Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 10:24 PM EDT

PDB ID	:	6OPE
Title	:	Crystal structure of tRNA^ Ala(GGC) U32-A38 bound to near-cognate 70S A site
Authors	:	Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on	:	2019-04-24
Resolution	:	3.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

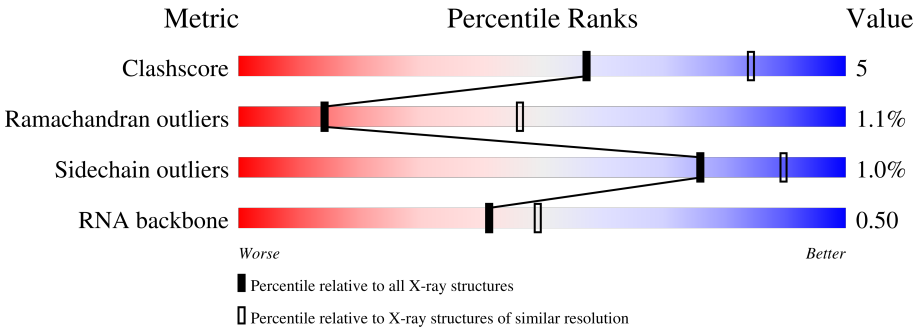
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1522	63% 29% 6% ••
1	XA	1522	64% 28% 6% ••
2	QB	256	74% 18% 7%
2	XB	256	74% 19% 7%
3	QC	239	67% 17% • 14%
3	XC	239	74% 12% 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	81% 17%
4	XD	209	85% 14%
5	QE	162	75% 18% 7%
5	XE	162	83% 10% 7%
6	QF	101	87% 13%
6	XF	101	87% 13%
7	QG	156	88% 12%
7	XG	156	91% 8%
8	QH	138	88% 12%
8	XH	138	77% 23%
9	QI	128	74% 23%
9	XI	128	73% 27%
10	QJ	105	70% 25% 6%
10	XJ	105	77% 17% 6%
11	QK	129	71% 21% 8%
11	XK	129	82% 9% 8%
12	QL	131	75% 19% 5%
12	XL	131	76% 18% 5%
13	QM	126	67% 28%
13	XM	126	78% 18%
14	QN	61	75% 23%
14	XN	61	85% 13%
15	QO	89	84% 13%
15	XO	89	92% 7%
16	QP	88	70% 24% 5%

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Mol	Chain	Length	Quality of chain
16	XP	88	80% 15% • 5%
17	QQ	105	78% 17% 5%
17	XQ	105	83% 12% 5%
18	QR	88	63% 15% • 20%
18	XR	88	66% 14% 20%
19	QS	93	66% 23% • 10%
19	XS	93	69% 19% •• 10%
20	QT	106	85% 8% 7%
20	XT	106	75% 15% •• 7%
21	QU	27	70% 22% 7%
21	XU	27	78% 15% 7%
22	QV	77	70% 26% •
22	XV	77	74% 22% •
23	QX	19	26% 63% 5% 5%
23	XX	19	42% 42% 11% 5%
24	QY	76	42% 37% 17% • •
24	XY	76	54% 32% 12% ••
25	R0	85	78% 18% • •
25	Y0	85	74% 22% •
26	R1	98	81% 16% ••
26	Y1	98	80% 19% •
27	R2	72	65% 29% • •
27	Y2	72	69% 26% •
28	R3	60	83% 15% •
28	Y3	60	87% 12% •

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Mol	Chain	Length	Quality of chain
29	R4	71	58% 32% 8%
29	Y4	71	68% 30%
30	R5	60	78% 17%
30	Y5	60	82% 17%
31	R6	54	61% 24% 9%
31	Y6	54	61% 24% 9%
32	R7	49	86% 14%
32	Y7	49	86% 14%
33	R8	65	66% 29%
33	Y8	65	69% 25% 5%
34	R9	37	81% 19%
34	Y9	37	78% 22%
35	RA	2915	62% 28% 7%
35	YA	2915	62% 29% 7%
36	RB	122	66% 22% 7%
36	YB	122	69% 24% 6%
37	RD	276	76% 21%
37	YD	276	73% 24%
38	RE	206	67% 32%
38	YE	206	76% 22%
39	RF	210	77% 20%
39	YF	210	68% 28%
40	RG	182	83% 16%
40	YG	182	81% 18%
41	RH	180	77% 17% 6%

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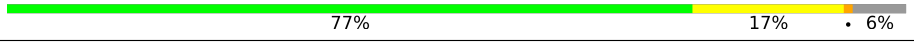
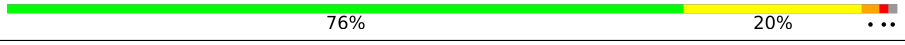
Mol	Chain	Length	Quality of chain
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	
52	YW	113	
53	RX	96	
53	YX	96	

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Mol	Chain	Length	Quality of chain
54	RY	110	76% 15% • 7%
54	YY	110	81% 12% 7%
55	RZ	206	65% 22% • 11%
55	YZ	206	67% 20% • 11%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 294981 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	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	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
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	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	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- 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	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- 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	99	Total 801	C 504	N 157	O 139	S 1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total 964	C 597	N 199	O 166	S 2	0	0	0
13	XM	121	Total 964	C 597	N 199	O 166	S 2	0	0	0

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

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

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

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

- 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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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 217	C 134	N 52	O 31	0	0	0
21	XU	25	Total 217	C 134	N 52	O 31	0	0	0

- Molecule 22 is a RNA chain called P-site tRNAfMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0
22	XV	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total 396	C 177	N 82	O 119	P 18	0	0	0
23	XX	18	Total 396	C 177	N 82	O 119	P 18	0	0	0

- Molecule 24 is a RNA chain called A-site tRNAAla(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	75	Total 1602	C 714	N 288	O 525	P 75	0	0	0
24	XY	75	Total 1602	C 714	N 288	O 525	P 75	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	82	Total 648	C 401	N 138	O 108	S 1	0	0	0
25	Y0	82	Total 648	C 401	N 138	O 108	S 1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total 763	C 481	N 150	O 131	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
29	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
31	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
32	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
35	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 36 is a RNA chain called 5S rRNA.

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

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
41	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
47	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	102	Total 785	C 505	N 150	O 125	S 5	0	0	0
54	YY	102	Total 785	C 505	N 150	O 125	S 5	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total 1461	C 933	N 260	O 265	S 3	0	0	0
55	YZ	183	Total 1461	C 933	N 260	O 265	S 3	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	73	Total 73	Mg 73	0	0
56	QF	1	Total 1	Mg 1	0	0
56	QM	1	Total 1	Mg 1	0	0
56	QV	1	Total 1	Mg 1	0	0
56	QX	2	Total 2	Mg 2	0	0
56	R0	1	Total 1	Mg 1	0	0
56	R5	1	Total 1	Mg 1	0	0
56	R8	1	Total 1	Mg 1	0	0
56	R9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RA	281	Total Mg 281 281	0	0
56	RB	4	Total Mg 4 4	0	0
56	RD	1	Total Mg 1 1	0	0
56	RE	4	Total Mg 4 4	0	0
56	RF	1	Total Mg 1 1	0	0
56	RP	3	Total Mg 3 3	0	0
56	RR	1	Total Mg 1 1	0	0
56	RU	1	Total Mg 1 1	0	0
56	XA	91	Total Mg 91 91	0	0
56	XF	1	Total Mg 1 1	0	0
56	XM	1	Total Mg 1 1	0	0
56	XV	2	Total Mg 2 2	0	0
56	XX	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	Y1	1	Total Mg 1 1	0	0
56	Y2	1	Total Mg 1 1	0	0
56	Y5	1	Total Mg 1 1	0	0
56	Y6	2	Total Mg 2 2	0	0
56	Y8	1	Total Mg 1 1	0	0
56	Y9	1	Total Mg 1 1	0	0
56	YA	347	Total Mg 347 347	0	0

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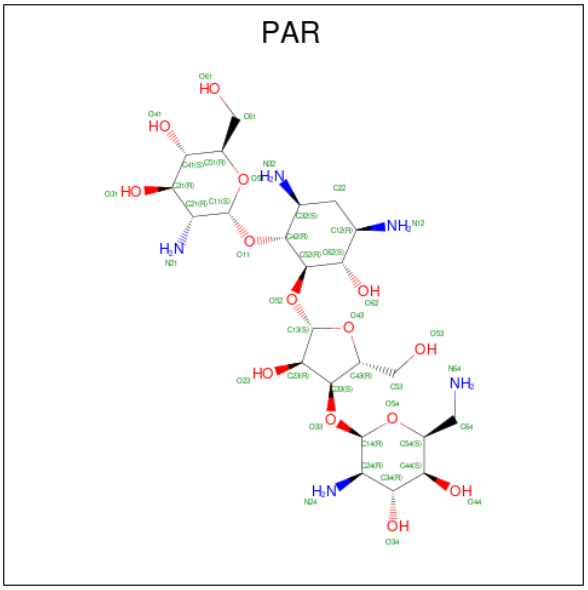
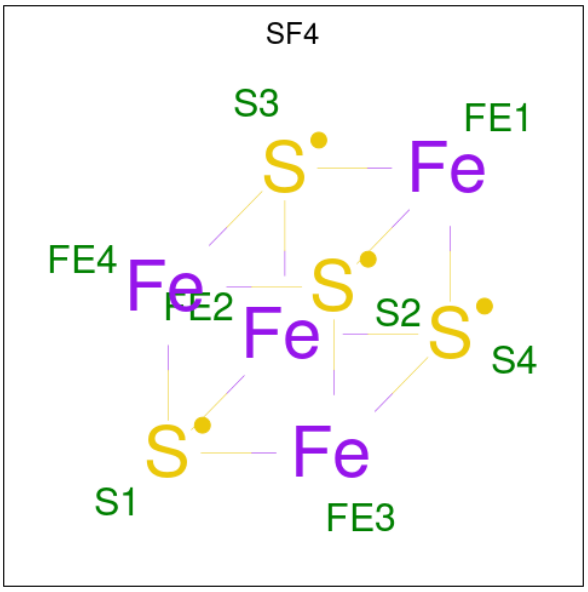
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	YB	6	Total Mg 6 6	0	0
56	YE	3	Total Mg 3 3	0	0
56	YN	1	Total Mg 1 1	0	0
56	YP	3	Total Mg 3 3	0	0
56	YQ	3	Total Mg 3 3	0	0
56	YR	1	Total Mg 1 1	0	0
56	YX	1	Total Mg 1 1	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QA	1	Total C N O 42 23 5 14	0	0
57	XA	1	Total C N O 42 23 5 14	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QN	1	Total Zn 1 1	0	0
59	R9	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0
59	Y9	1	Total Zn 1 1	0	0

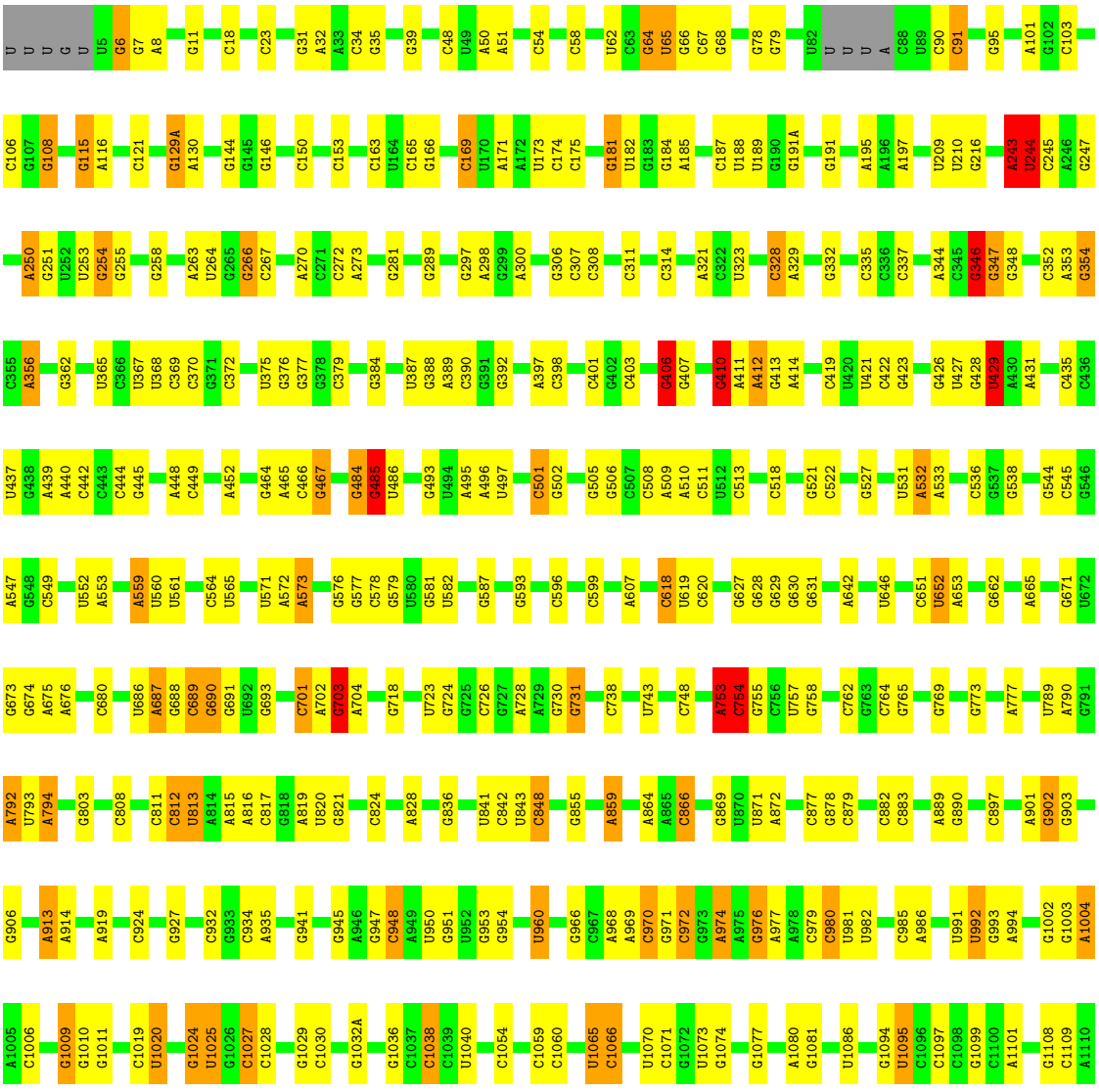
3 Residue-property plots (i)

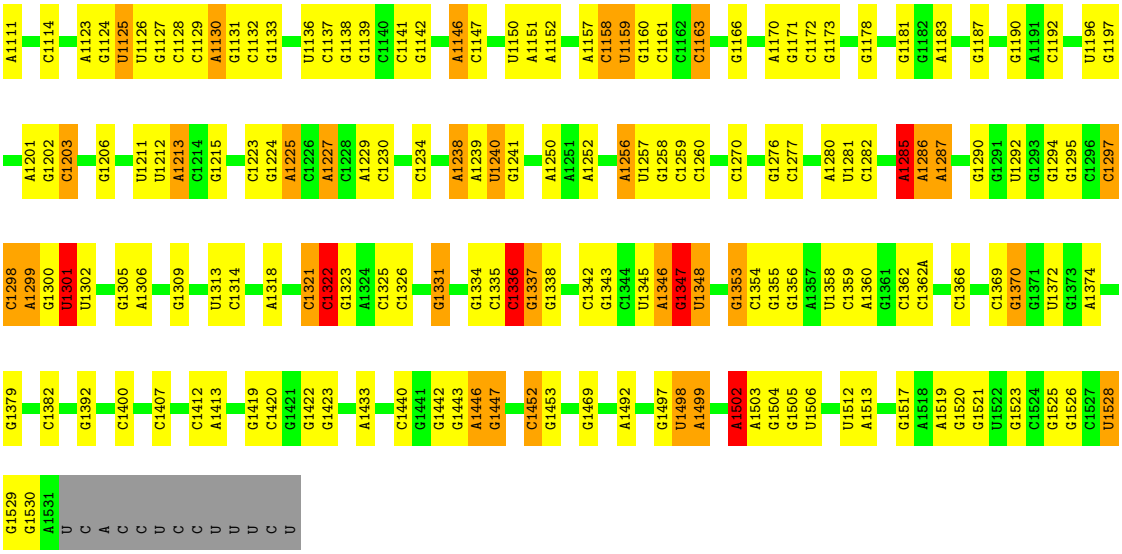
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: 16S rRNA

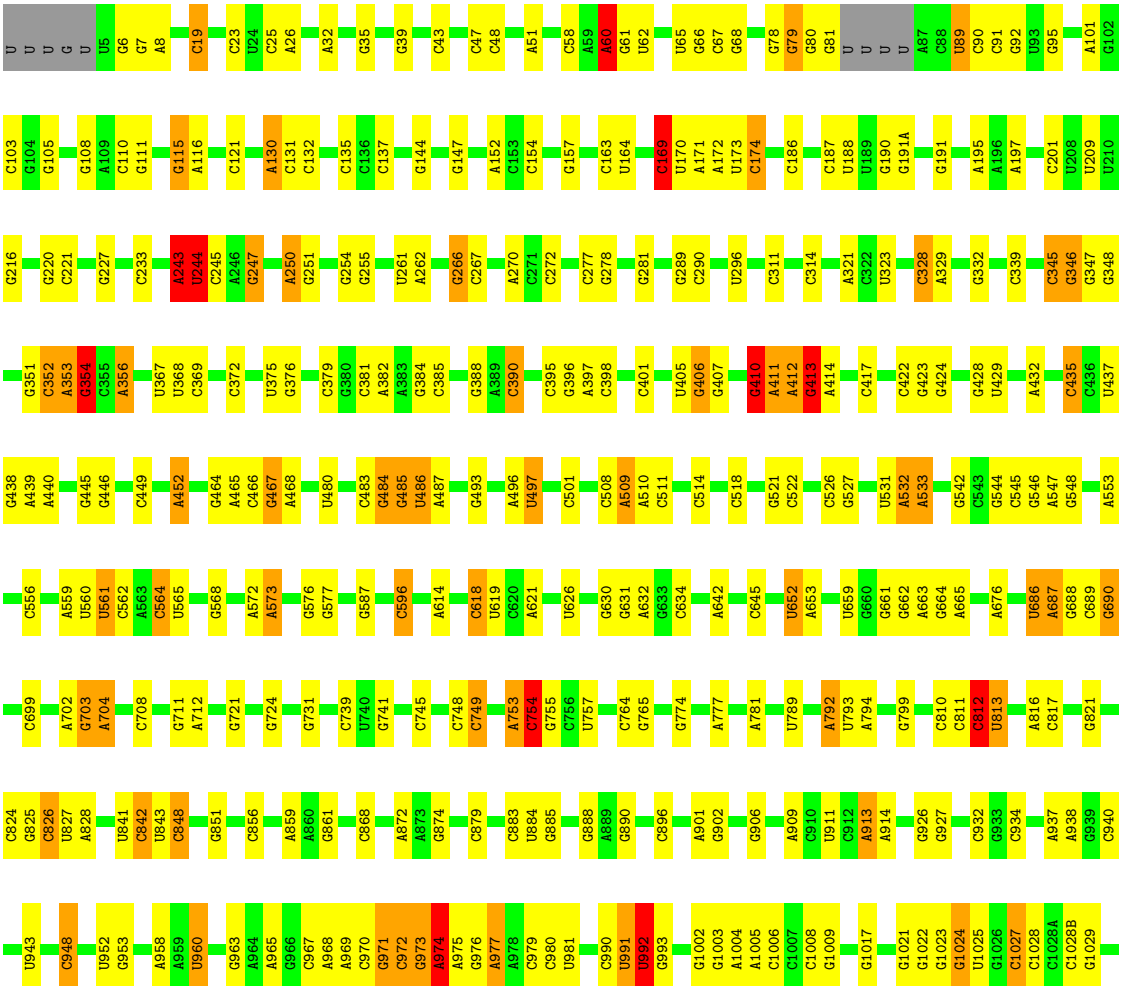
Chain QA:

