%)	76	88
33	XB	204/220 (93%)	204 (100%)	0	100	100
34	QC	159/188 (85%)	159 (100%)	0	100	100
34	XC	159/188 (85%)	157 (99%)	2 (1%)	69	84
35	QD	180/181 (99%)	178 (99%)	2 (1%)	73	86
35	XD	180/181 (99%)	173 (96%)	7 (4%)	32	61
36	QE	116/123 (94%)	113 (97%)	3 (3%)	46	72
36	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
37	QF	90/90 (100%)	90 (100%)	0	100	100
37	XF	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	QG	126/127 (99%)	124 (98%)	2 (2%)	62	81
38	XG	126/127 (99%)	124 (98%)	2 (2%)	62	81
39	QH	118/119 (99%)	118 (100%)	0	100	100
39	XH	118/119 (99%)	118 (100%)	0	100	100
40	QI	98/99 (99%)	97 (99%)	1 (1%)	76	88
40	XI	97/99 (98%)	97 (100%)	0	100	100
41	QJ	89/92 (97%)	86 (97%)	3 (3%)	37	65
41	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	85
42	QK	88/99 (89%)	87 (99%)	1 (1%)	73	86
42	XK	88/99 (89%)	88 (100%)	0	100	100
43	QL	104/109 (95%)	104 (100%)	0	100	100
43	XL	103/109 (94%)	103 (100%)	0	100	100
44	QM	96/101 (95%)	93 (97%)	3 (3%)	40	68
44	XM	95/101 (94%)	92 (97%)	3 (3%)	39	67
45	QN	49/50 (98%)	49 (100%)	0	100	100
45	XN	49/50 (98%)	49 (100%)	0	100	100
46	QO	79/80 (99%)	78 (99%)	1 (1%)	69	84
46	XO	79/80 (99%)	79 (100%)	0	100	100
47	QP	72/74 (97%)	70 (97%)	2 (3%)	43	70
47	XP	72/74 (97%)	70 (97%)	2 (3%)	43	70
48	QQ	95/97 (98%)	95 (100%)	0	100	100
48	XQ	95/97 (98%)	95 (100%)	0	100	100
49	QR	61/77 (79%)	61 (100%)	0	100	100
49	XR	61/77 (79%)	61 (100%)	0	100	100
50	QS	72/80 (90%)	72 (100%)	0	100	100
50	XS	73/80 (91%)	71 (97%)	2 (3%)	44	70
51	QT	76/82 (93%)	76 (100%)	0	100	100
51	XT	76/82 (93%)	76 (100%)	0	100	100
52	QU	20/22 (91%)	18 (90%)	2 (10%)	7	27
52	XU	20/22 (91%)	20 (100%)	0	100	100
All	All	9712/10066 (96%)	9607 (99%)	105 (1%)	73	86

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	RE	21	VAL
4	RE	159	HIS
5	RF	204	ASN
6	RG	172	LEU
8	RI	77	LEU
8	RI	85	GLU
8	RI	86	THR
8	RI	91	SER
8	RI	96	ASP
8	RI	97	ILE
8	RI	103	ARG
8	RI	117	GLU
8	RI	118	LYS
8	RI	120	ILE
8	RI	121	LYS
8	RI	123	LEU
8	RI	138	ILE
9	RN	137	LYS
11	RP	29	LYS
11	RP	70	GLN
12	RQ	21	THR
12	RQ	58	PHE
12	RQ	60	ARG
12	RQ	83	MET
15	RT	62	THR
17	RV	7	THR
19	RX	66	LEU
21	RZ	9	TYR
21	RZ	156	LYS
21	RZ	180	VAL
21	RZ	182	LYS
21	RZ	185	GLU
22	R0	14	ARG
25	R3	30	ARG
25	R3	36	VAL
26	R4	40	HIS
26	R4	51	ASP
30	R8	61	LEU
33	QB	21	ARG
33	QB	230	VAL
35	QD	31	CYS
35	QD	33	MET

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Mol	Chain	Res	Type
36	QE	24	ARG
36	QE	51	VAL
36	QE	63	ARG
38	QG	36	LYS
38	QG	94	ARG
40	QI	53	VAL
41	QJ	29	ARG
41	QJ	42	THR
41	QJ	58	ASP
42	QK	33	THR
44	QM	7	VAL
44	QM	45	VAL
44	QM	86	CYS
46	QO	79	ARG
47	QP	1	MET
47	QP	67	THR
52	QU	8	THR
52	QU	24	ARG
3	YD	273	ARG
3	YD	274	ARG
4	YE	201	THR
5	YF	46	ARG
5	YF	183	VAL
6	YG	33	ARG
6	YG	117	PHE
7	YH	2	SER
7	YH	3	ARG
8	YI	118	LYS
9	YN	120	LEU
11	YP	71	VAL
12	YQ	21	THR
12	YQ	59	ARG
16	YU	91	ASP
19	YX	27	THR
19	YX	57	LEU
19	YX	59	VAL
20	YY	23	ARG
21	YZ	1	MET
21	YZ	183	LEU
22	Y0	14	ARG
25	Y3	30	ARG
28	Y6	9	LEU

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Mol	Chain	Res	Type
28	Y6	52	VAL
34	XC	11	ARG
34	XC	126	ARG
35	XD	8	VAL
35	XD	18	LYS
35	XD	19	LEU
35	XD	21	LEU
35	XD	22	LYS
35	XD	33	MET
35	XD	159	ARG
36	XE	116	THR
38	XG	37	ASN
38	XG	94	ARG
41	XJ	66	ARG
44	XM	3	ARG
44	XM	7	VAL
44	XM	59	TYR
47	XP	1	MET
47	XP	67	THR
50	XS	11	VAL
50	XS	78	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
4	RE	48	GLN
5	RF	40	GLN
21	RZ	34	ASN
24	R2	46	GLN
24	R2	47	ASN
26	R4	6	HIS
30	R8	31	HIS
41	QJ	69	ASN
6	YG	40	ASN
36	XE	127	ASN
39	XH	78	GLN
50	XS	53	ASN
50	XS	83	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2877/2915 (98%)	581 (20%)	41 (1%)
1	YA	2880/2915 (98%)	558 (19%)	40 (1%)
2	RB	119/122 (97%)	19 (15%)	1 (0%)
2	YB	119/122 (97%)	23 (19%)	2 (1%)
32	QA	1510/1521 (99%)	292 (19%)	37 (2%)
32	XA	1509/1521 (99%)	277 (18%)	29 (1%)
53	QV	16/17 (94%)	1 (6%)	0
53	XV	14/17 (82%)	0	0
54	QX	17/19 (89%)	5 (29%)	1 (5%)
54	XX	18/19 (94%)	9 (50%)	1 (5%)
All	All	9079/9188 (98%)	1765 (19%)	152 (1%)

