



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2020 – 03:05 AM EDT

PDB ID : 6NWY  
Title : Modified tRNA(Pro) bound to Thermus thermophilus 70S (near-cognate)  
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2019-02-07  
Resolution : 3.50 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

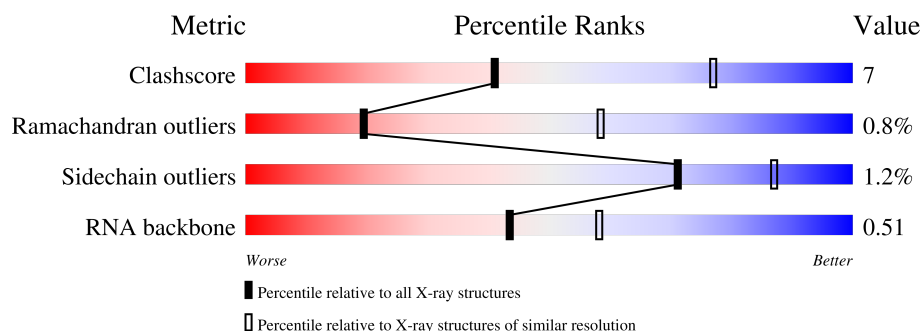
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)


























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	QA	1521	52% 38% 9% ..
1	XA	1521	52% 38% 9% .
2	QB	256	66% 26% 8%
2	XB	256	68% 24% 8%
3	QC	239	65% 20% 14%
3	XC	239	71% 15% 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	


























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Mol	Chain	Length	Quality of chain
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	
28	R4	71	
28	Y4	71	


























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Mol	Chain	Length	Quality of chain
29	R5	60	 68% 25% 5% .
29	Y5	60	 67% 27% . . .
30	R6	54	 72% 22% . . .
30	Y6	54	 65% 26% 6% . .
31	R7	49	 67% 29% .
31	Y7	49	 86% 12% .
32	R8	65	 69% 23% 6% .
32	Y8	65	 72% 26% .
33	R9	37	 70% 24% 5%
33	Y9	37	 68% 27% 5%
34	RA	2915	 53% 36% 9% . .
34	YA	2915	 53% 35% 10% . .
35	RB	122	 57% 37% . . .
35	YB	122	 53% 36% 7% . .
36	RD	276	 76% 21% . .
36	YD	276	 80% 18% . .
37	RE	206	 72% 25% .
37	YE	206	 75% 24%
38	RF	210	 75% 20% . .
38	YF	210	 73% 23% .
39	RG	182	 76% 23% . .
39	YG	182	 78% 21% .
40	RH	180	 64% 27% 6% .
40	YH	180	 77% 18% . . .
41	RI	148	 72% 23% . .

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Mol	Chain	Length	Quality of chain
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	
53	RY	110	
53	YY	110	

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Mol	Chain	Length	Quality of chain
54	RZ	206	
54	YZ	206	

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
56	SF4	QD	301	-	-	X	-

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 292039 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
1	XA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.



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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a RNA chain called E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			
23	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	45	Total	C	N	O	S	0	0	0
			348	224	57	62	5			
28	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
36	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

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

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
44	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
46	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 47 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
47	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			



- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
52	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
54	YZ	193	Total	C	N	O	S	0	0	0
			1529	973	270	283	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	87	Total	Mg	0	0
			87	87		
55	RP	1	Total	Mg	0	0
			1	1		
55	YA	439	Total	Mg	0	0
			439	439		
55	Y5	1	Total	Mg	0	0
			1	1		
55	YR	2	Total	Mg	0	0
			2	2		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	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	Y8	1	Total	Mg	0	0
			1	1		
55	XA	89	Total	Mg	0	0
			89	89		
55	RQ	1	Total	Mg	0	0
			1	1		
55	R0	2	Total	Mg	0	0
			2	2		
55	QL	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	YU	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	QH	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	YX	1	Total 1	Mg 1	0	0
55	RD	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	RA	429	Total 429	Mg 429	0	0
55	YF	1	Total 1	Mg 1	0	0
55	RE	4	Total 4	Mg 4	0	0
55	YB	8	Total 8	Mg 8	0	0
55	RB	11	Total 11	Mg 11	0	0
55	Y2	1	Total 1	Mg 1	0	0
55	RF	2	Total 2	Mg 2	0	0
55	R3	1	Total 1	Mg 1	0	0
55	YE	2	Total 2	Mg 2	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

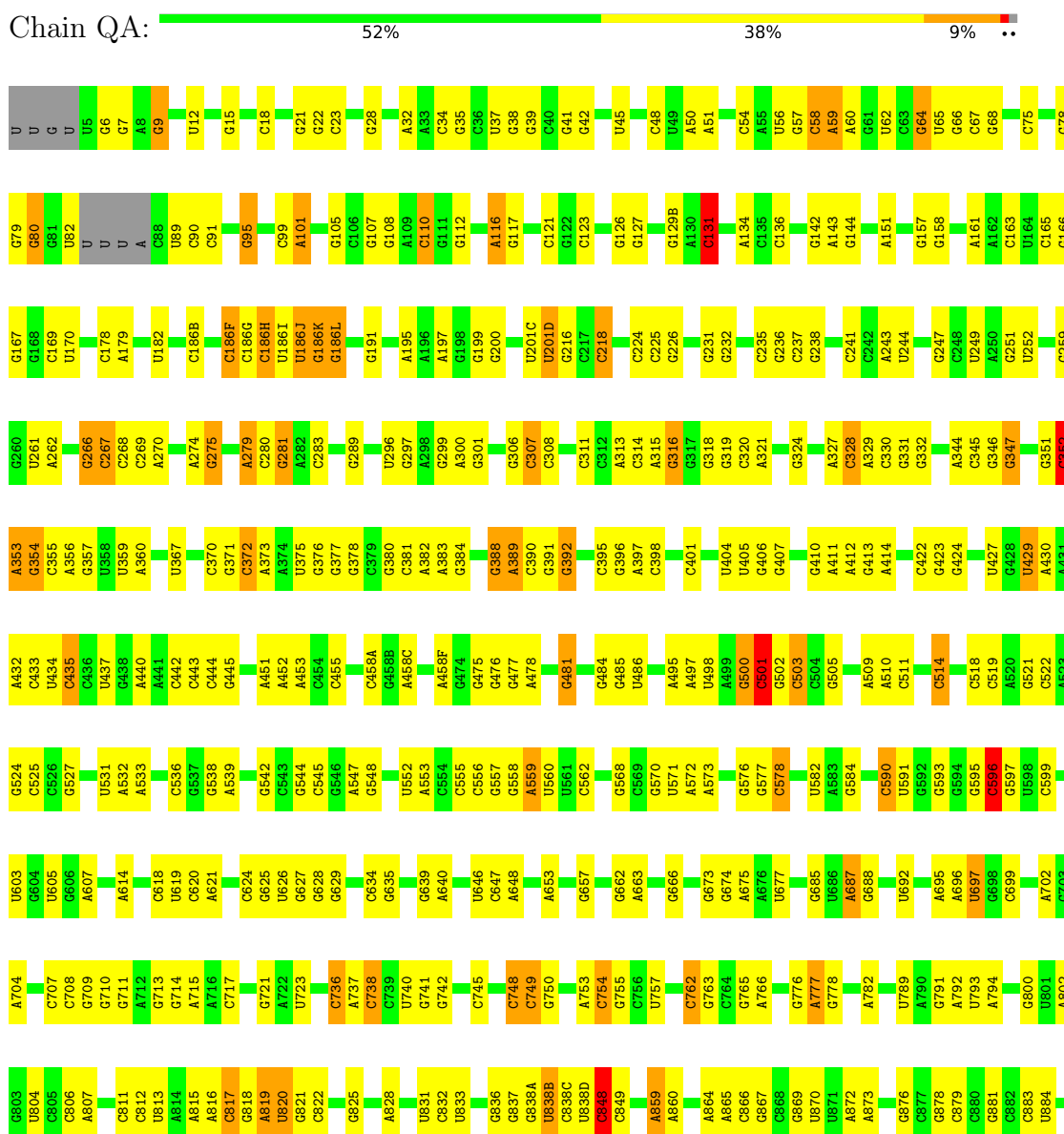
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	QN	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0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

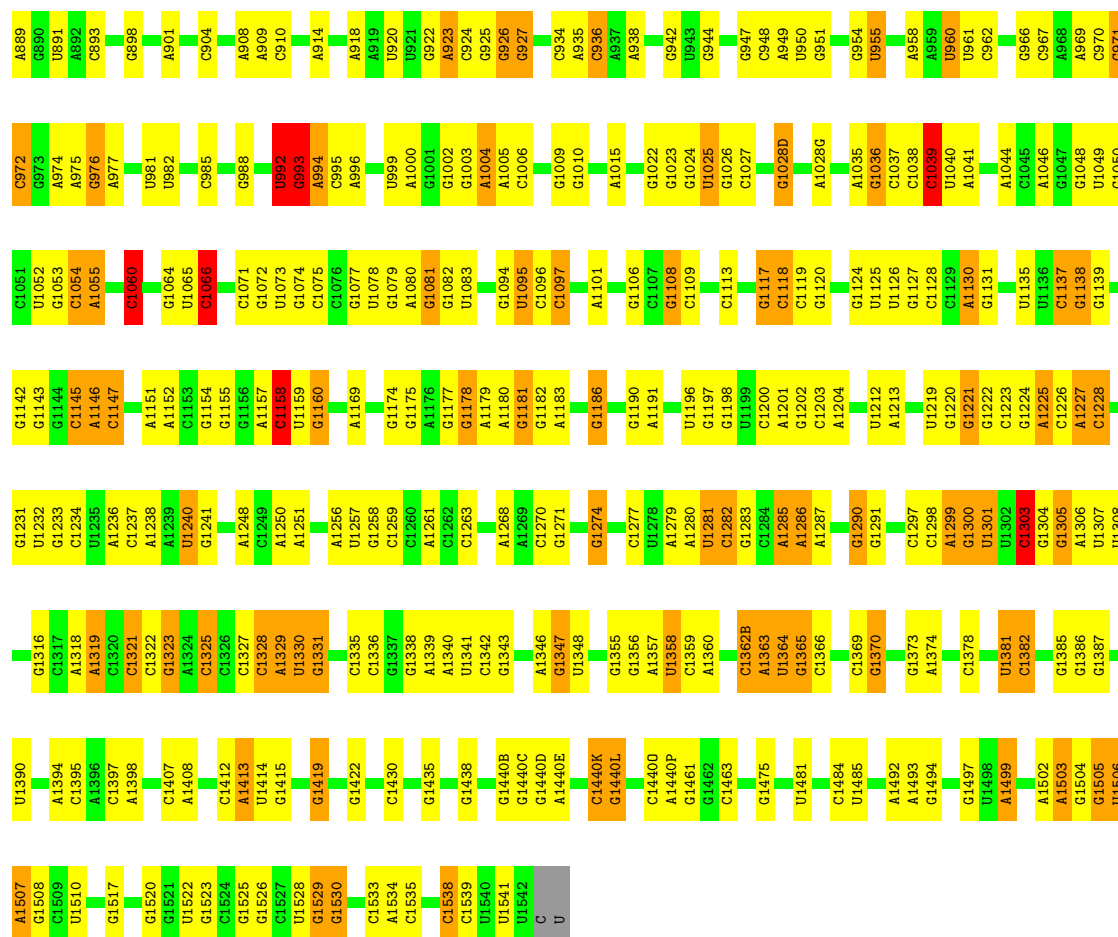
### 3 Residue-property plots [i](#)

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.

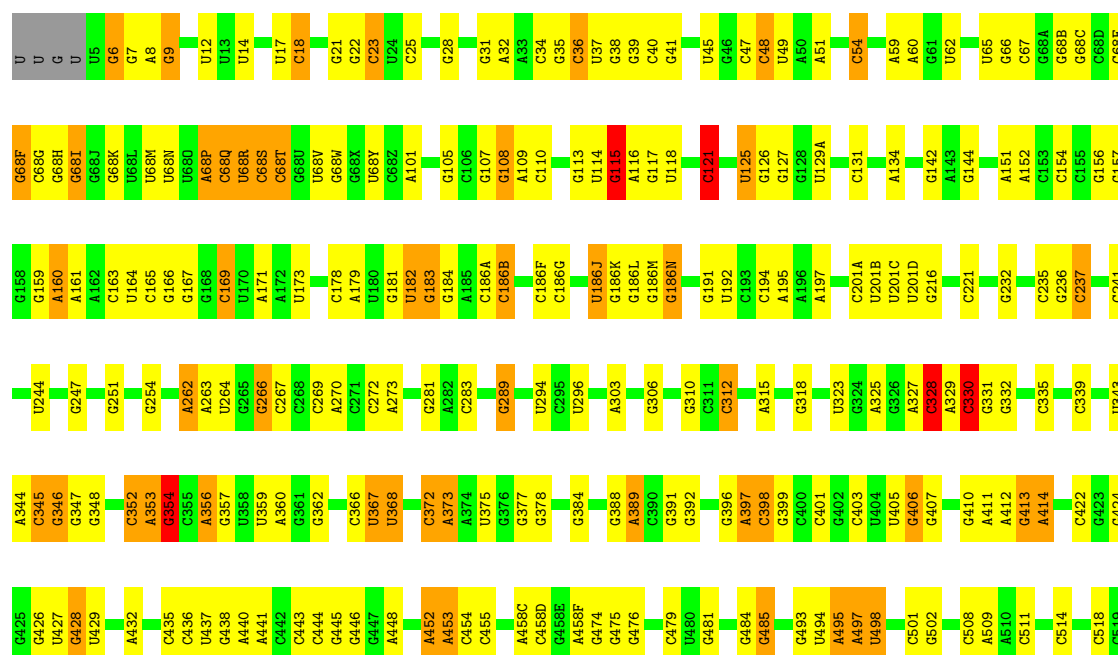
#### • Molecule 1: 16S rRNA

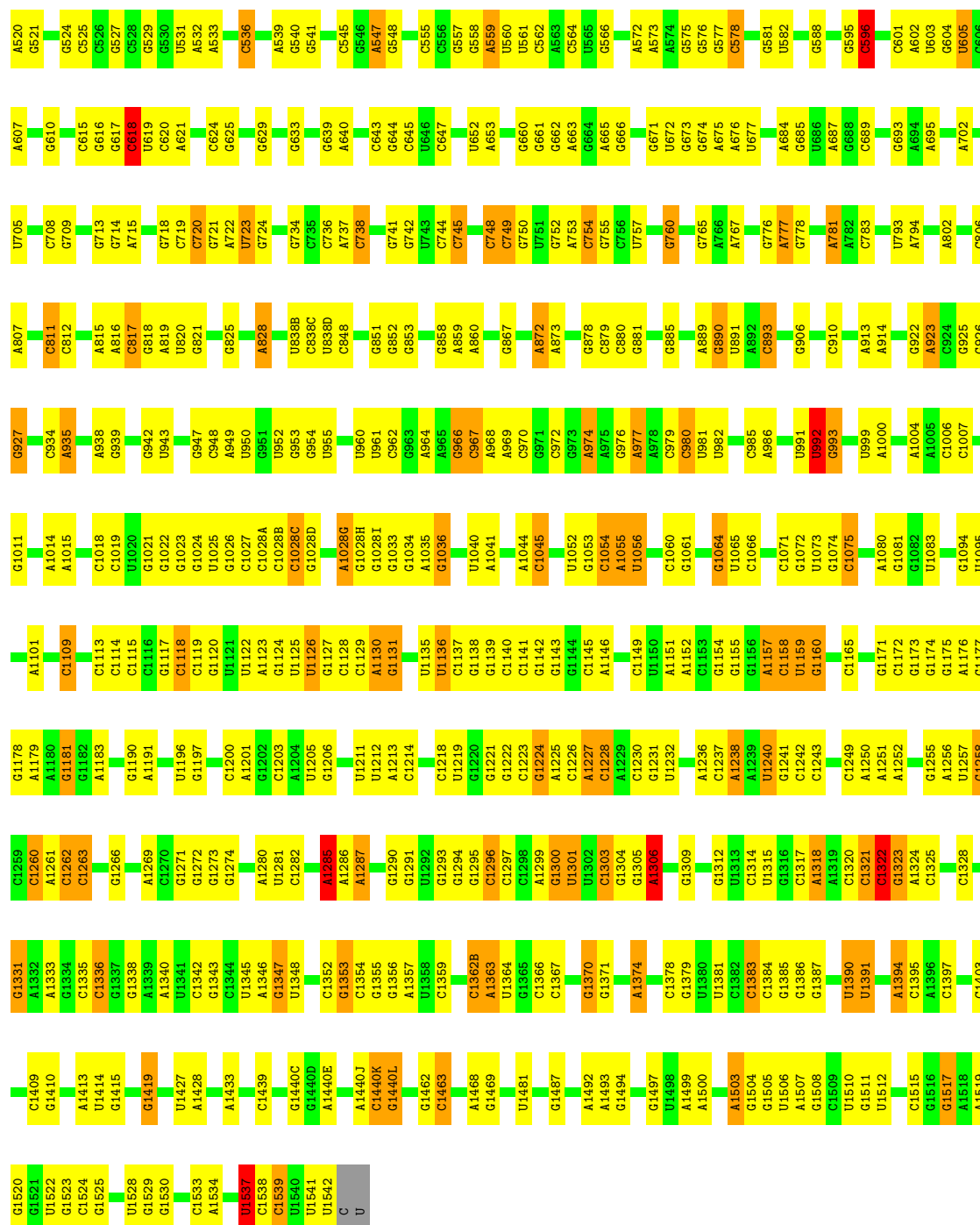




### • Molecule 1: 16S rRNA

Chain XA: 52% 38% 9% .





THR  
GLU  
THR  
PRO  
GLY  
GLU  
SER  
VAL  
GLU  
ALA

- Molecule 2: 30S ribosomal protein S2

Chain XB:  68% 24% 8%

MET PRO VAL I5 R21 K27 R30 Y31 I32 Y33 H40 D43 T47 T54 T67 I68 V71 K75 E84 R87 A88 G89 N104 I108 L115 L118 E119 A120 S124 P125 E126 R130 P131 K132 K133 E134 Q135 V136 R137 L142

L145 L155 A161 I162 F163 V164 P167 A171 R175 E176 A177 R178 K179 I182 P183 V184 I185 A186 L187 A188 D189 T190 D191 S192 D193 D198 Y199 I200 I201 N204 D205 D206 A207 I208 E209 S210 L215 V219 R226 Q240 GLU ALA GLU ALA THR THR

PRO  
GLU  
GLY  
SER  
VAL  
GLU  
ALA

- Molecule 3: 30S ribosomal protein S3

Chain QC:  65% 20% 14%

MET G2 H6 P7 I8 R11 L12 V18 W22 Y23 A24 Y29 L32 L33 L34 E35 D36 Q37 R38 L43 E44 E47 A50 G51 L52 D56 L57 E58 R59 V66 T67 P73 G74 V75 V76 L87 R88 L91 L101 N102 V103 M108 L111

S112 L115 V120 I124 R127 R131 I134 R140 E143 S144 K150 R172 T177 Y184 A200 Y201 E205 VAL ILE GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU ARG PRO ARG ARG ARG ARG PRO ALA VAL

LYS  
LYS  
GLU  
GLU


- Molecule 3: 30S ribosomal protein S3

Chain XC:  71% 15% 14%

MET G2 I8 G9 L12 G13 I14 T15 R16 D17 W18 E19 S20 W22 L32 E35 D36 R40 L43 L47 E58 R59 V64 A65 V66 L91 K97 L101 R119 R140 V153 I157 E161 Q162 A163 R164 H176 Y184 A187

L196 G197 V198 E205 VAL ILE GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA ARG ARG ARG ARG ARG PRO ALA VAL VAL VAL LYS GLU GLU

- Molecule 4: 30S ribosomal protein S4

Chain QD:  76% 22% 2%

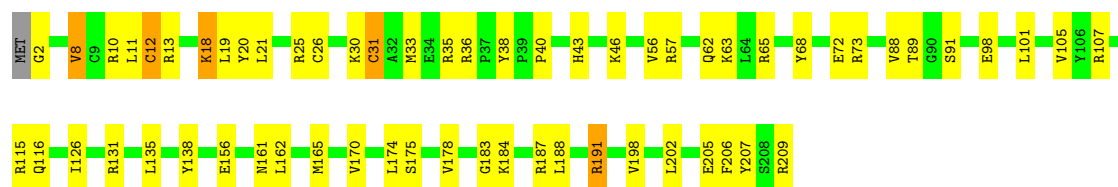
MET G2 R3 V8 C9 R10 L11 G12 R13 R14 E15 K18 L21 K22 S28 P29 R30 C31 A32 N33 R57 L58 R59 E60 K61 K62 K63 L64 R65 R66 E72 R73 F79 K85 E98 S99 R100 N103 I108 G109 R115 R118 Q119 L120 V121 R122

I126 D134 S137 E156 Q160 M165 K166 G167 R168 K169 L174 R191 T204 E205 F206 Y207 S208 R209


- Molecule 4: 30S ribosomal protein S4

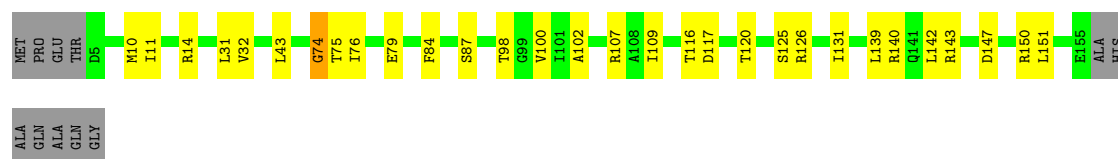


Chain XD:  70% 27% .



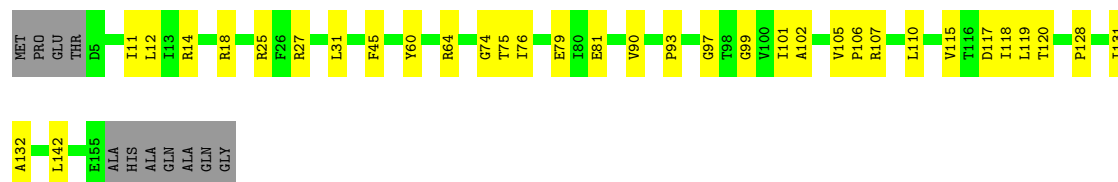
- Molecule 5: 30S ribosomal protein S5

Chain QE:  75% 18% 7% .




- Molecule 5: 30S ribosomal protein S5

Chain XE:  72% 21% 7% .




- Molecule 6: 30S ribosomal protein S6

Chain QF:  84% 16% .




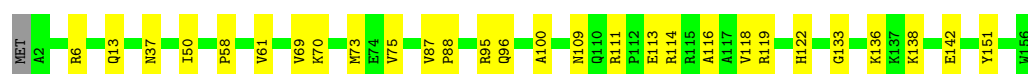
- Molecule 6: 30S ribosomal protein S6

Chain XF:  82% 18% .

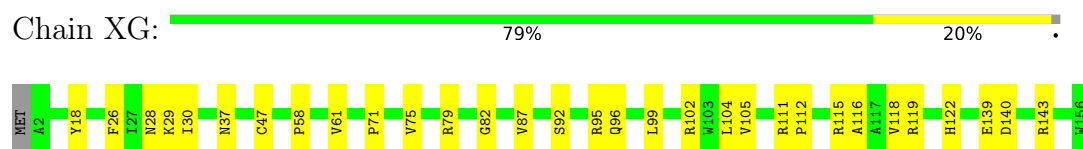


- Molecule 7: 30S ribosomal protein S7

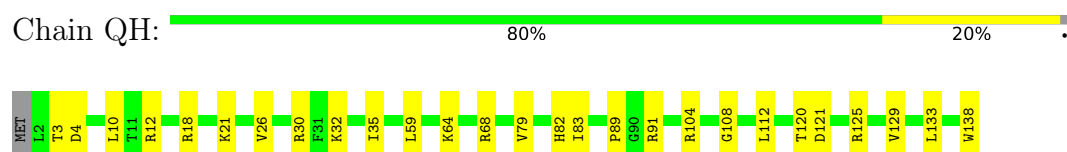
Chain QG:  81% 18% .



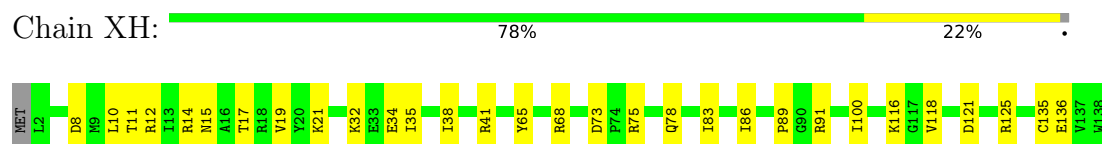
- Molecule 7: 30S ribosomal protein S7



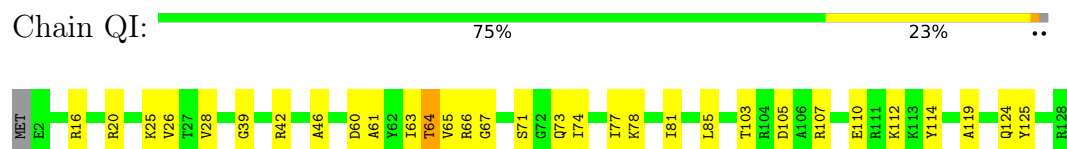
- Molecule 8: 30S ribosomal protein S8



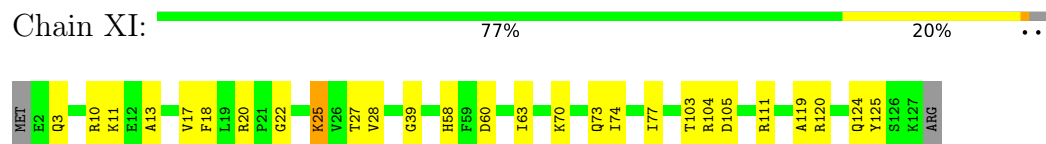
- Molecule 8: 30S ribosomal protein S8



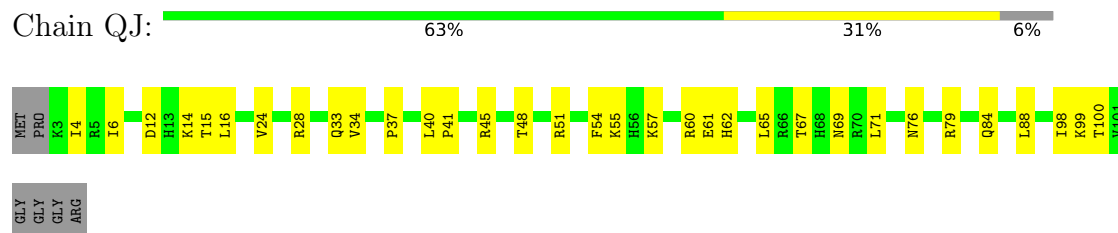
- Molecule 9: 30S ribosomal protein S9



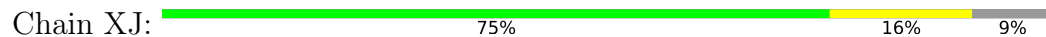
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

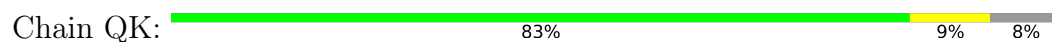


- Molecule 10: 30S ribosomal protein S10

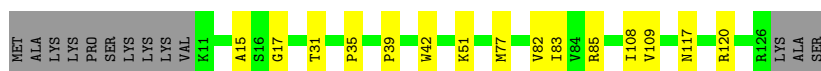
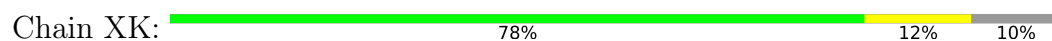




- Molecule 11: 30S ribosomal protein S11



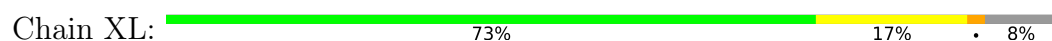
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



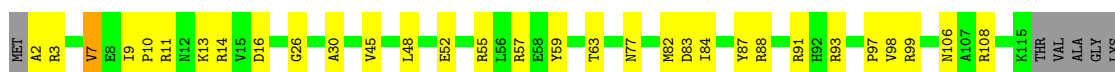
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



LYS  
LYS  
ALA  
PRO  
ARG  
LYS

- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  70% 25% 5% 0%

MET A2 R3 L6 K9 R12 T13 P14 K17 V18 R23 C24 G28 R35 C40 R41 I42 C43 L44 R45 P54 W61

- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  62% 31% 5% 2%

MET A2 K9 R12 R19 R23 C24 C37 G28 R29 C40 R41 I42 C43 L44 E46 R45 L47 Q52 L53 P54 G55 V56 R57 K58 W61

- Molecule 15: 30S ribosomal protein S15

Chain QO:  89% 10% 1% 0%


MET F2 T22 E26 Q27 V29 L39 L56 R64 R72 I87 R88 G89

- Molecule 15: 30S ribosomal protein S15

Chain XO:  83% 15% 2% 0%


MET F2 K10 Q13 E26 R35 L39 H53 L56 R64 R65 R68 R72 L81 R88 GLY

- Molecule 16: 30S ribosomal protein S16

Chain QP:  74% 22% 5% 0%


H1 I4 R5 R8 M14 P15 H16 V21 R25 I33 G37 D40 K43 K50 V53 E54 R55 W59 V62 T69 R75 V79 A84 ARG GLU GLY ALA

- Molecule 16: 30S ribosomal protein S16

Chain XP:  76% 19% 5% 0%

H1 I4 R5 L6 Y17 R18 I19 V20 V21 T22 D23 K27 K35 I36 G37 D40 W48 L49 K50 P66 R75 Q82 E83 A84 ARG GLU GLY ALA

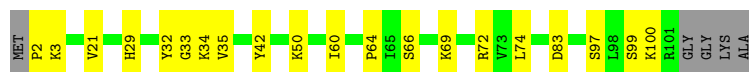
- Molecule 17: 30S ribosomal protein S17

Chain QQ:  83% 12% 5% 0%



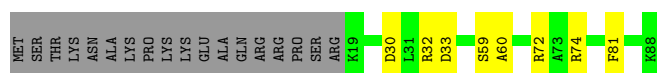
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 76% 19% 5%



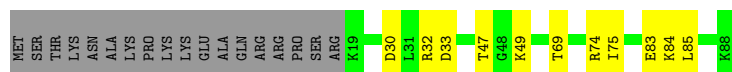
- Molecule 18: 30S ribosomal protein S18

Chain QR: 70% 9% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR: 67% 13% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS: 73% 15% 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS: 68% 23% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT: 70% 22% 7%



- Molecule 20: 30S ribosomal protein S20

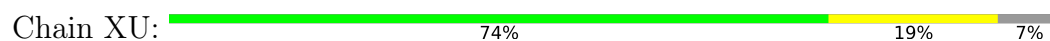
Chain XT: 69% 21% 7%



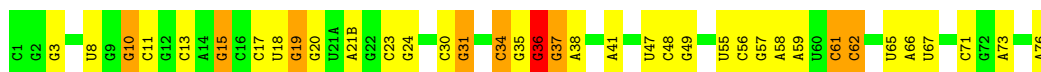
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



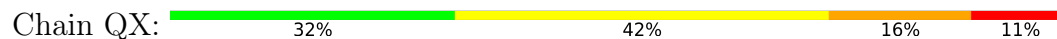
- Molecule 22: E-site tRNA-Pro



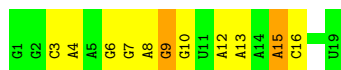
- Molecule 22: E-site tRNA-Pro



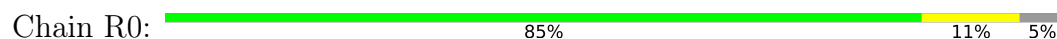
- Molecule 23: mRNA



- Molecule 23: mRNA



- Molecule 24: 50S ribosomal protein L27





- Molecule 24: 50S ribosomal protein L27

Chain Y0: 80% 16%



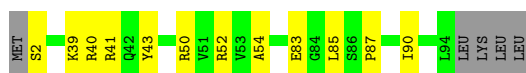
- Molecule 25: 50S ribosomal protein L28

Chain R1: 80% 17%



- Molecule 25: 50S ribosomal protein L28

Chain Y1: 83% 12% 5%



- Molecule 26: 50S ribosomal protein L29

Chain R2: 82% 14%



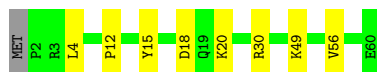
- Molecule 26: 50S ribosomal protein L29

Chain Y2: 82% 13% 6%



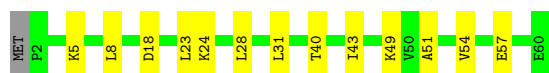
- Molecule 27: 50S ribosomal protein L30

Chain R3: 85% 13%

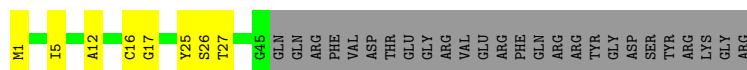


- Molecule 27: 50S ribosomal protein L30

Chain Y3: 77% 22%



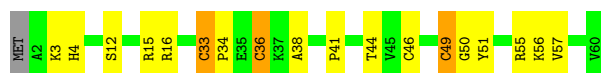
- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



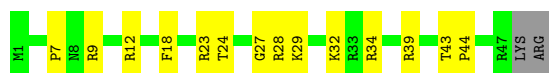
- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34







- Molecule 31: 50S ribosomal protein L34

Chain Y7: 86% 12% .



- Molecule 32: 50S ribosomal protein L35

Chain R8: 69% 23% 6% .



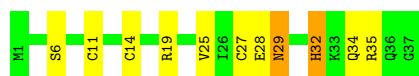
- Molecule 32: 50S ribosomal protein L35

Chain Y8: 72% 26% .



- Molecule 33: 50S ribosomal protein L36

Chain R9: 70% 24% 5%



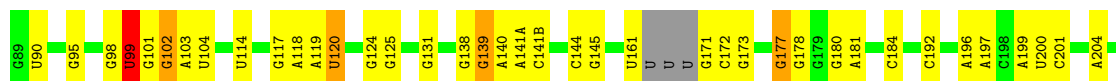
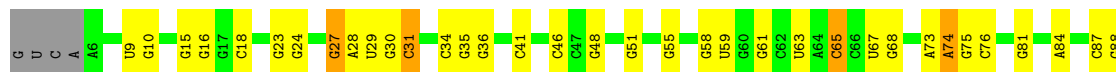
- Molecule 33: 50S ribosomal protein L36

Chain Y9: 68% 27% 5%



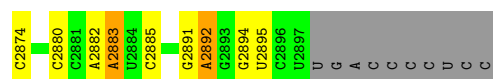
- Molecule 34: 23S rRNA

Chain RA: 53% 36% 9% ..



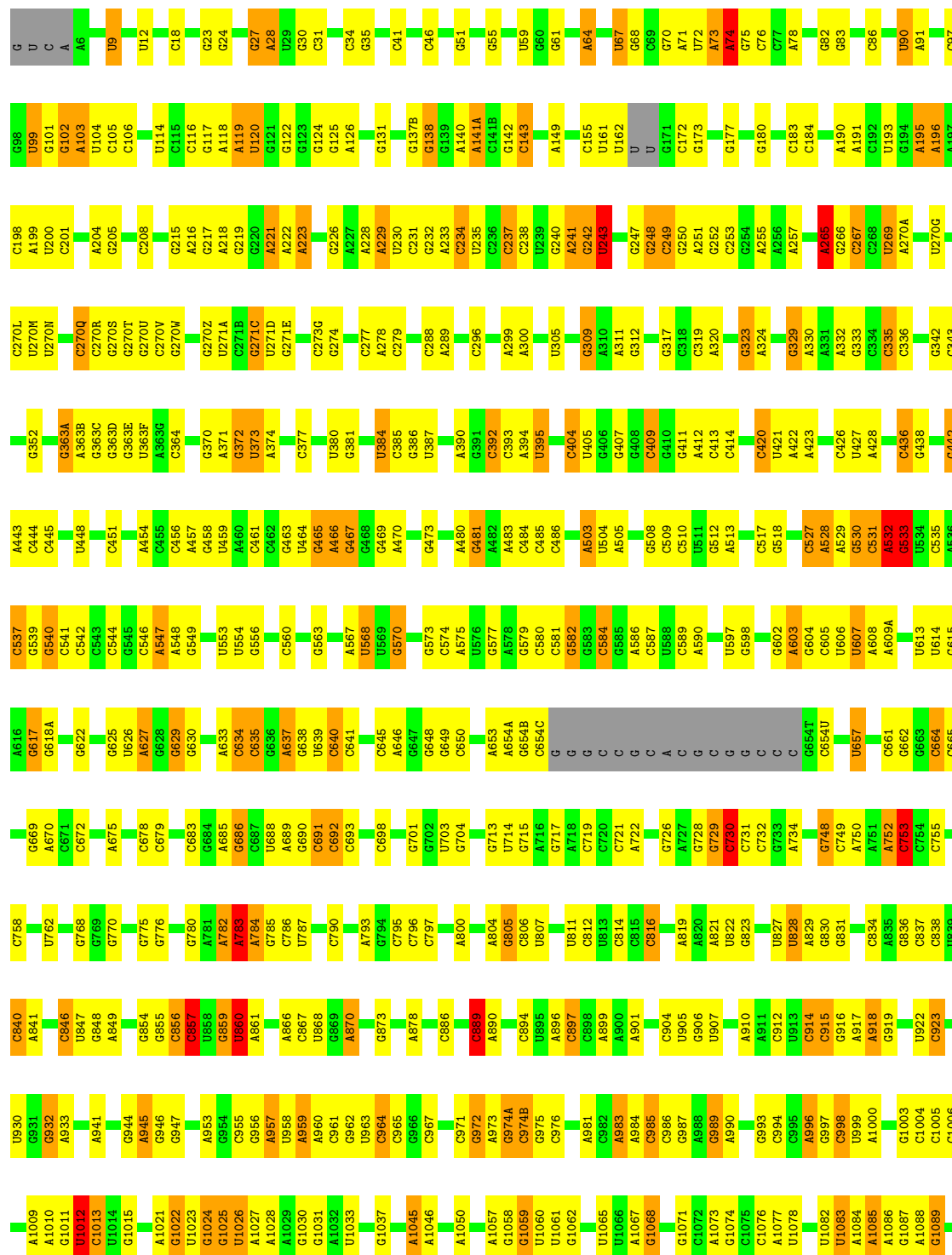
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G1407	C1407	A1308	G1225	G1136	G1058	A983	C904	G808	G707	G642	U566	A482	A371	G272	C209
C1407	C1407	A1307	G1226	G1137	G1062	A984	U907	G809	G708	A646	A567	A483	G372	C273E	G214
C1407	C1407	A1306	G1227	G1138	G1063	A985	A910	G810	G715	G645	U568	A483	A374	G275	G215
C1407	C1407	A1305	G1228	G1139	G1064	A986	A911	G811	G716	G646	A571	A484	U380	G276	A216
C1407	C1407	A1304	G1229	G1140	G1065	A987	A912	G812	G717	G647	A572	A485	U381	G277	G217
C1407	C1407	A1303	G1230	G1141	G1066	A988	A913	G813	G718	G648	A573	A486	U382	A278	A221
C1407	C1407	A1302	G1231	G1142	G1067	A989	U914	G814	G719	G649	A574	A487	U383	A279	A222
C1407	C1407	A1301	G1232	G1143	G1068	A990	C915	G815	G720	G650	A575	A488	U384	A280	A223
C1407	C1407	A1300	G1233	G1144	G1069	A991	G916	G816	G721	G651	A576	A489	U385	A281	A224
C1407	C1407	A1299	G1234	G1145	G1070	A992	G917	G817	G722	G652	A577	A490	U386	A282	A225
C1407	C1407	A1298	G1235	G1146	G1071	A993	A918	G818	G723	G653	A578	A491	U387	A283	A226
C1407	C1407	A1297	G1236	G1147	G1072	A994	A919	G819	G724	G654	A579	A492	U388	A284	A227
C1407	C1407	A1296	G1237	G1148	G1073	A995	A920	G820	G725	G655	A580	A493	U389	A285	A228
C1407	C1407	A1295	G1238	G1149	G1074	A996	A921	G821	G726	G656	A581	A494	U390	A286	A229
C1407	C1407	A1294	G1239	G1150	G1075	A997	A922	G822	G727	G657	A582	A495	U391	A287	A230
C1407	C1407	A1293	G1240	G1151	G1076	A998	C923	G823	G728	G658	A583	A496	U392	A288	A231
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C1407	C1407	A1291	G1242	G1153	G1078	A1000	C925	G825	G730	G660	A585	A498	U394	A290	A233
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C1407	C1407	A1232	G1301	G1212	G1137	A1059	A984	G884	G789	G719	A644	A557	U453	A349	A292
C1407	C1407	A1231	G1302	G1213	G1138	A1060	A985	G885	G790	G720	A645	A558	U454	A350	A293
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C1407	C1407	A1229	G1304	G1215	G1140	A1062	A987	G887	G792	G722	A647	A560	U456	A352	A295
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C1407	C1407	A1226	G1307	G1218	G1143	A1065	A990	G890	G795	G725	A650	A563	U459	A355	A298
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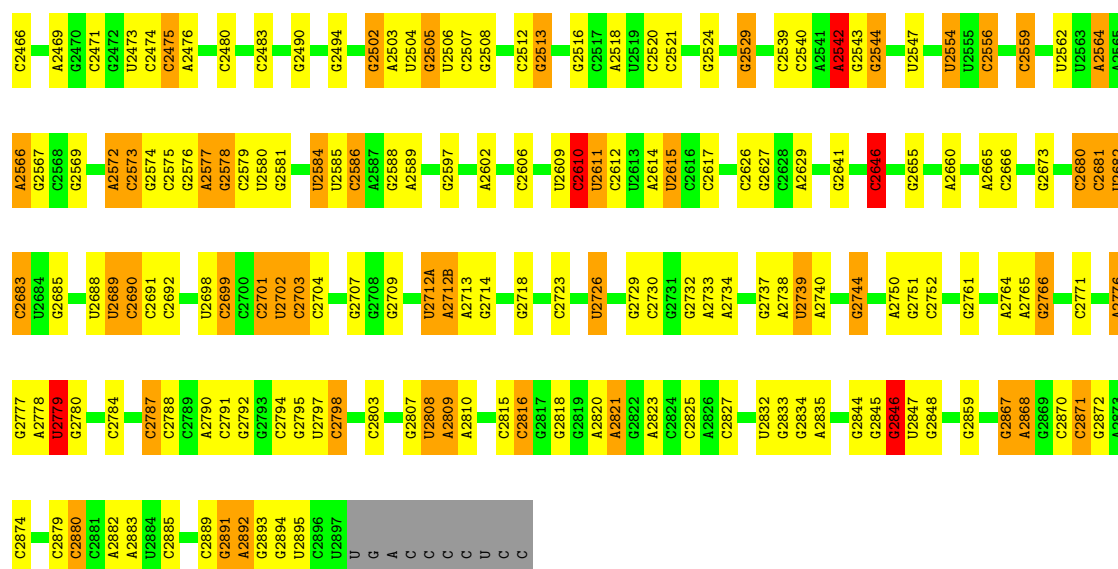


• Molecule 34: 23S rRNA

Chain YA: 53% 35% 10% ..

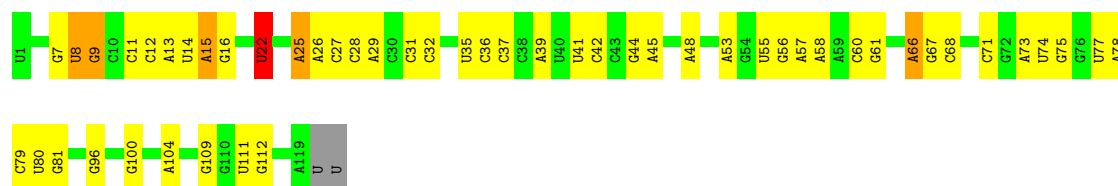


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G2385	G2215	G2213	G2131	G2061	A1972		C1781	G1674		G1473			U1188	U1096
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G2390	G2312	G2226	C2137			C1887	A1786	G1682	A1585				C1196	U1101
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G2448	G2387	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2449	G2388	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2450	G2389	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2451	G2390	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2452	G2391	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2453	G2392	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2454	G2393	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2455	G2394	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2456	G2395	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2457	G2396	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2458	G2397	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2459	G2398	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2460	G2399	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2461	G2400	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2462	G2401	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2463	G2402	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2464	G2403	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2465	G2404	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2466	G2405	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2467	G2406	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2468	G2407	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2469	G2408	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2470	G2409	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2471	G2410	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A1669	G1560	C1463	G1369	C1270	C1180
G2472	G2411	A2199	A2199	G2127	G2055	C1967	U1864	U1775	A					



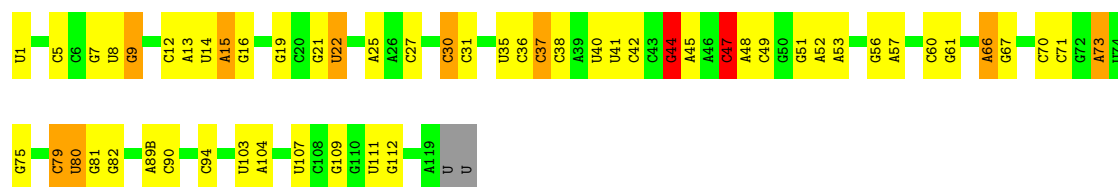
• Molecule 35: 5S rRNA

Chain RB: 57% 37% ..



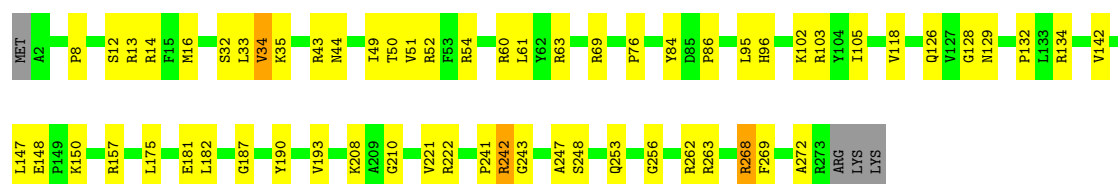
• Molecule 35: 5S rRNA

Chain YB: 53% 36% 7% ..



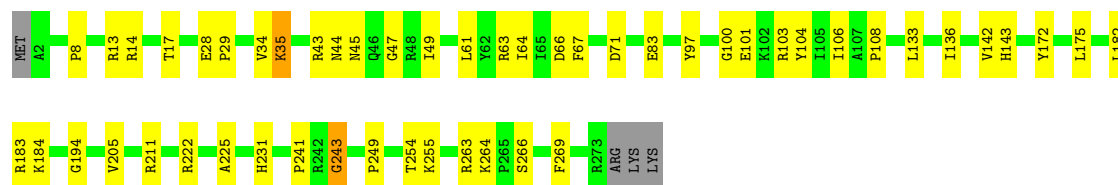
• Molecule 36: 50S ribosomal protein L2

Chain RD: 76% 21% ..

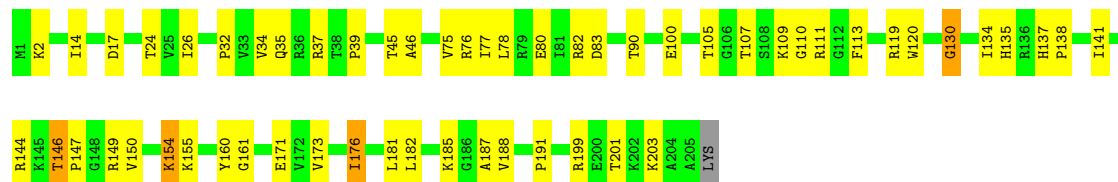
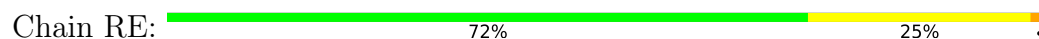


• Molecule 36: 50S ribosomal protein L2

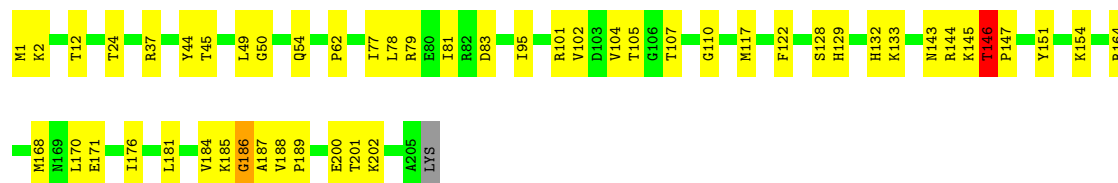
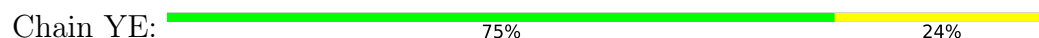
Chain YD: 80% 18% ..



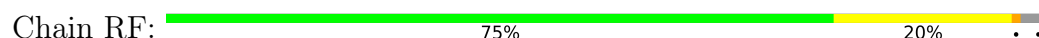
- Molecule 37: 50S ribosomal protein L3



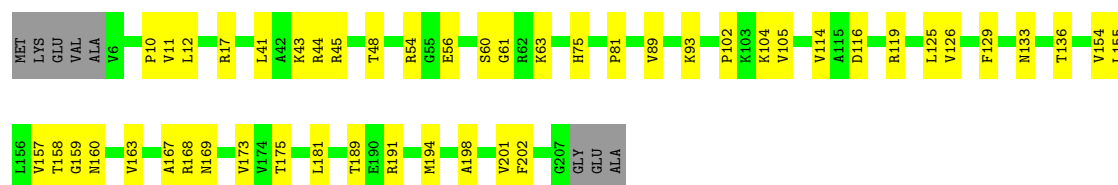
- Molecule 37: 50S ribosomal protein L3



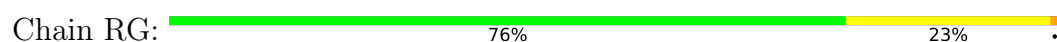
- Molecule 38: 50S ribosomal protein L4

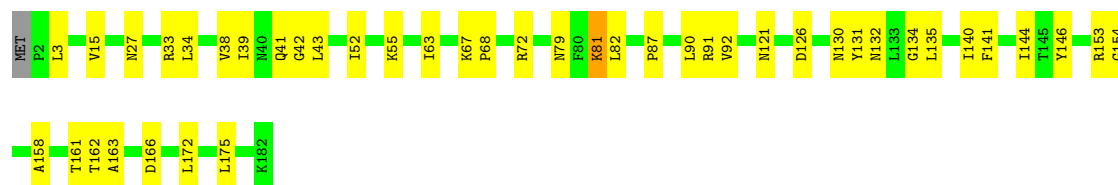


- Molecule 38: 50S ribosomal protein L4



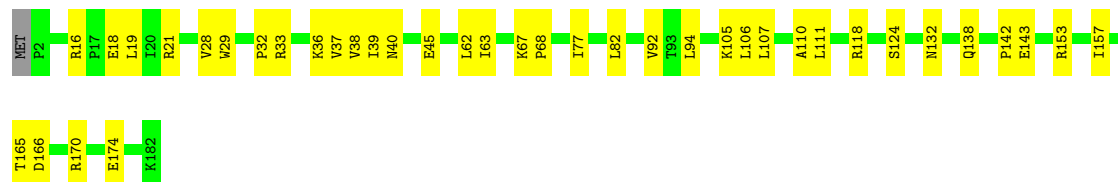
- Molecule 39: 50S ribosomal protein L5





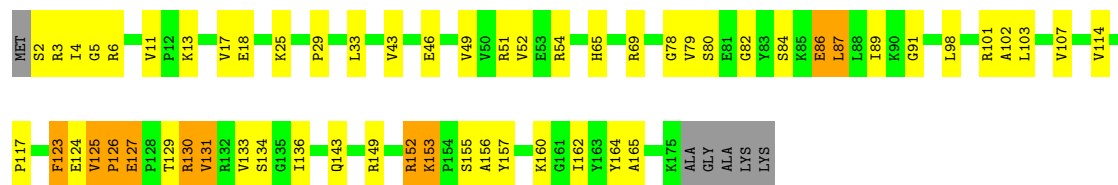
- Molecule 39: 50S ribosomal protein L5

Chain YG: 78% 21% .



- Molecule 40: 50S ribosomal protein L6

Chain RH: 64% 27% 6% .



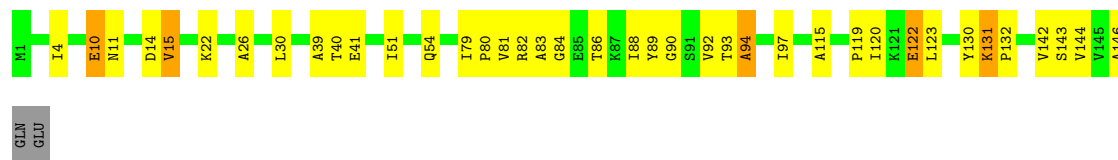
- Molecule 40: 50S ribosomal protein L6

Chain YH: 77% 18% . . .



- Molecule 41: 50S ribosomal protein L9

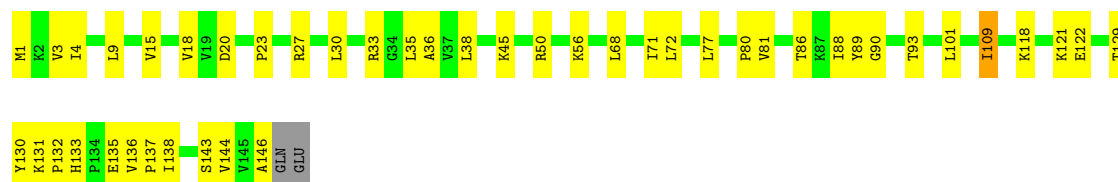
Chain RI: 72% 23% . .



- Molecule 41: 50S ribosomal protein L9

Chain YI: 68% 30% . .





- Molecule 42: 50S ribosomal protein L13

Chain RN: 82% 16% ..



- Molecule 42: 50S ribosomal protein L13

Chain YN: 79% 20% .



- Molecule 43: 50S ribosomal protein L14

Chain RO: 75% 25%



- Molecule 43: 50S ribosomal protein L14

Chain YO: 84% 16%



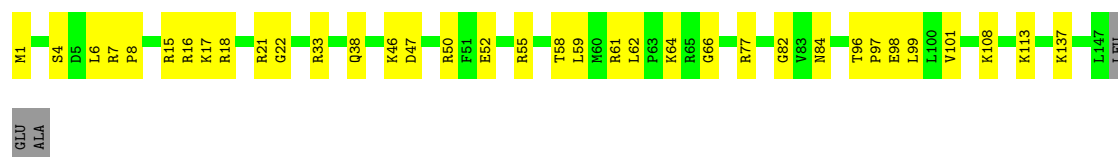
- Molecule 44: 50S ribosomal protein L15

Chain YP: 77% 21%




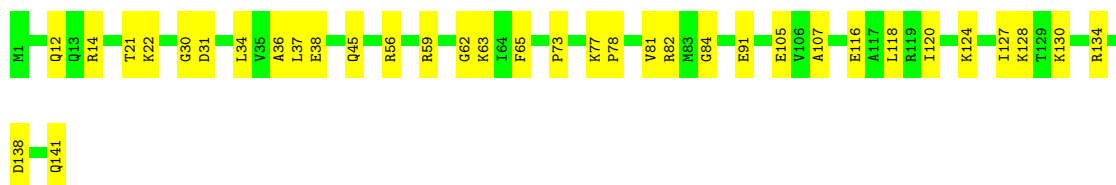
- Molecule 44: 50S ribosomal protein L15

Chain YP: 75% 23%




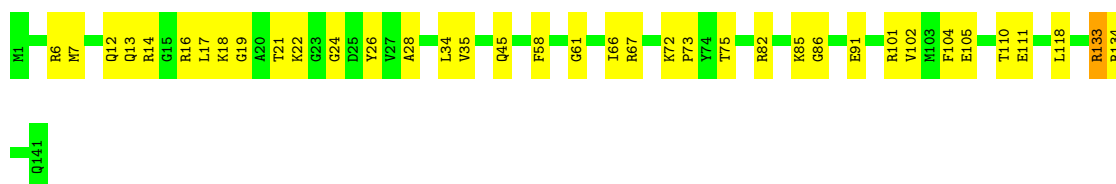
- Molecule 45: 50S ribosomal protein L16

Chain RQ:  75% 25%



- Molecule 45: 50S ribosomal protein L16

Chain YQ:  74% 26%




- Molecule 46: 50S ribosomal protein L17

Chain RR:  69% 28%




- Molecule 46: 50S ribosomal protein L17

Chain YR:  75% 24%




- Molecule 47: 50S ribosomal protein L18

Chain RS:  75% 24%




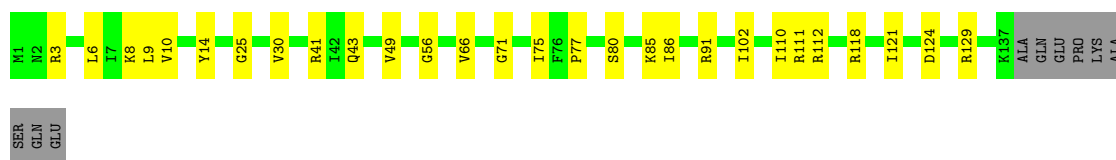
- Molecule 47: 50S ribosomal protein L18

Chain YS:  79% 18%



- Molecule 48: 50S ribosomal protein L19

Chain RT:  75% 19% 6%




- Molecule 48: 50S ribosomal protein L19

Chain YT:  66% 27% 6%




- Molecule 49: 50S ribosomal protein L20

Chain RU:  77% 19% ..




- Molecule 49: 50S ribosomal protein L20

Chain YU:  79% 19% ..




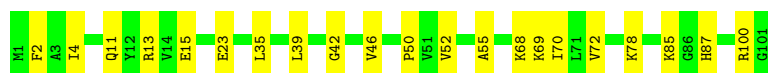
- Molecule 50: 50S ribosomal protein L21

Chain RV:  78% 22%




- Molecule 50: 50S ribosomal protein L21

Chain YV:  79% 21%

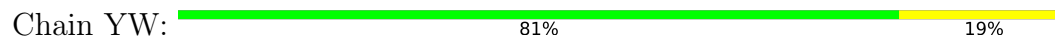


- Molecule 51: 50S ribosomal protein L22

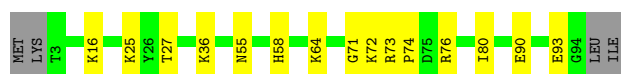
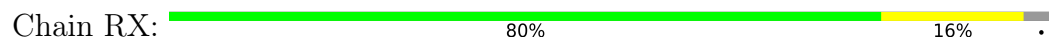
Chain RW:  79% 21%



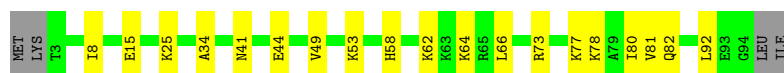
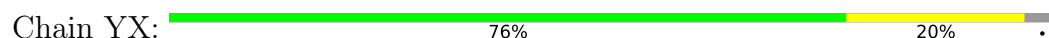
- Molecule 51: 50S ribosomal protein L22



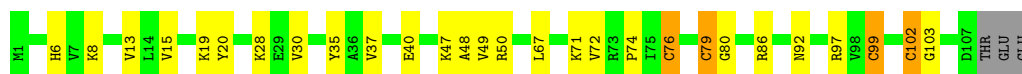
- Molecule 52: 50S ribosomal protein L23



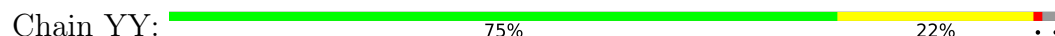
- Molecule 52: 50S ribosomal protein L23



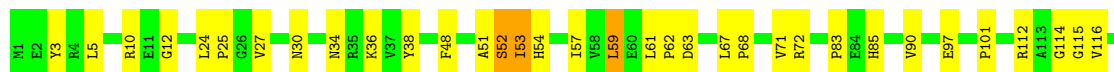
- Molecule 53: 50S ribosomal protein L24



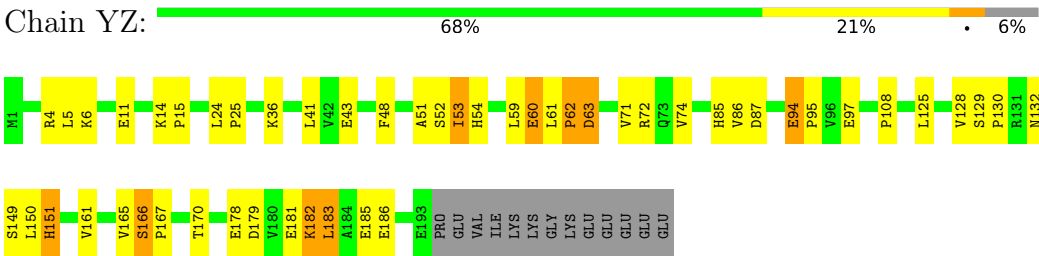
- Molecule 53: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L25



- Molecule 54: 50S ribosomal protein L25



## 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, $\alpha$ , $\beta$ , $\gamma$	210.74Å 450.26Å 626.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.50	Depositor
% Data completeness (in resolution range)	97.6 (49.94-3.50)	Depositor
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.240 , 0.258	Depositor
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.423	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	292039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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	QA	0.69	1/36343 (0.0%)	1.14	198/56720 (0.3%)
1	XA	0.77	0/36435	1.15	194/56865 (0.3%)
2	QB	0.35	0/1942	0.67	0/2619
2	XB	0.37	0/1950	0.64	1/2630 (0.0%)
3	QC	0.36	0/1629	0.66	0/2195
3	XC	0.37	0/1629	0.61	0/2195
4	QD	0.45	1/1733 (0.1%)	0.65	0/2318
4	XD	0.52	2/1733 (0.1%)	0.70	2/2318 (0.1%)
5	QE	0.37	0/1171	0.67	0/1576
5	XE	0.43	0/1171	0.62	0/1576
6	QF	0.39	0/856	0.68	0/1154
6	XF	0.41	0/856	0.62	0/1154
7	QG	0.35	0/1276	0.63	1/1709 (0.1%)
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1128	0.62	0/1517
8	XH	0.42	0/1128	0.66	0/1517
9	QI	0.42	0/1029	0.74	0/1379
9	XI	0.36	0/1017	0.70	0/1365
10	QJ	0.35	0/814	0.67	0/1095
10	XJ	0.34	0/790	0.59	0/1063
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/879	0.59	0/1187
12	QL	0.41	0/991	0.70	1/1327 (0.1%)
12	XL	0.45	0/972	0.77	2/1301 (0.2%)
13	QM	0.35	0/965	0.78	0/1292
13	XM	0.37	0/924	0.66	0/1238
14	QN	0.67	1/501 (0.2%)	0.84	3/664 (0.5%)
14	XN	0.68	1/501 (0.2%)	0.88	2/664 (0.3%)
15	QO	0.38	0/745	0.57	0/992
15	XO	0.40	0/740	0.56	0/987
16	QP	0.40	0/721	0.64	0/970
16	XP	0.38	0/721	0.66	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.39	0/847	0.62	0/1131
17	XQ	0.47	0/847	0.64	0/1131
18	QR	0.37	0/579	0.56	0/768
18	XR	0.39	0/579	0.58	0/768
19	QS	0.35	0/680	0.72	1/915 (0.1%)
19	XS	0.36	0/689	0.70	0/926
20	QT	0.77	2/765 (0.3%)	1.14	8/1007 (0.8%)
20	XT	0.37	0/765	0.75	2/1007 (0.2%)
21	QU	0.34	0/221	0.58	0/288
21	XU	0.32	0/221	0.54	0/288
22	QV	0.70	2/1813 (0.1%)	1.39	32/2825 (1.1%)
22	XV	0.66	0/1813	1.20	13/2825 (0.5%)
23	QX	0.99	1/459 (0.2%)	2.11	25/715 (3.5%)
23	XX	0.63	0/459	1.26	1/715 (0.1%)
24	R0	0.40	0/652	0.63	0/867
24	Y0	0.59	0/657	0.60	0/874
25	R1	0.54	0/753	0.68	0/1000
25	Y1	0.59	0/736	0.73	0/978
26	R2	0.37	0/583	0.62	0/771
26	Y2	0.47	0/577	0.62	0/764
27	R3	0.39	0/474	0.59	0/635
27	Y3	0.62	0/474	0.59	0/635
28	R4	0.33	0/357	0.60	0/483
28	Y4	1.56	2/366 (0.5%)	1.47	8/495 (1.6%)
29	R5	0.88	3/473 (0.6%)	0.79	2/639 (0.3%)
29	Y5	0.94	2/473 (0.4%)	0.77	1/639 (0.2%)
30	R6	0.96	3/460 (0.7%)	0.78	2/613 (0.3%)
30	Y6	1.33	6/460 (1.3%)	1.01	3/613 (0.5%)
31	R7	0.53	0/417	0.62	0/550
31	Y7	0.63	0/426	0.66	0/561
32	R8	0.43	0/525	0.88	3/691 (0.4%)
32	Y8	0.59	0/525	0.84	0/691
33	R9	0.62	1/310 (0.3%)	0.72	1/407 (0.2%)
33	Y9	0.63	0/310	0.73	0/407
34	RA	0.91	2/69520 (0.0%)	1.22	576/108527 (0.5%)
34	YA	1.27	23/69543 (0.0%)	1.33	807/108563 (0.7%)
35	RB	0.71	0/2878	1.14	18/4490 (0.4%)
35	YB	1.08	0/2878	1.32	38/4490 (0.8%)
36	RD	0.52	0/2165	0.71	3/2919 (0.1%)
36	YD	0.64	0/2165	0.74	4/2919 (0.1%)
37	RE	0.50	0/1601	0.83	3/2160 (0.1%)
37	YE	0.66	0/1601	0.84	3/2160 (0.1%)
38	RF	0.49	0/1620	0.70	1/2194 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YF	0.67	0/1620	0.65	1/2194 (0.0%)
39	RG	0.40	0/1499	0.69	0/2016
39	YG	0.43	0/1499	0.68	0/2016
40	RH	0.39	0/1362	0.83	5/1841 (0.3%)
40	YH	0.58	0/1362	0.82	4/1841 (0.2%)
41	RI	0.48	2/1151 (0.2%)	0.86	6/1558 (0.4%)
41	YI	0.45	1/1151 (0.1%)	0.79	0/1558
42	RN	0.45	0/1131	0.68	1/1525 (0.1%)
42	YN	0.63	0/1131	0.70	2/1525 (0.1%)
43	RO	0.51	0/943	0.65	0/1269
43	YO	0.60	0/943	0.63	0/1269
44	RP	0.44	0/1162	0.76	1/1544 (0.1%)
44	YP	0.54	0/1139	0.83	1/1514 (0.1%)
45	RQ	0.45	0/1143	0.73	0/1527
45	YQ	0.61	0/1143	0.77	2/1527 (0.1%)
46	RR	0.48	0/974	0.68	0/1302
46	YR	0.57	0/974	0.70	0/1302
47	RS	0.39	0/892	0.66	0/1187
47	YS	0.52	0/892	0.67	0/1187
48	RT	0.43	0/1155	0.69	0/1542
48	YT	0.54	0/1155	0.72	1/1542 (0.1%)
49	RU	0.49	0/982	0.62	0/1306
49	YU	0.70	0/982	0.61	0/1306
50	RV	0.47	0/790	0.74	1/1057 (0.1%)
50	YV	0.63	0/790	0.76	1/1057 (0.1%)
51	RW	0.52	0/911	0.63	0/1220
51	YW	0.68	0/911	0.64	0/1220
52	RX	0.52	0/739	0.60	0/993
52	YX	0.66	0/739	0.68	0/993
53	RY	0.72	4/831 (0.5%)	0.66	2/1108 (0.2%)
53	YY	0.73	1/831 (0.1%)	0.72	2/1108 (0.2%)
54	RZ	0.43	0/1493	0.89	6/2026 (0.3%)
54	YZ	0.51	0/1561	0.85	5/2119 (0.2%)
All	All	0.87	61/316163 (0.0%)	1.12	2000/472822 (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
28	Y4	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	1	7