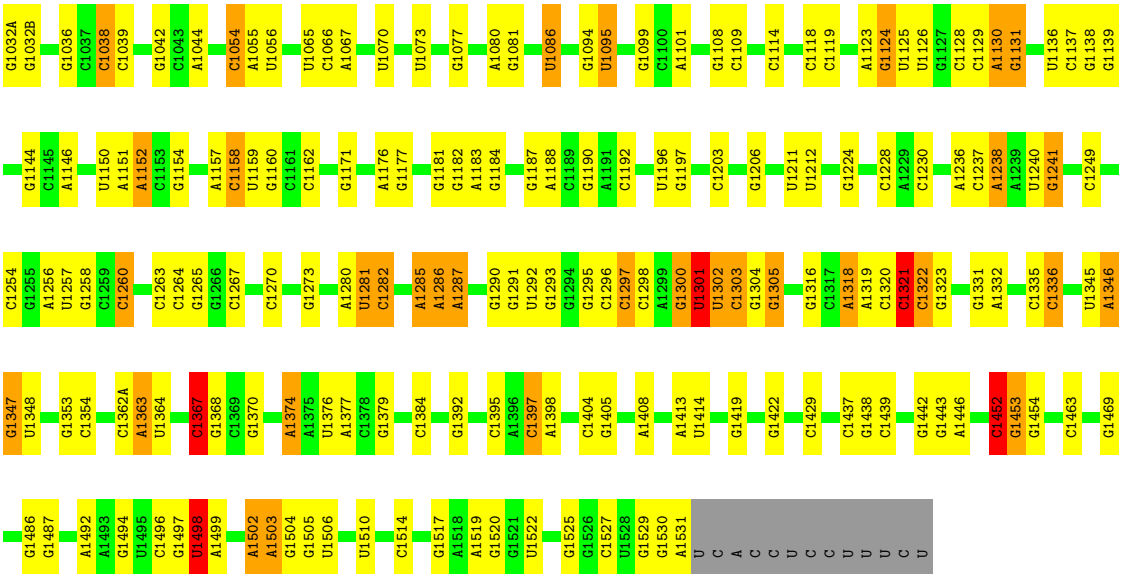




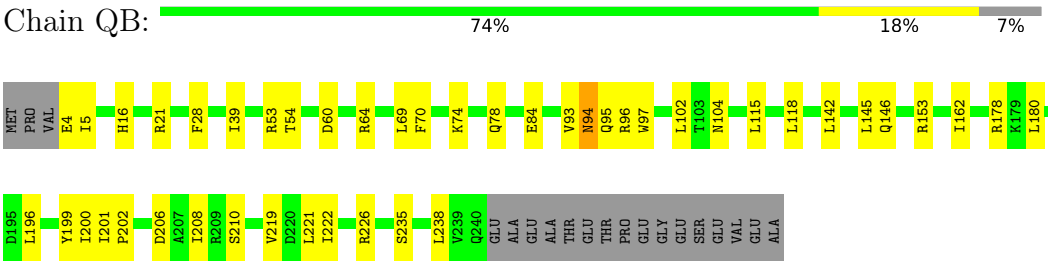
• Molecule 1: 16S rRNA

Chain XA:

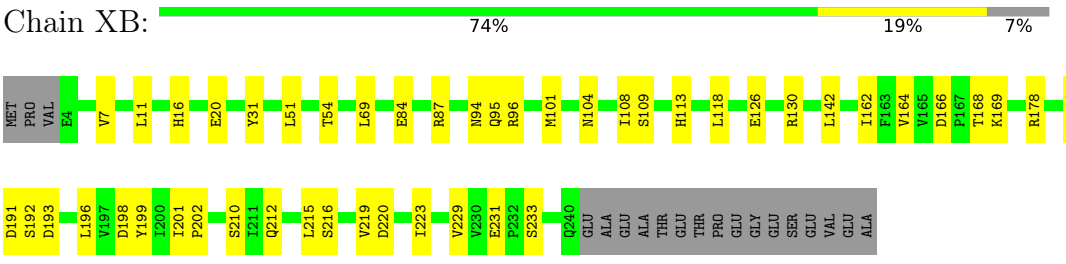




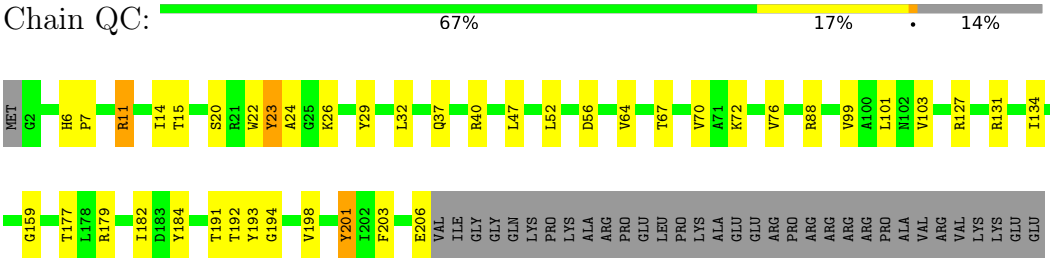
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

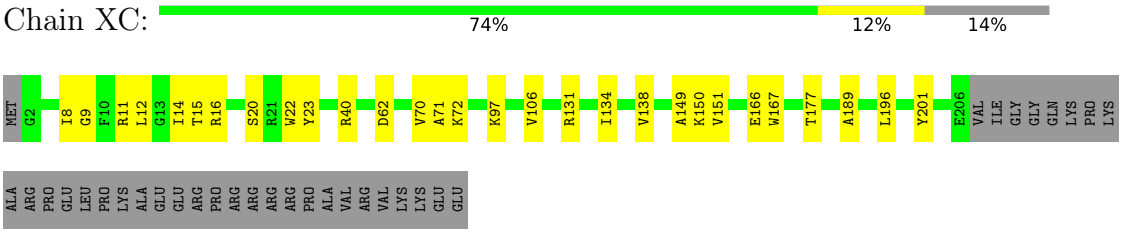


• Molecule 3: 30S ribosomal protein S3



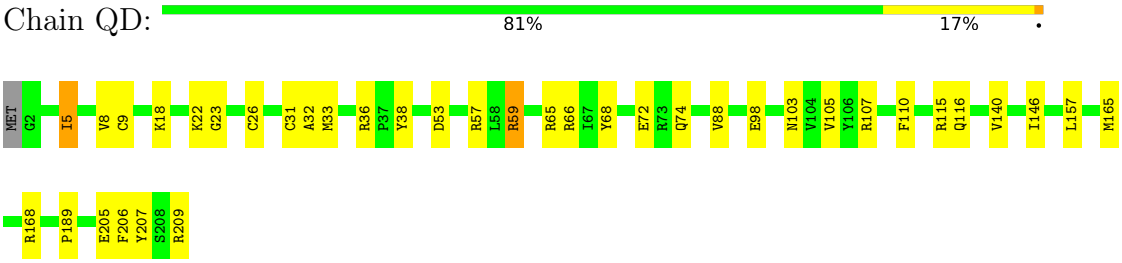
• Molecule 3: 30S ribosomal protein S3

Chain XC:



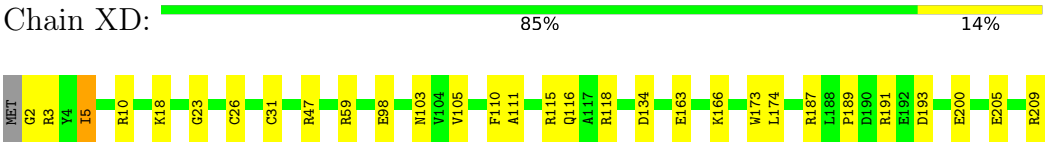
• Molecule 4: 30S ribosomal protein S4

Chain QD:



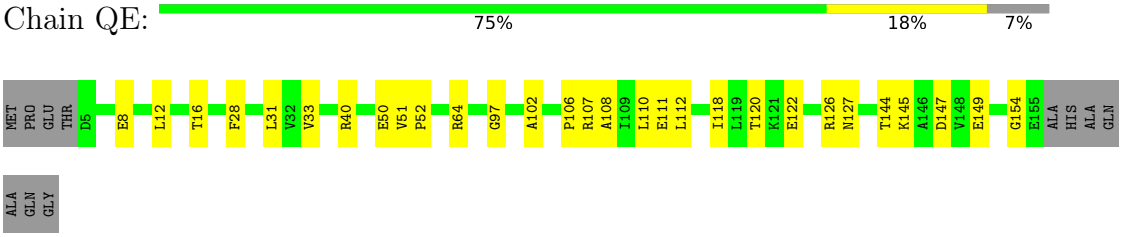
• Molecule 4: 30S ribosomal protein S4

Chain XD:



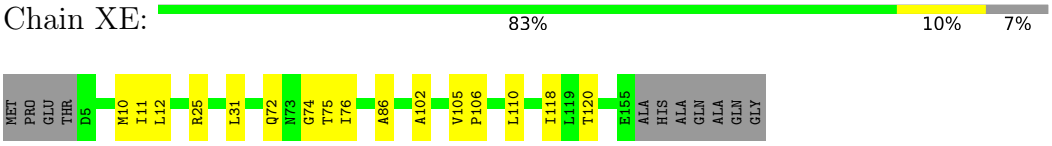
• Molecule 5: 30S ribosomal protein S5

Chain QE:



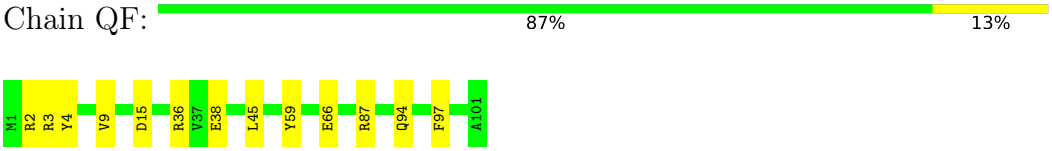
• Molecule 5: 30S ribosomal protein S5

Chain XE:



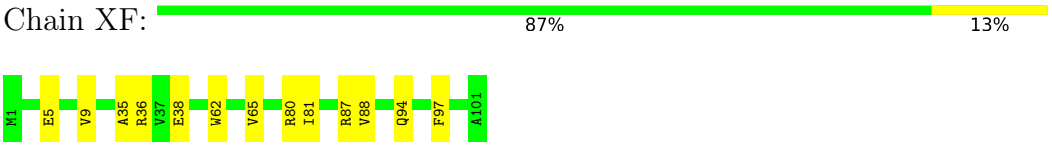
• Molecule 6: 30S ribosomal protein S6

Chain QF:



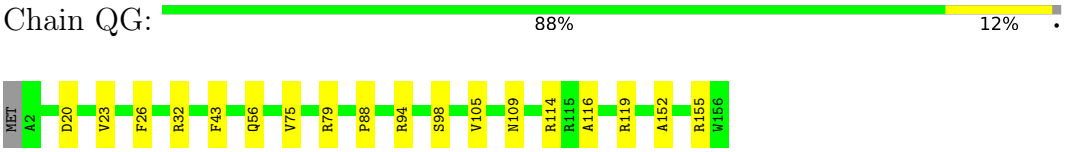
• Molecule 6: 30S ribosomal protein S6

Chain XF:



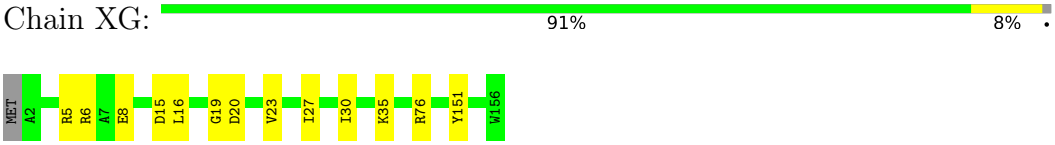
• Molecule 7: 30S ribosomal protein S7

Chain QG:



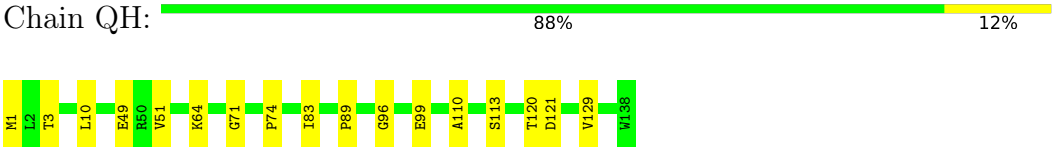
• Molecule 7: 30S ribosomal protein S7

Chain XG:



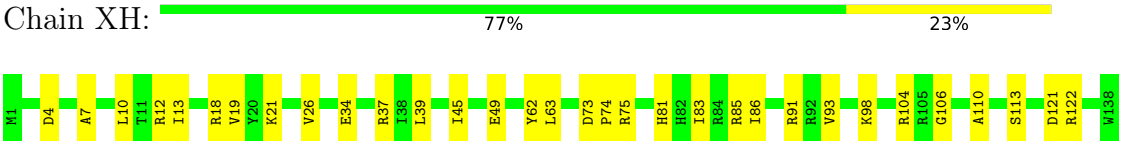
• Molecule 8: 30S ribosomal protein S8

Chain QH:



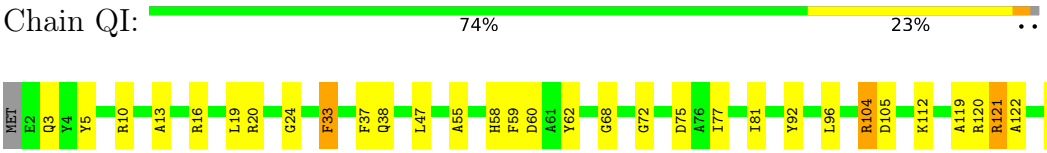
• Molecule 8: 30S ribosomal protein S8

Chain XH:



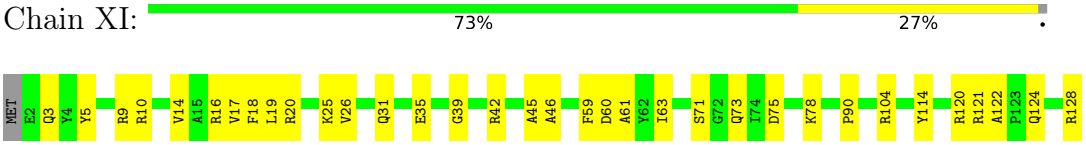
• Molecule 9: 30S ribosomal protein S9

Chain QI:



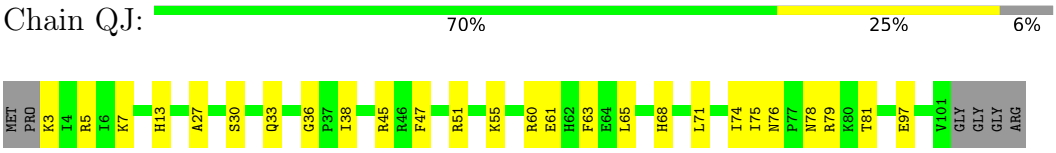
• Molecule 9: 30S ribosomal protein S9

Chain XI:



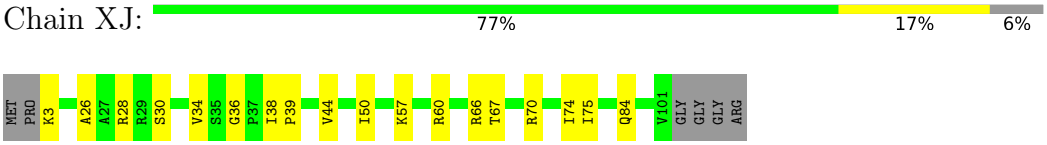
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



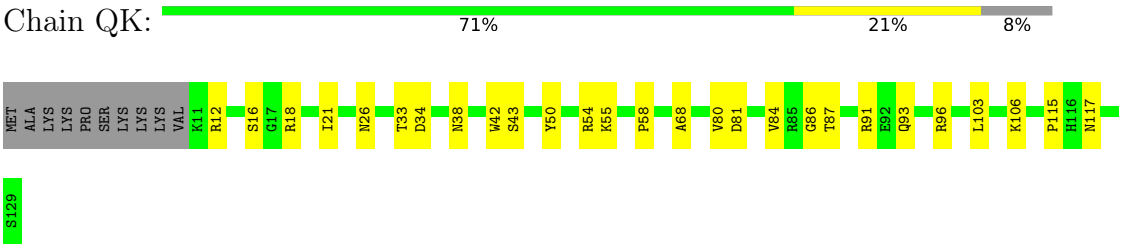
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



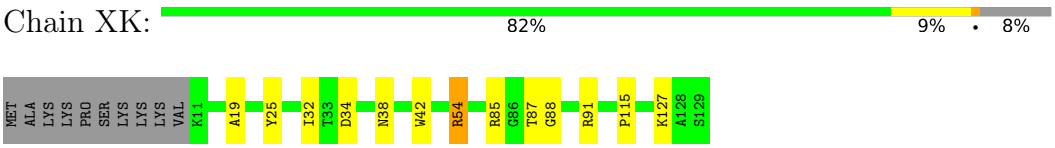
• Molecule 11: 30S ribosomal protein S11