All (1765) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	9	U
1	RA	15	G
1	RA	34	C
1	RA	35	G
1	RA	46	C
1	RA	51	G
1	RA	55	G
1	RA	63	U
1	RA	72	U
1	RA	73	A
1	RA	74	A
1	RA	75	G
1	RA	82	G
1	RA	83	G
1	RA	90	U
1	RA	95	G
1	RA	101	G
1	RA	103	A
1	RA	118	A
1	RA	120	U
1	RA	131	G
1	RA	140	A
1	RA	177	G
1	RA	181	A
1	RA	196	A
1	RA	199	A
1	RA	214	G
1	RA	215	G

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Mol	Chain	Res	Type
1	RA	216	A
1	RA	221	A
1	RA	222	A
1	RA	223	A
1	RA	229	A
1	RA	230	U
1	RA	248	G
1	RA	249	C
1	RA	252	G
1	RA	265	A
1	RA	266	G
1	RA	269	U
1	RA	270(L)	U
1	RA	270(M)	U
1	RA	270(N)	G
1	RA	270(P)	C
1	RA	271(C)	U
1	RA	273(F)	C
1	RA	275	G
1	RA	276	A
1	RA	277	C
1	RA	299	A
1	RA	311	A
1	RA	316	C
1	RA	323	G
1	RA	324	A
1	RA	329	G
1	RA	330	A
1	RA	342	G
1	RA	346	A
1	RA	352	G
1	RA	363(F)	A
1	RA	364	C
1	RA	371	A
1	RA	372	G
1	RA	373	U
1	RA	386	G
1	RA	395	U
1	RA	405	U
1	RA	411	G
1	RA	412	A
1	RA	428	A

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Mol	Chain	Res	Type
1	RA	435	C
1	RA	444	C
1	RA	448	U
1	RA	454	A
1	RA	455	C
1	RA	456	C
1	RA	457	A
1	RA	458	G
1	RA	470	A
1	RA	481	G
1	RA	501	A
1	RA	503	A
1	RA	504	U
1	RA	505	A
1	RA	509	C
1	RA	513	A
1	RA	528	A
1	RA	529	A
1	RA	530	G
1	RA	531	C
1	RA	532	A
1	RA	533	G
1	RA	537	C
1	RA	539	G
1	RA	540	G
1	RA	546	C
1	RA	547	A
1	RA	556	G
1	RA	563	G
1	RA	573	G
1	RA	574	C
1	RA	575	A
1	RA	583	G
1	RA	588	U
1	RA	603	A
1	RA	607	U
1	RA	614	U
1	RA	615	G
1	RA	616	A
1	RA	617	G
1	RA	626	U
1	RA	627	A

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Mol	Chain	Res	Type
1	RA	631	A
1	RA	637	A
1	RA	638	G
1	RA	645	C
1	RA	646	A
1	RA	647	G
1	RA	650	C
1	RA	651	G
1	RA	652	C
1	RA	654	A
1	RA	654(A)	G
1	RA	669	G
1	RA	670	A
1	RA	686	G
1	RA	702	G
1	RA	717	G
1	RA	722	A
1	RA	726	G
1	RA	730	C
1	RA	752	A
1	RA	753	C
1	RA	765	G
1	RA	776	G
1	RA	782	A
1	RA	783	A
1	RA	784	A
1	RA	785	G
1	RA	790	C
1	RA	791	C
1	RA	792	G
1	RA	805	G
1	RA	812	C
1	RA	819	A
1	RA	827	U
1	RA	828	U
1	RA	830	G
1	RA	831	G
1	RA	846	C
1	RA	847	U
1	RA	856	C
1	RA	857	C
1	RA	859	G

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Mol	Chain	Res	Type
1	RA	866	A
1	RA	869	G
1	RA	882	G
1	RA	884	C
1	RA	885	C
1	RA	886	C
1	RA	888	C
1	RA	889	C
1	RA	896	A
1	RA	897	C
1	RA	900	A
1	RA	901	A
1	RA	907	U
1	RA	910	A
1	RA	914	C
1	RA	915	C
1	RA	917	A
1	RA	932	G
1	RA	941	A
1	RA	945	A
1	RA	946	G
1	RA	953	A
1	RA	957	A
1	RA	959	A
1	RA	961	C
1	RA	973	A
1	RA	974	G
1	RA	974(A)	C
1	RA	980	A
1	RA	983	A
1	RA	996	A
1	RA	1003	G
1	RA	1005	C
1	RA	1008	C
1	RA	1012	U
1	RA	1013	C
1	RA	1020	A
1	RA	1022	G
1	RA	1023	U
1	RA	1025	G
1	RA	1026	U
1	RA	1027	A

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Mol	Chain	Res	Type
1	RA	1033	U
1	RA	1042	G
1	RA	1045	A
1	RA	1046	A
1	RA	1047	G
1	RA	1048	A
1	RA	1052	C
1	RA	1054	A
1	RA	1058	G
1	RA	1060	U
1	RA	1063	G
1	RA	1064	C
1	RA	1065	U
1	RA	1066	U
1	RA	1067	A
1	RA	1068	G
1	RA	1069	A
1	RA	1070	A
1	RA	1071	G
1	RA	1073	A
1	RA	1074	G
1	RA	1076	C
1	RA	1078	U
1	RA	1079	C
1	RA	1082	U
1	RA	1083	U
1	RA	1084	A
1	RA	1085	A
1	RA	1086	A
1	RA	1088	A
1	RA	1090	U
1	RA	1091	G
1	RA	1092	C
1	RA	1093	G
1	RA	1094	U
1	RA	1109	C
1	RA	1110	G
1	RA	1111	A
1	RA	1112	G
1	RA	1122	G
1	RA	1129	A
1	RA	1130	U

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Mol	Chain	Res	Type
1	RA	1135	C
1	RA	1136	G
1	RA	1139	G
1	RA	1140	C
1	RA	1142	U
1	RA	1142(A)	A
1	RA	1173	G
1	RA	1174	A
1	RA	1175	U
1	RA	1176	G
1	RA	1178	C
1	RA	1181	C
1	RA	1195	G
1	RA	1204	A
1	RA	1205	U
1	RA	1210	A
1	RA	1211	U
1	RA	1220	A
1	RA	1236	G
1	RA	1238	G
1	RA	1248	G
1	RA	1250	G
1	RA	1253	A
1	RA	1256	G
1	RA	1265	A
1	RA	1272	A
1	RA	1281	G
1	RA	1300	U
1	RA	1301	A
1	RA	1312	U
1	RA	1313	U
1	RA	1314	C
1	RA	1321	A
1	RA	1329	U
1	RA	1349	A
1	RA	1352	U
1	RA	1365	A
1	RA	1370	C
1	RA	1379	A
1	RA	1384	A
1	RA	1385	G
1	RA	1386	C