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-21.70	1.04	1.54
28	Y4	4	GLY	N-CA	-18.70	1.18	1.46
30	R6	16	CYS	CB-SG	14.24	2.06	1.82
30	Y6	16	CYS	CB-SG	-14.07	1.58	1.82
20	QT	74	LYS	CA-CB	-13.71	1.23	1.53
29	Y5	32	PRO	N-CA	13.22	1.69	1.47
30	Y6	13	CYS	CB-SG	-13.08	1.60	1.82
20	QT	73	HIS	N-CA	-12.34	1.21	1.46
14	QN	43	CYS	CB-SG	11.14	2.01	1.82
4	XD	12	CYS	CB-SG	10.96	2.00	1.82
14	XN	43	CYS	CB-SG	10.95	2.00	1.82
53	RY	102	CYS	CB-SG	-10.82	1.63	1.82
29	R5	34	PRO	N-CD	10.57	1.62	1.47
53	YY	79	CYS	CB-SG	-10.37	1.64	1.82
29	R5	33	CYS	C-N	8.95	1.51	1.34
30	Y6	40	CYS	CB-SG	8.88	1.97	1.82
30	Y6	40	CYS	C-N	8.73	1.50	1.34
33	R9	29	ASN	C-N	8.41	1.50	1.34
53	RY	79	CYS	CB-SG	8.22	1.96	1.82
30	R6	13	CYS	CB-SG	-7.94	1.68	1.82
30	R6	41	PRO	N-CD	7.50	1.58	1.47
34	RA	74	A	N9-C4	-7.27	1.33	1.37
41	RI	94	ALA	C-N	7.08	1.50	1.34
30	Y6	41	PRO	N-CD	7.04	1.57	1.47
41	RI	82	ARG	C-N	-6.80	1.18	1.34
4	QD	8	VAL	CB-CG1	6.80	1.67	1.52
34	YA	1021	A	N9-C4	-6.67	1.33	1.37
23	QX	16	C	N1-C6	6.17	1.40	1.37
53	RY	99	CYS	CB-SG	-6.08	1.72	1.82
34	RA	1601	G	O3'-P	-6.06	1.53	1.61
22	QV	36	G	N7-C5	-6.02	1.35	1.39
22	QV	34	C	N1-C2	6.00	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	YA	74	A	N9-C4	-5.98	1.34	1.37
29	Y5	31	VAL	C-N	5.92	1.45	1.34
34	YA	198	C	C4-C5	-5.86	1.38	1.43
53	RY	76	CYS	CB-SG	-5.84	1.72	1.81
1	QA	1499	A	O3'-P	5.79	1.68	1.61
4	XD	31	CYS	CB-SG	5.55	1.91	1.82
34	YA	1210	A	N9-C4	-5.52	1.34	1.37
34	YA	390	A	N9-C4	-5.47	1.34	1.37
34	YA	783	A	N9-C4	-5.41	1.34	1.37
34	YA	528	A	N9-C4	-5.40	1.34	1.37
30	Y6	51	GLU	CG-CD	-5.35	1.44	1.51
34	YA	1021	A	N3-C4	-5.35	1.31	1.34
34	YA	804	A	N9-C4	-5.33	1.34	1.37
34	YA	2015	A	N7-C5	-5.30	1.36	1.39
34	YA	582	G	N7-C5	-5.29	1.36	1.39
41	YI	109	ILE	C-N	5.28	1.46	1.34
34	YA	1253	A	N9-C4	-5.26	1.34	1.37
34	YA	2453	A	C5-C4	-5.25	1.35	1.38
34	YA	528	A	C5-C6	-5.15	1.36	1.41
29	R5	33	CYS	CB-SG	-5.15	1.73	1.81
34	YA	981	A	N7-C5	-5.12	1.36	1.39
34	YA	2025	C	N1-C6	-5.12	1.34	1.37
34	YA	451	C	N1-C6	-5.09	1.34	1.37
34	YA	2564	A	N9-C4	-5.08	1.34	1.37
34	YA	1658	C	N1-C6	-5.07	1.34	1.37
34	YA	532	A	N7-C5	-5.05	1.36	1.39
34	YA	567	A	N9-C4	-5.03	1.34	1.37
34	YA	2030	A	N9-C4	-5.03	1.34	1.37
34	YA	2542	A	N3-C4	5.01	1.37	1.34