Chain QK:



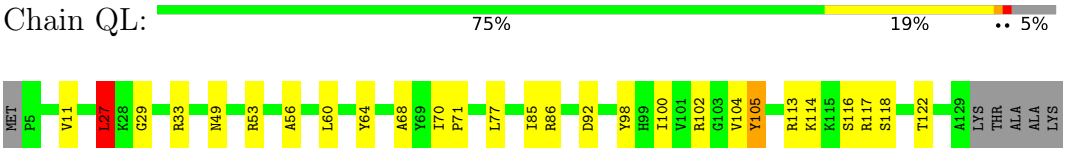
• Molecule 11: 30S ribosomal protein S11

Chain XK:



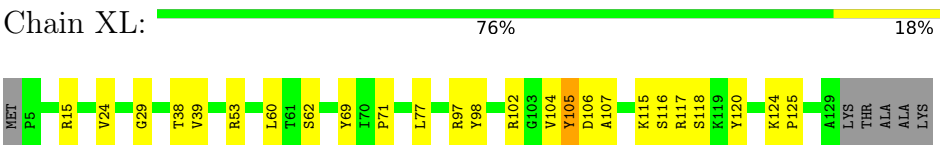
• Molecule 12: 30S ribosomal protein S12

Chain QL:



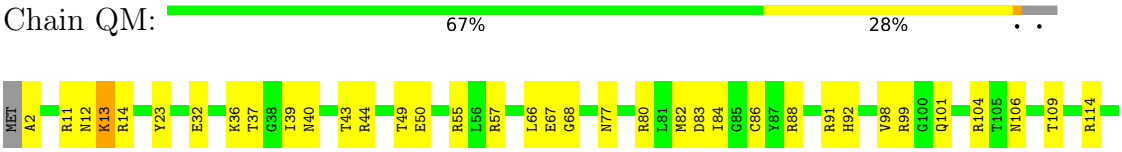
• Molecule 12: 30S ribosomal protein S12

Chain XL:



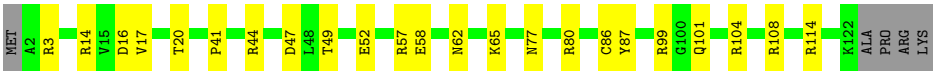
• Molecule 13: 30S ribosomal protein S13

Chain QM:



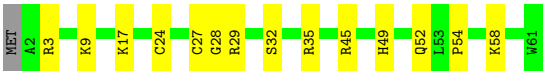
• Molecule 13: 30S ribosomal protein S13

Chain XM:



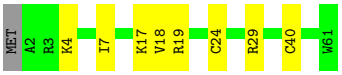
• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



• Molecule 15: 30S ribosomal protein S15

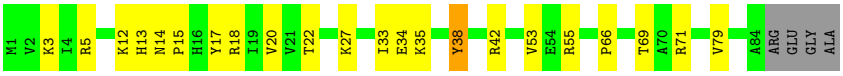
Chain QO:

• Molecule 15: 30S ribosomal protein S15

Chain XO:

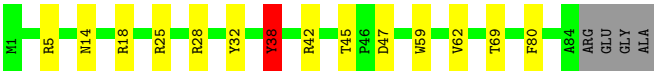
• Molecule 16: 30S ribosomal protein S16

Chain QP:



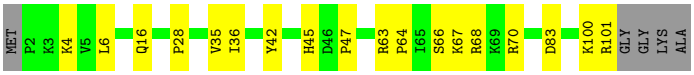
• Molecule 16: 30S ribosomal protein S16

Chain XP:



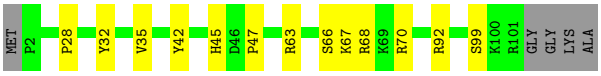
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



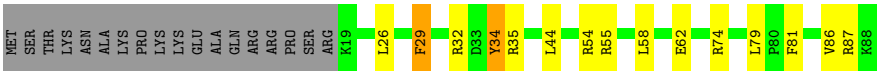
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



• Molecule 18: 30S ribosomal protein S18

Chain QR:

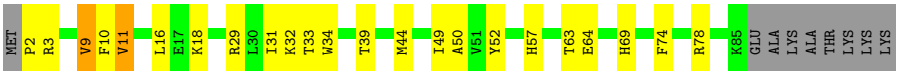


• Molecule 18: 30S ribosomal protein S18

Chain XR:

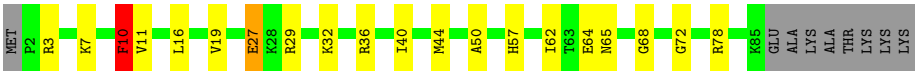
• Molecule 19: 30S ribosomal protein S19

Chain QS:



• Molecule 19: 30S ribosomal protein S19

Chain XS:

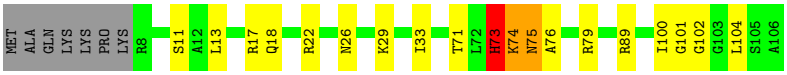


• Molecule 20: 30S ribosomal protein S20

Chain QT:

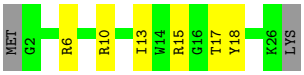
• Molecule 20: 30S ribosomal protein S20

Chain XT:



• Molecule 21: 30S ribosomal protein Thx

Chain QU:

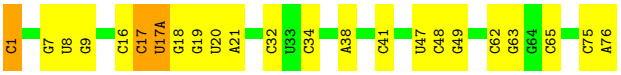


• Molecule 21: 30S ribosomal protein Thx

Chain XU:

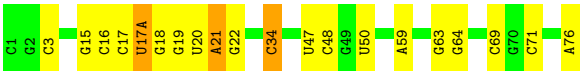
• Molecule 22: P-site tRNAfMet

Chain QV:



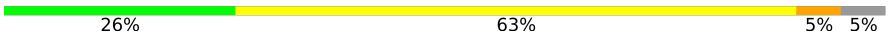
• Molecule 22: P-site tRNAfMet

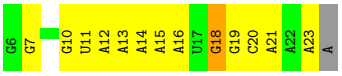
Chain XV:



• Molecule 23: mRNA

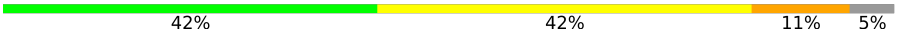
Chain QX:

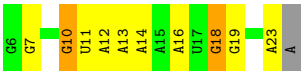




• Molecule 23: mRNA

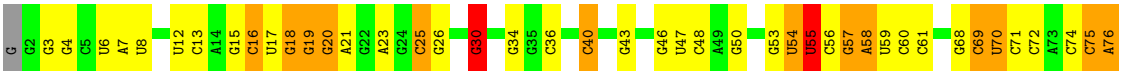
Chain XX:





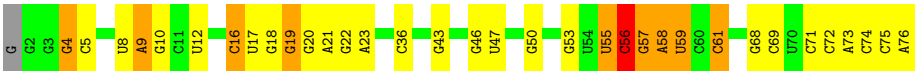
• Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain QY:



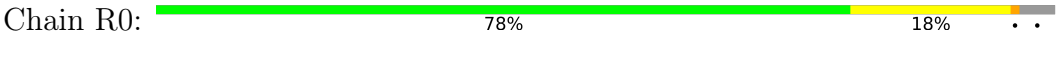
• Molecule 24: A-site tRNAAla(GGC) U32-A38

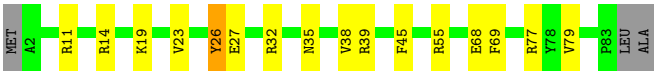
Chain XY:



• Molecule 25: 50S ribosomal protein L27

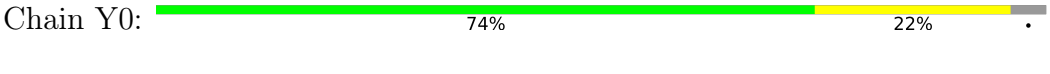
Chain R0:





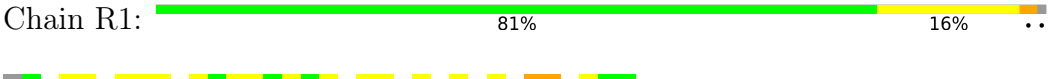
• Molecule 25: 50S ribosomal protein L27

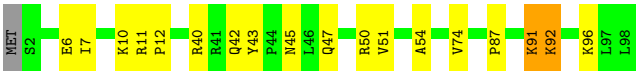
Chain Y0:



• Molecule 26: 50S ribosomal protein L28

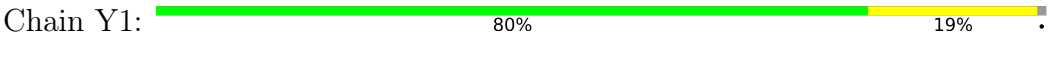
Chain R1:

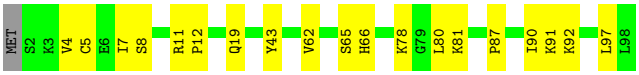




• Molecule 26: 50S ribosomal protein L28

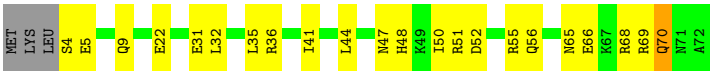
Chain Y1:





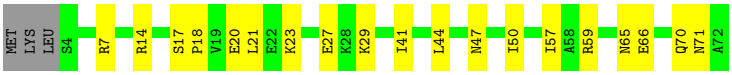
• Molecule 27: 50S ribosomal protein L29

Chain R2:



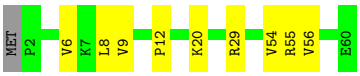
• Molecule 27: 50S ribosomal protein L29

Chain Y2: 



• Molecule 28: 50S ribosomal protein L30

Chain R3: 

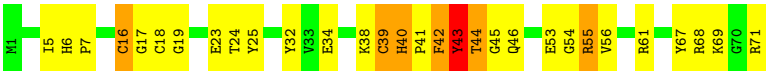


• Molecule 28: 50S ribosomal protein L30

Chain Y3: 

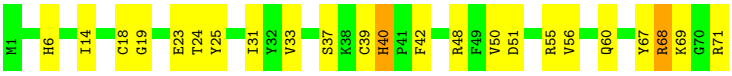
• Molecule 29: 50S ribosomal protein L31

Chain R4: 



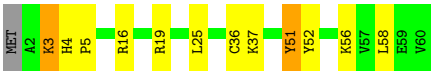
• Molecule 29: 50S ribosomal protein L31

Chain Y4: 



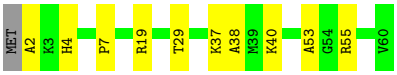
• Molecule 30: 50S ribosomal protein L32

Chain R5: 



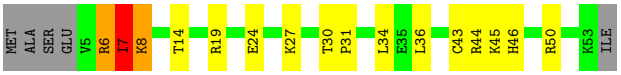
• Molecule 30: 50S ribosomal protein L32

Chain Y5: 



• Molecule 31: 50S ribosomal protein L33

Chain R6:



• Molecule 31: 50S ribosomal protein L33

Chain Y6:

• Molecule 32: 50S ribosomal protein L34

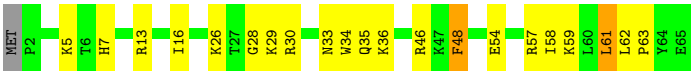
Chain R7:

• Molecule 32: 50S ribosomal protein L34

Chain Y7:

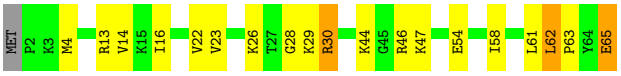
• Molecule 33: 50S ribosomal protein L35

Chain R8:



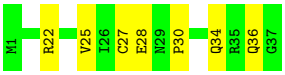
• Molecule 33: 50S ribosomal protein L35

Chain Y8:



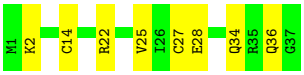
• Molecule 34: 50S ribosomal protein L36

Chain R9:



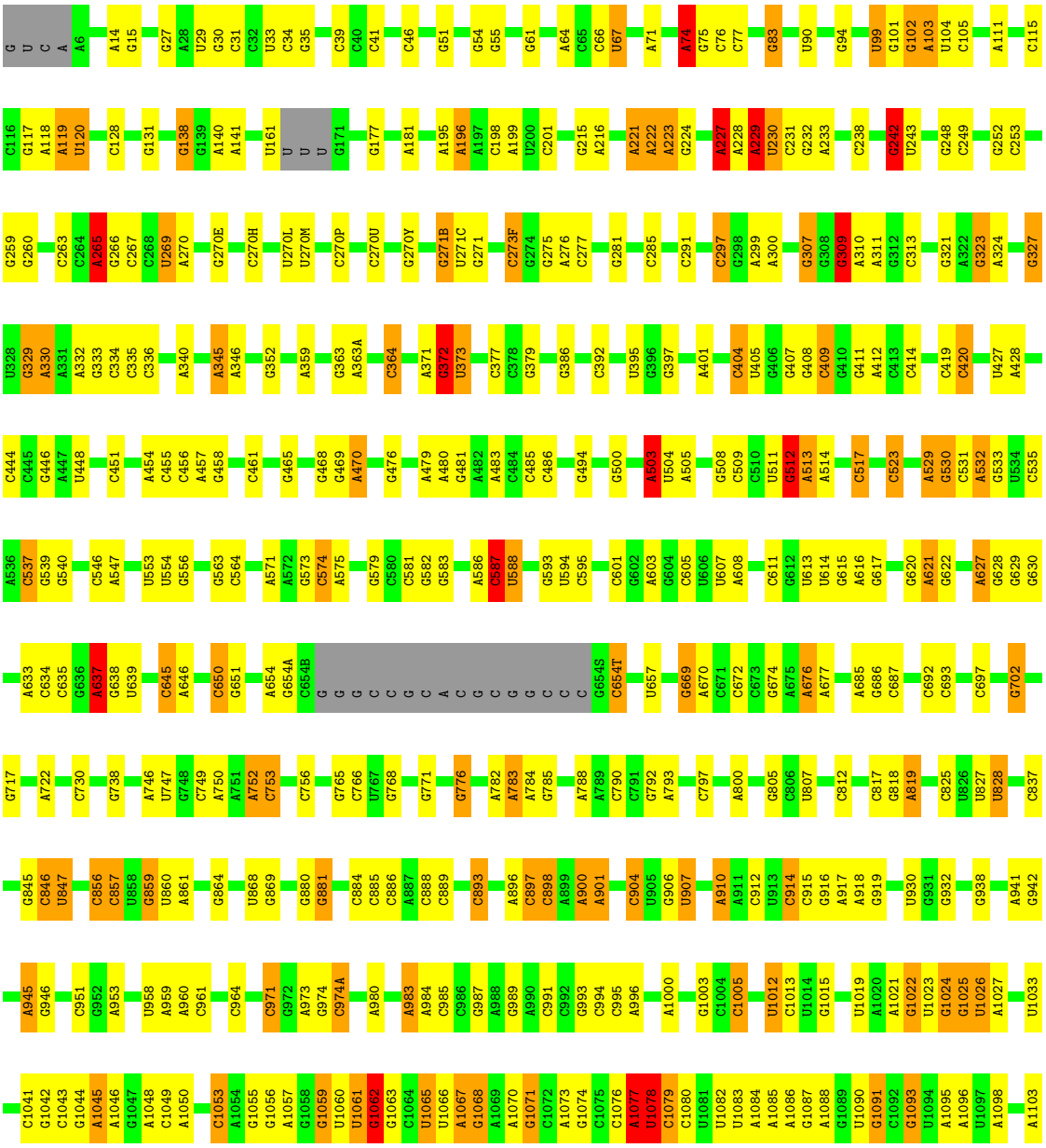
• Molecule 34: 50S ribosomal protein L36

Chain Y9:



• Molecule 35: 23S rRNA

Chain RA:



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G1122 C1123 C1124
U1130 G1131
C1135 G1136 G1137
G1138 G1139 C1140
A1142A
A1155
G1168 G1169 G1170 G1171
G1173 A1174 U1175 G1176 A1177 C1178
C1179 C1180
G1183
G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195
A1204 U1205 G1206
A1210 U1211 G1212 A1213 A1214
C1217
A1220
G1228
C1233
G1236 A1237 G1238 G1239 U1240
G1244
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G1271 A1272 U1273
A1278
A1284
C1290
C1295 G1296
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G1309
U1312 U1313 C1314
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U1329
G1332
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C1403 C1404 U1405 U1406 C1407
C1411
G1416
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C1437
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C1458 G1459 A1460 G1461
C1467 C1468
A1471
C1474
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A1490
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G1525
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A1566 A1567 G1568 A1569
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U1578
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G2358
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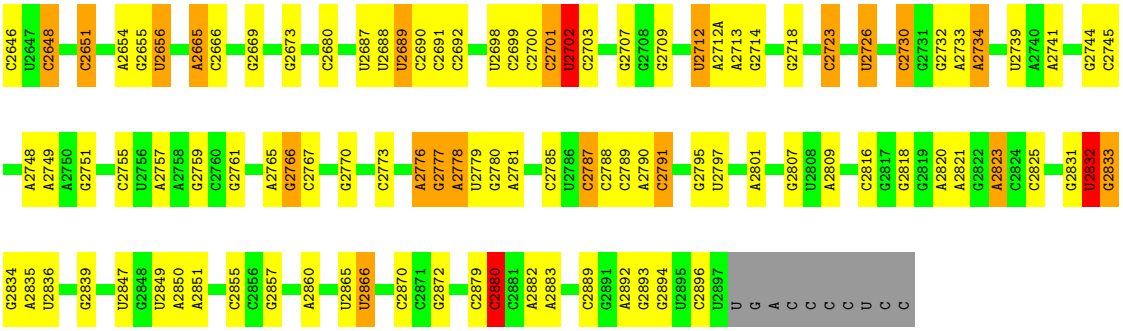
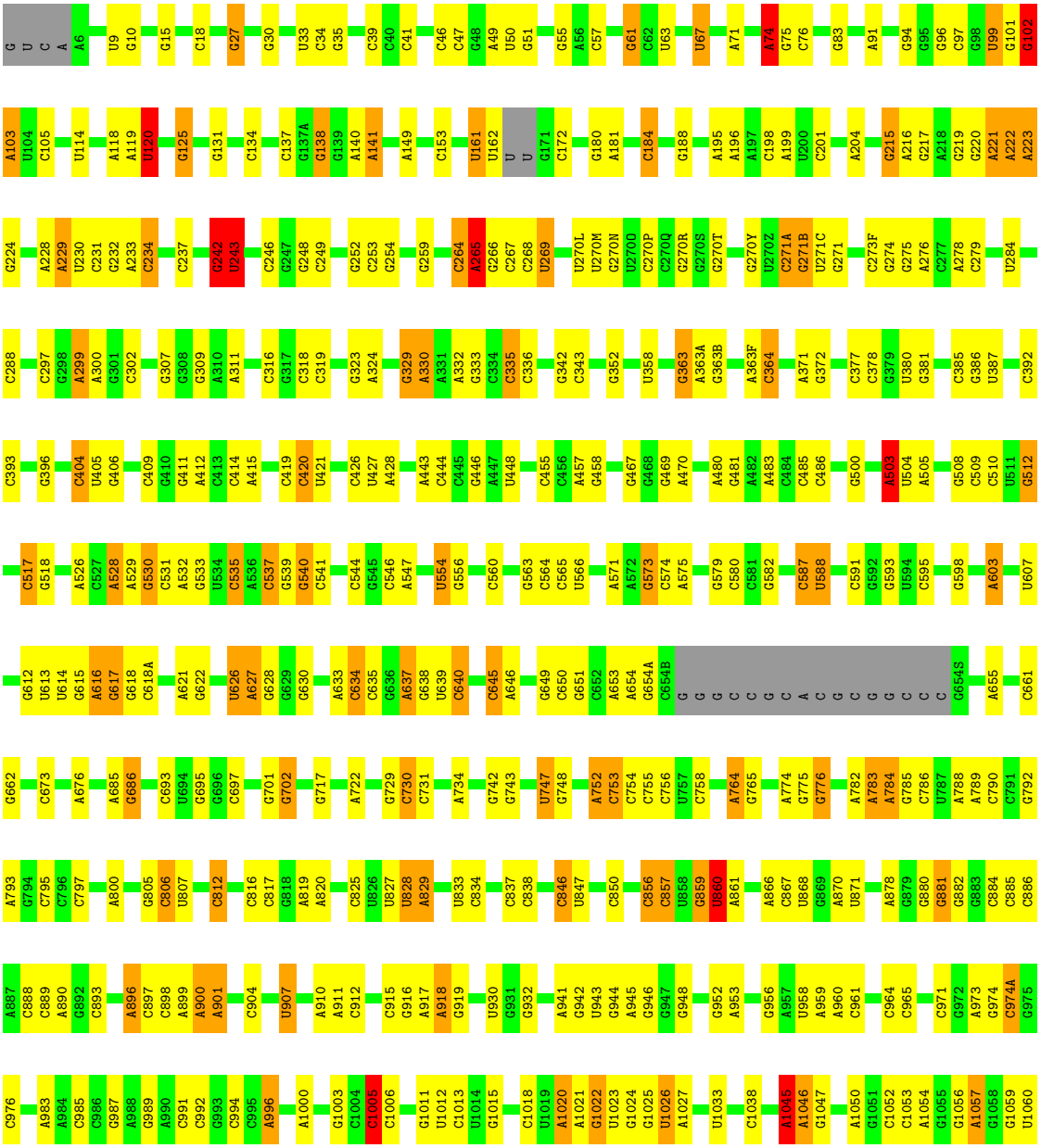


• Molecule 35: 23S rRNA

Chain YA:



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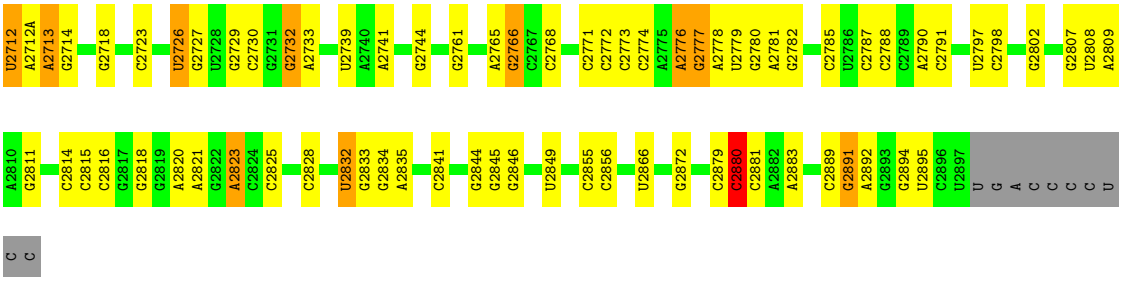
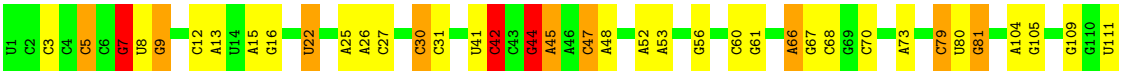
A1732 G1733 C1742 G1743 C1754 A1755 G1756 A1762 G1763 G1764 C1765 G1769 A1773 G1776 U1779 A1780 C1781 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 C1797 U1798 G1799 C1800 G1801 C1804 U1805 U1808 G1811 G1816 G1817 U1818 A1819 U1820 G1824 A1825 G1826 C1827 G1828 A1829
G1835 C1836 A1847 A1853 G1858 A1859 G1869 A1872 G1878 C1879 C1880 C1881 C1882 G1883 A1884 G1888 A1889 C1892 C1893 G1896 G1899 A1900 A1901 C1902 C1905 G1906 C1914 A1919 C1920 G1929 G1930 U1931 A1937 A1938 U1939 U1940 C1947 G1950 U1955 U1956 C1957 C1958
U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 C1979 G1980 A1981 C1982 C1988 U1991 G1992 U1993 C1994 U1995 C1996 C2006 G2010 U2011 G2012 A2013 A2014 A2015 U2016 A2019 A2020 C2021 U2022 G2023 A2031 G2032 A2033 U2034 G2035 C2039 C2043 C2044 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060
G2061 A2062 C2065 C2066 G2067 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 U2076 U2079 G2080 G2090 G2093 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 C2138 C2146 G2147 G2148 G2149 U2150 G2151
A2158 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 A2176 C2177 C2178 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 G2210 G2211 A2212 U2213 G2215 A2225 U2233 G2234 G2235 C2236 G2237 G2238 G2239 U2243 G2246 U2249 G2253 C2258 C2261 A2269
C2275 C2283 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 A2298 G2304 G2307 G2308 A2309 A2310 A2311 U2312 G2315 C2316 C2317 G2318 G2319 A2320 G2321 G2325 A2328 G2334 A2335 A2336 C2342 C2343 U2344 G2345 A2346 C2347 C2350 G2354 C2355 C2368 G2373 C2374 A2377
G2383 G2384 C2385 G2391 A2392 A2393 C2394 C2402 C2403 C2404 G2405 U2406 G2410 C2416 C2420 U2423 G2424 A2425 A2426 C2427 G2428 G2429 A2430 A2435 A2439 C2440 C2441 C2442 C2443 G2444 G2445 G2447 A2448 U2449 C2452 C2465 G2468 A2469 G2470 C2471 G2472 U2473 C2474 C2475 A2478 G2479
C2480 G2481 G2482 C2483 G2490 U2491 G2494 C2298 G2502 A2503 U2504 G2505 U2506 A2518 G2524 G2525 G2529 A2542 G2543 G2544 U2547 U2554 C2559 C2560 A2561 U2562 U2563 A2564 A2565 A2566 G2567 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 U2584 U2585 C2586 G2592 G2597
A2602 U2609 C2610 U2611 C2612 U2615 C2616 C2617 C2618 C2619 A2629 G2630 G2631 A2632 C2646 U2653 A2654 C2655 U2656 C2659 A2660 G2661 A2662 A2665 C2666 C2667 C2673 A2679 C2680 C2681 U2682 C2683 U2687 U2688 U2689 C2690 C2691 C2692 U2698 C2701 U2702 G2707 G2708 G2709 C2710 A2711



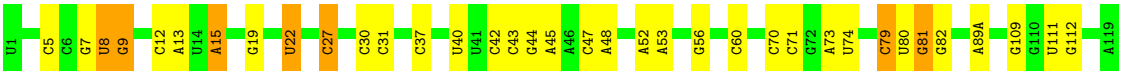
• Molecule 36: 5S rRNA

Chain RB:



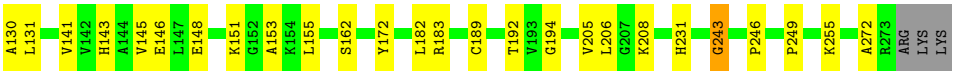
• Molecule 36: 5S rRNA

Chain YB:



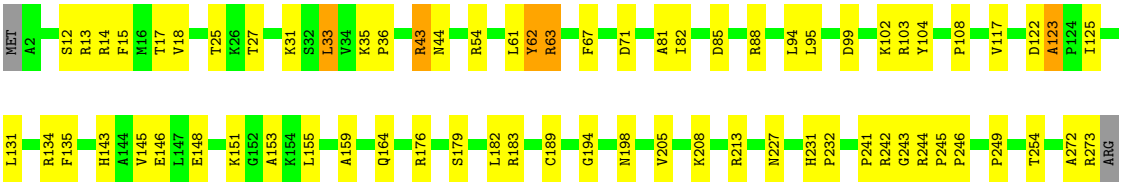
• Molecule 37: 50S ribosomal protein L2

Chain RD:



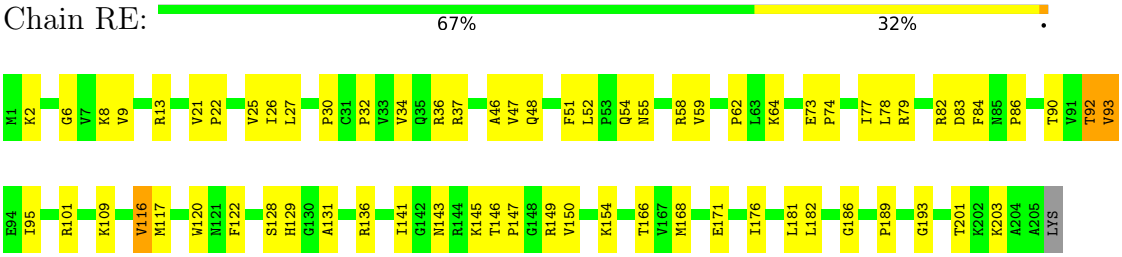
• Molecule 37: 50S ribosomal protein L2

Chain YD:



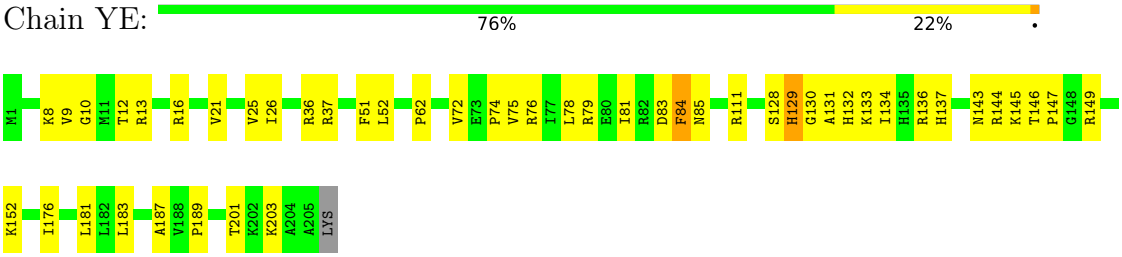
• Molecule 38: 50S ribosomal protein L3

Chain RE:



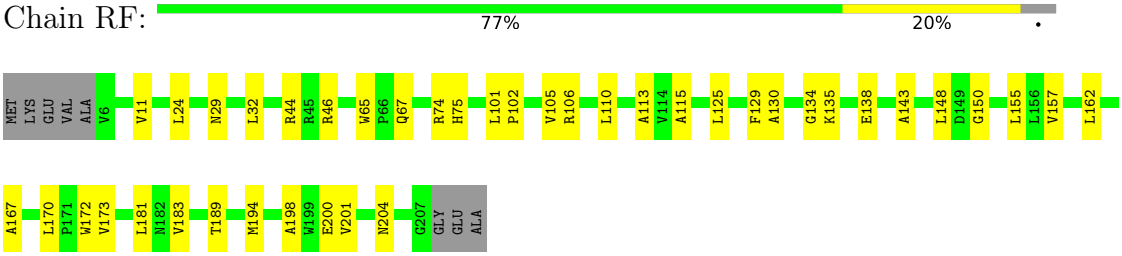
• Molecule 38: 50S ribosomal protein L3

Chain YE:



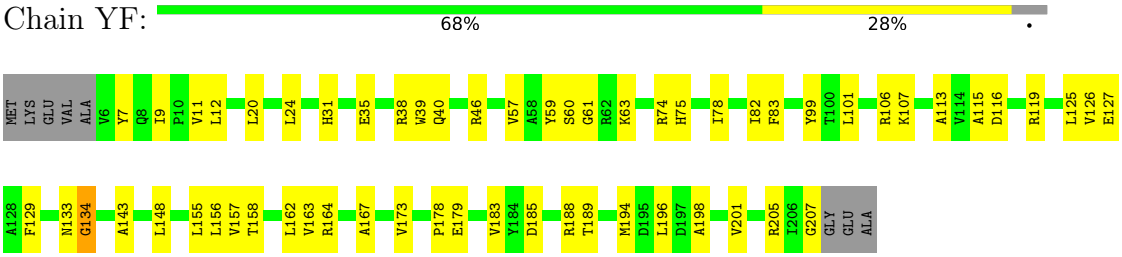
• Molecule 39: 50S ribosomal protein L4

Chain RF:



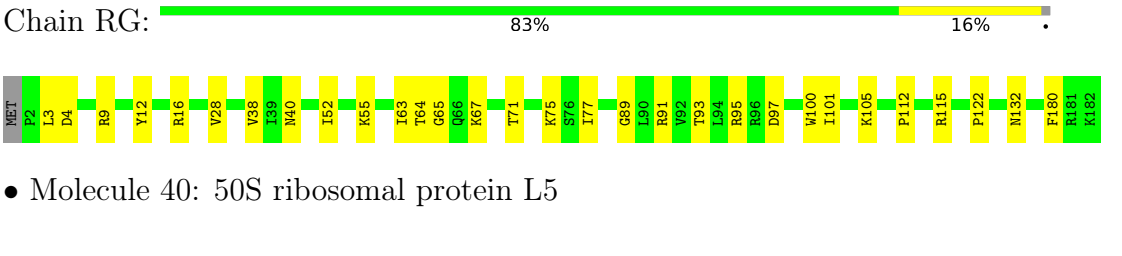
• Molecule 39: 50S ribosomal protein L4

Chain YF:



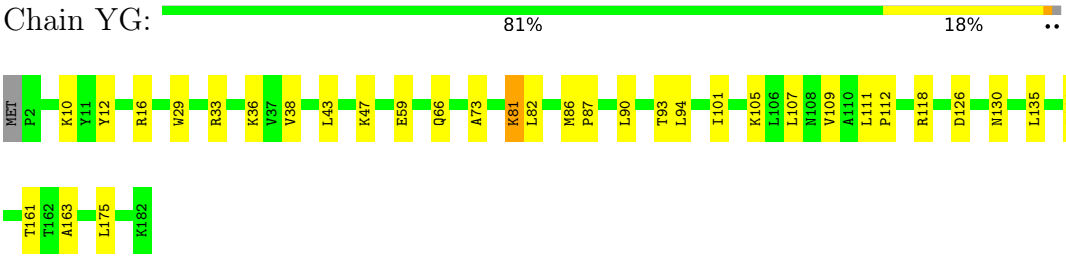
• Molecule 40: 50S ribosomal protein L5

Chain RG:



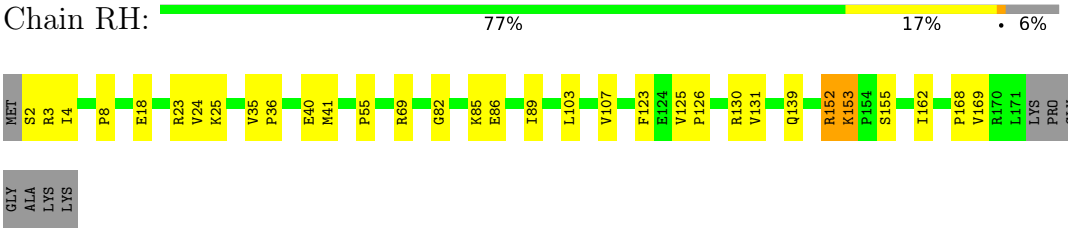
• Molecule 40: 50S ribosomal protein L5

Chain YG:



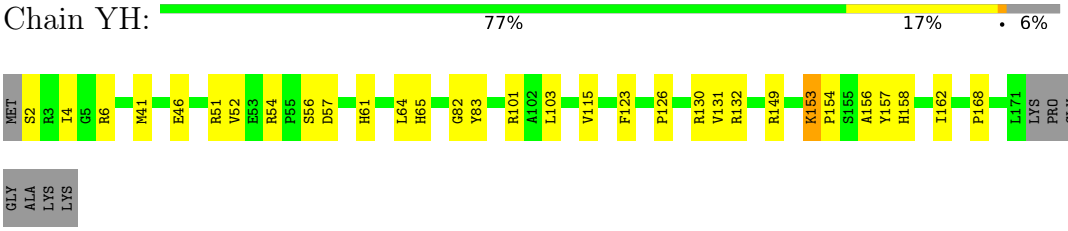
• Molecule 41: 50S ribosomal protein L6

Chain RH:



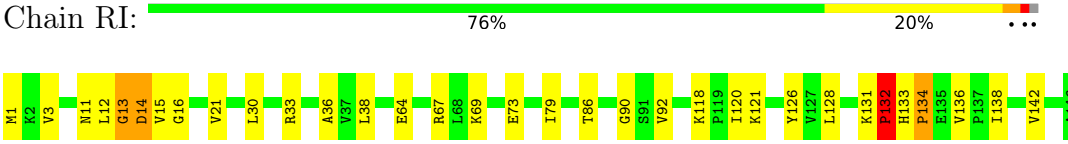
• Molecule 41: 50S ribosomal protein L6

Chain YH:



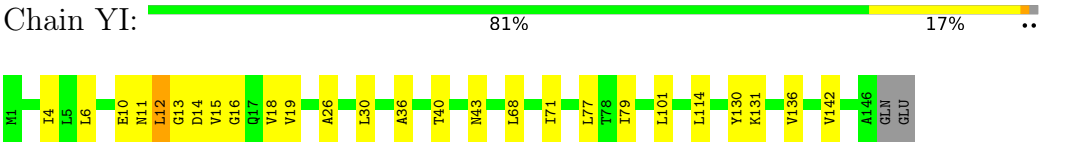
• Molecule 42: 50S ribosomal protein L9

Chain RI:



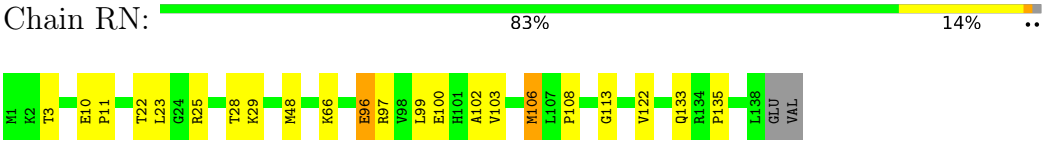
• Molecule 42: 50S ribosomal protein L9

Chain YI:



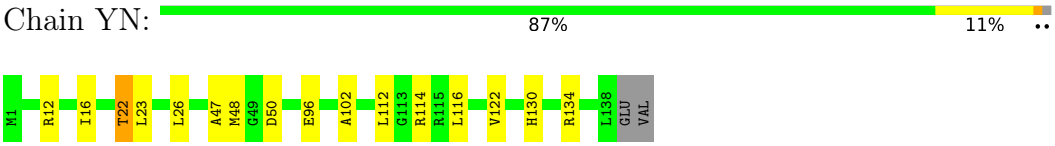
• Molecule 43: 50S ribosomal protein L13

Chain RN:



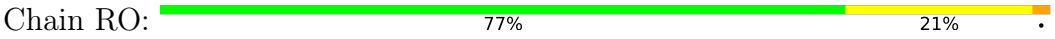
• Molecule 43: 50S ribosomal protein L13

Chain YN:



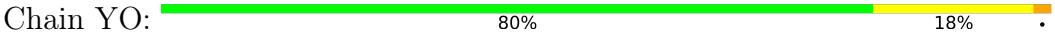
• Molecule 44: 50S ribosomal protein L14

Chain RO:



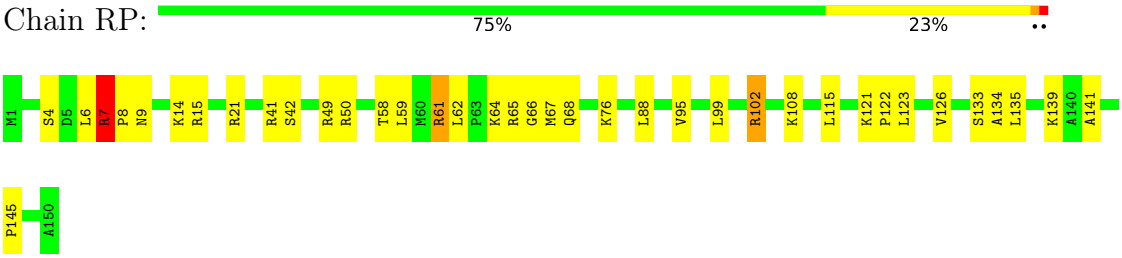
• Molecule 44: 50S ribosomal protein L14

Chain YO:



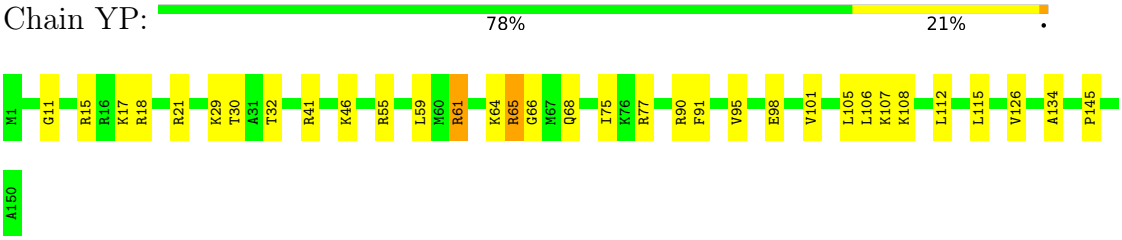
• Molecule 45: 50S ribosomal protein L15

Chain RP:



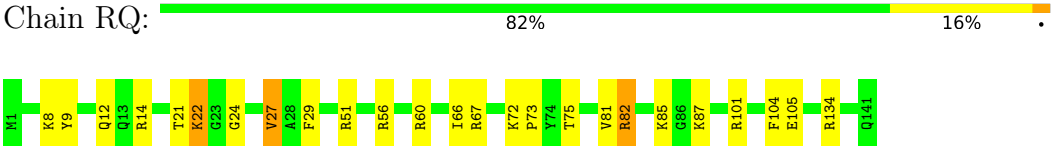
• Molecule 45: 50S ribosomal protein L15

Chain YP:



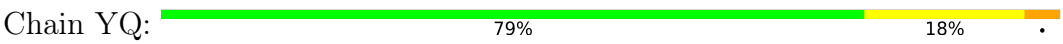
• Molecule 46: 50S ribosomal protein L16

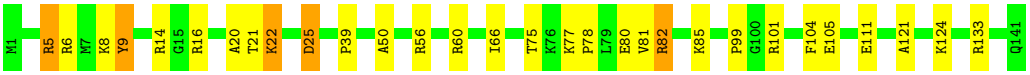
Chain RQ:



• Molecule 46: 50S ribosomal protein L16

Chain YQ:





• Molecule 47: 50S ribosomal protein L17

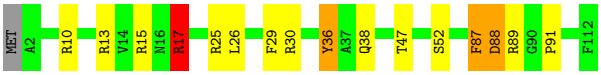
Chain RR:

• Molecule 47: 50S ribosomal protein L17

Chain YR:

• Molecule 48: 50S ribosomal protein L18

Chain RS:

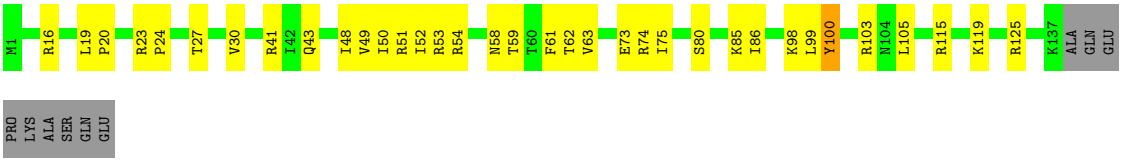


• Molecule 48: 50S ribosomal protein L18

Chain YS:

• Molecule 49: 50S ribosomal protein L19

Chain RT:

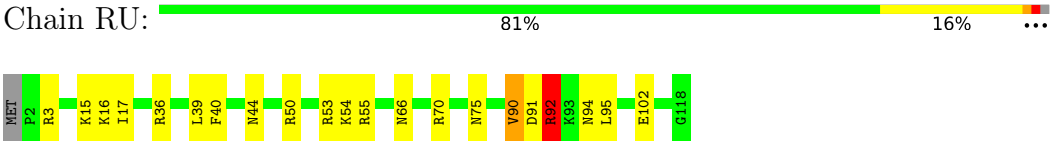


• Molecule 49: 50S ribosomal protein L19

Chain YT:

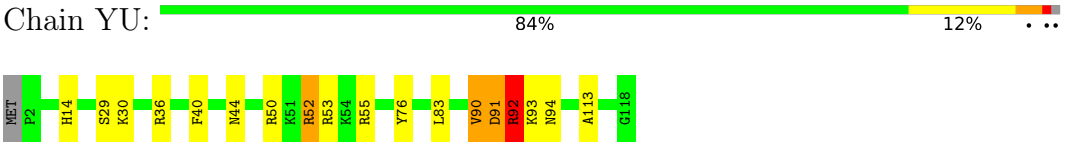
• Molecule 50: 50S ribosomal protein L20

Chain RU:



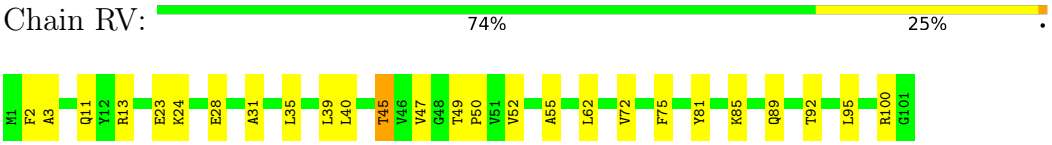
• Molecule 50: 50S ribosomal protein L20

Chain YU:



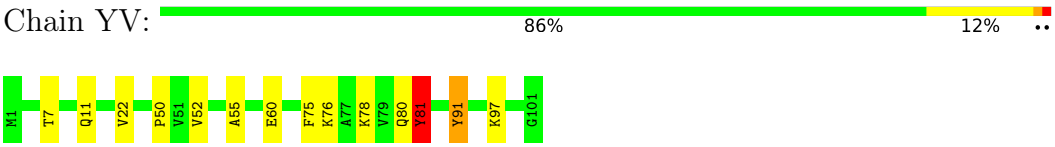
• Molecule 51: 50S ribosomal protein L21

Chain RV:



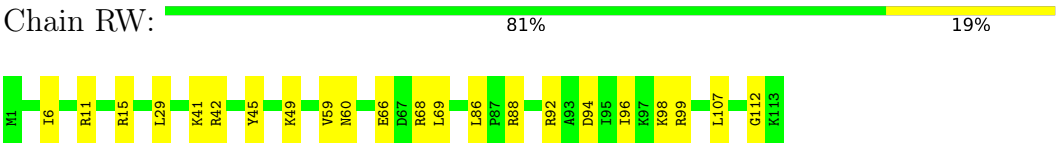
• Molecule 51: 50S ribosomal protein L21

Chain YV:



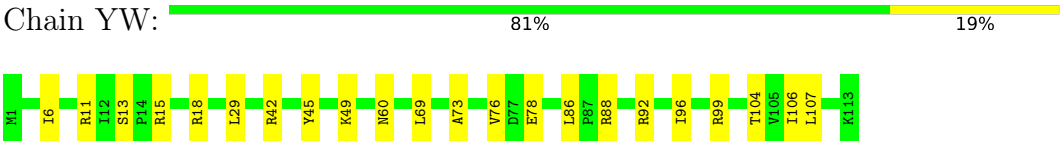
• Molecule 52: 50S ribosomal protein L22

Chain RW:



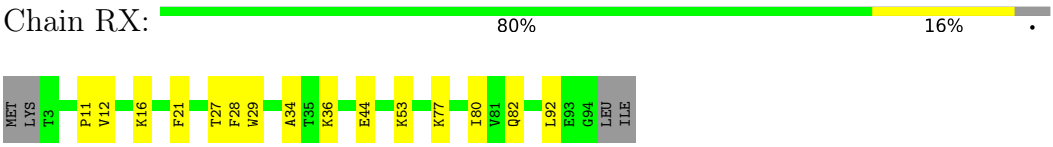
• Molecule 52: 50S ribosomal protein L22

Chain YW:



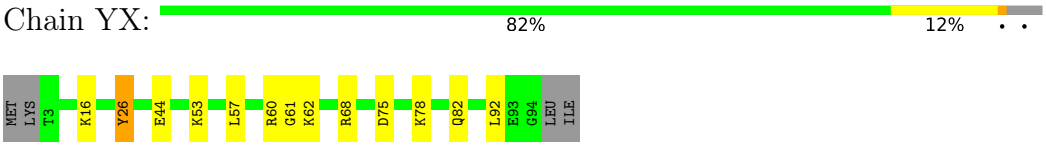
• Molecule 53: 50S ribosomal protein L23

Chain RX:



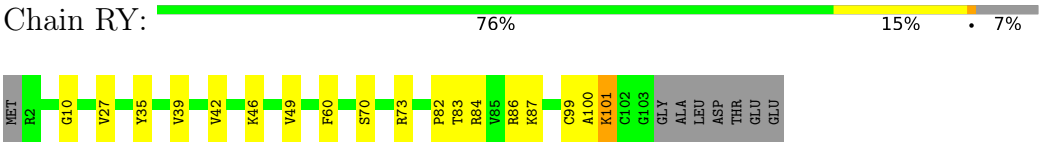
• Molecule 53: 50S ribosomal protein L23

Chain YX:



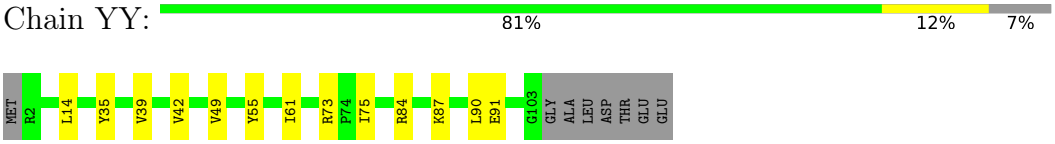
• Molecule 54: 50S ribosomal protein L24

Chain RY:



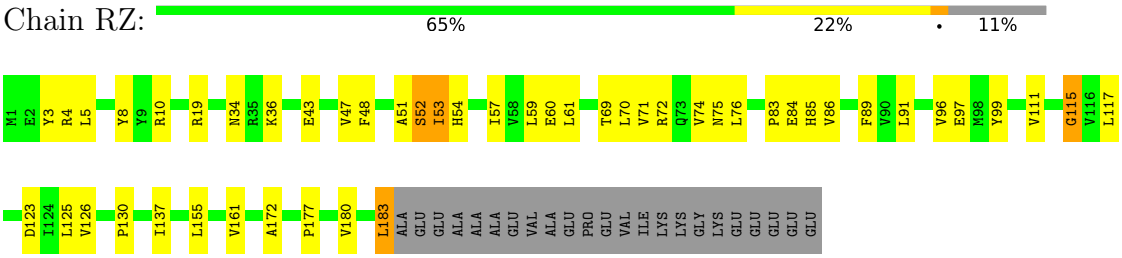
• Molecule 54: 50S ribosomal protein L24

Chain YY:



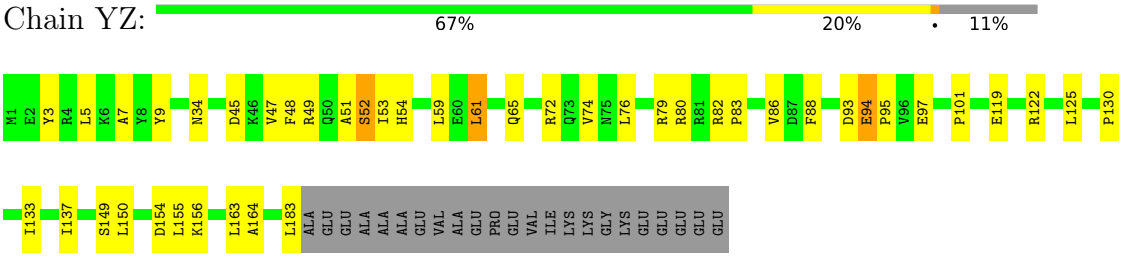
• Molecule 55: 50S ribosomal protein L25

Chain RZ:



• Molecule 55: 50S ribosomal protein L25

Chain YZ:



4 Data and refinement statistics (i)

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, α, β, γ	209.38Å 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10	Depositor
% Data completeness (in resolution range)	97.2 (49.74-3.10)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266	Depositor
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.328	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, ZN, PAR, MG