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Mol	Chain	Res	Type
1	RA	1390	U
1	RA	1391	U
1	RA	1395	A
1	RA	1407	C
1	RA	1408	C
1	RA	1411	C
1	RA	1416	G
1	RA	1419	A
1	RA	1420	U
1	RA	1421	G
1	RA	1428	C
1	RA	1444(A)	A
1	RA	1445	C
1	RA	1449	A
1	RA	1449(A)	G
1	RA	1455	G
1	RA	1460	A
1	RA	1461	G
1	RA	1471	A
1	RA	1480	G
1	RA	1482	U
1	RA	1483	G
1	RA	1487	G
1	RA	1493	C
1	RA	1494	A
1	RA	1495	A
1	RA	1497	U
1	RA	1504	C
1	RA	1505	C
1	RA	1506	C
1	RA	1507	A
1	RA	1508	A
1	RA	1509	C
1	RA	1510	A
1	RA	1511	A
1	RA	1513	C
1	RA	1514	U
1	RA	1515	C
1	RA	1519	G
1	RA	1522	G
1	RA	1533	C
1	RA	1535	U

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Mol	Chain	Res	Type
1	RA	1536	A
1	RA	1537	C
1	RA	1538	G
1	RA	1543	A
1	RA	1544	C
1	RA	1545	A
1	RA	1547	C
1	RA	1558	A
1	RA	1559	G
1	RA	1566	A
1	RA	1569	A
1	RA	1578	U
1	RA	1580	A
1	RA	1586	A
1	RA	1587	A
1	RA	1598	C
1	RA	1599	C
1	RA	1608	A
1	RA	1609	A
1	RA	1616	A
1	RA	1617	C
1	RA	1634	A
1	RA	1640	C
1	RA	1648	C
1	RA	1654	A
1	RA	1667	G
1	RA	1674	G
1	RA	1678	G
1	RA	1725	G
1	RA	1728	G
1	RA	1729	A
1	RA	1730	U
1	RA	1731	G
1	RA	1733	G
1	RA	1742	C
1	RA	1743	G
1	RA	1750	G
1	RA	1756	G
1	RA	1762	A
1	RA	1763	G
1	RA	1764	G
1	RA	1773	A

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Mol	Chain	Res	Type
1	RA	1776	G
1	RA	1780	A
1	RA	1782	C
1	RA	1787	A
1	RA	1791	A
1	RA	1799	G
1	RA	1800	C
1	RA	1801	G
1	RA	1816	G
1	RA	1820	U
1	RA	1829	A
1	RA	1835	G
1	RA	1847	A
1	RA	1848	A
1	RA	1858	G
1	RA	1869	G
1	RA	1870	C
1	RA	1872	A
1	RA	1878	G
1	RA	1882	C
1	RA	1888	G
1	RA	1889	A
1	RA	1900	A
1	RA	1903	G
1	RA	1906	G
1	RA	1909	C
1	RA	1913	A
1	RA	1914	C
1	RA	1929	G
1	RA	1930	G
1	RA	1936	A
1	RA	1939	U
1	RA	1955	U
1	RA	1963	U
1	RA	1967	C
1	RA	1969	A
1	RA	1970	A
1	RA	1971	A
1	RA	1972	A
1	RA	1982	C
1	RA	1991	U
1	RA	1992	G

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Mol	Chain	Res	Type
1	RA	1993	U
1	RA	2020	A
1	RA	2023	G
1	RA	2030	A
1	RA	2031	A
1	RA	2032	G
1	RA	2033	A
1	RA	2043	C
1	RA	2055	C
1	RA	2056	G
1	RA	2059	A
1	RA	2060	A
1	RA	2061	G
1	RA	2062	A
1	RA	2069	G
1	RA	2089	U
1	RA	2093	G
1	RA	2099	U
1	RA	2101	G
1	RA	2107	C
1	RA	2111	C
1	RA	2113	U
1	RA	2114	A
1	RA	2115	G
1	RA	2116	G
1	RA	2117	A
1	RA	2118	U
1	RA	2126	A
1	RA	2127	G
1	RA	2128	C
1	RA	2131	G
1	RA	2132	U
1	RA	2133	G
1	RA	2135	A
1	RA	2141	G
1	RA	2145	C
1	RA	2146	C
1	RA	2147	G
1	RA	2148	G
1	RA	2158	A
1	RA	2160	G
1	RA	2166	G

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Mol	Chain	Res	Type
1	RA	2168	G
1	RA	2169	A
1	RA	2170	A
1	RA	2173	A
1	RA	2181	G
1	RA	2189	U
1	RA	2190	G
1	RA	2191	G
1	RA	2192	G
1	RA	2198	A
1	RA	2210	G
1	RA	2211	G
1	RA	2212	A
1	RA	2215	G
1	RA	2225	A
1	RA	2238	G
1	RA	2239	G
1	RA	2243	U
1	RA	2266	A
1	RA	2275	C
1	RA	2278	A
1	RA	2280	G
1	RA	2283	C
1	RA	2287	A
1	RA	2288	A
1	RA	2305	A
1	RA	2307	G
1	RA	2308	G
1	RA	2309	A
1	RA	2311	A
1	RA	2312	U
1	RA	2320	A
1	RA	2325	G
1	RA	2334	G
1	RA	2336	A
1	RA	2345	G
1	RA	2346	A
1	RA	2347	C
1	RA	2350	C
1	RA	2383	G
1	RA	2385	C
1	RA	2403	C

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Mol	Chain	Res	Type
1	RA	2406	U
1	RA	2424	C
1	RA	2425	A
1	RA	2427	C
1	RA	2429	G
1	RA	2430	A
1	RA	2435	A
1	RA	2439	A
1	RA	2440	C
1	RA	2441	C
1	RA	2448	A
1	RA	2465	C
1	RA	2469	A
1	RA	2473	U
1	RA	2475	C
1	RA	2480	C
1	RA	2482	G
1	RA	2494	G
1	RA	2502	G
1	RA	2505	G
1	RA	2518	A
1	RA	2519	U
1	RA	2529	G
1	RA	2542	A
1	RA	2543	G
1	RA	2554	U
1	RA	2564	A
1	RA	2566	A
1	RA	2567	G
1	RA	2569	G
1	RA	2572	A
1	RA	2573	C
1	RA	2602	A
1	RA	2609	U
1	RA	2611	U
1	RA	2612	C
1	RA	2615	U
1	RA	2623	G
1	RA	2629	A
1	RA	2636	U
1	RA	2641	G
1	RA	2654	A

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Mol	Chain	Res	Type
1	RA	2655	G
1	RA	2665	A
1	RA	2673	G
1	RA	2689	U
1	RA	2690	C
1	RA	2702	U
1	RA	2703	C
1	RA	2707	G
1	RA	2712(A)	A
1	RA	2713	A
1	RA	2714	G
1	RA	2726	U
1	RA	2732	G
1	RA	2733	A
1	RA	2744	G
1	RA	2748	A
1	RA	2751	G
1	RA	2757	A
1	RA	2758	A
1	RA	2761	G
1	RA	2762	G
1	RA	2764	A
1	RA	2765	A
1	RA	2766	G
1	RA	2778	A
1	RA	2779	U
1	RA	2780	G
1	RA	2789	C
1	RA	2790	A
1	RA	2791	C
1	RA	2797	U
1	RA	2798	C
1	RA	2799	A
1	RA	2807	G
1	RA	2813	A
1	RA	2818	G
1	RA	2820	A
1	RA	2821	A
1	RA	2833	G
1	RA	2834	G
1	RA	2847	U
1	RA	2867	G