All (2000) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	QT	74	LYS	N-CA-CB	21.28	148.91	110.60
23	QX	17	C	C6-N1-C2	-19.01	112.70	120.30
22	QV	35	G	C8-N9-C4	-16.76	99.70	106.40
28	Y4	5	ILE	CB-CA-C	16.14	143.88	111.60
34	YA	2453	A	N1-C2-N3	-15.63	121.48	129.30
23	QX	18	C	O5'-P-OP1	-15.31	91.92	105.70
37	RE	146	THR	C-N-CD	-15.29	86.97	120.60
54	RZ	166	SER	C-N-CD	-14.13	89.52	120.60
37	YE	146	THR	C-N-CD	-14.12	89.53	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	15	A	P-O3'-C3'	-13.61	103.37	119.70
40	RH	86	GLU	CB-CA-C	-12.84	84.72	110.40
54	YZ	166	SER	C-N-CD	-12.60	92.88	120.60
1	XA	1301	U	C2-N1-C1'	12.40	132.58	117.70
1	XA	1158	C	N1-C2-O2	11.98	126.09	118.90
1	QA	1301	U	C2-N1-C1'	11.78	131.84	117.70
23	QX	18	C	N1-C2-O2	11.78	125.97	118.90
1	QA	754	C	C2-N1-C1'	11.76	131.74	118.80
1	QA	754	C	N1-C2-O2	11.76	125.96	118.90
1	XA	1158	C	C2-N1-C1'	11.73	131.70	118.80
23	QX	18	C	C2-N1-C1'	11.72	131.69	118.80
22	QV	35	G	O5'-P-OP1	-11.31	95.52	105.70
34	YA	856	C	C6-N1-C2	-11.28	115.79	120.30
22	QV	35	G	N7-C8-N9	11.26	118.73	113.10
23	QX	18	C	C6-N1-C1'	-11.00	107.60	120.80
1	XA	1301	U	N1-C2-O2	10.97	130.48	122.80
34	YA	2542	A	N9-C4-C5	-10.95	101.42	105.80
34	RA	856	C	C6-N1-C2	-10.75	116.00	120.30
1	QA	1301	U	N1-C2-O2	10.56	130.20	122.80
34	RA	828	U	C2-N1-C1'	10.38	130.15	117.70
1	XA	754	C	C2-N1-C1'	10.29	130.12	118.80
23	QX	17	C	C5-C6-N1	10.27	126.13	121.00
34	RA	1313	U	C2-N1-C1'	10.17	129.91	117.70
34	RA	1407	C	C6-N1-C2	-10.17	116.23	120.30
34	YA	1658	C	C5-C6-N1	10.05	126.03	121.00
34	YA	537	C	C5-C6-N1	10.04	126.02	121.00
34	RA	120	U	N3-C2-O2	-10.00	115.20	122.20
34	YA	2063	C	N1-C2-O2	10.00	124.90	118.90
34	RA	1762	A	C6-N1-C2	-9.99	112.61	118.60
34	RA	828	U	N1-C2-O2	9.94	129.76	122.80
34	YA	1653	G	N1-C6-O6	-9.92	113.95	119.90
1	XA	1301	U	N3-C2-O2	-9.90	115.27	122.20
30	Y6	43	CYS	N-CA-CB	-9.84	92.89	110.60
1	XA	121	C	C2-N3-C4	-9.83	114.98	119.90
1	QA	1301	U	N3-C2-O2	-9.80	115.34	122.20
34	RA	120	U	N1-C2-O2	9.70	129.59	122.80
34	YA	2032	G	C5-N7-C8	-9.66	99.47	104.30
34	YA	1956	U	N3-C2-O2	-9.64	115.45	122.20
1	QA	754	C	N3-C2-O2	-9.60	115.18	121.90
34	YA	1914	C	N1-C2-O2	9.55	124.63	118.90
34	RA	1407	C	C2-N1-C1'	9.52	129.28	118.80
37	YE	146	THR	C-N-CA	9.52	161.97	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	17	C	C2-N1-C1'	9.48	129.23	118.80
34	YA	1788	C	C5-C6-N1	9.47	125.74	121.00
34	RA	1314	C	C2-N1-C1'	9.44	129.18	118.80
1	XA	618	C	N1-C2-O2	9.44	124.56	118.90
34	YA	1535	U	N1-C2-O2	9.39	129.37	122.80
1	XA	1158	C	N3-C2-O2	-9.37	115.34	121.90
34	YA	1653	G	N3-C4-C5	-9.31	123.95	128.60
34	YA	837	C	C6-N1-C2	-9.23	116.61	120.30
34	YA	1914	C	C2-N1-C1'	9.20	128.92	118.80
34	YA	860	U	N3-C2-O2	-9.19	115.77	122.20
34	RA	1640	C	N1-C2-O2	9.16	124.40	118.90
34	RA	2143	C	N3-C2-O2	-9.16	115.49	121.90
23	QX	18	C	N3-C4-N4	9.15	124.41	118.00
1	QA	1358	U	N3-C2-O2	-9.15	115.80	122.20
54	RZ	166	SER	C-N-CA	9.14	160.39	122.00
34	YA	2544	G	C5-N7-C8	-9.13	99.73	104.30
34	RA	856	C	C5-C6-N1	9.11	125.56	121.00
30	R6	16	CYS	CA-CB-SG	9.10	130.39	114.00
34	YA	2868	A	N7-C8-N9	9.10	118.35	113.80
20	QT	74	LYS	N-CA-C	-9.09	86.46	111.00
20	QT	73	HIS	N-CA-C	9.07	135.49	111.00
1	QA	618	C	N1-C2-O2	9.07	124.34	118.90
22	QV	34	C	N1-C2-O2	8.99	124.30	118.90
34	RA	1417	C	C5-C6-N1	8.99	125.50	121.00
1	QA	1358	U	N1-C2-O2	8.96	129.07	122.80
34	YA	120	U	N3-C2-O2	-8.95	115.93	122.20
1	QA	90	C	C2-N1-C1'	8.93	128.62	118.80
34	YA	856	C	C5-C6-N1	8.93	125.46	121.00
34	YA	1314	C	C2-N1-C1'	8.91	128.60	118.80
1	XA	1301	U	C5-C6-N1	8.91	127.15	122.70
28	Y4	39	CYS	C-N-CA	8.90	143.96	121.70
34	YA	1313	U	C2-N1-C1'	8.89	128.37	117.70
34	RA	1632	A	C5-N7-C8	-8.89	99.45	103.90
28	Y4	5	ILE	N-CA-C	-8.88	87.02	111.00
34	YA	2544	G	C4-C5-N7	8.87	114.35	110.80
35	YB	31	C	N1-C2-O2	8.85	124.21	118.90
1	QA	1395	C	C2-N1-C1'	8.83	128.51	118.80
34	RA	1535	U	C2-N1-C1'	8.79	128.25	117.70
34	YA	1535	U	C2-N1-C1'	8.79	128.25	117.70
34	YA	753	C	C5-C6-N1	8.77	125.38	121.00
34	YA	2063	C	N3-C2-O2	-8.75	115.78	121.90
1	XA	1019	C	N3-C2-O2	-8.70	115.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	136	C	C2-N1-C1'	8.66	128.33	118.80
34	YA	1640	C	N1-C2-O2	8.64	124.09	118.90
34	YA	198	C	C5-C6-N1	8.63	125.31	121.00
34	YA	795	C	C6-N1-C2	-8.62	116.85	120.30
34	RA	1882	C	C2-N1-C1'	8.61	128.28	118.80
35	RB	11	C	N1-C2-O2	8.61	124.06	118.90
34	YA	31	C	C5-C6-N1	8.61	125.30	121.00
34	RA	828	U	N3-C2-O2	-8.60	116.18	122.20
34	RA	889	C	O4'-C1'-N1	8.58	115.06	108.20
34	RA	456	C	C2-N1-C1'	8.57	128.23	118.80
34	YA	343	C	C6-N1-C2	-8.56	116.88	120.30
34	RA	1135	C	N1-C2-O2	8.55	124.03	118.90
34	YA	1407	C	C2-N1-C1'	8.55	128.20	118.80
34	YA	1658	C	C6-N1-C2	-8.54	116.88	120.30
34	RA	613	U	N1-C2-O2	8.54	128.78	122.80
1	XA	221	C	N1-C2-O2	8.51	124.00	118.90
54	YZ	166	SER	C-N-CA	8.51	157.72	122.00
1	XA	1539	C	N3-C2-O2	-8.50	115.95	121.90
2	XB	89	GLY	C-N-CA	8.49	142.92	121.70
34	RA	1407	C	C5-C6-N1	8.45	125.23	121.00
34	YA	2808	U	N3-C2-O2	-8.45	116.28	122.20
30	Y6	43	CYS	CB-CA-C	8.43	127.27	110.40
37	RE	146	THR	C-N-CA	8.43	157.41	122.00
22	QV	35	G	N9-C4-C5	8.43	108.77	105.40
34	RA	669	G	C4-N9-C1'	8.39	137.41	126.50
34	YA	1653	G	C6-N1-C2	-8.38	120.07	125.10
34	YA	2712(B)	A	N7-C8-N9	8.34	117.97	113.80
34	YA	1535	U	N3-C2-O2	-8.34	116.36	122.20
34	YA	2726	U	N3-C2-O2	-8.32	116.38	122.20
34	RA	613	U	N3-C2-O2	-8.31	116.38	122.20
1	XA	1383	C	N1-C2-O2	8.31	123.89	118.90
4	XD	18	LYS	CD-CE-NZ	8.30	130.79	111.70
34	YA	97	C	C6-N1-C2	-8.29	116.98	120.30
34	YA	2542	A	C8-N9-C4	8.29	109.12	105.80
22	QV	35	G	C4-N9-C1'	8.26	137.24	126.50
34	YA	120	U	N1-C2-O2	8.24	128.57	122.80
1	XA	1348	U	N1-C2-O2	8.24	128.57	122.80
34	YA	343	C	C5-C6-N1	8.24	125.12	121.00
34	YA	661	C	C6-N1-C2	-8.23	117.01	120.30
34	YA	1264	G	C8-N9-C4	-8.22	103.11	106.40
34	YA	1313	U	N3-C2-O2	-8.21	116.45	122.20
1	XA	1019	C	N1-C2-O2	8.20	123.82	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	754	C	C6-N1-C1'	-8.19	110.97	120.80
34	YA	2453	A	C2-N3-C4	8.18	114.69	110.60
1	XA	498	U	N3-C2-O2	-8.18	116.48	122.20
34	RA	1535	U	N3-C2-O2	-8.17	116.48	122.20
1	XA	312	C	N3-C2-O2	-8.14	116.20	121.90
36	YD	34	VAL	N-CA-C	-8.14	89.02	111.00
22	XV	15	G	C4-N9-C1'	8.13	137.07	126.50
34	YA	2868	A	C8-N9-C4	-8.12	102.55	105.80
35	YB	27	C	N1-C2-O2	8.12	123.77	118.90
1	QA	1348	U	N1-C2-O2	8.12	128.48	122.80
34	RA	1535	U	N1-C2-O2	8.09	128.46	122.80
34	RA	1804	C	C6-N1-C2	-8.07	117.07	120.30
34	YA	749	C	N1-C2-O2	8.07	123.74	118.90
34	RA	1914	C	C2-N1-C1'	8.05	127.65	118.80
1	XA	1158	C	C6-N1-C2	-8.05	117.08	120.30
1	XA	738	C	C5-C6-N1	8.04	125.02	121.00
1	XA	1301	U	C6-N1-C1'	-8.03	109.95	121.20
22	QV	36	G	C5'-C4'-O4'	8.03	118.74	109.10
29	Y5	32	PRO	CA-N-CD	-8.03	100.26	111.50
34	YA	1135	C	N1-C2-O2	8.02	123.71	118.90
34	YA	2739	U	N3-C2-O2	-8.01	116.59	122.20
34	RA	1313	U	N1-C2-O2	8.01	128.41	122.80
40	RH	152	ARG	C-N-CA	7.99	141.68	121.70
34	YA	1788	C	C6-N1-C2	-7.99	117.10	120.30
23	QX	19	U	C4-C5-C6	7.99	124.50	119.70
34	RA	1313	U	N3-C2-O2	-7.99	116.61	122.20
1	XA	1158	C	C6-N1-C1'	-7.99	111.21	120.80
40	YH	151	ILE	N-CA-C	-7.98	89.45	111.00
34	YA	2542	A	C2-N3-C4	-7.98	106.61	110.60
34	RA	856	C	C2-N1-C1'	7.98	127.58	118.80
34	YA	2465	C	C5-C6-N1	7.98	124.99	121.00
34	YA	373	U	N3-C2-O2	-7.97	116.62	122.20
34	YA	2712(B)	A	C8-N9-C4	-7.94	102.63	105.80
1	QA	307	C	N1-C2-O2	7.93	123.66	118.90
34	YA	198	C	C6-N1-C2	-7.93	117.13	120.30
34	YA	1407	C	C6-N1-C2	-7.92	117.13	120.30
34	YA	795	C	C5-C6-N1	7.92	124.96	121.00
34	RA	613	U	C2-N1-C1'	7.91	127.20	117.70
34	YA	2726	U	C2-N1-C1'	7.91	127.19	117.70
34	YA	2815	C	C6-N1-C2	-7.90	117.14	120.30
34	YA	856	C	C2-N1-C1'	7.89	127.48	118.80
34	YA	2465	C	C6-N1-C2	-7.88	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	753	C	C5-C6-N1	7.88	124.94	121.00
34	RA	1804	C	C5-C6-N1	7.88	124.94	121.00
34	YA	915	C	C2-N1-C1'	7.87	127.46	118.80
34	RA	2210	G	C4-N9-C1'	7.87	136.73	126.50
34	YA	837	C	C5-C6-N1	7.87	124.94	121.00
34	YA	1979	C	C6-N1-C2	-7.87	117.15	120.30
34	RA	1417	C	C2-N1-C1'	7.87	127.45	118.80
1	XA	754	C	C6-N1-C1'	-7.87	111.36	120.80
22	QV	30	C	C6-N1-C2	-7.86	117.16	120.30
34	YA	392	C	C6-N1-C2	-7.86	117.16	120.30
34	YA	1882	C	C6-N1-C2	-7.85	117.16	120.30
34	YA	2416	C	C6-N1-C2	-7.85	117.16	120.30
34	RA	31	C	C5-C6-N1	7.84	124.92	121.00
34	RA	2542	A	C2-N3-C4	-7.84	106.68	110.60
34	RA	1406	U	C2-N1-C1'	7.84	127.10	117.70
34	YA	889	C	O4'-C1'-N1	7.84	114.47	108.20
34	YA	2808	U	N1-C2-O2	7.84	128.29	122.80
34	YA	2210	G	C4-N9-C1'	7.83	136.67	126.50
1	XA	1328	C	N3-C2-O2	-7.82	116.43	121.90
34	YA	930	U	C2-N1-C1'	7.82	127.08	117.70
34	YA	120	U	C2-N1-C1'	7.81	127.07	117.70
34	YA	1640	C	C2-N1-C1'	7.81	127.39	118.80
34	YA	97	C	C5-C6-N1	7.80	124.90	121.00
34	RA	2847	U	N1-C2-O2	7.80	128.26	122.80
34	YA	2416	C	C5-C6-N1	7.79	124.90	121.00
34	RA	1914	C	N1-C2-O2	7.78	123.56	118.90
34	YA	530	G	O4'-C1'-N9	7.77	114.42	108.20
34	YA	1640	C	C6-N1-C2	-7.75	117.20	120.30
28	Y4	5	ILE	N-CA-CB	7.75	128.62	110.80
28	Y4	3	GLU	C-N-CA	-7.75	106.03	122.30
1	XA	618	C	N3-C2-O2	-7.73	116.49	121.90
34	RA	1180	C	C2-N1-C1'	7.72	127.29	118.80
1	QA	1301	U	C6-N1-C1'	-7.71	110.40	121.20
1	XA	1383	C	N3-C2-O2	-7.70	116.51	121.90
34	YA	1437	C	C6-N1-C2	-7.69	117.22	120.30
34	YA	2712(A)	U	N3-C2-O2	-7.69	116.82	122.20
41	RI	82	ARG	C-N-CA	-7.69	102.48	121.70
34	YA	1313	U	N1-C2-O2	7.68	128.18	122.80
34	RA	1078	U	N1-C2-O2	7.68	128.18	122.80
34	RA	456	C	N1-C2-O2	7.67	123.50	118.90
34	YA	2666	C	N1-C2-O2	7.67	123.50	118.90
1	QA	330	C	N1-C2-O2	7.66	123.50	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1914	C	N3-C2-O2	-7.66	116.54	121.90
34	RA	912	C	C2-N1-C1'	7.65	127.21	118.80
34	YA	2063	C	C2-N1-C1'	7.64	127.20	118.80
34	YA	2394	C	N1-C2-O2	7.64	123.48	118.90
34	RA	2295	C	C5-C6-N1	7.64	124.82	121.00
35	YB	37	C	N3-C2-O2	-7.64	116.56	121.90
34	YA	1598	C	C2-N1-C1'	7.63	127.20	118.80
34	YA	1375	C	C5-C6-N1	7.62	124.81	121.00
34	YA	12	U	N3-C2-O2	-7.62	116.87	122.20
34	YA	860	U	C2-N1-C1'	7.62	126.84	117.70
14	QN	24	CYS	CA-CB-SG	7.61	127.70	114.00
1	XA	125	U	N1-C2-N3	7.58	119.45	114.90
35	RB	11	C	N3-C2-O2	-7.58	116.59	121.90
34	RA	676	A	N7-C8-N9	7.58	117.59	113.80
1	XA	1322	C	N1-C2-O2	7.57	123.44	118.90
1	QA	1358	U	C2-N1-C1'	7.56	126.77	117.70
34	YA	930	U	N1-C2-O2	7.56	128.09	122.80
34	YA	1534	G	N3-C4-C5	-7.55	124.82	128.60
20	QT	73	HIS	N-CA-CB	7.54	124.18	110.60
34	RA	2847	U	N3-C2-O2	-7.54	116.92	122.20
1	XA	221	C	N3-C2-O2	-7.54	116.62	121.90
34	YA	2787	C	C2-N1-C1'	7.54	127.09	118.80
1	QA	754	C	C6-N1-C2	-7.53	117.29	120.30
35	YB	47	C	N1-C2-O2	7.53	123.42	118.90
34	YA	1640	C	N3-C2-O2	-7.52	116.63	121.90
34	YA	806	C	N1-C2-O2	7.52	123.41	118.90
34	YA	1180	C	C5-C6-N1	7.51	124.76	121.00
34	YA	2044	C	C6-N1-C2	-7.51	117.30	120.30
34	RA	1474	C	C6-N1-C2	-7.50	117.30	120.30
34	RA	2179	C	N1-C2-O2	7.50	123.40	118.90
34	YA	1892	C	C6-N1-C2	-7.49	117.30	120.30
34	YA	1534	G	N3-C4-N9	7.48	130.49	126.00
34	YA	183	C	C6-N1-C2	-7.47	117.31	120.30
34	YA	797	C	C5-C6-N1	7.47	124.73	121.00
34	RA	120	U	C2-N1-C1'	7.46	126.66	117.70
23	QX	19	U	N3-C4-C5	-7.46	110.12	114.60
34	RA	749	C	N1-C2-O2	7.46	123.38	118.90
34	RA	456	C	C6-N1-C2	-7.46	117.32	120.30
34	RA	1881	C	C2-N1-C1'	7.46	127.00	118.80
34	YA	860	U	N1-C2-O2	7.45	128.02	122.80
34	YA	856	C	N1-C2-O2	7.45	123.37	118.90
34	YA	2321	G	C4-N9-C1'	7.43	136.16	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	2168	G	C4-N9-C1'	7.43	136.16	126.50
34	YA	1882	C	C2-N1-C1'	7.43	126.97	118.80
34	YA	640	C	C5-C6-N1	7.43	124.71	121.00
34	YA	753	C	C6-N1-C2	-7.41	117.33	120.30
34	RA	1640	C	N3-C2-O2	-7.41	116.71	121.90
1	QA	1301	U	C5-C6-N1	7.40	126.40	122.70
36	RD	34	VAL	N-CA-C	-7.39	91.04	111.00
34	YA	930	U	N3-C2-O2	-7.39	117.02	122.20
34	YA	2032	G	C8-N9-C1'	7.39	136.61	127.00
35	YB	30	C	C6-N1-C2	-7.39	117.34	120.30
34	YA	2108	C	N1-C2-O2	7.39	123.33	118.90
34	YA	1180	C	C6-N1-C2	-7.38	117.35	120.30
1	QA	307	C	N3-C2-O2	-7.37	116.74	121.90
34	YA	41	C	C6-N1-C2	-7.37	117.35	120.30
34	RA	1180	C	C5-C6-N1	7.35	124.68	121.00
34	YA	2044	C	C5-C6-N1	7.35	124.67	121.00
34	RA	1774	C	N1-C2-O2	7.34	123.31	118.90
23	QX	18	C	O5'-P-OP2	7.34	119.51	110.70
34	RA	1406	U	C5-C6-N1	7.34	126.37	122.70
1	XA	115	G	P-O3'-C3'	7.33	128.50	119.70
34	RA	2712(A)	U	C2'-C3'-O3'	7.33	125.63	109.50
34	RA	2814	C	N1-C2-O2	7.33	123.30	118.90
34	YA	1656	C	C6-N1-C2	-7.32	117.37	120.30
34	RA	1741	C	N1-C2-O2	7.32	123.29	118.90
34	YA	1314	C	C6-N1-C2	-7.31	117.38	120.30
1	XA	1348	U	N3-C2-O2	-7.31	117.09	122.20
34	RA	2143	C	C6-N1-C2	-7.30	117.38	120.30
34	RA	2701	C	C6-N1-C2	-7.30	117.38	120.30
34	YA	2726	U	N1-C2-O2	7.30	127.91	122.80
34	RA	1267	U	N3-C2-O2	-7.30	117.09	122.20
1	QA	136	C	N1-C2-O2	7.29	123.28	118.90
1	XA	1149	C	N3-C2-O2	-7.29	116.80	121.90
34	YA	1774	C	C2-N1-C1'	7.29	126.81	118.80
1	QA	618	C	N3-C2-O2	-7.28	116.80	121.90
34	RA	1956	U	N3-C2-O2	-7.28	117.10	122.20
34	YA	1598	C	N1-C2-O2	7.28	123.27	118.90
34	RA	63	U	O4'-C1'-N1	7.27	114.02	108.20
34	YA	974(B)	C	C2-N1-C1'	7.27	126.79	118.80
34	RA	1774	C	C6-N1-C2	-7.26	117.40	120.30
1	QA	1263	C	C2-N1-C1'	7.25	126.78	118.80
34	RA	669	G	C8-N9-C1'	-7.23	117.60	127.00
34	RA	2703	C	C2-N1-C1'	7.23	126.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	125	U	C6-N1-C2	-7.23	116.66	121.00
1	QA	620	C	N1-C2-O2	7.23	123.24	118.90
35	YB	31	C	N3-C2-O2	-7.22	116.84	121.90
34	YA	1375	C	C6-N1-C2	-7.22	117.41	120.30
34	RA	721	C	C2-N1-C1'	7.22	126.74	118.80
1	XA	514	C	C2-N1-C1'	7.22	126.74	118.80
34	YA	640	C	C6-N1-C2	-7.22	117.41	120.30
34	RA	114	U	C2-N1-C1'	7.21	126.36	117.70
34	YA	114	U	C2-N1-C1'	7.21	126.35	117.70
34	YA	2870	C	C6-N1-C2	-7.20	117.42	120.30
34	YA	1956	U	N1-C2-O2	7.19	127.84	122.80
1	XA	1306	A	C8-N9-C4	-7.19	102.92	105.80
34	YA	1407	C	C5-C6-N1	7.19	124.60	121.00
1	XA	1395	C	C2-N1-C1'	7.18	126.70	118.80
34	RA	2006	C	C2-N1-C1'	7.18	126.69	118.80
1	QA	136	C	C6-N1-C2	-7.17	117.43	120.30
35	YB	37	C	N1-C2-O2	7.16	123.20	118.90
22	QV	35	G	N3-C4-C5	-7.16	125.02	128.60
34	YA	650	C	C5-C6-N1	7.16	124.58	121.00
34	YA	1636	C	C6-N1-C2	-7.16	117.44	120.30
34	RA	2321	G	C4-N9-C1'	7.16	135.80	126.50
34	YA	265	A	O4'-C1'-N9	7.15	113.92	108.20
34	YA	1267	U	C2-N1-C1'	7.15	126.28	117.70
34	YA	1882	C	C5-C6-N1	7.15	124.58	121.00
34	YA	466	A	C8-N9-C4	-7.15	102.94	105.80
34	YA	1804	C	C6-N1-C2	-7.15	117.44	120.30
23	QX	17	C	N3-C2-O2	-7.15	116.90	121.90
36	YD	35	LYS	CA-CB-CG	7.14	129.12	113.40
22	QV	30	C	C2-N1-C1'	7.14	126.66	118.80
34	YA	2211	G	C4-N9-C1'	7.14	135.78	126.50
34	RA	1498	C	C2-N1-C1'	7.14	126.65	118.80
34	YA	2666	C	N3-C2-O2	-7.14	116.90	121.90
34	YA	1306	C	C5-C6-N1	7.13	124.57	121.00
34	RA	828	U	C5-C6-N1	7.13	126.26	122.70
1	QA	1228	C	C2-N1-C1'	7.12	126.64	118.80
1	XA	1537	U	OP1-P-O3'	7.12	120.86	105.20
34	YA	140	A	N7-C8-N9	7.12	117.36	113.80
34	RA	139	G	O4'-C1'-N9	-7.12	102.51	108.20
34	YA	1830	C	C2-N1-C1'	7.12	126.63	118.80
34	YA	806	C	C6-N1-C2	-7.10	117.46	120.30
34	YA	2666	C	C6-N1-C2	-7.10	117.46	120.30
34	RA	753	C	C6-N1-C2	-7.09	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1534	G	C4-N9-C1'	7.09	135.72	126.50
34	YA	2063	C	C6-N1-C2	-7.09	117.46	120.30
34	YA	2584	U	C2-N1-C1'	7.09	126.21	117.70
1	XA	498	U	N1-C2-O2	7.08	127.76	122.80
34	YA	1793	C	C6-N1-C2	-7.08	117.47	120.30
34	YA	31	C	C6-N1-C2	-7.08	117.47	120.30
1	QA	1027	C	C2-N1-C1'	7.08	126.58	118.80
1	QA	241	C	C2-N1-C1'	7.08	126.58	118.80
34	RA	2726	U	C2-N1-C1'	7.08	126.19	117.70
34	RA	1774	C	N3-C2-O2	-7.07	116.95	121.90
34	YA	231	C	C2-N1-C1'	7.06	126.57	118.80
34	RA	2580	U	C2-N1-C1'	7.06	126.17	117.70
34	YA	1506	C	C2-N1-C1'	7.05	126.56	118.80
22	XV	15	G	N3-C4-C5	-7.05	125.07	128.60
34	YA	1830	C	C5-C6-N1	7.05	124.53	121.00
34	RA	2832	U	P-O3'-C3'	7.05	128.16	119.70
34	YA	1407	C	N1-C2-O2	7.05	123.13	118.90
34	YA	2542	A	C4-C5-N7	7.04	114.22	110.70
1	QA	435	C	C5-C6-N1	7.04	124.52	121.00
34	YA	2559	C	C2-N1-C1'	7.04	126.54	118.80
1	XA	962	C	C6-N1-C2	-7.03	117.49	120.30
34	YA	721	C	C2-N1-C1'	7.03	126.53	118.80
1	QA	748	C	P-O3'-C3'	7.02	128.12	119.70
34	RA	2874	C	C2-N1-C1'	7.01	126.51	118.80
34	YA	2185	C	C6-N1-C2	-7.01	117.50	120.30
34	RA	2210	G	C8-N9-C1'	-7.00	117.90	127.00
34	YA	607	U	N1-C2-O2	7.00	127.70	122.80
34	YA	1370	C	C2-N1-C1'	7.00	126.50	118.80
34	YA	2041	U	C5-C6-N1	7.00	126.20	122.70
34	YA	537	C	C6-N1-C2	-7.00	117.50	120.30
34	YA	2032	G	N3-C4-N9	-7.00	121.80	126.00
34	RA	2683	C	N1-C2-O2	6.99	123.10	118.90
41	RI	82	ARG	O-C-N	6.99	133.89	122.70
1	XA	368	U	N3-C2-O2	-6.99	117.31	122.20
34	YA	1474	C	C2-N1-C1'	6.99	126.49	118.80
34	RA	795	C	C6-N1-C2	-6.99	117.50	120.30
34	RA	537	C	C5-C6-N1	6.97	124.48	121.00
34	YA	1332	G	C6-C5-N7	-6.97	126.22	130.40
34	YA	2712(A)	U	P-O3'-C3'	6.97	128.06	119.70
1	XA	1260	C	N1-C2-O2	6.97	123.08	118.90
34	RA	2211	G	C4-N9-C1'	6.96	135.55	126.50
35	YB	1	U	N3-C2-O2	-6.96	117.33	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1915	U	N1-C2-O2	6.96	127.67	122.80
34	YA	1105	U	C2-N1-C1'	6.96	126.05	117.70
1	QA	1066	C	N1-C2-O2	6.95	123.07	118.90
34	YA	1741	C	C2-N1-C1'	6.95	126.44	118.80
34	YA	2507	C	C6-N1-C2	-6.95	117.52	120.30
34	RA	2814	C	N3-C2-O2	-6.94	117.05	121.90
1	QA	1036	G	N3-C4-N9	6.93	130.16	126.00
34	YA	1830	C	C6-N1-C2	-6.93	117.53	120.30
34	YA	1306	C	C6-N1-C2	-6.93	117.53	120.30
1	QA	186(H)	C	C6-N1-C2	-6.93	117.53	120.30
34	RA	2229	C	C6-N1-C2	-6.93	117.53	120.30
20	QT	73	HIS	CB-CA-C	-6.93	96.55	110.40
34	YA	2712(A)	U	C6-N1-C2	-6.92	116.84	121.00
34	YA	1506	C	N1-C2-O2	6.92	123.05	118.90
34	YA	2617	C	N1-C2-O2	6.92	123.05	118.90
34	YA	2559	C	C6-N1-C2	-6.92	117.53	120.30
1	XA	992	U	P-O3'-C3'	6.91	127.99	119.70
34	RA	1135	C	C2-N1-C1'	6.90	126.39	118.80
35	YB	30	C	N1-C2-O2	6.90	123.04	118.90
34	RA	1686	C	C2-N1-C1'	6.90	126.39	118.80
34	YA	2083	G	N3-C4-N9	6.89	130.13	126.00
34	YA	1022	G	P-O3'-C3'	6.89	127.97	119.70
22	QV	36	G	C6-C5-N7	-6.88	126.27	130.40
34	YA	1135	C	C2-N1-C1'	6.88	126.37	118.80
34	RA	2128	C	C2-N1-C1'	6.88	126.36	118.80
34	YA	607	U	N3-C2-O2	-6.88	117.39	122.20
34	YA	1026	U	P-O3'-C3'	6.88	127.95	119.70
34	RA	904	C	N1-C2-O2	6.87	123.03	118.90
1	XA	1260	C	N3-C2-O2	-6.87	117.09	121.90
23	QX	18	C	C5-C4-N4	-6.87	115.39	120.20
34	RA	2559	C	N1-C2-O2	6.87	123.02	118.90
41	RI	131	LYS	N-CA-C	6.87	129.54	111.00
34	RA	721	C	N1-C2-O2	6.86	123.02	118.90
23	QX	18	C	N1-C2-N3	-6.86	114.40	119.20
34	RA	2703	C	C5-C6-N1	6.86	124.43	121.00
34	YA	2196	C	C2-N1-C1'	6.86	126.34	118.80
34	RA	1267	U	N1-C2-O2	6.86	127.60	122.80
34	YA	537	C	C2-N1-C1'	6.85	126.34	118.80
34	YA	2688	U	C2-N1-C1'	6.85	125.92	117.70
1	XA	1537	U	P-O3'-C3'	6.85	127.92	119.70
34	RA	372	G	OP2-P-O3'	6.85	120.27	105.20
34	RA	1314	C	C6-N1-C2	-6.85	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1781	C	N1-C2-O2	6.85	123.01	118.90
34	YA	2065	C	C6-N1-C2	-6.85	117.56	120.30
34	YA	2889	C	N1-C2-O2	6.85	123.01	118.90
35	YB	27	C	C6-N1-C2	-6.85	117.56	120.30
34	YA	1656	C	C5-C6-N1	6.84	124.42	121.00
1	XA	1149	C	N1-C2-O2	6.84	123.00	118.90
34	YA	271(C)	G	P-O3'-C3'	6.84	127.91	119.70
34	RA	1694	C	P-O3'-C3'	6.84	127.91	119.70
34	RA	1632	A	C4-C5-N7	6.83	114.11	110.70
34	RA	343	C	C6-N1-C2	-6.83	117.57	120.30
1	XA	962	C	C5-C6-N1	6.83	124.41	121.00
34	RA	828	U	C6-N1-C1'	-6.82	111.65	121.20
34	YA	141(A)	A	N7-C8-N9	6.82	117.21	113.80
34	YA	1558	A	P-O3'-C3'	6.82	127.89	119.70
34	RA	1314	C	N1-C2-O2	6.82	122.99	118.90
34	YA	846	C	P-O3'-C3'	6.82	127.88	119.70
34	YA	2210	G	C8-N9-C1'	-6.82	118.14	127.00
1	QA	1036	G	C4-N9-C1'	6.81	135.36	126.50
34	RA	1598	C	N1-C2-O2	6.81	122.98	118.90
34	RA	2544	G	C5-N7-C8	-6.80	100.90	104.30
34	YA	1892	C	C5-C6-N1	6.80	124.40	121.00
1	QA	330	C	C6-N1-C2	-6.80	117.58	120.30
1	XA	1064	G	P-O3'-C3'	6.80	127.86	119.70
1	XA	645	C	N1-C2-O2	6.80	122.98	118.90
34	YA	1920	C	C5-C6-N1	6.79	124.39	121.00
34	RA	1836	C	C6-N1-C2	-6.79	117.58	120.30
34	YA	2739	U	N1-C2-O2	6.79	127.55	122.80
34	RA	1914	C	N3-C2-O2	-6.78	117.15	121.90
34	YA	1516	U	C2-N1-C1'	6.78	125.84	117.70
23	QX	19	U	C5-C4-O4	6.78	129.97	125.90
34	YA	2666	C	C2-N1-C1'	6.78	126.26	118.80
35	YB	27	C	N3-C2-O2	-6.78	117.16	121.90
34	RA	2321	G	N3-C4-C5	-6.78	125.21	128.60
34	RA	456	C	C5-C6-N1	6.77	124.39	121.00
1	QA	992	U	P-O3'-C3'	6.77	127.82	119.70
34	RA	837	C	C5-C6-N1	6.77	124.38	121.00
34	YA	1881	C	C2-N1-C1'	6.77	126.24	118.80
35	YB	1	U	N1-C2-O2	6.77	127.54	122.80
1	XA	1296	C	N1-C2-O2	6.76	122.96	118.90
1	QA	330	C	C5-C6-N1	6.76	124.38	121.00
34	YA	41	C	C5-C6-N1	6.76	124.38	121.00
34	YA	1830	C	N1-C2-O2	6.76	122.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1064	C	C6-N1-C2	-6.76	117.60	120.30
1	XA	368	U	N1-C2-O2	6.76	127.53	122.80
34	RA	2507	C	C5-C6-N1	6.75	124.38	121.00
34	RA	2043	C	C5-C6-N1	6.75	124.38	121.00
34	RA	2499	C	C2-N3-C4	-6.75	116.53	119.90
1	XA	1325	C	C2-N1-C1'	6.75	126.22	118.80
34	RA	2064	C	C6-N1-C2	-6.75	117.60	120.30
42	YN	114	ARG	N-CA-C	-6.75	92.78	111.00
34	YA	537	C	N1-C2-O2	6.74	122.94	118.90
35	YB	79	C	C6-N1-C2	-6.74	117.60	120.30
34	RA	976	C	C6-N1-C2	-6.74	117.61	120.30
34	YA	985	C	C5-C6-N1	6.74	124.37	121.00
35	RB	11	C	C2-N1-C1'	6.73	126.20	118.80
1	XA	221	C	C6-N1-C2	-6.73	117.61	120.30
34	YA	1774	C	C6-N1-C2	-6.73	117.61	120.30
34	YA	2465	C	C2-N1-C1'	6.73	126.20	118.80
34	YA	141(A)	A	C5-N7-C8	-6.72	100.54	103.90
1	QA	972	C	C6-N1-C2	-6.72	117.61	120.30
34	RA	459	U	N1-C2-O2	6.72	127.50	122.80
34	YA	650	C	C6-N1-C2	-6.71	117.61	120.30
34	RA	1762	A	C5-C6-N1	6.71	121.05	117.70
34	YA	1332	G	N7-C8-N9	6.71	116.45	113.10
34	RA	2394	C	N1-C2-O2	6.70	122.92	118.90
1	XA	121	C	C5-C4-N4	-6.70	115.51	120.20
34	YA	465	G	C8-N9-C4	-6.70	103.72	106.40
22	QV	30	C	C5-C6-N1	6.70	124.35	121.00
34	RA	1417	C	C6-N1-C2	-6.69	117.62	120.30
40	YH	152	ARG	C-N-CA	6.68	138.41	121.70
34	YA	637	A	P-O3'-C3'	6.68	127.72	119.70
35	RB	27	C	N1-C2-O2	6.68	122.91	118.90
34	YA	1498	C	C2-N1-C1'	6.67	126.14	118.80
34	RA	2814	C	C2-N1-C1'	6.67	126.14	118.80
20	QT	74	LYS	CA-C-O	6.67	134.10	120.10
1	XA	1036	G	N3-C4-C5	-6.66	125.27	128.60
34	RA	1078	U	C2-N1-C1'	6.66	125.69	117.70
35	YB	80	U	N3-C2-O2	-6.66	117.54	122.20
34	RA	1558	A	P-O3'-C3'	6.65	127.69	119.70
34	RA	1882	C	C6-N1-C2	-6.65	117.64	120.30
34	RA	234	C	N1-C2-O2	6.65	122.89	118.90
34	RA	537	C	C2-N1-C1'	6.65	126.11	118.80
34	YA	2032	G	N7-C8-N9	6.65	116.42	113.10
1	QA	91	C	C2-N1-C1'	6.65	126.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	596	C	C6-N1-C2	-6.65	117.64	120.30
34	YA	1914	C	C6-N1-C1'	-6.65	112.82	120.80
34	RA	1506	C	N1-C2-O2	6.64	122.89	118.90
34	YA	2032	G	C4-C5-N7	6.64	113.46	110.80
34	YA	2701	C	C6-N1-C2	-6.64	117.64	120.30
34	YA	758	C	C6-N1-C2	-6.64	117.64	120.30
1	QA	90	C	N1-C2-O2	6.64	122.88	118.90
34	YA	1332	G	C4-N9-C1'	6.64	135.13	126.50
34	YA	2703	C	C2-N1-C1'	6.64	126.10	118.80
1	QA	1075	C	N1-C2-O2	6.63	122.88	118.90
22	QV	34	C	C2-N1-C1'	6.63	126.10	118.80
34	RA	676	A	C8-N9-C4	-6.63	103.15	105.80
34	YA	2610	C	P-O3'-C3'	6.63	127.66	119.70
1	QA	501	C	C6-N1-C2	-6.63	117.65	120.30
34	YA	857	C	C2-N1-C1'	6.63	126.09	118.80
1	XA	754	C	N1-C2-O2	6.62	122.87	118.90
34	YA	2681	C	P-O3'-C3'	6.62	127.64	119.70
34	RA	2442	C	C6-N1-C2	-6.61	117.66	120.30
34	RA	1304	C	C6-N1-C2	-6.61	117.66	120.30
34	RA	67	U	C5-C6-N1	6.61	126.00	122.70
1	XA	962	C	C2-N1-C1'	6.61	126.07	118.80
34	YA	1411	C	C6-N1-C2	-6.61	117.66	120.30
22	QV	34	C	C6-N1-C1'	-6.60	112.88	120.80
34	YA	373	U	N1-C2-O2	6.60	127.42	122.80
1	QA	308	C	N1-C2-O2	6.60	122.86	118.90
34	RA	2847	U	C2-N1-C1'	6.60	125.62	117.70
1	QA	1158	C	C6-N1-C2	-6.60	117.66	120.30
19	QS	41	VAL	N-CA-C	6.60	128.82	111.00
34	YA	1474	C	C6-N1-C2	-6.60	117.66	120.30
34	YA	2779	U	C2-N1-C1'	6.60	125.62	117.70
34	YA	2460	U	C5-C6-N1	6.59	126.00	122.70
34	RA	1306	C	C5-C6-N1	6.58	124.29	121.00
34	RA	2559	C	C2-N1-C1'	6.58	126.04	118.80
34	YA	974(B)	C	N1-C2-O2	6.58	122.84	118.90
34	RA	1102	C	N1-C2-O2	6.57	122.84	118.90
34	YA	2453	A	N9-C4-C5	-6.57	103.17	105.80
34	YA	635	C	C6-N1-C2	-6.57	117.67	120.30
34	RA	1533	C	C2-N1-C1'	6.57	126.03	118.80
35	YB	1	U	C2-N1-C1'	6.57	125.58	117.70
34	YA	634	C	C6-N1-C2	-6.57	117.67	120.30
34	YA	12	U	N1-C2-O2	6.57	127.39	122.80
1	QA	1060	C	C2-N1-C1'	6.56	126.02	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	637	A	P-O3'-C3'	6.56	127.57	119.70
34	YA	544	C	C6-N1-C2	-6.56	117.68	120.30
34	YA	1805	U	C6-N1-C2	-6.55	117.07	121.00
1	QA	838(B)	U	N3-C2-O2	-6.55	117.61	122.20
34	RA	856	C	N1-C2-O2	6.55	122.83	118.90
1	XA	201(A)	C	C2-N1-C1'	6.55	126.00	118.80
34	YA	466	A	N7-C8-N9	6.55	117.07	113.80
34	RA	2128	C	C5-C6-N1	6.54	124.27	121.00
14	XN	28	GLY	N-CA-C	6.54	129.46	113.10
34	RA	1306	C	C6-N1-C2	-6.54	117.68	120.30
34	YA	2584	U	N3-C2-O2	-6.54	117.62	122.20
1	XA	443	C	C2-N1-C1'	6.54	125.99	118.80
34	YA	856	C	N3-C2-O2	-6.54	117.32	121.90
34	YA	392	C	C5-C6-N1	6.54	124.27	121.00
34	YA	1012	U	P-O3'-C3'	6.54	127.54	119.70
34	RA	426	C	N1-C2-O2	6.53	122.82	118.90
34	YA	363(F)	U	C2-N1-C1'	6.53	125.54	117.70
1	XA	514	C	C5-C6-N1	6.53	124.27	121.00
20	QT	74	LYS	CA-C-N	-6.53	102.84	117.20
34	YA	1445	C	C6-N1-C2	-6.53	117.69	120.30
34	YA	2043	C	C5-C6-N1	6.53	124.26	121.00
34	YA	998	C	C6-N1-C2	-6.53	117.69	120.30
34	RA	2043	C	C6-N1-C2	-6.52	117.69	120.30
34	YA	1264	G	N7-C8-N9	6.52	116.36	113.10
34	RA	1267	U	C2-N1-C1'	6.52	125.52	117.70
22	QV	15	G	N3-C4-C5	-6.51	125.34	128.60
34	YA	834	C	C6-N1-C2	-6.51	117.69	120.30
1	QA	503	C	C6-N1-C2	-6.51	117.69	120.30
1	QA	1348	U	C2-N1-C1'	6.51	125.51	117.70
34	RA	2683	C	N3-C2-O2	-6.50	117.35	121.90
34	YA	384	U	N3-C2-O2	-6.50	117.65	122.20
23	QX	19	U	N1-C1'-C2'	-6.49	104.86	112.00
34	RA	846	C	P-O3'-C3'	6.49	127.49	119.70
1	QA	58	C	C5-C6-N1	6.49	124.24	121.00
34	YA	2506	U	N1-C2-O2	6.49	127.34	122.80
34	RA	1294	U	N3-C2-O2	-6.49	117.66	122.20
1	XA	1322	C	C2-N1-C1'	6.49	125.93	118.80
34	YA	1881	C	C6-N1-C2	-6.49	117.71	120.30
34	RA	1474	C	C2-N1-C1'	6.48	125.93	118.80
34	RA	1640	C	C2-N1-C1'	6.48	125.93	118.80
34	YA	2588	G	C4-C5-N7	6.48	113.39	110.80
34	YA	2816	C	C6-N1-C2	-6.48	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YB	27	C	C2-N1-C1'	6.48	125.92	118.80
1	QA	267	C	N1-C2-O2	6.47	122.78	118.90
34	RA	2559	C	C6-N1-C2	-6.47	117.71	120.30
54	RZ	62	PRO	C-N-CA	6.47	137.86	121.70
1	XA	110	C	N1-C2-O2	6.47	122.78	118.90
34	RA	2580	U	N3-C2-O2	-6.46	117.68	122.20
1	QA	443	C	N1-C2-O2	6.46	122.78	118.90
1	QA	1395	C	N1-C2-O2	6.46	122.78	118.90
34	YA	2439	A	P-O3'-C3'	6.46	127.45	119.70
1	QA	962	C	C2-N1-C1'	6.45	125.90	118.80
34	RA	2825	C	N1-C2-O2	6.45	122.77	118.90
34	YA	2784	C	C5-C6-N1	6.45	124.22	121.00
34	YA	672	C	C6-N1-C2	-6.44	117.72	120.30
1	QA	618	C	C2-N1-C1'	6.44	125.89	118.80
34	YA	2646	C	C5-C6-N1	6.44	124.22	121.00
34	YA	1804	C	C5-C6-N1	6.44	124.22	121.00
34	RA	2507	C	C6-N1-C2	-6.44	117.72	120.30
1	XA	121	C	N3-C4-C5	6.44	124.47	121.90
34	RA	459	U	N3-C2-O2	-6.43	117.70	122.20
34	YA	459	U	C2-N1-C1'	6.43	125.42	117.70
1	QA	699	C	C6-N1-C2	-6.43	117.73	120.30
34	YA	1234	U	N3-C2-O2	-6.43	117.70	122.20
34	YA	1404	C	C6-N1-C2	-6.43	117.73	120.30
34	YA	749	C	N3-C2-O2	-6.43	117.40	121.90
1	QA	91	C	N1-C2-O2	6.42	122.75	118.90
34	YA	806	C	N3-C2-O2	-6.42	117.40	121.90
34	YA	2064	C	C6-N1-C2	-6.42	117.73	120.30
1	QA	1325	C	N1-C2-O2	6.42	122.75	118.90
34	YA	2032	G	C8-N9-C4	-6.42	103.83	106.40
34	YA	2825	C	C6-N1-C2	-6.42	117.73	120.30
1	QA	754	C	C5-C6-N1	6.42	124.21	121.00
34	RA	1313	U	C6-N1-C1'	-6.42	112.22	121.20
34	YA	484	C	C6-N1-C2	-6.42	117.73	120.30
22	QV	36	G	C5-C6-O6	-6.41	124.75	128.60
42	RN	114	ARG	N-CA-C	-6.41	93.69	111.00
34	YA	140	A	C8-N9-C4	-6.41	103.24	105.80
34	YA	1045	A	P-O3'-C3'	6.41	127.39	119.70
34	RA	755	C	C5-C6-N1	6.41	124.20	121.00
34	YA	533	G	C8-N9-C4	-6.41	103.84	106.40
22	QV	36	G	N1-C6-O6	6.40	123.74	119.90
1	QA	838(B)	U	N1-C2-O2	6.40	127.28	122.80
34	RA	837	C	C6-N1-C2	-6.40	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1881	C	C5-C6-N1	6.40	124.20	121.00
34	RA	229	A	P-O3'-C3'	6.40	127.38	119.70
30	R6	13	CYS	CA-CB-SG	-6.39	102.49	114.00
34	YA	183	C	C2-N1-C1'	6.39	125.83	118.80
34	RA	1314	C	C6-N1-C1'	-6.39	113.13	120.80
34	RA	31	C	C6-N1-C2	-6.39	117.74	120.30
34	RA	758	C	C6-N1-C2	-6.39	117.74	120.30
34	YA	1653	G	C5-C6-N1	6.39	114.69	111.50
53	RY	99	CYS	CA-CB-SG	6.39	125.50	114.00
1	XA	738	C	C6-N1-C2	-6.39	117.75	120.30
34	YA	613	U	C2-N1-C1'	6.38	125.36	117.70
1	QA	307	C	C6-N1-C2	-6.38	117.75	120.30
1	XA	68(S)	C	C6-N1-C2	-6.38	117.75	120.30
1	XA	368	U	C2-N1-C1'	6.38	125.36	117.70
1	QA	1348	U	N3-C2-O2	-6.38	117.73	122.20
34	YA	2065	C	C5-C6-N1	6.38	124.19	121.00
34	YA	183	C	N1-C2-O2	6.38	122.73	118.90
1	QA	1036	G	N3-C4-C5	-6.38	125.41	128.60
34	RA	1882	C	C5-C6-N1	6.38	124.19	121.00
22	XV	15	G	N3-C4-N9	6.38	129.83	126.00
34	YA	1498	C	N1-C2-O2	6.38	122.72	118.90
34	RA	1544	C	N1-C2-O2	6.37	122.72	118.90
34	YA	2107	C	N1-C2-O2	6.37	122.72	118.90
34	YA	1333	C	C5-C6-N1	6.37	124.18	121.00
1	QA	1263	C	N1-C2-O2	6.36	122.72	118.90
1	QA	1538	C	P-O3'-C3'	6.36	127.34	119.70
34	RA	208	C	C6-N1-C2	-6.36	117.75	120.30
23	QX	18	C	C2-N3-C4	6.36	123.08	119.90
34	RA	1022	G	C2'-C3'-O3'	6.36	123.88	113.70
34	YA	783	A	C5-N7-C8	-6.36	100.72	103.90
34	YA	1013	C	C6-N1-C2	-6.36	117.76	120.30
34	YA	2688	U	N3-C2-O2	-6.36	117.75	122.20
1	QA	1395	C	C6-N1-C2	-6.36	117.76	120.30
34	RA	2126	A	P-O3'-C3'	6.36	127.33	119.70
34	RA	1078	U	N3-C2-O2	-6.35	117.75	122.20
1	QA	1109	C	N1-C2-O2	6.35	122.71	118.90
34	YA	528	A	C5-N7-C8	-6.35	100.72	103.90
22	XV	15	G	C8-N9-C1'	-6.35	118.74	127.00
34	RA	2814	C	C6-N1-C2	-6.35	117.76	120.30
34	YA	661	C	C5-C6-N1	6.35	124.17	121.00
34	RA	1474	C	N1-C2-O2	6.35	122.71	118.90
34	RA	2043	C	C2-N1-C1'	6.34	125.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1325	C	N3-C2-O2	-6.34	117.46	121.90
1	XA	221	C	C2-N1-C1'	6.33	125.77	118.80
34	YA	1893	C	N1-C2-O2	6.33	122.70	118.90
34	RA	343	C	C5-C6-N1	6.33	124.16	121.00
34	YA	1408	C	C6-N1-C2	-6.33	117.77	120.30
1	XA	618	C	C2-N1-C1'	6.33	125.76	118.80
34	RA	965	C	C2-N1-C1'	6.32	125.75	118.80
1	QA	936	C	N1-C2-O2	6.32	122.69	118.90
34	YA	1402	C	C6-N1-C2	-6.32	117.77	120.30
34	RA	1956	U	N1-C2-O2	6.32	127.22	122.80
34	RA	2785	C	C6-N1-C2	-6.32	117.77	120.30
34	RA	459	U	C2-N1-C1'	6.32	125.28	117.70
34	YA	384	U	N1-C2-O2	6.32	127.22	122.80
34	RA	1180	C	C6-N1-C2	-6.31	117.78	120.30
34	YA	392	C	C2-N1-C1'	6.31	125.74	118.80
34	YA	242	G	P-O3'-C3'	6.31	127.27	119.70
34	YA	1653	G	P-O3'-C3'	6.31	127.27	119.70
34	YA	1406	U	C2-N1-C1'	6.31	125.27	117.70
40	YH	82	GLY	N-CA-C	6.31	128.87	113.10
34	RA	1915	U	N3-C2-O2	-6.30	117.79	122.20
42	YN	48	MET	CG-SD-CE	-6.30	90.11	100.20
34	RA	2168	G	N3-C4-C5	-6.30	125.45	128.60
1	QA	433	C	C6-N1-C2	-6.30	117.78	120.30
34	YA	1180	C	C2-N1-C1'	6.30	125.73	118.80
34	YA	1404	C	C2-N1-C1'	6.30	125.73	118.80
12	QL	104	VAL	C-N-CA	6.29	137.43	121.70
34	RA	242	G	P-O3'-C3'	6.29	127.25	119.70
34	RA	1899	G	N3-C4-N9	6.29	129.78	126.00
1	XA	972	C	C6-N1-C2	-6.29	117.78	120.30
34	YA	404	C	P-O3'-C3'	6.29	127.25	119.70
34	YA	752	A	P-O3'-C3'	6.29	127.24	119.70
1	XA	1306	A	N7-C8-N9	6.28	116.94	113.80
34	YA	985	C	C2-N1-C1'	6.28	125.71	118.80
1	QA	90	C	C6-N1-C2	-6.28	117.79	120.30
34	YA	2559	C	C5-C6-N1	6.28	124.14	121.00
1	XA	18	C	C5-C6-N1	6.28	124.14	121.00
1	XA	1383	C	C6-N1-C2	-6.28	117.79	120.30
34	RA	2295	C	C6-N1-C2	-6.27	117.79	120.30
34	YA	1026	U	OP1-P-O3'	6.27	119.00	105.20
34	YA	1774	C	C5-C6-N1	6.27	124.14	121.00
1	QA	962	C	N1-C2-O2	6.27	122.66	118.90
34	YA	1915	U	N3-C2-O2	-6.27	117.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	271(C)	G	P-O3'-C3'	6.27	127.22	119.70
1	XA	1260	C	C6-N1-C2	-6.27	117.79	120.30
34	RA	915	C	C2-N1-C1'	6.26	125.69	118.80
34	RA	104	U	N1-C2-O2	6.26	127.18	122.80
1	XA	1290	G	C4-N9-C1'	6.26	134.64	126.50
1	XA	736	C	C6-N1-C2	-6.26	117.80	120.30
34	YA	1833	U	N3-C2-O2	-6.26	117.82	122.20
34	RA	1950	G	C4-N9-C1'	6.26	134.63	126.50
34	RA	2179	C	N3-C2-O2	-6.26	117.52	121.90
34	YA	1411	C	C5-C6-N1	6.25	124.13	121.00
34	RA	1087	G	O4'-C1'-N9	-6.25	103.20	108.20
34	RA	229	A	OP2-P-O3'	6.25	118.94	105.20
34	RA	537	C	C6-N1-C2	-6.25	117.80	120.30
34	RA	2439	A	P-O3'-C3'	6.25	127.20	119.70
34	RA	456	C	N3-C2-O2	-6.25	117.53	121.90
34	YA	985	C	N1-C2-O2	6.24	122.64	118.90
34	YA	691	C	C6-N1-C2	-6.24	117.80	120.30
34	YA	2766	G	C4-N9-C1'	6.24	134.61	126.50
35	RB	27	C	N3-C2-O2	-6.24	117.53	121.90
1	QA	455	C	N1-C2-O2	6.24	122.64	118.90
1	XA	1158	C	C5-C6-N1	6.24	124.12	121.00
34	YA	2211	G	C8-N9-C1'	-6.24	118.89	127.00
1	XA	54	C	N1-C2-O2	6.23	122.64	118.90
34	RA	2542	A	N9-C4-C5	-6.23	103.31	105.80
34	YA	377	C	C5-C6-N1	6.23	124.11	121.00
1	QA	1097	C	N1-C2-O2	6.23	122.64	118.90
34	YA	1982	C	C2-N1-C1'	6.23	125.65	118.80
35	YB	30	C	C2-N1-C1'	6.23	125.65	118.80
34	RA	1920	C	C5-C6-N1	6.22	124.11	121.00
34	YA	834	C	C5-C6-N1	6.22	124.11	121.00
34	YA	1437	C	C5-C6-N1	6.22	124.11	121.00
34	YA	393	C	C6-N1-C2	-6.22	117.81	120.30
34	YA	1950	G	C4-N9-C1'	6.22	134.59	126.50
22	QV	36	G	N7-C8-N9	6.22	116.21	113.10
1	QA	960	U	C2-N1-C1'	6.22	125.16	117.70
1	QA	1228	C	N1-C2-O2	6.22	122.63	118.90
34	RA	269	U	N3-C2-O2	-6.22	117.85	122.20
22	XV	31	G	C4-N9-C1'	6.22	134.58	126.50
34	YA	904	C	N3-C2-O2	-6.22	117.55	121.90
34	RA	1983	C	C6-N1-C2	-6.21	117.81	120.30
38	RF	197	ASP	N-CA-C	-6.21	94.22	111.00
34	YA	1992	G	P-O3'-C3'	6.21	127.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RB	22	U	C2-N1-C1'	6.21	125.16	117.70
34	YA	915	C	C6-N1-C2	-6.21	117.82	120.30
22	QV	30	C	N1-C2-O2	6.21	122.62	118.90
34	RA	1304	C	C2-N1-C1'	6.21	125.63	118.80
34	YA	613	U	N1-C2-O2	6.21	127.14	122.80
34	YA	2211	G	N3-C4-N9	6.21	129.72	126.00
34	YA	2099	U	C5-C6-N1	6.20	125.80	122.70
34	YA	2108	C	N3-C2-O2	-6.20	117.56	121.90
34	YA	1178	C	C6-N1-C2	-6.20	117.82	120.30
1	QA	328	C	P-O3'-C3'	6.20	127.13	119.70
34	YA	420	C	C2-N1-C1'	6.20	125.61	118.80
1	XA	893	C	N1-C2-O2	6.19	122.62	118.90
34	YA	1653	G	N3-C4-N9	6.19	129.71	126.00
34	YA	2006	C	N1-C2-O2	6.19	122.61	118.90
1	QA	252	U	N3-C2-O2	-6.18	117.87	122.20
34	RA	2128	C	N1-C2-O2	6.18	122.61	118.90
7	QG	73	MET	N-CA-CB	-6.18	99.47	110.60
34	YA	2126	A	P-O3'-C3'	6.18	127.12	119.70
1	QA	620	C	C2-N1-C1'	6.18	125.59	118.80
1	XA	241	C	C2-N1-C1'	6.18	125.59	118.80
35	RB	66	A	P-O3'-C3'	6.17	127.11	119.70
34	RA	1533	C	N1-C2-O2	6.17	122.60	118.90
34	RA	1498	C	N1-C2-O2	6.17	122.60	118.90
34	RA	1312	U	P-O3'-C3'	6.16	127.10	119.70
1	XA	68(R)	U	N1-C2-O2	6.16	127.11	122.80
34	RA	2825	C	N3-C2-O2	-6.16	117.59	121.90
34	YA	974(B)	C	P-O3'-C3'	6.15	127.08	119.70
35	YB	47	C	N3-C2-O2	-6.15	117.59	121.90
1	QA	90	C	C6-N1-C1'	-6.15	113.42	120.80
35	RB	11	C	C6-N1-C2	-6.15	117.84	120.30
22	QV	36	G	C4-C5-N7	6.15	113.26	110.80
34	RA	200	U	N3-C2-O2	-6.15	117.90	122.20
34	YA	114	U	C5-C6-N1	6.15	125.77	122.70
34	YA	229	A	P-O3'-C3'	6.14	127.07	119.70
34	YA	1982	C	C5-C6-N1	6.14	124.07	121.00
34	YA	198	C	C2-N1-C1'	6.14	125.55	118.80
34	YA	420	C	N1-C2-O2	6.14	122.58	118.90
22	QV	15	G	C4-N9-C1'	6.14	134.48	126.50
1	XA	18	C	C6-N1-C2	-6.13	117.85	120.30
34	YA	985	C	C6-N1-C2	-6.13	117.85	120.30
34	YA	1267	U	N3-C2-O2	-6.13	117.91	122.20
34	YA	669	G	C4-N9-C1'	6.13	134.47	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	RI	10	GLU	C-N-CA	6.13	137.02	121.70
1	XA	618	C	C6-N1-C2	-6.13	117.85	120.30
1	XA	620	C	N1-C2-O2	6.12	122.58	118.90
34	RA	923	C	C5-C6-N1	6.12	124.06	121.00
34	RA	2703	C	N1-C2-O2	6.12	122.57	118.90
34	YA	2320	A	C2-N3-C4	6.12	113.66	110.60
34	RA	222	A	P-O3'-C3'	6.12	127.04	119.70
1	XA	237	C	N3-C4-C5	-6.12	119.45	121.90
1	XA	525	C	C5-C6-N1	6.12	124.06	121.00
23	QX	16	C	C6-N1-C2	-6.12	117.85	120.30
34	RA	269	U	N1-C2-O2	6.12	127.08	122.80
34	RA	2480	C	N3-C2-O2	-6.11	117.62	121.90
1	QA	1036	G	C8-N9-C1'	-6.11	119.06	127.00
1	QA	1039	C	N3-C2-O2	-6.11	117.62	121.90
1	QA	91	C	C6-N1-C2	-6.11	117.86	120.30
1	QA	1395	C	C6-N1-C1'	-6.11	113.47	120.80
34	RA	385	C	C6-N1-C2	-6.11	117.86	120.30
35	YB	27	C	C5-C6-N1	6.11	124.05	121.00
34	YA	2889	C	C6-N1-C2	-6.10	117.86	120.30
34	RA	2295	C	C2-N1-C1'	6.10	125.51	118.80
23	QX	17	C	N1-C2-N3	6.10	123.47	119.20
34	RA	1549	C	C2-N1-C1'	6.10	125.51	118.80
34	RA	1882	C	N1-C2-O2	6.10	122.56	118.90
1	XA	514	C	C6-N1-C2	-6.10	117.86	120.30
34	YA	2787	C	N1-C2-O2	6.10	122.56	118.90
1	QA	381	C	N1-C2-O2	6.09	122.56	118.90
34	RA	2043	C	N1-C2-O2	6.09	122.56	118.90
22	QV	62	C	C5-C6-N1	6.09	124.05	121.00
1	QA	1109	C	N3-C2-O2	-6.09	117.64	121.90
34	RA	912	C	N1-C2-O2	6.09	122.56	118.90
34	RA	1915	U	N1-C2-O2	6.09	127.06	122.80
34	RA	1314	C	C5-C6-N1	6.09	124.05	121.00
34	RA	1427	A	P-O3'-C3'	6.09	127.01	119.70
36	RD	33	LEU	CA-CB-CG	6.09	129.31	115.30
34	YA	1314	C	C5-C6-N1	6.09	124.05	121.00
34	YA	2776	A	P-O3'-C3'	6.09	127.01	119.70
34	RA	2471	C	C6-N1-C2	-6.09	117.87	120.30
34	RA	1742	C	C6-N1-C2	-6.08	117.87	120.30
1	XA	68(S)	C	C5-C6-N1	6.08	124.04	121.00
1	QA	90	C	C5-C6-N1	6.08	124.04	121.00
34	RA	2456	C	C6-N1-C2	-6.08	117.87	120.30
34	RA	2776	A	P-O3'-C3'	6.08	126.99	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	2260	C	C6-N1-C2	-6.08	117.87	120.30
1	QA	1113	C	C6-N1-C2	-6.08	117.87	120.30
34	RA	1462	C	N3-C2-O2	-6.08	117.65	121.90
22	XV	40	G	C4-N9-C1'	6.08	134.40	126.50
34	RA	912	C	C6-N1-C2	-6.08	117.87	120.30
34	RA	2168	G	C8-N9-C1'	-6.07	119.10	127.00
1	XA	54	C	N3-C2-O2	-6.07	117.65	121.90
34	YA	2889	C	C5-C6-N1	6.07	124.04	121.00
34	YA	456	C	N1-C2-O2	6.07	122.54	118.90
34	RA	2471	C	C2-N1-C1'	6.07	125.47	118.80
1	XA	201(A)	C	N1-C2-O2	6.07	122.54	118.90
34	YA	1506	C	C5-C6-N1	6.07	124.03	121.00
34	YA	2474	C	N1-C2-O2	6.07	122.54	118.90
34	YA	1121	C	C6-N1-C2	-6.06	117.88	120.30
1	QA	736	C	C6-N1-C2	-6.06	117.88	120.30
34	RA	372	G	P-O3'-C3'	6.06	126.97	119.70
34	RA	876	C	N1-C2-O2	6.06	122.53	118.90
34	RA	1658	C	C5-C6-N1	6.06	124.03	121.00
34	YA	2506	U	C2-N1-C1'	6.06	124.97	117.70
34	RA	2210	G	N3-C4-N9	6.05	129.63	126.00
34	RA	2512	C	C5-C6-N1	6.05	124.03	121.00
34	RA	2254	C	C6-N1-C2	-6.05	117.88	120.30
34	YA	1544	C	N1-C2-O2	6.05	122.53	118.90
34	YA	2041	U	C6-N1-C2	-6.05	117.37	121.00
1	QA	1027	C	N1-C2-O2	6.05	122.53	118.90
34	YA	2712(A)	U	N1-C2-O2	6.05	127.03	122.80
1	QA	1075	C	C2-N1-C1'	6.05	125.45	118.80
34	YA	1894	C	C6-N1-C2	-6.05	117.88	120.30
1	QA	687	A	P-O3'-C3'	6.04	126.95	119.70
1	QA	1325	C	C2-N1-C1'	6.04	125.45	118.80
1	XA	1322	C	N3-C2-O2	-6.04	117.67	121.90
34	RA	2544	G	C4-C5-N7	6.04	113.21	110.80
40	RH	87	LEU	N-CA-CB	-6.04	98.33	110.40
1	XA	582	U	N3-C2-O2	-6.04	117.97	122.20
34	YA	1535	U	C6-N1-C1'	-6.04	112.75	121.20
34	RA	1950	G	O4'-C1'-N9	6.03	113.02	108.20
34	YA	333	G	C4-N9-C1'	6.03	134.34	126.50
34	YA	200	U	N3-C2-O2	-6.02	117.98	122.20
34	RA	2307	G	C4-N9-C1'	6.02	134.32	126.50
1	XA	723	U	N1-C2-O2	6.02	127.01	122.80
34	YA	1799	G	P-O3'-C3'	6.02	126.92	119.70
34	YA	1462	C	N1-C2-O2	6.02	122.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	634	C	C5-C6-N1	6.01	124.01	121.00
34	RA	2006	C	C6-N1-C2	-6.01	117.89	120.30
1	XA	1395	C	C6-N1-C2	-6.01	117.90	120.30
34	YA	1636	C	N3-C2-O2	-6.01	117.69	121.90
34	RA	1899	G	N1-C2-N2	-6.01	110.79	116.20
34	RA	2053	G	C4-C5-N7	6.01	113.20	110.80
34	RA	1135	C	N3-C2-O2	-6.01	117.70	121.90
34	RA	2032	G	C5-N7-C8	-6.00	101.30	104.30
1	QA	697	U	N3-C2-O2	-6.00	118.00	122.20
34	RA	9	U	N3-C2-O2	-6.00	118.00	122.20
41	RI	130	TYR	C-N-CA	6.00	136.70	121.70
34	YA	2210	G	N3-C4-N9	6.00	129.60	126.00
1	XA	1114	C	C6-N1-C2	-5.99	117.90	120.30
34	YA	755	C	C6-N1-C2	-5.99	117.90	120.30
22	QV	31	G	C4-N9-C1'	5.99	134.28	126.50
34	RA	1982	C	N1-C2-O2	5.99	122.49	118.90
34	YA	2868	A	C5-N7-C8	-5.99	100.91	103.90
1	QA	455	C	C2-N1-C1'	5.98	125.38	118.80
34	RA	904	C	N3-C2-O2	-5.98	117.71	121.90
1	XA	455	C	C2-N1-C1'	5.98	125.38	118.80
34	YA	1893	C	N3-C2-O2	-5.98	117.71	121.90
35	YB	66	A	P-O3'-C3'	5.98	126.88	119.70
1	QA	960	U	N1-C2-O2	5.98	126.98	122.80
34	RA	669	G	N3-C4-N9	5.98	129.59	126.00
34	YA	806	C	C5-C6-N1	5.97	123.99	121.00
34	YA	1427	A	P-O3'-C3'	5.97	126.87	119.70
35	YB	31	C	C2-N1-C1'	5.97	125.37	118.80
34	RA	1370	C	N1-C2-O2	5.96	122.48	118.90
34	YA	923	C	C5-C6-N1	5.96	123.98	121.00
34	YA	1297	C	C6-N1-C2	-5.96	117.92	120.30
34	YA	1417	C	C5-C6-N1	5.96	123.98	121.00
34	RA	1799	G	P-O3'-C3'	5.96	126.85	119.70
34	RA	2766	G	C4-N9-C1'	5.95	134.24	126.50
41	RI	82	ARG	CA-C-N	-5.95	104.10	117.20
34	RA	766	C	C6-N1-C2	-5.95	117.92	120.30
34	RA	1741	C	C2-N1-C1'	5.95	125.35	118.80
34	YA	2226	C	N1-C2-O2	5.95	122.47	118.90
1	QA	993	G	N3-C4-N9	5.95	129.57	126.00
34	RA	1533	C	C5-C6-N1	5.95	123.97	121.00
34	RA	74	A	N3-C4-N9	-5.95	122.64	127.40
34	YA	74	A	O4'-C1'-N9	-5.95	103.44	108.20
34	YA	1534	G	C2-N3-C4	5.94	114.87	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	752	A	P-O3'-C3'	5.94	126.83	119.70
1	XA	1301	U	C6-N1-C2	-5.94	117.43	121.00
34	YA	104	U	N3-C2-O2	-5.94	118.04	122.20
34	RA	1130	U	P-O3'-C3'	5.94	126.83	119.70
34	RA	1468	C	C6-N1-C2	-5.94	117.92	120.30
1	XA	328	C	P-O3'-C3'	5.94	126.83	119.70
35	YB	47	C	C2-N1-C1'	5.94	125.33	118.80
1	QA	186(H)	C	C6-N1-C1'	5.94	127.92	120.80
34	RA	806	C	C6-N1-C2	-5.94	117.92	120.30
34	RA	41	C	C2-N1-C1'	5.93	125.33	118.80
1	XA	498	U	C2-N1-C1'	5.93	124.82	117.70
34	YA	1333	C	C6-N1-C2	-5.93	117.93	120.30
34	RA	2726	U	N1-C2-O2	5.93	126.95	122.80
34	RA	2229	C	N3-C4-C5	-5.93	119.53	121.90
34	RA	1774	C	C2-N1-C1'	5.93	125.32	118.80
34	RA	2784	C	C5-C6-N1	5.93	123.96	121.00
34	YA	99	U	P-O3'-C3'	5.93	126.81	119.70
34	RA	1462	C	N1-C2-O2	5.92	122.45	118.90
22	QV	31	G	N3-C4-C5	-5.92	125.64	128.60
35	YB	30	C	C5-C6-N1	5.92	123.96	121.00
34	RA	2065	C	C5-C6-N1	5.92	123.96	121.00
34	YA	530	G	N1-C6-O6	-5.92	116.35	119.90
34	YA	2321	G	C8-N9-C4	-5.92	104.03	106.40
34	RA	1644	C	C6-N1-C2	-5.92	117.93	120.30
34	RA	63	U	C4'-C3'-O3'	5.91	124.82	113.00
34	YA	1362	C	C6-N1-C2	-5.91	117.94	120.30
28	Y4	5	ILE	CA-CB-CG1	5.91	122.22	111.00
34	YA	198	C	N1-C2-O2	5.91	122.44	118.90
34	YA	2483	C	C6-N1-C2	-5.91	117.94	120.30
1	QA	1060	C	C6-N1-C2	-5.90	117.94	120.30
1	XA	1036	G	N3-C4-N9	5.90	129.54	126.00
34	YA	2507	C	C5-C6-N1	5.90	123.95	121.00
34	RA	1833	U	N3-C2-O2	-5.90	118.07	122.20
34	YA	1694	C	P-O3'-C3'	5.90	126.78	119.70
34	YA	2544	G	N7-C8-N9	5.90	116.05	113.10
1	QA	955	U	C5-C6-N1	5.90	125.65	122.70
34	RA	2580	U	N1-C2-O2	5.90	126.93	122.80
34	RA	1779	U	C2-N1-C1'	5.89	124.77	117.70
34	YA	377	C	C6-N1-C2	-5.89	117.94	120.30
34	RA	544	C	C2-N1-C1'	5.89	125.28	118.80
34	RA	141(B)	C	C6-N1-C2	-5.89	117.94	120.30
34	RA	624	C	C2-N1-C1'	5.89	125.28	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1013	C	C5-C6-N1	5.89	123.94	121.00
34	YA	974(B)	C	N3-C2-O2	-5.88	117.78	121.90
34	YA	2566	A	P-O3'-C3'	5.88	126.76	119.70
34	YA	967	C	C6-N1-C2	-5.88	117.95	120.30
1	QA	866	C	C5-C6-N1	5.88	123.94	121.00
34	YA	97	C	C2-N1-C1'	5.88	125.27	118.80
34	RA	1045	A	P-O3'-C3'	5.88	126.75	119.70
34	RA	138	G	O4'-C1'-N9	5.87	112.90	108.20
34	RA	634	C	C6-N1-C2	-5.87	117.95	120.30
34	RA	2006	C	N1-C2-O2	5.87	122.42	118.90
34	YA	143	C	C5-C6-N1	5.87	123.94	121.00
34	YA	957	A	C5-C6-N6	-5.87	119.00	123.70
34	RA	1741	C	N3-C2-O2	-5.87	117.79	121.90
34	RA	209	C	C5-C6-N1	5.87	123.93	121.00
34	YA	731	C	C6-N1-C2	-5.86	117.95	120.30
34	RA	1376	C	C5-C6-N1	5.86	123.93	121.00
34	YA	528	A	C4-C5-N7	5.86	113.63	110.70
1	XA	962	C	N1-C2-O2	5.86	122.42	118.90
34	YA	2703	C	C5-C6-N1	5.86	123.93	121.00
1	QA	1228	C	C6-N1-C2	-5.86	117.96	120.30
1	XA	1539	C	N3-C4-N4	-5.86	113.90	118.00
54	RZ	59	LEU	CA-CB-CG	5.86	128.77	115.30
34	YA	2243	U	N3-C2-O2	-5.85	118.10	122.20
34	RA	676	A	C5-N7-C8	-5.85	100.97	103.90
1	XA	1260	C	C2-N1-C1'	5.85	125.24	118.80
34	YA	67	U	C5-C6-N1	5.85	125.63	122.70
34	RA	2666	C	C6-N1-C2	-5.85	117.96	120.30
34	YA	1920	C	C6-N1-C2	-5.85	117.96	120.30
34	YA	2243	U	N1-C2-N3	5.85	118.41	114.90
34	YA	2504	U	N1-C2-O2	5.85	126.89	122.80
34	YA	976	C	C6-N1-C2	-5.85	117.96	120.30
4	XD	8	VAL	CG1-CB-CG2	5.84	120.25	110.90
34	YA	195	A	P-O3'-C3'	5.84	126.71	119.70
34	RA	2689	U	P-O3'-C3'	5.84	126.71	119.70
34	YA	267	C	C5-C6-N1	5.84	123.92	121.00
34	RA	512	G	P-O3'-C3'	5.84	126.71	119.70
34	RA	1644	C	N3-C2-O2	-5.84	117.81	121.90
34	YA	221	A	P-O3'-C3'	5.84	126.71	119.70
34	YA	2321	G	N3-C4-C5	-5.84	125.68	128.60
34	YA	1915	U	C2-N1-C1'	5.84	124.71	117.70
1	QA	1323	G	N3-C4-N9	5.83	129.50	126.00
34	RA	834	C	C6-N1-C2	-5.83	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	891	U	N3-C2-O2	-5.83	118.12	122.20
1	QA	1303	C	C2-N1-C1'	5.83	125.22	118.80
1	QA	1290	G	C4-N9-C1'	5.83	134.08	126.50
34	RA	2517	C	C6-N1-C2	-5.83	117.97	120.30
1	XA	993	G	C4-N9-C1'	5.83	134.08	126.50
34	YA	2779	U	N3-C2-O2	-5.83	118.12	122.20
1	XA	1113	C	C6-N1-C2	-5.83	117.97	120.30
1	XA	1296	C	N3-C2-O2	-5.83	117.82	121.90
1	QA	136	C	C5-C6-N1	5.83	123.91	121.00
34	RA	650	C	C6-N1-C2	-5.82	117.97	120.30
34	YA	486	C	C6-N1-C2	-5.82	117.97	120.30
34	YA	503	A	OP2-P-O3'	5.82	118.01	105.20
34	YA	1437	C	C2-N1-C1'	5.82	125.21	118.80
34	YA	2211	G	N3-C4-C5	-5.82	125.69	128.60
34	YA	2254	C	C6-N1-C2	-5.82	117.97	120.30
32	R8	62	LEU	CA-CB-CG	5.82	128.69	115.30
34	YA	1293	C	C5-C6-N1	5.82	123.91	121.00
34	RA	2582	G	C4-N9-C1'	5.82	134.06	126.50
34	YA	1314	C	N1-C2-O2	5.82	122.39	118.90
34	YA	2615	U	C2-N1-C1'	5.82	124.68	117.70
34	YA	2815	C	C5-C6-N1	5.82	123.91	121.00
28	Y4	5	ILE	CA-CB-CG2	-5.82	99.27	110.90
1	QA	582	U	N3-C2-O2	-5.81	118.13	122.20
34	RA	2688	U	C2-N1-C1'	5.81	124.67	117.70
34	YA	580	C	C5-C6-N1	5.81	123.91	121.00
34	YA	930	U	C5-C6-N1	5.81	125.61	122.70
34	YA	967	C	C5-C6-N1	5.81	123.91	121.00
34	YA	1234	U	N1-C2-O2	5.81	126.87	122.80
1	QA	1285	A	P-O3'-C3'	5.81	126.67	119.70
34	YA	672	C	C5-C6-N1	5.81	123.91	121.00
34	YA	859	G	P-O3'-C3'	5.81	126.67	119.70
34	RA	1819	A	P-O3'-C3'	5.81	126.67	119.70
34	RA	2785	C	C5-C6-N1	5.80	123.90	121.00
34	YA	234	C	N1-C2-O2	5.80	122.38	118.90
34	YA	503	A	P-O3'-C3'	5.80	126.66	119.70
1	QA	1060	C	C5-C6-N1	5.80	123.90	121.00
34	RA	209	C	C6-N1-C2	-5.80	117.98	120.30
34	RA	776	G	C4-N9-C1'	5.80	134.04	126.50
34	YA	1293	C	C6-N1-C2	-5.80	117.98	120.30
12	XL	47	LYS	N-CA-C	5.80	126.66	111.00
34	YA	556	G	C6-C5-N7	-5.80	126.92	130.40
34	YA	2808	U	C2-N1-C1'	5.80	124.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1474	C	C5-C6-N1	5.79	123.90	121.00
1	QA	1499	A	P-O3'-C3'	5.79	126.65	119.70
34	YA	485	C	C6-N1-C2	-5.79	117.98	120.30
34	YA	1534	G	C8-N9-C1'	-5.79	119.47	127.00
34	RA	392	C	C2-N1-C1'	5.79	125.17	118.80
34	RA	1920	C	C6-N1-C2	-5.79	117.98	120.30
34	YA	114	U	N1-C2-O2	5.79	126.85	122.80
34	YA	758	C	N3-C2-O2	-5.79	117.85	121.90
34	YA	1519	G	C4-N9-C1'	5.79	134.03	126.50
34	YA	1537	C	C6-N1-C2	-5.78	117.99	120.30
1	QA	433	C	N3-C2-O2	-5.78	117.85	121.90
34	YA	2739	U	C6-N1-C2	-5.78	117.53	121.00
1	XA	1322	C	C6-N1-C2	-5.78	117.99	120.30
34	RA	2175	C	C5-C6-N1	5.78	123.89	121.00
34	YA	1988	C	C6-N1-C2	-5.78	117.99	120.30
34	RA	9	U	N1-C2-O2	5.77	126.84	122.80
34	RA	1658	C	C6-N1-C2	-5.77	117.99	120.30
34	RA	2646	C	C6-N1-C2	-5.77	117.99	120.30
34	RA	797	C	C5-C6-N1	5.77	123.88	121.00
34	RA	1881	C	N1-C2-O2	5.77	122.36	118.90
34	RA	669	G	N3-C4-C5	-5.76	125.72	128.60
34	RA	1430	C	C5-C6-N1	5.76	123.88	121.00
1	QA	618	C	C6-N1-C2	-5.76	118.00	120.30
34	YA	426	C	N1-C2-O2	5.76	122.36	118.90
34	RA	1430	C	C6-N1-C2	-5.76	118.00	120.30
34	YA	1188	U	N1-C2-O2	5.76	126.83	122.80
34	YA	1468	C	C6-N1-C2	-5.76	118.00	120.30
34	RA	1762	A	N1-C2-N3	5.75	132.18	129.30
34	YA	1314	C	C6-N1-C1'	-5.75	113.89	120.80
1	QA	1066	C	C2-N1-C1'	5.75	125.13	118.80
34	YA	155	C	C6-N1-C2	-5.75	118.00	120.30
34	YA	2784	C	C6-N1-C2	-5.75	118.00	120.30
34	YA	140	A	C5-N7-C8	-5.75	101.03	103.90
34	YA	613	U	N3-C2-O2	-5.75	118.18	122.20
1	QA	620	C	N3-C2-O2	-5.75	117.88	121.90
34	YA	2504	U	N3-C2-O2	-5.75	118.18	122.20
34	RA	1258	C	C6-N1-C2	-5.74	118.00	120.30
22	XV	56	C	N1-C2-O2	5.74	122.35	118.90
34	YA	196	A	O4'-C1'-N9	5.74	112.80	108.20
34	YA	267	C	C6-N1-C2	-5.74	118.00	120.30
34	YA	721	C	C6-N1-C2	-5.74	118.00	120.30
34	YA	1474	C	C5-C6-N1	5.74	123.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1979	C	C5-C6-N1	5.74	123.87	121.00
1	QA	838(B)	U	C2-N1-C1'	5.74	124.59	117.70
34	RA	1304	C	C5-C6-N1	5.74	123.87	121.00
34	YA	234	C	N3-C2-O2	-5.74	117.88	121.90
34	YA	1313	U	C6-N1-C1'	-5.74	113.16	121.20
34	YA	2576	G	C4-N9-C1'	5.74	133.96	126.50
1	XA	312	C	C6-N1-C2	-5.74	118.00	120.30
1	XA	1149	C	C6-N1-C2	-5.74	118.00	120.30
1	XA	596	C	C6-N1-C2	-5.73	118.01	120.30
22	XV	15	G	C8-N9-C4	-5.73	104.11	106.40
34	YA	1012	U	OP2-P-O3'	5.73	117.81	105.20
34	YA	2089	U	C5-C6-N1	5.73	125.57	122.70
34	YA	2870	C	N3-C2-O2	-5.73	117.89	121.90
34	YA	1102	C	N1-C2-O2	5.73	122.34	118.90
1	QA	136	C	N3-C2-O2	-5.73	117.89	121.90
34	RA	976	C	C5-C6-N1	5.73	123.86	121.00
34	RA	1078	U	C5-C6-N1	5.73	125.56	122.70
34	RA	1404	C	N1-C2-O2	5.73	122.34	118.90
34	YA	1140	C	N1-C2-O2	5.73	122.34	118.90
14	QN	43	CYS	CB-CA-C	5.72	121.85	110.40
34	RA	384	U	N1-C2-O2	5.72	126.81	122.80
34	RA	1075	C	N3-C2-O2	-5.72	117.89	121.90
35	RB	27	C	C2-N1-C1'	5.72	125.10	118.80
34	YA	2506	U	N3-C2-O2	-5.72	118.19	122.20
34	YA	1679	U	N3-C2-O2	-5.72	118.19	122.20
34	RA	856	C	P-O3'-C3'	5.72	126.56	119.70
34	RA	1406	U	N1-C2-O2	5.72	126.80	122.80
34	YA	485	C	C5-C6-N1	5.72	123.86	121.00
34	RA	234	C	N3-C2-O2	-5.71	117.90	121.90
34	RA	1882	C	C6-N1-C1'	-5.71	113.95	120.80
34	RA	1899	G	N3-C2-N2	5.71	123.90	119.90
34	YA	2490	G	C4-N9-C1'	5.71	133.92	126.50
34	RA	640	C	C5-C6-N1	5.71	123.86	121.00
34	RA	2060	A	P-O3'-C3'	5.70	126.54	119.70
34	RA	2584	U	N3-C2-O2	-5.70	118.21	122.20
1	XA	330	C	N1-C2-O2	5.70	122.32	118.90
1	QA	353	A	OP2-P-O3'	5.70	117.74	105.20
34	RA	2321	G	C8-N9-C4	-5.70	104.12	106.40
34	YA	640	C	C2-N1-C1'	5.70	125.07	118.80
34	YA	965	C	C5-C6-N1	5.70	123.85	121.00
34	RA	1914	C	C6-N1-C2	-5.70	118.02	120.30
35	YB	60	C	C6-N1-C2	-5.70	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1233	C	C6-N1-C2	-5.70	118.02	120.30
34	RA	1404	C	C6-N1-C2	-5.69	118.02	120.30
1	XA	596	C	N1-C2-O2	5.69	122.31	118.90
1	XA	736	C	C5-C6-N1	5.69	123.84	121.00
34	YA	1819	A	P-O3'-C3'	5.69	126.53	119.70
34	YA	1982	C	N1-C2-O2	5.69	122.31	118.90
1	QA	960	U	N3-C2-O2	-5.68	118.22	122.20
34	RA	2226	C	N1-C2-O2	5.68	122.31	118.90
35	RB	60	C	C5-C6-N1	5.68	123.84	121.00
34	YA	363(F)	U	N1-C2-O2	5.68	126.78	122.80
34	RA	2566	A	P-O3'-C3'	5.68	126.51	119.70
34	RA	2512	C	C6-N1-C2	-5.68	118.03	120.30
34	RA	2584	U	C2-N1-C1'	5.67	124.51	117.70
34	YA	2584	U	N1-C2-O2	5.67	126.77	122.80
34	RA	1005	C	C2-N1-C1'	5.67	125.04	118.80
34	YA	2588	G	C6-C5-N7	-5.67	127.00	130.40
34	RA	1295	C	C6-N1-C2	-5.67	118.03	120.30
1	XA	993	G	C8-N9-C1'	-5.67	119.63	127.00
34	YA	1775	U	C5-C4-O4	-5.67	122.50	125.90
34	RA	65	C	N1-C2-O2	5.67	122.30	118.90
34	YA	2098	U	N1-C2-O2	5.67	126.77	122.80
45	YQ	19	GLY	N-CA-C	-5.67	98.93	113.10
1	XA	1262	C	C5-C6-N1	5.67	123.83	121.00
34	RA	271(C)	G	OP2-P-O3'	5.66	117.66	105.20
34	YA	1399	C	C6-N1-C2	-5.66	118.03	120.30
34	YA	231	C	C6-N1-C1'	-5.66	114.01	120.80
34	YA	1774	C	N1-C2-O2	5.66	122.30	118.90
34	YA	1930	G	OP2-P-O3'	5.66	117.65	105.20
34	YA	2048	G	C4-N9-C1'	5.66	133.86	126.50
34	RA	2726	U	N3-C2-O2	-5.66	118.24	122.20
34	YA	1267	U	N1-C2-O2	5.66	126.76	122.80
22	QV	62	C	C6-N1-C2	-5.66	118.04	120.30
34	YA	1806	C	C6-N1-C2	-5.66	118.04	120.30
35	YB	30	C	N3-C2-O2	-5.66	117.94	121.90
34	YA	1686	C	C2-N1-C1'	5.65	125.02	118.80
34	YA	2723	C	C6-N1-C2	-5.65	118.04	120.30
34	RA	1632	A	N7-C8-N9	5.64	116.62	113.80
1	XA	23	C	C5-C6-N1	5.64	123.82	121.00
22	QV	31	G	C8-N9-C4	-5.64	104.14	106.40
34	RA	2701	C	C5-C6-N1	5.64	123.82	121.00
34	YA	1992	G	OP2-P-O3'	5.64	117.61	105.20
34	RA	104	U	N3-C2-O2	-5.64	118.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1513	C	C5-C6-N1	5.64	123.82	121.00
34	YA	183	C	N3-C2-O2	-5.64	117.95	121.90
34	YA	544	C	C5-C6-N1	5.64	123.82	121.00
34	YA	1407	C	N3-C2-O2	-5.64	117.95	121.90
1	QA	936	C	N3-C2-O2	-5.63	117.96	121.90
1	XA	68(R)	U	N3-C2-O2	-5.63	118.26	122.20
1	XA	1285	A	P-O3'-C3'	5.63	126.46	119.70
34	YA	106	C	C6-N1-C2	-5.63	118.05	120.30
37	YE	186	GLY	N-CA-C	5.63	127.18	113.10
34	YA	363(F)	U	N3-C2-O2	-5.63	118.26	122.20
34	YA	2294	C	N1-C2-O2	5.63	122.28	118.90
34	RA	2168	G	N3-C4-N9	5.63	129.38	126.00
1	XA	1203	C	N1-C2-O2	5.63	122.28	118.90
35	YB	70	C	C6-N1-C2	-5.63	118.05	120.30
34	RA	1407	C	N1-C2-O2	5.63	122.28	118.90
34	YA	384	U	C2-N1-C1'	5.63	124.45	117.70
34	YA	1085	A	P-O3'-C3'	5.63	126.45	119.70
35	YB	71	C	N1-C2-O2	5.63	122.28	118.90
36	YD	241	PRO	C-N-CA	5.62	135.76	121.70
1	XA	1290	G	N3-C4-N9	5.62	129.37	126.00
34	YA	1844	C	C6-N1-C2	-5.62	118.05	120.30
20	QT	73	HIS	CA-CB-CG	5.62	123.15	113.60
34	RA	689	A	C5-C6-N1	5.62	120.51	117.70
34	YA	2368	C	C6-N1-C2	-5.62	118.05	120.30
1	XA	68(T)	C	N1-C2-O2	5.62	122.27	118.90
34	YA	584	C	C2-N1-C1'	5.62	124.98	118.80
34	YA	243	U	C5-C6-N1	5.62	125.51	122.70
34	YA	1398	C	N1-C2-O2	5.62	122.27	118.90
1	QA	1225	A	C4-N9-C1'	5.62	136.41	126.30
34	YA	1535	U	O4'-C1'-N1	5.62	112.69	108.20
1	QA	23	C	C6-N1-C2	-5.61	118.05	120.30
35	RB	60	C	C6-N1-C2	-5.61	118.06	120.30
34	YA	319	C	N1-C2-O2	5.61	122.27	118.90
1	QA	267	C	N3-C2-O2	-5.61	117.97	121.90
1	XA	748	C	P-O3'-C3'	5.61	126.43	119.70
34	YA	964	C	C6-N1-C2	-5.61	118.06	120.30
34	RA	2211	G	C8-N9-C1'	-5.61	119.71	127.00
1	XA	68(R)	U	C2-N1-C1'	5.61	124.43	117.70
34	YA	1786	A	C4-N9-C1'	5.61	136.39	126.30
34	RA	2542	A	C8-N9-C4	5.60	108.04	105.80
34	YA	2457	U	N3-C2-O2	-5.60	118.28	122.20
44	RP	59	LEU	CA-CB-CG	5.60	128.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	435	C	C5-C6-N1	5.60	123.80	121.00
34	RA	1417	C	N1-C2-O2	5.60	122.26	118.90
34	RA	1982	C	C2-N1-C1'	5.60	124.96	118.80
34	RA	1934	C	N1-C2-O2	5.60	122.26	118.90
34	YA	231	C	N1-C2-O2	5.60	122.26	118.90
34	YA	2559	C	N1-C2-O2	5.60	122.26	118.90
1	QA	525	C	C5-C6-N1	5.60	123.80	121.00
22	XV	31	G	N3-C4-C5	-5.60	125.80	128.60
22	QV	15	G	N3-C4-N9	5.59	129.35	126.00
22	XV	15	G	N7-C8-N9	5.59	115.90	113.10
34	RA	1881	C	C6-N1-C2	-5.59	118.06	120.30
34	YA	1742	C	C6-N1-C2	-5.59	118.06	120.30
35	YB	38	C	C6-N1-C2	-5.59	118.06	120.30
35	YB	60	C	C5-C6-N1	5.59	123.79	121.00
34	RA	420	C	C2-N1-C1'	5.59	124.94	118.80
35	YB	37	C	C6-N1-C2	-5.58	118.07	120.30
35	YB	94	C	C6-N1-C2	-5.58	118.07	120.30
34	YA	1430	C	C5-C6-N1	5.58	123.79	121.00
1	XA	154	C	N1-C2-O2	5.58	122.25	118.90
34	YA	1683	C	C5-C6-N1	5.58	123.79	121.00
1	QA	891	U	N3-C2-O2	-5.58	118.30	122.20
34	RA	2065	C	C6-N1-C2	-5.58	118.07	120.30
34	YA	2460	U	N1-C2-O2	5.58	126.70	122.80
1	QA	503	C	C2-N1-C1'	5.57	124.93	118.80
34	RA	76	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	797	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	2008	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	2516	G	N3-C4-C5	-5.57	125.81	128.60
34	RA	2128	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	409	C	N1-C2-O2	5.57	122.24	118.90
34	YA	2032	G	N3-C4-C5	5.57	131.38	128.60
34	YA	1644	C	N3-C2-O2	-5.57	118.00	121.90
34	RA	102	G	P-O3'-C3'	5.56	126.37	119.70
34	RA	2559	C	N3-C2-O2	-5.56	118.01	121.90
34	RA	1881	C	C5-C6-N1	5.56	123.78	121.00
1	XA	645	C	N3-C2-O2	-5.56	118.01	121.90
34	YA	2832	U	OP2-P-O3'	5.55	117.42	105.20
1	QA	241	C	C6-N1-C2	-5.55	118.08	120.30
34	YA	385	C	C2-N1-C1'	5.55	124.91	118.80
1	QA	993	G	C4-N9-C1'	5.55	133.72	126.50
34	YA	1398	C	C6-N1-C2	-5.55	118.08	120.30
1	XA	1113	C	C5-C6-N1	5.55	123.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R5	34	PRO	CA-N-CD	-5.55	103.73	111.50
34	YA	2099	U	N1-C2-O2	5.55	126.68	122.80
28	Y4	39	CYS	N-CA-C	-5.54	96.03	111.00
32	R8	61	LEU	C-N-CA	5.54	135.56	121.70
34	RA	384	U	C2-N1-C1'	5.54	124.35	117.70
34	YA	1383	C	N1-C2-O2	5.54	122.23	118.90
34	YA	2161	C	N1-C2-O2	5.54	122.23	118.90
1	XA	455	C	N1-C2-O2	5.54	122.22	118.90
34	YA	2321	G	C8-N9-C1'	-5.54	119.80	127.00
34	YA	2889	C	C2-N1-C1'	5.54	124.90	118.80
34	RA	99	U	P-O3'-C3'	5.54	126.35	119.70
34	RA	1264	G	C8-N9-C4	-5.54	104.18	106.40
1	QA	458(A)	C	C6-N1-C2	-5.54	118.08	120.30
34	RA	624	C	C6-N1-C2	-5.54	118.08	120.30
34	YA	2061	G	C4-N9-C1'	5.54	133.70	126.50
1	QA	762	C	C6-N1-C2	-5.54	118.09	120.30
1	QA	381	C	N3-C2-O2	-5.53	118.03	121.90
1	XA	1322	C	C5-C6-N1	5.53	123.77	121.00
34	YA	544	C	C2-N1-C1'	5.53	124.88	118.80
34	YA	1290	C	C6-N1-C2	-5.53	118.09	120.30
34	YA	2846	G	C8-N9-C4	-5.53	104.19	106.40
54	YZ	62	PRO	C-N-CA	5.53	135.52	121.70
34	YA	2827	C	C5-C6-N1	5.53	123.77	121.00
34	RA	1857	G	C8-N9-C4	-5.53	104.19	106.40
34	RA	2559	C	C5-C6-N1	5.53	123.76	121.00
34	RA	2874	C	N1-C2-O2	5.53	122.22	118.90
1	XA	125	U	O4'-C1'-N1	5.53	112.62	108.20
1	XA	811	C	N3-C2-O2	-5.53	118.03	121.90
40	RH	153	LYS	N-CA-C	5.53	125.92	111.00
34	YA	267	C	N1-C2-O2	5.53	122.22	118.90
34	YA	2453	A	C5-C6-N6	-5.53	119.28	123.70
1	QA	443	C	C2-N1-C1'	5.52	124.88	118.80
34	YA	9	U	N1-C2-O2	5.52	126.67	122.80
34	YA	1658	C	C2-N1-C1'	5.52	124.88	118.80
34	YA	2107	C	N3-C2-O2	-5.52	118.03	121.90
34	YA	1549	C	C6-N1-C2	-5.52	118.09	120.30
34	YA	904	C	N1-C2-O2	5.52	122.21	118.90
1	QA	455	C	C5-C6-N1	5.52	123.76	121.00
34	YA	104	U	N1-C2-O2	5.52	126.66	122.80
34	YA	1653	G	C4-N9-C1'	5.52	133.67	126.50
44	YP	59	LEU	CA-CB-CG	5.52	127.99	115.30
34	RA	1742	C	N1-C2-O2	5.51	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	102	G	P-O3'-C3'	5.51	126.32	119.70
34	YA	2506	U	C5-C6-N1	5.51	125.46	122.70
34	YA	2871	C	C6-N1-C2	-5.51	118.09	120.30
1	QA	597	G	C4-C5-N7	5.51	113.00	110.80
1	QA	136	C	C6-N1-C1'	-5.51	114.19	120.80
34	RA	1376	C	C2-N1-C1'	5.51	124.86	118.80
34	RA	1632	A	C8-N9-C4	-5.51	103.59	105.80
34	RA	1786	A	N7-C8-N9	5.51	116.56	113.80
34	RA	2295	C	N1-C2-O2	5.51	122.21	118.90
1	XA	353	A	OP2-P-O3'	5.51	117.33	105.20
34	YA	1598	C	N3-C2-O2	-5.51	118.04	121.90
1	QA	697	U	N1-C2-O2	5.51	126.66	122.80
1	QA	1158	C	C2-N1-C1'	5.51	124.86	118.80
34	RA	1611	C	C6-N1-C2	-5.51	118.10	120.30
34	RA	2226	C	C6-N1-C2	-5.51	118.10	120.30
34	RA	2591	C	C6-N1-C2	-5.51	118.10	120.30
1	XA	1290	G	C8-N9-C1'	-5.51	119.84	127.00
34	RA	1549	C	N1-C2-O2	5.50	122.20	118.90
34	YA	2098	U	N3-C2-O2	-5.50	118.35	122.20
34	YA	2771	C	N1-C2-O2	5.50	122.20	118.90
34	RA	2316	C	C5-C6-N1	5.50	123.75	121.00
1	XA	525	C	C6-N1-C2	-5.50	118.10	120.30
34	YA	923	C	C6-N1-C2	-5.50	118.10	120.30
34	YA	998	C	C5-C6-N1	5.50	123.75	121.00
34	YA	1947	C	C6-N1-C2	-5.50	118.10	120.30
34	YA	2048	G	C8-N9-C1'	-5.50	119.84	127.00
34	YA	2576	G	N3-C4-N9	5.50	129.30	126.00
34	RA	974(B)	C	P-O3'-C3'	5.50	126.30	119.70
34	YA	641	C	N1-C2-O2	5.50	122.20	118.90
34	YA	2512	C	C5-C6-N1	5.50	123.75	121.00
23	QX	17	C	N3-C4-C5	-5.50	119.70	121.90
34	YA	1295	C	N3-C2-O2	-5.50	118.05	121.90
34	YA	1140	C	C2-N1-C1'	5.50	124.84	118.80
34	YA	2099	U	C2-N1-C1'	5.50	124.29	117.70
34	RA	2666	C	N1-C2-O2	5.49	122.20	118.90
1	QA	1181	G	N1-C6-O6	-5.49	116.61	119.90
34	YA	1290	C	C5-C6-N1	5.49	123.75	121.00
34	YA	2048	G	N3-C4-N9	5.49	129.29	126.00
23	QX	19	U	O4'-C1'-N1	5.49	112.59	108.20
34	RA	2053	G	N9-C4-C5	-5.49	103.20	105.40
1	QA	64	G	P-O3'-C3'	5.49	126.28	119.70
34	RA	856	C	N3-C2-O2	-5.48	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	988	G	N1-C6-O6	-5.48	116.61	119.90
1	XA	1297	C	N1-C2-O2	5.48	122.19	118.90
1	QA	548	G	C6-C5-N7	-5.48	127.11	130.40
34	YA	657	U	N3-C2-O2	-5.48	118.36	122.20
34	RA	1064	C	C5-C6-N1	5.48	123.74	121.00
34	RA	2720	U	N3-C2-O2	-5.48	118.37	122.20
34	YA	510	C	N1-C2-O2	5.48	122.19	118.90
1	QA	1407	C	C6-N1-C2	-5.47	118.11	120.30
1	XA	1403	C	C6-N1-C2	-5.47	118.11	120.30
34	RA	1786	A	C4-N9-C1'	5.47	136.15	126.30
34	RA	2784	C	C6-N1-C2	-5.47	118.11	120.30
34	RA	1180	C	N1-C2-O2	5.47	122.18	118.90
34	RA	1611	C	C5-C6-N1	5.47	123.73	121.00
34	YA	413	C	N1-C2-O2	5.47	122.18	118.90
34	RA	665	C	C6-N1-C2	-5.47	118.11	120.30
34	YA	1575	C	C5-C6-N1	5.47	123.73	121.00
34	RA	825	C	C6-N1-C2	-5.46	118.11	120.30
34	RA	1644	C	N1-C2-O2	5.46	122.18	118.90
34	YA	2317	C	C6-N1-C2	-5.46	118.11	120.30
1	XA	1539	C	C5-C4-N4	5.46	124.02	120.20
34	YA	1775	U	N3-C4-O4	5.46	123.22	119.40
1	QA	1366	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	590	C	C2-N1-C1'	5.46	124.80	118.80
1	QA	1430	C	C6-N1-C2	-5.46	118.12	120.30
34	RA	120	U	C6-N1-C2	-5.46	117.72	121.00
34	RA	1075	C	N1-C2-O2	5.46	122.17	118.90
34	RA	2254	C	C5-C6-N1	5.46	123.73	121.00
34	YA	1844	C	C5-C6-N1	5.46	123.73	121.00
34	RA	641	C	C2-N1-C1'	5.45	124.80	118.80
34	RA	1535	U	C6-N1-C1'	-5.45	113.57	121.20
34	RA	1741	C	C6-N1-C2	-5.45	118.12	120.30
34	YA	1363	C	C6-N1-C2	-5.45	118.12	120.30
34	RA	456	C	C6-N1-C1'	-5.45	114.27	120.80
34	RA	2142	C	N1-C2-O2	5.45	122.17	118.90
1	XA	514	C	N1-C2-O2	5.45	122.17	118.90
34	YA	986	C	C6-N1-C2	-5.45	118.12	120.30
34	YA	1549	C	C2-N1-C1'	5.45	124.79	118.80
34	RA	1762	A	C8-N9-C4	-5.44	103.62	105.80
34	YA	393	C	C5-C6-N1	5.44	123.72	121.00
34	YA	1157	G	C6-C5-N7	-5.44	127.13	130.40
34	YA	2683	C	N1-C2-O2	5.44	122.17	118.90
50	RV	48	GLY	C-N-CA	5.44	135.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1135	C	N3-C2-O2	-5.44	118.09	121.90
34	RA	208	C	C5-C6-N1	5.44	123.72	121.00
34	YA	30	G	N3-C4-N9	5.44	129.26	126.00
34	RA	74	A	C4-C5-C6	-5.44	114.28	117.00
34	YA	2294	C	C5-C6-N1	5.44	123.72	121.00
34	RA	2064	C	C2-N1-C1'	5.43	124.78	118.80
1	XA	1190	G	C6-N1-C2	-5.43	121.84	125.10
34	YA	584	C	N1-C2-O2	5.43	122.16	118.90
34	RA	2579	C	C6-N1-C2	-5.43	118.13	120.30
34	YA	2043	C	C6-N1-C2	-5.43	118.13	120.30
23	XX	16	C	O5'-P-OP2	-5.43	100.81	105.70
34	YA	669	G	C8-N9-C1'	-5.43	119.94	127.00
1	QA	54	C	N3-C2-O2	-5.43	118.10	121.90
1	XA	1539	C	C6-N1-C1'	5.43	127.31	120.80
34	RA	1774	C	C5-C6-N1	5.42	123.71	121.00
34	YA	208	C	C5-C6-N1	5.42	123.71	121.00
34	YA	2254	C	C5-C6-N1	5.42	123.71	121.00
1	QA	1263	C	C6-N1-C1'	-5.42	114.30	120.80
34	RA	265	A	O4'-C1'-N9	5.42	112.53	108.20
1	XA	943	U	N1-C2-O2	5.42	126.59	122.80
1	QA	1301	U	C6-N1-C2	-5.42	117.75	121.00
34	RA	676	A	O4'-C1'-N9	5.42	112.53	108.20
34	RA	2073	C	C6-N1-C2	-5.42	118.13	120.30
34	YA	335	C	C6-N1-C2	-5.42	118.13	120.30
34	RA	1506	C	N3-C2-O2	-5.41	118.11	121.90
34	RA	1836	C	C5-C6-N1	5.41	123.71	121.00
1	XA	993	G	C6-C5-N7	-5.41	127.15	130.40
34	YA	1233	C	C5-C6-N1	5.41	123.71	121.00
34	RA	1437	C	C6-N1-C2	-5.41	118.14	120.30
34	RA	2008	C	C6-N1-C2	-5.41	118.14	120.30
34	YA	657	U	N1-C2-O2	5.41	126.59	122.80
34	RA	221	A	P-O3'-C3'	5.41	126.19	119.70
12	XL	46	LYS	C-N-CA	-5.41	108.18	121.70
34	RA	2456	C	C5-C6-N1	5.40	123.70	121.00
34	YA	691	C	C5-C6-N1	5.40	123.70	121.00
34	YA	1781	C	N3-C2-O2	-5.40	118.12	121.90
34	YA	2474	C	N3-C2-O2	-5.40	118.12	121.90
1	QA	58	C	C6-N1-C2	-5.40	118.14	120.30
1	QA	738	C	C5-C6-N1	5.40	123.70	121.00
34	YA	957	A	C4-C5-N7	5.40	113.40	110.70
34	YA	1343	G	C4-N9-C1'	5.40	133.52	126.50
1	QA	522	C	N1-C2-O2	5.40	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	13	C	N1-C2-O2	5.40	122.14	118.90
34	RA	2108	C	N1-C2-O2	5.40	122.14	118.90
35	YB	71	C	C2-N1-C1'	5.40	124.74	118.80
34	YA	1402	C	C5-C6-N1	5.40	123.70	121.00
34	RA	1914	C	C6-N1-C1'	-5.39	114.33	120.80
22	XV	40	G	C8-N9-C1'	-5.39	119.99	127.00
34	RA	1407	C	C6-N1-C1'	-5.39	114.33	120.80
34	YA	1640	C	C5-C6-N1	5.39	123.70	121.00
48	YT	114	LEU	CA-CB-CG	5.39	127.70	115.30
34	YA	1021	A	C8-N9-C4	-5.39	103.64	105.80
34	YA	1468	C	C5-C6-N1	5.39	123.70	121.00
34	RA	634	C	N1-C2-O2	5.39	122.13	118.90
34	RA	1126	A	C6-N1-C2	5.39	121.83	118.60
34	RA	1830	C	N1-C2-O2	5.39	122.13	118.90
34	YA	2036	C	C2-N1-C1'	5.39	124.73	118.80
40	YH	155	SER	N-CA-C	5.39	125.55	111.00
34	YA	461	C	C5-C6-N1	5.39	123.69	121.00
34	RA	420	C	N1-C2-O2	5.38	122.13	118.90
34	RA	2496	C	O5'-P-OP1	-5.38	100.86	105.70
34	YA	897	C	C2-N1-C1'	5.38	124.72	118.80
34	YA	2576	G	C8-N9-C1'	-5.38	120.00	127.00
34	YA	2787	C	C6-N1-C1'	-5.38	114.34	120.80
34	RA	270(L)	C	N1-C2-O2	5.38	122.13	118.90
34	RA	1598	C	C2-N1-C1'	5.38	124.72	118.80
34	YA	2646	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	2779	U	N1-C2-O2	5.38	126.57	122.80
34	RA	1762	A	N3-C4-C5	-5.38	123.03	126.80
34	RA	2063	C	N1-C2-O2	5.38	122.13	118.90
1	XA	455	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	445	C	C6-N1-C2	-5.38	118.15	120.30
34	RA	1640	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	2032	G	C4-C5-C6	-5.38	115.57	118.80
1	XA	615	C	C6-N1-C2	-5.37	118.15	120.30
1	XA	723	U	N3-C2-O2	-5.37	118.44	122.20
34	YA	2107	C	C6-N1-C2	-5.37	118.15	120.30
35	YB	51	G	N1-C6-O6	-5.37	116.68	119.90
1	QA	218	C	C6-N1-C2	-5.37	118.15	120.30
1	XA	1045	C	N1-C2-O2	5.37	122.12	118.90
34	YA	1644	C	N1-C2-O2	5.37	122.12	118.90
34	RA	2517	C	N3-C4-C5	-5.37	119.75	121.90
34	YA	1598	C	C5-C6-N1	5.37	123.69	121.00
34	YA	2043	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	2809	A	N7-C8-N9	5.37	116.48	113.80
1	XA	443	C	C6-N1-C2	-5.37	118.15	120.30
34	YA	183	C	C5-C6-N1	5.37	123.68	121.00
1	QA	514	C	N1-C2-O2	5.37	122.12	118.90
14	QN	43	CYS	CA-CB-SG	-5.37	104.34	114.00
34	RA	1158	C	N1-C2-O2	5.37	122.12	118.90
34	RA	1534	G	N3-C4-N9	5.37	129.22	126.00
34	YA	1679	U	C2-N1-C1'	5.37	124.14	117.70
34	YA	2320	A	N3-C4-N9	5.37	131.69	127.40
22	QV	36	G	C8-N9-C4	-5.36	104.25	106.40
34	RA	1513	C	C6-N1-C2	-5.36	118.16	120.30
14	XN	58	LYS	N-CA-C	-5.36	96.52	111.00
34	YA	2008	C	C5-C6-N1	5.36	123.68	121.00
23	QX	19	U	C2-N1-C1'	-5.36	111.27	117.70
34	YA	729	G	N3-C2-N2	-5.36	116.15	119.90
1	QA	1395	C	C5-C6-N1	5.36	123.68	121.00
34	RA	1788	C	C6-N1-C2	-5.36	118.16	120.30
1	XA	891	U	N1-C2-O2	5.36	126.55	122.80
34	YA	541	C	C6-N1-C2	-5.36	118.16	120.30
34	YA	2210	G	N3-C4-C5	-5.36	125.92	128.60
34	YA	2471	C	C2-N1-C1'	5.36	124.69	118.80
34	YA	2681	C	OP2-P-O3'	5.36	116.99	105.20
35	RB	22	U	N3-C2-O2	-5.36	118.45	122.20
34	YA	1411	C	C2-N1-C1'	5.36	124.69	118.80
1	QA	1066	C	C5-C6-N1	5.36	123.68	121.00
34	RA	1306	C	C2-N1-C1'	5.36	124.69	118.80
34	RA	2089	U	N1-C2-O2	5.36	126.55	122.80
34	YA	1021	A	C5-N7-C8	-5.36	101.22	103.90
34	RA	1544	C	N3-C2-O2	-5.36	118.15	121.90
34	RA	1988	C	C5-C6-N1	5.36	123.68	121.00
34	YA	12	U	C2-N1-C1'	5.36	124.13	117.70
34	YA	2032	G	C4-N9-C1'	-5.36	119.54	126.50
34	RA	1313	U	C5-C6-N1	5.35	125.38	122.70
34	RA	1947	C	C6-N1-C2	-5.35	118.16	120.30
34	YA	2395	C	C5-C6-N1	5.35	123.68	121.00
34	RA	1445	C	C5-C6-N1	5.35	123.67	121.00
1	XA	1056	U	N3-C2-O2	-5.35	118.46	122.20
34	YA	1957	C	N3-C2-O2	-5.35	118.16	121.90
34	YA	2889	C	N3-C2-O2	-5.35	118.16	121.90
1	QA	54	C	C6-N1-C2	-5.35	118.16	120.30
1	QA	241	C	N1-C2-O2	5.35	122.11	118.90
34	RA	797	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1797	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	2115	G	C4-N9-C1'	5.35	133.45	126.50
34	RA	2703	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	1375	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	2307	G	O4'-C1'-N9	5.35	112.48	108.20
34	YA	1793	C	C5-C6-N1	5.34	123.67	121.00
34	YA	2542	A	N1-C6-N6	5.34	121.81	118.60
1	QA	131	C	N3-C2-O2	-5.34	118.16	121.90
34	RA	487	C	N1-C2-O2	5.34	122.10	118.90
34	RA	1741	C	C5-C6-N1	5.34	123.67	121.00
20	XT	10	LEU	CA-CB-CG	5.34	127.58	115.30
34	YA	1166	C	C5-C6-N1	5.34	123.67	121.00
34	YA	2033	A	O5'-P-OP2	-5.34	100.89	105.70
34	RA	1526	G	C4-N9-C1'	5.34	133.44	126.50
34	YA	2026	C	C5-C6-N1	5.34	123.67	121.00
34	RA	721	C	C5-C6-N1	5.34	123.67	121.00
34	RA	817	C	C6-N1-C2	-5.34	118.17	120.30
1	XA	1348	U	C2-N1-C1'	5.34	124.10	117.70
34	RA	1049	C	C6-N1-C2	-5.33	118.17	120.30
1	QA	848	C	N1-C2-O2	5.33	122.10	118.90
34	RA	200	U	N1-C2-O2	5.33	126.53	122.80
34	RA	384	U	N3-C2-O2	-5.33	118.47	122.20
34	RA	2321	G	C8-N9-C1'	-5.33	120.07	127.00
1	XA	354	G	C4-N9-C1'	5.33	133.43	126.50
34	YA	459	U	N1-C2-O2	5.33	126.53	122.80
34	YA	1102	C	N3-C2-O2	-5.33	118.17	121.90
33	R9	32	HIS	CB-CA-C	5.33	121.06	110.40
1	QA	1158	C	N3-C2-O2	-5.33	118.17	121.90
34	RA	721	C	C6-N1-C1'	-5.33	114.41	120.80
1	XA	1109	C	N1-C2-O2	5.33	122.10	118.90
34	YA	2359	C	C5-C6-N1	5.33	123.66	121.00
34	RA	67	U	C2-N1-C1'	5.33	124.09	117.70
34	YA	1004	C	C5-C6-N1	5.33	123.66	121.00
34	RA	2115	G	N3-C4-N9	5.32	129.19	126.00
1	QA	352	C	N1-C2-O2	5.32	122.09	118.90
34	YA	1506	C	C6-N1-C2	-5.32	118.17	120.30
34	RA	580	C	C6-N1-C2	-5.32	118.17	120.30
34	RA	1691	C	C5-C6-N1	5.32	123.66	121.00
34	YA	2043	C	C2-N1-C1'	5.32	124.65	118.80
34	RA	2568	C	C5-C6-N1	5.32	123.66	121.00
34	RA	1781	C	C2-N1-C1'	5.32	124.65	118.80
1	XA	1390	U	N3-C2-O2	-5.32	118.48	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	535	C	C5-C6-N1	5.32	123.66	121.00
34	YA	1157	G	C4-N9-C1'	5.32	133.41	126.50
34	RA	665	C	C5-C6-N1	5.31	123.66	121.00
1	XA	1296	C	C6-N1-C2	-5.31	118.17	120.30
35	YB	22	U	N1-C2-O2	5.31	126.52	122.80
35	RB	22	U	N1-C2-O2	5.31	126.52	122.80
34	YA	1805	U	C5-C6-N1	5.31	125.36	122.70
34	YA	2874	C	N1-C2-O2	5.31	122.09	118.90
34	RA	634	C	C5-C6-N1	5.31	123.66	121.00
34	RA	141(B)	C	C5-C6-N1	5.31	123.65	121.00
1	XA	110	C	N3-C2-O2	-5.31	118.19	121.90
34	YA	241	A	OP1-P-O3'	5.31	116.88	105.20
35	YB	44	G	C4-N9-C1'	-5.31	119.60	126.50
45	YQ	17	LEU	CB-CA-C	-5.31	100.11	110.20
34	YA	2395	C	C6-N1-C2	-5.31	118.18	120.30
1	XA	910	C	C5-C6-N1	5.30	123.65	121.00
34	YA	248	G	C8-N9-C4	-5.30	104.28	106.40
34	YA	542	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	1990	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	2236	C	N1-C2-O2	5.30	122.08	118.90
34	RA	503	A	P-O3'-C3'	5.30	126.06	119.70
34	YA	641	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	2320	A	C4-N9-C1'	5.30	135.84	126.30
34	YA	481	G	O4'-C1'-N9	5.30	112.44	108.20
1	QA	904	C	N1-C2-O2	5.30	122.08	118.90
1	QA	252	U	N1-C2-O2	5.30	126.51	122.80
34	RA	1445	C	C6-N1-C2	-5.30	118.18	120.30
1	QA	435	C	C6-N1-C2	-5.29	118.18	120.30
34	RA	2089	U	C5-C6-N1	5.29	125.35	122.70
34	YA	556	G	C4-N9-C1'	5.29	133.38	126.50
1	QA	514	C	C6-N1-C2	-5.29	118.18	120.30
22	QV	36	G	C5-N7-C8	-5.29	101.66	104.30
34	RA	537	C	N1-C2-O2	5.29	122.08	118.90
34	YA	836	G	C8-N9-C4	-5.29	104.28	106.40
34	YA	1398	C	C5-C6-N1	5.29	123.65	121.00
34	RA	1506	C	C6-N1-C2	-5.29	118.18	120.30
34	YA	2682	U	N1-C2-O2	5.29	126.50	122.80
34	RA	1611	C	C2-N1-C1'	5.29	124.62	118.80
34	YA	1385	G	O4'-C1'-N9	5.29	112.43	108.20
34	RA	2089	U	N3-C2-O2	-5.28	118.50	122.20
34	YA	2236	C	C5-C6-N1	5.28	123.64	121.00
34	YA	420	C	N3-C2-O2	-5.28	118.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1463	C	C6-N1-C2	-5.28	118.19	120.30
34	RA	1437	C	C2-N1-C1'	5.28	124.61	118.80
1	XA	68(S)	C	C2-N1-C1'	5.28	124.61	118.80
34	YA	556	G	N3-C4-N9	5.28	129.17	126.00
34	YA	692	C	C6-N1-C2	-5.28	118.19	120.30
34	RA	192	C	N3-C2-O2	-5.28	118.21	121.90
34	RA	846	C	OP2-P-O3'	5.28	116.81	105.20
34	RA	1313	U	C6-N1-C2	-5.28	117.83	121.00
34	YA	1407	C	C6-N1-C1'	-5.28	114.47	120.80
34	YA	1864	U	N1-C2-O2	5.28	126.49	122.80
34	YA	2350	C	C2-N1-C1'	5.28	124.61	118.80
35	YB	51	G	C5-C6-O6	5.28	131.77	128.60
34	RA	1982	C	C5-C6-N1	5.28	123.64	121.00
1	XA	186(B)	C	C5-C6-N1	5.28	123.64	121.00
34	YA	1267	U	C5-C6-N1	5.28	125.34	122.70
34	YA	1766	U	N3-C2-O2	-5.28	118.51	122.20
34	YA	2798	C	N1-C2-O2	5.28	122.06	118.90
35	RB	27	C	C6-N1-C2	-5.27	118.19	120.30
34	YA	1370	C	N1-C2-O2	5.27	122.06	118.90
1	QA	1234	C	C6-N1-C2	-5.27	118.19	120.30
34	RA	1526	G	C8-N9-C1'	-5.27	120.15	127.00
34	YA	692	C	C5-C6-N1	5.27	123.64	121.00
34	YA	1257	C	C6-N1-C2	-5.27	118.19	120.30
34	YA	1920	C	C2-N1-C1'	5.27	124.60	118.80
1	QA	597	G	N9-C4-C5	-5.27	103.29	105.40
34	RA	2615	U	C2-N1-C1'	5.27	124.03	117.70
34	YA	229	A	OP2-P-O3'	5.27	116.80	105.20
34	YA	840	C	C6-N1-C2	-5.27	118.19	120.30
34	RA	1509	C	OP1-P-O3'	5.27	116.80	105.20
34	YA	1135	C	C6-N1-C1'	-5.27	114.48	120.80
34	YA	1742	C	C5-C6-N1	5.27	123.63	121.00
34	YA	2699	C	N1-C2-O2	5.27	122.06	118.90
1	XA	723	U	C2-N1-C1'	5.27	124.02	117.70
34	YA	1298	C	C5-C6-N1	5.27	123.63	121.00
34	YA	2539	C	N1-C2-O2	5.27	122.06	118.90
54	YZ	151	HIS	N-CA-C	5.27	125.22	111.00
34	RA	650	C	C2-N1-C1'	5.26	124.59	118.80
34	RA	692	C	C2-N1-C1'	5.26	124.59	118.80
34	RA	74	A	C4-N9-C1'	-5.26	116.83	126.30
34	RA	2666	C	C2-N1-C1'	5.26	124.59	118.80
1	XA	689	C	C2-N1-C1'	5.26	124.59	118.80
34	RA	1153	C	C6-N1-C2	-5.26	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	283	C	C6-N1-C2	-5.26	118.20	120.30
34	YA	2556	C	N1-C2-O2	5.26	122.05	118.90
1	QA	555	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	745	C	C6-N1-C2	-5.25	118.20	120.30
1	XA	266	G	P-O3'-C3'	5.25	126.00	119.70
34	YA	2798	C	C6-N1-C2	-5.25	118.20	120.30
35	YB	31	C	C6-N1-C2	-5.25	118.20	120.30
34	RA	1549	C	C6-N1-C2	-5.25	118.20	120.30
34	YA	1295	C	N1-C2-O2	5.25	122.05	118.90
34	YA	1931	U	N3-C2-O2	-5.25	118.53	122.20
34	RA	2179	C	C2-N1-C1'	5.25	124.57	118.80
1	XA	966	G	C4-N9-C1'	-5.25	119.68	126.50
1	QA	962	C	C6-N1-C2	-5.25	118.20	120.30
34	RA	1830	C	C6-N1-C2	-5.24	118.20	120.30
1	XA	37	U	N3-C2-O2	-5.24	118.53	122.20
34	YA	1653	G	C8-N9-C4	-5.24	104.30	106.40
34	RA	1708	C	C6-N1-C2	-5.24	118.20	120.30
54	RZ	178	GLU	C-N-CA	5.24	134.81	121.70
34	YA	2063	C	C5-C6-N1	5.24	123.62	121.00
34	YA	1779	U	C2-N1-C1'	5.24	123.98	117.70
34	RA	1332	G	C4-N9-C1'	5.24	133.31	126.50
34	RA	1971	A	C2-N3-C4	5.24	113.22	110.60
1	XA	993	G	N3-C4-N9	5.24	129.14	126.00
1	QA	519	C	N1-C2-O2	5.23	122.04	118.90
34	YA	2129	C	N1-C2-O2	5.23	122.04	118.90
34	YA	664	C	C6-N1-C2	-5.23	118.21	120.30
34	YA	752	A	OP2-P-O3'	5.23	116.71	105.20
34	YA	856	C	C2-N3-C4	5.23	122.52	119.90
34	RA	666	G	N3-C4-N9	5.23	129.14	126.00
34	RA	1102	C	C5-C6-N1	5.23	123.61	121.00
34	YA	1957	C	N1-C2-O2	5.23	122.03	118.90
1	XA	328	C	OP2-P-O3'	5.22	116.69	105.20
34	YA	2787	C	C5-C6-N1	5.22	123.61	121.00
34	RA	876	C	N3-C2-O2	-5.22	118.24	121.90
34	RA	2646	C	C5-C6-N1	5.22	123.61	121.00
1	XA	536	C	C6-N1-C2	-5.22	118.21	120.30
34	YA	1526	G	C4-N9-C1'	5.22	133.29	126.50
34	RA	2755	C	C5-C6-N1	5.22	123.61	121.00
34	RA	31	C	C2-N1-C1'	5.22	124.54	118.80
34	RA	613	U	C6-N1-C1'	-5.22	113.90	121.20
34	RA	1930	G	P-O3'-C3'	5.22	125.96	119.70
34	YA	1083	U	N3-C2-O2	-5.22	118.55	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	2588	G	C4-C5-N7	5.21	112.89	110.80
34	YA	273(G)	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1463	C	C6-N1-C2	-5.21	118.22	120.30
34	YA	1598	C	C6-N1-C1'	-5.21	114.55	120.80
34	YA	528	A	N1-C6-N6	5.21	121.72	118.60
34	RA	2137	C	C2-N1-C1'	5.21	124.53	118.80
1	XA	970	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1539	C	C2-N1-C1'	-5.21	113.07	118.80
34	YA	635	C	C5-C6-N1	5.21	123.60	121.00
35	YB	44	G	C8-N9-C1'	5.21	133.77	127.00
1	XA	1306	A	O4'-C1'-N9	5.20	112.36	108.20
34	YA	1145	C	C6-N1-C2	-5.20	118.22	120.30
34	RA	2582	G	C8-N9-C1'	-5.20	120.24	127.00
1	XA	1383	C	C2-N1-C1'	5.20	124.52	118.80
34	RA	2874	C	C6-N1-C1'	-5.20	114.56	120.80
34	RA	2544	G	N7-C8-N9	5.20	115.70	113.10
1	XA	943	U	N3-C2-O2	-5.20	118.56	122.20
34	YA	530	G	C4-C5-N7	-5.20	108.72	110.80
34	RA	2063	C	C6-N1-C2	-5.19	118.22	120.30
34	YA	816	C	C5-C6-N1	5.19	123.60	121.00
34	YA	1178	C	C5-C6-N1	5.19	123.60	121.00
1	QA	891	U	N1-C2-O2	5.19	126.43	122.80
34	YA	1021	A	C2-N3-C4	-5.19	108.00	110.60
34	YA	1652	A	N1-C6-N6	5.19	121.71	118.60
34	YA	2685	G	N3-C4-N9	-5.19	122.89	126.00
53	YY	79	CYS	N-CA-CB	5.19	119.94	110.60
34	RA	339	U	N3-C2-O2	-5.18	118.57	122.20
22	XV	15	G	C2-N3-C4	5.18	114.49	111.90
34	YA	915	C	C6-N1-C1'	-5.18	114.58	120.80
34	RA	915	C	C6-N1-C2	-5.18	118.23	120.30
34	RA	976	C	C2-N1-C1'	5.18	124.50	118.80
34	YA	721	C	C5-C6-N1	5.18	123.59	121.00
34	YA	730	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	1519	G	C6-C5-N7	-5.18	127.29	130.40
34	YA	2299	G	C4-N9-C1'	5.18	133.24	126.50
1	QA	110	C	N1-C2-O2	5.18	122.01	118.90
1	QA	590	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	2544	G	C5-C6-O6	-5.18	125.49	128.60
34	YA	2456	C	C6-N1-C2	-5.18	118.23	120.30
34	RA	510	C	C5-C6-N1	5.18	123.59	121.00
34	YA	2798	C	C2-N1-C1'	5.18	124.50	118.80
35	RB	31	C	C6-N1-C2	-5.18	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1598	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	1684	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	1839	G	C4-N9-C1'	5.18	133.23	126.50
34	RA	1474	C	N3-C2-O2	-5.17	118.28	121.90
1	XA	620	C	N3-C2-O2	-5.17	118.28	121.90
34	RA	1776	G	N3-C4-N9	5.17	129.10	126.00
34	RA	1806	C	C6-N1-C2	-5.17	118.23	120.30
1	XA	241	C	N1-C2-O2	5.17	122.00	118.90
34	RA	1899	G	N3-C4-C5	-5.17	126.02	128.60
34	RA	1950	G	C8-N9-C1'	-5.17	120.28	127.00
34	RA	1294	U	N1-C2-O2	5.16	126.42	122.80
1	XA	1054	C	N1-C2-O2	5.16	122.00	118.90
36	YD	243	GLY	N-CA-C	5.16	126.01	113.10
34	RA	1526	G	N3-C4-N9	5.16	129.10	126.00
34	YA	2006	C	N3-C2-O2	-5.16	118.29	121.90
34	RA	9	U	C2-N1-C1'	5.16	123.89	117.70
34	RA	1830	C	C2-N1-C1'	5.16	124.48	118.80
34	YA	1256	G	N3-C4-N9	5.16	129.10	126.00
34	YA	2442	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	330	C	N3-C2-O2	-5.16	118.29	121.90
1	QA	442	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	833	U	N3-C2-O2	-5.16	118.59	122.20
34	YA	105	C	C6-N1-C2	-5.16	118.24	120.30
34	RA	2307	G	C8-N9-C1'	-5.16	120.30	127.00
34	YA	1881	C	N1-C2-O2	5.16	121.99	118.90
1	QA	224	C	N1-C2-O2	5.16	121.99	118.90
34	RA	1130	U	OP1-P-O3'	5.16	116.54	105.20
34	YA	333	G	C8-N9-C1'	-5.16	120.30	127.00
34	YA	2584	U	O4'-C1'-N1	5.16	112.32	108.20
34	RA	1788	C	C2-N1-C1'	5.15	124.47	118.80
34	YA	2006	C	C6-N1-C2	-5.15	118.24	120.30
1	QA	1440(O)	C	N3-C2-O2	-5.15	118.29	121.90
34	YA	1683	C	C6-N1-C2	-5.15	118.24	120.30
1	QA	308	C	N3-C2-O2	-5.15	118.30	121.90
34	RA	41	C	C6-N1-C2	-5.15	118.24	120.30
34	RA	1467	C	C6-N1-C2	-5.15	118.24	120.30
34	YA	634	C	N1-C2-O2	5.15	121.99	118.90
34	RA	2089	U	C2-N1-C1'	5.15	123.88	117.70
34	RA	2142	C	N3-C2-O2	-5.15	118.30	121.90
34	YA	9	U	C2-N1-C1'	5.15	123.88	117.70
34	RA	635	C	C6-N1-C2	-5.15	118.24	120.30
34	RA	1506	C	C2-N1-C1'	5.14	124.46	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	XT	72	LEU	CA-CB-CG	5.14	127.13	115.30
1	XA	68(S)	C	N1-C2-O2	5.14	121.98	118.90
34	YA	2689	U	P-O3'-C3'	5.14	125.87	119.70
50	YV	35	LEU	CA-CB-CG	5.14	127.13	115.30
1	QA	1097	C	C5-C6-N1	5.14	123.57	121.00
34	RA	2306	C	C6-N1-C2	-5.14	118.24	120.30
34	YA	1157	G	C8-N9-C1'	-5.14	120.32	127.00
34	YA	1950	G	C6-C5-N7	-5.14	127.32	130.40
34	YA	2420	C	C5-C6-N1	5.14	123.57	121.00
34	YA	2579	C	N1-C2-O2	5.14	121.98	118.90
34	YA	1767	C	C5-C6-N1	5.14	123.57	121.00
34	YA	2460	U	C2-N1-C1'	5.14	123.87	117.70
53	RY	99	CYS	CB-CA-C	-5.14	100.13	110.40
34	YA	1218	C	C6-N1-C2	-5.14	118.25	120.30
34	YA	1533	C	N1-C2-O2	5.14	121.98	118.90
34	RA	74	A	N3-C4-C5	5.13	130.40	126.80
34	YA	531	C	O5'-P-OP1	-5.13	101.08	105.70
34	YA	976	C	C5-C6-N1	5.13	123.57	121.00
34	YA	1950	G	C8-N9-C1'	-5.13	120.33	127.00
1	QA	1290	G	C8-N9-C1'	-5.13	120.33	127.00
34	RA	1505	C	N3-C2-O2	-5.13	118.31	121.90
36	RD	241	PRO	C-N-CA	5.13	134.53	121.70
34	YA	689	A	C5-C6-N1	5.13	120.27	117.70
34	YA	2137	C	N1-C2-O2	5.13	121.98	118.90
34	YA	2704	C	C2-N1-C1'	5.13	124.44	118.80
34	RA	1157	G	N3-C4-N9	5.13	129.08	126.00
32	R8	28	GLY	N-CA-C	5.13	125.92	113.10
34	RA	640	C	C6-N1-C2	-5.13	118.25	120.30
34	YA	894	C	N1-C2-O2	5.13	121.98	118.90
34	YA	99	U	OP2-P-O3'	5.13	116.48	105.20
34	YA	1158	C	N1-C2-O2	5.13	121.97	118.90
34	YA	1914	C	C6-N1-C2	-5.13	118.25	120.30
34	YA	2453	A	C6-N1-C2	5.13	121.68	118.60
34	YA	2040	C	C5-C6-N1	5.12	123.56	121.00
34	YA	2680	C	C2-N1-C1'	5.12	124.44	118.80
34	RA	659	C	C6-N1-C2	-5.12	118.25	120.30
34	RA	806	C	C2-N1-C1'	5.12	124.44	118.80
34	RA	1404	C	C2-N1-C1'	5.12	124.44	118.80
34	RA	2551	C	N1-C2-O2	5.12	121.97	118.90
34	YA	459	U	N3-C2-O2	-5.12	118.61	122.20
34	YA	1101	U	N1-C2-O2	5.12	126.39	122.80
34	YA	2844	G	C4-N9-C1'	5.12	133.16	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	2885	C	C6-N1-C2	-5.12	118.25	120.30
34	YA	749	C	C2-N1-C1'	5.12	124.43	118.80
34	YA	2712(A)	U	C5-C6-N1	5.12	125.26	122.70
1	XA	1439	C	C6-N1-C2	-5.12	118.25	120.30
34	YA	1417	C	C2-N1-C1'	5.12	124.43	118.80
1	QA	514	C	C5-C6-N1	5.12	123.56	121.00
34	RA	63	U	OP1-P-O3'	5.12	116.46	105.20
1	XA	744	C	C6-N1-C2	-5.12	118.25	120.30
29	R5	34	PRO	N-CA-CB	5.12	109.44	103.30
34	RA	1370	C	N3-C2-O2	-5.12	118.32	121.90
1	XA	1391	U	N3-C2-O2	-5.12	118.62	122.20
30	Y6	13	CYS	CA-CB-SG	-5.11	104.80	114.00
34	YA	1332	G	C8-N9-C1'	-5.11	120.35	127.00
22	QV	10	G	P-O3'-C3'	5.11	125.83	119.70
34	RA	974(B)	C	C2-N1-C1'	5.11	124.42	118.80
34	YA	838	C	C6-N1-C2	-5.11	118.26	120.30
34	YA	868	U	C2-N1-C1'	5.11	123.83	117.70
34	YA	2108	C	C6-N1-C2	-5.11	118.26	120.30
34	YA	1157	G	C4-C5-N7	5.11	112.84	110.80
34	RA	2784	C	N1-C2-O2	5.11	121.96	118.90
1	XA	328	C	C2-N1-C1'	5.11	124.42	118.80
1	XA	738	C	C2-N1-C1'	5.11	124.42	118.80
34	YA	2885	C	C5-C6-N1	5.11	123.55	121.00
34	RA	1178	C	P-O3'-C3'	5.11	125.83	119.70
34	RA	1516	U	C2-N1-C1'	5.11	123.83	117.70
34	YA	1516	U	N3-C2-O2	-5.11	118.63	122.20
34	YA	1982	C	C6-N1-C2	-5.11	118.26	120.30
34	YA	2326	C	C6-N1-C2	-5.11	118.26	120.30
38	YF	133	ASN	N-CA-C	-5.11	97.22	111.00
1	QA	18	C	C5-C6-N1	5.10	123.55	121.00
34	RA	691	C	C6-N1-C2	-5.10	118.26	120.30
34	YA	999	U	N3-C2-O2	-5.10	118.63	122.20
34	YA	2424	C	C5-C4-N4	-5.10	116.63	120.20
34	YA	2794	C	N1-C2-O2	5.10	121.96	118.90
34	YA	404	C	OP2-P-O3'	5.10	116.42	105.20
1	QA	1290	G	N3-C4-N9	5.10	129.06	126.00
34	RA	2636	U	N3-C2-O2	-5.10	118.63	122.20
35	RB	71	C	C2-N1-C1'	5.10	124.41	118.80
34	YA	1330	C	C6-N1-C2	-5.10	118.26	120.30
22	XV	31	G	C8-N9-C4	-5.10	104.36	106.40
1	XA	647	C	C6-N1-C2	-5.09	118.26	120.30
1	XA	754	C	C5-C6-N1	5.09	123.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1147	C	C6-N1-C2	-5.09	118.26	120.30
34	YA	1899	G	N1-C2-N2	-5.09	111.61	116.20
1	QA	1060	C	N1-C2-O2	5.09	121.96	118.90
1	XA	1165	C	C6-N1-C2	-5.09	118.26	120.30
34	YA	237	C	N1-C2-O2	5.09	121.95	118.90
1	QA	1358	U	C5-C6-N1	5.09	125.25	122.70
34	RA	1333	C	N1-C2-O2	5.09	121.95	118.90
34	RA	1417	C	N3-C4-N4	5.09	121.56	118.00
1	XA	955	U	C5-C6-N1	5.09	125.25	122.70
34	YA	914	C	C6-N1-C2	-5.09	118.26	120.30
34	YA	1370	C	C6-N1-C1'	-5.09	114.69	120.80
34	RA	231	C	N1-C2-O2	5.09	121.95	118.90
34	RA	1233	C	C6-N1-C2	-5.09	118.27	120.30
1	XA	1290	G	N3-C4-C5	-5.09	126.06	128.60
23	QX	18	C	C5'-C4'-O4'	5.08	115.20	109.10
34	YA	2044	C	C2-N1-C1'	5.08	124.39	118.80
22	QV	34	C	C5-C4-N4	-5.08	116.64	120.20
34	RA	766	C	C5-C6-N1	5.08	123.54	121.00
34	YA	177	G	C4-N9-C1'	5.08	133.11	126.50
34	YA	683	C	N1-C2-O2	5.08	121.95	118.90
34	YA	1864	U	N3-C2-O2	-5.08	118.64	122.20
1	QA	1285	A	OP2-P-O3'	5.08	116.38	105.20
1	XA	1075	C	C6-N1-C2	-5.08	118.27	120.30
34	YA	1332	G	C4-C5-N7	5.08	112.83	110.80
34	RA	904	C	C2-N1-C1'	5.08	124.39	118.80
34	RA	2210	G	N3-C4-C5	-5.08	126.06	128.60
34	RA	2636	U	N1-C2-O2	5.08	126.35	122.80
34	YA	465	G	N3-C4-C5	-5.08	126.06	128.60
34	RA	1526	G	C6-C5-N7	-5.08	127.36	130.40
54	RZ	12	GLY	N-CA-C	-5.08	100.41	113.10
1	XA	1018	C	N1-C2-O2	5.08	121.95	118.90
34	YA	719	C	C6-N1-C2	-5.07	118.27	120.30
1	QA	201(D)	U	C2-N1-C1'	5.07	123.79	117.70
34	RA	1830	C	C5-C6-N1	5.07	123.54	121.00
1	XA	241	C	C5-C6-N1	5.07	123.54	121.00
34	RA	2480	C	N1-C2-O2	5.07	121.94	118.90
1	XA	1336	C	OP2-P-O3'	5.07	116.36	105.20
34	YA	372	G	C4-N9-C1'	-5.07	119.91	126.50
34	YA	2036	C	C6-N1-C2	-5.07	118.27	120.30
1	QA	500	G	C4-N9-C1'	5.07	133.09	126.50
34	RA	319	C	C2-N1-C1'	5.07	124.37	118.80
34	RA	1312	U	OP2-P-O3'	5.07	116.35	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	372	G	O4'-C1'-N9	5.07	112.25	108.20
34	YA	753	C	N1-C2-O2	5.07	121.94	118.90
34	YA	2816	C	C5-C6-N1	5.07	123.53	121.00
1	QA	1440(O)	C	N1-C2-O2	5.07	121.94	118.90
34	RA	2320	A	C2-N3-C4	5.07	113.13	110.60
34	RA	2579	C	C5-C6-N1	5.07	123.53	121.00
34	YA	641	C	C2-N1-C1'	5.07	124.37	118.80
34	YA	1394	U	C6-N1-C1'	5.07	128.29	121.20
34	YA	76	C	C6-N1-C2	-5.06	118.27	120.30
34	YA	533	G	N3-C4-C5	-5.06	126.07	128.60
34	RA	2471	C	N1-C2-O2	5.06	121.94	118.90
34	YA	537	C	C4-C5-C6	-5.06	114.87	117.40
34	RA	1178	C	N1-C2-O2	5.06	121.94	118.90
34	YA	114	U	N3-C2-O2	-5.06	118.66	122.20
34	YA	242	G	OP2-P-O3'	5.06	116.33	105.20
34	YA	436	C	C6-N1-C2	-5.06	118.28	120.30
34	YA	1741	C	C6-N1-C2	-5.06	118.28	120.30
1	QA	201(D)	U	N1-C2-O2	5.06	126.34	122.80
40	RH	155	SER	N-CA-C	5.06	124.66	111.00
34	YA	1398	C	C2-N1-C1'	5.06	124.36	118.80
34	YA	2870	C	C5-C6-N1	5.06	123.53	121.00
34	RA	2186	G	C4-N9-C1'	5.06	133.07	126.50
1	QA	1054	C	N1-C2-O2	5.05	121.93	118.90
1	QA	1225	A	N3-C4-N9	5.05	131.44	127.40
34	RA	1611	C	N1-C2-O2	5.05	121.93	118.90
37	RE	146	THR	N-CA-C	5.05	124.64	111.00
34	YA	2461	C	C2-N1-C1'	5.05	124.36	118.80
34	YA	1318	C	C5-C6-N1	5.05	123.53	121.00
34	RA	856	C	C2-N3-C4	5.05	122.42	119.90
34	YA	1958	C	C5-C6-N1	5.05	123.52	121.00
34	RA	2115	G	N3-C4-C5	-5.05	126.08	128.60
35	RB	68	C	C6-N1-C2	-5.05	118.28	120.30
1	XA	36	C	C6-N1-C2	-5.05	118.28	120.30
34	YA	626	U	C5-C6-N1	5.05	125.22	122.70
34	YA	1383	C	N3-C2-O2	-5.05	118.37	121.90
34	YA	2083	G	C5-C6-O6	-5.05	125.57	128.60
34	RA	2870	C	C6-N1-C2	-5.04	118.28	120.30
34	RA	1187	G	C8-N9-C4	-5.04	104.38	106.40
34	YA	2056	G	C4-N9-C1'	5.04	133.05	126.50
34	YA	2261	C	C2-N1-C1'	5.04	124.34	118.80
1	QA	1027	C	C6-N1-C1'	-5.04	114.75	120.80
34	RA	1686	C	C6-N1-C2	-5.04	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	2103	C	N1-C2-O2	5.04	121.92	118.90
34	RA	2116	G	C8-N9-C4	-5.04	104.39	106.40
34	YA	510	C	C2-N1-C1'	5.04	124.34	118.80
34	RA	1345	C	C6-N1-C2	-5.04	118.29	120.30
34	RA	2350	C	C5-C6-N1	5.04	123.52	121.00
34	YA	857	C	C6-N1-C2	-5.04	118.29	120.30
35	RB	22	U	C5-C6-N1	5.03	125.22	122.70
34	RA	2343	C	C2-N1-C1'	5.03	124.33	118.80
34	RA	2724	C	N1-C2-O2	5.03	121.92	118.90
34	YA	486	C	C5-C6-N1	5.03	123.52	121.00
34	YA	2703	C	N1-C2-O2	5.03	121.92	118.90
34	RA	1258	C	C5-C6-N1	5.03	123.52	121.00
34	YA	1306	C	N1-C2-O2	5.03	121.92	118.90
34	YA	1432	C	C5-C6-N1	5.03	123.52	121.00
34	RA	1241	A	O4'-C1'-N9	5.03	112.22	108.20
34	RA	2164	C	N1-C2-O2	5.03	121.92	118.90
34	YA	1887	C	C6-N1-C2	-5.03	118.29	120.30
34	RA	1742	C	C5-C6-N1	5.03	123.51	121.00
34	YA	755	C	C5-C6-N1	5.03	123.51	121.00
34	YA	2083	G	C6-C5-N7	-5.03	127.38	130.40
23	QX	16	C	C5-C4-N4	5.02	123.72	120.20
34	YA	2752	C	N1-C2-O2	5.02	121.91	118.90
1	XA	330	C	C5-C6-N1	5.02	123.51	121.00
1	XA	1539	C	O4'-C1'-N1	5.02	112.22	108.20
34	YA	732	C	C5-C6-N1	5.02	123.51	121.00
1	QA	1075	C	C5-C6-N1	5.02	123.51	121.00
34	RA	267	C	C6-N1-C2	-5.02	118.29	120.30
34	YA	1533	C	C2-N1-C1'	5.02	124.32	118.80
1	XA	745	C	C6-N1-C2	-5.02	118.29	120.30
34	YA	560	C	C6-N1-C2	-5.02	118.29	120.30
34	YA	731	C	C5-C6-N1	5.02	123.51	121.00
34	YA	1404	C	N1-C2-O2	5.02	121.91	118.90
1	QA	514	C	C2-N1-C1'	5.02	124.32	118.80
34	RA	1417	C	C6-N1-C1'	-5.02	114.78	120.80
34	YA	974(B)	C	C6-N1-C1'	-5.02	114.78	120.80
34	RA	2149	G	N1-C2-N2	-5.01	111.69	116.20
54	YZ	63	ASP	CB-CG-OD1	5.01	122.81	118.30
34	RA	1375	C	C5-C6-N1	5.01	123.51	121.00
34	YA	1675	C	N3-C2-O2	-5.01	118.39	121.90
34	YA	731	C	C2-N1-C1'	5.01	124.31	118.80
34	YA	1882	C	N1-C2-O2	5.01	121.91	118.90
34	YA	2342	C	C2-N1-C1'	5.01	124.31	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	YY	79	CYS	CA-CB-SG	5.01	123.02	114.00
34	RA	392	C	C6-N1-C2	-5.01	118.30	120.30
34	YA	1786	A	C8-N9-C1'	-5.01	118.68	127.70
34	YA	2286	A	N7-C8-N9	5.01	116.30	113.80
1	QA	910	C	C6-N1-C2	-5.01	118.30	120.30
34	YA	540	G	C4-N9-C1'	5.01	133.01	126.50
34	RA	392	C	C5-C6-N1	5.01	123.50	121.00
34	YA	1406	U	N1-C2-O2	5.01	126.31	122.80
34	YA	783	A	C4-C5-N7	5.00	113.20	110.70
34	YA	944	G	C4-N9-C1'	5.00	133.01	126.50
34	YA	2803	C	N1-C2-O2	5.00	121.90	118.90
34	RA	231	C	C2-N1-C1'	5.00	124.30	118.80
34	RA	976	C	N1-C2-O2	5.00	121.90	118.90
34	YA	253	C	C5-C6-N1	5.00	123.50	121.00
34	RA	1178	C	C6-N1-C2	-5.00	118.30	120.30
34	YA	1544	C	N3-C2-O2	-5.00	118.40	121.90
34	YA	2474	C	C6-N1-C2	-5.00	118.30	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	Y4	5	ILE	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
28	Y4	5	ILE	Mainchain
37	YE	146	THR	Peptide
54	YZ	166	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	QA	32469	0	16393	389	0
1	XA	32551	0	16433	382	1
2	QB	1907	0	1958	40	0
2	XB	1915	0	1968	37	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	22	0
4	QD	1703	0	1763	55	0
4	XD	1703	0	1763	47	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	22	0
6	QF	843	0	857	9	0
6	XF	843	0	857	11	0
7	QG	1257	0	1296	21	0
7	XG	1257	0	1296	23	0
8	QH	1108	0	1165	20	0
8	XH	1108	0	1165	23	0
9	QI	1010	0	1037	22	0
9	XI	998	0	1024	21	0
10	QJ	801	0	849	22	0
10	XJ	777	0	816	13	0
11	QK	885	0	904	7	0
11	XK	864	0	881	11	0
12	QL	975	0	1062	23	0
12	XL	956	0	1046	14	0
13	QM	955	0	1021	27	0
13	XM	914	0	971	23	0
14	QN	492	0	532	18	0
14	XN	492	0	531	16	0
15	QO	734	0	771	5	0
15	XO	729	0	768	10	0
16	QP	705	0	725	13	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	5	0
18	XR	574	0	644	11	0
19	QS	665	0	686	14	0
19	XS	674	0	699	16	0
20	QT	763	0	861	17	0
20	XT	763	0	861	17	0
21	QU	217	0	234	8	0
21	XU	217	0	234	4	0
22	QV	1647	0	834	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	XV	1647	0	834	18	0
23	QX	409	0	209	13	0
23	XX	409	0	209	6	0
24	R0	643	0	667	6	0
24	Y0	648	0	672	14	0
25	R1	746	0	826	21	0
25	Y1	729	0	802	7	0
26	R2	581	0	629	7	0
26	Y2	575	0	624	5	0
27	R3	469	0	518	6	0
27	Y3	469	0	518	10	0
28	R4	348	0	354	6	0
28	Y4	357	0	362	12	0
29	R5	459	0	477	23	0
29	Y5	459	0	476	17	0
30	R6	453	0	474	7	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	9	0
31	Y7	418	0	467	7	0
32	R8	517	0	582	19	0
32	Y8	517	0	582	16	0
33	R9	307	0	335	9	0
33	Y9	307	0	336	17	0
34	RA	62070	0	31284	607	0
34	YA	62091	0	31294	489	0
35	RB	2573	0	1306	26	0
35	YB	2573	0	1306	24	0
36	RD	2115	0	2195	50	0
36	YD	2115	0	2195	39	0
37	RE	1568	0	1634	36	0
37	YE	1568	0	1633	34	0
38	RF	1585	0	1632	30	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	32	0
39	YG	1474	0	1535	24	0
40	RH	1336	0	1418	57	0
40	YH	1336	0	1418	21	0
41	RI	1136	0	1223	32	1
41	YI	1136	0	1223	25	0
42	RN	1104	0	1180	14	0
42	YN	1104	0	1180	15	0
43	RO	933	0	996	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	YO	933	0	996	14	0
44	RP	1145	0	1228	27	0
44	YP	1122	0	1206	28	0
45	RQ	1122	0	1179	23	0
45	YQ	1122	0	1179	25	0
46	RR	960	0	1021	31	0
46	YR	960	0	1021	19	0
47	RS	882	0	943	20	0
47	YS	882	0	943	18	0
48	RT	1141	0	1202	17	0
48	YT	1141	0	1202	27	0
49	RU	964	0	1022	25	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	14	0
50	YV	779	0	852	12	0
51	RW	900	0	964	17	0
51	YW	900	0	964	16	0
52	RX	725	0	778	9	0
52	YX	725	0	778	14	0
53	RY	818	0	911	24	0
53	YY	818	0	910	21	0
54	RZ	1461	0	1493	32	0
54	YZ	1529	0	1551	29	0
55	QA	87	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	1	0	0	0	0
55	R0	2	0	0	0	0
55	R1	1	0	0	0	0
55	R3	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	429	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	89	0	0	0	0
55	XE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Y1	1	0	0	0	0
55	Y2	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	439	0	0	0	0
55	YB	8	0	0	0	0
55	YD	1	0	0	0	0
55	YE	2	0	0	0	0
55	YF	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	1	0
All	All	292039	0	197760	3309	1