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	1.05	0/36098	1.14	177/56341 (0.3%)
1	XA	1.14	0/36101	1.18	234/56346 (0.4%)
2	QB	0.48	0/1959	0.68	0/2642
2	XB	0.55	0/1959	0.68	0/2642
3	QC	0.50	0/1629	0.69	2/2195 (0.1%)
3	XC	0.52	0/1629	0.66	0/2195
4	QD	0.58	0/1704	0.63	0/2284
4	XD	0.58	0/1704	0.65	0/2284
5	QE	0.55	1/1171 (0.1%)	0.67	0/1576
5	XE	0.54	0/1171	0.65	1/1576 (0.1%)
6	QF	0.60	0/856	0.62	0/1154
6	XF	0.58	0/856	0.66	0/1154
7	QG	0.51	0/1276	0.65	1/1709 (0.1%)
7	XG	0.52	0/1276	0.65	0/1709
8	QH	0.51	0/1136	0.66	0/1527
8	XH	0.59	0/1136	0.66	0/1527
9	QI	0.53	0/1029	0.77	0/1379
9	XI	0.53	0/1029	0.72	0/1379
10	QJ	0.46	0/814	0.64	0/1095
10	XJ	0.53	0/814	0.63	0/1095
11	QK	0.55	0/900	0.64	0/1213
11	XK	0.53	0/900	0.63	0/1213
12	QL	0.56	0/991	0.76	3/1327 (0.2%)
12	XL	0.63	0/991	0.75	1/1327 (0.1%)
13	QM	0.52	0/974	0.79	1/1303 (0.1%)
13	XM	0.50	0/974	0.72	0/1303
14	QN	0.55	0/501	0.67	0/664
14	XN	0.62	0/501	0.75	0/664
15	QO	0.50	0/745	0.59	0/992
15	XO	0.48	0/745	0.59	0/992
16	QP	0.58	0/721	0.75	2/970 (0.2%)
16	XP	0.55	0/721	0.76	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.60	0/847	0.65	1/1131 (0.1%)
17	XQ	0.59	0/847	0.64	1/1131 (0.1%)
18	QR	0.59	0/579	0.73	0/768
18	XR	0.57	0/579	0.65	0/768
19	QS	0.47	0/689	0.70	0/926
19	XS	0.62	0/689	0.97	2/926 (0.2%)
20	QT	0.48	0/765	0.66	0/1007
20	XT	0.44	0/765	0.71	1/1007 (0.1%)
21	QU	0.59	0/221	0.73	0/288
21	XU	0.67	0/221	0.81	1/288 (0.3%)
22	QV	0.91	0/1832	1.23	17/2855 (0.6%)
22	XV	1.07	0/1832	1.13	7/2855 (0.2%)
23	QX	0.77	0/446	1.06	2/695 (0.3%)
23	XX	0.87	0/446	1.17	1/695 (0.1%)
24	QY	0.74	0/1790	1.20	15/2789 (0.5%)
24	XY	0.78	0/1790	1.20	10/2789 (0.4%)
25	R0	0.59	0/657	0.68	1/874 (0.1%)
25	Y0	0.69	0/657	0.69	0/874
26	R1	0.63	0/770	0.79	2/1022 (0.2%)
26	Y1	0.64	0/770	0.76	1/1022 (0.1%)
27	R2	0.52	0/583	0.68	0/771
27	Y2	0.56	0/583	0.75	0/771
28	R3	0.50	0/474	0.57	0/635
28	Y3	0.57	0/474	0.58	0/635
29	R4	0.61	0/594	1.05	2/795 (0.3%)
29	Y4	0.56	0/594	1.05	3/795 (0.4%)
30	R5	0.60	0/473	0.92	2/639 (0.3%)
30	Y5	0.68	0/473	0.74	0/639
31	R6	0.70	0/431	1.14	2/575 (0.3%)
31	Y6	0.73	0/431	1.04	2/575 (0.3%)
32	R7	0.66	0/438	0.66	0/575
32	Y7	0.71	0/438	0.71	0/575
33	R8	0.64	0/525	0.86	1/691 (0.1%)
33	Y8	0.78	1/525 (0.2%)	0.84	0/691
34	R9	0.61	0/310	0.54	0/407
34	Y9	0.67	0/310	0.60	0/407
35	RA	1.23	8/69521 (0.0%)	1.22	496/108529 (0.5%)
35	YA	1.38	19/69543 (0.0%)	1.26	627/108563 (0.6%)
36	RB	0.99	0/2878	1.19	16/4490 (0.4%)
36	YB	1.23	0/2878	1.22	17/4490 (0.4%)
37	RD	0.71	0/2165	0.76	1/2919 (0.0%)
37	YD	0.75	0/2165	0.78	2/2919 (0.1%)
38	RE	0.63	0/1601	0.82	4/2160 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YE	0.71	0/1601	0.85	1/2160 (0.0%)
39	RF	0.65	0/1620	0.67	0/2194
39	YF	0.72	1/1620 (0.1%)	0.71	1/2194 (0.0%)
40	RG	0.51	0/1499	0.72	0/2016
40	YG	0.55	0/1499	0.70	1/2016 (0.0%)
41	RH	0.50	0/1332	0.81	2/1802 (0.1%)
41	YH	0.63	0/1332	0.84	3/1802 (0.2%)
42	RI	0.59	2/1151 (0.2%)	0.90	7/1558 (0.4%)
42	YI	0.52	0/1151	0.83	2/1558 (0.1%)
43	RN	0.57	0/1131	0.71	1/1525 (0.1%)
43	YN	0.63	0/1131	0.74	2/1525 (0.1%)
44	RO	0.62	0/943	0.66	1/1269 (0.1%)
44	YO	0.72	0/943	0.76	2/1269 (0.2%)
45	RP	0.59	0/1162	0.89	0/1544
45	YP	0.61	0/1162	0.85	1/1544 (0.1%)
46	RQ	0.63	0/1143	0.83	2/1527 (0.1%)
46	YQ	0.71	0/1143	0.87	3/1527 (0.2%)
47	RR	0.62	0/982	0.69	0/1312
47	YR	0.64	0/982	0.72	0/1312
48	RS	0.55	0/892	0.92	5/1187 (0.4%)
48	YS	0.59	0/892	0.78	1/1187 (0.1%)
49	RT	0.61	0/1155	0.78	3/1542 (0.2%)
49	YT	0.66	0/1155	0.82	4/1542 (0.3%)
50	RU	0.61	0/982	0.67	1/1306 (0.1%)
50	YU	0.70	0/982	0.69	1/1306 (0.1%)
51	RV	0.58	0/790	0.82	2/1057 (0.2%)
51	YV	0.76	0/790	0.88	2/1057 (0.2%)
52	RW	0.66	0/911	0.70	0/1220
52	YW	0.64	0/911	0.66	0/1220
53	RX	0.66	0/739	0.70	0/993
53	YX	0.71	0/739	0.67	0/993
54	RY	0.59	0/798	0.69	0/1064
54	YY	0.70	0/798	0.76	0/1064
55	RZ	0.52	0/1493	0.81	4/2026 (0.2%)
55	YZ	0.56	0/1493	0.78	2/2026 (0.1%)
All	All	1.08	32/319657 (0.0%)	1.11	1714/478147 (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
48	RS	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Y8	23	VAL	CB-CG1	-8.00	1.36	1.52
35	YA	528	A	N9-C4	-7.92	1.33	1.37
35	YA	1021	A	N9-C4	-7.85	1.33	1.37
35	YA	1142(A)	A	N9-C4	-7.78	1.33	1.37
35	YA	2287	A	N9-C4	-7.34	1.33	1.37
35	YA	27	G	N9-C4	-6.99	1.32	1.38
42	RI	133	HIS	C-N	6.98	1.47	1.34
35	RA	2448	A	N9-C4	-6.50	1.33	1.37
35	RA	1204	A	N9-C4	-6.20	1.34	1.37
35	YA	27	G	N3-C4	-6.14	1.31	1.35
35	RA	586	A	N9-C4	-6.03	1.34	1.37
5	QE	8	GLU	CG-CD	6.02	1.60	1.51
35	YA	1095	A	N9-C4	5.91	1.41	1.37
35	YA	2058	A	N9-C4	-5.69	1.34	1.37
35	YA	1020	A	N9-C4	-5.62	1.34	1.37
35	YA	783	A	N7-C5	-5.57	1.35	1.39
35	RA	1786	A	N7-C5	-5.48	1.35	1.39
35	YA	774	A	N9-C4	-5.43	1.34	1.37
35	YA	2561	A	N9-C4	-5.43	1.34	1.37
35	YA	829	A	N9-C4	-5.40	1.34	1.37
35	YA	1021	A	N3-C4	-5.39	1.31	1.34
35	RA	783	A	N9-C4	-5.37	1.34	1.37
35	YA	74	A	N9-C4	-5.35	1.34	1.37
35	YA	71	A	N9-C4	-5.27	1.34	1.37
35	YA	627	A	N9-C4	-5.24	1.34	1.37
35	YA	2452	C	N1-C6	-5.21	1.34	1.37
42	RI	134	PRO	N-CD	-5.19	1.40	1.47
35	RA	1142(A)	A	N9-C4	-5.13	1.34	1.37
35	RA	2378	A	N9-C4	-5.12	1.34	1.37
35	YA	1571	A	N9-C4	-5.10	1.34	1.37
35	RA	685	A	N9-C4	-5.06	1.34	1.37
39	YF	57	VAL	CB-CG1	-5.03	1.42	1.52