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Mol	Chain	Res	Type
1	RA	2868	A
1	RA	2872	G
1	RA	2880	C
1	RA	2892	A
1	RA	2894	G
1	RA	2895	U
1	RA	2897	U
2	RB	2	C
2	RB	8	U
2	RB	13	A
2	RB	15	A
2	RB	16	G
2	RB	19	G
2	RB	21	G
2	RB	25	A
2	RB	31	C
2	RB	41	U
2	RB	42	C
2	RB	44	G
2	RB	45	A
2	RB	52	A
2	RB	56	G
2	RB	67	G
2	RB	73	A
2	RB	108	C
2	RB	109	G
32	QA	6	G
32	QA	7	G
32	QA	9	G
32	QA	32	A
32	QA	39	G
32	QA	47	C
32	QA	48	C
32	QA	51	A
32	QA	59	A
32	QA	64	G
32	QA	65	U
32	QA	66	G
32	QA	76	G
32	QA	82	U
32	QA	90	C
32	QA	91	C

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Mol	Chain	Res	Type
32	QA	95	G
32	QA	101	A
32	QA	116	A
32	QA	120	A
32	QA	121	C
32	QA	129(A)	G
32	QA	144	G
32	QA	146	G
32	QA	158	G
32	QA	159	G
32	QA	162	A
32	QA	163	C
32	QA	169	C
32	QA	173	U
32	QA	174	C
32	QA	182	U
32	QA	187	C
32	QA	188	U
32	QA	190	G
32	QA	191(A)	G
32	QA	195	A
32	QA	197	A
32	QA	208	U
32	QA	209	U
32	QA	210	U
32	QA	216	G
32	QA	220	G
32	QA	244	U
32	QA	245	C
32	QA	247	G
32	QA	250	A
32	QA	251	G
32	QA	267	C
32	QA	270	A
32	QA	281	G
32	QA	289	G
32	QA	298	A
32	QA	306	G
32	QA	321	A
32	QA	328	C
32	QA	329	A
32	QA	332	G

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Mol	Chain	Res	Type
32	QA	344	A
32	QA	346	G
32	QA	347	G
32	QA	352	C
32	QA	353	A
32	QA	354	G
32	QA	356	A
32	QA	367	U
32	QA	372	C
32	QA	373	A
32	QA	389	A
32	QA	390	C
32	QA	397	A
32	QA	398	C
32	QA	406	G
32	QA	411	A
32	QA	412	A
32	QA	413	G
32	QA	414	A
32	QA	421	U
32	QA	422	C
32	QA	423	G
32	QA	424	G
32	QA	429	U
32	QA	430	A
32	QA	435	C
32	QA	439	A
32	QA	442	C
32	QA	466	C
32	QA	482	A
32	QA	485	G
32	QA	486	U
32	QA	495	A
32	QA	496	A
32	QA	497	U
32	QA	505	G
32	QA	508	C
32	QA	509	A
32	QA	510	A
32	QA	511	C
32	QA	518	C
32	QA	521	G

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Mol	Chain	Res	Type
32	QA	527	G
32	QA	532	A
32	QA	533	A
32	QA	545	C
32	QA	547	A
32	QA	559	A
32	QA	564	C
32	QA	568	G
32	QA	572	A
32	QA	573	A
32	QA	576	G
32	QA	577	G
32	QA	596	C
32	QA	618	C
32	QA	630	G
32	QA	631	G
32	QA	632	A
32	QA	633	G
32	QA	653	A
32	QA	657	G
32	QA	665	A
32	QA	666	G
32	QA	686	U
32	QA	688	G
32	QA	701	C
32	QA	702	A
32	QA	703	G
32	QA	704	A
32	QA	722	A
32	QA	724	G
32	QA	731	G
32	QA	748	C
32	QA	749	C
32	QA	754	C
32	QA	755	G
32	QA	760	G
32	QA	777	A
32	QA	786	G
32	QA	792	A
32	QA	793	U
32	QA	794	A
32	QA	812	C

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Mol	Chain	Res	Type
32	QA	813	U
32	QA	817	C
32	QA	819	A
32	QA	821	G
32	QA	828	A
32	QA	841	U
32	QA	842	C
32	QA	843	U
32	QA	848	C
32	QA	859	A
32	QA	870	U
32	QA	871	U
32	QA	872	A
32	QA	885	G
32	QA	889	A
32	QA	902	G
32	QA	914	A
32	QA	927	G
32	QA	934	C
32	QA	935	A
32	QA	960	U
32	QA	961	U
32	QA	968	A
32	QA	969	A
32	QA	971	G
32	QA	974	A
32	QA	976	G
32	QA	977	A
32	QA	982	U
32	QA	991	U
32	QA	992	U
32	QA	993	G
32	QA	994	A
32	QA	1004	A
32	QA	1005	A
32	QA	1006	C
32	QA	1008	C
32	QA	1009	G
32	QA	1020	U
32	QA	1024	G
32	QA	1025	U
32	QA	1027	C

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Mol	Chain	Res	Type
32	QA	1029	G
32	QA	1030	C
32	QA	1031	G
32	QA	1032(A)	G
32	QA	1033	G
32	QA	1034	G
32	QA	1042	G
32	QA	1054	C
32	QA	1064	G
32	QA	1065	U
32	QA	1066	C
32	QA	1080	A
32	QA	1081	G
32	QA	1094	G
32	QA	1095	U
32	QA	1101	A
32	QA	1108	G
32	QA	1124	G
32	QA	1125	U
32	QA	1126	U
32	QA	1130	A
32	QA	1131	G
32	QA	1136	U
32	QA	1137	C
32	QA	1138	G
32	QA	1139	G
32	QA	1140	C
32	QA	1146	A
32	QA	1157	A
32	QA	1158	C
32	QA	1159	U
32	QA	1160	G
32	QA	1181	G
32	QA	1183	A
32	QA	1184	G
32	QA	1187	G
32	QA	1190	G
32	QA	1196	U
32	QA	1201	A
32	QA	1202	G
32	QA	1212	U
32	QA	1213	A

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Mol	Chain	Res	Type
32	QA	1215	G
32	QA	1224	G
32	QA	1240	U
32	QA	1241	G
32	QA	1256	A
32	QA	1257	U
32	QA	1258	G
32	QA	1260	C
32	QA	1270	C
32	QA	1279	A
32	QA	1280	A
32	QA	1281	U
32	QA	1286	A
32	QA	1287	A
32	QA	1297	C
32	QA	1298	C
32	QA	1299	A
32	QA	1301	U
32	QA	1302	U
32	QA	1303	C
32	QA	1305	G
32	QA	1317	C
32	QA	1321	C
32	QA	1322	C
32	QA	1323	G
32	QA	1331	G
32	QA	1334	G
32	QA	1335	C
32	QA	1336	C
32	QA	1337	G
32	QA	1347	G
32	QA	1348	U
32	QA	1362(A)	C
32	QA	1370	G
32	QA	1379	G
32	QA	1397	C
32	QA	1398	A
32	QA	1419	G
32	QA	1439	C
32	QA	1442	G
32	QA	1446	A
32	QA	1447	G