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 (3309) 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)
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.78
40:RH:98:LEU:CD2	40:RH:125:VAL:HG11	1.44	1.45
29:Y5:32:PRO:CA	29:Y5:32:PRO:N	1.69	1.44
30:R6:16:CYS:CB	30:R6:16:CYS:SG	2.06	1.44
14:QN:24:CYS:SG	14:QN:40:CYS:CB	2.14	1.35
34:RA:1789:A:OP1	36:RD:222:ARG:HG3	1.26	1.29
46:RR:12:ARG:CG	46:RR:16:HIS:CD2	2.17	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QL:104:VAL:O	12:QL:105:TYR:CD2	1.90	1.24
40:RH:98:LEU:HD21	40:RH:125:VAL:CG1	1.66	1.23
40:RH:103:LEU:HD11	40:RH:123:PHE:CZ	1.72	1.22
46:RR:12:ARG:HD3	46:RR:16:HIS:NE2	1.53	1.21
46:RR:12:ARG:CG	46:RR:16:HIS:HD2	1.50	1.19
46:RR:12:ARG:HG2	46:RR:16:HIS:CD2	1.76	1.19
46:RR:12:ARG:HD3	46:RR:16:HIS:CD2	1.82	1.14
46:RR:12:ARG:CD	46:RR:16:HIS:CD2	2.31	1.14
1:XA:372:C:N4	1:XA:389:A:H62	1.48	1.11
34:YA:2611:U:H6	34:YA:2611:U:H5'	1.15	1.11
25:R1:90:ILE:HG22	25:R1:94:LEU:HD11	1.19	1.09
4:XD:18:LYS:NZ	4:XD:31:CYS:SG	2.26	1.06
14:YN:27:CYS:SG	14:YN:28:GLY:N	2.28	1.06
1:XA:372:C:H42	1:XA:389:A:N6	1.51	1.06
40:RH:87:LEU:O	40:RH:131:VAL:HG23	1.54	1.05
26:R2:48:HIS:HE2	26:R2:49:LYS:HE2	1.21	1.02
34:RA:1093:G:N2	34:RA:1098:A:H62	1.58	1.01
26:R2:48:HIS:NE2	26:R2:49:LYS:HE2	1.74	1.00
46:RR:12:ARG:HG2	46:RR:16:HIS:HD2	1.12	0.99
34:RA:1542:G:O6	34:RA:1543:A:N6	1.97	0.98
25:R1:95:LEU:O	25:R1:95:LEU:HD23	1.64	0.97
34:RA:1247:A:N1	34:RA:1249:U:O2	1.99	0.96
30:R6:13:CYS:SG	30:R6:14:THR:N	2.39	0.96
1:QA:372:C:N4	1:QA:389:A:H62	1.64	0.95
35:RB:22:U:H3	35:RB:61:G:H1	1.08	0.95
34:RA:2808:U:H3	34:RA:2892:A:H62	0.97	0.95
34:YA:2611:U:H5'	34:YA:2611:U:C6	2.02	0.95
29:R5:16:ARG:CD	34:RA:1263:U:H5''	1.97	0.94
1:QA:62:U:H3	1:QA:105:G:H1	0.95	0.94
34:RA:1093:G:H21	34:RA:1098:A:N6	1.66	0.94
34:YA:1652:A:N6	34:YA:1653:G:N1	2.17	0.93
22:XV:8:U:H3	22:XV:14:A:N6	1.66	0.93
34:RA:1035:U:H3	34:RA:1120:G:H1	1.14	0.93
1:XA:1238:A:N6	1:XA:1301:U:H3	1.66	0.93
34:RA:2094:G:OP1	41:RI:22:LYS:HE3	1.70	0.91
34:YA:2099:U:H3	34:YA:2190:G:H1	1.00	0.91
1:QA:372:C:H42	1:QA:389:A:N6	1.69	0.91
1:XA:45:U:H3	1:XA:396:G:H1	1.19	0.90
1:XA:927:G:H1	1:XA:1390:U:H3	1.10	0.90
25:R1:90:ILE:HA	25:R1:94:LEU:CD1	2.00	0.90
34:YA:1165:U:H3	34:YA:1184:G:H1	1.15	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2068:U:H3	34:YA:2430:A:H2	1.15	0.90
22:XV:8:U:H3	22:XV:14:A:H62	1.20	0.89
1:XA:1304:G:H21	1:XA:1333:A:H62	1.15	0.89
25:R1:90:ILE:CG2	25:R1:94:LEU:HD11	2.03	0.89
29:Y5:48:GLU:OE2	51:YW:37:ARG:NH1	2.05	0.88
1:XA:741:G:P	15:XO:35:ARG:HH21	1.96	0.88
34:RA:855:G:H1	34:RA:922:U:H3	1.20	0.88
34:RA:2508:G:H1	34:RA:2580:U:H3	1.21	0.88
1:XA:152:A:N6	1:XA:169:C:C4	2.43	0.87
1:QA:1066:C:H42	1:QA:1191:A:N6	1.72	0.87
34:RA:2680:C:OP2	37:RE:111:ARG:NH2	2.08	0.87
34:RA:2808:U:H3	34:RA:2892:A:N6	1.73	0.86
34:RA:585:G:N2	34:RA:1256:G:C6	2.42	0.86
33:Y9:13:LYS:HD2	33:Y9:13:LYS:O	1.76	0.86
1:QA:249:U:H3	1:QA:275:G:H1	1.19	0.86
1:XA:12:U:H3	1:XA:22:G:H1	1.24	0.86
40:RH:103:LEU:HD11	40:RH:123:PHE:CE1	2.09	0.85
1:XA:157:G:H1	1:XA:164:U:H3	1.21	0.85
34:YA:270(A):A:N6	34:YA:271(A):U:O2	2.09	0.85
1:XA:437:U:H3	1:XA:495:A:H62	1.21	0.85
34:YA:1419:A:H62	34:YA:1578:U:H3	1.23	0.85
34:RA:1482:U:H3	34:RA:1512:G:H1	1.25	0.85
34:RA:2475:C:H42	34:RA:2529:G:H22	1.22	0.84
4:QD:61:LYS:HE2	4:QD:206:PHE:CE2	2.11	0.84
16:QP:37:GLY:HA3	16:QP:50:LYS:O	1.77	0.84
34:RA:139:G:N2	34:RA:141(A):A:C6	2.45	0.84
34:RA:2542:A:O2'	34:RA:2543:G:H8	1.60	0.84
40:YH:9:ILE:HG21	40:YH:49:VAL:HB	1.56	0.84
1:QA:372:C:H42	1:QA:389:A:H62	0.88	0.84
34:RA:1093:G:H21	34:RA:1098:A:H62	0.86	0.84
35:RB:8:U:H3	35:RB:112:G:H1	1.21	0.84
34:YA:2542:A:H2	34:YA:2544:G:O6	1.61	0.84
40:RH:103:LEU:CD1	40:RH:123:PHE:CZ	2.61	0.84
1:XA:244:U:H3	1:XA:893:C:H42	1.22	0.84
35:YB:73:A:H62	35:YB:103:U:H3	1.26	0.83
34:RA:1247:A:C6	34:RA:1249:U:O2	2.31	0.83
29:R5:16:ARG:HD2	34:RA:1263:U:H5''	1.57	0.83
34:RA:2475:C:H42	34:RA:2529:G:N2	1.75	0.83
34:RA:2123:G:H1	34:RA:2175:C:H42	1.26	0.83
1:QA:401:C:C5	4:QD:73:ARG:NH2	2.48	0.82
1:QA:782:A:H62	1:QA:800:G:H21	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2751:G:C4	40:RH:3:ARG:HB3	2.14	0.82
1:XA:560:U:H5'	1:XA:566:G:N2	1.95	0.82
34:RA:586:A:H5'	38:RF:89:VAL:HG21	1.63	0.81
4:QD:61:LYS:HE2	4:QD:206:PHE:HE2	1.45	0.81
1:QA:15:G:H1	1:QA:920:U:H3	1.25	0.81
29:Y5:45:VAL:HG21	29:Y5:58:LEU:HD21	1.63	0.81
34:YA:1652:A:N6	34:YA:1653:G:C6	2.49	0.81
40:YH:9:ILE:CG2	40:YH:49:VAL:HB	2.11	0.80
40:RH:98:LEU:HD21	40:RH:125:VAL:HG11	0.81	0.80
1:XA:289:G:N2	1:XA:312:C:O2	2.14	0.80
25:R1:90:ILE:HG22	25:R1:94:LEU:CD1	2.06	0.80
46:RR:12:ARG:HG3	46:RR:16:HIS:HD2	1.47	0.80
34:RA:1632:A:N6	34:RA:1762:A:C2	2.49	0.80
34:RA:2852:G:H1	34:RA:2865:U:H3	1.26	0.80
40:RH:89:ILE:CD1	40:RH:131:VAL:HG22	2.12	0.80
41:RI:84:GLY:HA3	41:RI:89:TYR:OH	1.82	0.80
29:R5:16:ARG:HD3	34:RA:1263:U:H5''	1.63	0.79
35:RB:35:U:OP2	35:RB:36:C:OP2	1.98	0.79
34:RA:978:G:N2	34:RA:986:C:C2	2.50	0.79
1:QA:766:A:H62	1:QA:813:U:H3	1.27	0.79
4:QD:18:LYS:NZ	56:QD:301:SF4:S4	2.55	0.79
40:RH:98:LEU:CG	40:RH:125:VAL:HG11	2.13	0.78
1:QA:80:G:H1	1:QA:89:U:H3	1.30	0.78
1:QA:401:C:H5	4:QD:73:ARG:NH2	1.82	0.78
34:YA:59:U:H3	34:YA:68:G:H1	1.32	0.78
34:RA:2094:G:OP1	41:RI:22:LYS:CE	2.32	0.77
34:RA:676:A:H8	34:RA:2069:G:H21	1.33	0.77
34:RA:2291:U:H3	34:RA:2341:G:H1	1.28	0.77
34:RA:990:A:OP2	34:RA:991:C:OP2	2.03	0.77
40:RH:98:LEU:CD2	40:RH:125:VAL:CG1	2.41	0.77
34:RA:585:G:C2	34:RA:1256:G:C6	2.73	0.77
40:RH:87:LEU:O	40:RH:131:VAL:CG2	2.32	0.77
34:RA:1276:A:O2'	46:RR:12:ARG:NH1	2.18	0.77
1:XA:575:G:N2	1:XA:880:C:O2	2.17	0.77
34:YA:2508:G:H1	34:YA:2580:U:H3	1.31	0.77
50:RV:45:THR:O	50:RV:45:THR:HG22	1.83	0.77
25:R1:90:ILE:HA	25:R1:94:LEU:HD12	1.67	0.76
1:QA:819:A:N7	1:QA:1529:G:N1	2.34	0.76
41:RI:92:VAL:O	41:RI:120:ILE:HB	1.85	0.76
54:YZ:183:LEU:HD23	54:YZ:183:LEU:O	1.85	0.76
34:RA:2475:C:N4	34:RA:2529:G:H22	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:526:A:OP1	34:RA:527:C:OP1	2.03	0.75
34:RA:2747:G:H21	34:RA:2757:A:H62	1.32	0.75
41:RI:92:VAL:HB	41:RI:120:ILE:CG2	2.16	0.75
10:QJ:79:ARG:O	10:QJ:79:ARG:NH1	2.20	0.75
33:Y9:27:CYS:SG	33:Y9:29:ASN:N	2.58	0.75
33:Y9:29:ASN:ND2	33:Y9:32:HIS:NE2	2.35	0.75
34:RA:1789:A:OP1	36:RD:222:ARG:CG	2.21	0.74
34:RA:2641:G:N2	34:RA:2774:C:C2	2.55	0.74
34:YA:2245:U:H6	34:YA:2245:U:H5''	1.52	0.74
34:YA:855:G:H1	34:YA:922:U:H3	1.34	0.74
32:R8:35:GLN:NE2	32:R8:36:LYS:HE2	2.02	0.74
34:RA:1165:U:H3	34:RA:1184:G:H1	1.35	0.74
34:RA:1234:U:C2'	34:RA:1235:G:H5'	2.17	0.74
1:XA:244:U:H3	1:XA:893:C:N4	1.85	0.74
1:XA:1304:G:N2	1:XA:1333:A:H62	1.85	0.74
1:QA:1066:C:H42	1:QA:1191:A:H62	1.32	0.74
1:QA:1066:C:N4	1:QA:1191:A:H62	1.84	0.73
1:QA:663:A:H61	1:QA:742:G:H1	1.36	0.73
1:XA:152:A:N6	1:XA:169:C:N4	2.36	0.73
34:RA:139:G:N2	34:RA:141(A):A:N6	2.36	0.73
34:YA:1215:G:H1	34:YA:1234:U:H3	1.36	0.73
34:RA:2542:A:O2'	34:RA:2543:G:C8	2.37	0.73
34:RA:2061:G:H5''	34:RA:2503:A:C2	2.24	0.72
34:RA:1632:A:N6	34:RA:1762:A:H2	1.87	0.72
2:QB:172:ILE:O	2:QB:176:GLU:HB2	1.88	0.72
34:YA:2611:U:H6	34:YA:2611:U:C5'	1.99	0.72
34:RA:141(A):A:H8	34:RA:1595:G:H21	1.37	0.72
1:QA:60:A:H62	1:QA:110:C:N4	1.88	0.72
36:RD:96:HIS:CE1	36:RD:102:LYS:HE2	2.24	0.71
1:XA:765:G:H1	1:XA:812:C:HO2'	1.37	0.71
1:QA:778:G:H1	1:QA:804:U:H3	1.38	0.71
34:YA:1612:C:C2	34:YA:1620:G:N2	2.59	0.71
9:QI:16:ARG:HB3	9:QI:64:THR:HG23	1.73	0.71
45:RQ:65:PHE:HB2	45:RQ:105:GLU:HB2	1.72	0.71
34:YA:1433:U:H3	34:YA:1560:G:H1	1.37	0.71
34:YA:574:C:N3	37:YE:145:LYS:NZ	2.35	0.71
1:XA:323:U:H3	1:XA:327:A:H62	1.39	0.71
34:RA:978:G:C2	34:RA:986:C:C2	2.79	0.70
2:XB:120:ALA:O	2:XB:124:SER:HB2	1.92	0.70
34:RA:1768:U:H3	34:RA:1984:G:H1	1.40	0.70
34:YA:2403:C:N4	34:YA:2415:G:C6	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:152:A:H62	1:XA:169:C:N4	1.90	0.70
12:QL:104:VAL:O	12:QL:105:TYR:HD2	1.68	0.70
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.74	0.69
4:XD:57:ARG:HB3	4:XD:206:PHE:HB2	1.72	0.69
34:RA:1632:A:H61	34:RA:1762:A:H2	1.39	0.69
4:XD:12:CYS:SG	4:XD:19:LEU:HB2	2.33	0.69
4:QD:61:LYS:CE	4:QD:206:PHE:CE2	2.75	0.69
14:QN:24:CYS:SG	14:QN:40:CYS:CA	2.81	0.69
40:RH:103:LEU:CD1	40:RH:123:PHE:CE1	2.75	0.69
1:QA:819:A:N7	1:QA:1529:G:C2	2.61	0.69
34:RA:1234:U:O2'	34:RA:1235:G:H5'	1.93	0.69
29:R5:15:ARG:NH2	34:RA:2022:U:OP2	2.26	0.69
36:YD:35:LYS:HB2	36:YD:63:ARG:HA	1.75	0.69
1:QA:927:G:H1	1:QA:1390:U:H3	1.40	0.68
36:RD:8:PRO:HB3	36:RD:14:ARG:HB3	1.75	0.68
30:Y6:6:ARG:NH1	34:YA:2285:C:OP2	2.25	0.68
1:XA:289:G:N1	1:XA:312:C:N3	2.41	0.68
34:RA:1791:A:N6	34:RA:1828:G:O2'	2.25	0.68
42:RN:16:ILE:HB	42:RN:54:VAL:HG12	1.75	0.68
53:RY:99:CYS:HB2	53:RY:103:GLY:H	1.58	0.68
1:XA:68(F):G:H1	1:XA:68(V):U:H3	1.39	0.68
34:YA:2392:A:H2	34:YA:2424:C:H42	1.41	0.68
1:QA:60:A:N6	1:QA:110:C:N4	2.41	0.68
3:XC:43:LEU:O	3:XC:47:LEU:HB2	1.93	0.68
22:XV:8:U:N3	22:XV:14:A:N6	2.34	0.68
34:YA:2185:C:H2'	34:YA:2186:G:H8	1.58	0.68
41:RI:81:VAL:HG21	41:RI:88:ILE:HD12	1.75	0.68
45:RQ:38:GLU:HG2	45:RQ:127:ILE:HG23	1.74	0.68
34:YA:2245:U:C6	34:YA:2245:U:H5''	2.29	0.67
34:YA:2542:A:C2	34:YA:2544:G:O6	2.46	0.67
4:QD:3:ARG:HH22	4:QD:100:ARG:HH22	1.42	0.67
34:RA:2576:G:N3	34:RA:2576:G:H3'	2.09	0.67
34:YA:1154:G:OP2	49:YU:58:ARG:NH2	2.27	0.67
38:RF:154:VAL:HG12	38:RF:191:ARG:HB2	1.77	0.67
1:XA:1238:A:H62	1:XA:1301:U:H3	0.80	0.67
1:QA:437:U:H3	1:QA:495:A:H62	1.42	0.67
42:YN:131:GLN:OE1	42:YN:134:ARG:NH2	2.27	0.67
1:XA:107:G:N7	20:XT:15:ARG:NH2	2.43	0.67
45:YQ:16:ARG:HH21	45:YQ:18:LYS:HD3	1.59	0.67
5:QE:139:LEU:HA	5:QE:142:LEU:HD12	1.77	0.67
34:RA:784:A:OP2	34:RA:2589:A:OP1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:92:VAL:HB	41:RI:120:ILE:HG21	1.74	0.67
34:RA:2343:C:HO2'	34:RA:2373:G:HO2'	1.37	0.67
40:RH:101:ARG:HH12	40:RH:123:PHE:H	1.43	0.67
54:RZ:52:SER:O	54:RZ:54:HIS:N	2.28	0.67
22:QV:37:1MG:HM13	23:QX:16:C:C6	2.30	0.67
4:QD:31:CYS:SG	4:QD:33:MET:HB2	2.35	0.66
33:Y9:13:LYS:HD2	33:Y9:13:LYS:C	2.14	0.66
54:RZ:112:ARG:HG3	54:RZ:114:GLY:H	1.59	0.66
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.60	0.66
1:XA:1238:A:N7	1:XA:1301:U:O4	2.27	0.66
22:XV:65:U:H2'	22:XV:66:A:H8	1.59	0.66
32:Y8:8:LYS:NZ	34:YA:243:U:OP1	2.28	0.66
53:YY:79:CYS:SG	57:YY:201:ZN:ZN	1.84	0.66
1:XA:1512:U:H3	1:XA:1523:G:H1	1.43	0.66
34:RA:139:G:N3	34:RA:141(A):A:N1	2.43	0.66
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.78	0.66
1:QA:765:G:H1	1:QA:812:C:HO2'	1.42	0.66
34:RA:981:A:H2	34:RA:2027:G:N3	1.93	0.66
1:XA:1300:G:O2'	1:XA:1303:C:N4	2.29	0.66
34:YA:1187:G:O5'	34:YA:1187:G:H8	1.79	0.66
34:RA:2751:G:N3	40:RH:3:ARG:HG2	2.10	0.66
1:XA:186(G):C:H42	1:XA:186(M):G:H1	1.43	0.66
1:QA:815:A:O4'	1:QA:817:C:N4	2.29	0.66
34:RA:27:G:N2	34:RA:513:A:OP2	2.29	0.66
40:RH:18:GLU:HB2	40:RH:25:LYS:HB2	1.78	0.66
1:XA:1320:C:H42	19:XS:36:ARG:HG3	1.59	0.66
1:XA:560:U:H5'	1:XA:566:G:H21	1.60	0.66
40:YH:84:SER:HB2	40:YH:132:ARG:HD2	1.78	0.66
9:XI:18:PHE:HB3	9:XI:20:ARG:HH12	1.60	0.66
34:RA:1052:C:H6	34:RA:1052:C:O5'	1.79	0.65
29:Y5:16:ARG:NH2	34:YA:517:C:OP1	2.28	0.65
2:QB:167:PRO:O	2:QB:171:ALA:HB2	1.96	0.65
34:RA:2508:G:O6	34:RA:2580:U:O4	2.15	0.65
34:RA:2641:G:C2	34:RA:2774:C:N3	2.65	0.65
34:RA:2641:G:N1	34:RA:2774:C:N3	2.43	0.65
1:QA:1127:G:N3	1:QA:1147:C:N4	2.44	0.65
1:QA:266:G:H5'	1:QA:268:C:H41	1.60	0.65
1:QA:766:A:N6	1:QA:813:U:H3	1.94	0.65
34:RA:1824:G:HO2'	36:RD:248:SER:HG	1.40	0.65
34:RA:962:G:OP1	34:RA:963:U:OP2	2.13	0.65
51:RW:88:ARG:HB2	51:RW:92:ARG:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:674:G:H2'	1:XA:675:A:H8	1.61	0.65
20:XT:86:ARG:O	20:XT:90:GLN:NE2	2.30	0.65
34:YA:530:G:O2'	34:YA:532:A:N7	2.29	0.65
50:RV:62:LEU:HD11	50:RV:95:LEU:HB2	1.77	0.65
1:QA:401:C:OP2	4:QD:73:ARG:NE	2.29	0.65
38:RF:147:GLY:O	38:RF:191:ARG:NH1	2.29	0.65
40:RH:89:ILE:HD11	40:RH:131:VAL:HG22	1.76	0.65
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.61	0.65
1:XA:375:U:H4'	16:XP:6:LEU:HD11	1.78	0.65
1:XA:438:G:H21	1:XA:497:A:H62	1.45	0.65
34:YA:2680:C:H5'	37:YE:189:PRO:HA	1.79	0.65
13:QM:14:ARG:HG2	13:QM:44:ARG:HD3	1.78	0.65
34:RA:2641:G:N1	34:RA:2774:C:C4	2.65	0.65
34:RA:675:A:O2'	38:RF:67:GLN:NE2	2.29	0.65
29:Y5:48:GLU:CD	51:YW:37:ARG:HH12	1.99	0.65
1:QA:982:U:H3	1:QA:1223:C:H42	1.44	0.65
4:QD:121:VAL:HG22	4:QD:126:ILE:HG13	1.79	0.65
34:RA:229:A:H4'	34:RA:230:U:H5'	1.78	0.65
34:YA:703:U:H3	34:YA:728:G:H1	1.44	0.65
1:QA:942:G:H1	1:QA:1341:U:H3	1.45	0.65
1:XA:1261:A:H62	1:XA:1274:G:H21	1.45	0.65
54:RZ:10:ARG:HD2	54:RZ:38:TYR:HB3	1.79	0.65
4:XD:20:TYR:HA	4:XD:26:CYS:SG	2.37	0.65
22:XV:8:U:O4	22:XV:14:A:N7	2.30	0.65
47:YS:106:ARG:HB2	47:YS:110:LEU:HD23	1.78	0.65
34:RA:811:U:HO2'	34:RA:1250:G:HO2'	1.35	0.64
37:RE:75:VAL:HG23	37:RE:76:ARG:HG2	1.79	0.64
2:QB:177:ALA:HB1	2:QB:182:ILE:HB	1.78	0.64
1:QA:860:A:N3	8:QH:18:ARG:NH1	2.44	0.64
34:RA:331:A:N6	34:RA:1210:A:OP2	2.30	0.64
8:XH:14:ARG:HB3	8:XH:83:ILE:HD11	1.79	0.64
35:YB:90:C:H5'	45:YQ:18:LYS:HA	1.80	0.64
41:RI:92:VAL:HB	41:RI:120:ILE:HB	1.80	0.64
29:Y5:16:ARG:NH1	29:Y5:17:ASP:OD1	2.30	0.64
34:YA:2402:C:H6	34:YA:2402:C:O5'	1.80	0.64
34:YA:1252:G:N3	49:YU:33:ARG:NH1	2.45	0.64
34:YA:1392:A:N6	52:YX:15:GLU:OE2	2.30	0.64
4:QD:18:LYS:HG3	4:QD:33:MET:HG3	1.78	0.64
25:Y1:87:PRO:HA	25:Y1:90:ILE:HG22	1.80	0.64
4:QD:9:CYS:SG	4:QD:22:LYS:NZ	2.71	0.64
1:QA:1291:G:H4'	9:QL:39:GLY:HA3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2542:A:C2	34:RA:2544:G:O6	2.50	0.64
1:QA:1074:G:H1	1:QA:1083:U:H3	1.45	0.64
1:QA:624:C:H2'	1:QA:625:G:H8	1.62	0.64
9:XI:17:VAL:HG12	9:XI:63:ILE:HD12	1.79	0.64
32:R8:8:LYS:NZ	34:RA:243:U:OP1	2.29	0.64
1:XA:1323:G:H5''	13:XM:99:ARG:HH21	1.61	0.64
34:YA:2086:U:OP2	36:YD:263:ARG:NH1	2.29	0.64
34:YA:414:C:O2	34:YA:1864:U:O2'	2.16	0.64
34:YA:138:G:N2	52:YX:44:GLU:OE2	2.29	0.64
1:QA:12:U:H3	1:QA:22:G:H1	1.46	0.64
34:RA:1654:A:H5''	34:RA:1654:A:H8	1.61	0.64
34:RA:811:U:H3'	44:RP:22:GLY:HA2	1.80	0.64
34:YA:1270:C:H5''	34:YA:1271:G:H5'	1.79	0.64
34:YA:1307:A:C6	34:YA:1622:G:O6	2.51	0.64
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	1.78	0.64
34:RA:1026:U:H1'	34:RA:1027:A:H5''	1.80	0.64
34:YA:2425:A:H4'	34:YA:2426:A:H5''	1.79	0.64
1:QA:1415:G:H1	1:QA:1485:U:H3	1.44	0.64
34:RA:1818:U:OP2	36:RD:157:ARG:NH1	2.31	0.64
40:RH:6:ARG:HH22	40:RH:54:ARG:HD3	1.62	0.64
10:XJ:50:ILE:HA	10:XJ:60:ARG:HB2	1.79	0.64
36:RD:60:ARG:HD3	36:RD:86:PRO:HB2	1.80	0.63
45:RQ:81:VAL:HG12	45:RQ:82:ARG:HG2	1.80	0.63
1:XA:160:A:N1	1:XA:343:U:O2'	2.30	0.63
1:QA:1221:G:OP1	1:QA:1321:C:N4	2.31	0.63
54:RZ:52:SER:O	54:RZ:54:HIS:ND1	2.32	0.63
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.81	0.63
32:Y8:22:VAL:HB	32:Y8:53:PRO:HB3	1.80	0.63
5:QE:140:ARG:O	5:QE:143:ARG:NH1	2.32	0.63
34:RA:1012:U:OP1	49:RU:75:ASN:ND2	2.31	0.63
40:RH:78:GLY:HA2	40:RH:82:GLY:HA3	1.79	0.63
41:RI:84:GLY:HA3	41:RI:89:TYR:CZ	2.33	0.63
34:YA:2701:C:H3'	34:YA:2702:U:H5''	1.80	0.63
34:YA:1695:G:N7	36:YD:14:ARG:NH2	2.47	0.63
44:YP:4:SER:O	44:YP:7:ARG:NH2	2.32	0.63
1:QA:346:G:OP1	48:RT:41:ARG:NH2	2.32	0.63
5:QE:79:GLU:O	8:QH:104:ARG:NH1	2.32	0.63
17:XQ:29:HIS:HB3	17:XQ:33:GLY:H	1.64	0.63
28:Y4:22:ILE:HG22	28:Y4:23:GLU:HG3	1.80	0.63
34:RA:1022:G:N7	34:RA:1140:C:N4	2.46	0.63
24:Y0:72:ARG:HE	24:Y0:75:LEU:HD12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:109:LYS:HE3	37:RE:191:PRO:HA	1.79	0.63
1:XA:166:G:H2'	1:XA:167:G:H8	1.64	0.63
34:YA:2006:C:O2'	34:YA:2823:A:N3	2.31	0.63
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.30	0.63
34:RA:1247:A:OP2	44:RP:15:ARG:NH2	2.32	0.63
4:XD:8:VAL:HA	4:XD:11:LEU:HD13	1.81	0.63
32:R8:35:GLN:HE22	32:R8:36:LYS:HE2	1.62	0.62
34:YA:1186:G:H8	34:YA:1186:G:O5'	1.82	0.62
34:YA:1607:C:N4	34:YA:1622:G:OP2	2.32	0.62
34:YA:1995:U:O2	43:YO:3:GLN:NE2	2.32	0.62
1:QA:674:G:H2'	1:QA:675:A:H8	1.64	0.62
21:QU:12:LYS:HB3	21:QU:22:ARG:HD2	1.80	0.62
34:RA:998:C:OP2	49:RU:58:ARG:NH1	2.32	0.62
37:RE:119:ARG:HG3	37:RE:160:TYR:CD1	2.34	0.62
34:RA:2102:U:H3	34:RA:2187:G:H1	1.46	0.62
34:YA:627:A:N7	44:YP:84:ASN:ND2	2.46	0.62
54:YZ:52:SER:O	54:YZ:54:HIS:N	2.32	0.62
34:RA:139:G:C2	34:RA:141(A):A:N6	2.67	0.62
34:RA:2641:G:C2	34:RA:2774:C:C2	2.88	0.62
47:RS:83:LYS:HG3	47:RS:84:GLN:HG3	1.81	0.62
1:XA:345:C:O2'	1:XA:346:G:N2	2.33	0.62
7:QG:118:VAL:O	7:QG:122:HIS:ND1	2.32	0.62
1:QA:1198:G:H21	10:QJ:54:PHE:HE1	1.48	0.62
29:R5:51:TYR:CE1	29:R5:56:LYS:HB3	2.35	0.62
45:RQ:37:LEU:HD11	45:RQ:130:LYS:HG2	1.81	0.62
53:RY:99:CYS:CB	53:RY:103:GLY:H	2.12	0.62
1:QA:1066:C:N4	1:QA:1191:A:N6	2.43	0.62
27:R3:49:LYS:NZ	34:RA:851:U:OP1	2.31	0.62
34:YA:2547:U:O2	43:YO:23:ARG:NH2	2.33	0.62
34:YA:270(A):A:OP2	34:YA:270(Z):G:N2	2.28	0.62
41:YI:80:PRO:HB2	41:YI:146:ALA:HB2	1.81	0.62
34:RA:1314:C:OP1	34:RA:1332:G:OP1	2.17	0.62
1:XA:1510:U:H3	1:XA:1525:G:H1	1.48	0.62
1:XA:954:G:H21	1:XA:1227:A:H62	1.48	0.62
1:XA:1179:A:H4'	9:XI:103:THR:HA	1.80	0.62
34:YA:1612:C:C2	34:YA:1620:G:C2	2.88	0.62
34:YA:780:G:H21	34:YA:783:A:H62	1.48	0.62
36:YD:264:LYS:HG2	36:YD:266:SER:H	1.64	0.62
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.33	0.62
1:QA:262:A:H5''	20:QT:76:ALA:HB2	1.82	0.62
1:QA:553:A:H5''	12:QL:24:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:570:G:H2'	1:QA:571:U:H6	1.64	0.62
47:YS:23:ARG:NH2	47:YS:84:GLN:OE1	2.33	0.62
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.32	0.62
29:R5:3:LYS:O	34:RA:2056:G:N2	2.30	0.62
1:XA:1007:C:N3	1:XA:1023:G:N2	2.48	0.62
1:XA:289:G:N2	1:XA:312:C:C2	2.68	0.62
38:YF:160:ASN:HB3	38:YF:163:VAL:HG12	1.81	0.62
22:QV:19:G:H1'	22:QV:56:C:H42	1.65	0.61
25:R1:95:LEU:O	25:R1:95:LEU:CD2	2.45	0.61
54:RZ:72:ARG:NH2	54:RZ:97:GLU:O	2.33	0.61
34:YA:269:U:C5	34:YA:271(A):U:C4	2.88	0.61
34:YA:768:G:O2'	34:YA:1379:A:N6	2.32	0.61
37:RE:141:ILE:O	37:RE:154:LYS:NZ	2.33	0.61
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.32	0.61
32:Y8:11:LYS:HB3	32:Y8:60:LEU:HD11	1.82	0.61
34:YA:2126:A:N6	34:YA:2163:C:O2'	2.34	0.61
50:YV:72:VAL:HB	50:YV:85:LYS:HB3	1.82	0.61
27:R3:12:PRO:HB2	27:R3:20:LYS:HD3	1.82	0.61
34:RA:1664:A:H61	34:RA:1996:C:N4	1.99	0.61
34:RA:1859:A:N6	34:RA:1883:G:O2'	2.33	0.61
34:RA:259:G:H21	34:RA:621:A:H8	1.48	0.61
1:XA:1157:A:H2'	1:XA:1181:G:H22	1.65	0.61
1:XA:749:C:H2'	1:XA:750:G:H8	1.64	0.61
15:XO:88:ARG:NH1	34:YA:713:G:OP2	2.33	0.61
34:YA:814:C:O2'	34:YA:1225:C:N3	2.33	0.61
1:XA:339:C:OP2	43:YO:97:ARG:NH1	2.33	0.61
44:RP:47:ASP:OD2	44:RP:50:ARG:NH2	2.33	0.61
16:XP:6:LEU:HB2	16:XP:17:TYR:HB3	1.82	0.61
42:YN:112:LEU:O	42:YN:116:LEU:HB2	1.99	0.61
28:R4:16:CYS:SG	28:R4:17:GLY:N	2.73	0.61
1:XA:437:U:H3	1:XA:495:A:N6	1.96	0.61
36:RD:96:HIS:HE1	36:RD:102:LYS:HE2	1.64	0.61
41:YI:30:LEU:HB3	41:YI:36:ALA:HB3	1.80	0.61
34:YA:955:C:OP1	45:YQ:85:LYS:NZ	2.33	0.61
1:QA:992:U:H3	1:QA:1044:A:H62	1.47	0.61
1:QA:1316:G:H4'	14:QN:18:VAL:HG11	1.83	0.61
45:RQ:63:LYS:HD2	54:RZ:175:VAL:HG21	1.82	0.61
1:XA:881:G:OP2	12:XL:9:GLN:NE2	2.33	0.61
32:Y8:12:LYS:NZ	34:YA:249:C:O2	2.32	0.61
16:QP:53:VAL:HG12	16:QP:79:VAL:HG12	1.82	0.61
34:RA:300:A:OP1	53:RY:86:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RR:74:LYS:HD3	46:RR:77:ARG:HH21	1.66	0.61
1:XA:1324:A:OP2	13:XM:99:ARG:NH2	2.33	0.61
54:YZ:181:GLU:O	54:YZ:182:LYS:O	2.19	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
1:QA:766:A:N7	1:QA:813:U:O4	2.34	0.61
34:RA:1638:C:O3'	34:RA:2709:G:N2	2.34	0.61
53:RY:76:CYS:SG	53:RY:80:GLY:N	2.74	0.61
34:YA:265:A:N6	34:YA:427:U:O2'	2.34	0.61
35:YB:37:C:O2	47:YS:95:HIS:NE2	2.27	0.61
7:QG:133:GLY:HA2	7:QG:136:LYS:HE2	1.83	0.60
7:QG:138:LYS:HE2	7:QG:142:GLU:HG3	1.83	0.60
13:QM:57:ARG:O	13:QM:61:GLU:HB2	2.01	0.60
54:RZ:3:TYR:HB2	54:RZ:57:ILE:HG22	1.81	0.60
34:YA:2010:G:H5''	51:YW:42:ARG:HB2	1.81	0.60
34:RA:2641:G:H2'	34:RA:2642:G:H8	1.66	0.60
48:RT:77:PRO:HG2	48:RT:80:SER:HB3	1.82	0.60
1:XA:68(I):G:H21	1:XA:68(T):C:H41	1.47	0.60
34:YA:960:A:H61	45:YQ:82:ARG:HH12	1.48	0.60
34:RA:626:U:H3	44:RP:105:LEU:HA	1.66	0.60
34:RA:994:C:OP1	49:RU:53:ARG:NH2	2.35	0.60
4:XD:25:ARG:NE	4:XD:30:LYS:O	2.33	0.60
34:YA:2402:C:H6	34:YA:2402:C:C5'	2.14	0.60
34:YA:688:U:H6	34:YA:688:U:O5'	1.85	0.60
34:YA:750:A:C2	34:YA:753:C:C6	2.89	0.60
34:RA:2483:C:N3	45:RQ:124:LYS:NZ	2.49	0.60
39:RG:72:ARG:HA	39:RG:87:PRO:HA	1.82	0.60
34:YA:1093:G:H21	34:YA:1098:A:H62	1.48	0.60
34:YA:2572:A:OP1	34:YA:2574:G:O2'	2.20	0.60
35:YB:48:A:OP2	47:YS:30:ARG:NH2	2.34	0.60
37:YE:1:MET:HG3	37:YE:200:GLU:HG2	1.82	0.60
2:XB:163:PHE:HA	2:XB:185:ILE:O	2.01	0.60
34:YA:1669:A:N3	34:YA:1669:A:H2'	2.17	0.60
34:RA:2808:U:C2	34:RA:2892:A:N6	2.70	0.60
28:Y4:1:MET:N	35:YB:44:G:OP1	2.33	0.60
34:YA:1224:G:N2	34:YA:1227:A:OP2	2.31	0.60
41:RI:92:VAL:HB	41:RI:120:ILE:CB	2.30	0.60
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.34	0.60
39:YG:16:ARG:NH2	39:YG:28:VAL:O	2.35	0.60
44:YP:58:THR:O	44:YP:61:ARG:NH2	2.34	0.60
51:YW:6:ILE:HG12	51:YW:104:THR:HG23	1.84	0.60
51:YW:30:GLU:O	51:YW:34:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1234:U:H2'	34:RA:1235:G:H5'	1.83	0.60
34:RA:585:G:C2	34:RA:1256:G:O6	2.55	0.60
46:RR:97:VAL:HG22	46:RR:114:VAL:HG12	1.84	0.60
4:XD:13:ARG:HG3	4:XD:40:PRO:HD3	1.84	0.60
34:YA:987:G:O2'	34:YA:1000:A:N3	2.30	0.60
40:YH:89:ILE:O	40:YH:129:THR:OG1	2.19	0.60
1:QA:1261:A:H62	1:QA:1274:G:H21	1.50	0.60
32:R8:12:LYS:NZ	34:RA:249:C:O2	2.35	0.60
2:XB:126:GLU:OE2	2:XB:130:ARG:NH1	2.34	0.60
2:XB:67:THR:HG21	2:XB:155:LEU:HG	1.84	0.60
13:XM:3:ARG:O	13:XM:57:ARG:NH2	2.35	0.60
34:RA:1827:C:OP2	36:RD:222:ARG:NH1	2.35	0.60
1:XA:545:C:OP2	4:XD:65:ARG:NH2	2.35	0.60
34:YA:1340:U:OP2	52:YX:78:LYS:NZ	2.32	0.60
34:YA:811:U:O4	44:YP:21:ARG:NH2	2.34	0.60
38:YF:11:VAL:HG22	38:YF:125:LEU:HB2	1.84	0.60
10:QJ:6:ILE:HG22	10:QJ:98:ILE:HG22	1.84	0.59
32:R8:56:GLU:HA	32:R8:59:LYS:HE2	1.83	0.59
5:XE:79:GLU:HG3	5:XE:93:PRO:HD2	1.84	0.59
1:XA:760:G:N2	17:XQ:97:SER:OG	2.35	0.59
34:YA:2108:C:N3	34:YA:2182:G:N2	2.50	0.59
34:YA:782:A:O2'	36:YD:225:ALA:O	2.19	0.59
47:YS:4:LEU:HD11	47:YS:12:PHE:HE2	1.67	0.59
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.35	0.59
11:XK:17:GLY:HA2	11:XK:35:PRO:HD3	1.83	0.59
30:Y6:6:ARG:HH21	30:Y6:24:GLU:HG3	1.65	0.59
31:Y7:3:ARG:NE	34:YA:1613:G:O2'	2.36	0.59
1:QA:178:C:H2'	1:QA:179:A:H8	1.66	0.59
1:QA:545:C:OP2	4:QD:65:ARG:NH2	2.36	0.59
34:RA:2701:C:H3'	34:RA:2702:U:H5''	1.84	0.59
37:RE:201:THR:HG22	37:RE:203:LYS:H	1.66	0.59
41:RI:88:ILE:HG22	41:RI:90:GLY:H	1.66	0.59
34:RA:825:C:O2	44:RP:55:ARG:NH2	2.36	0.59
1:XA:520:A:H62	1:XA:529:G:H21	1.50	0.59
34:YA:1988:C:N4	34:YA:1989:G:O6	2.35	0.59
34:YA:994:C:OP1	49:YU:53:ARG:NH2	2.36	0.59
51:YW:33:ARG:NH2	51:YW:52:GLU:OE1	2.35	0.59
34:RA:2820:A:N3	34:RA:2820:A:H2'	2.17	0.59
46:RR:12:ARG:HG3	46:RR:16:HIS:CD2	2.25	0.59
28:Y4:5:ILE:N	28:Y4:5:ILE:HD13	2.17	0.59
34:YA:2055:C:O2	34:YA:2572:A:N6	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:530:G:O2'	34:RA:532:A:N7	2.34	0.59
40:RH:89:ILE:HD11	40:RH:131:VAL:CG2	2.32	0.59
1:XA:410:G:H21	1:XA:432:A:H62	1.50	0.59
8:XH:100:ILE:HD11	8:XH:125:ARG:HB3	1.84	0.59
34:YA:1216:G:OP1	49:YU:11:ARG:NH2	2.32	0.59
34:YA:1433:U:O4	34:YA:1560:G:O6	2.21	0.59
37:YE:143:ASN:N	37:YE:143:ASN:OD1	2.35	0.59
53:YY:79:CYS:HB2	53:YY:81:LYS:HG2	1.83	0.59
31:R7:9:ARG:NE	34:RA:1310:G:OP2	2.34	0.59
34:RA:572:A:H61	34:RA:2029:G:H21	1.50	0.59
34:RA:659:C:H2'	34:RA:660:G:H8	1.66	0.59
22:XV:30:C:H2'	22:XV:31:G:H8	1.66	0.59
36:YD:61:LEU:O	36:YD:63:ARG:NH1	2.36	0.59
41:YI:9:LEU:HD21	41:YI:35:LEU:HD12	1.84	0.59
34:RA:2085:C:H4'	36:RD:262:ARG:HH21	1.66	0.59
34:RA:2542:A:H2	34:RA:2544:G:O6	1.86	0.59
35:RB:37:C:O2	47:RS:95:HIS:NE2	2.35	0.59
41:RI:93:THR:O	41:RI:97:ILE:HG13	2.03	0.59
46:RR:51:LEU:HG	46:RR:66:VAL:HG23	1.85	0.59
8:XH:91:ARG:NH1	17:XQ:32:TYR:O	2.35	0.59
34:YA:83:G:N2	34:YA:103:A:OP2	2.34	0.59
25:Y1:39:LYS:NZ	34:YA:205:G:O6	2.35	0.59
1:QA:782:A:H62	1:QA:800:G:N2	1.98	0.59
4:QD:98:GLU:OE1	4:QD:103:ASN:ND2	2.36	0.59
34:RA:1066:U:N3	34:RA:1069:A:OP2	2.34	0.59
40:RH:107:VAL:O	40:RH:152:ARG:NH2	2.35	0.59
43:RO:88:ASN:ND2	43:RO:90:GLN:OE1	2.36	0.59
23:QX:8:A:H2'	23:QX:9:G:H8	1.68	0.59
10:XJ:10:GLY:HA3	10:XJ:16:LEU:HD21	1.84	0.59
34:YA:2475:C:H42	34:YA:2529:G:H22	1.50	0.59
34:YA:2502:G:H5''	34:YA:2503:A:H5''	1.85	0.59
38:YF:168:ARG:HG2	38:YF:175:THR:HG21	1.84	0.59
34:RA:2576:G:O2'	34:RA:2579:C:OP2	2.16	0.59
13:XM:3:ARG:HH12	13:XM:11:ARG:HH21	1.51	0.59
19:XS:63:THR:OG1	19:XS:65:ASN:OD1	2.21	0.59
34:YA:1800:C:OP2	36:YD:183:ARG:NH1	2.34	0.59
54:YZ:151:HIS:HB3	54:YZ:170:THR:HA	1.85	0.59
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.67	0.58
29:R5:33:CYS:CB	29:R5:46:CYS:SG	2.90	0.58
34:RA:2134:A:O2'	34:RA:2159:G:N3	2.36	0.58
34:RA:2448:A:OP2	34:RA:2499:C:OP2	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:152:ARG:HG2	40:RH:153:LYS:HG2	1.84	0.58
33:Y9:6:SER:HB3	34:YA:2466:C:H5''	1.85	0.58
3:QC:108:ASN:ND2	3:QC:144:SER:OG	2.36	0.58
5:QE:75:THR:OG1	5:QE:76:ILE:N	2.35	0.58
38:RF:148:LEU:HD13	38:RF:191:ARG:HH11	1.68	0.58
1:XA:406:G:H1	1:XA:436:C:H42	1.51	0.58
1:XA:578:C:H5''	1:XA:578:C:H6	1.68	0.58
34:YA:1930:G:N2	34:YA:1969:A:OP2	2.35	0.58
34:RA:309:G:N3	34:RA:329:G:O2'	2.36	0.58
34:YA:1789:A:OP2	36:YD:222:ARG:NH1	2.36	0.58
1:XA:1463:C:H4'	48:YT:112:ARG:HH21	1.68	0.58
1:QA:976:G:O4'	1:QA:1363:A:N6	2.36	0.58
2:QB:78:GLN:O	2:QB:94:ASN:ND2	2.37	0.58
34:RA:1637:A:H4'	34:RA:2711:A:O2'	2.03	0.58
34:RA:946:G:O6	34:RA:972:G:N2	2.36	0.58
1:XA:1130:A:O2'	9:XI:3:GLN:OE1	2.22	0.58
1:XA:49:U:H3	1:XA:362:G:H1'	1.69	0.58
34:YA:1667:G:O2'	34:YA:1991:U:O4	2.21	0.58
34:YA:27:G:N2	34:YA:513:A:OP2	2.36	0.58
34:YA:776:G:N7	34:YA:793:A:O2'	2.36	0.58
36:YD:35:LYS:H	36:YD:64:ILE:HG12	1.68	0.58
6:QF:23:LYS:NZ	6:QF:42:GLU:OE1	2.36	0.58
34:RA:2729:G:H1'	37:RE:187:ALA:HB2	1.86	0.58
34:RA:2086:U:OP2	36:RD:263:ARG:NH1	2.36	0.58
5:XE:18:ARG:NH1	5:XE:25:ARG:O	2.36	0.58
22:XV:49:G:H1	22:XV:65:U:H3	1.52	0.58
24:Y0:33:ALA:O	34:YA:2353:G:O2'	2.22	0.58
32:Y8:42:ARG:NH1	34:YA:2349:G:OP2	2.36	0.58
34:YA:269:U:C6	34:YA:271(A):U:C4	2.91	0.58
37:YE:128:SER:OG	37:YE:129:HIS:N	2.35	0.58
37:YE:50:GLY:HA2	37:YE:77:ILE:HA	1.85	0.58
43:YO:80:ASP:OD2	48:YT:64:ARG:NH2	2.34	0.58
30:R6:16:CYS:SG	30:R6:42:TRP:HB2	2.44	0.58
1:XA:578:C:H5''	1:XA:578:C:C6	2.38	0.58
1:XA:643:C:H2'	1:XA:644:G:H8	1.67	0.58
3:XC:9:GLY:HA2	3:XC:12:LEU:HD13	1.83	0.58
34:YA:180:G:N2	34:YA:215:G:O6	2.36	0.58
4:QD:59:ARG:HH12	4:QD:66:ARG:HH22	1.51	0.58
34:RA:654(B):G:N2	34:RA:654(U):C:O2	2.36	0.58
34:RA:863:A:O3'	35:RB:100:G:N2	2.37	0.58
50:RV:24:LYS:HA	50:RV:92:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RX:25:LYS:HD3	52:RX:80:ILE:HD11	1.86	0.58
53:RY:99:CYS:HB2	53:RY:103:GLY:N	2.18	0.58
34:YA:141(A):A:H8	34:YA:1595:G:H21	1.50	0.58
1:QA:736:C:OP1	18:QR:72:ARG:NH2	2.37	0.58
1:QA:1268:A:N3	21:QU:20:LYS:NZ	2.51	0.58
43:RO:1:MET:HB2	43:RO:32:TYR:HB3	1.84	0.58
54:RZ:30:ASN:HB3	54:RZ:90:VAL:HG22	1.86	0.58
13:XM:11:ARG:O	13:XM:13:LYS:NZ	2.35	0.58
17:XQ:99:SER:OG	17:XQ:100:LYS:N	2.37	0.58
20:XT:71:THR:OG1	20:XT:72:LEU:N	2.36	0.58
1:QA:1233:G:OP2	9:QI:124:GLN:NE2	2.36	0.58
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.69	0.58
10:QJ:40:LEU:HD11	10:QJ:71:LEU:HB2	1.86	0.58
22:QV:37:IMG:H3'	22:QV:38:A:H8	1.69	0.58
34:RA:197:A:N6	34:RA:2430:A:C8	2.72	0.58
34:RA:2431:U:N3	34:RA:2434:A:OP2	2.31	0.58
34:RA:2808:U:O4	34:RA:2892:A:N7	2.36	0.58
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.37	0.58
34:YA:2683:C:O2	43:YO:70:LYS:NZ	2.28	0.58
34:YA:392:C:H5''	34:YA:409:C:H5''	1.85	0.58
34:YA:442:G:H1'	38:YF:48:THR:HG21	1.86	0.58
41:YI:3:VAL:HG12	41:YI:38:LEU:HA	1.85	0.58
3:QC:91:LEU:HD12	3:QC:101:LEU:HD11	1.85	0.57
27:R3:30:ARG:NH1	34:RA:1184:G:OP1	2.37	0.57
34:RA:1653:G:N7	46:RR:9:LYS:HB2	2.18	0.57
34:RA:2314:C:H2'	34:RA:2315:G:H8	1.69	0.57
39:RG:15:VAL:HG22	39:RG:175:LEU:HD22	1.86	0.57
5:XE:11:ILE:HG21	5:XE:105:VAL:HG22	1.86	0.57
34:YA:1068:G:O2'	34:YA:1096:A:N3	2.37	0.57
34:YA:2118:U:H3	34:YA:2148:G:H4'	1.67	0.57
34:YA:2788:C:O2'	34:YA:2809:A:N3	2.32	0.57
34:YA:662:G:OP1	44:YP:15:ARG:NH1	2.36	0.57
34:RA:265:A:N6	34:RA:428:A:N7	2.52	0.57
34:RA:2712(A):U:O2	34:RA:2712(A):U:H5''	2.05	0.57
41:RI:115:ALA:HB2	41:RI:131:LYS:HE3	1.85	0.57
1:XA:1304:G:H21	1:XA:1333:A:N6	1.93	0.57
27:Y3:24:LYS:NZ	34:YA:933:A:OP1	2.36	0.57
34:YA:2131:G:H1'	34:YA:2158:A:H61	1.69	0.57
34:YA:2508:G:O6	34:YA:2580:U:O4	2.22	0.57
46:YR:56:LYS:O	46:YR:88:ARG:NH2	2.36	0.57
48:YT:36:GLU:OE1	48:YT:41:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:881:G:OP1	12:QL:13:LYS:NZ	2.37	0.57
4:QD:167:GLY:O	4:QD:169:LYS:NZ	2.36	0.57
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.68	0.57
34:RA:585:G:N2	34:RA:1256:G:C5	2.71	0.57
34:RA:1789:A:P	36:RD:222:ARG:HG3	2.40	0.57
37:RE:26:ILE:HG23	37:RE:182:LEU:HB3	1.86	0.57
35:RB:9:G:OP1	47:RS:15:ARG:NH1	2.37	0.57
49:RU:6:THR:OG1	49:RU:7:GLY:N	2.37	0.57
1:XA:1028(B):C:O2	1:XA:1028(I):G:N2	2.37	0.57
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.35	0.57
2:XB:115:LEU:HD12	2:XB:145:LEU:HB3	1.86	0.57
20:XT:30:LYS:HA	20:XT:33:ILE:HD12	1.87	0.57
34:YA:2134:A:H8	34:YA:2157:G:H21	1.53	0.57
34:YA:2880:C:O2'	46:YR:90:ARG:NH1	2.37	0.57
39:YG:29:TRP:O	39:YG:33:ARG:NH1	2.37	0.57
40:YH:9:ILE:HD12	40:YH:51:ARG:HG2	1.85	0.57
34:RA:1856:G:O6	34:RA:1857:G:N2	2.37	0.57
1:QA:1408:A:O2'	34:RA:1916:A:N6	2.34	0.57
40:RH:149:ARG:HA	40:RH:162:ILE:HD11	1.85	0.57
1:XA:1440(K):C:O2'	1:XA:1440(L):G:N2	2.37	0.57
1:XA:1507:A:H2'	1:XA:1508:G:H8	1.70	0.57
8:XH:11:THR:O	8:XH:15:ASN:ND2	2.37	0.57
34:YA:2312:U:O2	39:YG:40:ASN:ND2	2.35	0.57
1:QA:995:C:H2'	1:QA:996:A:H8	1.70	0.57
10:QJ:45:ARG:HB3	10:QJ:65:LEU:HB3	1.85	0.57
34:RA:1454:U:O2'	34:RA:1455:G:N7	2.36	0.57
8:XH:8:ASP:OD2	8:XH:12:ARG:NH2	2.37	0.57
34:YA:2871:C:OP1	46:YR:50:HIS:NE2	2.37	0.57
34:YA:2219:G:OP1	36:YD:172:TYR:OH	2.22	0.57
1:QA:1060:C:H4'	10:QJ:51:ARG:HB3	1.86	0.57
1:QA:677:U:O2	1:QA:777:A:O2'	2.22	0.57
2:QB:74:LYS:HG3	2:QB:77:ALA:HB3	1.87	0.57
1:QA:1240:U:O4	7:QG:109:ASN:ND2	2.37	0.57
7:QG:50:ILE:HG12	7:QG:61:VAL:HG11	1.86	0.57
9:QI:67:GLY:O	9:QI:73:GLN:NE2	2.38	0.57
26:R2:4:SER:OG	26:R2:5:GLU:N	2.37	0.57
34:RA:514:A:N3	34:RA:581:C:O2'	2.35	0.57
45:RQ:12:GLN:HB2	45:RQ:73:PRO:HD2	1.87	0.57
1:XA:1158:C:H2'	1:XA:1159:U:H4'	1.87	0.57
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.70	0.57
3:XC:17:ASP:OD1	3:XC:21:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1307:A:C6	34:YA:1622:G:C6	2.93	0.57
36:YD:28:GLU:HG2	36:YD:29:PRO:HD3	1.86	0.57
34:YA:1113:U:H5'	40:YH:2:SER:HB3	1.85	0.57
1:QA:1505:G:H4'	1:QA:1506:U:H5''	1.85	0.57
1:QA:237:C:H2'	1:QA:238:G:H8	1.69	0.57
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.85	0.57
10:QJ:24:VAL:HG21	10:QJ:37:PRO:HG3	1.87	0.57
32:R8:13:ARG:HG2	44:RP:63:PRO:HB3	1.85	0.57
34:RA:1528:A:OP2	34:RA:1542:G:O6	2.23	0.57
34:RA:2744:G:N2	40:RH:143:GLN:OE1	2.37	0.57
43:RO:71:ARG:NE	43:RO:105:GLU:OE2	2.36	0.57
1:XA:1252:A:H61	1:XA:1285:A:H61	1.53	0.57
34:YA:2882:A:OP1	46:YR:96:ARG:NH1	2.37	0.57
46:YR:57:ARG:NH1	46:YR:59:ASP:OD2	2.38	0.57
1:QA:944:G:H21	1:QA:1339:A:H62	1.52	0.57
34:RA:2683:C:N3	34:RA:2727:G:O2'	2.36	0.57
3:XC:36:ASP:OD1	3:XC:59:ARG:NH2	2.34	0.57
34:YA:1566:A:OP1	36:YD:211:ARG:NH1	2.37	0.57
36:YD:184:LYS:HB3	36:YD:269:PHE:HB3	1.86	0.57
53:YY:30:VAL:HG22	53:YY:37:VAL:HG12	1.87	0.57
1:QA:1440(K):C:O2'	1:QA:1440(L):G:N2	2.36	0.57
9:XI:10:ARG:HG3	9:XI:11:LYS:HG2	1.86	0.57
34:YA:974(A):G:C4	34:YA:989:G:N2	2.72	0.57
1:QA:570:G:O4'	1:QA:820:U:C6	2.58	0.57
1:QA:9:G:N7	1:QA:558:G:O2'	2.38	0.57
13:QM:91:ARG:HD2	13:QM:96:LEU:HD22	1.87	0.57
34:RA:2406:U:OP2	34:RA:2411:A:N6	2.38	0.57
1:XA:1131:G:H1	1:XA:1143:G:H21	1.53	0.57
34:YA:886:C:O2'	34:YA:889:C:N4	2.35	0.57
40:YH:155:SER:OG	40:YH:156:ALA:N	2.36	0.57
1:QA:401:C:C6	4:QD:73:ARG:NH2	2.73	0.56
17:XQ:3:LYS:HB2	17:XQ:60:ILE:HD11	1.86	0.56
30:Y6:3:SER:OG	30:Y6:4:GLU:N	2.37	0.56
30:Y6:19:ARG:HH21	30:Y6:52:VAL:HG21	1.68	0.56
34:YA:184:C:O2'	34:YA:217:G:N3	2.35	0.56
1:QA:1316:G:N1	1:QA:1319:A:OP2	2.37	0.56
1:QA:60:A:N6	1:QA:110:C:C4	2.73	0.56
2:QB:130:ARG:O	2:QB:135:GLN:NE2	2.37	0.56
9:QI:64:THR:OG1	9:QI:66:ARG:NH1	2.37	0.56
28:R4:1:MET:N	35:RB:39:A:N1	2.53	0.56
34:RA:1251:C:OP2	49:RU:10:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2816:C:O2	34:RA:2883:A:O2'	2.21	0.56
34:RA:495:G:N3	51:RW:61:ASN:ND2	2.53	0.56
39:RG:144:ILE:HG22	39:RG:146:TYR:H	1.69	0.56
1:XA:427:U:OP2	4:XD:36:ARG:NH1	2.38	0.56
11:XK:15:ALA:HA	11:XK:77:MET:HA	1.86	0.56
15:XO:88:ARG:NH2	34:YA:714:U:OP2	2.38	0.56
1:XA:1317:C:O2	19:XS:37:ARG:NH2	2.38	0.56
34:YA:1812:A:H2'	34:YA:1813:G:H8	1.69	0.56
2:QB:87:ARG:NH1	2:QB:220:ASP:OD2	2.38	0.56
25:R1:29:GLY:O	34:RA:2396:G:O2'	2.23	0.56
40:RH:29:PRO:HD2	40:RH:79:VAL:HB	1.86	0.56
44:RP:58:THR:O	44:RP:61:ARG:NH2	2.38	0.56
54:RZ:127:LYS:HB3	54:RZ:162:GLU:HB2	1.86	0.56
1:XA:413:G:H1'	1:XA:428:G:H21	1.70	0.56
1:XA:405:U:O4	4:XD:2:GLY:N	2.37	0.56
8:XH:73:ASP:OD1	8:XH:75:ARG:NH1	2.38	0.56
10:XJ:40:LEU:HD11	10:XJ:71:LEU:HB2	1.87	0.56
45:YQ:24:GLY:H	45:YQ:101:ARG:HD2	1.70	0.56
46:YR:14:SER:OG	46:YR:15:SER:N	2.38	0.56
1:QA:708:C:H2'	1:QA:709:G:H8	1.70	0.56
34:RA:1066:U:H2'	34:RA:1067:A:H3'	1.87	0.56
34:RA:978:G:C2	34:RA:986:C:N3	2.73	0.56
35:RB:35:U:OP2	35:RB:36:C:P	2.62	0.56
34:RA:2635:C:H5''	37:RE:78:LEU:HA	1.86	0.56
37:YE:49:LEU:HD22	37:YE:81:ILE:HD11	1.85	0.56
53:YY:76:CYS:HB3	53:YY:79:CYS:SG	2.45	0.56
33:R9:6:SER:HB2	34:RA:2466:C:H5''	1.88	0.56
1:XA:118:U:O5'	1:XA:118:U:H6	1.88	0.56
8:XH:32:LYS:HA	8:XH:35:ILE:HD12	1.86	0.56
9:XI:111:ARG:NH1	14:YN:61:TRP:O	2.33	0.56
1:XA:754:C:OP1	15:XO:72:ARG:NH2	2.38	0.56
34:YA:2068:U:N3	34:YA:2430:A:H2	1.95	0.56
1:QA:825:G:O2'	8:QH:12:ARG:NH2	2.37	0.56
8:QH:12:ARG:HD2	8:QH:26:VAL:HG12	1.88	0.56
31:R7:29:LYS:HA	31:R7:32:LYS:HG3	1.88	0.56
34:RA:768:G:O2'	34:RA:1379:A:N6	2.39	0.56
37:RE:34:VAL:HG21	37:RE:77:ILE:HD11	1.88	0.56
45:RQ:138:ASP:O	45:RQ:141:GLN:NE2	2.39	0.56
49:RU:50:ARG:O	49:RU:54:LYS:NZ	2.39	0.56
53:RY:30:VAL:HG12	53:RY:37:VAL:HG23	1.87	0.56
1:XA:272:C:H2'	1:XA:273:A:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:748:G:C8	34:YA:750:A:C8	2.94	0.56
34:RA:1035:U:O2	34:RA:1120:G:N2	2.31	0.56
37:RE:39:PRO:HD3	37:RE:45:THR:HG22	1.87	0.56
35:RB:104:A:OP1	54:RZ:72:ARG:NH1	2.38	0.56
1:XA:407:G:OP1	4:XD:115:ARG:NH1	2.38	0.56
34:YA:2847:U:OP1	48:YT:98:LYS:NZ	2.37	0.56
39:YG:37:VAL:HG13	39:YG:94:LEU:HB2	1.85	0.56
54:YZ:52:SER:O	54:YZ:54:HIS:ND1	2.38	0.56
34:RA:1297:C:H2'	34:RA:1298:C:H6	1.71	0.56
34:RA:2061:G:H5''	34:RA:2503:A:N1	2.20	0.56
34:RA:793:A:OP2	34:RA:2071:A:O2'	2.23	0.56
38:RF:195:ASP:N	38:RF:195:ASP:OD1	2.38	0.56
41:RI:26:ALA:HA	41:RI:30:LEU:HB2	1.88	0.56
43:YO:107:ARG:NH2	48:YT:36:GLU:O	2.39	0.56
1:QA:200:G:N2	1:QA:218:C:O2	2.38	0.56
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.39	0.56
13:QM:11:ARG:HG3	13:QM:12:ASN:H	1.71	0.56
38:RF:117:ARG:NH1	38:RF:120:GLU:OE2	2.38	0.56
1:XA:152:A:N6	1:XA:169:C:N3	2.54	0.56
1:XA:684:A:O2'	11:XK:39:PRO:O	2.21	0.56
24:Y0:23:VAL:HG21	34:YA:857:C:H4'	1.88	0.56
34:YA:1918:A:O2'	34:YA:1920:C:N4	2.38	0.56
42:YN:63:THR:OG1	42:YN:64:GLY:N	2.39	0.56
1:QA:186(J):U:O2'	17:QQ:63:ARG:NH2	2.38	0.56
34:RA:1022:G:N2	34:RA:1141:U:N3	2.54	0.56
42:RN:22:THR:OG1	42:RN:23:LEU:N	2.39	0.56
1:XA:605:U:H6	1:XA:605:U:O5'	1.88	0.56
1:XA:8:A:N1	4:XD:209:ARG:NH1	2.53	0.56
4:XD:205:GLU:OE1	5:XE:107:ARG:NH1	2.39	0.56
34:YA:2291:U:O2'	34:YA:2374:C:O2	2.24	0.56
1:QA:259:G:OP2	20:QT:83:ARG:NH1	2.38	0.56
1:XA:38:G:N2	1:XA:397:A:OP1	2.39	0.56
1:XA:776:G:N2	1:XA:802:A:OP2	2.38	0.56
3:XC:14:ILE:HG22	3:XC:15:THR:HG23	1.88	0.56
34:YA:664:C:OP1	44:YP:18:ARG:NH1	2.39	0.56
41:YI:130:TYR:HB3	41:YI:136:VAL:HG13	1.86	0.56
1:QA:1236:A:OP1	21:QU:10:ARG:NH1	2.39	0.55
34:RA:180:G:N2	34:RA:215:G:O6	2.39	0.55
34:RA:1658:C:OP1	37:RE:135:HIS:NE2	2.39	0.55
39:RG:126:ASP:OD2	39:RG:130:ASN:ND2	2.36	0.55
41:RI:86:THR:O	41:RI:122:GLU:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:566:U:H5''	44:RP:29:LYS:HE3	1.88	0.55
34:YA:2375:G:N2	34:YA:2378:A:OP2	2.34	0.55
39:YG:77:ILE:HG22	39:YG:82:LEU:HB2	1.89	0.55
1:QA:791:G:O6	1:QA:792:A:N6	2.39	0.55
1:QA:993:G:O2'	1:QA:994:A:N7	2.37	0.55
2:QB:195:ASP:O	8:QH:68:ARG:NH2	2.39	0.55
25:R1:90:ILE:CA	25:R1:94:LEU:HD12	2.35	0.55
35:RB:48:A:OP2	47:RS:30:ARG:NH2	2.39	0.55
34:RA:494:G:OP1	51:RW:8:ARG:NH1	2.39	0.55
53:RY:47:LYS:NZ	53:RY:48:ALA:O	2.37	0.55
34:YA:1728:G:N1	34:YA:1730:U:OP2	2.39	0.55
35:YB:90:C:OP2	45:YQ:16:ARG:NH1	2.38	0.55
34:RA:1025:G:N7	34:RA:1135:C:H1'	2.21	0.55
34:RA:815:C:OP2	50:RV:83:ARG:NH1	2.38	0.55
43:RO:106:LEU:HB3	43:RO:111:PHE:HB2	1.87	0.55
44:RP:90:ARG:HG3	44:RP:91:PHE:HD1	1.71	0.55
14:YN:23:ARG:NH1	14:YN:24:CYS:O	2.40	0.55
34:YA:527:C:N4	34:YA:2779:U:OP2	2.39	0.55
34:YA:956:G:OP2	45:YQ:14:ARG:NH2	2.39	0.55
28:Y4:24:THR:O	39:YG:105:LYS:NZ	2.38	0.55
42:YN:129:PRO:O	42:YN:134:ARG:NH1	2.33	0.55
1:QA:806:C:H2'	1:QA:807:A:H8	1.70	0.55
24:R0:74:ARG:NH2	34:RA:2334:G:O6	2.39	0.55
43:RO:19:ILE:HG22	43:RO:43:VAL:HG12	1.88	0.55
23:XX:6:G:H2'	23:XX:7:G:C8	2.42	0.55
34:YA:1246:A:OP1	44:YP:15:ARG:NH2	2.38	0.55
34:YA:335:C:OP2	53:YY:84:ARG:NH2	2.40	0.55
34:YA:2690:C:OP1	46:YR:17:ARG:NH2	2.40	0.55
48:YT:51:ARG:HD2	48:YT:100:TYR:HE1	1.72	0.55
1:QA:116:A:H61	1:QA:313:A:H1'	1.71	0.55
1:QA:677:U:H3	1:QA:713:G:H22	1.53	0.55
1:QA:1438:G:OP1	20:QT:34:LYS:NZ	2.40	0.55
40:RH:33:LEU:HD11	40:RH:136:ILE:HG13	1.87	0.55
43:RO:14:THR:HG21	43:RO:86:ILE:HD12	1.88	0.55
1:XA:323:U:O4	1:XA:327:A:N7	2.40	0.55
1:XA:890:G:O2'	1:XA:906:G:O6	2.24	0.55
1:XA:1291:G:OP1	7:XG:37:ASN:ND2	2.39	0.55
34:YA:2406:U:OP2	34:YA:2411:A:N6	2.39	0.55
32:Y8:12:LYS:NZ	34:YA:247:G:O6	2.36	0.55
43:YO:87:ILE:HD12	43:YO:91:LEU:HA	1.89	0.55
48:YT:3:ARG:HG3	48:YT:6:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:YU:92:ARG:HH11	50:YV:11:GLN:HB2	1.71	0.55
1:QA:673:G:H2'	1:QA:674:G:C8	2.42	0.55
9:QI:46:ALA:HA	9:QI:78:LYS:HB3	1.88	0.55
34:RA:1075:C:OP1	45:RQ:59:ARG:NH1	2.36	0.55
34:RA:2581:G:C6	34:RA:2610:C:N3	2.75	0.55
34:RA:288:C:H2'	34:RA:289:A:H8	1.71	0.55
38:RF:117:ARG:NH2	38:RF:189:THR:O	2.40	0.55
47:RS:106:ARG:HA	47:RS:110:LEU:HD21	1.88	0.55
4:QD:11:LEU:HD13	4:QD:66:ARG:HD2	1.88	0.55
29:R5:16:ARG:NH2	34:RA:517:C:OP1	2.40	0.55
34:RA:1660:C:H2'	34:RA:1661:G:H8	1.71	0.55
34:RA:1675:C:O5'	34:RA:1675:C:H6	1.89	0.55
34:RA:729:G:C6	36:RD:208:LYS:HB2	2.42	0.55
1:XA:927:G:N2	1:XA:1390:U:O2	2.32	0.55
33:Y9:14:CYS:HA	33:Y9:27:CYS:HB2	1.88	0.55
34:YA:1203:G:O6	34:YA:1204:A:N6	2.40	0.55
34:YA:998:C:OP2	49:YU:58:ARG:NH1	2.40	0.55
38:YF:56:GLU:OE2	38:YF:93:LYS:NZ	2.36	0.55
1:QA:1507:A:C2	1:QA:1530:G:C4	2.95	0.55
1:QA:626:U:H2'	1:QA:627:G:H8	1.71	0.55
3:QC:108:ASN:HB3	3:QC:111:LEU:HB2	1.89	0.55
34:RA:2463:C:C2	34:RA:2488:A:C2	2.95	0.55
40:RH:86:GLU:HG3	40:RH:165:ALA:HB3	1.89	0.55
43:RO:112:MET:HA	43:RO:115:VAL:HG22	1.88	0.55
1:XA:59:A:H2	1:XA:330:C:H42	1.54	0.55
41:YI:131:LYS:HG2	41:YI:135:GLU:HG3	1.87	0.55
26:R2:35:LEU:HD23	26:R2:50:ILE:HG12	1.88	0.55
47:RS:25:ARG:HH21	47:RS:40:ILE:HG13	1.70	0.55
24:Y0:19:LYS:NZ	34:YA:2261:C:OP1	2.34	0.55
34:YA:2403:C:C4	34:YA:2415:G:N1	2.75	0.55
34:YA:483:A:O2'	53:YY:49:VAL:O	2.25	0.55
1:QA:107:G:H3'	1:QA:108:G:H21	1.71	0.55
1:QA:542:G:OP1	4:QD:10:ARG:NH1	2.34	0.55
31:R7:23:ARG:O	31:R7:28:ARG:NH1	2.40	0.55
33:Y9:16:VAL:HG12	33:Y9:25:VAL:HG12	1.88	0.55
1:QA:578:C:H5''	1:QA:578:C:H6	1.71	0.54
1:QA:954:G:H4'	13:QM:121:LYS:HB3	1.89	0.54
34:RA:834:C:H2'	34:RA:835:A:H8	1.72	0.54
43:RO:104:ARG:NH2	43:RO:121:VAL:O	2.40	0.54
1:XA:1261:A:H62	1:XA:1274:G:N2	2.04	0.54
1:XA:45:U:O4	1:XA:396:G:O6	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:564:C:O2'	8:XH:91:ARG:NH2	2.39	0.54
1:XA:1312:G:H5'	19:XS:5:LEU:HD11	1.88	0.54
34:YA:219:G:N3	34:YA:234:C:O2'	2.35	0.54
34:YA:2473:U:OP1	34:YA:2529:G:N2	2.39	0.54
41:YI:129:THR:HA	41:YI:137:PRO:HA	1.89	0.54
53:YY:83:THR:HG21	53:YY:99:CYS:SG	2.48	0.54
8:QH:64:LYS:HG2	8:QH:79:VAL:HG11	1.90	0.54
13:QM:67:GLU:OE1	13:QM:71:ARG:NH1	2.40	0.54
14:QN:24:CYS:SG	14:QN:40:CYS:N	2.80	0.54
31:R7:7:PRO:HB2	34:RA:1309:G:H4'	1.89	0.54
34:RA:2511:U:O2'	37:RE:138:PRO:O	2.25	0.54
45:RQ:45:GLN:NE2	45:RQ:91:GLU:O	2.40	0.54
1:XA:398:C:H2'	1:XA:399:G:H8	1.72	0.54
54:YZ:149:SER:OG	54:YZ:150:LEU:N	2.40	0.54
1:QA:634:C:H2'	1:QA:635:G:H8	1.73	0.54
34:RA:2845:G:H2'	34:RA:2846:G:H8	1.72	0.54
34:RA:783:A:H8	34:RA:784:A:H4'	1.72	0.54
34:RA:982:C:H6	34:RA:982:C:O5'	1.90	0.54
43:RO:22:ILE:HB	43:RO:40:VAL:HG13	1.89	0.54
47:RS:34:HIS:ND1	47:RS:53:SER:OG	2.40	0.54
51:RW:67:ASP:N	51:RW:67:ASP:OD1	2.39	0.54
54:RZ:128:VAL:HG23	54:RZ:161:VAL:HG12	1.89	0.54
2:XB:187:LEU:HA	2:XB:201:ILE:HB	1.90	0.54
7:XG:29:LYS:HE2	7:XG:102:ARG:HB3	1.89	0.54
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.40	0.54
30:Y6:40:CYS:HB3	30:Y6:43:CYS:HB3	1.88	0.54
34:YA:116:C:O2'	34:YA:126:A:N3	2.33	0.54
34:YA:1328:G:H8	34:YA:1328:G:O5'	1.89	0.54
25:Y1:52:ARG:NH2	34:YA:2213:U:O2	2.41	0.54
5:QE:151:LEU:HD12	8:QH:79:VAL:HG12	1.89	0.54
12:QL:53:ARG:HB3	12:QL:69:TYR:HE1	1.73	0.54
1:QA:1360:A:OP2	14:QN:35:ARG:NH1	2.40	0.54
14:QN:6:LEU:HB3	14:QN:23:ARG:HH12	1.72	0.54
34:RA:819:A:OP2	34:RA:1187:G:N2	2.40	0.54
34:RA:2490:G:N3	34:RA:2490:G:H2'	2.22	0.54
34:RA:270(V):C:H2'	34:RA:270(W):G:H8	1.73	0.54
35:RB:22:U:O4	35:RB:61:G:O6	2.26	0.54
1:XA:1394:A:N6	1:XA:1500:A:O2'	2.30	0.54
1:XA:318:G:HO2'	1:XA:1468:A:HO2'	1.54	0.54
22:XV:31:G:H22	22:XV:39:C:H42	1.54	0.54
34:YA:24:G:O2'	51:YW:78:GLU:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2848:G:O2'	34:YA:2867:G:N2	2.38	0.54
34:YA:323:G:HO2'	34:YA:1205:U:H3	1.56	0.54
34:YA:867:C:N3	34:YA:912:C:O2'	2.40	0.54
34:YA:958:U:OP2	45:YQ:14:ARG:NH1	2.40	0.54
1:QA:231:G:H2'	1:QA:232:G:H8	1.73	0.54
1:QA:458(F):A:OP1	16:QP:75:ARG:NH1	2.39	0.54
34:RA:392:C:H5''	34:RA:409:C:H5''	1.89	0.54
37:RE:2:LYS:NZ	37:RE:100:GLU:OE2	2.40	0.54
34:YA:1657:C:H4'	37:YE:133:LYS:HB3	1.89	0.54
40:YH:2:SER:O	40:YH:2:SER:OG	2.24	0.54
54:YZ:97:GLU:HB3	54:YZ:125:LEU:HD11	1.90	0.54
1:QA:266:G:O2'	1:QA:268:C:OP2	2.21	0.54
3:QC:88:ARG:HG2	3:QC:101:LEU:HD13	1.90	0.54
33:R9:14:CYS:HA	33:R9:27:CYS:HB2	1.88	0.54
34:RA:687:C:H42	34:RA:787:U:H4'	1.73	0.54
50:RV:62:LEU:HB2	50:RV:93:GLU:HG3	1.88	0.54
34:RA:484:C:P	53:RY:50:ARG:HG2	2.48	0.54
1:XA:107:G:H3'	1:XA:108:G:H21	1.72	0.54
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.41	0.54
1:XA:356:A:O2'	1:XA:367:U:O2'	2.21	0.54
34:YA:581:C:H2'	34:YA:582:G:H8	1.72	0.54
34:YA:784:A:OP2	34:YA:2589:A:OP1	2.25	0.54
46:YR:104:ARG:NH1	46:YR:107:ASP:OD1	2.40	0.54
34:RA:1546:C:H5'	34:RA:1547:C:H5'	1.90	0.54
34:RA:2808:U:N3	34:RA:2892:A:N6	2.39	0.54
38:RF:63:LYS:NZ	38:RF:75:HIS:O	2.33	0.54
53:RY:6:HIS:O	53:RY:97:ARG:NH2	2.39	0.54
1:XA:1221:G:H4'	19:XS:77:THR:HG21	1.88	0.54
34:YA:579:G:O2'	34:YA:2019:A:OP1	2.25	0.54
34:YA:2577:A:H5''	34:YA:2578:G:H5'	1.88	0.54
51:YW:69:LEU:HD13	51:YW:107:LEU:HD23	1.89	0.54
26:Y2:36:ARG:NH2	52:YX:8:ILE:O	2.41	0.54
3:QC:11:ARG:NH2	3:QC:177:THR:O	2.40	0.54
1:QA:191:G:O2'	20:QT:101:GLY:O	2.22	0.54
22:QV:19:G:OP2	22:QV:20:G:N2	2.41	0.54
1:XA:453:A:H5'	16:XP:75:ARG:HH22	1.73	0.54
45:YQ:45:GLN:NE2	45:YQ:91:GLU:O	2.40	0.54
1:QA:1106:G:H4'	3:QC:172:ARG:HG3	1.89	0.54
1:QA:296:U:O2'	1:QA:556:C:O2	2.24	0.54
34:RA:1676:A:C2	34:RA:1993:U:H5'	2.43	0.54
34:RA:240:G:O2'	34:RA:257:A:N6	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1202:C:HO2'	38:RF:184:TYR:HH	1.56	0.54
1:XA:9:G:N7	1:XA:558:G:O2'	2.41	0.54
7:XG:71:PRO:O	7:XG:96:GLN:NE2	2.41	0.54
27:Y3:8:LEU:HD13	27:Y3:23:LEU:HD11	1.90	0.54
32:Y8:7:HIS:NE2	34:YA:251:A:OP1	2.38	0.54
34:YA:1709:U:O2'	34:YA:2859:G:N3	2.35	0.54
34:YA:602:G:HO2'	34:YA:604:G:HO2'	1.50	0.54
34:YA:861:A:N3	35:YB:79:C:O2'	2.40	0.54
34:YA:971:C:O2'	34:YA:983:A:N3	2.32	0.54
54:YZ:53:ILE:HG22	54:YZ:71:VAL:HG13	1.90	0.54
1:QA:938:A:O3'	7:QG:95:ARG:NH2	2.41	0.54
10:QJ:40:LEU:HD13	10:QJ:69:ASN:HB3	1.90	0.54
29:R5:33:CYS:N	29:R5:38:ALA:O	2.28	0.54
34:RA:987:G:O2'	34:RA:1000:A:N3	2.35	0.54
34:RA:1681:G:O2'	34:RA:1762:A:O2'	2.26	0.54
34:RA:2468:G:N2	34:RA:2468:G:OP2	2.41	0.54
34:RA:59:U:H3	34:RA:68:G:H1	1.55	0.54
46:RR:33:ARG:NH2	46:RR:115:GLU:OE1	2.41	0.54
34:YA:1664:A:H61	34:YA:1996:C:H42	1.56	0.54
39:YG:19:LEU:HD23	39:YG:32:PRO:HD2	1.89	0.54
54:YZ:108:PRO:HA	54:YZ:142:SER:HA	1.88	0.54
3:QC:108:ASN:HD22	3:QC:111:LEU:HD23	1.72	0.53
19:QS:4:SER:OG	19:QS:5:LEU:N	2.41	0.53
33:R9:25:VAL:HB	33:R9:34:GLN:HB2	1.90	0.53
34:RA:1068:G:N2	34:RA:1095:A:O2'	2.41	0.53
2:XB:192:SER:OG	2:XB:193:ASP:N	2.40	0.53
34:YA:1296:G:OP1	34:YA:2709:G:O2'	2.19	0.53
34:YA:270(G):U:H3	34:YA:270(U):G:H1	1.56	0.53
34:YA:2540:C:O2'	34:YA:2740:A:N3	2.34	0.53
29:R5:36:CYS:SG	29:R5:49:CYS:HB3	2.49	0.53
34:RA:1019:U:OP1	34:RA:1035:U:O2'	2.21	0.53
34:RA:662:G:OP1	44:RP:15:ARG:NH1	2.41	0.53
16:XP:37:GLY:HA3	16:XP:50:LYS:O	2.09	0.53
35:YB:73:A:N7	35:YB:103:U:O4	2.40	0.53
41:YI:68:LEU:HA	41:YI:71:ILE:HG22	1.90	0.53
1:QA:112:G:H1	1:QA:315:A:H61	1.57	0.53
34:RA:1247:A:C6	34:RA:1249:U:C2	2.96	0.53
34:RA:605:C:O2	34:RA:657:U:O2'	2.26	0.53
35:RB:57:A:OP2	35:RB:58:A:OP2	2.27	0.53
36:RD:44:ASN:OD1	36:RD:44:ASN:N	2.41	0.53
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:86:ILE:HD11	8:XH:136:GLU:HG2	1.89	0.53
25:Y1:2:SER:N	34:YA:1364:G:N7	2.56	0.53
29:Y5:3:LYS:HG3	34:YA:2611:U:C4	2.42	0.53
33:Y9:29:ASN:ND2	33:Y9:32:HIS:CD2	2.77	0.53
34:YA:2125:G:N1	34:YA:2172:U:OP1	2.42	0.53
45:YQ:28:ALA:N	45:YQ:105:GLU:OE2	2.41	0.53
54:YZ:11:GLU:O	54:YZ:36:LYS:NZ	2.36	0.53
1:QA:754:C:OP1	15:QO:72:ARG:NH2	2.40	0.53
34:RA:2291:U:O2'	34:RA:2374:C:O2	2.27	0.53
34:RA:918:A:N3	35:RB:80:U:O2'	2.39	0.53
1:XA:1306:A:N6	1:XA:1331:G:O2'	2.41	0.53
17:XQ:83:ASP:N	17:XQ:83:ASP:OD1	2.40	0.53
30:Y6:35:GLU:OE2	30:Y6:50:ARG:NH1	2.42	0.53
31:Y7:8:ASN:ND2	34:YA:770:G:OP1	2.40	0.53
34:YA:2403:C:N4	34:YA:2415:G:N1	2.57	0.53
54:YZ:129:SER:OG	54:YZ:132:ASN:OD1	2.24	0.53
46:RR:56:LYS:NZ	46:RR:90:ARG:O	2.41	0.53
1:XA:1028(D):G:O2'	1:XA:1028(G):A:N6	2.40	0.53
18:XR:47:THR:HG22	18:XR:85:LEU:HD13	1.90	0.53
24:Y0:20:ARG:HD3	34:YA:2356:C:H4'	1.91	0.53
34:YA:906:G:HO2'	45:YQ:67:ARG:HH21	1.56	0.53
6:QF:97:PHE:HB2	18:QR:32:ARG:HE	1.73	0.53
27:R3:12:PRO:HA	27:R3:15:TYR:HD2	1.73	0.53
29:R5:16:ARG:HD3	34:RA:1263:U:C5'	2.37	0.53
34:RA:2306:C:N4	39:RG:42:GLY:O	2.42	0.53
38:RF:185:ASP:OD1	38:RF:188:ARG:NH1	2.42	0.53
46:RR:103:ARG:NH1	46:RR:108:GLY:O	2.40	0.53
51:RW:14:PRO:HG2	51:RW:78:GLU:HG3	1.90	0.53
1:XA:860:A:H61	1:XA:872:A:H62	1.57	0.53
1:QA:357:G:O2'	41:YI:89:TYR:O	2.25	0.53
1:QA:320:C:HO2'	1:QA:1435:G:HO2'	1.57	0.53
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.73	0.53
1:QA:430:A:OP1	4:QD:9:CYS:HB2	2.08	0.53
25:R1:41:ARG:NH2	34:RA:1365:A:O4'	2.42	0.53
38:RF:107:LYS:HE3	38:RF:207:GLY:H	1.73	0.53
34:RA:23:G:N2	51:RW:77:ASP:OD1	2.36	0.53
1:XA:624:C:H2'	1:XA:625:G:H8	1.73	0.53
1:XA:719:C:N3	18:XR:74:ARG:NH2	2.51	0.53
28:Y4:11:PRO:HA	28:Y4:25:TYR:HA	1.90	0.53
34:YA:703:U:O4	34:YA:728:G:O6	2.27	0.53
28:Y4:7:PRO:HG3	39:YG:62:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:938:A:H4'	7:QG:95:ARG:HH12	1.74	0.53
1:QA:591:U:OP1	8:QH:30:ARG:NH1	2.42	0.53
34:RA:2784:C:O2'	37:RE:37:ARG:NH1	2.42	0.53
31:R7:39:ARG:NH1	34:RA:459:U:OP2	2.42	0.53
47:RS:18:ILE:HD13	47:RS:88:ASP:HA	1.90	0.53
1:XA:1232:U:OP1	9:XI:124:GLN:NE2	2.42	0.53
2:XB:132:LYS:HA	2:XB:135:GLN:HB2	1.89	0.53
7:XG:18:TYR:OH	7:XG:47:CYS:SG	2.64	0.53
29:Y5:57:VAL:O	46:YR:33:ARG:NH2	2.34	0.53
34:YA:1215:G:O6	34:YA:1234:U:O4	2.27	0.53
47:YS:26:LEU:HB3	47:YS:87:PHE:HA	1.90	0.53
9:QI:71:SER:HA	9:QI:74:ILE:HG12	1.90	0.53
34:RA:139:G:H22	34:RA:1596:A:H4'	1.73	0.53
34:RA:2328:A:H2'	34:RA:2329:G:C8	2.44	0.53
37:RE:171:GLU:HB3	37:RE:185:LYS:HE2	1.90	0.53
42:RN:39:ARG:NH1	42:RN:48:MET:SD	2.82	0.53
40:YH:103:LEU:HB3	40:YH:115:VAL:HG22	1.91	0.53
1:QA:570:G:H2'	1:QA:571:U:C6	2.44	0.53
7:QG:111:ARG:HH11	7:QG:119:ARG:HA	1.73	0.53
34:RA:2100:G:O5'	34:RA:2100:G:H8	1.92	0.53
34:RA:380:U:H2'	34:RA:381:G:H8	1.74	0.53
34:RA:468:G:O2'	38:RF:62:ARG:NH2	2.42	0.53
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.27	0.53
1:XA:548:G:H5'	4:XD:73:ARG:HH22	1.74	0.53
1:XA:977:A:N6	1:XA:1224:G:OP1	2.41	0.53
36:YD:17:THR:HB	36:YD:205:VAL:H	1.74	0.53
34:YA:2307:G:N1	39:YG:45:GLU:OE2	2.36	0.53
34:YA:86:C:OP1	53:YY:33:LYS:NZ	2.42	0.53
1:QA:373:A:O2'	1:QA:451:A:N6	2.42	0.52
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.41	0.52
22:QV:55:U:N3	22:QV:58:A:OP2	2.39	0.52
22:QV:65:U:H2'	22:QV:66:A:H8	1.74	0.52
32:R8:2:PRO:O	34:RA:666:G:N2	2.42	0.52
34:RA:1025:G:C8	34:RA:1135:C:H1'	2.43	0.52
34:RA:1782:C:H42	34:RA:2586:C:H42	1.57	0.52
34:RA:184:C:O2'	34:RA:217:G:N3	2.39	0.52
34:RA:2319:G:N1	34:RA:2334:G:OP2	2.39	0.52
50:RV:76:LYS:HB2	50:RV:81:TYR:HB3	1.90	0.52
1:XA:186(B):C:O2'	20:XT:89:ARG:NH2	2.42	0.52
1:XA:68(P):A:C5	1:XA:68(Q):C:H1'	2.44	0.52
11:XK:83:ILE:HD13	11:XK:109:VAL:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1473:G:H1	34:YA:1520:U:H3	1.57	0.52
1:QA:614:A:OP2	4:QD:85:LYS:NZ	2.34	0.52
1:QA:955:U:O2	19:QS:83:HIS:NE2	2.39	0.52
7:QG:114:ARG:O	7:QG:119:ARG:NH2	2.42	0.52
10:QJ:33:GLN:O	10:QJ:76:ASN:ND2	2.43	0.52
24:R0:23:VAL:HG21	34:RA:857:C:H4'	1.90	0.52
30:R6:9:LEU:HD13	30:R6:51:GLU:HB2	1.90	0.52
34:RA:48:G:N2	34:RA:177:G:OP2	2.37	0.52
34:RA:303:U:H2'	34:RA:304:G:H8	1.74	0.52
34:RA:664:C:OP1	44:RP:18:ARG:NH2	2.39	0.52
34:RA:1788:C:OP1	36:RD:222:ARG:NH2	2.43	0.52
39:RG:166:ASP:OD2	39:RG:166:ASP:N	2.42	0.52
34:YA:729:G:OP2	36:YD:13:ARG:NH1	2.42	0.52
49:YU:28:ARG:NH1	49:YU:38:THR:OG1	2.42	0.52
2:QB:209:ARG:NH1	2:QB:240:GLN:OE1	2.42	0.52
23:QX:17:C:C4	23:QX:18:C:C5	2.97	0.52
29:R5:49:CYS:SG	29:R5:50:GLY:N	2.82	0.52
34:RA:1116:C:H2'	34:RA:1117:G:H8	1.74	0.52
44:RP:29:LYS:HD3	44:RP:30:THR:HG23	1.92	0.52
1:XA:1295:G:O3'	13:XM:14:ARG:NH1	2.42	0.52
1:XA:947:G:HO2'	1:XA:1306:A:HO2'	1.57	0.52
3:XC:32:LEU:O	3:XC:59:ARG:NH2	2.42	0.52
47:YS:61:ASN:ND2	47:YS:64:GLU:OE1	2.42	0.52
23:QX:14:A:H8	23:QX:14:A:O5'	1.92	0.52
34:RA:1482:U:O4	34:RA:1512:G:O6	2.26	0.52
40:RH:125:VAL:O	40:RH:125:VAL:HG22	2.08	0.52
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.40	0.52