All (1714) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	XS	10	PHE	CB-CG-CD1	12.46	129.52	120.80
1	QA	1301	U	N1-C2-O2	11.86	131.10	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2506	U	C2-N1-C1'	11.85	131.92	117.70
1	QA	1301	U	C2-N1-C1'	11.78	131.83	117.70
35	YA	2506	U	C2-N1-C1'	11.73	131.77	117.70
35	RA	2506	U	N3-C2-O2	-11.66	114.04	122.20
1	QA	328	C	N1-C2-O2	11.60	125.86	118.90
19	XS	10	PHE	CB-CG-CD2	-11.54	112.72	120.80
35	RA	2506	U	N1-C2-O2	11.50	130.85	122.80
1	XA	1336	C	N1-C2-O2	11.40	125.74	118.90
22	QV	17	C	N1-C2-O2	11.36	125.72	118.90
35	YA	2506	U	N1-C2-O2	11.16	130.61	122.80
35	YA	2506	U	N3-C2-O2	-11.13	114.41	122.20
35	YA	2688	U	N3-C2-O2	-11.00	114.50	122.20
35	RA	613	U	N3-C2-O2	-10.78	114.65	122.20
29	R4	43	TYR	CA-CB-CG	10.64	133.61	113.40
1	QA	1301	U	N3-C2-O2	-10.56	114.81	122.20
35	YA	856	C	C6-N1-C2	-10.56	116.08	120.30
35	RA	828	U	N3-C2-O2	-10.55	114.81	122.20
35	YA	2474	C	N1-C2-O2	10.52	125.21	118.90
22	QV	17	C	C2-N1-C1'	10.45	130.30	118.80
46	YQ	5	ARG	CG-CD-NE	-10.41	89.94	111.80
35	YA	860	U	N3-C2-O2	-10.23	115.04	122.20
35	YA	27	G	N3-C4-N9	-10.13	119.92	126.00
1	XA	1336	C	C2-N1-C1'	10.02	129.82	118.80
35	YA	1313	U	C2-N1-C1'	10.01	129.72	117.70
35	RA	1914	C	N1-C2-O2	9.99	124.89	118.90
1	XA	1336	C	N3-C2-O2	-9.98	114.91	121.90
22	QV	17(A)	U	N3-C2-O2	-9.82	115.33	122.20
1	XA	1054	C	N1-C2-O2	9.81	124.78	118.90
29	Y4	39	CYS	C-N-CA	9.74	146.06	121.70
22	QV	17	C	C6-N1-C2	-9.62	116.45	120.30
22	QV	17	C	N3-C2-O2	-9.59	115.19	121.90
35	RA	613	U	N1-C2-O2	9.59	129.51	122.80
35	YA	1396	U	N1-C2-O2	9.57	129.50	122.80
35	YA	265	A	O4'-C1'-N9	9.46	115.77	108.20
35	RA	1914	C	N3-C2-O2	-9.35	115.36	121.90
1	QA	1158	C	C2-N1-C1'	9.32	129.06	118.80
35	YA	1396	U	C2-N1-C1'	9.28	128.84	117.70
35	RA	2712	U	N3-C2-O2	-9.23	115.74	122.20
1	XA	792	A	O4'-C1'-N9	9.21	115.57	108.20
35	RA	828	U	C2-N1-C1'	9.18	128.71	117.70
48	RS	17	ARG	CG-CD-NE	9.14	130.99	111.80
1	XA	963	G	C6-C5-N7	-9.13	124.92	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	1396	U	N3-C2-O2	-9.03	115.88	122.20
35	RA	2755	C	C5-C6-N1	8.99	125.50	121.00
35	YA	2712	U	N3-C2-O2	-8.96	115.93	122.20
35	RA	1313	U	N3-C2-O2	-8.94	115.94	122.20
35	RA	1882	C	C6-N1-C2	-8.94	116.72	120.30
36	YB	31	C	C6-N1-C2	-8.91	116.73	120.30
35	YA	2584	U	N3-C2-O2	-8.88	115.98	122.20
35	RA	1914	C	C2-N1-C1'	8.87	128.55	118.80
35	YA	1314	C	N1-C2-O2	8.86	124.22	118.90
24	XY	59	U	N1-C2-O2	8.82	128.98	122.80
35	YA	650	C	C6-N1-C2	-8.80	116.78	120.30
35	YA	271(A)	C	N1-C2-O2	8.77	124.16	118.90
30	R5	3	LYS	C-N-CA	8.75	143.58	121.70
1	XA	1336	C	C6-N1-C2	-8.72	116.81	120.30
35	RA	837	C	C6-N1-C2	-8.71	116.82	120.30
35	RA	1313	U	C2-N1-C1'	8.70	128.14	117.70
24	QY	54	U	C5-C6-N1	8.69	127.05	122.70
35	RA	860	U	N3-C2-O2	-8.69	116.12	122.20
44	YO	71	ARG	CG-CD-NE	8.68	130.03	111.80
35	RA	856	C	C5-C6-N1	8.68	125.34	121.00
35	YA	2474	C	N3-C2-O2	-8.67	115.83	121.90
1	XA	1054	C	N3-C2-O2	-8.64	115.85	121.90
35	RA	856	C	C6-N1-C2	-8.64	116.84	120.30
1	XA	812	C	P-O3'-C3'	8.63	130.06	119.70
26	R1	10	LYS	C-N-CA	8.63	143.27	121.70
35	RA	828	U	N1-C2-O2	8.62	128.84	122.80
35	YA	1204	A	O4'-C1'-N9	8.58	115.07	108.20
35	YA	1121	C	C6-N1-C2	-8.56	116.87	120.30
35	YA	120	U	C2-N1-C1'	8.53	127.94	117.70
1	QA	1158	C	N1-C2-O2	8.52	124.01	118.90
1	XA	827	U	N3-C2-O2	-8.52	116.24	122.20
35	RA	1543	A	O4'-C1'-N9	8.51	115.01	108.20
1	QA	328	C	N3-C2-O2	-8.50	115.95	121.90
35	RA	2712	U	N1-C2-O2	8.46	128.72	122.80
35	RA	1332	G	N7-C8-N9	8.46	117.33	113.10
1	XA	1301	U	N1-C2-O2	8.44	128.70	122.80
1	QA	1301	U	C6-N1-C1'	-8.43	109.40	121.20
35	RA	2286	A	N9-C4-C5	-8.40	102.44	105.80
51	YV	81	TYR	CA-CB-CG	8.38	129.33	113.40
35	YA	753	C	C6-N1-C2	-8.38	116.95	120.30
35	RA	1204	A	O4'-C1'-N9	8.37	114.90	108.20
1	XA	739	C	C6-N1-C2	-8.35	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	1163	C	C6-N1-C2	-8.27	116.99	120.30
22	QV	17(A)	U	N1-C2-O2	8.27	128.59	122.80
35	RA	1407	C	N1-C2-O2	8.24	123.84	118.90
35	RA	2205	C	C6-N1-C2	-8.21	117.01	120.30
1	XA	827	U	C2-N1-C1'	8.19	127.53	117.70
35	YA	856	C	C5-C6-N1	8.17	125.08	121.00
35	YA	120	U	N1-C2-O2	8.15	128.50	122.80
1	XA	346	G	N3-C4-N9	8.14	130.89	126.00
35	YA	860	U	C2-N1-C1'	8.12	127.45	117.70
35	YA	271(A)	C	N3-C2-O2	-8.12	116.22	121.90
35	YA	1931	U	N3-C2-O2	-8.11	116.52	122.20
35	RA	1407	C	C6-N1-C2	-8.10	117.06	120.30
35	YA	1914	C	C2-N1-C1'	8.09	127.69	118.80
35	YA	120	U	N3-C2-O2	-8.08	116.54	122.20
35	YA	860	U	N1-C2-O2	8.08	128.46	122.80
35	RA	915	C	C6-N1-C2	-8.07	117.07	120.30
35	YA	2856	C	C6-N1-C2	-8.07	117.07	120.30
12	QL	105	TYR	CA-CB-CG	8.07	128.73	113.40
35	RA	1404	C	N1-C2-O2	8.06	123.74	118.90
1	QA	254	G	O5'-P-OP1	-8.06	98.45	105.70
35	YA	1402	C	C6-N1-C2	-8.03	117.09	120.30
35	RA	2712	U	C2-N1-C1'	8.03	127.33	117.70
35	RA	1654	A	O5'-P-OP1	-8.02	98.49	105.70
35	YA	912	C	C6-N1-C2	-8.01	117.10	120.30
1	QA	328	C	C2-N1-C1'	8.00	127.60	118.80
35	YA	2688	U	N1-C2-O2	7.99	128.39	122.80
35	YA	1881	C	C6-N1-C2	-7.98	117.11	120.30
1	XA	1301	U	N3-C2-O2	-7.97	116.62	122.20
35	YA	560	C	N1-C2-O2	7.95	123.67	118.90
35	RA	2702	U	N1-C2-O2	7.94	128.36	122.80
1	XA	1158	C	C2-N1-C1'	7.92	127.51	118.80
35	RA	2506	U	C6-N1-C1'	-7.91	110.12	121.20
35	RA	595	C	C5-C6-N1	7.89	124.94	121.00
24	QY	70	U	N1-C2-O2	7.84	128.28	122.80
1	QA	960	U	N1-C2-O2	7.83	128.28	122.80
22	QV	17(A)	U	C2-N1-C1'	7.81	127.07	117.70
35	RA	2210	G	C4-N9-C1'	7.80	136.63	126.50
35	RA	2755	C	C6-N1-C2	-7.79	117.19	120.30
22	XV	17(A)	U	N3-C2-O2	-7.78	116.76	122.20
35	YA	1314	C	C6-N1-C2	-7.77	117.19	120.30
35	YA	2584	U	C2-N1-C1'	7.77	127.02	117.70
35	YA	528	A	C2-N3-C4	-7.75	106.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	1956	U	N3-C2-O2	-7.75	116.77	122.20
1	QA	1336	C	N1-C2-O2	7.74	123.55	118.90
35	YA	1178	C	C6-N1-C2	-7.74	117.20	120.30
35	YA	1313	U	N3-C2-O2	-7.73	116.79	122.20
35	YA	1879	C	C6-N1-C2	-7.73	117.21	120.30
35	RA	1804	C	C6-N1-C2	-7.73	117.21	120.30
35	RA	2584	U	N3-C2-O2	-7.69	116.81	122.20
35	RA	2591	C	C6-N1-C2	-7.69	117.22	120.30
35	YA	2832	U	P-O3'-C3'	7.69	128.93	119.70
35	YA	385	C	N3-C2-O2	-7.69	116.52	121.90
35	RA	650	C	C6-N1-C2	-7.68	117.23	120.30
22	QV	17(A)	U	C6-N1-C2	-7.68	116.39	121.00
35	YA	1376	C	N1-C2-O2	7.68	123.51	118.90
48	RS	17	ARG	CD-NE-CZ	7.67	134.34	123.60
1	QA	1322	C	N1-C2-O2	7.67	123.50	118.90
35	RA	1314	C	C5-C6-N1	7.66	124.83	121.00
35	YA	898	C	N1-C2-O2	7.66	123.50	118.90
1	XA	328	C	N1-C2-O2	7.65	123.49	118.90
35	YA	2506	U	C6-N1-C1'	-7.65	110.48	121.20
35	RA	2702	U	N3-C2-O2	-7.65	116.84	122.20
35	YA	1899	G	C4-N9-C1'	7.65	136.44	126.50
35	RA	1786	A	N7-C8-N9	7.65	117.62	113.80
35	YA	1306	C	C6-N1-C2	-7.65	117.24	120.30
35	YA	817	C	C6-N1-C2	-7.64	117.24	120.30
35	YA	1914	C	N1-C2-O2	7.64	123.48	118.90
35	RA	2703	C	N1-C2-O2	7.63	123.48	118.90
35	YA	1314	C	C2-N1-C1'	7.63	127.19	118.80
35	RA	650	C	C5-C6-N1	7.63	124.81	121.00
24	XY	59	U	N3-C2-O2	-7.63	116.86	122.20
36	YB	22	U	C5-C6-N1	7.62	126.51	122.70
35	RA	1899	G	C4-N9-C1'	7.62	136.40	126.50
35	YA	837	C	C6-N1-C2	-7.61	117.25	120.30
35	YA	1437	C	N1-C2-O2	7.61	123.46	118.90
35	RA	1992	G	C2'-C3'-O3'	7.60	126.23	109.50
35	RA	1882	C	C5-C6-N1	7.60	124.80	121.00
35	YA	930	U	C2-N1-C1'	7.59	126.81	117.70
35	YA	1950	G	C4-N9-C1'	7.59	136.36	126.50
31	Y6	7	ILE	C-N-CA	7.58	140.66	121.70
31	R6	7	ILE	C-N-CA	7.58	140.65	121.70
35	YA	2712	U	N1-C2-O2	7.58	128.11	122.80
35	YA	1021	A	C8-N9-C4	-7.58	102.77	105.80
1	XA	328	C	C2-N1-C1'	7.58	127.13	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	RB	70	C	C6-N1-C2	-7.55	117.28	120.30
1	XA	963	G	N3-C4-N9	7.55	130.53	126.00
35	YA	758	C	C6-N1-C2	-7.55	117.28	120.30
35	YA	97	C	C6-N1-C2	-7.53	117.29	120.30
35	YA	243	U	C5-C6-N1	7.53	126.47	122.70
35	RA	669	G	C4-N9-C1'	7.52	136.27	126.50
35	YA	1578	U	N3-C2-O2	-7.51	116.94	122.20
35	RA	613	U	C2-N1-C1'	7.51	126.71	117.70
24	XY	72	C	N1-C2-O2	7.51	123.40	118.90
35	YA	2210	G	C4-N9-C1'	7.51	136.26	126.50
1	XA	826	C	C6-N1-C2	-7.50	117.30	120.30
35	RA	912	C	C6-N1-C2	-7.49	117.30	120.30
35	YA	378	C	C6-N1-C2	-7.48	117.31	120.30
35	RA	2350	C	N1-C2-O2	7.48	123.39	118.90
35	RA	1407	C	C2-N1-C1'	7.47	127.02	118.80
35	RA	1332	G	C4-N9-C1'	7.47	136.21	126.50
35	YA	2559	C	C5-C6-N1	7.47	124.73	121.00
1	XA	1024	G	O5'-P-OP1	7.47	119.66	110.70
1	QA	1158	C	N3-C2-O2	-7.46	116.68	121.90
1	XA	749	C	C6-N1-C2	-7.46	117.31	120.30
35	RA	1644	C	C6-N1-C2	-7.45	117.32	120.30
35	RA	2210	G	C8-N9-C1'	-7.44	117.33	127.00
33	R8	61	LEU	C-N-CA	7.42	140.26	121.70
35	YA	2712	U	C2-N1-C1'	7.42	126.60	117.70
35	YA	1313	U	N1-C2-O2	7.41	127.99	122.80
1	QA	1066	C	N1-C2-O2	7.39	123.33	118.90
1	QA	1407	C	C5-C6-N1	7.38	124.69	121.00
1	QA	1297	C	P-O3'-C3'	7.38	128.56	119.70
35	YA	1955	U	N3-C2-O2	-7.38	117.03	122.20
35	RA	1558	A	P-O3'-C3'	7.35	128.52	119.70
1	XA	328	C	P-O3'-C3'	7.35	128.52	119.70
35	RA	227	A	P-O3'-C3'	7.34	128.51	119.70
1	XA	699	C	C6-N1-C2	-7.34	117.36	120.30
35	YA	2474	C	C2-N1-C1'	7.33	126.87	118.80
1	QA	960	U	C2-N1-C1'	7.33	126.50	117.70
35	YA	1332	G	N7-C8-N9	7.31	116.75	113.10
35	YA	2559	C	C6-N1-C2	-7.31	117.38	120.30
35	YA	1332	G	C6-C5-N7	-7.30	126.02	130.40
35	YA	2044	C	C6-N1-C2	-7.30	117.38	120.30
1	QA	1161	C	N1-C2-O2	7.30	123.28	118.90
1	XA	346	G	N3-C4-C5	-7.29	124.95	128.60
35	YA	783	A	N7-C8-N9	7.29	117.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2712	U	P-O3'-C3'	7.29	128.45	119.70
35	YA	1314	C	N3-C2-O2	-7.27	116.81	121.90
35	YA	634	C	C6-N1-C2	-7.27	117.39	120.30
1	XA	972	C	C6-N1-C2	-7.26	117.39	120.30
35	YA	783	A	C5-N7-C8	-7.26	100.27	103.90
35	YA	385	C	C2-N1-C1'	7.25	126.77	118.80
35	RA	2044	C	C6-N1-C2	-7.25	117.40	120.30
3	QC	23	TYR	CA-CB-CG	7.23	127.14	113.40
35	RA	420	C	C6-N1-C2	-7.23	117.41	120.30
35	RA	898	C	N1-C2-O2	7.23	123.24	118.90
35	YA	1026	U	P-O3'-C3'	7.23	128.38	119.70
35	RA	140	A	N7-C8-N9	7.23	117.42	113.80
24	XY	59	U	C2-N1-C1'	7.22	126.37	117.70
35	YA	560	C	N3-C2-O2	-7.22	116.84	121.90
35	YA	2646	C	N1-C2-O2	7.22	123.23	118.90
1	XA	254	G	O5'-P-OP1	-7.22	99.20	105.70
35	YA	161	U	N3-C2-O2	-7.22	117.15	122.20
1	XA	314	C	C6-N1-C2	-7.21	117.42	120.30
1	QA	789	U	N3-C2-O2	-7.21	117.16	122.20
35	RA	1313	U	N1-C2-O2	7.20	127.84	122.80
35	RA	2286	A	C8-N9-C4	7.19	108.68	105.80
35	YA	333	G	C4-N9-C1'	7.19	135.85	126.50
35	YA	1174	A	C2-N3-C4	7.19	114.20	110.60
1	QA	1407	C	C6-N1-C2	-7.19	117.42	120.30
1	XA	749	C	C5-C6-N1	7.19	124.59	121.00
35	YA	2403	C	N1-C2-O2	7.19	123.22	118.90
35	YA	2880	C	C6-N1-C2	-7.19	117.42	120.30
35	RA	2591	C	C5-C6-N1	7.18	124.59	121.00
35	RA	2787	C	N1-C2-O2	7.18	123.21	118.90
35	YA	385	C	N1-C2-O2	7.18	123.21	118.90
35	YA	846	C	O5'-P-OP1	-7.18	99.24	105.70
35	RA	1305	C	N1-C2-O2	7.17	123.20	118.90
1	QA	1440	C	N1-C2-O2	7.17	123.20	118.90
35	YA	2044	C	C5-C6-N1	7.16	124.58	121.00
35	YA	1914	C	N3-C2-O2	-7.15	116.89	121.90
1	XA	435	C	C6-N1-C2	-7.14	117.44	120.30
35	YA	2681	C	P-O3'-C3'	7.14	128.26	119.70
1	QA	328	C	P-O3'-C3'	7.13	128.26	119.70
35	RA	120	U	N1-C2-O2	7.12	127.79	122.80
35	RA	140	A	C8-N9-C4	-7.12	102.95	105.80
35	RA	1881	C	C6-N1-C2	-7.11	117.46	120.30
35	RA	1022	G	P-O3'-C3'	7.11	128.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2584	U	C2-N1-C1'	7.11	126.23	117.70
35	RA	1314	C	C6-N1-C2	-7.10	117.46	120.30
35	YA	1640	C	C5-C6-N1	7.10	124.55	121.00
35	RA	120	U	C2-N1-C1'	7.10	126.22	117.70
35	YA	27	G	N3-C2-N2	-7.08	114.94	119.90
55	RZ	183	LEU	CA-CB-CG	7.08	131.58	115.30
35	YA	537	C	C6-N1-C2	-7.07	117.47	120.30
35	YA	1535	U	C2-N1-C1'	7.07	126.18	117.70
35	RA	229	A	OP2-P-O3'	7.07	120.75	105.20
48	RS	36	TYR	CA-CB-CG	7.07	126.83	113.40
1	QA	346	G	N3-C4-N9	7.06	130.24	126.00
24	QY	70	U	C5-C6-N1	7.06	126.23	122.70
36	YB	31	C	C2-N1-C1'	7.06	126.56	118.80
36	YB	70	C	C6-N1-C2	-7.06	117.48	120.30
35	YA	1021	A	C2-N3-C4	-7.06	107.07	110.60
35	RA	1314	C	N1-C2-O2	7.05	123.13	118.90
35	RA	229	A	P-O3'-C3'	7.05	128.16	119.70
35	RA	1332	G	C8-N9-C4	-7.05	103.58	106.40
35	RA	1407	C	C5-C6-N1	7.05	124.52	121.00
1	QA	311	C	C6-N1-C2	-7.05	117.48	120.30
1	QA	1322	C	N3-C2-O2	-7.03	116.98	121.90
35	YA	528	A	N3-C4-N9	-7.03	121.78	127.40
35	RA	66	C	C6-N1-C2	-7.02	117.49	120.30
1	QA	337	C	C6-N1-C2	-7.02	117.49	120.30
1	XA	1109	C	C6-N1-C2	-7.02	117.49	120.30
35	RA	1658	C	C6-N1-C2	-7.00	117.50	120.30
1	XA	827	U	N1-C2-O2	7.00	127.70	122.80
35	YA	2403	C	C6-N1-C2	-7.00	117.50	120.30
35	RA	1332	G	C6-C5-N7	-7.00	126.20	130.40
35	RA	2559	C	N1-C2-O2	7.00	123.10	118.90
1	QA	1285	A	P-O3'-C3'	7.00	128.10	119.70
22	XV	17(A)	U	N1-C2-O2	6.99	127.69	122.80
22	QV	17	C	C5-C6-N1	6.98	124.49	121.00
35	RA	1407	C	N3-C2-O2	-6.98	117.01	121.90
35	YA	2688	U	C2-N1-C1'	6.98	126.07	117.70
1	QA	1203	C	C6-N1-C2	-6.98	117.51	120.30
35	YA	385	C	C6-N1-C2	-6.97	117.51	120.30
16	XP	38	TYR	CA-CB-CG	6.97	126.64	113.40
35	RA	1598	C	C6-N1-C2	-6.96	117.52	120.30
35	RA	2210	G	N3-C4-N9	6.96	130.18	126.00
35	YA	1095	A	C2-N3-C4	6.94	114.07	110.60
35	YA	528	A	N3-C4-C5	6.94	131.66	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	792	A	P-O3'-C3'	6.94	128.03	119.70
35	YA	930	U	N1-C2-O2	6.94	127.66	122.80
36	YB	31	C	N3-C2-O2	-6.93	117.05	121.90
35	YA	1314	C	C5-C6-N1	6.92	124.46	121.00
1	XA	812	C	OP2-P-O3'	6.92	120.41	105.20
35	YA	1407	C	C5-C6-N1	6.91	124.45	121.00
35	YA	1558	A	P-O3'-C3'	6.90	127.98	119.70
35	RA	2044	C	C5-C6-N1	6.89	124.44	121.00
35	YA	828	U	C2-N1-C1'	6.88	125.96	117.70
35	YA	1899	G	N3-C4-N9	6.88	130.13	126.00
1	XA	449	C	C2-N1-C1'	6.87	126.36	118.80
1	XA	963	G	N1-C2-N2	-6.87	110.02	116.20
1	QA	1065	U	P-O3'-C3'	6.87	127.94	119.70
39	YF	7	TYR	CA-CB-CG	6.87	126.45	113.40
1	XA	789	U	C2-N1-C1'	6.87	125.94	117.70
35	RA	1882	C	C2-N1-C1'	6.86	126.34	118.80
1	XA	789	U	N3-C2-O2	-6.85	117.40	122.20
35	YA	613	U	N3-C2-O2	-6.85	117.40	122.20
35	YA	1496	A	N7-C8-N9	6.85	117.22	113.80
35	YA	2889	C	C6-N1-C2	-6.85	117.56	120.30
35	YA	2321	G	C4-N9-C1'	6.85	135.40	126.50
1	XA	980	C	C6-N1-C2	-6.83	117.57	120.30
35	RA	753	C	C6-N1-C2	-6.83	117.57	120.30
35	YA	1686	C	C6-N1-C2	-6.83	117.57	120.30
35	YA	1022	G	P-O3'-C3'	6.82	127.89	119.70
35	RA	1793	C	C6-N1-C2	-6.82	117.57	120.30
35	RA	1124	C	C6-N1-C2	-6.82	117.57	120.30
1	QA	1066	C	C2-N1-C1'	6.81	126.30	118.80
35	RA	817	C	C6-N1-C2	-6.81	117.58	120.30
35	YA	2895	U	C5-C6-N1	6.81	126.10	122.70
1	QA	1024	G	O5'-P-OP1	6.80	118.86	110.70
43	YN	48	MET	CG-SD-CE	-6.80	89.32	100.20