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Mol	Chain	Res	Type
32	QA	1452	C
32	QA	1453	G
32	QA	1487	G
32	QA	1492	A
32	QA	1494	G
32	QA	1497	G
32	QA	1499	A
32	QA	1503	A
32	QA	1504	G
32	QA	1506	U
32	QA	1517	G
32	QA	1519	A
32	QA	1520	G
32	QA	1529	G
32	QA	1530	G
32	QA	1531	A
32	QA	1532	U
32	QA	1533	C
32	QA	1534	A
32	QA	1535	C
32	QA	1537	U
32	QA	1538	C
32	QA	1539	C
32	QA	1541	U
53	QV	43	G
54	QX	8	A
54	QX	12	A
54	QX	13	A
54	QX	14	A
54	QX	15	A
1	YA	9	U
1	YA	14	A
1	YA	15	G
1	YA	23	G
1	YA	26	G
1	YA	34	C
1	YA	35	G
1	YA	46	C
1	YA	55	G
1	YA	63	U
1	YA	64	A
1	YA	72	U

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Mol	Chain	Res	Type
1	YA	74	A
1	YA	75	G
1	YA	90	U
1	YA	95	G
1	YA	99	U
1	YA	101	G
1	YA	102	G
1	YA	118	A
1	YA	120	U
1	YA	125	G
1	YA	131	G
1	YA	140	A
1	YA	161	U
1	YA	162	U
1	YA	181	A
1	YA	196	A
1	YA	199	A
1	YA	204	A
1	YA	216	A
1	YA	221	A
1	YA	222	A
1	YA	223	A
1	YA	226	G
1	YA	228	A
1	YA	229	A
1	YA	230	U
1	YA	232	G
1	YA	233	A
1	YA	242	G
1	YA	243	U
1	YA	248	G
1	YA	252	G
1	YA	265	A
1	YA	266	G
1	YA	269	U
1	YA	270(L)	U
1	YA	270(M)	U
1	YA	270(N)	G
1	YA	270(P)	C
1	YA	271(C)	U
1	YA	271(D)	G
1	YA	274	G

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Mol	Chain	Res	Type
1	YA	275	G
1	YA	276	A
1	YA	278	A
1	YA	279	C
1	YA	299	A
1	YA	311	A
1	YA	323	G
1	YA	324	A
1	YA	327	G
1	YA	329	G
1	YA	330	A
1	YA	331	A
1	YA	332	A
1	YA	333	G
1	YA	352	G
1	YA	363(E)	U
1	YA	364	C
1	YA	371	A
1	YA	372	G
1	YA	386	G
1	YA	387	U
1	YA	396	G
1	YA	405	U
1	YA	411	G
1	YA	412	A
1	YA	428	A
1	YA	443	A
1	YA	444	C
1	YA	448	U
1	YA	457	A
1	YA	470	A
1	YA	481	G
1	YA	504	U
1	YA	505	A
1	YA	508	G
1	YA	509	C
1	YA	512	G
1	YA	530	G
1	YA	531	C
1	YA	532	A
1	YA	533	G
1	YA	537	C

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Mol	Chain	Res	Type
1	YA	539	G
1	YA	540	G
1	YA	546	C
1	YA	547	A
1	YA	563	G
1	YA	573	G
1	YA	574	C
1	YA	575	A
1	YA	586	A
1	YA	603	A
1	YA	607	U
1	YA	609(A)	G
1	YA	614	U
1	YA	617	G
1	YA	618	G
1	YA	622	G
1	YA	627	A
1	YA	634	C
1	YA	637	A
1	YA	638	G
1	YA	645	C
1	YA	646	A
1	YA	651	G
1	YA	654	A
1	YA	654(A)	G
1	YA	657	U
1	YA	669	G
1	YA	686	G
1	YA	701	G
1	YA	722	A
1	YA	730	C
1	YA	752	A
1	YA	753	C
1	YA	764	A
1	YA	782	A
1	YA	784	A
1	YA	785	G
1	YA	790	C
1	YA	791	C
1	YA	792	G
1	YA	805	G
1	YA	812	C

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Mol	Chain	Res	Type
1	YA	819	A
1	YA	827	U
1	YA	828	U
1	YA	831	G
1	YA	847	U
1	YA	856	C
1	YA	857	C
1	YA	860	U
1	YA	866	A
1	YA	878	A
1	YA	881	G
1	YA	882	G
1	YA	884	C
1	YA	886	C
1	YA	888	C
1	YA	889	C
1	YA	896	A
1	YA	897	C
1	YA	898	C
1	YA	900	A
1	YA	901	A
1	YA	904	C
1	YA	905	U
1	YA	907	U
1	YA	910	A
1	YA	915	C
1	YA	917	A
1	YA	918	A
1	YA	932	G
1	YA	938	G
1	YA	941	A
1	YA	945	A
1	YA	946	G
1	YA	953	A
1	YA	957	A
1	YA	959	A
1	YA	961	C
1	YA	974	G
1	YA	974(A)	C
1	YA	980	A
1	YA	983	A
1	YA	989	G

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Mol	Chain	Res	Type
1	YA	996	A
1	YA	1011	G
1	YA	1012	U
1	YA	1013	C
1	YA	1015	G
1	YA	1021	A
1	YA	1022	G
1	YA	1023	U
1	YA	1025	G
1	YA	1026	U
1	YA	1027	A
1	YA	1033	U
1	YA	1045	A
1	YA	1046	A
1	YA	1047	G
1	YA	1050	A
1	YA	1051	G
1	YA	1057	A
1	YA	1059	G
1	YA	1060	U
1	YA	1061	U
1	YA	1065	U
1	YA	1066	U
1	YA	1067	A
1	YA	1068	G
1	YA	1070	A
1	YA	1071	G
1	YA	1073	A
1	YA	1076	C
1	YA	1077	A
1	YA	1078	U
1	YA	1082	U
1	YA	1083	U
1	YA	1084	A
1	YA	1085	A
1	YA	1086	A
1	YA	1088	A
1	YA	1093	G
1	YA	1095	A
1	YA	1096	A
1	YA	1097	U
1	YA	1103	A