36:YD:67:PHE:HE1	36:YD:106:ILE:HD11	1.75	0.52
37:YE:176:ILE:HG13	37:YE:181:LEU:HB2	1.92	0.52
39:YG:170:ARG:NH1	39:YG:174:GLU:OE1	2.43	0.52
1:QA:352:C:O2'	1:QA:354:G:OP1	2.21	0.52
7:QG:13:GLN:OE1	9:QI:42:ARG:NH2	2.42	0.52
29:R5:46:CYS:HB3	29:R5:49:CYS:SG	2.50	0.52
34:RA:1026:U:C4	34:RA:1125:G:O6	2.62	0.52
34:RA:1815:A:OP2	36:RD:54:ARG:NH2	2.42	0.52
34:RA:2448:A:OP2	34:RA:2498:C:OP2	2.27	0.52
34:RA:979:G:N2	34:RA:985:C:N4	2.56	0.52
34:RA:2224:G:OP1	36:RD:268:ARG:HD3	2.10	0.52
39:RG:41:GLN:HB2	39:RG:90:LEU:HB2	1.92	0.52
48:RT:6:LEU:HA	48:RT:9:LEU:HB2	1.91	0.52
34:YA:1478:G:H2'	34:YA:1479:G:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1701:A:OP1	34:YA:1763:G:N1	2.37	0.52
34:YA:2099:U:O4	34:YA:2190:G:O6	2.27	0.52
34:YA:2573:C:OP1	34:YA:2575:C:OP2	2.26	0.52
34:YA:605:C:O2	34:YA:657:U:O2'	2.26	0.52
1:QA:1005:A:O2'	1:QA:1036:G:N2	2.43	0.52
1:QA:1358:U:H5''	14:QN:35:ARG:H	1.74	0.52
1:QA:864:A:H2'	1:QA:865:A:C8	2.45	0.52
38:RF:65:TRP:NE1	38:RF:73:ALA:O	2.42	0.52
43:RO:24:VAL:HG13	43:RO:33:ALA:HB2	1.91	0.52
54:RZ:24:LEU:HD11	54:RZ:83:PRO:HB2	1.90	0.52
54:RZ:27:VAL:HG22	54:RZ:85:HIS:HE1	1.74	0.52
1:XA:708:C:H2'	1:XA:709:G:H8	1.75	0.52
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.90	0.52
45:YQ:21:THR:OG1	45:YQ:22:LYS:N	2.42	0.52
1:QA:789:U:H6	1:QA:789:U:O5'	1.93	0.52
1:QA:859:A:OP2	1:QA:869:G:N1	2.39	0.52
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.92	0.52
24:R0:66:VAL:O	24:R0:81:VAL:HA	2.10	0.52
34:RA:1247:A:N6	34:RA:1249:U:O2	2.43	0.52
34:RA:2506:U:O2	34:RA:2506:U:H2'	2.10	0.52
34:RA:2641:G:H2'	34:RA:2642:G:C8	2.44	0.52
34:RA:615:G:N2	38:RF:44:ARG:O	2.43	0.52
34:RA:2208:U:O2'	36:RD:150:LYS:O	2.28	0.52
1:XA:719:C:H1'	18:XR:49:LYS:HB2	1.90	0.52
31:Y7:28:ARG:NH2	34:YA:1368:G:OP1	2.42	0.52
32:Y8:49:VAL:HG23	32:Y8:53:PRO:HD3	1.91	0.52
34:YA:617:G:OP2	38:YF:43:LYS:NZ	2.32	0.52
12:QL:85:ILE:HD11	12:QL:98:TYR:HB3	1.92	0.52
34:RA:2010:G:H5''	51:RW:42:ARG:HB2	1.92	0.52
34:RA:2258:C:O2'	34:RA:2427:C:OP2	2.28	0.52
34:RA:2375:G:N2	34:RA:2378:A:OP2	2.41	0.52
48:RT:30:VAL:HG12	48:RT:86:ILE:HG23	1.92	0.52
1:XA:8:A:N6	4:XD:205:GLU:O	2.43	0.52
8:XH:121:ASP:N	8:XH:121:ASP:OD1	2.42	0.52
1:XA:1345:U:H5''	9:XI:120:ARG:HH11	1.75	0.52
9:XI:25:LYS:HE3	9:XI:60:ASP:HB3	1.92	0.52
34:YA:2292:C:OP2	47:YS:17:ARG:NH1	2.42	0.52
34:YA:780:G:N2	34:YA:783:A:H62	2.08	0.52
34:YA:831:G:O2'	44:YP:38:GLN:OE1	2.28	0.52
2:QB:61:LEU:HD21	2:QB:68:ILE:HD11	1.91	0.52
5:QE:147:ASP:HA	5:QE:150:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:QR:30:ASP:HB3	18:QR:33:ASP:HB2	1.92	0.52
33:R9:27:CYS:SG	33:R9:28:GLU:N	2.83	0.52
34:RA:579:G:O2'	34:RA:2019:A:OP1	2.27	0.52
45:RQ:81:VAL:O	45:RQ:82:ARG:NE	2.34	0.52
1:XA:1172:C:H2'	1:XA:1173:G:H8	1.74	0.52
1:XA:1255:G:O2'	1:XA:1258:G:N3	2.36	0.52
1:XA:1080:A:H5'	5:XE:14:ARG:HH21	1.74	0.52
7:XG:92:SER:O	7:XG:96:GLN:HB2	2.10	0.52
34:YA:2019:A:O2'	49:YU:34:LYS:NZ	2.43	0.52
34:YA:873:G:N2	34:YA:905:U:O2	2.42	0.52
1:QA:1040:U:H2'	1:QA:1041:A:H8	1.75	0.52
4:QD:122:ARG:NH1	4:QD:122:ARG:O	2.43	0.52
34:RA:2144:U:O2'	34:RA:2147:G:O6	2.28	0.52
34:RA:372:G:N2	34:RA:401:A:OP2	2.37	0.52
34:RA:458:G:O2'	34:RA:469:G:O6	2.25	0.52
42:RN:35:ARG:HG3	42:RN:37:LYS:HG2	1.91	0.52
44:RP:84:ASN:ND2	44:RP:117:GLU:OE2	2.43	0.52
5:XE:76:ILE:HB	5:XE:142:LEU:HD21	1.92	0.52
1:QA:1022:G:H2'	1:QA:1023:G:H8	1.75	0.51
1:QA:1286:A:N6	1:QA:1355:G:OP1	2.44	0.51
1:QA:395:C:N4	1:QA:396:G:O6	2.43	0.51
4:QD:15:GLU:OE2	4:QD:66:ARG:NH2	2.42	0.51
14:QN:24:CYS:HB2	14:QN:28:GLY:H	1.73	0.51
34:RA:385:C:O2'	34:RA:388:G:N2	2.42	0.51
43:RO:23:ARG:NH2	43:RO:28:SER:O	2.43	0.51
47:RS:26:LEU:O	47:RS:88:ASP:HB3	2.10	0.51
53:RY:19:LYS:HZ1	53:RY:20:TYR:HE2	1.49	0.51
53:RY:76:CYS:HB2	53:RY:99:CYS:SG	2.51	0.51
1:XA:1266:G:N2	1:XA:1269:A:OP2	2.35	0.51
3:XC:22:TRP:HA	10:XJ:93:GLY:HA2	1.92	0.51
34:YA:2846:G:N1	34:YA:2871:C:O2	2.43	0.51
35:YB:44:G:O2'	35:YB:47:C:N4	2.43	0.51
36:YD:8:PRO:HB3	36:YD:14:ARG:HG2	1.92	0.51
38:YF:198:ALA:HA	38:YF:201:VAL:HG12	1.91	0.51
1:QA:313:A:H2'	1:QA:314:C:C6	2.46	0.51
1:QA:951:G:N3	1:QA:970:C:O2'	2.40	0.51
34:RA:981:A:C2	34:RA:2027:G:N3	2.75	0.51
53:RY:67:LEU:HD22	53:RY:71:LYS:HD2	1.91	0.51
1:XA:925:G:H1	1:XA:1391:U:H3	1.58	0.51
2:XB:43:ASP:O	2:XB:47:THR:OG1	2.23	0.51
13:XM:82:MET:O	13:XM:93:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:XP:4:ILE:HB	16:XP:66:PRO:HB3	1.92	0.51
37:YE:78:LEU:HG	37:YE:79:ARG:HD2	1.91	0.51
48:YT:19:LEU:HD22	48:YT:86:ILE:HD12	1.92	0.51
1:QA:377:G:H2'	1:QA:378:G:H8	1.75	0.51
1:QA:392:G:OP2	16:QP:8:ARG:NH2	2.37	0.51
2:QB:84:GLU:OE2	2:QB:87:ARG:NH2	2.43	0.51
20:QT:71:THR:OG1	20:QT:72:LEU:N	2.43	0.51
28:R4:26:SER:OG	28:R4:27:THR:N	2.43	0.51
34:RA:1216:G:OP2	49:RU:12:ARG:NH2	2.40	0.51
34:RA:1651:G:H4'	46:RR:39:PRO:HG2	1.92	0.51
40:RH:103:LEU:HG	40:RH:123:PHE:CE1	2.45	0.51
45:RQ:21:THR:OG1	45:RQ:22:LYS:N	2.43	0.51
1:XA:639:G:H2'	1:XA:640:A:H8	1.74	0.51
4:XD:187:ARG:NH1	4:XD:188:LEU:O	2.43	0.51
30:Y6:34:LEU:N	30:Y6:51:GLU:OE1	2.44	0.51
45:YQ:67:ARG:O	45:YQ:101:ARG:NH2	2.44	0.51
30:R6:6:ARG:NH1	30:R6:24:GLU:OE2	2.43	0.51
34:RA:1824:G:OP1	36:RD:52:ARG:NH2	2.38	0.51
34:RA:566:U:H5''	44:RP:29:LYS:CE	2.40	0.51
40:RH:103:LEU:CG	40:RH:123:PHE:CE1	2.94	0.51
41:RI:86:THR:HA	41:RI:123:LEU:CB	2.40	0.51
47:RS:6:ALA:HA	47:RS:9:ARG:HG2	1.92	0.51
1:XA:1074:G:H1	1:XA:1083:U:H3	1.58	0.51
1:XA:235:C:H2'	1:XA:236:G:H8	1.75	0.51
34:YA:1286:A:N6	34:YA:1289:C:C2	2.78	0.51
34:YA:1792:G:H5'	36:YD:205:VAL:HG13	1.93	0.51
34:YA:807:U:O2'	34:YA:2060:A:N1	2.40	0.51
34:YA:584:C:OP2	49:YU:10:ARG:NH2	2.43	0.51
1:QA:1238:A:H62	1:QA:1301:U:H3	1.59	0.51
1:QA:123:C:OP1	1:QA:311:C:O2'	2.27	0.51
1:QA:1259:C:O2'	1:QA:1283:G:N2	2.38	0.51
1:QA:427:U:OP1	4:QD:13:ARG:NH2	2.40	0.51
7:QG:69:VAL:HG13	7:QG:100:ALA:HB1	1.93	0.51
1:QA:1151:A:H5'	10:QJ:41:PRO:HA	1.92	0.51
1:XA:1367:C:H4'	10:XJ:48:THR:HG21	1.90	0.51
22:XV:55:U:N3	22:XV:58:A:OP2	2.38	0.51
28:Y4:6:HIS:CE1	39:YG:67:LYS:H	2.28	0.51
32:Y8:30:ARG:HE	44:YP:62:LEU:HD12	1.76	0.51
34:YA:2152:G:H2'	34:YA:2153:G:H8	1.75	0.51
53:YY:76:CYS:SG	53:YY:79:CYS:SG	3.08	0.51
25:R1:10:LYS:NZ	25:R1:65:SER:OG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1567:A:OP2	36:RD:84:TYR:OH	2.28	0.51
34:RA:2795:G:N2	34:RA:2799:A:OP2	2.44	0.51
34:RA:748:G:OP1	34:RA:2612:C:N4	2.44	0.51
41:RI:86:THR:HA	41:RI:123:LEU:HB2	1.92	0.51
41:RI:94:ALA:HA	41:RI:97:ILE:HD12	1.93	0.51
42:RN:3:THR:HG21	49:RU:61:TRP:HE1	1.75	0.51
1:XA:992:U:H3	1:XA:1044:A:H62	1.57	0.51
1:XA:935:A:O2'	1:XA:1383:C:N3	2.43	0.51
1:XA:59:A:H3'	1:XA:331:G:H22	1.74	0.51
10:XJ:26:ALA:O	10:XJ:84:GLN:NE2	2.43	0.51
36:YD:108:PRO:HB3	36:YD:143:HIS:CE1	2.46	0.51
52:YX:25:LYS:HA	52:YX:81:VAL:O	2.11	0.51
1:QA:15:G:O6	1:QA:920:U:O4	2.29	0.51
1:QA:778:G:O6	1:QA:804:U:O4	2.28	0.51
34:RA:1990:C:H2'	34:RA:1991:U:C6	2.45	0.51
34:RA:2169:A:N6	34:RA:2170:A:N1	2.59	0.51
37:RE:110:GLY:HA2	37:RE:161:GLY:HA3	1.92	0.51
39:RG:52:ILE:HG22	39:RG:55:LYS:HD2	1.92	0.51
1:XA:21:G:H2'	1:XA:22:G:C8	2.46	0.51
2:XB:198:ASP:OD1	8:XH:68:ARG:NH2	2.44	0.51
34:YA:1012:U:OP2	49:YU:70:ARG:NH2	2.39	0.51
34:YA:693:C:O2'	34:YA:1353:A:N3	2.37	0.51
34:YA:1435:G:N2	34:YA:1477:A:O2'	2.42	0.51
27:Y3:31:LEU:HG	34:YA:989:G:OP1	2.10	0.51
34:YA:1824:G:N3	36:YD:254:THR:OG1	2.44	0.51
42:YN:97:ARG:HA	42:YN:100:GLU:HB2	1.92	0.51
1:QA:1081:G:H2'	1:QA:1082:G:H8	1.75	0.51
1:QA:249:U:O4	1:QA:275:G:O6	2.28	0.51
8:QH:32:LYS:HA	8:QH:35:ILE:HD12	1.92	0.51
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.93	0.51
34:YA:1670:C:O5'	34:YA:1670:C:H6	1.94	0.51
1:QA:1233:G:O2'	1:QA:1365:G:OP1	2.28	0.51
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.92	0.51
32:R8:30:ARG:O	32:R8:30:ARG:HG2	2.11	0.51
34:RA:1041:C:H2'	34:RA:1042:G:H8	1.76	0.51
34:RA:2014:A:O3'	51:RW:92:ARG:NH2	2.44	0.51
34:RA:1759:A:HO2'	34:RA:2714:G:HO2'	1.59	0.51
36:RD:147:LEU:HD12	36:RD:148:GLU:HG3	1.93	0.51
39:RG:121:ASN:O	39:RG:131:TYR:OH	2.26	0.51
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.92	0.51
34:YA:960:A:C8	34:YA:962:G:C8	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YF:154:VAL:HG22	38:YF:191:ARG:HB2	1.93	0.51
38:YF:63:LYS:NZ	38:YF:75:HIS:O	2.33	0.51
1:QA:556:C:H2'	1:QA:557:G:H8	1.76	0.51
5:QE:10:MET:HA	5:QE:32:VAL:HG12	1.93	0.51
12:QL:104:VAL:O	12:QL:105:TYR:CG	2.57	0.51
12:QL:39:VAL:HG12	12:QL:57:LYS:HG2	1.93	0.51
22:QV:36:G:C2	23:QX:17:C:O2	2.64	0.51
34:RA:1288:U:O3'	34:RA:1647:G:N2	2.44	0.51
44:RP:57:THR:OG1	44:RP:58:THR:N	2.44	0.51
48:RT:3:ARG:HG3	48:RT:6:LEU:HB2	1.92	0.51
1:XA:352:C:O2'	1:XA:354:G:OP1	2.24	0.51
2:XB:167:PRO:O	2:XB:171:ALA:HB2	2.11	0.51
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.91	0.51
1:XA:1537:U:H3	23:XX:9:G:H1	1.59	0.51
34:YA:547:A:H2'	34:YA:548:A:C8	2.46	0.51
1:QA:235:C:H2'	1:QA:236:G:H8	1.75	0.50
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	1.93	0.50
32:R8:8:LYS:HB3	32:R8:12:LYS:HE3	1.94	0.50
34:RA:2397:G:O6	34:RA:2419:U:O2	2.29	0.50
36:RD:175:LEU:O	36:RD:182:LEU:HA	2.12	0.50
42:RN:39:ARG:NH2	42:RN:41:ASP:OD1	2.44	0.50
47:RS:35:ILE:HD11	47:RS:97:ARG:HD2	1.92	0.50
50:RV:8:GLY:O	50:RV:10:LYS:NZ	2.42	0.50
1:XA:1338:G:N3	22:XV:41:A:O2'	2.44	0.50
1:XA:428:G:OP2	4:XD:10:ARG:NH1	2.39	0.50
1:XA:672:U:H2'	1:XA:673:G:H8	1.76	0.50
1:XA:828:A:H62	1:XA:858:G:H21	1.59	0.50
4:XD:19:LEU:HB3	4:XD:21:LEU:HD23	1.92	0.50
7:XG:111:ARG:HD3	7:XG:112:PRO:HD2	1.93	0.50
34:YA:2508:G:O2'	34:YA:2554:U:O2'	2.29	0.50
41:YI:1:MET:HG2	41:YI:23:PRO:HB3	1.92	0.50
12:QL:46:LYS:HD2	12:QL:47:LYS:HB2	1.93	0.50
22:QV:49:G:H1	22:QV:65:U:H3	1.59	0.50
53:RY:19:LYS:NZ	53:RY:20:TYR:CE2	2.71	0.50
1:XA:1034:G:H2'	1:XA:1035:A:C8	2.47	0.50
1:XA:373:A:H61	1:XA:391:G:H1'	1.75	0.50
3:XC:157:ILE:HD12	3:XC:164:ARG:HG3	1.94	0.50
8:XH:21:LYS:O	8:XH:65:TYR:OH	2.28	0.50
34:YA:1286:A:C6	34:YA:1289:C:C2	2.99	0.50
2:QB:111:ARG:HH11	2:QB:114:ARG:HH12	1.60	0.50
2:QB:208:ILE:O	2:QB:212:GLN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:57:ILE:HG22	3:QC:66:VAL:HG22	1.93	0.50
34:RA:58:G:H5'	52:RX:74:PRO:HB3	1.92	0.50
1:XA:1500:A:H5''	1:XA:1508:G:H5''	1.93	0.50
40:YH:85:LYS:HB3	40:YH:133:VAL:HG13	1.93	0.50
34:RA:1953:A:O2'	34:RA:2559:C:O2	2.29	0.50
34:RA:2185:C:H2'	34:RA:2186:G:H8	1.77	0.50
34:RA:321:G:O2'	34:RA:340:A:N3	2.42	0.50
1:XA:410:G:N2	1:XA:432:A:H62	2.10	0.50
8:XH:38:ILE:HD12	8:XH:41:ARG:HH21	1.76	0.50
34:YA:530:G:C6	34:YA:2022:U:OP1	2.65	0.50
34:YA:662:G:H5''	44:YP:17:LYS:HG2	1.92	0.50
1:QA:603:U:H3	1:QA:635:G:H1	1.60	0.50
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.37	0.50
34:RA:1297:C:H2'	34:RA:1298:C:C6	2.46	0.50
34:RA:2178:C:H2'	34:RA:2179:C:H6	1.76	0.50
1:XA:1386:G:H2'	1:XA:1387:G:C8	2.43	0.50
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.44	0.50
20:XT:75:ASN:OD1	20:XT:75:ASN:N	2.44	0.50
24:Y0:41:ARG:NH2	34:YA:2387:U:O2'	2.45	0.50
34:YA:2148:G:H2'	34:YA:2149:G:H8	1.76	0.50
34:YA:581:C:H2'	34:YA:582:G:C8	2.47	0.50
40:YH:113:VAL:HG11	40:YH:151:ILE:HD12	1.94	0.50
52:YX:53:LYS:HG2	52:YX:82:GLN:HB3	1.93	0.50
1:QA:1261:A:H62	1:QA:1274:G:N2	2.09	0.50
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.47	0.50
1:QA:1484:C:HO2'	34:RA:1960:A:HO2'	1.53	0.50
13:QM:84:ILE:HG12	19:QS:66:MET:CE	2.41	0.50
22:QV:37:IMG:HM13	23:QX:16:C:N1	2.26	0.50
34:RA:2490:G:N2	34:RA:2490:G:OP2	2.45	0.50
31:R7:34:ARG:NH1	34:RA:466:A:OP1	2.45	0.50
34:RA:505:A:OP2	34:RA:1235:G:OP1	2.29	0.50
1:XA:159:G:H21	1:XA:161:A:H8	1.60	0.50
1:XA:181:G:N2	1:XA:182:U:O4	2.36	0.50
1:XA:745:C:OP1	1:XA:851:G:O2'	2.30	0.50
2:XB:118:LEU:HD23	2:XB:142:LEU:HB2	1.94	0.50
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.92	0.50
28:Y4:16:CYS:HB3	28:Y4:33:VAL:HB	1.93	0.50
34:YA:2076:U:OP2	34:YA:2238:G:N2	2.37	0.50
34:YA:2808:U:C2	34:YA:2892:A:N6	2.79	0.50
34:YA:458:G:O2'	34:YA:469:G:O6	2.29	0.50
34:YA:630:G:N2	34:YA:633:A:OP2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1338:G:N3	22:QV:41:A:O2'	2.44	0.50
34:RA:1422:G:H1	34:RA:1576:U:H3	1.60	0.50
34:RA:2751:G:C4	40:RH:3:ARG:CB	2.90	0.50
36:RD:69:ARG:NH1	36:RD:128:GLY:O	2.42	0.50
42:RN:112:LEU:O	42:RN:116:LEU:HB2	2.10	0.50
42:RN:9:VAL:HG11	42:RN:39:ARG:HH12	1.77	0.50
4:XD:107:ARG:HB3	4:XD:174:LEU:HD11	1.93	0.50
34:YA:305:U:O4	34:YA:312:G:O6	2.30	0.50
34:YA:255:A:O2'	34:YA:384:U:OP1	2.27	0.50
34:YA:919:G:N2	34:YA:2269:A:OP2	2.44	0.50
37:YE:101:ARG:NE	37:YE:171:GLU:OE2	2.41	0.50
38:YF:10:PRO:HB3	38:YF:17:ARG:HH21	1.76	0.50
19:QS:10:PHE:HZ	19:QS:15:LEU:HD11	1.76	0.50
34:RA:1405:U:H2'	34:RA:1406:U:H6	1.76	0.50
34:RA:1654:A:N1	34:RA:2048:G:O2'	2.44	0.50
34:RA:2572:A:OP1	34:RA:2574:G:O2'	2.25	0.50
34:RA:947:G:H2'	34:RA:948:G:H8	1.75	0.50
5:XE:81:GLU:HG2	5:XE:90:VAL:HG23	1.94	0.50
9:XI:22:GLY:N	9:XI:58:HIS:O	2.37	0.50
10:XJ:53:PRO:HB3	14:YN:42:ILE:HG12	1.94	0.50
33:Y9:27:CYS:HB3	33:Y9:32:HIS:HB2	1.94	0.50
34:YA:2692:C:O2	34:YA:2847:U:O2'	2.27	0.50
34:YA:28:A:HO2'	34:YA:582:G:HO2'	1.56	0.50
51:YW:86:LEU:HD22	51:YW:96:ILE:HD11	1.93	0.50
53:YY:28:LYS:NZ	53:YY:64:GLU:OE2	2.35	0.50
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.27	0.50
13:QM:84:ILE:HG12	19:QS:66:MET:HE3	1.94	0.50
34:RA:764:A:H5'	36:RD:210:GLY:HA2	1.93	0.50
36:RD:126:GLN:O	36:RD:129:ASN:ND2	2.41	0.50
1:XA:126:G:OP1	1:XA:633:G:N2	2.42	0.50
1:XA:444:C:H2'	1:XA:445:G:C8	2.46	0.50
20:XT:74:LYS:O	20:XT:76:ALA:N	2.44	0.50
34:YA:1682:G:OP1	34:YA:1699:G:N1	2.44	0.50
34:YA:962:G:H2'	34:YA:963:U:C6	2.47	0.50
1:QA:1305:G:OP2	21:QU:2:GLY:N	2.45	0.49
1:QA:1510:U:H3	1:QA:1525:G:H1	1.59	0.49
1:QA:243:A:N6	1:QA:281:G:O2'	2.43	0.49
2:QB:146:GLN:HG3	2:QB:153:ARG:HH22	1.77	0.49
2:QB:178:ARG:NH2	2:QB:198:ASP:OD1	2.39	0.49
13:QM:16:ASP:N	13:QM:16:ASP:OD1	2.44	0.49
34:RA:1882:C:H3'	34:RA:1883:G:H8	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:19:VAL:HG23	8:XH:21:LYS:HG3	1.94	0.49
29:Y5:25:LEU:HG	51:YW:19:LEU:HD12	1.94	0.49
35:YB:36:C:H42	35:YB:49:C:H1'	1.77	0.49
1:XA:1122:U:O4	1:XA:1123:A:N6	2.45	0.49
34:YA:1791:A:N6	34:YA:1828:G:O2'	2.44	0.49
34:YA:2729:G:H1'	37:YE:187:ALA:HB2	1.94	0.49
43:YO:63:VAL:HG12	43:YO:106:LEU:HD21	1.93	0.49
1:QA:1117:G:H21	1:QA:1180:A:H1'	1.76	0.49
1:QA:1203:C:H2'	1:QA:1204:A:H8	1.78	0.49
4:QD:61:LYS:HD3	4:QD:206:PHE:CD2	2.46	0.49
20:QT:66:ALA:O	20:QT:71:THR:OG1	2.28	0.49
20:QT:56:MET:HG3	20:QT:84:LEU:HD21	1.94	0.49
1:QA:1304:G:OP1	21:QU:10:ARG:NH2	2.45	0.49
28:R4:5:ILE:HB	39:RG:67:LYS:HD2	1.94	0.49
24:R0:12:ASN:ND2	34:RA:2278:A:OP2	2.45	0.49
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.76	0.49
1:XA:1124:G:H1'	10:XJ:38:ILE:HD12	1.95	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
4:XD:88:VAL:HG13	5:XE:97:GLY:HA3	1.94	0.49
5:XE:101:ILE:O	5:XE:120:THR:OG1	2.30	0.49
7:XG:58:PRO:HA	7:XG:61:VAL:HG12	1.92	0.49
33:Y9:27:CYS:SG	33:Y9:28:GLU:N	2.84	0.49
34:YA:124:G:N2	34:YA:126:A:O2'	2.46	0.49
34:YA:1653:G:O6	46:YR:11:ASN:N	2.43	0.49
34:YA:1901:A:OP2	36:YD:255:LYS:NZ	2.34	0.49
34:YA:2198:A:OP1	41:YI:33:ARG:NH2	2.46	0.49
1:QA:776:G:N2	1:QA:802:A:OP2	2.45	0.49
23:QX:3:C:H2'	23:QX:4:A:C8	2.47	0.49
24:R0:72:ARG:HE	24:R0:75:LEU:HD12	1.76	0.49
25:R1:90:ILE:HA	25:R1:94:LEU:CG	2.42	0.49
34:RA:1147:C:H2'	34:RA:1148:A:H8	1.77	0.49
1:XA:269:C:H2'	1:XA:270:A:H8	1.77	0.49
23:XX:6:G:H2'	23:XX:7:G:H8	1.75	0.49
34:YA:1668:A:H62	34:YA:1991:U:H3	1.60	0.49
37:YE:1:MET:N	37:YE:83:ASP:O	2.36	0.49
54:YZ:6:LYS:NZ	54:YZ:43:GLU:OE1	2.39	0.49
1:QA:1128:C:O2'	1:QA:1130:A:N7	2.45	0.49
30:R6:18:ARG:O	30:R6:20:ASN:ND2	2.44	0.49
34:RA:2148:G:H2'	34:RA:2149:G:C8	2.48	0.49
34:RA:2306:C:H2'	34:RA:2307:G:H21	1.76	0.49
34:RA:270(S):G:H2'	34:RA:270(T):G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:290:G:H1	34:RA:350:U:H3	1.60	0.49
34:RA:586:A:C5'	38:RF:89:VAL:HG21	2.37	0.49
40:RH:89:ILE:HD12	40:RH:131:VAL:HG22	1.94	0.49
7:XG:140:ASP:OD2	7:XG:143:ARG:NH1	2.45	0.49
36:YD:97:TYR:HB2	36:YD:101:GLU:O	2.13	0.49
1:QA:766:A:N6	1:QA:813:U:N3	2.48	0.49
13:QM:84:ILE:HG12	19:QS:66:MET:SD	2.53	0.49
1:QA:1268:A:H5'	21:QU:20:LYS:HG2	1.95	0.49
33:R9:11:CYS:SG	33:R9:14:CYS:N	2.85	0.49
34:RA:1668:A:N3	34:RA:1670:C:N4	2.60	0.49
25:R1:78:LYS:HZ3	34:RA:270(T):G:H1'	1.77	0.49
39:RG:135:LEU:O	39:RG:154:GLY:HA3	2.13	0.49
50:RV:45:THR:O	50:RV:45:THR:CG2	2.55	0.49
1:XA:652:U:O4	1:XA:752:G:O2'	2.28	0.49
7:XG:115:ARG:HB2	7:XG:118:VAL:HG12	1.94	0.49
7:XG:118:VAL:HG22	7:XG:122:HIS:CE1	2.48	0.49
20:XT:41:ILE:HD13	20:XT:87:LYS:HG2	1.95	0.49
1:XA:186(A):C:H5'	20:XT:78:ALA:HB1	1.95	0.49
26:Y2:16:LEU:O	26:Y2:67:LYS:NZ	2.45	0.49
32:Y8:10:ALA:O	32:Y8:14:VAL:HB	2.13	0.49
34:YA:2245:U:H5'	34:YA:2246:G:H5'	1.93	0.49
34:YA:793:A:OP2	34:YA:2071:A:O2'	2.30	0.49
34:YA:959:A:N3	34:YA:2457:U:O2'	2.36	0.49
28:Y4:31:ILE:HG21	39:YG:142:PRO:HB2	1.93	0.49
44:YP:52:GLU:OE1	44:YP:55:ARG:NH1	2.46	0.49
1:QA:475:G:H2'	1:QA:476:G:H8	1.78	0.49
1:QA:762:C:H2'	1:QA:763:G:H8	1.76	0.49
3:QC:35:GLU:HA	3:QC:38:ARG:HH21	1.77	0.49
6:QF:35:ALA:HB1	6:QF:65:VAL:HG21	1.95	0.49
34:RA:1652:A:C2	34:RA:2006:C:N3	2.80	0.49
34:RA:505:A:HO2'	34:RA:509:C:HO2'	1.58	0.49
34:RA:690:G:H21	36:RD:43:ARG:HH21	1.61	0.49
1:XA:557:G:H2'	1:XA:558:G:C8	2.48	0.49
1:XA:925:G:O2'	1:XA:927:G:OP1	2.24	0.49
6:XF:61:LEU:HD23	6:XF:63:TYR:HE2	1.77	0.49
19:XS:12:ASP:HB2	19:XS:37:ARG:HE	1.77	0.49
19:XS:40:ILE:HD13	19:XS:71:LEU:HD21	1.95	0.49
30:Y6:23:THR:OG1	30:Y6:24:GLU:N	2.42	0.49
34:YA:1153:C:H5'	49:YU:76:TYR:HE2	1.77	0.49
34:YA:1212:G:O2'	34:YA:1236:G:N2	2.39	0.49
34:YA:2092:U:OP2	41:YI:27:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2131:G:N3	34:YA:2158:A:N6	2.61	0.49
34:YA:288:C:H2'	34:YA:289:A:H8	1.77	0.49
34:YA:577:G:O2'	34:YA:1254:A:OP1	2.31	0.49
34:YA:71:A:N3	34:YA:73:A:N6	2.60	0.49
1:QA:1049:U:H4'	1:QA:1050:G:H5''	1.94	0.49
34:RA:1224:G:N2	34:RA:1227:A:OP2	2.36	0.49
34:RA:577:G:O2'	34:RA:1254:A:OP1	2.30	0.49
34:RA:1265:A:H61	34:RA:2013:A:H5''	1.77	0.49
34:RA:1837:C:O2'	34:RA:1927:A:N3	2.36	0.49
43:RO:88:ASN:HD21	43:RO:90:GLN:HB2	1.78	0.49
51:RW:22:ASP:OD1	51:RW:25:ARG:NH1	2.45	0.49
1:XA:474:G:H2'	1:XA:475:G:H8	1.77	0.49
4:XD:56:VAL:HG13	4:XD:57:ARG:HD2	1.94	0.49
4:XD:72:GLU:OE2	4:XD:207:TYR:OH	2.19	0.49
34:YA:2744:G:H21	40:YH:143:GLN:HE22	1.61	0.49
45:YQ:66:ILE:HA	45:YQ:104:PHE:HA	1.95	0.49
1:QA:1096:C:H2'	1:QA:1097:C:H6	1.78	0.49
1:QA:126:G:OP1	1:QA:605:U:O2'	2.25	0.49
3:QC:47:LEU:HD11	3:QC:87:LEU:HD21	1.95	0.49
4:QD:79:PHE:HE1	4:QD:204:ILE:HD13	1.77	0.49
34:RA:1116:C:H2'	34:RA:1117:G:C8	2.48	0.49
34:RA:1181:C:H2'	34:RA:1182:A:H8	1.78	0.49
34:RA:2581:G:OP2	34:RA:2581:G:N2	2.44	0.49
45:RQ:36:ALA:HB1	45:RQ:127:ILE:HG21	1.94	0.49
1:XA:107:G:OP1	1:XA:325:A:N6	2.46	0.49
1:XA:14:U:N3	1:XA:17:U:OP2	2.42	0.49
1:QA:1281:U:H5''	1:QA:1282:C:H5	1.78	0.49
1:QA:59:A:H5''	1:QA:60:A:H5''	1.95	0.49
5:QE:87:SER:OG	5:QE:125:SER:OG	2.27	0.49
34:RA:975:G:N2	34:RA:1156:A:O2'	2.46	0.49
34:RA:180:G:N1	34:RA:214:G:O6	2.46	0.49
34:RA:441:U:O2	38:RF:46:ARG:NH2	2.45	0.49
34:RA:848:G:H2'	34:RA:849:A:C8	2.48	0.49
53:RY:76:CYS:SG	53:RY:79:CYS:CA	2.94	0.49
1:XA:1384:C:H2'	1:XA:1385:G:H8	1.77	0.49
15:XO:10:LYS:HA	15:XO:13:GLN:HG2	1.95	0.49
1:XA:191:G:N2	20:XT:103:GLY:O	2.34	0.49
48:YT:28:VAL:HG12	48:YT:88:ILE:HA	1.95	0.49
1:QA:1270:C:H2'	1:QA:1271:G:C8	2.48	0.48
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.94	0.48
34:RA:1086:A:O2'	34:RA:1087:G:N7	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1454:U:O2	46:RR:64:ARG:NE	2.41	0.48
34:RA:820:A:N3	34:RA:943:U:O2'	2.39	0.48
34:RA:566:U:H5''	44:RP:29:LYS:NZ	2.28	0.48
54:RZ:163:LEU:HD22	54:RZ:167:PRO:HG3	1.95	0.48
1:XA:62:U:H3	1:XA:105:G:H1	1.61	0.48
1:XA:1500:A:OP1	1:XA:1508:G:OP1	2.31	0.48
1:XA:714:G:H2'	1:XA:715:A:C8	2.48	0.48
13:XM:88:ARG:HD2	13:XM:98:VAL:HB	1.95	0.48
13:XM:91:ARG:NE	13:XM:97:PRO:O	2.46	0.48
34:YA:1165:U:O4	34:YA:1184:G:O6	2.30	0.48
34:YA:587:C:O2	44:YP:33:ARG:NH2	2.36	0.48
1:QA:570:G:H1'	1:QA:820:U:H5	1.77	0.48
4:QD:72:GLU:OE2	4:QD:207:TYR:OH	2.29	0.48
5:QE:84:PHE:N	5:QE:87:SER:O	2.45	0.48
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.46	0.48
18:QR:59:SER:OG	18:QR:60:ALA:N	2.46	0.48
34:RA:1315:C:O2'	34:RA:1392:A:N3	2.40	0.48
34:RA:2291:U:O4	34:RA:2341:G:O6	2.31	0.48
34:RA:560:C:O2	49:RU:49:HIS:NE2	2.46	0.48
40:RH:3:ARG:HH12	40:RH:5:GLY:HA2	1.77	0.48
1:XA:1115:C:H1'	9:XI:111:ARG:HH21	1.78	0.48
1:XA:1175:G:H2'	1:XA:1176:A:H8	1.78	0.48
4:XD:20:TYR:HD1	4:XD:26:CYS:HB3	1.78	0.48
31:Y7:7:PRO:HA	34:YA:686:G:C8	2.47	0.48
33:Y9:14:CYS:HB3	33:Y9:27:CYS:HB2	1.95	0.48
34:YA:2403:C:C4	34:YA:2415:G:C2	3.01	0.48
34:YA:860:U:H1'	34:YA:2268:A:H5'	1.94	0.48
41:YI:129:THR:HG22	41:YI:137:PRO:HB3	1.95	0.48
54:YZ:24:LEU:HD23	54:YZ:41:LEU:HG	1.94	0.48
1:QA:1507:A:C2	1:QA:1530:G:N9	2.81	0.48
34:RA:1024:G:HO2'	34:RA:1144:G:HO2'	1.59	0.48
40:RH:3:ARG:HG3	40:RH:3:ARG:O	2.13	0.48
43:RO:15:GLY:O	43:RO:47:ILE:N	2.45	0.48
53:RY:15:VAL:HA	53:RY:72:VAL:HA	1.94	0.48
1:XA:922:G:H2'	1:XA:923:A:C8	2.48	0.48
48:YT:31:SER:OG	48:YT:85:LYS:NZ	2.44	0.48
1:QA:1137:C:O2'	1:QA:1138:G:N2	2.46	0.48
1:QA:1291:G:H5'	7:QG:37:ASN:HD21	1.77	0.48
1:QA:1357:A:H5'	10:QJ:45:ARG:HH12	1.78	0.48
34:RA:1608:A:C5	34:RA:1611:C:C4	3.01	0.48
34:RA:2195:C:H2'	34:RA:2196:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:358:U:H2'	34:RA:359:A:H8	1.79	0.48
34:RA:483:A:O2'	53:RY:49:VAL:O	2.30	0.48
44:RP:106:LEU:HD13	44:RP:112:LEU:HD13	1.95	0.48
34:RA:2295:C:OP1	47:RS:10:ARG:NH1	2.46	0.48
1:XA:1230:C:H2'	1:XA:1231:G:H8	1.77	0.48
1:XA:781:A:O2'	1:XA:1522:U:O2	2.30	0.48
6:XF:82:ARG:HB3	6:XF:85:VAL:HG12	1.95	0.48
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.47	0.48
34:YA:2099:U:O2	34:YA:2190:G:N2	2.37	0.48
34:YA:675:A:OP1	38:YF:63:LYS:NZ	2.39	0.48
36:YD:108:PRO:HB3	36:YD:143:HIS:HE1	1.77	0.48
41:YI:77:LEU:HD13	41:YI:101:LEU:HB3	1.96	0.48
54:YZ:130:PRO:HA	54:YZ:133:ILE:HD11	1.96	0.48
1:QA:117:G:H8	1:QA:117:G:O5'	1.96	0.48
7:QG:111:ARG:NH1	7:QG:113:GLU:OE1	2.43	0.48
10:QJ:4:ILE:HG12	10:QJ:100:THR:HG22	1.96	0.48
11:QK:82:VAL:HG13	11:QK:108:ILE:HA	1.95	0.48
20:QT:54:LYS:HE3	20:QT:100:ILE:HG21	1.95	0.48
20:QT:67:ALA:O	20:QT:73:HIS:ND1	2.39	0.48
34:RA:1525:G:H2'	34:RA:1526:G:H8	1.77	0.48
34:RA:2489:G:O2'	34:RA:2518:A:N6	2.47	0.48
35:RB:75:G:H4'	54:RZ:36:LYS:HE2	1.96	0.48
54:RZ:61:LEU:HD23	54:RZ:67:LEU:HD23	1.94	0.48
6:XF:5:GLU:HA	6:XF:63:TYR:O	2.14	0.48
16:XP:40:ASP:HB3	16:XP:48:TRP:HB2	1.94	0.48
19:XS:36:ARG:HB2	19:XS:72:GLY:HA3	1.94	0.48
34:YA:1193:G:OP2	44:YP:16:ARG:NH2	2.42	0.48
34:YA:1307:A:N1	34:YA:1622:G:C6	2.81	0.48
34:YA:1802:A:H2'	34:YA:1803:A:C8	2.48	0.48
34:YA:2816:C:O2	34:YA:2883:A:O2'	2.27	0.48
34:YA:363(B):A:H2'	34:YA:363(C):G:H8	1.78	0.48
32:Y8:13:ARG:HD2	44:YP:61:ARG:HG3	1.95	0.48
47:YS:4:LEU:HD22	47:YS:8:GLU:CD	2.34	0.48
48:YT:52:ILE:HG13	48:YT:61:PHE:HB3	1.96	0.48
1:QA:819:A:C8	1:QA:1529:G:N1	2.81	0.48
1:QA:976:G:OP2	1:QA:1358:U:O2'	2.30	0.48
1:QA:261:U:OP2	20:QT:80:ARG:NH2	2.47	0.48
34:RA:521:G:H2'	34:RA:522:G:H8	1.77	0.48
34:RA:571:A:O5'	34:RA:2030:A:N6	2.43	0.48
34:RA:2314:C:H5'	39:RG:38:VAL:HG11	1.96	0.48
4:XD:63:LYS:HD2	4:XD:198:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:3:ARG:HD2	13:XM:7:VAL:HG12	1.96	0.48
26:Y2:4:SER:OG	26:Y2:5:GLU:N	2.39	0.48
34:YA:1174:A:H2'	34:YA:1175:U:H4'	1.94	0.48
34:YA:2250:G:C4	45:YQ:82:ARG:HG3	2.48	0.48
1:QA:1342:C:H4'	9:QI:125:TYR:HB3	1.95	0.48
5:QE:74:GLY:O	5:QE:116:THR:OG1	2.31	0.48
34:RA:1586:A:H3'	34:RA:1587:A:H8	1.79	0.48
29:R5:4:HIS:O	34:RA:2056:G:N2	2.47	0.48
34:RA:2450:A:H62	34:RA:2501:C:H42	1.61	0.48
38:RF:48:THR:O	38:RF:48:THR:OG1	2.32	0.48
40:RH:46:GLU:HB2	40:RH:49:VAL:HG23	1.95	0.48
40:RH:43:VAL:HG23	40:RH:52:VAL:HG12	1.95	0.48
49:RU:90:VAL:O	49:RU:92:ARG:N	2.35	0.48
53:RY:13:VAL:HA	53:RY:74:PRO:HA	1.96	0.48
1:XA:28:G:O2'	1:XA:296:U:OP1	2.30	0.48
1:XA:372:C:H42	1:XA:389:A:H62	0.68	0.48
1:XA:520:A:H62	1:XA:529:G:N2	2.11	0.48
1:XA:693:G:H22	22:XV:37:1MG:HN21	1.60	0.48
4:XD:91:SER:HB2	4:XD:191:ARG:HD2	1.95	0.48
4:XD:89:THR:OG1	5:XE:97:GLY:O	2.27	0.48
34:YA:1087:G:O6	34:YA:1089:G:N2	2.44	0.48
34:YA:1419:A:N7	34:YA:1578:U:O4	2.47	0.48
34:YA:1980:G:O2'	34:YA:1982:C:OP2	2.25	0.48
32:Y8:13:ARG:NH2	34:YA:250:G:OP2	2.47	0.48
34:YA:993:G:N2	50:YV:23:GLU:OE2	2.46	0.48
39:YG:68:PRO:HB3	39:YG:92:VAL:HB	1.95	0.48
46:YR:3:HIS:O	46:YR:5:LYS:N	2.47	0.48
34:RA:514:A:H2'	34:RA:515:A:H8	1.79	0.48
34:RA:685:A:OP1	34:RA:686:G:N2	2.45	0.48
1:XA:114:U:H2'	1:XA:115:G:C8	2.48	0.48
1:XA:1223:C:H5''	1:XA:1224:G:H5''	1.95	0.48
1:XA:346:G:OP1	48:YT:41:ARG:NH2	2.39	0.48
1:XA:410:G:OP1	4:XD:30:LYS:NZ	2.47	0.48
1:XA:737:A:H2'	1:XA:738:C:H6	1.79	0.48
1:XA:938:A:O3'	7:XG:95:ARG:NH2	2.47	0.48
5:XE:60:TYR:OH	5:XE:64:ARG:NH2	2.47	0.48
24:Y0:11:ARG:O	24:Y0:14:ARG:NH2	2.43	0.48
25:Y1:83:GLU:HG3	25:Y1:85:LEU:H	1.78	0.48
34:YA:2787:C:H1'	37:YE:62:PRO:HG3	1.96	0.48
37:YE:117:MET:HA	37:YE:122:PHE:H	1.79	0.48
38:YF:116:ASP:OD2	44:YP:1:MET:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YG:107:LEU:HA	39:YG:111:LEU:HD12	1.95	0.48
1:QA:1299:A:H2'	1:QA:1301:U:H1'	1.96	0.48
1:QA:1318:A:H1'	19:QS:37:ARG:HE	1.79	0.48
25:R1:2:SER:N	34:RA:1364:G:OP2	2.46	0.48
34:RA:2245:U:H5''	34:RA:2246:G:H5'	1.96	0.48
34:RA:23:G:OP1	34:RA:504:U:N3	2.38	0.48
34:RA:2473:U:OP1	34:RA:2529:G:N2	2.46	0.48
34:RA:597:U:H2'	34:RA:598:G:C8	2.49	0.48
38:RF:159:GLY:O	38:RF:164:ARG:NH2	2.41	0.48
42:RN:60:ILE:HA	42:RN:60:ILE:HD12	1.81	0.48
1:XA:618:C:H5'	1:XA:619:U:H5''	1.96	0.48
2:XB:30:ARG:NH1	2:XB:31:TYR:OH	2.46	0.48
3:XC:153:VAL:HB	3:XC:196:LEU:HD21	1.95	0.48
15:XO:39:LEU:HG	15:XO:56:LEU:HD12	1.96	0.48
34:YA:1338:G:N7	52:YX:62:LYS:NZ	2.59	0.48
34:YA:2115:G:N2	34:YA:2164:C:OP2	2.47	0.48
34:YA:480:A:O2'	53:YY:46:LYS:O	2.32	0.48
40:YH:70:THR:O	40:YH:74:ASN:ND2	2.47	0.48
45:YQ:35:VAL:HG12	45:YQ:102:VAL:HG22	1.94	0.48
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.47	0.48
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.45	0.48
1:QA:1250:A:H4'	9:QI:67:GLY:HA2	1.96	0.48
34:RA:1052:C:H2'	34:RA:1053:C:C5	2.49	0.48
34:RA:2085:C:H4'	36:RD:262:ARG:NH2	2.29	0.48
34:RA:2156:G:O6	34:RA:2157:G:N2	2.47	0.48
34:RA:862:G:O2'	35:RB:78:A:N3	2.47	0.48
39:RG:126:ASP:OD1	39:RG:130:ASN:N	2.43	0.48
1:XA:949:A:O2'	1:XA:1363:A:OP2	2.31	0.48
1:XA:767:A:O2'	1:XA:1524:C:O2	2.27	0.48
1:XA:192:U:H4'	20:XT:57:ARG:HD3	1.96	0.48
1:XA:605:U:OP2	1:XA:605:U:H5	1.97	0.48
9:XI:73:GLN:O	9:XI:77:ILE:HG12	2.14	0.48
22:XV:8:U:C2	22:XV:14:A:N6	2.82	0.48
30:Y6:19:ARG:NH1	34:YA:2399:G:O2'	2.47	0.48
37:YE:37:ARG:O	37:YE:45:THR:HA	2.13	0.48
39:YG:63:ILE:HG22	39:YG:143:GLU:HB2	1.95	0.48
1:QA:815:A:H4'	1:QA:817:C:C5	2.48	0.47
2:QB:47:THR:HG23	2:QB:202:PRO:HG2	1.96	0.47
3:QC:50:ALA:HB2	3:QC:75:VAL:HB	1.96	0.47
1:QA:407:G:H5''	4:QD:115:ARG:HE	1.78	0.47
34:RA:1411:C:H42	34:RA:1591:G:H22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RT:91:ARG:NH2	48:RT:124:ASP:OD2	2.47	0.47
1:XA:1370:G:H2'	1:XA:1371:G:H8	1.79	0.47
17:XQ:66:SER:H	17:XQ:69:LYS:HB3	1.78	0.47
20:XT:61:SER:OG	20:XT:62:LEU:N	2.47	0.47
34:YA:2105:C:H2'	34:YA:2106:G:C8	2.49	0.47
34:YA:2427:C:H5'	34:YA:2429:G:H5'	1.96	0.47
34:YA:363(D):G:H2'	34:YA:363(E):G:H8	1.78	0.47
35:YB:12:C:O4'	35:YB:15:A:N6	2.47	0.47
37:YE:102:VAL:O	37:YE:170:LEU:N	2.45	0.47
1:QA:161:A:H2	1:QA:347:G:H21	1.62	0.47
3:QC:34:LEU:O	3:QC:38:ARG:NE	2.43	0.47
4:QD:108:LEU:HD22	4:QD:174:LEU:HD13	1.96	0.47
13:QM:26:GLY:O	13:QM:30:ALA:CB	2.62	0.47
34:RA:1058:G:H2'	34:RA:1059:G:C8	2.49	0.47
34:RA:2693:A:H2'	34:RA:2694:G:H8	1.78	0.47
34:RA:839:U:H3	34:RA:939:G:H1	1.62	0.47
47:RS:26:LEU:HB3	47:RS:87:PHE:HA	1.96	0.47
49:RU:17:ILE:HG13	49:RU:39:LEU:HD12	1.95	0.47
16:XP:6:LEU:HD13	16:XP:17:TYR:CG	2.49	0.47
19:XS:4:SER:HB2	19:XS:7:LYS:HG2	1.95	0.47
34:YA:2154:G:H2'	34:YA:2155:G:H8	1.79	0.47
35:YB:9:G:OP1	47:YS:25:ARG:NH1	2.40	0.47
50:YV:13:ARG:NH1	50:YV:15:GLU:OE2	2.45	0.47
50:YV:52:VAL:HG21	50:YV:55:ALA:HB3	1.95	0.47
53:YY:11:ASP:N	53:YY:11:ASP:OD1	2.43	0.47
1:QA:1318:A:H1'	19:QS:37:ARG:HH21	1.80	0.47
29:R5:12:SER:O	29:R5:16:ARG:HB2	2.14	0.47
38:RF:102:PRO:HB2	38:RF:105:VAL:HG23	1.95	0.47
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.28	0.47
2:XB:71:VAL:HB	2:XB:164:VAL:HG12	1.96	0.47
4:XD:175:SER:O	4:XD:183:GLY:HA2	2.15	0.47
4:XD:175:SER:HB3	4:XD:184:LYS:HB3	1.96	0.47
1:XA:458(F):A:HO2'	16:XP:82:GLN:H	1.60	0.47
47:YS:25:ARG:HG3	47:YS:88:ASP:HB2	1.96	0.47
1:QA:21:G:H2'	1:QA:22:G:C8	2.49	0.47
1:QA:269:C:H2'	1:QA:270:A:H8	1.79	0.47
1:QA:1186:G:O2'	9:QI:110:GLU:OE2	2.27	0.47
9:QI:20:ARG:HG3	9:QI:60:ASP:HB2	1.96	0.47
12:QL:7:ILE:HD11	17:QQ:32:TYR:HB3	1.94	0.47
25:R1:17:SER:O	25:R1:17:SER:OG	2.29	0.47
34:RA:1203:G:O6	34:RA:1204:A:N6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:442:G:N2	38:RF:48:THR:OG1	2.47	0.47
37:RE:105:THR:OG1	37:RE:199:ARG:NH1	2.48	0.47
34:RA:2845:G:OP1	48:RT:56:GLY:N	2.48	0.47
1:XA:974:A:OP2	14:XN:29:ARG:NH2	2.48	0.47
34:YA:1286:A:C6	34:YA:1289:C:N3	2.83	0.47
34:YA:1792:G:O2'	34:YA:1830:C:OP1	2.32	0.47
29:Y5:52:TYR:OH	34:YA:2883:A:OP1	2.20	0.47
45:YQ:75:THR:HB	45:YQ:86:GLY:HA3	1.96	0.47
1:QA:1052:U:O2'	1:QA:1055:A:OP2	2.28	0.47
31:R7:24:THR:HG23	31:R7:27:GLY:H	1.79	0.47
34:RA:1068:G:O6	34:RA:1069:A:N6	2.48	0.47
34:RA:1270:C:H5''	34:RA:1271:G:H5'	1.97	0.47
34:RA:1542:G:O6	34:RA:1543:A:C6	2.67	0.47
34:RA:2328:A:H2'	34:RA:2329:G:H8	1.79	0.47
41:RI:51:ILE:HA	41:RI:54:GLN:HG2	1.95	0.47
2:XB:204:ASN:OD1	2:XB:205:ASP:N	2.48	0.47
27:Y3:18:ASP:OD1	27:Y3:18:ASP:N	2.46	0.47
34:YA:974(A):G:C4	34:YA:1186:G:C2	3.03	0.47
34:YA:1535:U:H2'	34:YA:1536:A:C8	2.49	0.47
34:YA:28:A:N6	34:YA:512:G:O2'	2.47	0.47
34:YA:730:C:OP1	34:YA:1775:U:O2'	2.25	0.47
1:QA:1221:G:H5'	19:QS:36:ARG:HH22	1.78	0.47
11:QK:17:GLY:HA2	11:QK:35:PRO:HD3	1.97	0.47
12:QL:5:PRO:HG2	12:QL:10:LEU:HD21	1.96	0.47
34:RA:1148:A:H2'	34:RA:1149:G:H8	1.80	0.47
34:RA:534:U:H3	34:RA:559:G:H1	1.63	0.47
34:RA:99:U:O4	53:RY:8:LYS:NZ	2.46	0.47
1:XA:303:A:HO2'	1:XA:555:C:HO2'	1.59	0.47
2:XB:84:GLU:HG3	2:XB:215:LEU:HB3	1.96	0.47
7:XG:99:LEU:HD12	7:XG:102:ARG:HD2	1.96	0.47
13:XM:83:ASP:OD2	13:XM:84:ILE:N	2.46	0.47
1:XA:734:G:H21	18:XR:75:ILE:HD13	1.80	0.47
27:Y3:51:ALA:HA	27:Y3:54:VAL:HG12	1.96	0.47
34:YA:137(B):G:N3	52:YX:41:ASN:ND2	2.61	0.47
37:YE:105:THR:HG21	37:YE:164:ARG:HH21	1.78	0.47
41:YI:88:ILE:HG22	41:YI:90:GLY:H	1.80	0.47
1:QA:1328:C:H4'	13:QM:29:ARG:HD3	1.96	0.47
11:QK:27:ASN:OD1	11:QK:28:THR:N	2.47	0.47
34:RA:2751:G:N7	40:RH:2:SER:OG	2.46	0.47
34:RA:581:C:H2'	34:RA:582:G:H8	1.79	0.47
34:RA:1843:C:O2'	36:RD:256:GLY:O	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RR:26:LYS:O	46:RR:30:THR:OG1	2.24	0.47
49:RU:6:THR:HG21	49:RU:10:ARG:HH12	1.79	0.47
49:RU:90:VAL:HG13	50:RV:39:LEU:HD22	1.97	0.47
1:XA:1503:A:O2'	23:XX:15:A:N6	2.44	0.47
1:XA:403:C:H42	1:XA:547:A:H5'	1.80	0.47
1:XA:616:G:H2'	1:XA:617:G:H8	1.78	0.47
34:YA:1689:A:H62	34:YA:1698:A:H2	1.63	0.47
34:YA:821:A:N6	34:YA:972:G:O2'	2.47	0.47
34:YA:958:U:O2	35:YB:89(B):A:O2'	2.25	0.47
47:YS:11:LYS:HG3	47:YS:15:ARG:HE	1.80	0.47
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.46	0.47
17:QQ:83:ASP:OD1	17:QQ:83:ASP:N	2.47	0.47
33:R9:11:CYS:N	33:R9:14:CYS:SG	2.83	0.47
34:RA:2118:U:H3	34:RA:2148:G:H4'	1.80	0.47
34:RA:2096:U:H3	34:RA:2193:G:H1	1.61	0.47
34:RA:2749:A:H3'	34:RA:2750:A:H2'	1.96	0.47
34:RA:978:G:N1	34:RA:986:C:N3	2.62	0.47
52:RX:64:LYS:HD2	52:RX:73:ARG:HH12	1.77	0.47
22:XV:19:G:OP1	22:XV:20:G:N2	2.48	0.47
34:YA:2589:A:N1	34:YA:2606:C:N4	2.63	0.47
36:YD:35:LYS:HG3	36:YD:63:ARG:HG3	1.96	0.47
34:YA:586:A:H5'	38:YF:89:VAL:HG21	1.96	0.47
43:YO:120:GLU:OE1	48:YT:67:SER:OG	2.33	0.47
1:QA:1035:A:H2'	1:QA:1036:G:H8	1.80	0.47
1:QA:1237:C:H5''	1:QA:1238:A:C8	2.50	0.47
1:QA:749:C:H2'	1:QA:750:G:H8	1.80	0.47
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.47	0.47
16:QP:21:VAL:HG23	16:QP:33:ILE:HB	1.96	0.47
17:QQ:62:SER:OG	17:QQ:72:ARG:NE	2.47	0.47
1:QA:1329:A:H62	21:QU:7:ARG:HH12	1.62	0.47
34:RA:2150:U:H2'	34:RA:2151:G:H8	1.79	0.47
34:RA:2852:G:O6	34:RA:2865:U:O4	2.32	0.47
1:XA:1028(H):G:H2'	1:XA:1028(I):G:C8	2.50	0.47
1:XA:413:G:H21	1:XA:428:G:H1'	1.79	0.47
1:XA:427:U:O2'	1:XA:541:G:OP1	2.29	0.47
2:XB:184:VAL:HG23	2:XB:198:ASP:H	1.79	0.47
34:YA:1058:G:H2'	34:YA:1059:G:H8	1.80	0.47
34:YA:1728:G:H8	34:YA:1732:A:H62	1.62	0.47
34:YA:2584:U:H2'	34:YA:2585:U:H2'	1.96	0.47
34:YA:2611:U:C5'	34:YA:2611:U:C6	2.86	0.47
34:YA:422:A:O5'	34:YA:422:A:H8	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YH:18:GLU:HB3	40:YH:25:LYS:HG2	1.96	0.47
41:YI:20:ASP:N	41:YI:20:ASP:OD2	2.43	0.47
1:QA:316:G:OP2	1:QA:351:G:O2'	2.31	0.47
1:QA:542:G:O3'	4:QD:14:ARG:NH2	2.48	0.47
1:QA:982:U:H5''	14:QN:6:LEU:HD11	1.96	0.47
10:QJ:67:THR:O	10:QJ:67:THR:OG1	2.32	0.47
15:QO:26:GLU:HA	15:QO:29:VAL:HG12	1.97	0.47
40:RH:6:ARG:HE	40:RH:65:HIS:HB3	1.80	0.47
41:RI:83:ALA:C	41:RI:89:TYR:CE2	2.88	0.47
34:RA:2377:A:H4'	47:RS:112:PHE:HA	1.97	0.47
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.79	0.47
1:XA:942:G:N2	9:XI:124:GLN:OE1	2.44	0.47
13:XM:14:ARG:HG2	13:XM:16:ASP:H	1.79	0.47
14:XN:23:ARG:NH1	14:XN:28:GLY:HA2	2.29	0.47
28:Y4:23:GLU:O	28:Y4:25:TYR:N	2.46	0.47
34:YA:1779:U:OP2	34:YA:1784:A:N6	2.43	0.47
34:YA:2011:U:OP2	51:YW:16:LYS:NZ	2.35	0.47
34:YA:380:U:H2'	34:YA:381:G:H8	1.80	0.47
34:YA:223:A:O2'	34:YA:420:C:O2	2.25	0.47
38:YF:157:VAL:HG13	38:YF:194:MET:HB3	1.97	0.47
6:QF:24:GLU:OE1	6:QF:28:ARG:NH1	2.48	0.47
8:QH:108:GLY:HA3	8:QH:138:TRP:HB3	1.97	0.47
25:R1:2:SER:O	25:R1:61:ARG:NH1	2.47	0.47
34:RA:2249:U:N3	34:RA:2253:G:OP2	2.48	0.47
34:RA:414:C:O2	34:RA:1864:U:O2'	2.30	0.47
1:XA:925:G:O6	1:XA:1391:U:O4	2.33	0.47
1:XA:1525:G:OP1	11:XK:120:ARG:NH1	2.41	0.47
1:XA:967:C:O3'	9:XI:125:TYR:OH	2.27	0.47
12:XL:12:ARG:HH21	12:XL:13:LYS:HE3	1.79	0.47
17:XQ:21:VAL:N	17:XQ:42:TYR:O	2.40	0.47
22:XV:76:A:N6	34:YA:2422:A:O4'	2.47	0.47
34:YA:363(A):G:H2'	34:YA:363(B):A:H8	1.79	0.47
34:YA:238:C:O2'	34:YA:608:A:N3	2.34	0.47
34:YA:635:C:O2'	34:YA:639:U:OP1	2.29	0.47
38:YF:12:LEU:HB3	38:YF:126:VAL:HG12	1.95	0.47
1:QA:1048:G:O2'	1:QA:1050:G:OP1	2.34	0.46
2:QB:134:GLU:HA	2:QB:137:ARG:HG2	1.96	0.46
4:QD:156:GLU:O	4:QD:160:GLN:N	2.48	0.46
1:QA:1298:C:N4	7:QG:113:GLU:O	2.48	0.46
8:QH:91:ARG:NE	17:QQ:32:TYR:O	2.40	0.46
22:QV:37:1MG:C8	22:QV:38:A:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1102:C:H2'	34:RA:1103:A:H8	1.79	0.46
34:RA:1783:A:OP1	34:RA:1784:A:OP2	2.33	0.46
34:RA:659:C:H2'	34:RA:660:G:C8	2.49	0.46
34:RA:956:G:OP2	45:RQ:14:ARG:NH2	2.36	0.46
35:RB:15:A:H5'	35:RB:16:G:C8	2.49	0.46
37:RE:24:THR:HG21	37:RE:188:VAL:HG22	1.97	0.46
40:RH:11:VAL:HG12	40:RH:13:LYS:HG2	1.97	0.46
51:RW:68:ARG:NH2	51:RW:109:GLU:OE2	2.48	0.46
1:XA:1127:G:N2	1:XA:1145:C:O2	2.47	0.46
4:XD:18:LYS:HZ3	4:XD:33:MET:HG3	1.80	0.46
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.62	0.46
12:XL:8:ASN:O	12:XL:12:ARG:HB2	2.15	0.46
33:Y9:14:CYS:CA	33:Y9:27:CYS:HB2	2.44	0.46
22:XV:19:G:H2'	34:YA:2112:G:C6	2.50	0.46
34:YA:963:U:H1'	34:YA:2250:G:O6	2.15	0.46
34:YA:28:A:O2'	34:YA:582:G:O2'	2.30	0.46
42:YN:16:ILE:HG21	42:YN:26:LEU:HD11	1.97	0.46
1:QA:1004:A:N6	1:QA:1025:U:O3'	2.47	0.46
1:QA:407:G:H5'	4:QD:115:ARG:HH21	1.80	0.46
7:QG:70:LYS:HB2	7:QG:96:GLN:HB3	1.97	0.46
16:QP:40:ASP:OD1	16:QP:43:LYS:N	2.46	0.46
34:RA:144:C:H2'	34:RA:145:G:H8	1.80	0.46
34:RA:2151:G:H2'	34:RA:2152:G:H8	1.81	0.46
34:RA:2153:G:H2'	34:RA:2154:G:H8	1.80	0.46
34:RA:2185:C:H2'	34:RA:2186:G:C8	2.51	0.46
40:RH:126:PRO:HG2	40:RH:130:ARG:HG3	1.96	0.46
52:RX:72:LYS:NZ	52:RX:73:ARG:O	2.38	0.46
1:XA:1419:G:H1	1:XA:1481:U:H3	1.62	0.46
1:XA:413:G:H4'	1:XA:414:A:H5''	1.97	0.46
1:XA:673:G:H2'	1:XA:674:G:C8	2.51	0.46
2:XB:188:ALA:HB3	2:XB:200:ILE:HD11	1.97	0.46
16:XP:20:VAL:HG12	16:XP:35:LYS:HA	1.97	0.46
34:YA:373:U:H1'	34:YA:423:A:N3	2.30	0.46
31:Y7:33:ARG:NH1	34:YA:467:G:OP1	2.47	0.46
34:YA:805:G:N2	34:YA:829:A:OP1	2.47	0.46
41:YI:72:LEU:HD12	41:YI:138:ILE:HD12	1.97	0.46
34:YA:296:C:O3'	53:YY:95:LYS:NZ	2.48	0.46
1:QA:1097:C:O2'	1:QA:1169:A:N3	2.37	0.46
1:QA:976:G:N1	1:QA:1362(B):C:OP2	2.37	0.46
1:QA:75:C:H42	1:QA:95:G:H1	1.62	0.46
34:RA:1070:A:O2'	34:RA:1097:U:O3'	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:630:G:N2	34:RA:633:A:OP2	2.35	0.46
34:RA:979:G:N2	34:RA:985:C:C4	2.84	0.46
38:RF:24:LEU:HD12	38:RF:115:ALA:HB2	1.96	0.46
40:RH:123:PHE:HE2	40:RH:133:VAL:HG22	1.80	0.46
46:RR:28:LEU:HD23	46:RR:48:VAL:HG21	1.98	0.46
54:RZ:182:LYS:HD2	54:RZ:182:LYS:HA	1.75	0.46
1:XA:186(F):C:N3	1:XA:186(N):G:N2	2.63	0.46
7:XG:75:VAL:HA	7:XG:87:VAL:O	2.16	0.46
34:YA:2152:G:H2'	34:YA:2153:G:C8	2.49	0.46
34:YA:840:C:H2'	34:YA:841:A:H8	1.79	0.46
38:YF:60:SER:OG	38:YF:61:GLY:N	2.49	0.46
1:QA:1000:A:N1	1:QA:1041:A:N6	2.64	0.46
1:QA:1227:A:OP1	19:QS:80:TYR:OH	2.30	0.46
1:QA:599:C:O2'	8:QH:129:VAL:O	2.27	0.46
9:QI:28:VAL:HA	9:QI:63:ILE:HB	1.97	0.46
22:QV:61:C:H2'	22:QV:62:C:H6	1.80	0.46
25:R1:90:ILE:HA	25:R1:94:LEU:HD11	1.93	0.46
29:R5:12:SER:HB3	34:RA:2020:A:H5'	1.97	0.46
34:RA:1657:C:H2'	34:RA:1658:C:H6	1.80	0.46
32:R8:30:ARG:HH21	44:RP:62:LEU:HD12	1.81	0.46
1:XA:165:C:H2'	1:XA:166:G:C8	2.51	0.46
1:XA:6:G:H2'	5:XE:119:LEU:HD21	1.98	0.46
1:XA:948:C:H2'	1:XA:949:A:H8	1.80	0.46
1:XA:979:C:O2	14:XN:19:ARG:NH2	2.40	0.46
1:XA:640:A:O2'	8:XH:116:LYS:NZ	2.49	0.46
8:XH:86:ILE:HD12	8:XH:135:CYS:HA	1.97	0.46
34:YA:1753:G:N2	34:YA:1758:G:N7	2.62	0.46
34:YA:2403:C:N3	34:YA:2415:G:C2	2.83	0.46
34:YA:309:G:N3	34:YA:329:G:O2'	2.47	0.46
34:YA:363(C):G:H2'	34:YA:363(D):G:H8	1.80	0.46
34:YA:974(A):G:C6	34:YA:1186:G:N1	2.84	0.46
34:YA:984:A:H5''	34:YA:985:C:H5	1.81	0.46
44:YP:98:GLU:HA	44:YP:101:VAL:HG12	1.96	0.46
1:QA:186(H):C:O2	1:QA:186(L):G:N1	2.49	0.46
1:QA:324:G:N2	1:QA:327:A:OP2	2.48	0.46
1:QA:707:C:H2'	1:QA:708:C:H6	1.81	0.46
1:QA:898:G:N2	1:QA:901:A:OP2	2.45	0.46
3:QC:66:VAL:HB	3:QC:101:LEU:HG	1.98	0.46
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.97	0.46
9:QI:105:ASP:HB3	9:QI:107:ARG:HE	1.80	0.46
26:R2:48:HIS:ND1	34:RA:95:G:O2'	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R5:57:VAL:O	46:RR:33:ARG:NH1	2.39	0.46
34:RA:1363:C:O2'	34:RA:1809:A:N3	2.39	0.46
34:RA:2195:C:H2'	34:RA:2196:C:H6	1.80	0.46
1:XA:186(F):C:H42	1:XA:186(N):G:H1	1.61	0.46
10:XJ:78:ASN:HB2	10:XJ:81:THR:HG23	1.97	0.46
17:XQ:34:LYS:NZ	17:XQ:35:VAL:O	2.46	0.46
34:YA:1669:A:N3	34:YA:1669:A:C2'	2.78	0.46
34:YA:589:C:H2'	34:YA:590:A:C8	2.50	0.46
38:YF:41:LEU:HA	38:YF:44:ARG:HG2	1.98	0.46
1:QA:359:U:H2'	1:QA:360:A:H8	1.79	0.46
1:QA:410:G:H21	1:QA:432:A:H62	1.62	0.46
1:QA:628:G:H2'	1:QA:629:G:H8	1.80	0.46
1:QA:663:A:N6	1:QA:742:G:H1	2.10	0.46
8:QH:121:ASP:OD2	8:QH:125:ARG:NH1	2.48	0.46
1:QA:972:C:H4'	10:QJ:57:LYS:HB2	1.98	0.46
13:QM:91:ARG:HD2	13:QM:96:LEU:HB3	1.98	0.46
34:RA:1181:C:H2'	34:RA:1182:A:C8	2.49	0.46
34:RA:1316:U:H2'	34:RA:1317:A:H8	1.80	0.46
34:RA:2845:G:H2'	34:RA:2846:G:C8	2.51	0.46
34:RA:2882:A:OP1	46:RR:96:ARG:NH1	2.47	0.46
41:RI:88:ILE:HG22	41:RI:90:GLY:N	2.31	0.46
1:XA:1071:C:OP1	5:XE:27:ARG:NH2	2.49	0.46
1:XA:36:C:O2'	1:XA:501:C:OP1	2.33	0.46
1:XA:737:A:H2'	1:XA:738:C:C6	2.50	0.46
13:XM:59:TYR:O	13:XM:63:THR:OG1	2.25	0.46
34:YA:1363:C:O2'	34:YA:1809:A:N3	2.38	0.46
34:YA:2404:C:O3'	44:YP:77:ARG:NH2	2.49	0.46
34:YA:517:C:O2'	51:YW:18:ARG:NH2	2.48	0.46
40:YH:89:ILE:HD11	40:YH:94:TYR:HB3	1.98	0.46
2:QB:101:MET:HA	2:QB:108:ILE:HG13	1.97	0.46
13:QM:47:ASP:N	13:QM:47:ASP:OD1	2.48	0.46
34:RA:1543:A:H1'	34:RA:1545(A):A:H5''	1.97	0.46
34:RA:65:C:H1'	34:RA:456:C:H42	1.81	0.46
34:RA:971:C:O2'	34:RA:983:A:N3	2.38	0.46
37:RE:14:ILE:HD11	37:RE:173:VAL:HG11	1.97	0.46
38:RF:56:GLU:OE2	38:RF:93:LYS:NZ	2.49	0.46
49:RU:27:LEU:HD22	49:RU:31:SER:HB2	1.97	0.46
1:XA:1014:A:H2'	1:XA:1015:A:C8	2.50	0.46
1:XA:444:C:H2'	1:XA:445:G:H8	1.81	0.46
22:XV:1:C:H2'	22:XV:2:G:H8	1.81	0.46
34:YA:1652:A:N6	34:YA:1653:G:H1	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1255:U:N3	34:YA:2060:A:OP2	2.44	0.46
35:YB:73:A:N6	35:YB:103:U:H3	2.04	0.46
42:YN:47:ALA:HB2	42:YN:112:LEU:HD11	1.98	0.46
43:YO:78:ARG:NE	48:YT:73:GLU:OE1	2.45	0.46
1:QA:359:U:H2'	1:QA:360:A:C8	2.51	0.46
9:QI:26:VAL:HG12	9:QI:61:ALA:HB3	1.98	0.46
10:QJ:48:THR:HG22	10:QJ:62:HIS:HB3	1.98	0.46
20:QT:54:LYS:HZ3	20:QT:57:ARG:HE	1.64	0.46
32:R8:29:LYS:O	32:R8:31:HIS:N	2.45	0.46
34:RA:16:G:C6	34:RA:525:U:N3	2.84	0.46
34:RA:2812:G:H2'	34:RA:2813:A:H8	1.81	0.46
37:RE:14:ILE:HB	48:RT:14:TYR:HE2	1.81	0.46
34:RA:2635:C:O2'	37:RE:80:GLU:OE1	2.26	0.46
38:RF:182:ASN:N	38:RF:182:ASN:OD1	2.46	0.46
40:RH:84:SER:HA	40:RH:134:SER:HA	1.97	0.46
2:XB:118:LEU:HB3	2:XB:142:LEU:HD13	1.98	0.46
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.49	0.46
13:XM:45:VAL:HG23	13:XM:48:LEU:HD12	1.98	0.46
26:Y2:28:LYS:HD3	26:Y2:28:LYS:HA	1.77	0.46
34:YA:1953:A:O2'	34:YA:2559:C:O2	2.28	0.46
40:YH:137:ASP:OD2	40:YH:138:LYS:N	2.48	0.46
43:YO:64:ARG:HB2	43:YO:83:ALA:HB3	1.98	0.46
54:YZ:74:VAL:HG22	54:YZ:86:VAL:HG23	1.97	0.46
1:QA:864:A:O2'	1:QA:1078:U:O4	2.26	0.46
1:QA:1463:C:H5''	48:RT:112:ARG:HE	1.79	0.46
1:QA:373:A:H61	1:QA:391:G:H1'	1.80	0.46
1:QA:593:G:H1	1:QA:646:U:H3	1.64	0.46
1:QA:710:G:H2'	1:QA:711:G:H8	1.80	0.46
1:QA:883:C:N4	1:QA:884:U:O4	2.49	0.46
3:QC:184:TYR:HA	3:QC:200:ALA:O	2.15	0.46
16:QP:59:TRP:HA	16:QP:62:VAL:HG22	1.97	0.46
34:RA:1247:A:N1	34:RA:1249:U:C2	2.81	0.46
43:RO:104:ARG:NH2	48:RT:43:GLN:OE1	2.49	0.46
52:RX:90:GLU:HA	52:RX:93:GLU:HG2	1.97	0.46
54:RZ:67:LEU:HD13	54:RZ:68:PRO:HD2	1.96	0.46
1:XA:581:G:OP1	15:XO:65:ARG:NH1	2.33	0.46
2:XB:175:ARG:HH22	2:XB:179:LYS:HZ1	1.64	0.46
12:XL:53:ARG:HB3	12:XL:69:TYR:HE1	1.79	0.46
31:Y7:7:PRO:HA	34:YA:686:G:H8	1.80	0.46
34:YA:1891:G:O2'	34:YA:2235:G:O2'	2.32	0.46
34:YA:2314:C:H2'	34:YA:2315:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:YX:64:LYS:HZ2	52:YX:73:ARG:HE	1.63	0.46
1:QA:1385:G:H2'	1:QA:1386:G:H8	1.81	0.46
1:QA:157:G:H2'	1:QA:158:G:H8	1.81	0.46
5:QE:98:THR:N	5:QE:117:ASP:OD1	2.40	0.46
13:QM:26:GLY:O	13:QM:30:ALA:HB2	2.15	0.46
25:R1:90:ILE:CA	25:R1:94:LEU:CD1	2.84	0.46
34:RA:1048:A:N6	34:RA:1111:A:N3	2.64	0.46
34:RA:2514:U:H3	34:RA:2570:G:H1	1.63	0.46
37:RE:46:ALA:HB1	37:RE:80:GLU:HG2	1.98	0.46
34:RA:2310:A:N6	39:RG:79:ASN:HD22	2.14	0.46
46:RR:38:VAL:HG12	46:RR:112:ALA:HB2	1.96	0.46
1:XA:448:A:OP2	1:XA:485:G:N1	2.39	0.46
1:XA:603:U:H2'	1:XA:604:G:H8	1.80	0.46
1:XA:806:C:H2'	1:XA:807:A:H8	1.80	0.46
11:XK:31:THR:HA	11:XK:42:TRP:HA	1.97	0.46
21:XU:6:ARG:HH21	21:XU:15:ARG:HH22	1.64	0.46
41:YI:4:ILE:HG22	41:YI:18:VAL:HB	1.98	0.46
48:YT:91:ARG:NH2	48:YT:124:ASP:OD2	2.48	0.46
1:QA:666:G:H1	1:QA:740:U:H3	1.62	0.45
1:QA:949:A:HO2'	1:QA:971:G:H1	1.64	0.45
2:QB:73:THR:O	2:QB:75:LYS:NZ	2.50	0.45
5:QE:87:SER:OG	5:QE:125:SER:O	2.32	0.45
11:QK:57:THR:HG23	11:QK:60:ALA:H	1.81	0.45
1:QA:657:G:H4'	15:QO:28:GLN:HG2	1.97	0.45
18:QR:74:ARG:HD3	18:QR:81:PHE:HA	1.98	0.45
34:RA:2037:G:H2'	34:RA:2038:G:C8	2.51	0.45
34:RA:2618:G:H21	37:RE:150:VAL:HG21	1.80	0.45
34:RA:271(E):G:H2'	34:RA:272:G:H8	1.80	0.45
34:RA:414:C:H2'	34:RA:415:A:H8	1.81	0.45
34:RA:1654:A:O2'	37:RE:113:PHE:O	2.19	0.45
51:RW:86:LEU:HD22	51:RW:96:ILE:HD11	1.98	0.45
35:RB:74:U:H1'	54:RZ:34:ASN:HD21	1.81	0.45
1:XA:407:G:O2'	4:XD:116:GLN:OE1	2.33	0.45
1:XA:264:U:O2'	17:XQ:64:PRO:O	2.31	0.45
34:YA:597:U:H2'	34:YA:598:G:H8	1.81	0.45
45:YQ:133:ARG:HG3	45:YQ:134:ARG:H	1.80	0.45
48:YT:16:ARG:HH21	48:YT:81:PRO:HA	1.80	0.45
1:QA:1250:A:N3	1:QA:1370:G:O2'	2.44	0.45
1:QA:922:G:H2'	1:QA:923:A:C8	2.52	0.45
10:QJ:12:ASP:O	10:QJ:16:LEU:HB3	2.16	0.45
9:QI:114:TYR:HB2	10:QJ:60:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R0:43:THR:HG21	34:RA:2336:A:H61	1.81	0.45
34:RA:1147:C:H2'	34:RA:1148:A:C8	2.51	0.45
34:RA:513:A:O2'	34:RA:1217:C:OP1	2.30	0.45
34:RA:81:G:HO2'	34:RA:295:G:HO2'	1.50	0.45
39:RG:68:PRO:HB3	39:RG:92:VAL:HB	1.98	0.45
1:XA:1124:G:O2'	1:XA:1126:U:O4	2.28	0.45
2:XB:68:ILE:HG22	2:XB:161:ALA:HB3	1.98	0.45
34:YA:1174:A:H2	34:YA:1176:G:H4'	1.81	0.45
34:YA:1612:C:N3	34:YA:1620:G:N1	2.65	0.45
34:YA:2315:G:OP1	39:YG:36:LYS:NZ	2.40	0.45
34:YA:2730:C:O2'	37:YE:168:MET:O	2.32	0.45
44:YP:96:THR:HG22	44:YP:99:LEU:HD22	1.98	0.45
49:YU:90:VAL:HG22	50:YV:39:LEU:HB3	1.98	0.45
1:QA:1177:G:H2'	1:QA:1178:G:C4	2.51	0.45
4:QD:22:LYS:HG3	56:QD:301:SF4:S1	2.56	0.45
11:QK:101:SER:OG	11:QK:101:SER:O	2.30	0.45
15:QO:39:LEU:HD22	15:QO:56:LEU:HD13	1.97	0.45
34:RA:2463:C:C2	34:RA:2488:A:H2	2.35	0.45
34:RA:2722:G:H5''	34:RA:2820:A:N7	2.31	0.45
34:RA:589:C:H2'	34:RA:590:A:C8	2.52	0.45
1:XA:881:G:P	12:XL:12:ARG:HH22	2.40	0.45
2:XB:207:ALA:O	2:XB:210:SER:OG	2.28	0.45
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.98	0.45
34:YA:2151:G:H2'	34:YA:2152:G:H8	1.80	0.45
34:YA:2641:G:H5''	42:YN:76:SER:HB3	1.97	0.45
36:YD:133:LEU:HD23	36:YD:136:ILE:HD12	1.98	0.45
46:YR:33:ARG:HA	46:YR:114:VAL:O	2.17	0.45
1:QA:28:G:O2'	1:QA:296:U:OP1	2.31	0.45
1:QA:370:C:H2'	1:QA:371:G:C8	2.51	0.45
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.82	0.45
13:QM:108:ARG:HA	13:QM:111:LYS:HB2	1.97	0.45
34:RA:2308:G:H22	34:RA:2311:A:H2	1.64	0.45
34:RA:665:C:H2'	34:RA:666:G:H8	1.81	0.45
36:RD:247:ALA:HA	36:RD:253:GLN:HA	1.98	0.45
43:RO:63:VAL:HB	43:RO:102:VAL:HG13	1.98	0.45
49:RU:45:TYR:O	49:RU:49:HIS:ND1	2.49	0.45
1:XA:1304:G:OP1	21:XU:2:GLY:N	2.50	0.45
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.82	0.45
1:XA:603:U:H2'	1:XA:604:G:C8	2.51	0.45
2:XB:27:LYS:HD2	2:XB:193:ASP:HB2	1.97	0.45
4:XD:162:LEU:HD12	4:XD:178:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:46:LYS:HG3	12:XL:48:PRO:HD2	1.98	0.45
15:XO:64:ARG:HH12	15:XO:68:ARG:HH22	1.63	0.45
1:QA:1347:G:O2'	1:QA:1373:G:O6	2.33	0.45
1:QA:165:C:H2'	1:QA:166:G:H8	1.81	0.45
1:QA:99:C:H2'	1:QA:101:A:C8	2.51	0.45
34:RA:1230:C:H2'	34:RA:1231:G:H8	1.82	0.45
34:RA:809:G:H2'	34:RA:810:U:C6	2.51	0.45
34:RA:890:A:H2'	34:RA:892:G:H8	1.82	0.45
36:RD:13:ARG:NH1	36:RD:16:MET:SD	2.90	0.45
35:RB:7:G:H21	47:RS:38:GLN:HE22	1.64	0.45
53:RY:28:LYS:HG3	53:RY:40:GLU:HG2	1.99	0.45
1:XA:34:C:H2'	1:XA:35:G:H8	1.81	0.45
1:XA:595:G:H1'	1:XA:596:C:H5	1.81	0.45
4:XD:30:LYS:HB3	4:XD:35:ARG:HH22	1.81	0.45
20:XT:11:SER:OG	20:XT:11:SER:O	2.28	0.45
36:YD:71:ASP:HB2	36:YD:103:ARG:HH12	1.82	0.45
38:YF:155:LEU:HB2	38:YF:189:THR:HG21	1.99	0.45
1:QA:947:G:HO2'	1:QA:1306:A:HO2'	1.59	0.45
1:QA:244:U:H3	1:QA:893:C:H42	1.64	0.45
2:QB:233:SER:OG	2:QB:233:SER:O	2.34	0.45
34:RA:172:C:H2'	34:RA:173:G:C8	2.52	0.45
34:RA:581:C:H2'	34:RA:582:G:C8	2.51	0.45
34:RA:626:U:H5'	34:RA:627:A:H5''	1.97	0.45
36:RD:132:PRO:HA	36:RD:190:TYR:HA	1.99	0.45
41:RI:123:LEU:HD12	41:RI:142:VAL:HG13	1.98	0.45
34:RA:2641:G:P	42:RN:74:ARG:HE	2.39	0.45
50:RV:14:VAL:HB	50:RV:96:ILE:HG12	1.98	0.45
51:RW:76:VAL:HG22	51:RW:103:ILE:HG23	1.98	0.45
1:XA:1128:C:O2'	1:XA:1130:A:N7	2.50	0.45
1:XA:1151:A:H2'	1:XA:1152:A:H8	1.82	0.45
1:XA:269:C:H2'	1:XA:270:A:C8	2.52	0.45
1:XA:327:A:O2'	1:XA:328:C:O4'	2.29	0.45
4:XD:21:LEU:N	4:XD:26:CYS:SG	2.89	0.45
33:Y9:25:VAL:HG22	33:Y9:34:GLN:HB3	1.98	0.45
34:YA:122:G:OP1	34:YA:149:A:O2'	2.31	0.45
34:YA:1636:C:H2'	34:YA:1637:A:C8	2.51	0.45
34:YA:1657:C:H2'	34:YA:1658:C:C6	2.51	0.45
34:YA:606:U:OP2	38:YF:104:LYS:NZ	2.43	0.45
38:YF:54:ARG:HD2	38:YF:81:PRO:HD3	1.98	0.45
45:YQ:13:GLN:O	45:YQ:72:LYS:NZ	2.38	0.45
49:YU:8:VAL:HG22	49:YU:12:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:YW:46:PHE:O	51:YW:50:VAL:HG23	2.16	0.45
35:YB:104:A:OP1	54:YZ:72:ARG:NH1	2.49	0.45
1:QA:1174:G:H2'	1:QA:1175:G:H8	1.81	0.45
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.51	0.45
1:QA:950:U:H3	1:QA:1231:G:H1	1.65	0.45
4:QD:85:LYS:HD2	4:QD:85:LYS:HA	1.73	0.45
32:R8:13:ARG:HD2	44:RP:61:ARG:HE	1.81	0.45
34:RA:1400:G:H2'	34:RA:1401:G:H8	1.81	0.45
34:RA:1789:A:H5''	36:RD:221:VAL:HA	1.99	0.45
34:RA:249:C:O5'	34:RA:2394:C:O2'	2.35	0.45
36:RD:208:LYS:HG3	36:RD:210:GLY:H	1.82	0.45
48:RT:102:ILE:HD12	48:RT:110:ILE:HD12	1.99	0.45
1:XA:125:U:H2'	1:XA:126:G:C8	2.52	0.45
1:XA:619:U:H5'	4:XD:131:ARG:HH21	1.82	0.45
4:XD:43:HIS:HB3	4:XD:46:LYS:HD2	1.98	0.45
7:XG:139:GLU:OE1	7:XG:143:ARG:NH2	2.49	0.45
7:XG:26:PHE:O	7:XG:30:ILE:HG12	2.17	0.45
8:XH:121:ASP:HB2	8:XH:125:ARG:HH21	1.82	0.45
12:XL:110:VAL:H	12:XL:122:THR:HG22	1.82	0.45
25:Y1:40:ARG:HG2	25:Y1:41:ARG:H	1.81	0.45
28:Y4:5:ILE:N	28:Y4:5:ILE:CD1	2.79	0.45
34:YA:1682:G:OP2	34:YA:1699:G:N2	2.44	0.45
34:YA:172:C:H2'	34:YA:173:G:C8	2.52	0.45
34:YA:2162:G:H2'	34:YA:2163:C:C2	2.52	0.45
34:YA:748:G:C8	34:YA:750:A:N7	2.85	0.45
42:YN:137:LYS:HD3	42:YN:138:LEU:HG	1.99	0.45
42:YN:91:LEU:HD23	42:YN:91:LEU:HA	1.81	0.45
48:YT:54:ARG:HA	48:YT:59:THR:HG23	1.99	0.45
49:YU:17:ILE:HG13	49:YU:32:PHE:HE1	1.82	0.45
1:QA:1338:G:H21	22:QV:41:A:H1'	1.80	0.45
34:RA:1608:A:C8	34:RA:1611:C:N4	2.84	0.45
34:RA:1689:A:H2'	34:RA:1690:A:H8	1.82	0.45
34:RA:2448:A:OP1	34:RA:2499:C:OP1	2.34	0.45
34:RA:1662:C:O2'	34:RA:2687:U:OP1	2.34	0.45
34:RA:65:C:H5'	52:RX:71:GLY:HA3	1.98	0.45
37:RE:111:ARG:HD3	37:RE:160:TYR:CE2	2.52	0.45
39:RG:81:LYS:HA	39:RG:81:LYS:HD2	1.74	0.45
40:RH:124:GLU:O	40:RH:124:GLU:HG3	2.17	0.45
40:RH:98:LEU:CG	40:RH:125:VAL:CG1	2.91	0.45
50:RV:68:LYS:HA	50:RV:68:LYS:HD2	1.70	0.45
54:RZ:54:HIS:HB3	54:RZ:101:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:985:C:H2'	1:XA:986:A:C8	2.51	0.45
24:Y0:41:ARG:O	34:YA:2330:G:N2	2.47	0.45
34:YA:2031:A:O2'	34:YA:2454:G:N2	2.49	0.45
35:YB:14:U:O3'	35:YB:107:U:O2'	2.29	0.45
37:YE:171:GLU:HB2	37:YE:185:LYS:HG3	1.98	0.45
1:QA:62:U:O4	1:QA:105:G:O6	2.35	0.45
1:QA:765:G:N1	1:QA:812:C:O2'	2.44	0.45
16:QP:4:ILE:HD13	16:QP:21:VAL:HG12	1.97	0.45
17:QQ:59:ILE:HG22	17:QQ:73:VAL:HA	1.98	0.45
31:R7:18:PHE:HB2	31:R7:43:THR:HG21	1.99	0.45
34:RA:1518:C:H2'	34:RA:1519:G:H8	1.82	0.45
34:RA:1687:G:N2	34:RA:1702:G:O6	2.50	0.45
34:RA:1838:C:O2	34:RA:1898:U:C4	2.70	0.45
34:RA:1939:U:OP1	34:RA:2604:U:O2'	2.35	0.45
34:RA:2099:U:H2'	34:RA:2100:G:C8	2.51	0.45
39:RG:161:THR:HG22	39:RG:163:ALA:H	1.82	0.45
41:RI:80:PRO:HB2	41:RI:146:ALA:HB2	1.97	0.45
43:RO:106:LEU:HA	43:RO:109:LYS:HB2	1.99	0.45
48:RT:118:ARG:HH11	48:RT:121:ILE:HG21	1.81	0.45
53:RY:28:LYS:NZ	53:RY:40:GLU:OE2	2.38	0.45