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Mol	Chain	Res	Type
1	YA	1104	C
1	YA	1105	U
1	YA	1110	G
1	YA	1111	A
1	YA	1122	G
1	YA	1126	A
1	YA	1130	U
1	YA	1131	G
1	YA	1135	C
1	YA	1136	G
1	YA	1142	U
1	YA	1142(A)	A
1	YA	1143	A
1	YA	1168	G
1	YA	1173	G
1	YA	1174	A
1	YA	1175	U
1	YA	1176	G
1	YA	1177	A
1	YA	1179	C
1	YA	1204	A
1	YA	1205	U
1	YA	1211	U
1	YA	1220	A
1	YA	1221	C
1	YA	1238	G
1	YA	1244	G
1	YA	1253	A
1	YA	1256	G
1	YA	1265	A
1	YA	1271	G
1	YA	1272	A
1	YA	1273	U
1	YA	1300	U
1	YA	1301	A
1	YA	1329	U
1	YA	1341	U
1	YA	1345	C
1	YA	1349	A
1	YA	1352	U
1	YA	1365	A
1	YA	1368	G

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Mol	Chain	Res	Type
1	YA	1370	C
1	YA	1379	A
1	YA	1384	A
1	YA	1385	G
1	YA	1395	A
1	YA	1407	C
1	YA	1411	C
1	YA	1416	G
1	YA	1419	A
1	YA	1420	U
1	YA	1421	G
1	YA	1428	C
1	YA	1444(A)	A
1	YA	1445	C
1	YA	1449	A
1	YA	1449(A)	G
1	YA	1455	G
1	YA	1459	G
1	YA	1460	A
1	YA	1461	G
1	YA	1467	C
1	YA	1471	A
1	YA	1478	G
1	YA	1482	U
1	YA	1483	G
1	YA	1485	G
1	YA	1493	C
1	YA	1494	A
1	YA	1497	U
1	YA	1504	C
1	YA	1506	C
1	YA	1507	A
1	YA	1510	A
1	YA	1511	A
1	YA	1515	C
1	YA	1520	U
1	YA	1522	G
1	YA	1533	C
1	YA	1534	G
1	YA	1535	U
1	YA	1536	A
1	YA	1537	C

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Mol	Chain	Res	Type
1	YA	1538	G
1	YA	1540	G
1	YA	1543	A
1	YA	1544	C
1	YA	1545	A
1	YA	1558	A
1	YA	1559	G
1	YA	1566	A
1	YA	1569	A
1	YA	1578	U
1	YA	1585	C
1	YA	1586	A
1	YA	1598	C
1	YA	1607	C
1	YA	1608	A
1	YA	1609	A
1	YA	1610	A
1	YA	1617	C
1	YA	1618	A
1	YA	1640	C
1	YA	1648	C
1	YA	1654	A
1	YA	1674	G
1	YA	1675	C
1	YA	1687	G
1	YA	1693	U
1	YA	1695	G
1	YA	1725	G
1	YA	1728	G
1	YA	1729	A
1	YA	1730	U
1	YA	1731	G
1	YA	1743	G
1	YA	1754	C
1	YA	1756	G
1	YA	1762	A
1	YA	1763	G
1	YA	1764	G
1	YA	1773	A
1	YA	1780	A
1	YA	1787	A
1	YA	1791	A

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Mol	Chain	Res	Type
1	YA	1799	G
1	YA	1800	C
1	YA	1801	G
1	YA	1816	G
1	YA	1835	G
1	YA	1847	A
1	YA	1858	G
1	YA	1869	G
1	YA	1870	C
1	YA	1872	A
1	YA	1878	G
1	YA	1882	C
1	YA	1884	A
1	YA	1885	A
1	YA	1889	A
1	YA	1899	G
1	YA	1903	G
1	YA	1906	G
1	YA	1913	A
1	YA	1914	C
1	YA	1919	A
1	YA	1929	G
1	YA	1930	G
1	YA	1936	A
1	YA	1938	A
1	YA	1939	U
1	YA	1940	U
1	YA	1955	U
1	YA	1960	A
1	YA	1963	U
1	YA	1965	C
1	YA	1967	C
1	YA	1969	A
1	YA	1970	A
1	YA	1971	A
1	YA	1972	A
1	YA	1982	C
1	YA	1992	G
1	YA	1993	U
1	YA	2020	A
1	YA	2021	C
1	YA	2023	G

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Mol	Chain	Res	Type
1	YA	2031	A
1	YA	2033	A
1	YA	2039	C
1	YA	2043	C
1	YA	2051	A
1	YA	2052	G
1	YA	2055	C
1	YA	2056	G
1	YA	2059	A
1	YA	2060	A
1	YA	2061	G
1	YA	2062	A
1	YA	2069	G
1	YA	2093	G
1	YA	2099	U
1	YA	2105	C
1	YA	2111	C
1	YA	2112	G
1	YA	2113	U
1	YA	2114	A
1	YA	2115	G
1	YA	2116	G
1	YA	2118	U
1	YA	2119	A
1	YA	2120	G
1	YA	2122	U
1	YA	2126	A
1	YA	2127	G
1	YA	2128	C
1	YA	2131	G
1	YA	2132	U
1	YA	2136	C
1	YA	2146	C
1	YA	2156	G
1	YA	2158	A
1	YA	2159	G
1	YA	2160	G
1	YA	2166	G
1	YA	2168	G
1	YA	2169	A
1	YA	2173	A
1	YA	2176	A

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Mol	Chain	Res	Type
1	YA	2180	U
1	YA	2187	G
1	YA	2189	U
1	YA	2190	G
1	YA	2192	G
1	YA	2193	G
1	YA	2198	A
1	YA	2210	G
1	YA	2211	G
1	YA	2212	A
1	YA	2213	U
1	YA	2215	G
1	YA	2225	A
1	YA	2238	G
1	YA	2239	G
1	YA	2243	U
1	YA	2246	G
1	YA	2266	A
1	YA	2273	A
1	YA	2275	C
1	YA	2280	G
1	YA	2283	C
1	YA	2287	A
1	YA	2288	A
1	YA	2307	G
1	YA	2308	G
1	YA	2310	A
1	YA	2311	A
1	YA	2320	A
1	YA	2325	G
1	YA	2334	G
1	YA	2342	C
1	YA	2346	A
1	YA	2347	C
1	YA	2350	C
1	YA	2354	G
1	YA	2383	G
1	YA	2385	C
1	YA	2392	A
1	YA	2401	U
1	YA	2402	C
1	YA	2406	U

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Mol	Chain	Res	Type
1	YA	2410	G
1	YA	2423	U
1	YA	2424	C
1	YA	2425	A
1	YA	2429	G
1	YA	2430	A
1	YA	2435	A
1	YA	2439	A
1	YA	2441	C
1	YA	2448	A
1	YA	2450	A
1	YA	2465	C
1	YA	2469	A
1	YA	2470	G
1	YA	2473	U
1	YA	2474	C
1	YA	2475	C
1	YA	2480	C
1	YA	2494	G
1	YA	2502	G
1	YA	2504	U
1	YA	2505	G
1	YA	2518	A
1	YA	2525	G
1	YA	2529	G
1	YA	2542	A
1	YA	2554	U
1	YA	2567	G
1	YA	2573	C
1	YA	2578	G
1	YA	2585	U
1	YA	2586	C
1	YA	2602	A
1	YA	2609	U
1	YA	2611	U
1	YA	2612	C
1	YA	2615	U
1	YA	2629	A
1	YA	2654	A
1	YA	2655	G
1	YA	2665	A
1	YA	2666	C