1:XA:977:A:O2'	1:XA:979:C:OP2	2.28	0.45
1:XA:778:G:H21	11:XK:120:ARG:HB3	1.81	0.45
1:XA:1228:C:P	13:XM:108:ARG:HH12	2.40	0.45
27:Y3:23:LEU:HD12	27:Y3:28:LEU:HB2	1.98	0.45
36:YD:44:ASN:HB3	36:YD:49:ILE:HG22	1.98	0.45
34:YA:2032:G:N2	37:YE:146:THR:OG1	2.48	0.45
1:QA:1095:U:P	1:QA:1108:G:H1	2.40	0.45
1:QA:382:A:H2'	1:QA:383:A:H8	1.81	0.45
2:QB:193:ASP:OD2	2:QB:193:ASP:N	2.50	0.45
3:QC:24:ALA:HB1	3:QC:32:LEU:HD21	1.99	0.45
3:QC:6:HIS:HE1	3:QC:8:ILE:HD12	1.82	0.45
6:QF:12:PRO:HD3	6:QF:58:GLY:HA2	1.99	0.45
33:R9:35:ARG:NH2	34:RA:2539:C:O2'	2.49	0.45
39:RG:81:LYS:HB3	39:RG:82:LEU:H	1.59	0.45
40:RH:126:PRO:HG2	40:RH:130:ARG:CG	2.46	0.45
41:RI:79:ILE:HG23	41:RI:142:VAL:HA	1.99	0.45
1:XA:1342:C:H2'	1:XA:1343:G:C8	2.52	0.45
1:XA:186(M):G:H2'	1:XA:186(N):G:C8	2.52	0.45
1:XA:68(C):G:H1	1:XA:68(Y):U:H3	1.64	0.45
1:XA:741:G:H5'	1:XA:742:G:OP2	2.17	0.45
1:XA:985:C:H2'	1:XA:986:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:XS:53:ASN:ND2	19:XS:76:PRO:O	2.48	0.45
27:Y3:40:THR:HB	27:Y3:43:ILE:HG12	1.98	0.45
1:QA:237:C:H2'	1:QA:238:G:C8	2.51	0.44
1:QA:685:G:N1	1:QA:704:A:OP2	2.41	0.44
8:QH:112:LEU:HD11	8:QH:133:LEU:HD12	1.99	0.44
33:R9:19:ARG:NH2	34:RA:2754:U:O3'	2.50	0.44
34:RA:1127:A:N7	34:RA:2488:A:O2'	2.45	0.44
34:RA:139:G:C2	34:RA:141(A):A:C6	3.04	0.44
34:RA:18:C:O2'	34:RA:553:U:OP1	2.33	0.44
34:RA:2342:C:O2'	34:RA:2374:C:OP1	2.33	0.44
34:RA:2687:U:H3	34:RA:2722:G:H1	1.66	0.44
36:RD:95:LEU:HB2	36:RD:103:ARG:O	2.17	0.44
37:RE:32:PRO:HA	37:RE:90:THR:HA	1.99	0.44
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.36	0.44
1:XA:1414:U:H2'	1:XA:1415:G:C8	2.50	0.44
2:XB:33:TYR:HB2	2:XB:43:ASP:HB2	1.99	0.44
12:XL:24:VAL:HG13	12:XL:98:TYR:HE1	1.82	0.44
32:Y8:42:ARG:NH2	34:YA:2382:G:H21	2.14	0.44
33:Y9:27:CYS:SG	33:Y9:29:ASN:HB3	2.57	0.44
34:YA:1499:C:H2'	34:YA:1500:G:H8	1.82	0.44
34:YA:1266:G:O2'	34:YA:2012:G:O6	2.22	0.44
34:YA:2402:C:C6	34:YA:2402:C:C5'	2.97	0.44
34:YA:2809:A:H2'	34:YA:2810:A:C8	2.52	0.44
34:YA:775:G:H4'	34:YA:776:G:H5'	1.98	0.44
34:YA:783:A:H8	34:YA:784:A:H4'	1.82	0.44
43:YO:44:LYS:HD3	43:YO:44:LYS:HA	1.72	0.44
54:YZ:5:LEU:HB2	54:YZ:59:LEU:HD12	1.98	0.44
1:QA:166:G:H2'	1:QA:167:G:H8	1.82	0.44
1:QA:37:U:HO2'	1:QA:500:G:HO2'	1.64	0.44
1:QA:647:C:H2'	1:QA:648:A:H8	1.81	0.44
1:QA:948:C:H2'	1:QA:949:A:H8	1.82	0.44
34:RA:1509:C:N3	34:RA:1511:A:N6	2.65	0.44
34:RA:966:G:H4'	34:RA:2271:G:H22	1.83	0.44
22:QV:76:A:N6	34:RA:2422:A:O4'	2.50	0.44
34:RA:2630:G:H2'	34:RA:2631:G:C8	2.52	0.44
34:RA:2531:A:H61	34:RA:2662:A:H61	1.64	0.44
34:RA:780:G:H21	34:RA:783:A:H62	1.65	0.44
54:RZ:97:GLU:HB3	54:RZ:125:LEU:HD11	2.00	0.44
1:XA:1499:A:H8	1:XA:1499:A:O5'	2.00	0.44
7:XG:79:ARG:HH21	7:XG:82:GLY:HA2	1.82	0.44
34:YA:2005:A:O2'	34:YA:2049:G:OP1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:532:A:H4'	34:YA:533:G:C8	2.52	0.44
1:QA:626:U:H2'	1:QA:627:G:C8	2.51	0.44
1:QA:67:C:H2'	1:QA:68:G:C8	2.53	0.44
2:QB:178:ARG:NH1	2:QB:196:LEU:O	2.49	0.44
6:QF:47:ARG:HD2	6:QF:57:GLN:HB3	2.00	0.44
29:R5:41:PRO:O	29:R5:44:THR:OG1	2.27	0.44
34:RA:2498:C:OP2	34:RA:2499:C:OP2	2.36	0.44
34:RA:29:U:H2'	34:RA:30:G:C8	2.53	0.44
34:RA:494:G:H21	51:RW:57:ASN:HD21	1.63	0.44
34:RA:84:A:N1	34:RA:98:G:O2'	2.38	0.44
40:RH:86:GLU:O	40:RH:164:TYR:HB2	2.17	0.44
43:RO:76:ALA:HB3	48:RT:75:ILE:HG12	1.99	0.44
1:XA:1462:G:H5''	48:YT:111:ARG:HH22	1.81	0.44
1:XA:1499:A:C8	1:XA:1499:A:O5'	2.70	0.44
12:XL:88:GLY:H	12:XL:98:TYR:HA	1.82	0.44
24:Y0:38:VAL:HG22	24:Y0:59:LEU:HB2	1.98	0.44
29:Y5:32:PRO:N	29:Y5:32:PRO:C	2.61	0.44
34:YA:568:U:H6	34:YA:568:U:H5''	1.82	0.44
42:YN:21:LYS:HD2	42:YN:26:LEU:HD13	1.98	0.44
48:YT:25:GLY:N	48:YT:49:VAL:O	2.42	0.44
50:YV:2:PHE:H	50:YV:42:GLY:HA3	1.82	0.44
1:QA:269:C:H2'	1:QA:270:A:C8	2.52	0.44
1:QA:318:G:H2'	1:QA:319:G:H8	1.83	0.44
1:QA:1080:A:OP1	5:QE:14:ARG:NH2	2.47	0.44
34:RA:2319:G:N2	34:RA:2334:G:OP1	2.51	0.44
34:RA:2809:A:OP2	34:RA:2891:G:N1	2.45	0.44
34:RA:28:A:HO2'	34:RA:582:G:HO2'	1.58	0.44
34:RA:861:A:N3	35:RB:79:C:O2'	2.51	0.44
35:RB:25:A:H2'	35:RB:26:A:H8	1.83	0.44
41:RI:4:ILE:HG23	41:RI:39:ALA:HB2	2.00	0.44
48:RT:25:GLY:H	48:RT:49:VAL:HG13	1.82	0.44
54:RZ:115:GLY:H	54:RZ:177:PRO:HG3	1.83	0.44
1:XA:1354:C:H2'	1:XA:1355:G:C8	2.53	0.44
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.52	0.44
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.50	0.44
3:XC:18:TRP:CE2	14:YN:55:GLY:HA2	2.53	0.44
13:XM:2:ALA:HB3	13:XM:9:ILE:HG21	2.00	0.44
34:YA:1549:C:O2'	34:YA:1733:G:N2	2.42	0.44
34:YA:190:A:N3	34:YA:679:C:O2'	2.44	0.44
34:YA:2102:U:H3	34:YA:2187:G:H1	1.64	0.44
34:YA:2303:G:N3	39:YG:132:ASN:ND2	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:YR:100:LEU:HD11	46:YR:113:LEU:HG	2.00	0.44
1:QA:502:G:H2'	1:QA:503:C:O4'	2.18	0.44
4:QD:61:LYS:HD2	4:QD:207:TYR:CZ	2.53	0.44
1:QA:707:C:OP1	11:QK:85:ARG:NH1	2.51	0.44
34:RA:1796:U:H2'	34:RA:1797:C:H6	1.82	0.44
34:RA:1851:U:H3	34:RA:1891:G:H1	1.65	0.44
34:RA:1992:G:C5	34:RA:1997:G:C6	3.05	0.44
34:RA:299:A:N3	34:RA:319:C:O2'	2.38	0.44
34:RA:679:C:H2'	34:RA:680:G:H8	1.82	0.44
36:RD:61:LEU:HD23	36:RD:61:LEU:HA	1.83	0.44
39:RG:135:LEU:HD11	39:RG:140:ILE:HD11	2.00	0.44
51:RW:65:LEU:HD12	51:RW:68:ARG:HH21	1.83	0.44
1:XA:1427:U:H2'	1:XA:1428:A:C8	2.52	0.44
16:XP:22:THR:OG1	16:XP:23:ASP:N	2.50	0.44
18:XR:85:LEU:HA	18:XR:85:LEU:HD12	1.83	0.44
34:YA:1859:A:N6	34:YA:1883:G:O2'	2.51	0.44
34:YA:840:C:H2'	34:YA:841:A:C8	2.53	0.44
38:YF:167:ALA:HB1	38:YF:173:VAL:HG11	1.99	0.44
45:YQ:12:GLN:HB2	45:YQ:73:PRO:HD2	2.00	0.44
1:QA:476:G:H2'	1:QA:477:G:H8	1.82	0.44
2:QB:51:LEU:HD23	2:QB:201:ILE:HD12	1.99	0.44
27:R3:18:ASP:N	27:R3:18:ASP:OD1	2.48	0.44
34:RA:1441:G:H2'	34:RA:1442:G:H8	1.82	0.44
34:RA:1791:A:H61	34:RA:1828:G:HO2'	1.61	0.44
34:RA:2094:G:OP1	41:RI:22:LYS:HE2	2.13	0.44
34:RA:2580:U:H5'	37:RE:130:GLY:O	2.18	0.44
34:RA:373:U:H2'	34:RA:374:A:H8	1.83	0.44
36:RD:12:SER:HB2	36:RD:208:LYS:HB3	1.99	0.44
41:RI:84:GLY:CA	41:RI:89:TYR:OH	2.61	0.44
1:XA:1174:G:H2'	1:XA:1175:G:C8	2.53	0.44
1:XA:1271:G:H5'	1:XA:1314:C:H5''	1.99	0.44
2:XB:189:ASP:OD1	2:XB:189:ASP:N	2.49	0.44
4:XD:57:ARG:NH2	4:XD:205:GLU:OE1	2.51	0.44
30:Y6:29:ASN:ND2	34:YA:2286:A:OP1	2.50	0.44
34:YA:1853:A:N3	34:YA:2233:U:O2'	2.46	0.44
34:YA:2109:U:H2'	34:YA:2110:G:C8	2.52	0.44
34:YA:828:U:H3'	34:YA:828:U:O2	2.17	0.44
34:YA:1500:G:O2'	36:YD:100:GLY:O	2.27	0.44
34:YA:270(R):C:H5''	41:YI:45:LYS:HD3	1.99	0.44
34:YA:1006:C:H5'	42:YN:28:THR:HG23	1.99	0.44
45:YQ:58:PHE:HD2	45:YQ:61:GLY:HA3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YY:13:VAL:HG12	53:YY:74:PRO:HA	1.99	0.44
1:QA:1220:G:H2'	1:QA:1221:G:H8	1.82	0.44
1:QA:1440(B):G:H21	1:QA:1440(P):A:H62	1.65	0.44
1:QA:297:G:N2	1:QA:300:A:OP2	2.51	0.44
1:QA:59:A:H3'	1:QA:331:G:H22	1.82	0.44
1:QA:949:A:H2'	1:QA:950:U:H6	1.83	0.44
10:QJ:28:ARG:HE	10:QJ:34:VAL:HG12	1.83	0.44
13:QM:95:GLY:HA2	13:QM:110:ARG:HH21	1.83	0.44
22:QV:71:C:O2	34:RA:1851:U:O2'	2.36	0.44
34:RA:2294:C:H2'	34:RA:2295:C:H6	1.82	0.44
40:RH:4:ILE:HD12	40:RH:6:ARG:HB2	1.99	0.44
34:RA:1138:G:H21	42:RN:106:MET:HG2	1.83	0.44
1:XA:294:U:OP1	1:XA:610:G:O2'	2.32	0.44
1:XA:59:A:H5'	1:XA:60:A:H5''	1.99	0.44
1:XA:964:A:N3	10:XJ:55:LYS:NZ	2.62	0.44
4:XD:68:TYR:OH	4:XD:98:GLU:OE2	2.33	0.44
34:YA:2153:G:H2'	34:YA:2154:G:H8	1.82	0.44
46:YR:29:LEU:HD13	46:YR:79:LEU:HD22	1.99	0.44
34:YA:1151:G:O2'	49:YU:77:SER:O	2.33	0.44
1:QA:1022:G:H2'	1:QA:1023:G:C8	2.52	0.44
1:QA:927:G:N2	1:QA:1390:U:O2	2.33	0.44
1:QA:444:C:H2'	1:QA:445:G:C8	2.53	0.44
3:QC:112:SER:HB3	3:QC:115:LEU:HD12	2.00	0.44
34:RA:1053:C:H6	34:RA:1053:C:O5'	2.00	0.44
34:RA:2081:C:H2'	34:RA:2082:A:H8	1.83	0.44
34:RA:2097:C:OP2	34:RA:2097:C:C6	2.71	0.44
34:RA:2097:C:OP2	34:RA:2097:C:H6	2.00	0.44
34:RA:2287:A:N6	34:RA:2344:U:H3	2.16	0.44
34:RA:2850:A:OP2	34:RA:2866:U:N3	2.51	0.44
36:RD:181:GLU:HA	36:RD:272:ALA:HB3	1.99	0.44
34:RA:1695:G:H1'	36:RD:8:PRO:O	2.17	0.44
34:RA:1276:A:H1'	46:RR:16:HIS:HE1	1.83	0.44
1:XA:1230:C:H2'	1:XA:1231:G:C8	2.53	0.44
1:XA:40:C:H2'	1:XA:41:G:H8	1.82	0.44
26:Y2:58:ALA:O	26:Y2:62:THR:OG1	2.30	0.44
39:YG:124:SER:OG	39:YG:124:SER:O	2.35	0.44
39:YG:138:GLN:OE1	39:YG:153:ARG:N	2.43	0.44
1:QA:1203:C:H2'	1:QA:1204:A:C8	2.53	0.44
1:QA:538:G:H2'	1:QA:539:A:H8	1.83	0.44
1:QA:595:G:H1'	1:QA:596:C:H5	1.83	0.44
1:QA:401:C:O2'	1:QA:621:A:N3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:662:G:H2'	1:QA:663:A:C8	2.53	0.44
5:QE:43:LEU:HD13	5:QE:109:ILE:HD11	1.99	0.44
19:QS:50:ALA:HA	19:QS:58:VAL:O	2.17	0.44
22:QV:37:1MG:C5	22:QV:38:A:C4	3.06	0.44
34:RA:1068:G:N2	34:RA:1095:A:O3'	2.51	0.44
34:RA:31:C:O2'	34:RA:1238:G:OP1	2.35	0.44
34:RA:1790:C:OP2	34:RA:1828:G:N1	2.48	0.44
34:RA:1962:C:O2'	34:RA:1964:G:OP2	2.28	0.44
34:RA:2098:U:H2'	34:RA:2098:U:O2	2.17	0.44
34:RA:997:G:OP1	49:RU:93:LYS:HD3	2.18	0.44
36:RD:50:THR:OG1	36:RD:51:VAL:N	2.50	0.44
1:XA:1251:A:H2'	1:XA:1252:A:C8	2.53	0.44
1:XA:1342:C:H2'	1:XA:1343:G:H8	1.83	0.44
1:XA:1427:U:H2'	1:XA:1428:A:H8	1.83	0.44
1:XA:575:G:N1	1:XA:880:C:N3	2.55	0.44
3:XC:66:VAL:HB	3:XC:101:LEU:HD13	2.00	0.44
16:XP:19:ILE:HG13	16:XP:36:ILE:HD11	2.00	0.44
18:XR:47:THR:O	18:XR:83:GLU:N	2.51	0.44
20:XT:100:ILE:HG23	20:XT:102:GLY:H	1.81	0.44
34:YA:1853:A:H2'	34:YA:1854:A:C8	2.53	0.44
38:YF:102:PRO:HB2	38:YF:105:VAL:HG23	1.99	0.44
51:YW:35:ILE:O	51:YW:39:THR:OG1	2.27	0.44
53:YY:28:LYS:N	53:YY:38:ILE:O	2.45	0.44
1:QA:1204:A:OP1	14:QN:3:ARG:NH2	2.51	0.43
25:R1:90:ILE:HA	25:R1:94:LEU:HG	1.99	0.43
34:RA:117:G:OP1	34:RA:124:G:N1	2.44	0.43
34:RA:265:A:N7	34:RA:428:A:N6	2.65	0.43
34:RA:707:G:H1	34:RA:724:U:H3	1.66	0.43
45:RQ:34:LEU:HB2	45:RQ:118:LEU:HD12	1.99	0.43
51:RW:71:VAL:HA	51:RW:107:LEU:HD23	2.00	0.43
52:RX:55:ASN:HB2	52:RX:80:ILE:HG23	2.00	0.43
1:XA:1291:G:H4'	9:XI:39:GLY:HA3	1.99	0.43
1:XA:48:C:OP2	1:XA:115:G:OP1	2.35	0.43
5:XE:31:LEU:HD13	5:XE:45:PHE:HD1	1.83	0.43
15:XO:53:HIS:NE2	34:YA:715:G:O6	2.49	0.43
36:YD:142:VAL:HA	36:YD:194:GLY:H	1.83	0.43
37:YE:102:VAL:N	37:YE:170:LEU:O	2.46	0.43
5:QE:100:VAL:O	5:QE:107:ARG:NH1	2.48	0.43
16:QP:55:ARG:HD2	16:QP:55:ARG:HA	1.79	0.43
23:QX:14:A:OP2	23:QX:14:A:C8	2.70	0.43
1:QA:1503:A:N3	23:QX:15:A:N6	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R4:12:ALA:H	28:R4:25:TYR:HA	1.83	0.43
34:RA:1084:A:H2'	34:RA:1085:A:C4	2.53	0.43
34:RA:2246:G:H2'	34:RA:2247:A:H8	1.82	0.43
34:RA:2392:A:H2	34:RA:2424:C:H42	1.66	0.43
34:RA:2576:G:N3	34:RA:2576:G:C3'	2.80	0.43
41:RI:79:ILE:HD12	41:RI:80:PRO:HD2	2.00	0.43
3:XC:187:ALA:HB3	3:XC:198:VAL:HG13	2.00	0.43
5:XE:105:VAL:HG11	5:XE:132:ALA:HB2	1.99	0.43
12:XL:33:ARG:NH2	12:XL:61:THR:OG1	2.51	0.43
28:Y4:37:SER:HA	28:Y4:41:PRO:HD2	1.98	0.43
32:Y8:56:GLU:OE1	32:Y8:59:LYS:NZ	2.36	0.43
34:YA:2031:A:HO2'	34:YA:2454:G:H21	1.66	0.43
34:YA:2821:A:OP1	37:YE:110:GLY:N	2.47	0.43
34:YA:748:G:N9	34:YA:750:A:N7	2.66	0.43
35:YB:5:C:OP1	35:YB:61:G:O2'	2.28	0.43
37:YE:37:ARG:NH1	37:YE:44:TYR:OH	2.48	0.43
39:YG:106:LEU:HD12	39:YG:110:ALA:HB3	1.99	0.43
44:YP:21:ARG:HB3	44:YP:22:GLY:H	1.67	0.43
1:QA:355:C:O2'	1:QA:388:G:N3	2.36	0.43
1:QA:406:G:H21	4:QD:119:GLN:HE22	1.66	0.43
1:QA:559:A:H4'	1:QA:560:U:H5''	2.00	0.43
1:QA:673:G:O3'	6:QF:87:ARG:NH2	2.50	0.43
1:QA:881:G:P	12:QL:12:ARG:HH22	2.41	0.43
34:RA:1165:U:O4	34:RA:1184:G:O6	2.36	0.43
34:RA:1182:A:H2'	34:RA:1183:G:H8	1.83	0.43
34:RA:1385:G:O2'	34:RA:1396:U:O2	2.32	0.43
34:RA:691:C:H2'	34:RA:692:C:H6	1.82	0.43
37:RE:176:ILE:HG13	37:RE:181:LEU:HB2	2.00	0.43
34:RA:2313:C:H5''	39:RG:91:ARG:HH21	1.83	0.43
1:XA:1409:C:H2'	1:XA:1410:G:H8	1.82	0.43
29:Y5:48:GLU:CD	51:YW:37:ARG:NH1	2.67	0.43
30:Y6:3:SER:HB3	30:Y6:6:ARG:HB3	2.00	0.43
24:Y0:12:ASN:ND2	34:YA:2278:A:OP2	2.51	0.43
35:YB:75:G:H21	54:YZ:85:HIS:CD2	2.36	0.43
47:YS:4:LEU:HD11	47:YS:12:PHE:CE2	2.51	0.43
1:QA:57:G:H2'	1:QA:58:C:H6	1.84	0.43
2:QB:54:THR:O	2:QB:58:ILE:HG12	2.18	0.43
6:QF:14:LEU:HD12	6:QF:18:GLN:CD	2.38	0.43
29:R5:12:SER:O	29:R5:16:ARG:CB	2.67	0.43
34:RA:1525:G:H2'	34:RA:1526:G:C8	2.53	0.43
34:RA:273(E):C:N4	34:RA:363(D):G:O6	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:29:U:H2'	34:RA:30:G:H8	1.83	0.43
34:RA:922:U:H2'	34:RA:923:C:C6	2.54	0.43
37:RE:171:GLU:H	37:RE:185:LYS:HB2	1.84	0.43
34:RA:2311:A:C8	39:RG:82:LEU:HD21	2.53	0.43
40:RH:80:SER:OG	40:RH:80:SER:O	2.31	0.43
46:RR:35:THR:HG22	46:RR:113:LEU:HD13	2.01	0.43
46:RR:29:LEU:HD12	46:RR:70:LEU:HD21	1.99	0.43
34:RA:2294:C:OP2	47:RS:13:ARG:NH2	2.52	0.43
1:XA:1135:U:H4'	1:XA:1136:U:H5	1.83	0.43
1:XA:67:C:O2'	1:XA:171:A:N3	2.40	0.43
1:XA:25:C:C4	1:XA:558:G:N2	2.86	0.43
1:XA:605:U:OP2	1:XA:605:U:C5	2.70	0.43
27:Y3:18:ASP:HB2	27:Y3:49:LYS:HE2	1.99	0.43
31:Y7:34:ARG:NH1	34:YA:466:A:OP1	2.51	0.43
34:YA:530:G:N1	34:YA:2022:U:OP1	2.52	0.43
34:YA:2047:U:O2'	34:YA:2823:A:N1	2.47	0.43
34:YA:629:G:N3	34:YA:639:U:O2'	2.51	0.43
41:YI:81:VAL:HG11	41:YI:88:ILE:HD13	1.99	0.43
44:YP:97:PRO:O	44:YP:98:GLU:HG3	2.18	0.43
49:YU:55:ARG:O	49:YU:59:ARG:HG2	2.18	0.43
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.83	0.43
1:QA:501:C:H2'	1:QA:502:G:C8	2.54	0.43
1:QA:674:G:H2'	1:QA:675:A:C8	2.48	0.43
3:QC:131:ARG:HH11	3:QC:134:ILE:HG21	1.83	0.43
8:QH:82:HIS:N	8:QH:138:TRP:OXT	2.41	0.43
9:QI:65:VAL:HG11	9:QI:73:GLN:HG3	2.01	0.43
26:R2:16:LEU:H	26:R2:67:LYS:NZ	2.16	0.43
34:RA:1814:G:H5'	36:RD:51:VAL:HG11	2.01	0.43
34:RA:2315:G:H2'	34:RA:2316:C:C6	2.54	0.43
34:RA:2425:A:H4'	34:RA:2426:A:H5''	2.00	0.43
34:RA:2504:U:H6	34:RA:2504:U:O5'	2.02	0.43
34:RA:2584:U:H2'	34:RA:2585:U:H2'	2.00	0.43
34:RA:947:G:H2'	34:RA:948:G:C8	2.53	0.43
39:RG:43:LEU:HD21	39:RG:153:ARG:HB2	1.99	0.43
43:RO:15:GLY:HA3	43:RO:50:GLY:HA3	1.99	0.43
48:RT:6:LEU:O	48:RT:10:VAL:HG23	2.19	0.43
1:XA:713:G:H2'	1:XA:714:G:C8	2.53	0.43
1:XA:765:G:N1	1:XA:812:C:O2'	2.40	0.43
9:XI:70:LYS:O	9:XI:74:ILE:HG13	2.19	0.43
1:XA:186(J):U:O2	17:XQ:72:ARG:NH2	2.52	0.43
18:XR:49:LYS:HE2	18:XR:49:LYS:HB3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:320:A:N3	38:YF:169:ASN:ND2	2.67	0.43
34:YA:463:G:O2'	34:YA:465:G:O6	2.36	0.43
34:YA:90:U:H1'	34:YA:91:A:C8	2.54	0.43
39:YG:165:THR:OG1	39:YG:166:ASP:N	2.52	0.43
41:YI:101:LEU:HD11	41:YI:109:ILE:HD13	2.00	0.43
35:YB:9:G:P	47:YS:25:ARG:HH12	2.42	0.43
1:QA:1038:C:N3	1:QA:1039:C:N4	2.67	0.43
1:QA:865:A:N3	1:QA:918:A:O2'	2.42	0.43
3:QC:12:LEU:HG	3:QC:18:TRP:HE1	1.83	0.43
4:QD:191:ARG:HD2	4:QD:191:ARG:HA	1.72	0.43
20:QT:58:LYS:O	20:QT:61:SER:OG	2.26	0.43
44:RP:96:THR:HA	44:RP:126:VAL:HB	2.01	0.43
54:RZ:156:LYS:HE3	54:RZ:156:LYS:HB3	1.74	0.43
54:RZ:48:PHE:HA	54:RZ:51:ALA:HB3	2.01	0.43
54:RZ:53:ILE:HG22	54:RZ:71:VAL:HG13	1.99	0.43
1:XA:1374:A:O2'	7:XG:28:ASN:O	2.37	0.43
1:XA:377:G:H2'	1:XA:378:G:H8	1.83	0.43
1:XA:601:C:H2'	1:XA:602:A:H8	1.83	0.43
1:XA:7:G:O2'	5:XE:120:THR:O	2.36	0.43
12:XL:86:ARG:HH21	12:XL:99:HIS:CD2	2.37	0.43
14:XN:40:CYS:SG	14:XN:41:ARG:N	2.91	0.43
34:YA:2081:C:H2'	34:YA:2082:A:H8	1.83	0.43
34:YA:240:G:O2'	34:YA:257:A:N6	2.51	0.43
34:YA:2581:G:N1	34:YA:2610:C:O2'	2.47	0.43
34:YA:2646:C:OP2	34:YA:2732:G:O2'	2.24	0.43
44:YP:64:LYS:O	44:YP:66:GLY:N	2.51	0.43
48:YT:19:LEU:HD21	48:YT:83:ILE:HD11	2.00	0.43
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.83	0.43
1:QA:131:C:OP2	1:QA:186(K):G:O2'	2.35	0.43
1:QA:382:A:H2'	1:QA:383:A:C8	2.54	0.43
1:QA:736:C:H2'	1:QA:737:A:C8	2.53	0.43
2:QB:188:ALA:HB1	2:QB:192:SER:HB2	2.01	0.43
23:QX:14:A:C8	23:QX:14:A:O5'	2.70	0.43
34:RA:1148:A:H2'	34:RA:1149:G:C8	2.54	0.43
34:RA:1528:A:H2'	34:RA:1529:A:H8	1.84	0.43
38:RF:152:GLU:OE1	38:RF:191:ARG:NE	2.52	0.43
42:RN:28:THR:O	42:RN:32:THR:OG1	2.24	0.43
49:RU:91:ASP:O	49:RU:93:LYS:N	2.50	0.43
1:XA:1205:U:H2'	1:XA:1206:G:H8	1.83	0.43
1:XA:129(A):U:H3	1:XA:232:G:H1	1.67	0.43
1:XA:262:A:H2'	1:XA:263:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XK:82:VAL:HB	11:XK:108:ILE:HA	2.01	0.43
24:Y0:72:ARG:CB	24:Y0:75:LEU:HB2	2.49	0.43
33:Y9:10:ILE:N	33:Y9:14:CYS:SG	2.84	0.43
34:YA:974(A):G:C5	34:YA:1186:G:C2	3.07	0.43
34:YA:947:G:N3	34:YA:984:A:C2	2.87	0.43
36:YD:143:HIS:ND1	36:YD:194:GLY:O	2.40	0.43
39:YG:18:GLU:OE1	39:YG:21:ARG:NH2	2.50	0.43
48:YT:120:ARG:HA	48:YT:123:GLN:HB2	2.01	0.43
53:YY:76:CYS:CB	53:YY:79:CYS:SG	3.07	0.43
1:QA:1003:G:H2'	1:QA:1004:A:H4'	2.00	0.43
1:QA:451:A:N7	1:QA:481:G:N1	2.67	0.43
1:QA:819:A:N7	1:QA:1529:G:C6	2.87	0.43
7:QG:75:VAL:HA	7:QG:88:PRO:HA	2.00	0.43
12:QL:76:ASN:HD21	12:QL:108:ALA:HB3	1.84	0.43
13:QM:29:ARG:HH21	13:QM:64:TRP:HE1	1.67	0.43
13:QM:87:TYR:OH	13:QM:91:ARG:NH2	2.47	0.43
14:QN:6:LEU:HD23	14:QN:9:LYS:HD3	2.00	0.43
34:RA:1140:C:O3'	42:RN:25:ARG:NH2	2.44	0.43
34:RA:1732:A:H3'	34:RA:1733:G:H8	1.82	0.43
34:RA:2133:G:N2	34:RA:2157:G:H2'	2.33	0.43
34:RA:578:A:OP1	34:RA:1255:U:O2'	2.36	0.43
43:RO:15:GLY:HA2	43:RO:47:ILE:HG22	2.00	0.43
3:XC:64:VAL:HG13	3:XC:97:LYS:HD2	2.01	0.43
32:Y8:60:LEU:HA	32:Y8:60:LEU:HD12	1.81	0.43
34:YA:2148:G:H2'	34:YA:2149:G:C8	2.54	0.43
34:YA:363(B):A:H2'	34:YA:363(C):G:C8	2.52	0.43
47:YS:14:VAL:O	47:YS:18:ILE:HG12	2.18	0.43
48:YT:16:ARG:NH2	48:YT:83:ILE:O	2.51	0.43
1:QA:380:G:N2	1:QA:383:A:OP2	2.42	0.43
1:QA:401:C:H5	4:QD:73:ARG:HH22	1.60	0.43
1:QA:411:A:OP1	4:QD:30:LYS:NZ	2.49	0.43
1:QA:708:C:H2'	1:QA:709:G:C8	2.53	0.43
3:QC:43:LEU:HG	3:QC:47:LEU:HD22	2.00	0.43
13:QM:34:LEU:HA	13:QM:37:THR:HG22	2.01	0.43
19:QS:70:LYS:N	19:QS:73:GLU:OE1	2.52	0.43
22:QV:23:C:H2'	22:QV:24:G:C8	2.54	0.43
34:RA:1370:C:O2'	34:RA:1811:G:O2'	2.34	0.43
34:RA:1995:U:H3'	34:RA:1996:C:H2'	2.01	0.43
34:RA:2630:G:H2'	34:RA:2631:G:H8	1.84	0.43
35:RB:8:U:O2	35:RB:112:G:N2	2.43	0.43
1:XA:851:G:H2'	1:XA:852:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y0:26:TYR:N	24:Y0:29:GLN:OE1	2.52	0.43
34:YA:2140:C:H2'	34:YA:2141:G:H8	1.83	0.43
34:YA:688:U:H1'	34:YA:786:C:O2'	2.19	0.43
38:YF:158:THR:OG1	38:YF:159:GLY:N	2.51	0.43
40:YH:152:ARG:HD3	40:YH:152:ARG:HA	1.80	0.43
34:RA:1179:C:H2'	34:RA:1180:C:H6	1.84	0.43
34:RA:1539:G:H2'	34:RA:1540:G:H8	1.83	0.43
34:RA:2470:G:OP1	45:RQ:56:ARG:NH2	2.43	0.43
37:RE:35:GLN:HB2	37:RE:37:ARG:HH21	1.84	0.43
40:RH:46:GLU:OE1	40:RH:51:ARG:NH1	2.52	0.43
54:RZ:130:PRO:HA	54:RZ:133:ILE:HD11	2.01	0.43
1:XA:445:G:H2'	1:XA:446:G:H8	1.84	0.43
7:XG:102:ARG:HA	7:XG:105:VAL:HG22	2.01	0.43
11:XK:109:VAL:HG11	18:XR:84:LYS:HD2	2.01	0.43
27:Y3:5:LYS:HE3	27:Y3:57:GLU:HB3	1.99	0.43
34:YA:1600:C:OP1	52:YX:58:HIS:NE2	2.42	0.43
34:YA:2249:U:N3	34:YA:2253:G:OP2	2.46	0.43
34:YA:964:C:O2'	34:YA:2273:A:N3	2.37	0.43
34:YA:18:C:O2'	34:YA:553:U:OP1	2.31	0.43
38:YF:48:THR:OG1	38:YF:48:THR:O	2.36	0.43
54:YZ:85:HIS:NE2	54:YZ:87:ASP:OD1	2.52	0.43
1:QA:1145:C:O2'	1:QA:1146:A:N7	2.47	0.42
1:QA:908:A:H2'	1:QA:909:A:H8	1.84	0.42
2:QB:150:SER:HA	2:QB:153:ARG:HH21	1.83	0.42
3:QC:140:ARG:HA	3:QC:143:GLU:HG2	2.01	0.42
6:QF:78:GLU:HA	6:QF:81:ILE:HG12	2.01	0.42
10:QJ:61:GLU:HG3	14:QN:45:ARG:HH12	1.84	0.42
34:RA:532:A:H4'	34:RA:533:G:C8	2.53	0.42
15:QO:64:ARG:NH1	34:RA:715:G:OP1	2.52	0.42
34:RA:807:U:OP1	44:RP:36:LYS:HD3	2.19	0.42
37:RE:134:ILE:HD12	37:RE:134:ILE:HA	1.85	0.42
45:RQ:77:LYS:NZ	45:RQ:84:GLY:O	2.40	0.42
53:RY:79:CYS:N	53:RY:102:CYS:SG	2.92	0.42
1:XA:17:U:H2'	1:XA:18:C:H6	1.83	0.42
1:XA:815:A:O4'	1:XA:817:C:N4	2.52	0.42
10:XJ:99:LYS:HA	10:XJ:99:LYS:HD2	1.73	0.42
34:YA:2808:U:N3	34:YA:2892:A:N6	2.67	0.42
34:YA:603:A:N1	34:YA:625:G:O2'	2.49	0.42
54:YZ:48:PHE:HA	54:YZ:51:ALA:HB3	2.00	0.42
1:QA:757:U:O2'	1:QA:879:C:O2	2.35	0.42
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:100:ARG:HG3	4:QD:137:SER:HA	2.00	0.42
8:QH:10:LEU:HG	8:QH:83:ILE:HD11	1.99	0.42
12:QL:57:LYS:HA	12:QL:67:THR:HA	2.00	0.42
34:RA:30:G:H2'	34:RA:31:C:C6	2.53	0.42
36:RD:13:ARG:HD2	36:RD:13:ARG:HA	1.80	0.42
37:RE:120:TRP:CD2	37:RE:155:LYS:HB3	2.54	0.42
37:RE:109:LYS:HG2	37:RE:191:PRO:HB3	2.00	0.42
44:RP:65:ARG:O	44:RP:68:GLN:NE2	2.52	0.42
1:XA:1314:C:H2'	1:XA:1315:U:H6	1.84	0.42
1:XA:1384:C:H2'	1:XA:1385:G:C8	2.54	0.42
7:XG:116:ALA:HA	7:XG:119:ARG:HE	1.83	0.42
1:XA:948:C:OP2	13:XM:106:ASN:ND2	2.48	0.42
34:YA:1935:G:H1'	34:YA:1964:G:N2	2.34	0.42
29:Y5:8:LYS:NZ	34:YA:2055:C:OP1	2.45	0.42
34:YA:2446:G:H2'	34:YA:2447:G:H5''	2.01	0.42
34:YA:691:C:H2'	34:YA:692:C:H6	1.85	0.42
37:YE:144:ARG:HG3	37:YE:145:LYS:H	1.84	0.42
1:QA:1071:C:H2'	1:QA:1072:G:C8	2.52	0.42
3:QC:22:TRP:HH2	3:QC:32:LEU:HD13	1.85	0.42
5:QE:102:ALA:H	5:QE:107:ARG:NH2	2.18	0.42
22:QV:19:G:H4'	22:QV:57:G:H1	1.85	0.42
23:QX:14:A:C8	23:QX:14:A:P	3.12	0.42
34:RA:1021:A:H62	34:RA:1022:G:H21	1.67	0.42
1:XA:1052:U:O2'	1:XA:1055:A:OP2	2.29	0.42
1:XA:1314:C:H2'	1:XA:1315:U:C6	2.55	0.42
1:XA:662:G:H2'	1:XA:663:A:C8	2.54	0.42
2:XB:87:ARG:HH21	2:XB:219:VAL:HG13	1.84	0.42
13:XM:9:ILE:HA	13:XM:10:PRO:HD3	1.90	0.42
13:XM:52:GLU:HA	13:XM:55:ARG:HG2	2.00	0.42
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.52	0.42
20:XT:17:ARG:HE	20:XT:17:ARG:HB3	1.73	0.42
34:YA:1782:C:H42	34:YA:2586:C:N4	2.16	0.42
34:YA:2151:G:H2'	34:YA:2152:G:C8	2.54	0.42
34:YA:816:C:O2'	34:YA:932:G:O6	2.36	0.42
35:YB:111:U:H2'	35:YB:112:G:H8	1.85	0.42
40:YH:159:GLU:HG2	40:YH:169:VAL:HG21	2.01	0.42
51:YW:57:ASN:O	51:YW:61:ASN:HB2	2.19	0.42
1:QA:1028(D):G:N2	1:QA:1028(G):A:OP2	2.53	0.42
1:QA:1219:U:H2'	1:QA:1220:G:C8	2.54	0.42
1:QA:477:G:H2'	1:QA:478:A:H8	1.83	0.42
4:QD:15:GLU:HG2	4:QD:63:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:126:ARG:HA	5:QE:131:ILE:HD11	2.01	0.42
7:QG:75:VAL:HG12	7:QG:88:PRO:HB3	2.01	0.42
12:QL:79:GLU:OE2	12:QL:80:HIS:NE2	2.53	0.42
17:QQ:45:HIS:H	17:QQ:72:ARG:HA	1.84	0.42
19:QS:39:THR:HG22	19:QS:41:VAL:HG22	2.01	0.42
22:QV:61:C:H2'	22:QV:62:C:C6	2.53	0.42
23:QX:15:A:O2'	23:QX:17:C:OP2	2.37	0.42
34:RA:2378:A:O3'	47:RS:23:ARG:NH1	2.52	0.42
34:RA:894:C:H2'	34:RA:895:U:C6	2.55	0.42
46:RR:8:ARG:HD2	46:RR:10:LEU:HD21	2.01	0.42
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.54	0.42
3:XC:8:ILE:HG12	3:XC:184:TYR:HB3	2.02	0.42
14:XN:23:ARG:NH1	14:XN:24:CYS:HB3	2.34	0.42
33:Y9:32:HIS:CD2	33:Y9:32:HIS:N	2.87	0.42
34:YA:117:G:OP2	34:YA:119:A:O2'	2.27	0.42
34:YA:2245:U:H6	34:YA:2245:U:C5'	2.29	0.42
34:YA:690:G:O2'	36:YD:43:ARG:NH1	2.53	0.42
53:YY:79:CYS:SG	53:YY:81:LYS:HE2	2.60	0.42
13:QM:66:LEU:HB3	13:QM:67:GLU:H	1.71	0.42
34:RA:511:U:H4'	34:RA:1235:G:H4'	2.00	0.42
34:RA:1728:G:H8	34:RA:1732:A:H62	1.67	0.42
34:RA:2748:A:H62	34:RA:2754:U:H3	1.67	0.42
34:RA:2853:C:H2'	34:RA:2854:G:H8	1.84	0.42
34:RA:504:U:H5''	34:RA:505:A:H5'	2.02	0.42
35:RB:28:C:H2'	35:RB:29:A:H8	1.85	0.42
35:RB:28:C:H2'	35:RB:29:A:C8	2.54	0.42
36:RD:49:ILE:HD11	36:RD:52:ARG:HA	2.00	0.42
51:RW:13:SER:HA	51:RW:99:ARG:HB2	2.01	0.42
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.85	0.42
1:XA:501:C:H2'	1:XA:502:G:C8	2.54	0.42
1:XA:401:C:O2'	1:XA:621:A:N3	2.43	0.42
1:XA:674:G:H2'	1:XA:675:A:C8	2.49	0.42
7:XG:99:LEU:HA	7:XG:99:LEU:HD12	1.93	0.42
1:XA:878:G:H5'	8:XH:89:PRO:HG2	2.00	0.42
19:XS:19:VAL:HA	19:XS:22:LEU:HB2	2.01	0.42
32:Y8:4:MET:HG3	32:Y8:61:LEU:HD11	2.01	0.42
34:YA:639:U:H3	34:YA:649:G:H1	1.67	0.42
34:YA:750:A:C2	34:YA:753:C:N1	2.88	0.42
40:YH:9:ILE:HG22	40:YH:49:VAL:HB	1.96	0.42
42:YN:40:PRO:HB3	49:YU:68:ALA:HB2	2.02	0.42
44:YP:82:GLY:HA2	44:YP:113:LYS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:YR:35:THR:HA	46:YR:112:ALA:O	2.19	0.42
1:QA:1118:C:H1'	1:QA:1179:A:C5	2.54	0.42
1:QA:1220:G:O3'	19:QS:36:ARG:NH2	2.53	0.42
2:QB:175:ARG:O	2:QB:179:LYS:HG3	2.20	0.42
9:QL:103:THR:O	9:QL:103:THR:OG1	2.37	0.42
14:QN:41:ARG:HG3	14:QN:42:ILE:HG13	2.01	0.42
20:QT:14:LYS:HA	20:QT:17:ARG:HG2	2.02	0.42
34:RA:1051:G:C5	34:RA:1052:C:C4	3.08	0.42
34:RA:2014:A:H2	34:RA:2613:U:N3	2.17	0.42
34:RA:2105:C:H2'	34:RA:2106:G:C8	2.55	0.42
34:RA:2710:C:H2'	34:RA:2711:A:C8	2.55	0.42
34:RA:863:A:H2'	34:RA:864:G:C8	2.55	0.42
49:RU:85:LYS:HE2	49:RU:116:ALA:HA	2.01	0.42
34:RA:24:G:O2'	51:RW:78:GLU:O	2.24	0.42
34:RA:336:C:HO2'	53:RY:35:TYR:HH	1.67	0.42
54:RZ:67:LEU:HD12	54:RZ:90:VAL:HB	2.02	0.42
1:XA:1517:G:N3	34:YA:1919:A:O2'	2.47	0.42
1:XA:17:U:H2'	1:XA:18:C:C6	2.54	0.42
1:XA:186(A):C:H2'	1:XA:186(B):C:C6	2.54	0.42
6:XF:27:GLN:HA	6:XF:30:LEU:HD12	2.02	0.42
34:YA:2521:C:O2'	34:YA:2564:A:N3	2.38	0.42
34:YA:664:C:H2'	34:YA:665:C:H6	1.85	0.42
34:YA:750:A:H2	34:YA:753:C:C6	2.34	0.42
34:YA:906:G:OP1	45:YQ:26:TYR:OH	2.34	0.42
47:YS:34:HIS:O	47:YS:97:ARG:NH2	2.52	0.42
1:QA:1381:U:H1'	1:QA:1382:C:H5'	2.01	0.42
1:QA:375:U:OP1	16:QP:69:THR:OG1	2.29	0.42
1:QA:56:U:H2'	1:QA:57:G:C8	2.55	0.42
1:QA:926:G:O6	23:QX:19:U:H3'	2.19	0.42
1:QA:1158:C:H1'	2:QB:132:LYS:HD3	2.02	0.42
4:QD:59:ARG:HH12	4:QD:66:ARG:NH2	2.16	0.42
1:QA:502:G:OP1	12:QL:117:ARG:N	2.53	0.42
1:QA:552:U:O2'	12:QL:86:ARG:O	2.31	0.42
31:R7:12:ARG:HH21	31:R7:44:PRO:HB3	1.84	0.42
34:RA:1518:C:H2'	34:RA:1519:G:C8	2.54	0.42
34:RA:589:C:H2'	34:RA:590:A:H8	1.84	0.42
36:RD:142:VAL:HG23	36:RD:193:VAL:HA	2.02	0.42
34:RA:2296:U:OP2	47:RS:9:ARG:NH1	2.52	0.42
1:XA:411:A:OP1	4:XD:30:LYS:NZ	2.45	0.42
2:XB:177:ALA:HB1	2:XB:182:ILE:HB	2.01	0.42
3:XC:119:ARG:HG2	3:XC:140:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:XE:99:GLY:N	5:XE:117:ASP:OD1	2.47	0.42
14:YN:53:LEU:HD12	14:YN:54:PRO:HD2	2.01	0.42
1:XA:693:G:N2	22:XV:37:1MG:HN21	2.17	0.42
34:YA:1858:G:O2'	34:YA:1884:A:N6	2.53	0.42
34:YA:848:G:H2'	34:YA:849:A:C8	2.55	0.42
38:YF:114:VAL:HG11	38:YF:202:PHE:CZ	2.55	0.42
48:YT:6:LEU:HA	48:YT:9:LEU:HB2	2.02	0.42
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.41	0.42
1:QA:737:A:H2'	1:QA:738:C:C6	2.55	0.42
7:QG:58:PRO:HA	7:QG:61:VAL:HG12	2.01	0.42
8:QH:21:LYS:HE2	8:QH:21:LYS:HB2	1.91	0.42
22:QV:56:C:N4	22:QV:57:G:O6	2.53	0.42
32:R8:61:LEU:HD12	32:R8:62:LEU:HG	2.02	0.42
34:RA:2308:G:H1	34:RA:2311:A:H2	1.68	0.42
32:R8:39:LYS:NZ	34:RA:2351:G:O6	2.49	0.42
34:RA:2712(A):U:H3'	34:RA:2712(A):U:O2	2.19	0.42
34:RA:514:A:H2'	34:RA:515:A:C8	2.54	0.42
36:RD:32:SER:C	36:RD:34:VAL:H	2.23	0.42
53:RY:92:ASN:OD1	53:RY:92:ASN:N	2.53	0.42
1:XA:178:C:H2'	1:XA:179:A:H8	1.84	0.42
1:XA:183:G:H2'	1:XA:184:G:H8	1.84	0.42
1:XA:454:C:H41	1:XA:479:C:H42	1.65	0.42
9:XI:13:ALA:HB1	9:XI:73:GLN:HG3	2.01	0.42
12:XL:42:THR:HA	12:XL:53:ARG:O	2.19	0.42
1:XA:1060:C:OP1	14:YN:45:ARG:NH2	2.53	0.42
21:XU:6:ARG:NH2	21:XU:15:ARG:HH22	2.16	0.42
30:Y6:40:CYS:HB3	30:Y6:43:CYS:CB	2.50	0.42
34:YA:2291:U:H2'	34:YA:2292:C:C6	2.55	0.42
36:YD:83:GLU:OE1	36:YD:104:TYR:OH	2.31	0.42
37:YE:102:VAL:HG23	37:YE:200:GLU:HA	2.02	0.42
44:YP:46:LYS:HB3	44:YP:46:LYS:HE3	1.78	0.42
45:YQ:110:THR:OG1	45:YQ:111:GLU:N	2.53	0.42
52:YX:25:LYS:HB3	52:YX:80:ILE:HD11	2.00	0.42
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.85	0.42
1:QA:324:G:OP1	20:QT:70:SER:OG	2.35	0.42
1:QA:570:G:O4'	1:QA:820:U:H6	2.02	0.42
1:QA:762:C:H2'	1:QA:763:G:C8	2.54	0.42
2:QB:34:ALA:H	2:QB:41:ILE:HB	1.84	0.42
1:QA:1307:U:OP1	13:QM:101:GLN:NE2	2.53	0.42
20:QT:10:LEU:HA	20:QT:10:LEU:HD23	1.86	0.42
33:R9:29:ASN:HB3	33:R9:32:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1779:U:OP2	34:RA:1784:A:N6	2.35	0.42
34:RA:2431:U:P	34:RA:2432:A:OP2	2.77	0.42
34:RA:2474:C:H5''	34:RA:2475:C:H5	1.84	0.42
34:RA:2646:C:OP2	34:RA:2732:G:O2'	2.25	0.42
34:RA:303:U:H2'	34:RA:304:G:C8	2.55	0.42
34:RA:30:G:H2'	34:RA:31:C:H6	1.85	0.42
34:RA:587:C:C2	34:RA:671:C:O4'	2.73	0.42
38:RF:8:GLN:NE2	38:RF:19:GLU:OE1	2.51	0.42
38:RF:70:THR:HG23	38:RF:72:ARG:H	1.85	0.42
40:RH:126:PRO:HB2	40:RH:127:GLU:H	1.68	0.42
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.34	0.42
1:XA:156:G:H2'	1:XA:157:G:H8	1.85	0.42
1:XA:624:C:H2'	1:XA:625:G:C8	2.55	0.42
7:XG:104:LEU:HA	7:XG:104:LEU:HD23	1.90	0.42
19:XS:30:LEU:HD13	19:XS:48:THR:HG23	2.01	0.42
21:XU:10:ARG:HA	21:XU:13:ILE:HG22	2.01	0.42
22:XV:9:G:O2'	22:XV:10:G:N7	2.53	0.42
34:YA:513:A:O2'	34:YA:1217:C:OP1	2.38	0.42
34:YA:2096:U:H3	34:YA:2193:G:H1	1.68	0.42
34:YA:648:G:O2'	34:YA:2351:G:OP1	2.26	0.42
34:YA:320:A:H2'	38:YF:136:THR:HG21	2.02	0.42
34:YA:654(C):C:H42	34:YA:654(U):C:N4	2.18	0.42
44:YP:15:ARG:HA	44:YP:15:ARG:HD3	1.85	0.42
45:YQ:34:LEU:HB2	45:YQ:118:LEU:HD22	2.01	0.42
1:QA:1232:U:H5''	9:QL:124:GLN:HG3	2.02	0.42
1:QA:142:G:H2'	1:QA:143:A:C8	2.54	0.42
1:QA:1440(B):G:N2	1:QA:1461:G:O6	2.52	0.42
1:QA:406:G:H21	4:QD:119:GLN:NE2	2.18	0.42
1:QA:41:G:H2'	1:QA:42:G:H8	1.84	0.42
1:QA:56:U:H2'	1:QA:57:G:H8	1.85	0.42
1:QA:714:G:H2'	1:QA:715:A:C8	2.55	0.42
2:QB:231:GLU:HA	2:QB:232:PRO:HD3	1.87	0.42
1:QA:404:U:O4	4:QD:2:GLY:N	2.53	0.42
12:QL:102:ARG:HB3	12:QL:109:GLY:HA2	2.01	0.42
13:QM:29:ARG:HA	13:QM:29:ARG:HD2	1.79	0.42
32:R8:49:VAL:HG23	32:R8:53:PRO:HD3	2.02	0.42
32:R8:64:TYR:HB3	34:RA:625:G:P	2.60	0.42
36:RD:76:PRO:HB3	36:RD:118:VAL:HG22	2.02	0.42
39:RG:34:LEU:HD21	39:RG:172:LEU:HD21	2.02	0.42
1:XA:335:C:O2'	1:XA:1433:A:N3	2.46	0.42
1:XA:310:G:OP2	16:XP:27:LYS:NZ	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:950:U:H3	1:XA:1231:G:H1	1.67	0.42
34:YA:1024:G:OP2	34:YA:1025:G:C2'	2.68	0.42
29:Y5:9:LYS:NZ	34:YA:2019:A:OP2	2.34	0.42
34:YA:2105:C:H2'	34:YA:2106:G:H8	1.85	0.42
34:YA:2282:G:H5''	34:YA:2283:C:O4'	2.20	0.42
34:YA:2314:C:H5'	39:YG:38:VAL:HG21	2.01	0.42
34:YA:442:G:N2	38:YF:48:THR:OG1	2.53	0.42
34:YA:822:U:H2'	34:YA:823:G:H8	1.85	0.42
37:YE:24:THR:HG22	37:YE:186:GLY:H	1.83	0.42
37:YE:2:LYS:HD2	37:YE:95:ILE:HG22	2.02	0.42
46:YR:87:TYR:OH	46:YR:117:VAL:O	2.31	0.42
47:YS:18:ILE:HG21	47:YS:88:ASP:HA	2.02	0.42
49:YU:94:ASN:HD22	49:YU:94:ASN:C	2.23	0.42
1:QA:815:A:O4'	1:QA:817:C:C4	2.72	0.41
3:QC:120:VAL:O	3:QC:124:ILE:HG12	2.20	0.41
7:QG:87:VAL:HG23	7:QG:151:TYR:HB3	2.02	0.41
1:QA:376:G:H5''	16:QP:5:ARG:HB2	2.01	0.41
34:RA:2562:U:H4'	43:RO:25:LEU:HD21	2.02	0.41
34:RA:2576:G:P	34:RA:2576:G:N2	2.93	0.41
34:RA:2577:A:H5''	34:RA:2578:G:H5'	2.01	0.41
34:RA:414:C:H2'	34:RA:415:A:C8	2.54	0.41
38:RF:178:PRO:HB3	38:RF:198:ALA:HB2	2.02	0.41
41:RI:84:GLY:N	41:RI:89:TYR:CE2	2.89	0.41
45:RQ:62:GLY:HA2	54:RZ:116:VAL:HG21	2.01	0.41
1:XA:1040:U:H2'	1:XA:1041:A:C8	2.55	0.41
1:XA:121:C:N4	1:XA:237:C:H41	2.18	0.41
1:XA:22:G:H2'	1:XA:23:C:C6	2.55	0.41
1:XA:272:C:H2'	1:XA:273:A:C8	2.54	0.41
1:XA:475:G:H2'	1:XA:476:G:H8	1.84	0.41
1:XA:741:G:H3'	1:XA:742:G:H8	1.84	0.41
2:XB:75:LYS:HA	2:XB:75:LYS:HD3	1.85	0.41
4:XD:105:VAL:HG21	4:XD:126:ILE:HD13	2.02	0.41
5:XE:128:PRO:HA	5:XE:131:ILE:HG12	2.02	0.41
6:XF:22:GLU:OE2	6:XF:84:ASN:ND2	2.40	0.41
34:YA:2086:U:H2'	34:YA:2087:G:C8	2.55	0.41
34:YA:2306:C:H3'	34:YA:2307:G:H5''	2.01	0.41
34:YA:2845:G:H2'	34:YA:2846:G:C8	2.54	0.41
34:YA:467:G:O2'	34:YA:796:C:O2'	2.27	0.41
34:YA:191:A:HO2'	34:YA:678:C:HO2'	1.67	0.41
36:YD:45:ASN:O	36:YD:47:GLY:N	2.52	0.41
42:YN:5:VAL:HA	42:YN:6:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:YP:47:ASP:OD2	44:YP:50:ARG:NH1	2.53	0.41
46:YR:104:ARG:HD2	46:YR:109:ALA:HB3	2.01	0.41
1:QA:1154:G:H2'	1:QA:1155:G:H8	1.85	0.41
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.55	0.41
1:QA:60:A:N6	1:QA:110:C:H42	2.14	0.41
3:QC:73:PRO:HA	3:QC:76:VAL:HG22	2.01	0.41
7:QG:6:ARG:HA	7:QG:6:ARG:HD3	1.75	0.41
34:RA:1225:C:O2'	50:RV:86:GLY:N	2.36	0.41
34:RA:1600:C:OP1	52:RX:58:HIS:NE2	2.51	0.41
34:RA:87:C:H5''	34:RA:88:G:H5'	2.01	0.41
34:RA:997:G:H3'	49:RU:58:ARG:HH12	1.85	0.41
39:RG:39:ILE:HB	39:RG:92:VAL:HG13	2.02	0.41
44:RP:84:ASN:HA	44:RP:115:LEU:O	2.20	0.41
46:RR:13:HIS:O	46:RR:17:ARG:HB2	2.20	0.41
47:RS:50:SER:O	47:RS:76:LYS:NZ	2.41	0.41
1:XA:1028(C):C:H42	1:XA:1028(I):G:H1	1.68	0.41
1:XA:1318:A:H4'	19:XS:11:VAL:HG11	2.02	0.41
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.55	0.41
5:XE:75:THR:HG22	5:XE:117:ASP:O	2.21	0.41
34:YA:1028:A:OP2	34:YA:1126:A:N6	2.51	0.41
34:YA:2475:C:H42	34:YA:2529:G:N2	2.17	0.41
34:YA:2698:U:H2'	34:YA:2699:C:C6	2.54	0.41
34:YA:639:U:H2'	34:YA:640:C:C6	2.54	0.41
36:YD:66:ASP:OD1	36:YD:103:ARG:NH1	2.53	0.41
37:YE:201:THR:OG1	37:YE:202:LYS:N	2.53	0.41
39:YG:39:ILE:HG12	39:YG:157:ILE:HD12	2.02	0.41
41:YI:50:ARG:HA	41:YI:50:ARG:HD3	1.80	0.41
43:YO:70:LYS:HE2	43:YO:70:LYS:HB3	1.81	0.41
54:YZ:185:GLU:O	54:YZ:186:GLU:C	2.58	0.41
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.56	0.41
1:QA:1160:G:OP1	2:QB:132:LYS:NZ	2.48	0.41
1:QA:1308:U:OP1	13:QM:98:VAL:N	2.54	0.41
1:QA:370:C:H2'	1:QA:371:G:H8	1.84	0.41
1:QA:37:U:O2'	1:QA:500:G:O2'	2.30	0.41
1:QA:584:G:H1	1:QA:757:U:H3	1.69	0.41
1:QA:924:C:H2'	1:QA:925:G:C8	2.55	0.41
1:QA:958:A:N3	1:QA:985:C:O2'	2.42	0.41
4:QD:109:GLY:HA3	4:QD:165:MET:HG2	2.02	0.41
1:QA:7:G:O2'	5:QE:120:THR:O	2.34	0.41
28:R4:25:TYR:HE2	39:RG:3:LEU:HG	1.85	0.41
34:RA:1999:C:OP1	34:RA:2723:C:O2'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2145:C:H2'	34:RA:2147:G:C2	2.55	0.41
34:RA:2309:A:H2'	34:RA:2310:A:C4	2.56	0.41
34:RA:674:G:H1'	38:RF:74:ARG:HD2	2.02	0.41
45:RQ:116:GLU:O	45:RQ:120:ILE:HG12	2.20	0.41
49:RU:107:ALA:HA	49:RU:110:VAL:HG12	2.01	0.41
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.85	0.41
1:XA:1242:C:H2'	1:XA:1243:C:H6	1.85	0.41
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.85	0.41
1:XA:493:G:N2	1:XA:494:U:O4	2.53	0.41
1:XA:676:A:H2'	1:XA:677:U:H6	1.84	0.41
4:XD:101:LEU:HD22	4:XD:138:TYR:HB3	2.01	0.41
4:XD:161:ASN:O	4:XD:165:MET:HB2	2.21	0.41
6:XF:39:LYS:HB2	6:XF:64:GLN:HB3	2.01	0.41
33:Y9:7:VAL:O	34:YA:1031:G:O2'	2.25	0.41
34:YA:1210:A:H5''	34:YA:1211:U:H3'	2.02	0.41
34:YA:142:G:H2'	34:YA:143:C:C6	2.56	0.41
34:YA:1791:A:H3'	34:YA:1792:G:H8	1.85	0.41
44:YP:7:ARG:HA	44:YP:8:PRO:HD2	1.97	0.41
49:YU:50:ARG:O	49:YU:54:LYS:NZ	2.38	0.41
53:YY:102:CYS:SG	53:YY:103:GLY:N	2.94	0.41
1:QA:707:C:H2'	1:QA:708:C:C6	2.55	0.41
9:QL:77:ILE:O	9:QL:81:ILE:HG12	2.20	0.41
12:QL:104:VAL:O	12:QL:105:TYR:CE2	2.63	0.41
14:QN:6:LEU:HA	14:QN:6:LEU:HD23	1.84	0.41
21:QU:3:LYS:HD3	21:QU:14:TRP:CG	2.55	0.41
34:RA:1636:C:H2'	34:RA:1637:A:C8	2.55	0.41
34:RA:2174:C:H2'	34:RA:2175:C:C6	2.55	0.41
29:R5:3:LYS:HG2	34:RA:2611:U:C5	2.56	0.41
34:RA:2641:G:C6	34:RA:2774:C:N4	2.89	0.41
39:RG:63:ILE:HD13	39:RG:141:PHE:HB3	2.02	0.41
50:RV:32:THR:O	50:RV:32:THR:OG1	2.37	0.41
1:XA:1222:G:OP1	19:XS:78:ARG:NH1	2.53	0.41
1:XA:605:U:C6	1:XA:605:U:O5'	2.70	0.41
1:XA:22:G:O2'	1:XA:913:A:N1	2.46	0.41
1:XA:999:U:H2'	1:XA:1000:A:C8	2.55	0.41
2:XB:115:LEU:HB2	2:XB:145:LEU:HD23	2.02	0.41
3:XC:8:ILE:HD11	3:XC:184:TYR:H	1.84	0.41
14:YN:24:CYS:SG	14:YN:40:CYS:N	2.93	0.41
14:YN:47:LEU:HA	14:YN:47:LEU:HD23	1.86	0.41
24:Y0:72:ARG:HB3	24:Y0:75:LEU:HB2	2.02	0.41
34:YA:223:A:N6	34:YA:374:A:O2'	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:685:A:C2	34:YA:787:U:H1'	2.55	0.41
34:YA:996:A:O3'	49:YU:92:ARG:NH2	2.53	0.41
37:YE:132:HIS:O	37:YE:132:HIS:CD2	2.73	0.41
34:YA:1252:G:H21	49:YU:33:ARG:HH11	1.68	0.41
1:QA:186(J):U:H3	17:QQ:63:ARG:HG2	1.85	0.41
1:QA:34:C:H2'	1:QA:35:G:H8	1.85	0.41
1:QA:696:A:H2'	1:QA:697:U:H6	1.86	0.41
1:QA:831:U:H2'	1:QA:832:C:H6	1.86	0.41
13:QM:37:THR:O	13:QM:55:ARG:NH2	2.53	0.41
27:R3:4:LEU:HD21	27:R3:56:VAL:HB	2.02	0.41
34:RA:1234:U:H2'	34:RA:1235:G:C5'	2.48	0.41
34:RA:1716:U:O2	34:RA:1743:G:O6	2.38	0.41
34:RA:1841:U:H2'	34:RA:1842:G:H8	1.85	0.41
34:RA:2191:G:H2'	34:RA:2191:G:N3	2.35	0.41
32:R8:12:LYS:NZ	34:RA:247:G:O6	2.38	0.41
41:RI:143:SER:HB2	41:RI:144:VAL:H	1.64	0.41
44:RP:137:LYS:HD3	44:RP:137:LYS:HA	1.86	0.41
44:RP:41:ARG:HD3	44:RP:41:ARG:HA	1.82	0.41
49:RU:27:LEU:O	49:RU:31:SER:HB3	2.20	0.41
53:RY:99:CYS:HB3	53:RY:102:CYS:H	1.85	0.41
54:RZ:24:LEU:HA	54:RZ:25:PRO:HD3	1.92	0.41
1:XA:1236:A:H4'	1:XA:1304:G:H4'	2.02	0.41
1:XA:1237:C:H5''	1:XA:1238:A:C8	2.56	0.41
1:XA:1440(K):C:OP1	1:XA:1440(L):G:N1	2.54	0.41
1:XA:718:G:OP2	1:XA:720:C:N4	2.52	0.41
11:XK:51:LYS:HB2	11:XK:51:LYS:HE2	1.93	0.41
14:XN:47:LEU:HD22	14:XN:52:GLN:HB2	2.02	0.41
23:XX:8:A:H2'	23:XX:9:G:C8	2.55	0.41
34:YA:1173:G:H4'	34:YA:1174:A:C8	2.55	0.41
40:YH:86:GLU:H	40:YH:86:GLU:HG2	1.51	0.41
54:YZ:6:LYS:O	54:YZ:62:PRO:HD3	2.20	0.41
1:QA:1009:G:H2'	1:QA:1010:G:H8	1.86	0.41
1:QA:225:C:H2'	1:QA:226:G:H8	1.84	0.41
1:QA:377:G:H2'	1:QA:378:G:C8	2.55	0.41
1:QA:475:G:H2'	1:QA:476:G:C8	2.56	0.41
3:QC:76:VAL:HG21	3:QC:103:VAL:HG11	2.03	0.41
8:QH:3:THR:OG1	8:QH:4:ASP:N	2.54	0.41
1:QA:127:G:HO2'	17:QQ:2:PRO:N	2.17	0.41
29:R5:33:CYS:SG	29:R5:46:CYS:HB2	2.60	0.41
34:RA:1149:G:H2'	34:RA:1150:C:H6	1.86	0.41
34:RA:1664:A:H61	34:RA:1996:C:H42	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:QV:3:G:O2'	34:RA:1851:U:OP1	2.38	0.41
34:RA:2183:C:H2'	34:RA:2184:G:H8	1.85	0.41
36:RD:268:ARG:HG3	36:RD:269:PHE:CD2	2.55	0.41
40:RH:91:GLY:HA2	40:RH:160:LYS:HG2	2.03	0.41
1:XA:1160:G:O6	1:XA:1177:G:N2	2.53	0.41
1:XA:501:C:H2'	1:XA:502:G:H8	1.86	0.41
13:XM:9:ILE:HA	13:XM:9:ILE:HD13	1.93	0.41
27:Y3:31:LEU:HA	27:Y3:31:LEU:HD23	1.87	0.41
34:YA:1889:A:N3	34:YA:2086:U:O2'	2.52	0.41
34:YA:305:U:C4	34:YA:312:G:O6	2.73	0.41
34:YA:67:U:H3	34:YA:74:A:H2	1.69	0.41
35:YB:30:C:H1'	35:YB:57:A:H61	1.85	0.41
1:QA:1300:G:O2'	1:QA:1303:C:N4	2.47	0.41
1:QA:405:U:P	4:QD:118:ARG:HH12	2.43	0.41
1:QA:628:G:H2'	1:QA:629:G:C8	2.56	0.41
2:QB:75:LYS:HA	2:QB:75:LYS:HD3	1.83	0.41
13:QM:77:ASN:O	13:QM:81:LEU:HG	2.21	0.41
34:RA:1029:A:OP1	45:RQ:128:LYS:NZ	2.43	0.41
34:RA:1537:C:H2'	34:RA:1538:G:C8	2.56	0.41
34:RA:271(E):G:H2'	34:RA:272:G:C8	2.55	0.41
34:RA:2751:G:N3	40:RH:3:ARG:CB	2.84	0.41
34:RA:642:G:H21	34:RA:646:A:H2	1.67	0.41
37:RE:134:ILE:HD12	37:RE:137:HIS:HB2	2.02	0.41
39:RG:141:PHE:HB2	39:RG:144:ILE:HD13	2.03	0.41
48:RT:66:VAL:HA	48:RT:71:GLY:HA2	2.02	0.41
49:RU:39:LEU:HA	49:RU:39:LEU:HD23	1.93	0.41
49:RU:58:ARG:HH11	49:RU:93:LYS:NZ	2.18	0.41
1:XA:1028(C):C:N4	1:XA:1028(I):G:H1	2.18	0.41
1:XA:1250:A:N3	1:XA:1370:G:O2'	2.46	0.41
1:XA:359:U:H2'	1:XA:360:A:H8	1.84	0.41
1:XA:605:U:H6	1:XA:605:U:C5'	2.33	0.41
29:Y5:11:THR:HG23	29:Y5:15:ARG:HD2	2.02	0.41
29:Y5:58:LEU:HD23	46:YR:113:LEU:HD11	2.03	0.41
34:YA:2867:G:O2'	34:YA:2868:A:H8	2.04	0.41
34:YA:336:C:HO2'	53:YY:35:TYR:HH	1.68	0.41
34:YA:698:C:O2'	34:YA:734:A:N6	2.53	0.41
34:YA:945:A:N3	34:YA:945:A:H2'	2.36	0.41
36:YD:44:ASN:OD1	36:YD:44:ASN:N	2.53	0.41
37:YE:104:VAL:HG11	37:YE:188:VAL:HG12	2.03	0.41
48:YT:3:ARG:O	48:YT:7:ILE:HG12	2.21	0.41
54:YZ:178:GLU:HB3	54:YZ:179:ASP:H	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.39	0.41
1:QA:434:U:H2'	1:QA:435:C:C6	2.56	0.41
2:QB:167:PRO:O	2:QB:171:ALA:CB	2.67	0.41
2:QB:20:GLU:HG3	2:QB:191:ASP:HB2	2.02	0.41
4:QD:122:ARG:HA	4:QD:122:ARG:HD2	1.90	0.41
34:RA:1569:A:H2'	34:RA:1570:A:C8	2.56	0.41
34:RA:171:G:H2'	34:RA:172:C:C6	2.56	0.41
34:RA:690:G:H21	36:RD:43:ARG:NH2	2.18	0.41
34:RA:946:G:H2'	34:RA:947:G:H8	1.85	0.41
42:RN:97:ARG:HA	42:RN:100:GLU:HB2	2.02	0.41
45:RQ:31:ASP:OD2	45:RQ:134:ARG:NH2	2.54	0.41
45:RQ:34:LEU:HD13	45:RQ:118:LEU:HD12	2.03	0.41
46:RR:96:ARG:HB2	46:RR:117:VAL:HG12	2.02	0.41
48:RT:8:LYS:HE2	48:RT:8:LYS:HB2	1.86	0.41
54:RZ:5:LEU:H	54:RZ:59:LEU:HA	1.85	0.41
1:XA:539:A:H2'	1:XA:540:G:H8	1.85	0.41
2:XB:40:HIS:HB2	2:XB:190:THR:HG21	2.01	0.41
5:XE:110:LEU:HB3	5:XE:115:VAL:HB	2.03	0.41
13:XM:87:TYR:OH	13:XM:91:ARG:NH1	2.53	0.41
15:XO:26:GLU:HG3	15:XO:81:LEU:HD22	2.03	0.41
34:YA:2475:C:N4	34:YA:2529:G:H22	2.17	0.41
34:YA:270(V):C:H2'	34:YA:270(W):G:H8	1.86	0.41
34:YA:2810:A:H61	34:YA:2891:G:H2'	1.86	0.41
34:YA:922:U:H2'	34:YA:923:C:C6	2.56	0.41
34:YA:993:G:H4'	50:YV:70:ILE:HD11	2.02	0.41
36:YD:231:HIS:CD2	36:YD:249:PRO:HG3	2.56	0.41
1:QA:1330:U:H4'	13:QM:23:TYR:CD2	2.56	0.41
1:QA:186(B):C:OP1	20:QT:82:SER:OG	2.33	0.41
1:QA:757:U:OP1	1:QA:822:C:O2'	2.38	0.41
3:QC:36:ASP:OD1	3:QC:59:ARG:NH2	2.53	0.41
9:QI:25:LYS:O	9:QI:60:ASP:HA	2.21	0.41
1:QA:110:C:O2'	16:QP:25:ARG:O	2.29	0.41
22:QV:23:C:H2'	22:QV:24:G:H8	1.85	0.41
25:R1:8:SER:HB3	25:R1:66:HIS:CD2	2.55	0.41
26:R2:45:SER:OG	26:R2:46:GLN:N	2.53	0.41
34:RA:1400:G:H2'	34:RA:1401:G:C8	2.55	0.41
34:RA:177:G:H5'	34:RA:178:G:C8	2.56	0.41
34:RA:2128:C:O2'	34:RA:2173:A:N3	2.43	0.41
34:RA:2581:G:C5	34:RA:2610:C:C4	3.09	0.41
34:RA:270(F):G:H1	34:RA:270(V):C:H42	1.69	0.41
34:RA:2788:C:O2'	34:RA:2809:A:N3	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RD:35:LYS:HB3	36:RD:63:ARG:HA	2.03	0.41
41:RI:14:ASP:HB3	41:RI:15:VAL:H	1.65	0.41
49:RU:34:LYS:HA	49:RU:34:LYS:HD3	1.72	0.41
1:XA:1109:C:OP2	3:XC:176:HIS:ND1	2.54	0.41
1:XA:1324:A:H5'	1:XA:1362(B):C:H5'	2.02	0.41
1:XA:1366:C:O3'	10:XJ:60:ARG:NH2	2.53	0.41
1:XA:559:A:H4'	1:XA:560:U:H3'	2.03	0.41
3:XC:35:GLU:HB3	3:XC:59:ARG:HH22	1.85	0.41
9:XI:10:ARG:CZ	9:XI:105:ASP:HB2	2.51	0.41
13:XM:26:GLY:O	13:XM:30:ALA:HB2	2.20	0.41
20:XT:18:GLN:HE21	20:XT:22:ARG:NH2	2.19	0.41
34:YA:1196:C:O2'	34:YA:1228:G:O2'	2.24	0.41
34:YA:2103:C:H2'	34:YA:2104:G:H8	1.86	0.41
34:YA:218:A:N1	34:YA:235:U:H4'	2.36	0.41
34:YA:270(Q):C:H1'	41:YI:50:ARG:HH22	1.86	0.41
34:YA:363(C):G:H2'	34:YA:363(D):G:C8	2.55	0.41
34:YA:589:C:H2'	34:YA:590:A:H8	1.85	0.41
34:YA:860:U:OP2	34:YA:916:G:N1	2.53	0.41
34:YA:870:A:OP1	45:YQ:6:ARG:NH2	2.37	0.41
35:YB:48:A:H2'	35:YB:49:C:C6	2.56	0.41
48:YT:19:LEU:HA	48:YT:20:PRO:HD3	1.91	0.41
1:QA:936:C:H1'	1:QA:1382:C:H42	1.86	0.41
1:QA:186(F):C:H2'	1:QA:186(G):C:C6	2.56	0.41
1:QA:639:G:H2'	1:QA:640:A:C8	2.56	0.41
3:QC:12:LEU:HG	3:QC:18:TRP:NE1	2.36	0.41
4:QD:8:VAL:HG13	4:QD:21:LEU:HD12	2.02	0.41
25:R1:80:LEU:HD12	25:R1:81:LYS:HB2	2.03	0.41
29:R5:51:TYR:HD1	29:R5:55:ARG:O	2.03	0.41
34:RA:747:U:O2	34:RA:2014:A:H1'	2.21	0.41
34:RA:851:U:H2'	34:RA:852:G:H8	1.86	0.41
40:RH:123:PHE:HA	40:RH:123:PHE:HD2	1.77	0.41
34:RA:2684:U:O2'	43:RO:68:GLU:OE2	2.32	0.41
54:RZ:151:HIS:HB2	54:RZ:170:THR:HA	2.02	0.41
35:RB:75:G:H21	54:RZ:85:HIS:HD1	1.68	0.41
1:XA:396:G:O2'	1:XA:398:C:OP1	2.28	0.41
1:XA:445:G:H2'	1:XA:446:G:C8	2.55	0.41
1:XA:452:A:O2'	1:XA:453:A:O5'	2.36	0.41
1:XA:548:G:H5'	4:XD:73:ARG:NH2	2.36	0.41
1:XA:1055:A:O2'	3:XC:161:GLU:O	2.26	0.41
6:XF:12:PRO:HD3	6:XF:58:GLY:HA2	2.02	0.41
24:Y0:23:VAL:HA	24:Y0:38:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y5:49:CYS:SG	29:Y5:50:GLY:N	2.93	0.41
30:Y6:46:HIS:ND1	34:YA:2371:G:O2'	2.42	0.41
34:YA:1853:A:N6	34:YA:1889:A:N7	2.68	0.41
25:Y1:43:TYR:HD2	34:YA:2230:G:H5''	1.85	0.41
38:YF:157:VAL:HG21	38:YF:181:LEU:HD13	2.03	0.41
41:YI:143:SER:HB2	41:YI:144:VAL:H	1.60	0.41
52:YX:34:ALA:O	52:YX:77:LYS:NZ	2.54	0.41
1:QA:318:G:H2'	1:QA:319:G:C8	2.56	0.41
1:QA:57:G:H2'	1:QA:58:C:C6	2.56	0.41
1:QA:737:A:H2'	1:QA:738:C:H6	1.86	0.41
1:QA:838(A):G:H1	1:QA:848:C:H42	1.68	0.41
1:QA:999:U:O4	1:QA:1000:A:N6	2.54	0.41
4:QD:28:SER:HA	4:QD:29:PRO:HD3	1.96	0.41
29:R5:36:CYS:HG	29:R5:49:CYS:HB3	1.86	0.41
32:R8:35:GLN:NE2	32:R8:36:LYS:CE	2.80	0.41
34:RA:1130:U:O2	37:RE:149:ARG:NH2	2.38	0.41
34:RA:1405:U:H2'	34:RA:1406:U:C6	2.56	0.41
34:RA:1669:A:N3	34:RA:1669:A:H2'	2.34	0.41
34:RA:1853:A:N6	34:RA:1889:A:N7	2.69	0.41
34:RA:1773:A:HO2'	34:RA:1978:A:H61	1.69	0.41
34:RA:2194:G:C2'	34:RA:2195:C:H5'	2.50	0.41
34:RA:2696:U:H2'	34:RA:2697:G:C8	2.56	0.41
34:RA:557:U:H2'	34:RA:558:G:H8	1.86	0.41
39:RG:33:ARG:H	39:RG:162:THR:HG22	1.85	0.41
1:XA:23:C:OP2	1:XA:561:U:N3	2.40	0.41
1:XA:40:C:H2'	1:XA:41:G:C8	2.55	0.41
3:XC:91:LEU:HD22	3:XC:101:LEU:HD21	2.03	0.41
4:XD:170:VAL:HB	4:XD:174:LEU:HD12	2.02	0.41
12:XL:56:ALA:HB2	12:XL:70:ILE:HD11	2.03	0.41
34:YA:2513:G:O2'	37:YE:151:TYR:OH	2.20	0.41
34:YA:82:G:H5''	34:YA:296:C:H5'	2.03	0.41
34:YA:64:A:OP1	52:YX:73:ARG:NH1	2.54	0.41
38:YF:116:ASP:OD1	38:YF:119:ARG:NH2	2.52	0.41
44:YP:137:LYS:HD3	44:YP:137:LYS:HA	1.86	0.41
46:YR:56:LYS:NZ	46:YR:90:ARG:O	2.53	0.41
52:YX:92:LEU:HD23	52:YX:92:LEU:HA	1.86	0.41
53:YY:39:VAL:HG23	53:YY:42:VAL:HB	2.01	0.41
54:YZ:4:ARG:NH1	54:YZ:60:GLU:OE2	2.54	0.41
1:QA:1525:G:H2'	1:QA:1526:G:H8	1.85	0.40
1:QA:836:G:H2'	1:QA:837:G:C8	2.56	0.40
12:QL:32:PHE:HB3	12:QL:84:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:QN:12:ARG:HE	14:QN:14:PRO:HD2	1.86	0.40
17:QQ:75:ARG:HD2	17:QQ:75:ARG:HA	1.88	0.40
34:RA:2688:U:OP1	34:RA:2713:A:N6	2.54	0.40
34:RA:270(A):A:OP2	34:RA:270(Z):G:N2	2.54	0.40
34:RA:2810:A:H61	34:RA:2891:G:H2'	1.87	0.40
35:RB:55:U:O2'	39:RG:27:ASN:ND2	2.51	0.40
39:RG:132:ASN:HD22	39:RG:158:ALA:HA	1.86	0.40
40:RH:103:LEU:HD11	40:RH:123:PHE:CE2	2.45	0.40
40:RH:126:PRO:HD2	40:RH:131:VAL:HA	2.03	0.40
47:RS:59:LYS:HA	47:RS:59:LYS:HD2	1.94	0.40
34:RA:1598:C:H5'	52:RX:36:LYS:HB2	2.02	0.40
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.51	0.40
1:XA:1309:G:O3'	13:XM:77:ASN:ND2	2.48	0.40
1:XA:939:G:H4'	7:XG:102:ARG:NH2	2.36	0.40
8:XH:10:LEU:HD12	8:XH:83:ILE:HD12	2.03	0.40
34:YA:1307:A:N6	34:YA:1622:G:O6	2.54	0.40
34:YA:2578:G:OP1	34:YA:2614:A:N6	2.51	0.40
34:YA:394:A:H2'	34:YA:395:U:O4'	2.21	0.40
34:YA:423:A:H8	34:YA:423:A:O5'	2.03	0.40
34:YA:974(A):G:C5	34:YA:1186:G:N2	2.89	0.40
34:YA:443:A:N7	38:YF:45:ARG:HD3	2.36	0.40
43:YO:71:ARG:HH21	43:YO:77:ILE:HG21	1.86	0.40
48:YT:130:ALA:HA	48:YT:133:GLU:HG2	2.04	0.40
54:YZ:24:LEU:HA	54:YZ:25:PRO:HD3	1.87	0.40
1:QA:1096:C:H2'	1:QA:1097:C:C6	2.56	0.40
1:QA:819:A:C5	1:QA:1529:G:C6	3.10	0.40
1:QA:838(A):G:N2	1:QA:849:C:O2	2.54	0.40
10:QJ:99:LYS:HD3	10:QJ:99:LYS:HA	1.79	0.40
22:QV:37:1MG:C2	22:QV:38:A:H1'	2.56	0.40
34:RA:1798:U:O2'	34:RA:1802:A:N3	2.48	0.40
34:RA:2844:G:H3'	34:RA:2845:G:H8	1.87	0.40
34:RA:2853:C:H2'	34:RA:2854:G:C8	2.56	0.40
34:RA:925:C:H2'	34:RA:926:A:H8	1.86	0.40
36:RD:105:ILE:HD12	36:RD:105:ILE:HA	1.91	0.40
36:RD:134:ARG:N	36:RD:187:GLY:O	2.54	0.40
40:RH:103:LEU:O	40:RH:114:VAL:HA	2.22	0.40
44:RP:28:GLY:C	44:RP:30:THR:H	2.24	0.40
50:RV:73:SER:OG	50:RV:74:LYS:N	2.53	0.40
1:XA:1320:C:H2'	1:XA:1321:C:C6	2.57	0.40
1:XA:68(B):G:H2'	1:XA:68(C):G:H8	1.87	0.40
8:XH:34:GLU:O	8:XH:38:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1009:A:OP2	34:YA:1010:A:OP2	2.40	0.40
34:YA:237:C:O2	34:YA:609(A):A:O2'	2.35	0.40
34:YA:2503:A:O2'	34:YA:2505:G:OP2	2.31	0.40
34:YA:270(S):G:H2'	34:YA:270(T):G:H8	1.86	0.40
34:YA:436:C:H2'	34:YA:438:G:C8	2.56	0.40
34:YA:918:A:N3	35:YB:80:U:O2'	2.53	0.40
36:YD:172:TYR:HB3	36:YD:184:LYS:HG2	2.04	0.40
34:YA:2052:G:O2'	37:YE:144:ARG:O	2.38	0.40
37:YE:154:LYS:HD2	37:YE:154:LYS:HA	1.87	0.40
40:YH:115:VAL:HG21	40:YH:148:ILE:HD11	2.02	0.40
41:YI:121:LYS:HA	41:YI:121:LYS:HD3	1.67	0.40
44:YP:6:LEU:HA	44:YP:6:LEU:HD23	1.90	0.40
53:YY:12:THR:HA	53:YY:26:LYS:HA	2.03	0.40
54:YZ:94:GLU:HA	54:YZ:95:PRO:HD2	1.75	0.40
1:QA:1077:G:N2	1:QA:1079:G:H3'	2.36	0.40
1:QA:1142:G:H3'	1:QA:1143:G:H8	1.86	0.40
1:QA:1277:C:HO2'	1:QA:1279:A:H8	1.66	0.40
1:QA:1419:G:H1	1:QA:1481:U:H3	1.69	0.40
1:QA:157:G:H2'	1:QA:158:G:C8	2.56	0.40
5:QE:11:ILE:HG21	5:QE:31:LEU:HD23	2.02	0.40
10:QJ:14:LYS:HD3	10:QJ:15:THR:HG23	2.02	0.40
16:QP:14:ASN:OD1	16:QP:16:HIS:NE2	2.54	0.40
32:R8:3:LYS:H	32:R8:3:LYS:HG2	1.71	0.40
34:RA:1053:C:H2'	34:RA:1054:A:C8	2.56	0.40
34:RA:1418:G:N1	34:RA:1579:A:OP2	2.42	0.40
34:RA:172:C:H2'	34:RA:173:G:H8	1.85	0.40
34:RA:949:C:H2'	34:RA:950:G:C8	2.56	0.40
34:RA:2304:G:O2'	39:RG:134:GLY:N	2.53	0.40
40:RH:102:ALA:HA	40:RH:117:PRO:HD3	2.03	0.40
45:RQ:30:GLY:HA2	45:RQ:107:ALA:HB2	2.03	0.40
49:RU:58:ARG:O	49:RU:62:ILE:HG12	2.20	0.40
1:XA:1028(I):G:H2'	1:XA:1033:G:C8	2.56	0.40
1:XA:1321:C:H5''	1:XA:1322:C:H5''	2.02	0.40
1:XA:165:C:H2'	1:XA:166:G:H8	1.86	0.40
1:XA:68(G):C:H2'	1:XA:68(H):G:C8	2.56	0.40
1:XA:783:C:OP1	1:XA:1515:C:O2'	2.37	0.40
2:XB:104:ASN:O	2:XB:108:ILE:HG12	2.21	0.40
2:XB:134:GLU:HG3	2:XB:137:ARG:NE	2.37	0.40
34:YA:2074:U:O2'	34:YA:2597:G:O2'	2.33	0.40
34:YA:2626:C:H2'	34:YA:2627:G:C8	2.57	0.40
34:YA:2737:G:H2'	34:YA:2738:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YB:48:A:H4'	47:YS:95:HIS:HD2	1.85	0.40
50:YV:68:LYS:HA	50:YV:68:LYS:HD3	1.75	0.40
1:QA:1363:A:H4'	1:QA:1364:U:H5''	2.03	0.40
1:QA:45:U:H5''	1:QA:307:C:H1'	2.03	0.40
1:QA:429:U:H3'	4:QD:9:CYS:SG	2.62	0.40
1:QA:736:C:H2'	1:QA:737:A:H8	1.85	0.40
3:QC:56:ASP:HB3	3:QC:67:THR:HG23	2.02	0.40
10:QJ:84:GLN:O	10:QJ:88:LEU:HB2	2.22	0.40
34:RA:1364:G:N2	34:RA:1367:A:OP2	2.37	0.40
34:RA:1375:C:H2'	34:RA:1376:C:H6	1.87	0.40
34:RA:1388:G:O2'	34:RA:1525:G:O2'	2.27	0.40
34:RA:2364:C:H2'	34:RA:2365:G:O4'	2.21	0.40
46:RR:3:HIS:HB3	46:RR:4:LEU:H	1.64	0.40
1:XA:113:G:H2'	1:XA:114:U:C6	2.56	0.40
1:XA:1152:A:H5''	10:XJ:13:HIS:CD2	2.57	0.40
1:XA:1154:G:H2'	1:XA:1155:G:H8	1.87	0.40
1:XA:1262:C:H2'	1:XA:1263:C:C6	2.56	0.40
1:XA:1293:G:H2'	1:XA:1294:G:H8	1.87	0.40
1:XA:677:U:O2	1:XA:777:A:O2'	2.37	0.40
1:XA:952:U:H2'	1:XA:953:G:H8	1.85	0.40
2:XB:188:ALA:HB1	2:XB:192:SER:HB3	2.03	0.40
2:XB:88:ALA:O	2:XB:226:ARG:NH1	2.46	0.40
4:XD:202:LEU:HA	4:XD:205:GLU:HB2	2.03	0.40
8:XH:34:GLU:HB3	8:XH:118:VAL:HG11	2.03	0.40
12:XL:70:ILE:HG13	12:XL:100:ILE:HG13	2.03	0.40
34:YA:2197:U:H1'	34:YA:2198:A:C8	2.56	0.40
34:YA:828:U:C2'	34:YA:828:U:O2	2.70	0.40
36:YD:61:LEU:HA	36:YD:61:LEU:HD23	1.94	0.40
50:YV:69:LYS:HA	50:YV:87:HIS:O	2.21	0.40
54:YZ:14:LYS:HA	54:YZ:15:PRO:HD3	1.93	0.40
1:QA:1306:A:N6	1:QA:1331:G:HO2'	2.20	0.40
1:QA:1385:G:H2'	1:QA:1386:G:C8	2.56	0.40
1:QA:299:G:H2'	1:QA:300:A:C8	2.57	0.40
3:QC:44:GLU:HA	3:QC:52:LEU:HD21	2.03	0.40
4:QD:3:ARG:HE	4:QD:118:ARG:HD2	1.85	0.40
20:QT:74:LYS:O	20:QT:76:ALA:N	2.55	0.40
30:R6:29:ASN:HD22	34:RA:2286:A:P	2.44	0.40
34:RA:1358:G:H21	34:RA:1373:A:H62	1.69	0.40
34:RA:1352:U:O2'	34:RA:1570:A:N3	2.52	0.40
34:RA:2150:U:H2'	34:RA:2151:G:C8	2.56	0.40
34:RA:2310:A:H61	39:RG:79:ASN:HD22	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:848:G:C2	34:RA:933:A:H1'	2.57	0.40
35:RB:111:U:H2'	35:RB:112:G:H8	1.85	0.40
38:RF:160:ASN:OD1	38:RF:160:ASN:N	2.54	0.40
41:RI:40:THR:OG1	41:RI:41:GLU:N	2.54	0.40
44:RP:64:LYS:O	44:RP:66:GLY:N	2.55	0.40
1:XA:1021:G:H2'	1:XA:1022:G:C8	2.57	0.40
1:XA:21:G:H2'	1:XA:22:G:H8	1.87	0.40
1:XA:685:G:N2	1:XA:705:U:O4	2.55	0.40
1:XA:980:C:O3'	14:YN:9:LYS:NZ	2.43	0.40
18:XR:30:ASP:OD2	18:XR:33:ASP:N	2.54	0.40
19:XS:66:MET:HB3	19:XS:66:MET:HE2	2.00	0.40
23:XX:3:C:H2'	23:XX:4:A:C8	2.56	0.40
34:YA:1309:G:HO2'	34:YA:1611:C:HO2'	1.56	0.40
34:YA:172:C:H2'	34:YA:173:G:H8	1.86	0.40
34:YA:570:G:H2'	34:YA:2030:A:C5	2.57	0.40
36:YD:175:LEU:O	36:YD:182:LEU:HA	2.22	0.40
42:YN:34:LEU:O	42:YN:49:GLY:HA3	2.21	0.40
48:YT:80:SER:HA	48:YT:81:PRO:HD3	1.96	0.40
50:YV:100:ARG:HB2	50:YV:100:ARG:HE	1.70	0.40
49:YU:95:LEU:HG	50:YV:4:ILE:HD13	2.02	0.40
54:YZ:128:VAL:HG22	54:YZ:161:VAL:HG22	2.04	0.40
54:YZ:5:LEU:HB3	54:YZ:6:LYS:H	1.72	0.40