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Mol	Chain	Res	Type
1	YA	2673	G
1	YA	2675	A
1	YA	2682	U
1	YA	2689	U
1	YA	2702	U
1	YA	2707	G
1	YA	2712	U
1	YA	2712(A)	A
1	YA	2713	A
1	YA	2714	G
1	YA	2726	U
1	YA	2733	A
1	YA	2739	U
1	YA	2744	G
1	YA	2751	G
1	YA	2757	A
1	YA	2758	A
1	YA	2762	G
1	YA	2764	A
1	YA	2765	A
1	YA	2766	G
1	YA	2777	G
1	YA	2778	A
1	YA	2779	U
1	YA	2789	C
1	YA	2790	A
1	YA	2791	C
1	YA	2797	U
1	YA	2798	C
1	YA	2808	U
1	YA	2820	A
1	YA	2821	A
1	YA	2833	G
1	YA	2834	G
1	YA	2867	G
1	YA	2868	A
1	YA	2872	G
1	YA	2880	C
1	YA	2891	G
1	YA	2892	A
1	YA	2893	G
1	YA	2894	G

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Mol	Chain	Res	Type
2	YB	7	G
2	YB	8	U
2	YB	9	G
2	YB	12	C
2	YB	13	A
2	YB	15	A
2	YB	16	G
2	YB	19	G
2	YB	21	G
2	YB	25	A
2	YB	31	C
2	YB	41	U
2	YB	42	C
2	YB	44	G
2	YB	45	A
2	YB	52	A
2	YB	56	G
2	YB	67	G
2	YB	73	A
2	YB	81	G
2	YB	82	G
2	YB	108	C
2	YB	109	G
32	XA	6	G
32	XA	32	A
32	XA	39	G
32	XA	48	C
32	XA	51	A
32	XA	59	A
32	XA	61	G
32	XA	64	G
32	XA	65	U
32	XA	66	G
32	XA	79	G
32	XA	89	U
32	XA	92	G
32	XA	95	G
32	XA	101	A
32	XA	108	G
32	XA	116	A
32	XA	120	A
32	XA	121	C

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Mol	Chain	Res	Type
32	XA	130	A
32	XA	144	G
32	XA	163	C
32	XA	169	C
32	XA	172	A
32	XA	174	C
32	XA	188	U
32	XA	190	G
32	XA	195	A
32	XA	197	A
32	XA	209	U
32	XA	210	U
32	XA	231	G
32	XA	244	U
32	XA	245	C
32	XA	247	G
32	XA	251	G
32	XA	267	C
32	XA	281	G
32	XA	289	G
32	XA	298	A
32	XA	306	G
32	XA	321	A
32	XA	328	C
32	XA	329	A
32	XA	332	G
32	XA	344	A
32	XA	345	C
32	XA	347	G
32	XA	348	G
32	XA	351	G
32	XA	352	C
32	XA	353	A
32	XA	354	G
32	XA	356	A
32	XA	367	U
32	XA	372	C
32	XA	389	A
32	XA	397	A
32	XA	398	C
32	XA	411	A
32	XA	412	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	413	G
32	XA	414	A
32	XA	421	U
32	XA	422	C
32	XA	423	G
32	XA	424	G
32	XA	429	U
32	XA	430	A
32	XA	435	C
32	XA	438	G
32	XA	439	A
32	XA	465	A
32	XA	466	C
32	XA	467	G
32	XA	482	A
32	XA	484	G
32	XA	485	G
32	XA	486	U
32	XA	496	A
32	XA	497	U
32	XA	509	A
32	XA	510	A
32	XA	511	C
32	XA	518	C
32	XA	519	C
32	XA	527	G
32	XA	531	U
32	XA	532	A
32	XA	533	A
32	XA	547	A
32	XA	548	G
32	XA	559	A
32	XA	561	U
32	XA	564	C
32	XA	568	G
32	XA	572	A
32	XA	573	A
32	XA	576	G
32	XA	577	G
32	XA	579	G
32	XA	618	C
32	XA	630	G

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Mol	Chain	Res	Type
32	XA	631	G
32	XA	632	A
32	XA	633	G
32	XA	653	A
32	XA	657	G
32	XA	665	A
32	XA	686	U
32	XA	688	G
32	XA	703	G
32	XA	704	A
32	XA	721	G
32	XA	723	U
32	XA	731	G
32	XA	734	G
32	XA	749	C
32	XA	753	A
32	XA	754	C
32	XA	755	G
32	XA	777	A
32	XA	792	A
32	XA	793	U
32	XA	794	A
32	XA	799	G
32	XA	816	A
32	XA	817	C
32	XA	821	G
32	XA	828	A
32	XA	841	U
32	XA	842	C
32	XA	843	U
32	XA	848	C
32	XA	855	G
32	XA	859	A
32	XA	870	U
32	XA	871	U
32	XA	872	A
32	XA	902	G
32	XA	914	A
32	XA	926	G
32	XA	927	G
32	XA	934	C
32	XA	935	A

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Mol	Chain	Res	Type
32	XA	960	U
32	XA	966	G
32	XA	968	A
32	XA	969	A
32	XA	972	C
32	XA	974	A
32	XA	975	A
32	XA	976	G
32	XA	977	A
32	XA	981	U
32	XA	982	U
32	XA	991	U
32	XA	992	U
32	XA	993	G
32	XA	1004	A
32	XA	1006	C
32	XA	1009	G
32	XA	1024	G
32	XA	1025	U
32	XA	1028	C
32	XA	1028(A)	C
32	XA	1029	G
32	XA	1030	C
32	XA	1031	G
32	XA	1032	A
32	XA	1032(A)	G
32	XA	1038	C
32	XA	1039	C
32	XA	1040	U
32	XA	1042	G
32	XA	1053	G
32	XA	1054	C
32	XA	1064	G
32	XA	1066	C
32	XA	1081	G
32	XA	1094	G
32	XA	1101	A
32	XA	1108	G
32	XA	1124	G
32	XA	1125	U
32	XA	1126	U
32	XA	1127	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	1129	C
32	XA	1130	A
32	XA	1136	U
32	XA	1137	C
32	XA	1138	G
32	XA	1139	G
32	XA	1145	C
32	XA	1146	A
32	XA	1157	A
32	XA	1158	C
32	XA	1159	U
32	XA	1160	G
32	XA	1162	C
32	XA	1176	A
32	XA	1177	G
32	XA	1181	G
32	XA	1183	A
32	XA	1196	U
32	XA	1212	U
32	XA	1224	G
32	XA	1225	A
32	XA	1226	C
32	XA	1236	A
32	XA	1238	A
32	XA	1240	U
32	XA	1241	G
32	XA	1256	A
32	XA	1257	U
32	XA	1258	G
32	XA	1260	C
32	XA	1263	C
32	XA	1270	C
32	XA	1273	G
32	XA	1278	U
32	XA	1280	A
32	XA	1281	U
32	XA	1286	A
32	XA	1287	A
32	XA	1290	G
32	XA	1298	C
32	XA	1300	G
32	XA	1301	U