All (1) 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)
41:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	1.70	0.50

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	72
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	68
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	68
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	22	61
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	61
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	13 (10%)	1 (1%)	19	58
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	54
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	19	58
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	9	42
13	XM	112/126 (89%)	101 (90%)	10 (9%)	1 (1%)	17	56
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
14	XN	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	28
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	30
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	4	30
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	14	52
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	13 (30%)	3 (7%)	1	13
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	4	29
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	22	61
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	34	72
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YE	203/206 (98%)	163 (80%)	38 (19%)	2 (1%)	15	54
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	15	54
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	29	68
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25	64
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	9	42
40	YH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	4	31
41	RI	144/148 (97%)	115 (80%)	23 (16%)	6 (4%)	3	23
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	5	32
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	61
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	22	61
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
43	YO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	7	39
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	22	61
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	22	61
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	61
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	17	56
47	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	17	56
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100	100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	5	33
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	54
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	54
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	6	37
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	3	26
All	All	11414/12128 (94%)	10111 (89%)	1217 (11%)	86 (1%)	19	58

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR
41	RI	11	ASN
44	RP	108	LYS
49	RU	91	ASP
49	RU	92	ARG
54	RZ	53	ILE
4	XD	156	GLU
20	XT	74	LYS
20	XT	75	ASN
28	Y4	5	ILE
28	Y4	24	THR
37	YE	147	PRO
40	YH	157	TYR
44	YP	108	LYS
50	YV	50	PRO
54	YZ	53	ILE
54	YZ	182	LYS
14	QN	17	LYS
32	R8	29	LYS
36	RD	243	GLY
39	RG	81	LYS
40	RH	126	PRO
41	RI	132	PRO
42	RN	22	THR
44	RP	22	GLY
49	RU	90	VAL
54	RZ	167	PRO
14	XN	57	ARG

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Mol	Chain	Res	Type
36	YD	243	GLY
40	YH	47	GLU
41	YI	122	GLU
41	YI	132	PRO
47	YS	110	LEU
54	YZ	60	GLU
54	YZ	167	PRO
13	QM	118	ALA
20	QT	74	LYS
36	RD	242	ARG
37	RE	130	GLY
38	RF	67	GLN
38	RF	129	PHE
38	YF	129	PHE
46	YR	4	LEU
10	QJ	55	LYS
29	R5	49	CYS
37	RE	17	ASP
37	RE	83	ASP
41	RI	10	GLU
41	RI	122	GLU
44	RP	29	LYS
54	RZ	52	SER
54	RZ	63	ASP
13	XM	7	VAL
20	XT	73	HIS
28	Y4	40	HIS
29	Y5	49	CYS
40	YH	152	ARG
41	YI	15	VAL
54	YZ	183	LEU
20	QT	98	PRO
37	RE	82	ARG
40	RH	156	ALA
50	RV	53	GLU
5	XE	74	GLY
14	XN	56	VAL
40	YH	156	ALA
42	YN	22	THR
54	YZ	61	LEU
4	QD	156	GLU
13	QM	13	LYS

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Mol	Chain	Res	Type
41	RI	15	VAL
9	XI	119	ALA
25	Y1	54	ALA
37	YE	54	GLN
45	YQ	7	MET
54	YZ	94	GLU
5	QE	74	GLY
2	XB	208	ILE
45	RQ	78	PRO
41	YI	133	HIS
41	RI	119	PRO
40	YH	12	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	200 (98%)	3 (2%)	65	84
2	XB	204/220 (93%)	203 (100%)	1 (0%)	88	94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	86
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	86
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	94
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	88
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	88
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	91
8	XH	118/119 (99%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	79
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	79
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	88
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	88
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	99 (96%)	4 (4%)	32	64
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	XN	49/50 (98%)	46 (94%)	3 (6%)	18	51
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	75
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	86
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	58
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	R0	65/67 (97%)	64 (98%)	1 (2%)	65	84
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	47	75
25	Y1	78/83 (94%)	77 (99%)	1 (1%)	69	86
26	R2	64/67 (96%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	83
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	51 (100%)	0	100	100
28	R4	40/63 (64%)	40 (100%)	0	100	100
28	Y4	41/63 (65%)	39 (95%)	2 (5%)	25	59
29	R5	51/52 (98%)	50 (98%)	1 (2%)	55	79
29	Y5	51/52 (98%)	47 (92%)	4 (8%)	12	42
30	R6	51/52 (98%)	48 (94%)	3 (6%)	19	53
30	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	64
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	54 (100%)	0	100	100
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	53
36	RD	214/218 (98%)	212 (99%)	2 (1%)	78	90
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	161 (98%)	4 (2%)	49	76
37	YE	165/166 (99%)	162 (98%)	3 (2%)	59	81
38	RF	161/166 (97%)	158 (98%)	3 (2%)	57	80
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	155 (100%)	0	100	100
39	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
40	RH	145/148 (98%)	137 (94%)	8 (6%)	21	54
40	YH	145/148 (98%)	142 (98%)	3 (2%)	53	79
41	RI	122/124 (98%)	122 (100%)	0	100	100
41	YI	122/124 (98%)	118 (97%)	4 (3%)	38	68
42	RN	117/119 (98%)	116 (99%)	1 (1%)	78	90
42	YN	117/119 (98%)	115 (98%)	2 (2%)	60	82
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	97 (97%)	3 (3%)	41	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RP	116/116 (100%)	115 (99%)	1 (1%)	78	90
44	YP	114/116 (98%)	114 (100%)	0	100	100
45	RQ	111/111 (100%)	111 (100%)	0	100	100
45	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	90
46	RR	100/101 (99%)	98 (98%)	2 (2%)	55	79
46	YR	100/101 (99%)	99 (99%)	1 (1%)	76	88
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	RT	120/127 (94%)	117 (98%)	3 (2%)	47	75
48	YT	120/127 (94%)	118 (98%)	2 (2%)	60	82
49	RU	93/94 (99%)	93 (100%)	0	100	100
49	YU	93/94 (99%)	91 (98%)	2 (2%)	52	78
50	RV	82/82 (100%)	82 (100%)	0	100	100
50	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
51	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	71 (96%)	3 (4%)	30	63
52	YX	74/78 (95%)	72 (97%)	2 (3%)	44	73
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	87 (99%)	1 (1%)	73	88
54	RZ	162/179 (90%)	162 (100%)	0	100	100
54	YZ	167/179 (93%)	165 (99%)	2 (1%)	71	87
All	All	9648/10066 (96%)	9536 (99%)	112 (1%)	71	87

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	36	ARG
2	QB	149	LEU
2	QB	217	ARG
3	QC	38	ARG
3	QC	127	ARG
4	QD	18	LYS
8	QH	59	LEU

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Mol	Chain	Res	Type
9	QI	64	THR
9	QI	85	LEU
11	QK	41	THR
14	QN	43	CYS
15	QO	22	THR
15	QO	87	ILE
20	QT	73	HIS
21	QU	6	ARG
24	R0	14	ARG
25	R1	73	LEU
25	R1	92	LYS
29	R5	36	CYS
30	R6	13	CYS
30	R6	23	THR
30	R6	53	LYS
36	RD	242	ARG
36	RD	268	ARG
37	RE	107	THR
37	RE	144	ARG
37	RE	154	LYS
37	RE	176	ILE
38	RF	89	VAL
38	RF	144	LYS
38	RF	195	ASP
40	RH	17	VAL
40	RH	69	ARG
40	RH	123	PHE
40	RH	125	VAL
40	RH	127	GLU
40	RH	129	THR
40	RH	130	ARG
40	RH	131	VAL
42	RN	34	LEU
44	RP	16	ARG
46	RR	10	LEU
46	RR	12	ARG
48	RT	85	LYS
48	RT	111	ARG
48	RT	129	ARG
51	RW	52	GLU
52	RX	16	LYS
52	RX	27	THR

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Mol	Chain	Res	Type
52	RX	76	ARG
2	XB	21	ARG
3	XC	12	LEU
3	XC	162	GLN
4	XD	135	LEU
4	XD	191	ARG
5	XE	12	LEU
6	XF	80	ARG
9	XI	25	LYS
9	XI	27	THR
11	XK	117	ASN
12	XL	8	ASN
12	XL	41	ARG
12	XL	89	ARG
12	XL	105	TYR
14	XN	12	ARG
14	XN	27	CYS
14	XN	56	VAL
17	XQ	50	LYS
17	XQ	74	LEU
25	Y1	50	ARG
26	Y2	47	ASN
28	Y4	5	ILE
28	Y4	16	CYS
29	Y5	37	LYS
29	Y5	40	LYS
29	Y5	45	VAL
29	Y5	49	CYS
30	Y6	13	CYS
30	Y6	43	CYS
33	Y9	13	LYS
33	Y9	27	CYS
37	YE	12	THR
37	YE	107	THR
37	YE	184	VAL
39	YG	118	ARG
40	YH	11	VAL
40	YH	67	LEU
40	YH	69	ARG
41	YI	56	LYS
41	YI	86	THR
41	YI	93	THR

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Mol	Chain	Res	Type
41	YI	118	LYS
42	YN	96	GLU
42	YN	115	ARG
43	YO	24	VAL
43	YO	34	THR
43	YO	49	ARG
45	YQ	133	ARG
46	YR	2	ARG
47	YS	4	LEU
47	YS	110	LEU
48	YT	105	LEU
48	YT	129	ARG
49	YU	92	ARG
49	YU	94	ASN
50	YV	46	VAL
50	YV	78	LYS
52	YX	49	VAL
52	YX	66	LEU
53	YY	79	CYS
54	YZ	63	ASP
54	YZ	165	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
7	QG	37	ASN
7	QG	64	GLN
24	R0	12	ASN
32	R8	35	GLN
36	RD	253	GLN
39	RG	79	ASN
46	RR	16	HIS
47	RS	38	GLN
50	RV	11	GLN
4	XD	119	GLN
11	XK	117	ASN
37	YE	132	HIS
39	YG	132	ASN
50	YV	11	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	309 (20%)	9 (0%)
1	XA	1514/1521 (99%)	322 (21%)	10 (0%)
22	QV	76/77 (98%)	17 (22%)	2 (2%)
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QX	18/19 (94%)	4 (22%)	1 (5%)
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2878/2915 (98%)	617 (21%)	40 (1%)
34	YA	2880/2915 (98%)	634 (22%)	44 (1%)
35	RB	119/122 (97%)	21 (17%)	1 (0%)
35	YB	119/122 (97%)	25 (21%)	1 (0%)
All	All	9207/9308 (98%)	1975 (21%)	109 (1%)

All (1975) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	38	G
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	59	A
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	78	G
1	QA	79	G
1	QA	80	G
1	QA	82	U
1	QA	95	G
1	QA	101	A
1	QA	116	A
1	QA	121	C
1	QA	129(B)	G
1	QA	131	C
1	QA	134	A
1	QA	144	G
1	QA	151	A
1	QA	163	C
1	QA	169	C
1	QA	170	U

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Mol	Chain	Res	Type
1	QA	182	U
1	QA	186(F)	C
1	QA	186(I)	U
1	QA	186(J)	U
1	QA	186(K)	G
1	QA	186(L)	G
1	QA	195	A
1	QA	197	A
1	QA	199	G
1	QA	201(C)	U
1	QA	201(D)	U
1	QA	216	G
1	QA	247	G
1	QA	251	G
1	QA	267	C
1	QA	274	A
1	QA	275	G
1	QA	279	A
1	QA	280	C
1	QA	281	G
1	QA	283	C
1	QA	289	G
1	QA	301	G
1	QA	306	G
1	QA	316	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	344	A
1	QA	345	C
1	QA	347	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	384	G
1	QA	388	G
1	QA	389	A
1	QA	390	C

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Mol	Chain	Res	Type
1	QA	392	G
1	QA	397	A
1	QA	398	C
1	QA	412	A
1	QA	413	G
1	QA	414	A
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	440	A
1	QA	452	A
1	QA	453	A
1	QA	458(C)	A
1	QA	481	G
1	QA	484	G
1	QA	485	G
1	QA	486	U
1	QA	497	A
1	QA	498	U
1	QA	501	C
1	QA	505	G
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	514	C
1	QA	518	C
1	QA	521	G
1	QA	524	G
1	QA	527	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	536	C
1	QA	547	A
1	QA	559	A
1	QA	562	C
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G

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Mol	Chain	Res	Type
1	QA	578	C
1	QA	590	C
1	QA	596	C
1	QA	607	A
1	QA	653	A
1	QA	687	A
1	QA	688	G
1	QA	695	A
1	QA	702	A
1	QA	717	C
1	QA	721	G
1	QA	723	U
1	QA	741	G
1	QA	749	C
1	QA	753	A
1	QA	755	G
1	QA	777	A
1	QA	793	U
1	QA	794	A
1	QA	811	C
1	QA	816	A
1	QA	817	C
1	QA	818	G
1	QA	819	A
1	QA	820	U
1	QA	821	G
1	QA	828	A
1	QA	838(B)	U
1	QA	838(C)	C
1	QA	838(D)	U
1	QA	848	C
1	QA	859	A
1	QA	867	G
1	QA	870	U
1	QA	872	A
1	QA	873	A
1	QA	876	G
1	QA	889	A
1	QA	914	A
1	QA	923	A
1	QA	926	G
1	QA	927	G

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Mol	Chain	Res	Type
1	QA	934	C
1	QA	935	A
1	QA	960	U
1	QA	961	U
1	QA	966	G
1	QA	967	C
1	QA	969	A
1	QA	971	G
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1002	G
1	QA	1004	A
1	QA	1006	C
1	QA	1015	A
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1028(D)	G
1	QA	1037	C
1	QA	1039	C
1	QA	1046	A
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1060	C
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1117	G
1	QA	1118	C
1	QA	1124	G

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Mol	Chain	Res	Type
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1135	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1145	C
1	QA	1146	A
1	QA	1147	C
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1186	G
1	QA	1190	G
1	QA	1196	U
1	QA	1197	G
1	QA	1200	C
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1221	G
1	QA	1222	G
1	QA	1224	G
1	QA	1225	A
1	QA	1226	C
1	QA	1227	A
1	QA	1228	C
1	QA	1240	U
1	QA	1241	G
1	QA	1248	A
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1274	G

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Mol	Chain	Res	Type
1	QA	1280	A
1	QA	1281	U
1	QA	1282	C
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1290	G
1	QA	1297	C
1	QA	1299	A
1	QA	1300	G
1	QA	1303	C
1	QA	1305	G
1	QA	1319	A
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1325	C
1	QA	1327	C
1	QA	1328	C
1	QA	1329	A
1	QA	1330	U
1	QA	1331	G
1	QA	1335	C
1	QA	1336	C
1	QA	1340	A
1	QA	1346	A
1	QA	1347	G
1	QA	1359	C
1	QA	1362(B)	C
1	QA	1363	A
1	QA	1364	U
1	QA	1365	G
1	QA	1370	G
1	QA	1378	C
1	QA	1381	U
1	QA	1382	C
1	QA	1394	A
1	QA	1397	C
1	QA	1398	A
1	QA	1413	A
1	QA	1419	G
1	QA	1422	G

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Mol	Chain	Res	Type
1	QA	1440(C)	G
1	QA	1440(D)	G
1	QA	1440(E)	A
1	QA	1440(K)	C
1	QA	1440(L)	G
1	QA	1475	G
1	QA	1492	A
1	QA	1493	A
1	QA	1494	G
1	QA	1497	G
1	QA	1499	A
1	QA	1502	A
1	QA	1503	A
1	QA	1504	G
1	QA	1505	G
1	QA	1506	U
1	QA	1507	A
1	QA	1508	G
1	QA	1517	G
1	QA	1520	G
1	QA	1528	U
1	QA	1529	G
1	QA	1530	G
1	QA	1533	C
1	QA	1534	A
1	QA	1535	C
1	QA	1538	C
1	QA	1539	C
1	QA	1541	U
22	QV	8	U
22	QV	10	G
22	QV	11	C
22	QV	15	G
22	QV	17	C
22	QV	18	U
22	QV	19	G
22	QV	21(B)	A
22	QV	31	G
22	QV	34	C
22	QV	36	G
22	QV	47	U
22	QV	48	C

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Mol	Chain	Res	Type
22	QV	59	A
22	QV	61	C
22	QV	67	U
22	QV	73	A
23	QX	10	G
23	QX	12	A
23	QX	13	A
23	QX	18	C
34	RA	10	G
34	RA	15	G
34	RA	27	G
34	RA	34	C
34	RA	35	G
34	RA	36	G
34	RA	46	C
34	RA	51	G
34	RA	55	G
34	RA	61	G
34	RA	73	A
34	RA	74	A
34	RA	75	G
34	RA	90	U
34	RA	101	G
34	RA	102	G
34	RA	103	A
34	RA	118	A
34	RA	119	A
34	RA	120	U
34	RA	125	G
34	RA	131	G
34	RA	140	A
34	RA	161	U
34	RA	177	G
34	RA	181	A
34	RA	196	A
34	RA	199	A
34	RA	201	C
34	RA	204	A
34	RA	216	A
34	RA	221	A
34	RA	222	A
34	RA	223	A

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Mol	Chain	Res	Type
34	RA	229	A
34	RA	230	U
34	RA	232	G
34	RA	233	A
34	RA	241	A
34	RA	242	G
34	RA	243	U
34	RA	248	G
34	RA	249	C
34	RA	252	G
34	RA	265	A
34	RA	266	G
34	RA	267	C
34	RA	270(M)	U
34	RA	270(N)	U
34	RA	270(O)	G
34	RA	270(Q)	C
34	RA	270(Z)	G
34	RA	271(D)	U
34	RA	275	G
34	RA	276	A
34	RA	277	C
34	RA	278	A
34	RA	299	A
34	RA	311	A
34	RA	323	G
34	RA	324	A
34	RA	329	G
34	RA	330	A
34	RA	332	A
34	RA	342	G
34	RA	346	A
34	RA	352	G
34	RA	362	U
34	RA	364	C
34	RA	371	A
34	RA	372	G
34	RA	386	G
34	RA	387	U
34	RA	404	C
34	RA	405	U
34	RA	411	G

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Mol	Chain	Res	Type
34	RA	412	A
34	RA	423	A
34	RA	428	A
34	RA	435	C
34	RA	444	C
34	RA	448	U
34	RA	453	C
34	RA	454	A
34	RA	456	C
34	RA	457	A
34	RA	458	G
34	RA	467	G
34	RA	470	A
34	RA	481	G
34	RA	494	G
34	RA	501	A
34	RA	504	U
34	RA	505	A
34	RA	508	G
34	RA	509	C
34	RA	510	C
34	RA	512	G
34	RA	513	A
34	RA	529	A
34	RA	531	C
34	RA	532	A
34	RA	533	G
34	RA	537	C
34	RA	539	G
34	RA	540	G
34	RA	546	C
34	RA	547	A
34	RA	556	G
34	RA	563	G
34	RA	568	U
34	RA	573	G
34	RA	575	A
34	RA	603	A
34	RA	604	G
34	RA	607	U
34	RA	614	U
34	RA	615	G

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Mol	Chain	Res	Type
34	RA	616	A
34	RA	617	G
34	RA	618(A)	G
34	RA	621	A
34	RA	622	G
34	RA	626	U
34	RA	627	A
34	RA	631	A
34	RA	634	C
34	RA	637	A
34	RA	638	G
34	RA	645	C
34	RA	646	A
34	RA	651	G
34	RA	652	C
34	RA	654(A)	A
34	RA	654(B)	G
34	RA	657	U
34	RA	668	G
34	RA	669	G
34	RA	670	A
34	RA	686	G
34	RA	702	G
34	RA	717	G
34	RA	722	A
34	RA	726	G
34	RA	730	C
34	RA	747	U
34	RA	748	G
34	RA	753	C
34	RA	762	U
34	RA	764	A
34	RA	765	G
34	RA	776	G
34	RA	782	A
34	RA	784	A
34	RA	785	G
34	RA	790	C
34	RA	792	G
34	RA	800	A
34	RA	805	G
34	RA	810	U

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Mol	Chain	Res	Type
34	RA	812	C
34	RA	819	A
34	RA	826	U
34	RA	827	U
34	RA	828	U
34	RA	830	G
34	RA	845	G
34	RA	847	U
34	RA	856	C
34	RA	857	C
34	RA	859	G
34	RA	860	U
34	RA	877	U
34	RA	887	A
34	RA	889	C
34	RA	890	A
34	RA	896	A
34	RA	907	U
34	RA	910	A
34	RA	914	C
34	RA	915	C
34	RA	917	A
34	RA	918	A
34	RA	932	G
34	RA	941	A
34	RA	945	A
34	RA	946	G
34	RA	959	A
34	RA	961	C
34	RA	973	A
34	RA	974(A)	G
34	RA	974(B)	C
34	RA	975	G
34	RA	981	A
34	RA	983	A
34	RA	996	A
34	RA	1003	G
34	RA	1005	C
34	RA	1008	C
34	RA	1011	G
34	RA	1012	U
34	RA	1013	C

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Mol	Chain	Res	Type
34	RA	1015	G
34	RA	1020	A
34	RA	1022	G
34	RA	1023	U
34	RA	1024	G
34	RA	1025	G
34	RA	1026	U
34	RA	1027	A
34	RA	1033	U
34	RA	1044	G
34	RA	1045	A
34	RA	1046	A
34	RA	1050	A
34	RA	1052	C
34	RA	1062	G
34	RA	1065	U
34	RA	1067	A
34	RA	1070	A
34	RA	1071	G
34	RA	1072	C
34	RA	1073	A
34	RA	1075	C
34	RA	1076	C
34	RA	1082	U
34	RA	1083	U
34	RA	1087	G
34	RA	1088	A
34	RA	1090	U
34	RA	1091	G
34	RA	1097	U
34	RA	1102	C
34	RA	1103	A
34	RA	1104	C
34	RA	1110	G
34	RA	1112	G
34	RA	1126	A
34	RA	1129	A
34	RA	1130	U
34	RA	1131	G
34	RA	1135	C
34	RA	1136	G
34	RA	1139	G

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Mol	Chain	Res	Type
34	RA	1141	U
34	RA	1142(A)	U
34	RA	1142(B)	A
34	RA	1155	A
34	RA	1170	G
34	RA	1173	G
34	RA	1174	A
34	RA	1175	U
34	RA	1176	G
34	RA	1179	C
34	RA	1181	C
34	RA	1195	G
34	RA	1204	A
34	RA	1205	U
34	RA	1206	G
34	RA	1210	A
34	RA	1212	G
34	RA	1220	A
34	RA	1238	G
34	RA	1248	G
34	RA	1250	G
34	RA	1252	G
34	RA	1253	A
34	RA	1256	G
34	RA	1265	A
34	RA	1272	A
34	RA	1273	U
34	RA	1286	A
34	RA	1300	U
34	RA	1301	A
34	RA	1308	A
34	RA	1313	U
34	RA	1314	C
34	RA	1325	G
34	RA	1329	U
34	RA	1341	U
34	RA	1349	A
34	RA	1352	U
34	RA	1365	A
34	RA	1368	G
34	RA	1370	C
34	RA	1378	A

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Mol	Chain	Res	Type
34	RA	1379	A
34	RA	1384	A
34	RA	1385	G
34	RA	1395	A
34	RA	1407	C
34	RA	1411	C
34	RA	1416	G
34	RA	1419	A
34	RA	1420	U
34	RA	1421	G
34	RA	1427	A
34	RA	1428	C
34	RA	1444(B)	A
34	RA	1449(A)	A
34	RA	1449(B)	G
34	RA	1455	G
34	RA	1461	G
34	RA	1467	C
34	RA	1471	A
34	RA	1474	C
34	RA	1480	G
34	RA	1482	U
34	RA	1483	G
34	RA	1485	G
34	RA	1493	C
34	RA	1494	A
34	RA	1495	A
34	RA	1496	A
34	RA	1497	U
34	RA	1504	C
34	RA	1506	C
34	RA	1507	A
34	RA	1508	A
34	RA	1510	A
34	RA	1533	C
34	RA	1534	G
34	RA	1535	U
34	RA	1536	A
34	RA	1537	C
34	RA	1538	G
34	RA	1543	A
34	RA	1544	C

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Mol	Chain	Res	Type
34	RA	1545(A)	A
34	RA	1547	C
34	RA	1558	A
34	RA	1559	G
34	RA	1566	A
34	RA	1569	A
34	RA	1578	U
34	RA	1579	A
34	RA	1586	A
34	RA	1598	C
34	RA	1602	U
34	RA	1603	A
34	RA	1607	C
34	RA	1608	A
34	RA	1609	A
34	RA	1610	A
34	RA	1617	C
34	RA	1618	A
34	RA	1622	G
34	RA	1634	A
34	RA	1640	C
34	RA	1646	C
34	RA	1648	C
34	RA	1653	G
34	RA	1654	A
34	RA	1667	G
34	RA	1668	A
34	RA	1672	C
34	RA	1674	G
34	RA	1688	U
34	RA	1695	G
34	RA	1698	A
34	RA	1725	G
34	RA	1729	A
34	RA	1731	G
34	RA	1742	C
34	RA	1743	G
34	RA	1756	G
34	RA	1762	A
34	RA	1763	G
34	RA	1764	G
34	RA	1773	A

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Mol	Chain	Res	Type
34	RA	1780	A
34	RA	1781	C
34	RA	1784	A
34	RA	1791	A
34	RA	1799	G
34	RA	1800	C
34	RA	1801	G
34	RA	1811	G
34	RA	1816	G
34	RA	1820	U
34	RA	1829	A
34	RA	1835	G
34	RA	1847	A
34	RA	1848	A
34	RA	1858	G
34	RA	1869	G
34	RA	1870	C
34	RA	1872	A
34	RA	1878	G
34	RA	1882	C
34	RA	1888	G
34	RA	1889	A
34	RA	1896	G
34	RA	1905	C
34	RA	1906	G
34	RA	1919	A
34	RA	1930	G
34	RA	1931	U
34	RA	1936	A
34	RA	1937	A
34	RA	1938	A
34	RA	1939	U
34	RA	1955	U
34	RA	1963	U
34	RA	1965	C
34	RA	1966	A
34	RA	1967	C
34	RA	1969	A
34	RA	1970	A
34	RA	1971	A
34	RA	1972	A
34	RA	1981	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	RA	1982	C
34	RA	1991	U
34	RA	1992	G
34	RA	1993	U
34	RA	1994	C
34	RA	2021	C
34	RA	2023	G
34	RA	2030	A
34	RA	2031	A
34	RA	2032	G
34	RA	2033	A
34	RA	2043	C
34	RA	2055	C
34	RA	2056	G
34	RA	2059	A
34	RA	2060	A
34	RA	2061	G
34	RA	2062	A
34	RA	2069	G
34	RA	2077	A
34	RA	2080	G
34	RA	2089	U
34	RA	2092	U
34	RA	2093	G
34	RA	2094	G
34	RA	2095	C
34	RA	2096	U
34	RA	2097	C
34	RA	2099	U
34	RA	2100	G
34	RA	2111	C
34	RA	2113	U
34	RA	2114	A
34	RA	2115	G
34	RA	2116	G
34	RA	2118	U
34	RA	2119	A
34	RA	2120	G
34	RA	2126	A
34	RA	2127	G
34	RA	2128	C
34	RA	2131	G

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Mol	Chain	Res	Type
34	RA	2132	U
34	RA	2133	G
34	RA	2137	C
34	RA	2145	C
34	RA	2146	C
34	RA	2147	G
34	RA	2148	G
34	RA	2158	A
34	RA	2164	C
34	RA	2166	G
34	RA	2167	U
34	RA	2169	A
34	RA	2172	U
34	RA	2173	A
34	RA	2176	A
34	RA	2190	G
34	RA	2191	G
34	RA	2194	G
34	RA	2195	C
34	RA	2198	A
34	RA	2210	G
34	RA	2211	G
34	RA	2212	A
34	RA	2215	G
34	RA	2225	A
34	RA	2238	G
34	RA	2239	G
34	RA	2243	U
34	RA	2245	U
34	RA	2266	A
34	RA	2275	C
34	RA	2280	G
34	RA	2283	C
34	RA	2287	A
34	RA	2288	A
34	RA	2297	C
34	RA	2304	G
34	RA	2305	A
34	RA	2307	G
34	RA	2308	G
34	RA	2310	A
34	RA	2311	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	RA	2319	G
34	RA	2320	A
34	RA	2322	A
34	RA	2325	G
34	RA	2334	G
34	RA	2335	A
34	RA	2342	C
34	RA	2345	G
34	RA	2346	A
34	RA	2347	C
34	RA	2350	C
34	RA	2372	G
34	RA	2383	G
34	RA	2385	C
34	RA	2388	A
34	RA	2391	G
34	RA	2392	A
34	RA	2394	C
34	RA	2402	C
34	RA	2403	C
34	RA	2406	U
34	RA	2410	G
34	RA	2423	U
34	RA	2425	A
34	RA	2428	G
34	RA	2429	G
34	RA	2430	A
34	RA	2431	U
34	RA	2435	A
34	RA	2439	A
34	RA	2440	C
34	RA	2441	C
34	RA	2448	A
34	RA	2460	U
34	RA	2469	A
34	RA	2470	G
34	RA	2478	A
34	RA	2482	G
34	RA	2494	G
34	RA	2502	G
34	RA	2503	A
34	RA	2504	U

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Mol	Chain	Res	Type
34	RA	2505	G
34	RA	2506	U
34	RA	2518	A
34	RA	2520	C
34	RA	2542	A
34	RA	2543	G
34	RA	2553	G
34	RA	2554	U
34	RA	2562	U
34	RA	2567	G
34	RA	2569	G
34	RA	2572	A
34	RA	2577	A
34	RA	2580	U
34	RA	2602	A
34	RA	2609	U
34	RA	2610	C
34	RA	2611	U
34	RA	2612	C
34	RA	2614	A
34	RA	2629	A
34	RA	2646	C
34	RA	2654	A
34	RA	2655	G
34	RA	2665	A
34	RA	2673	G
34	RA	2686	G
34	RA	2689	U
34	RA	2690	C
34	RA	2691	C
34	RA	2702	U
34	RA	2707	G
34	RA	2711	A
34	RA	2712(A)	U
34	RA	2712(B)	A
34	RA	2713	A
34	RA	2714	G
34	RA	2726	U
34	RA	2733	A
34	RA	2739	U
34	RA	2744	G
34	RA	2748	A

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Mol	Chain	Res	Type
34	RA	2750	A
34	RA	2757	A
34	RA	2761	G
34	RA	2764	A
34	RA	2765	A
34	RA	2766	G
34	RA	2777	G
34	RA	2778	A
34	RA	2779	U
34	RA	2780	G
34	RA	2789	C
34	RA	2790	A
34	RA	2791	C
34	RA	2792	G
34	RA	2793	G
34	RA	2794	C
34	RA	2797	U
34	RA	2798	C
34	RA	2807	G
34	RA	2808	U
34	RA	2818	G
34	RA	2820	A
34	RA	2821	A
34	RA	2822	G
34	RA	2825	C
34	RA	2830	G
34	RA	2833	G
34	RA	2834	G
34	RA	2849	U
34	RA	2867	G
34	RA	2872	G
34	RA	2880	C
34	RA	2883	A
34	RA	2885	C
34	RA	2892	A
34	RA	2894	G
34	RA	2895	U
35	RB	8	U
35	RB	9	G
35	RB	12	C
35	RB	13	A
35	RB	14	U

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Mol	Chain	Res	Type
35	RB	15	A
35	RB	22	U
35	RB	25	A
35	RB	32	C
35	RB	41	U
35	RB	42	C
35	RB	44	G
35	RB	45	A
35	RB	53	A
35	RB	56	G
35	RB	67	G
35	RB	73	A
35	RB	77	U
35	RB	81	G
35	RB	96	G
35	RB	109	G
1	XA	6	G
1	XA	9	G
1	XA	31	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	54	C
1	XA	65	U
1	XA	66	G
1	XA	68(E)	C
1	XA	68(F)	G
1	XA	68(I)	G
1	XA	68(K)	G
1	XA	68(M)	U
1	XA	68(N)	U
1	XA	68(P)	A
1	XA	68(Q)	C
1	XA	68(R)	U
1	XA	68(S)	C
1	XA	68(W)	G
1	XA	101	A
1	XA	108	G
1	XA	109	A
1	XA	116	A

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Mol	Chain	Res	Type
1	XA	117	G
1	XA	121	C
1	XA	131	C
1	XA	134	A
1	XA	142	G
1	XA	144	G
1	XA	151	A
1	XA	160	A
1	XA	163	C
1	XA	169	C
1	XA	173	U
1	XA	182	U
1	XA	183	G
1	XA	186(J)	U
1	XA	186(K)	G
1	XA	186(L)	G
1	XA	186(N)	G
1	XA	194	C
1	XA	195	A
1	XA	197	A
1	XA	201(B)	U
1	XA	201(C)	U
1	XA	201(D)	U
1	XA	216	G
1	XA	247	G
1	XA	251	G
1	XA	254	G
1	XA	262	A
1	XA	266	G
1	XA	267	C
1	XA	281	G
1	XA	289	G
1	XA	306	G
1	XA	315	A
1	XA	328	C
1	XA	329	A
1	XA	330	C
1	XA	332	G
1	XA	344	A
1	XA	345	C
1	XA	346	G
1	XA	347	G

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Mol	Chain	Res	Type
1	XA	348	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	366	C
1	XA	368	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	389	A
1	XA	392	G
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	422	C
1	XA	424	G
1	XA	428	G
1	XA	429	U
1	XA	440	A
1	XA	441	A
1	XA	452	A
1	XA	453	A
1	XA	458(C)	A
1	XA	458(D)	C
1	XA	481	G
1	XA	484	G
1	XA	485	G
1	XA	495	A
1	XA	497	A
1	XA	498	U
1	XA	508	C
1	XA	509	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	524	G
1	XA	527	G

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Mol	Chain	Res	Type
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	536	C
1	XA	547	A
1	XA	559	A
1	XA	562	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	578	C
1	XA	588	G
1	XA	596	C
1	XA	605	U
1	XA	607	A
1	XA	618	C
1	XA	629	G
1	XA	653	A
1	XA	660	G
1	XA	661	G
1	XA	665	A
1	XA	666	G
1	XA	671	G
1	XA	687	A
1	XA	695	A
1	XA	702	A
1	XA	720	C
1	XA	721	G
1	XA	722	A
1	XA	723	U
1	XA	724	G
1	XA	749	C
1	XA	753	A
1	XA	755	G
1	XA	760	G
1	XA	777	A
1	XA	781	A
1	XA	793	U
1	XA	794	A
1	XA	811	C
1	XA	816	A

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Mol	Chain	Res	Type
1	XA	817	C
1	XA	818	G
1	XA	819	A
1	XA	820	U
1	XA	821	G
1	XA	828	A
1	XA	838(B)	U
1	XA	838(C)	C
1	XA	838(D)	U
1	XA	848	C
1	XA	853	G
1	XA	859	A
1	XA	867	G
1	XA	872	A
1	XA	873	A
1	XA	885	G
1	XA	889	A
1	XA	890	G
1	XA	914	A
1	XA	923	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	960	U
1	XA	961	U
1	XA	966	G
1	XA	967	C
1	XA	968	A
1	XA	969	A
1	XA	974	A
1	XA	976	G
1	XA	977	A
1	XA	980	C
1	XA	981	U
1	XA	982	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	1004	A
1	XA	1006	C
1	XA	1011	G

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Mol	Chain	Res	Type
1	XA	1024	G
1	XA	1025	U
1	XA	1026	G
1	XA	1027	C
1	XA	1028(A)	C
1	XA	1028(C)	C
1	XA	1028(G)	A
1	XA	1036	G
1	XA	1045	C
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1056	U
1	XA	1064	G
1	XA	1065	U
1	XA	1066	C
1	XA	1075	C
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1117	G
1	XA	1118	C
1	XA	1125	U
1	XA	1126	U
1	XA	1129	C
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1146	A
1	XA	1157	A
1	XA	1159	U
1	XA	1160	G
1	XA	1171	G
1	XA	1178	G
1	XA	1181	G
1	XA	1183	A
1	XA	1191	A

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Mol	Chain	Res	Type
1	XA	1196	U
1	XA	1197	G
1	XA	1200	C
1	XA	1201	A
1	XA	1211	U
1	XA	1212	U
1	XA	1213	A
1	XA	1214	C
1	XA	1224	G
1	XA	1225	A
1	XA	1226	C
1	XA	1227	A
1	XA	1228	C
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1263	C
1	XA	1272	G
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1296	C
1	XA	1299	A
1	XA	1300	G
1	XA	1303	C
1	XA	1305	G
1	XA	1306	A
1	XA	1318	A
1	XA	1321	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1335	C
1	XA	1336	C
1	XA	1340	A

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Mol	Chain	Res	Type
1	XA	1346	A
1	XA	1347	G
1	XA	1352	C
1	XA	1353	G
1	XA	1359	C
1	XA	1362(B)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1370	G
1	XA	1374	A
1	XA	1378	C
1	XA	1379	G
1	XA	1381	U
1	XA	1394	A
1	XA	1397	C
1	XA	1413	A
1	XA	1419	G
1	XA	1440(C)	G
1	XA	1440(E)	A
1	XA	1440(J)	A
1	XA	1440(K)	C
1	XA	1440(L)	G
1	XA	1469	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1494	G
1	XA	1497	G
1	XA	1503	A
1	XA	1504	G
1	XA	1505	G
1	XA	1506	U
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1528	U
1	XA	1529	G
1	XA	1530	G
1	XA	1533	C
1	XA	1534	A
1	XA	1538	C
1	XA	1539	C

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Mol	Chain	Res	Type
1	XA	1541	U
1	XA	1542	U
22	XV	8	U
22	XV	11	C
22	XV	17	C
22	XV	18	U
22	XV	19	G
22	XV	21(A)	U
22	XV	21(B)	A
22	XV	34	C
22	XV	37	1MG
22	XV	38	A
22	XV	40	G
22	XV	42	A
22	XV	43	G
22	XV	46	G
22	XV	47	U
22	XV	48	C
22	XV	58	A
22	XV	61	C
22	XV	69	A
22	XV	72	G
22	XV	73	A
23	XX	9	G
23	XX	10	G
23	XX	12	A
23	XX	13	A
23	XX	15	A
34	YA	9	U
34	YA	23	G
34	YA	27	G
34	YA	28	A
34	YA	34	C
34	YA	35	G
34	YA	46	C
34	YA	51	G
34	YA	55	G
34	YA	61	G
34	YA	64	A
34	YA	70	G
34	YA	72	U
34	YA	73	A

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Mol	Chain	Res	Type
34	YA	74	A
34	YA	75	G
34	YA	78	A
34	YA	90	U
34	YA	101	G
34	YA	102	G
34	YA	103	A
34	YA	118	A
34	YA	119	A
34	YA	120	U
34	YA	125	G
34	YA	131	G
34	YA	138	G
34	YA	161	U
34	YA	162	U
34	YA	193	U
34	YA	196	A
34	YA	199	A
34	YA	201	C
34	YA	204	A
34	YA	216	A
34	YA	221	A
34	YA	222	A
34	YA	223	A
34	YA	226	G
34	YA	228	A
34	YA	229	A
34	YA	230	U
34	YA	232	G
34	YA	233	A
34	YA	241	A
34	YA	242	G
34	YA	243	U
34	YA	248	G
34	YA	249	C
34	YA	252	G
34	YA	265	A
34	YA	266	G
34	YA	267	C
34	YA	269	U
34	YA	270(L)	C
34	YA	270(M)	U

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Mol	Chain	Res	Type
34	YA	270(N)	U
34	YA	270(Q)	C
34	YA	271(D)	U
34	YA	271(E)	G
34	YA	274	G
34	YA	277	C
34	YA	278	A
34	YA	279	C
34	YA	299	A
34	YA	300	A
34	YA	309	G
34	YA	311	A
34	YA	317	G
34	YA	323	G
34	YA	324	A
34	YA	329	G
34	YA	330	A
34	YA	332	A
34	YA	342	G
34	YA	352	G
34	YA	363(A)	G
34	YA	364	C
34	YA	370	G
34	YA	371	A
34	YA	372	G
34	YA	386	G
34	YA	387	U
34	YA	395	U
34	YA	405	U
34	YA	407	G
34	YA	411	G
34	YA	412	A
34	YA	421	U
34	YA	428	A
34	YA	442	G
34	YA	444	C
34	YA	448	U
34	YA	454	A
34	YA	457	A
34	YA	464	U
34	YA	467	G
34	YA	470	A

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Mol	Chain	Res	Type
34	YA	473	G
34	YA	481	G
34	YA	504	U
34	YA	505	A
34	YA	508	G
34	YA	509	C
34	YA	518	G
34	YA	527	C
34	YA	528	A
34	YA	529	A
34	YA	531	C
34	YA	532	A
34	YA	533	G
34	YA	537	C
34	YA	539	G
34	YA	540	G
34	YA	546	C
34	YA	547	A
34	YA	549	G
34	YA	554	U
34	YA	563	G
34	YA	568	U
34	YA	570	G
34	YA	573	G
34	YA	575	A
34	YA	603	A
34	YA	607	U
34	YA	614	U
34	YA	615	G
34	YA	617	G
34	YA	618(A)	G
34	YA	622	G
34	YA	627	A
34	YA	629	G
34	YA	634	C
34	YA	637	A
34	YA	638	G
34	YA	645	C
34	YA	646	A
34	YA	654(A)	A
34	YA	654(B)	G
34	YA	670	A

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Mol	Chain	Res	Type
34	YA	686	G
34	YA	701	G
34	YA	704	G
34	YA	717	G
34	YA	722	A
34	YA	726	G
34	YA	730	C
34	YA	748	G
34	YA	753	C
34	YA	762	U
34	YA	782	A
34	YA	783	A
34	YA	784	A
34	YA	785	G
34	YA	790	C
34	YA	800	A
34	YA	805	G
34	YA	812	C
34	YA	819	A
34	YA	827	U
34	YA	828	U
34	YA	830	G
34	YA	847	U
34	YA	854	G
34	YA	856	C
34	YA	857	C
34	YA	860	U
34	YA	866	A
34	YA	870	A
34	YA	878	A
34	YA	889	C
34	YA	890	A
34	YA	896	A
34	YA	897	C
34	YA	899	A
34	YA	901	A
34	YA	907	U
34	YA	910	A
34	YA	914	C
34	YA	915	C
34	YA	917	A
34	YA	918	A

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Mol	Chain	Res	Type
34	YA	932	G
34	YA	941	A
34	YA	945	A
34	YA	946	G
34	YA	953	A
34	YA	957	A
34	YA	959	A
34	YA	961	C
34	YA	972	G
34	YA	973	A
34	YA	974(A)	G
34	YA	974(B)	C
34	YA	975	G
34	YA	983	A
34	YA	989	G
34	YA	990	A
34	YA	996	A
34	YA	997	G
34	YA	1003	G
34	YA	1005	C
34	YA	1011	G
34	YA	1012	U
34	YA	1013	C
34	YA	1015	G
34	YA	1022	G
34	YA	1023	U
34	YA	1024	G
34	YA	1025	G
34	YA	1026	U
34	YA	1027	A
34	YA	1030	G
34	YA	1033	U
34	YA	1037	G
34	YA	1045	A
34	YA	1046	A
34	YA	1050	A
34	YA	1057	A
34	YA	1059	G
34	YA	1060	U
34	YA	1061	U
34	YA	1062	G
34	YA	1065	U

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Mol	Chain	Res	Type
34	YA	1067	A
34	YA	1068	G
34	YA	1071	G
34	YA	1073	A
34	YA	1074	G
34	YA	1076	C
34	YA	1077	A
34	YA	1078	U
34	YA	1082	U
34	YA	1083	U
34	YA	1084	A
34	YA	1085	A
34	YA	1086	A
34	YA	1088	A
34	YA	1089	G
34	YA	1093	G
34	YA	1095	A
34	YA	1096	A
34	YA	1097	U
34	YA	1099	G
34	YA	1103	A
34	YA	1104	C
34	YA	1110	G
34	YA	1111	A
34	YA	1112	G
34	YA	1122	G
34	YA	1126	A
34	YA	1131	G
34	YA	1135	C
34	YA	1136	G
34	YA	1139	G
34	YA	1142(A)	U
34	YA	1142(B)	A
34	YA	1173	G
34	YA	1174	A
34	YA	1175	U
34	YA	1176	G
34	YA	1177	A
34	YA	1179	C
34	YA	1180	C
34	YA	1195	G
34	YA	1204	A

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Mol	Chain	Res	Type
34	YA	1205	U
34	YA	1206	G
34	YA	1210	A
34	YA	1218	C
34	YA	1220	A
34	YA	1225	C
34	YA	1236	G
34	YA	1238	G
34	YA	1244	G
34	YA	1250	G
34	YA	1252	G
34	YA	1253	A
34	YA	1256	G
34	YA	1265	A
34	YA	1271	G
34	YA	1272	A
34	YA	1273	U
34	YA	1275	A
34	YA	1289	C
34	YA	1300	U
34	YA	1301	A
34	YA	1313	U
34	YA	1325	G
34	YA	1326	U
34	YA	1329	U
34	YA	1330	C
34	YA	1341	U
34	YA	1349	A
34	YA	1352	U
34	YA	1365	A
34	YA	1368	G
34	YA	1370	C
34	YA	1378	A
34	YA	1379	A
34	YA	1384	A
34	YA	1385	G
34	YA	1395	A
34	YA	1403	C
34	YA	1404	C
34	YA	1407	C
34	YA	1410	G
34	YA	1416	G

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Mol	Chain	Res	Type
34	YA	1417	C
34	YA	1419	A
34	YA	1420	U
34	YA	1421	G
34	YA	1427	A
34	YA	1428	C
34	YA	1433	U
34	YA	1444(B)	A
34	YA	1449(A)	A
34	YA	1449(B)	G
34	YA	1455	G
34	YA	1461	G
34	YA	1467	C
34	YA	1471	A
34	YA	1482	U
34	YA	1483	G
34	YA	1485	G
34	YA	1490	A
34	YA	1493	C
34	YA	1497	U
34	YA	1506	C
34	YA	1507	A
34	YA	1508	A
34	YA	1509	C
34	YA	1510	A
34	YA	1511	A
34	YA	1512	G
34	YA	1533	C
34	YA	1534	G
34	YA	1535	U
34	YA	1536	A
34	YA	1537	C
34	YA	1538	G
34	YA	1543	A
34	YA	1544	C
34	YA	1545(A)	A
34	YA	1554	A
34	YA	1558	A
34	YA	1559	G
34	YA	1566	A
34	YA	1567	A
34	YA	1569	A

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Mol	Chain	Res	Type
34	YA	1578	U
34	YA	1585	C
34	YA	1586	A
34	YA	1598	C
34	YA	1608	A
34	YA	1610	A
34	YA	1616	A
34	YA	1617	C
34	YA	1618	A
34	YA	1640	C
34	YA	1646	C
34	YA	1647	G
34	YA	1648	C
34	YA	1651	G
34	YA	1654	A
34	YA	1665	A
34	YA	1671	U
34	YA	1672	C
34	YA	1674	G
34	YA	1695	G
34	YA	1700	A
34	YA	1725	G
34	YA	1729	A
34	YA	1730	U
34	YA	1731	G
34	YA	1742	C
34	YA	1743	G
34	YA	1750	G
34	YA	1753	G
34	YA	1754	C
34	YA	1756	G
34	YA	1763	G
34	YA	1764	G
34	YA	1769	G
34	YA	1773	A
34	YA	1774	C
34	YA	1776	G
34	YA	1780	A
34	YA	1781	C
34	YA	1783	A
34	YA	1784	A
34	YA	1787	A

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Mol	Chain	Res	Type
34	YA	1791	A
34	YA	1799	G
34	YA	1800	C
34	YA	1801	G
34	YA	1802	A
34	YA	1815	A
34	YA	1816	G
34	YA	1820	U
34	YA	1828	G
34	YA	1829	A
34	YA	1847	A
34	YA	1858	G
34	YA	1864	U
34	YA	1869	G
34	YA	1870	C
34	YA	1872	A
34	YA	1878	G
34	YA	1882	C
34	YA	1888	G
34	YA	1889	A
34	YA	1905	C
34	YA	1906	G
34	YA	1913	A
34	YA	1929	G
34	YA	1930	G
34	YA	1931	U
34	YA	1936	A
34	YA	1938	A
34	YA	1939	U
34	YA	1955	U
34	YA	1963	U
34	YA	1965	C
34	YA	1966	A
34	YA	1967	C
34	YA	1969	A
34	YA	1970	A
34	YA	1971	A
34	YA	1972	A
34	YA	1982	C
34	YA	1992	G
34	YA	1993	U
34	YA	2023	G

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Mol	Chain	Res	Type
34	YA	2030	A
34	YA	2031	A
34	YA	2033	A
34	YA	2039	C
34	YA	2043	C
34	YA	2049	G
34	YA	2052	G
34	YA	2055	C
34	YA	2056	G
34	YA	2059	A
34	YA	2060	A
34	YA	2061	G
34	YA	2062	A
34	YA	2069	G
34	YA	2093	G
34	YA	2094	G
34	YA	2099	U
34	YA	2111	C
34	YA	2112	G
34	YA	2113	U
34	YA	2114	A
34	YA	2115	G
34	YA	2116	G
34	YA	2117	A
34	YA	2118	U
34	YA	2119	A
34	YA	2120	G
34	YA	2126	A
34	YA	2127	G
34	YA	2128	C
34	YA	2131	G
34	YA	2132	U
34	YA	2133	G
34	YA	2134	A
34	YA	2135	A
34	YA	2136	C
34	YA	2145	C
34	YA	2148	G
34	YA	2158	A
34	YA	2159	G
34	YA	2161	C
34	YA	2164	C

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Mol	Chain	Res	Type
34	YA	2165	G
34	YA	2166	G
34	YA	2168	G
34	YA	2169	A
34	YA	2172	U
34	YA	2173	A
34	YA	2176	A
34	YA	2190	G
34	YA	2191	G
34	YA	2198	A
34	YA	2199	A
34	YA	2210	G
34	YA	2211	G
34	YA	2212	A
34	YA	2213	U
34	YA	2215	G
34	YA	2225	A
34	YA	2234	G
34	YA	2238	G
34	YA	2239	G
34	YA	2243	U
34	YA	2246	G
34	YA	2249	U
34	YA	2266	A
34	YA	2267	A
34	YA	2275	C
34	YA	2278	A
34	YA	2280	G
34	YA	2283	C
34	YA	2287	A
34	YA	2288	A
34	YA	2307	G
34	YA	2308	G
34	YA	2311	A
34	YA	2318	G
34	YA	2319	G
34	YA	2320	A
34	YA	2325	G
34	YA	2327	A
34	YA	2328	A
34	YA	2329	G
34	YA	2334	G

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Mol	Chain	Res	Type
34	YA	2335	A
34	YA	2340	G
34	YA	2343	C
34	YA	2345	G
34	YA	2346	A
34	YA	2347	C
34	YA	2350	C
34	YA	2354	G
34	YA	2358	G
34	YA	2383	G
34	YA	2384	G
34	YA	2385	C
34	YA	2392	A
34	YA	2394	C
34	YA	2402	C
34	YA	2403	C
34	YA	2405	G
34	YA	2406	U
34	YA	2410	G
34	YA	2423	U
34	YA	2425	A
34	YA	2426	A
34	YA	2427	C
34	YA	2428	G
34	YA	2429	G
34	YA	2430	A
34	YA	2435	A
34	YA	2439	A
34	YA	2440	C
34	YA	2441	C
34	YA	2448	A
34	YA	2469	A
34	YA	2475	C
34	YA	2476	A
34	YA	2480	C
34	YA	2494	G
34	YA	2502	G
34	YA	2505	G
34	YA	2513	G
34	YA	2518	A
34	YA	2520	C
34	YA	2524	G

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Mol	Chain	Res	Type
34	YA	2529	G
34	YA	2542	A
34	YA	2543	G
34	YA	2554	U
34	YA	2556	C
34	YA	2562	U
34	YA	2567	G
34	YA	2569	G
34	YA	2572	A
34	YA	2573	C
34	YA	2577	A
34	YA	2578	G
34	YA	2586	C
34	YA	2602	A
34	YA	2609	U
34	YA	2611	U
34	YA	2612	C
34	YA	2615	U
34	YA	2629	A
34	YA	2646	C
34	YA	2655	G
34	YA	2660	A
34	YA	2665	A
34	YA	2673	G
34	YA	2682	U
34	YA	2689	U
34	YA	2690	C
34	YA	2691	C
34	YA	2702	U
34	YA	2703	C
34	YA	2707	G
34	YA	2712(A)	U
34	YA	2712(B)	A
34	YA	2713	A
34	YA	2714	G
34	YA	2718	G
34	YA	2726	U
34	YA	2733	A
34	YA	2734	A
34	YA	2739	U
34	YA	2744	G
34	YA	2750	A

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Mol	Chain	Res	Type
34	YA	2751	G
34	YA	2761	G
34	YA	2764	A
34	YA	2765	A
34	YA	2766	G
34	YA	2777	G
34	YA	2778	A
34	YA	2779	U
34	YA	2780	G
34	YA	2790	A
34	YA	2791	C
34	YA	2792	G
34	YA	2795	G
34	YA	2797	U
34	YA	2798	C
34	YA	2807	G
34	YA	2818	G
34	YA	2820	A
34	YA	2821	A
34	YA	2833	G
34	YA	2834	G
34	YA	2835	A
34	YA	2846	G
34	YA	2867	G
34	YA	2872	G
34	YA	2879	C
34	YA	2880	C
34	YA	2891	G
34	YA	2892	A
34	YA	2893	G
34	YA	2894	G
34	YA	2895	U
35	YB	7	G
35	YB	8	U
35	YB	9	G
35	YB	13	A
35	YB	15	A
35	YB	16	G
35	YB	19	G
35	YB	21	G
35	YB	22	U
35	YB	25	A

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Mol	Chain	Res	Type
35	YB	35	U
35	YB	40	U
35	YB	41	U
35	YB	42	C
35	YB	44	G
35	YB	45	A
35	YB	47	C
35	YB	52	A
35	YB	53	A
35	YB	56	G
35	YB	67	G
35	YB	73	A
35	YB	81	G
35	YB	82	G
35	YB	109	G

All (109) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	64	G
1	QA	266	G
1	QA	328	C
1	QA	687	A
1	QA	748	C
1	QA	819	A
1	QA	992	U
1	QA	1285	A
1	QA	1538	C
22	QV	10	G
22	QV	36	G
23	QX	17	C
34	RA	99	U
34	RA	102	G
34	RA	221	A
34	RA	222	A
34	RA	229	A
34	RA	242	G
34	RA	271(C)	G
34	RA	404	C
34	RA	503	A
34	RA	512	G
34	RA	637	A

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Mol	Chain	Res	Type
34	RA	752	A
34	RA	790	C
34	RA	846	C
34	RA	856	C
34	RA	974(B)	C
34	RA	1022	G
34	RA	1026	U
34	RA	1045	A
34	RA	1130	U
34	RA	1178	C
34	RA	1312	U
34	RA	1427	A
34	RA	1558	A
34	RA	1653	G
34	RA	1694	C
34	RA	1799	G
34	RA	1819	A
34	RA	1930	G
34	RA	1992	G
34	RA	2022	U
34	RA	2060	A
34	RA	2126	A
34	RA	2439	A
34	RA	2566	A
34	RA	2610	C
34	RA	2689	U
34	RA	2712(A)	U
34	RA	2776	A
34	RA	2832	U
35	RB	66	A
1	XA	115	G
1	XA	266	G
1	XA	328	C
1	XA	367	U
1	XA	748	C
1	XA	992	U
1	XA	1064	G
1	XA	1285	A
1	XA	1504	G
1	XA	1537	U
22	XV	10	G
34	YA	99	U

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Mol	Chain	Res	Type
34	YA	102	G
34	YA	195	A
34	YA	221	A
34	YA	229	A
34	YA	242	G
34	YA	271(C)	G
34	YA	278	A
34	YA	404	C
34	YA	503	A
34	YA	637	A
34	YA	653	A
34	YA	752	A
34	YA	846	C
34	YA	856	C
34	YA	859	G
34	YA	974(A)	G
34	YA	974(B)	C
34	YA	1012	U
34	YA	1022	G
34	YA	1026	U
34	YA	1045	A
34	YA	1085	A
34	YA	1178	C
34	YA	1427	A
34	YA	1508	A
34	YA	1558	A
34	YA	1653	G
34	YA	1694	C
34	YA	1799	G
34	YA	1819	A
34	YA	1930	G
34	YA	1992	G
34	YA	2126	A
34	YA	2319	G
34	YA	2402	C
34	YA	2439	A
34	YA	2566	A
34	YA	2610	C
34	YA	2611	U
34	YA	2681	C
34	YA	2689	U
34	YA	2712(A)	U

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Mol	Chain	Res	Type
34	YA	2776	A
35	YB	66	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$
22	1MG	XV	37	22	18,26,27	1.40	3 (16%)	19,39,42	1.97	3 (15%)
22	1MG	QV	37	22	18,26,27	2.26	4 (22%)	19,39,42	2.47	3 (15%)

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
22	1MG	XV	37	22	-	2/3/25/26	0/3/3/3
22	1MG	QV	37	22	-	2/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C6-C5	6.87	1.52	1.41
22	XV	37	1MG	C6-C5	4.58	1.48	1.41
22	QV	37	1MG	C5-C4	3.99	1.51	1.40
22	QV	37	1MG	C2-N3	2.72	1.38	1.34
22	QV	37	1MG	C6-N1	2.70	1.42	1.38
22	XV	37	1MG	C5-C4	2.39	1.47	1.40
22	XV	37	1MG	C6-N1	2.27	1.41	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	37	1MG	C2-N3-C4	8.22	124.75	115.36
22	XV	37	1MG	C2-N3-C4	6.46	122.73	115.36
22	QV	37	1MG	C1'-N9-C4	5.07	135.56	126.64
22	XV	37	1MG	C6-C5-C4	-3.44	117.75	119.96
22	QV	37	1MG	C4-C5-N7	-3.16	106.10	109.40
22	XV	37	1MG	C4-C5-N7	-3.04	106.23	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	37	1MG	O4'-C4'-C5'-O5'
22	XV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	XV	37	1MG	2	0
22	QV	37	1MG	6	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1110 ligands modelled in this entry, 1108 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
56	SF4	QD	301	4	0,12,12	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	SF4	XD	301	4	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
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	RI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RI	82:ARG	C	83:ALA	N	1.18

## 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.