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Mol	Chain	Res	Type
32	XA	1302	U
32	XA	1303	C
32	XA	1305	G
32	XA	1310	G
32	XA	1311	G
32	XA	1320	C
32	XA	1322	C
32	XA	1323	G
32	XA	1331	G
32	XA	1332	A
32	XA	1335	C
32	XA	1336	C
32	XA	1347	G
32	XA	1348	U
32	XA	1357	A
32	XA	1362(A)	C
32	XA	1364	U
32	XA	1378	C
32	XA	1399	C
32	XA	1419	G
32	XA	1442	G
32	XA	1446	A
32	XA	1447	G
32	XA	1452	C
32	XA	1453	G
32	XA	1454	G
32	XA	1487	G
32	XA	1492	A
32	XA	1493	A
32	XA	1497	G
32	XA	1499	A
32	XA	1502	A
32	XA	1503	A
32	XA	1504	G
32	XA	1506	U
32	XA	1517	G
32	XA	1520	G
32	XA	1529	G
32	XA	1530	G
32	XA	1532	U
32	XA	1533	C
32	XA	1534	A

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Mol	Chain	Res	Type
32	XA	1536	C
32	XA	1537	U
32	XA	1538	C
32	XA	1539	C
32	XA	1541	U
32	XA	1542	U
54	XX	2	G
54	XX	7	G
54	XX	10	G
54	XX	11	U
54	XX	12	A
54	XX	13	A
54	XX	14	A
54	XX	15	A
54	XX	19	U

All (152) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	RA	74	A
1	RA	99	U
1	RA	221	A
1	RA	222	A
1	RA	229	A
1	RA	271(B)	G
1	RA	345	A
1	RA	372	G
1	RA	404	C
1	RA	503	A
1	RA	508	G
1	RA	512	G
1	RA	587	C
1	RA	637	A
1	RA	752	A
1	RA	846	C
1	RA	856	C
1	RA	1022	G
1	RA	1053	C
1	RA	1057	A
1	RA	1065	U
1	RA	1067	A
1	RA	1073	A

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Mol	Chain	Res	Type
1	RA	1204	A
1	RA	1210	A
1	RA	1312	U
1	RA	1427	A
1	RA	1508	A
1	RA	1558	A
1	RA	1653	G
1	RA	1819	A
1	RA	1992	G
1	RA	2060	A
1	RA	2126	A
1	RA	2439	A
1	RA	2566	A
1	RA	2610	C
1	RA	2689	U
1	RA	2756	U
1	RA	2832	U
1	RA	2867	G
2	RB	66	A
32	QA	5	U
32	QA	64	G
32	QA	115	G
32	QA	119	A
32	QA	181	G
32	QA	243	A
32	QA	244	U
32	QA	250	A
32	QA	266	G
32	QA	328	C
32	QA	410	G
32	QA	412	A
32	QA	428	G
32	QA	429	U
32	QA	481	G
32	QA	484	G
32	QA	485	G
32	QA	509	A
32	QA	687	A
32	QA	703	G
32	QA	753	A
32	QA	792	A
32	QA	812	C

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Mol	Chain	Res	Type
32	QA	913	A
32	QA	960	U
32	QA	992	U
32	QA	1065	U
32	QA	1200	C
32	QA	1201	A
32	QA	1285	A
32	QA	1297	C
32	QA	1336	C
32	QA	1346	A
32	QA	1347	G
32	QA	1446	A
32	QA	1498	U
32	QA	1528	U
54	QX	13	A
1	YA	99	U
1	YA	196	A
1	YA	221	A
1	YA	229	A
1	YA	242	G
1	YA	271(B)	G
1	YA	278	A
1	YA	404	C
1	YA	503	A
1	YA	508	G
1	YA	637	A
1	YA	752	A
1	YA	846	C
1	YA	856	C
1	YA	859	G
1	YA	1012	U
1	YA	1022	G
1	YA	1026	U
1	YA	1085	A
1	YA	1109	C
1	YA	1130	U
1	YA	1178	C
1	YA	1204	A
1	YA	1210	A
1	YA	1427	A
1	YA	1460	A
1	YA	1558	A

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Mol	Chain	Res	Type
1	YA	1653	G
1	YA	1694	C
1	YA	1799	G
1	YA	1913	A
1	YA	1992	G
1	YA	2406	U
1	YA	2566	A
1	YA	2681	C
1	YA	2712	U
1	YA	2756	U
1	YA	2776	A
1	YA	2832	U
1	YA	2867	G
2	YB	24	G
2	YB	66	A
32	XA	60	A
32	XA	78	G
32	XA	115	G
32	XA	243	A
32	XA	244	U
32	XA	250	A
32	XA	266	G
32	XA	328	C
32	XA	388	G
32	XA	410	G
32	XA	412	A
32	XA	429	U
32	XA	481	G
32	XA	484	G
32	XA	485	G
32	XA	509	A
32	XA	560	U
32	XA	687	A
32	XA	703	G
32	XA	753	A
32	XA	913	A
32	XA	992	U
32	XA	1027	C
32	XA	1285	A
32	XA	1297	C
32	XA	1310	G
32	XA	1446	A

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Mol	Chain	Res	Type
32	XA	1498	U
32	XA	1537	U
54	XX	12	A

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

2 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	$\# Z  > 2$
53	1MG	XV	37	53	18,26,27	1.25	2 (11%)	19,39,42	1.65	2 (10%)
53	1MG	QV	37	53	18,26,27	1.24	2 (11%)	19,39,42	1.53	2 (10%)

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
53	1MG	XV	37	53	-	0/3/25/26	0/3/3/3
53	1MG	QV	37	53	-	0/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	37	1MG	C6-C5	4.28	1.48	1.41
53	QV	37	1MG	C6-C5	4.17	1.47	1.41
53	QV	37	1MG	C5-C4	2.35	1.47	1.40
53	XV	37	1MG	C5-C4	2.28	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	XV	37	1MG	C2-N3-C4	5.94	122.14	115.36
53	QV	37	1MG	C2-N3-C4	5.14	121.23	115.36
53	QV	37	1MG	C4-C5-N7	-2.93	106.35	109.40
53	XV	37	1MG	C4-C5-N7	-2.65	106.64	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	XV	37	1MG	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	SF4	QD	301	35	0,12,12	0.00	-	-		
57	SF4	XD	301	35	0,12,12	0.00	-	-		

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
57	SF4	QD	301	35	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	XD	301	35	-	-	0/6/5/5

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QD	301	SF4	1	0
57	XD	301	SF4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.