22	QV	17(A)	U	C5-C6-N1	6.79	126.10	122.70
1	XA	58	C	C6-N1-C2	-6.79	117.58	120.30
35	RA	2688	U	N3-C2-O2	-6.79	117.45	122.20
35	YA	404	C	P-O3'-C3'	6.79	127.84	119.70
35	RA	1908	C	C6-N1-C2	-6.78	117.59	120.30
35	YA	661	C	C6-N1-C2	-6.77	117.59	120.30
1	QA	812	C	P-O3'-C3'	6.77	127.83	119.70
21	XU	18	TYR	CA-CB-CG	6.77	126.27	113.40
35	YA	846	C	P-O3'-C3'	6.77	127.82	119.70
35	RA	1233	C	C6-N1-C2	-6.76	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	828	U	N3-C2-O2	-6.76	117.46	122.20
35	RA	1437	C	C6-N1-C2	-6.76	117.59	120.30
1	XA	1297	C	P-O3'-C3'	6.76	127.81	119.70
35	YA	27	G	N3-C4-C5	6.76	131.98	128.60
35	RA	313	C	C6-N1-C2	-6.75	117.60	120.30
1	XA	1027	C	P-O3'-C3'	6.75	127.80	119.70
35	YA	930	U	N3-C2-O2	-6.75	117.47	122.20
35	RA	1404	C	N3-C2-O2	-6.74	117.18	121.90
1	XA	328	C	C6-N1-C2	-6.73	117.61	120.30
35	YA	1899	G	N3-C4-C5	-6.73	125.24	128.60
35	YA	27	G	N9-C4-C5	6.72	108.09	105.40
35	RA	263	C	C6-N1-C2	-6.72	117.61	120.30
35	RA	1045	A	P-O3'-C3'	6.72	127.77	119.70
1	QA	328	C	C6-N1-C2	-6.72	117.61	120.30
1	XA	1367	C	C6-N1-C2	-6.72	117.61	120.30
35	YA	1899	G	C8-N9-C1'	-6.72	118.26	127.00
1	QA	789	U	C2-N1-C1'	6.72	125.76	117.70
22	QV	62	C	N1-C2-O2	6.72	122.93	118.90
35	RA	846	C	P-O3'-C3'	6.71	127.76	119.70
35	RA	1804	C	C5-C6-N1	6.71	124.36	121.00
35	YA	222	A	P-O3'-C3'	6.70	127.74	119.70
35	YA	268	C	N1-C2-O2	6.70	122.92	118.90
35	RA	120	U	N3-C2-O2	-6.70	117.51	122.20
20	XT	73	HIS	C-N-CA	6.69	138.44	121.70
1	XA	1354	C	C6-N1-C2	-6.69	117.62	120.30
16	QP	38	TYR	CA-CB-CG	6.69	126.11	113.40
35	YA	1788	C	C6-N1-C2	-6.69	117.62	120.30
35	YA	753	C	C5-C6-N1	6.69	124.34	121.00
35	RA	635	C	C6-N1-C2	-6.68	117.63	120.30
35	RA	1914	C	C6-N1-C2	-6.68	117.63	120.30
1	XA	992	U	P-O3'-C3'	6.67	127.71	119.70
35	YA	1982	C	C6-N1-C2	-6.67	117.63	120.30
35	YA	1021	A	C5-N7-C8	-6.66	100.57	103.90
35	YA	1797	C	C5-C6-N1	6.66	124.33	121.00
35	RA	242	G	P-O3'-C3'	6.66	127.69	119.70
35	YA	1528	A	N7-C8-N9	6.66	117.13	113.80
35	YA	2667	C	C6-N1-C2	-6.65	117.64	120.30
35	YA	1005	C	N1-C2-O2	6.65	122.89	118.90
1	QA	1161	C	N3-C2-O2	-6.65	117.25	121.90
1	XA	449	C	N1-C2-O2	6.65	122.89	118.90
35	RA	2576	G	C4-N9-C1'	6.64	135.14	126.50
35	YA	1881	C	N1-C2-O2	6.64	122.89	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	1544	C	N1-C2-O2	6.64	122.88	118.90
1	QA	1347	G	P-O3'-C3'	6.64	127.67	119.70
35	YA	2350	C	N1-C2-O2	6.64	122.88	118.90
1	QA	1528	U	P-O3'-C3'	6.63	127.66	119.70
1	XA	1498	U	P-O3'-C3'	6.63	127.66	119.70
35	YA	1955	U	P-O3'-C3'	6.63	127.66	119.70
1	XA	687	A	P-O3'-C3'	6.63	127.66	119.70
1	XA	314	C	N1-C2-O2	6.63	122.88	118.90
1	XA	60	A	P-O3'-C3'	6.63	127.66	119.70
1	QA	992	U	P-O3'-C3'	6.63	127.66	119.70
35	RA	307	G	O5'-P-OP1	-6.63	99.74	105.70
35	YA	613	U	C2-N1-C1'	6.63	125.65	117.70
35	YA	114	U	C2-N1-C1'	6.62	125.65	117.70
1	QA	410	G	P-O3'-C3'	6.62	127.65	119.70
35	YA	783	A	C8-N9-C4	-6.62	103.15	105.80
35	YA	2702	U	O5'-P-OP2	-6.62	99.74	105.70
48	RS	88	ASP	C-N-CA	6.62	138.25	121.70
1	XA	963	G	N3-C2-N2	6.62	124.53	119.90
1	QA	250	A	P-O3'-C3'	6.62	127.64	119.70
1	QA	1038	C	N1-C2-O2	6.62	122.87	118.90
1	XA	1285	A	P-O3'-C3'	6.62	127.64	119.70
1	XA	1301	U	C2-N1-C1'	6.62	125.64	117.70
35	RA	2403	C	C5-C6-N1	6.61	124.31	121.00
35	YA	420	C	N1-C2-O2	6.61	122.87	118.90
35	RA	2688	U	C2-N1-C1'	6.61	125.63	117.70
1	XA	1439	C	C6-N1-C2	-6.61	117.66	120.30
35	YA	1332	G	C4-N9-C1'	6.60	135.08	126.50
35	RA	1053	C	C6-N1-C2	-6.60	117.66	120.30
36	RB	31	C	N1-C2-O2	6.60	122.86	118.90
35	YA	1021	A	N7-C8-N9	6.60	117.10	113.80
36	YB	79	C	C6-N1-C2	-6.60	117.66	120.30
1	QA	1158	C	C6-N1-C2	-6.59	117.66	120.30
1	XA	913	A	P-O3'-C3'	6.59	127.61	119.70
48	YS	110	LEU	CA-CB-CG	6.59	130.46	115.30
35	RA	1078	U	P-O3'-C3'	6.59	127.61	119.70
1	XA	1114	C	N1-C2-O2	6.59	122.85	118.90
35	YA	912	C	N3-C2-O2	-6.59	117.29	121.90
35	RA	2712	U	P-O3'-C3'	6.59	127.60	119.70
1	QA	687	A	P-O3'-C3'	6.58	127.60	119.70
35	RA	1496	A	N7-C8-N9	6.58	117.09	113.80
35	YA	97	C	N1-C2-O2	6.58	122.85	118.90
35	YA	1712	C	C6-N1-C2	-6.58	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	404	C	P-O3'-C3'	6.57	127.59	119.70
1	QA	1027	C	P-O3'-C3'	6.57	127.58	119.70
1	XA	1367	C	C5-C6-N1	6.57	124.28	121.00
35	YA	2403	C	N3-C2-O2	-6.56	117.31	121.90
35	RA	2043	C	N1-C2-O2	6.56	122.84	118.90
1	XA	509	A	C8-N9-C4	-6.56	103.17	105.80
1	QA	1498	U	P-O3'-C3'	6.56	127.57	119.70
35	YA	2210	G	C8-N9-C1'	-6.56	118.47	127.00
35	YA	269	U	N3-C2-O2	-6.56	117.61	122.20
35	YA	335	C	C6-N1-C2	-6.56	117.68	120.30
1	XA	1024	G	O5'-P-OP2	-6.55	99.80	105.70
1	QA	484	G	P-O3'-C3'	6.55	127.56	119.70
35	YA	806	C	C6-N1-C2	-6.55	117.68	120.30
1	QA	106	C	C6-N1-C2	-6.55	117.68	120.30
35	RA	1549	C	C6-N1-C2	-6.55	117.68	120.30
48	RS	17	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	QA	346	G	N3-C4-C5	-6.55	125.33	128.60
35	RA	115	C	C6-N1-C2	-6.55	117.68	120.30
1	XA	1158	C	C6-N1-C2	-6.55	117.68	120.30
35	YA	1363	C	N1-C2-O2	6.54	122.82	118.90
35	RA	1411	C	C6-N1-C2	-6.54	117.69	120.30
36	RB	42	C	C6-N1-C2	-6.53	117.69	120.30
35	RA	837	C	C5-C6-N1	6.52	124.26	121.00
1	XA	545	C	N3-C2-O2	-6.52	117.34	121.90
35	YA	1950	G	O4'-C1'-N9	6.52	113.42	108.20
46	RQ	9	TYR	CA-CB-CG	6.52	125.79	113.40
35	RA	2112	G	N3-C4-C5	-6.52	125.34	128.60
35	RA	1295	C	C6-N1-C2	-6.51	117.69	120.30
1	XA	1367	C	C2-N1-C1'	6.51	125.96	118.80
35	YA	2785	C	C6-N1-C2	-6.51	117.70	120.30
35	RA	537	C	N1-C2-O2	6.51	122.81	118.90
35	RA	2060	A	P-O3'-C3'	6.51	127.51	119.70
35	RA	2073	C	C6-N1-C2	-6.51	117.70	120.30
1	QA	1346	A	P-O3'-C3'	6.51	127.51	119.70
35	RA	2321	G	C4-N9-C1'	6.50	134.96	126.50
35	RA	2832	U	OP2-P-O3'	6.50	119.51	105.20
1	XA	1260	C	C6-N1-C2	-6.50	117.70	120.30
35	RA	1795	C	C6-N1-C2	-6.50	117.70	120.30
35	YA	1578	U	N1-C2-O2	6.50	127.35	122.80
1	QA	314	C	C6-N1-C2	-6.49	117.70	120.30
35	YA	2210	G	N3-C4-N9	6.49	129.89	126.00
35	RA	1376	C	N1-C2-O2	6.49	122.79	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	1514	C	C6-N1-C2	-6.49	117.70	120.30
35	RA	1204	A	C2-N3-C4	-6.48	107.36	110.60
1	XA	545	C	N1-C2-O2	6.48	122.79	118.90
35	YA	1827	C	C6-N1-C2	-6.48	117.71	120.30
1	XA	1038	C	N1-C2-O2	6.48	122.79	118.90
35	YA	67	U	C5-C6-N1	6.48	125.94	122.70
24	XY	72	C	N3-C2-O2	-6.47	117.37	121.90
35	RA	1786	A	C8-N9-C4	-6.47	103.21	105.80
1	XA	221	C	C5-C6-N1	6.47	124.23	121.00
35	YA	271(B)	G	P-O3'-C3'	6.47	127.46	119.70
1	XA	1158	C	N3-C2-O2	-6.47	117.37	121.90
35	RA	1686	C	N1-C2-O2	6.46	122.78	118.90
35	YA	1799	G	P-O3'-C3'	6.46	127.46	119.70
1	XA	137	C	N1-C2-O2	6.46	122.78	118.90
35	RA	530	G	O4'-C1'-N9	6.46	113.37	108.20
35	YA	1463	C	C6-N1-C2	-6.46	117.72	120.30
1	XA	328	C	N3-C2-O2	-6.46	117.38	121.90
1	QA	328	C	C5-C6-N1	6.46	124.23	121.00
35	YA	2701	C	C6-N1-C2	-6.45	117.72	120.30
24	QY	36	C	C6-N1-C2	-6.45	117.72	120.30
35	YA	1445	C	C6-N1-C2	-6.45	117.72	120.30
1	XA	1384	C	N1-C2-O2	6.45	122.77	118.90
1	XA	972	C	N3-C2-O2	-6.45	117.39	121.90
35	YA	2342	C	C6-N1-C2	-6.44	117.72	120.30
35	YA	974(A)	C	N1-C2-O2	6.44	122.76	118.90
35	YA	2584	U	N1-C2-O2	6.44	127.31	122.80
35	YA	859	G	P-O3'-C3'	6.43	127.42	119.70
35	RA	637	A	P-O3'-C3'	6.43	127.42	119.70
35	RA	669	G	C8-N9-C1'	-6.43	118.64	127.00
1	XA	484	G	P-O3'-C3'	6.43	127.42	119.70
12	XL	120	TYR	CA-CB-CG	6.43	125.62	113.40
1	QA	1336	C	C2-N1-C1'	6.43	125.87	118.80
35	YA	1218	C	C6-N1-C2	-6.43	117.73	120.30
1	QA	401	C	C6-N1-C2	-6.43	117.73	120.30
35	RA	41	C	N1-C2-O2	6.43	122.76	118.90
35	RA	1178	C	C6-N1-C2	-6.43	117.73	120.30
24	QY	25	C	C6-N1-C2	-6.43	117.73	120.30
35	YA	1988	C	C6-N1-C2	-6.43	117.73	120.30
22	QV	17	C	C6-N1-C1'	-6.42	113.09	120.80
22	XV	71	C	C6-N1-C2	-6.42	117.73	120.30
35	YA	1549	C	N1-C2-O2	6.42	122.75	118.90
35	YA	915	C	N1-C2-O2	6.42	122.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	76	C	N1-C2-O2	6.42	122.75	118.90
35	YA	2416	C	C5-C6-N1	6.41	124.21	121.00
35	YA	637	A	P-O3'-C3'	6.41	127.39	119.70
49	YT	100	TYR	CA-CB-CG	6.41	125.57	113.40
1	XA	960	U	C2-N1-C1'	6.40	125.39	117.70
35	YA	2236	C	C5-C6-N1	6.40	124.20	121.00
35	YA	41	C	C5-C6-N1	6.40	124.20	121.00
35	RA	2723	C	C6-N1-C2	-6.40	117.74	120.30
1	XA	135	C	C6-N1-C2	-6.39	117.74	120.30
1	QA	687	A	N1-C6-N6	-6.38	114.77	118.60
35	YA	1694	C	P-O3'-C3'	6.38	127.36	119.70
35	YA	1363	C	N3-C2-O2	-6.38	117.43	121.90
35	YA	1882	C	N1-C2-O2	6.38	122.73	118.90
35	YA	834	C	C6-N1-C2	-6.38	117.75	120.30
35	RA	860	U	C2-N1-C1'	6.37	125.35	117.70
35	RA	1352	U	N3-C2-O2	-6.37	117.74	122.20
1	QA	1163	C	C5-C6-N1	6.37	124.19	121.00
35	YA	1797	C	C6-N1-C2	-6.37	117.75	120.30
1	QA	1066	C	N3-C2-O2	-6.37	117.44	121.90
35	YA	755	C	C6-N1-C2	-6.36	117.75	120.30
35	YA	161	U	N1-C2-O2	6.36	127.25	122.80
35	YA	269	U	N1-C2-O2	6.36	127.25	122.80
35	YA	2129	C	N1-C2-O2	6.36	122.71	118.90
35	RA	2137	C	N1-C2-O2	6.35	122.71	118.90
1	QA	410	G	OP1-P-O3'	6.34	119.15	105.20
1	XA	1336	C	C6-N1-C1'	-6.34	113.19	120.80
35	RA	1314	C	C2-N1-C1'	6.33	125.77	118.80
1	XA	410	G	OP1-P-O3'	6.33	119.12	105.20
35	RA	2870	C	C6-N1-C2	-6.33	117.77	120.30
35	YA	1534	G	N3-C4-N9	6.33	129.80	126.00
1	QA	932	C	N1-C2-O2	6.32	122.69	118.90
35	RA	752	A	P-O3'-C3'	6.32	127.28	119.70
35	RA	253	C	N1-C2-O2	6.32	122.69	118.90
35	RA	1233	C	C5-C6-N1	6.32	124.16	121.00
35	RA	1306	C	N1-C2-O2	6.32	122.69	118.90
35	YA	2662	A	C8-N9-C4	-6.32	103.27	105.80
35	YA	1656	C	C6-N1-C2	-6.31	117.78	120.30
35	YA	1827	C	N3-C2-O2	-6.31	117.48	121.90
35	YA	2825	C	C6-N1-C2	-6.31	117.78	120.30
35	YA	816	C	N1-C2-O2	6.31	122.68	118.90
36	RB	47	C	N3-C4-C5	6.30	124.42	121.90
42	RI	134	PRO	C-N-CA	6.30	137.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	1158	C	C6-N1-C1'	-6.30	113.24	120.80
1	QA	1097	C	C6-N1-C2	-6.30	117.78	120.30
1	QA	948	C	N1-C2-O2	6.30	122.68	118.90
1	XA	826	C	C5-C6-N1	6.29	124.14	121.00
38	RE	27	LEU	CA-CB-CG	6.29	129.76	115.30
1	QA	913	A	P-O3'-C3'	6.29	127.25	119.70
35	YA	1076	C	N1-C2-O2	6.28	122.67	118.90
35	YA	1411	C	C6-N1-C2	-6.28	117.79	120.30
35	YA	1892	C	C6-N1-C2	-6.28	117.79	120.30
35	YA	1881	C	C5-C6-N1	6.28	124.14	121.00
1	XA	754	C	C2-N1-C1'	6.28	125.70	118.80
35	RA	828	U	C6-N1-C2	-6.28	117.23	121.00
35	YA	229	A	P-O3'-C3'	6.27	127.23	119.70
35	YA	1534	G	N3-C4-C5	-6.27	125.46	128.60
35	YA	1905	C	C6-N1-C2	-6.27	117.79	120.30
1	XA	345	C	P-O3'-C3'	6.27	127.22	119.70
24	XY	36	C	C6-N1-C2	-6.27	117.79	120.30
35	RA	1077	A	C2-N3-C4	6.27	113.73	110.60
35	YA	114	U	N1-C2-O2	6.27	127.19	122.80
35	YA	2889	C	N1-C2-O2	6.27	122.66	118.90
35	RA	1899	G	C8-N9-C4	-6.26	103.89	106.40
35	RA	1786	A	C5-N7-C8	-6.26	100.77	103.90
1	XA	89	U	P-O3'-C3'	6.26	127.21	119.70
35	YA	242	G	P-O3'-C3'	6.26	127.21	119.70
35	YA	2774	C	N1-C2-O2	6.26	122.66	118.90
1	QA	449	C	C2-N1-C1'	6.26	125.68	118.80
1	XA	1158	C	N1-C2-O2	6.26	122.65	118.90
35	YA	1437	C	N3-C2-O2	-6.25	117.53	121.90
1	QA	753	A	P-O3'-C3'	6.25	127.19	119.70
35	RA	1312	U	P-O3'-C3'	6.25	127.19	119.70
35	YA	1956	U	N1-C2-O2	6.24	127.17	122.80
35	RA	1653	G	P-O3'-C3'	6.24	127.19	119.70
35	RA	2350	C	N3-C2-O2	-6.24	117.53	121.90
35	RA	222	A	P-O3'-C3'	6.24	127.19	119.70
35	RA	1799	G	P-O3'-C3'	6.24	127.19	119.70
1	QA	1440	C	N3-C2-O2	-6.23	117.54	121.90
35	YA	1955	U	N1-C2-O2	6.23	127.16	122.80
1	XA	990	C	C6-N1-C2	-6.23	117.81	120.30
35	YA	1776	G	C4-N9-C1'	6.23	134.60	126.50
1	XA	963	G	N7-C8-N9	6.23	116.21	113.10
1	XA	1336	C	C5-C6-N1	6.23	124.11	121.00
35	RA	1711	C	C6-N1-C2	-6.22	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	1399	C	C6-N1-C2	-6.22	117.81	120.30
35	RA	2726	U	N3-C2-O2	-6.22	117.84	122.20
35	YA	2881	C	C6-N1-C2	-6.22	117.81	120.30
35	YA	1662	C	C6-N1-C2	-6.22	117.81	120.30
35	YA	2726	U	N3-C2-O2	-6.21	117.85	122.20
35	YA	1882	C	C5-C6-N1	6.21	124.11	121.00
35	YA	2416	C	C6-N1-C2	-6.21	117.82	120.30
35	RA	1892	C	C6-N1-C2	-6.21	117.82	120.30
35	RA	912	C	N1-C2-O2	6.20	122.62	118.90
35	YA	1535	U	N1-C2-O2	6.20	127.14	122.80
35	RA	1781	C	C2-N1-C1'	6.20	125.62	118.80
35	RA	2832	U	P-O3'-C3'	6.20	127.14	119.70
35	YA	618(A)	C	N1-C2-O2	6.19	122.61	118.90
35	YA	1950	G	C8-N9-C1'	-6.19	118.95	127.00
35	YA	1218	C	C5-C6-N1	6.19	124.09	121.00
35	RA	2417	C	C6-N1-C2	-6.19	117.83	120.30
35	YA	1804	C	N1-C2-O2	6.19	122.61	118.90
35	YA	634	C	N3-C2-O2	-6.18	117.57	121.90
35	RA	1999	C	C6-N1-C2	-6.18	117.83	120.30
22	XV	34	C	N1-C2-O2	6.18	122.61	118.90
35	RA	766	C	C6-N1-C2	-6.18	117.83	120.30
35	YA	510	C	N1-C2-O2	6.18	122.61	118.90
35	YA	2039	C	C6-N1-C2	-6.18	117.83	120.30
35	YA	838	C	C6-N1-C2	-6.17	117.83	120.30
43	YN	114	ARG	N-CA-C	-6.17	94.33	111.00
1	XA	412	A	P-O3'-C3'	6.17	127.11	119.70
35	YA	1712	C	C5-C6-N1	6.17	124.09	121.00
55	YZ	9	TYR	CA-CB-CG	6.17	125.13	113.40
1	QA	485	G	P-O3'-C3'	6.16	127.10	119.70
35	YA	2295	C	C6-N1-C2	-6.16	117.84	120.30
1	XA	58	C	C5-C6-N1	6.16	124.08	121.00
23	XX	18	G	P-O3'-C3'	6.16	127.09	119.70
1	QA	1059	C	C6-N1-C2	-6.16	117.84	120.30
35	RA	2478	A	O5'-P-OP2	-6.16	100.16	105.70
35	YA	1427	A	P-O3'-C3'	6.16	127.09	119.70
35	RA	31	C	C6-N1-C2	-6.15	117.84	120.30
35	YA	2681	C	OP2-P-O3'	6.15	118.73	105.20
35	RA	2439	A	P-O3'-C3'	6.15	127.08	119.70
35	YA	2844	G	C4-N9-C1'	6.15	134.49	126.50
35	RA	645	C	C5-C6-N1	6.15	124.07	121.00
24	XY	59	U	C5-C6-N1	6.14	125.77	122.70
35	RA	372	G	P-O3'-C3'	6.13	127.06	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1694	C	P-O3'-C3'	6.13	127.06	119.70
41	YH	82	GLY	N-CA-C	6.13	128.43	113.10
24	QY	72	C	N1-C2-O2	6.12	122.57	118.90
35	RA	2691	C	C5-C6-N1	6.12	124.06	121.00
1	XA	244	U	P-O3'-C3'	6.12	127.04	119.70
23	QX	18	G	P-O3'-C3'	6.12	127.04	119.70
35	RA	231	C	N1-C2-O2	6.12	122.57	118.90
35	RA	2471	C	N1-C2-O2	6.12	122.57	118.90
1	XA	1260	C	N1-C2-O2	6.12	122.57	118.90
35	YA	1313	U	C6-N1-C1'	-6.12	112.63	121.20
35	YA	1765	C	N1-C2-O2	6.12	122.57	118.90
35	YA	2402	C	P-O3'-C3'	6.12	127.04	119.70
35	RA	99	U	P-O3'-C3'	6.12	127.04	119.70
35	YA	1881	C	C2-N1-C1'	6.12	125.53	118.80
35	YA	2610	C	P-O3'-C3'	6.12	127.04	119.70
35	RA	2880	C	N3-C2-O2	-6.11	117.62	121.90
35	RA	2043	C	C5-C6-N1	6.11	124.06	121.00
35	YA	1306	C	C5-C6-N1	6.11	124.06	121.00
35	RA	2073	C	C5-C6-N1	6.11	124.05	121.00
35	RA	2084	C	C6-N1-C2	-6.11	117.86	120.30
35	YA	134	C	N3-C2-O2	-6.11	117.63	121.90
35	RA	1427	A	P-O3'-C3'	6.10	127.02	119.70
35	RA	503	A	P-O3'-C3'	6.10	127.02	119.70
35	YA	2662	A	N7-C8-N9	6.10	116.85	113.80
35	RA	273(F)	C	C6-N1-C2	-6.10	117.86	120.30
22	QV	75	C	C6-N1-C2	-6.09	117.86	120.30
35	YA	795	C	C6-N1-C2	-6.09	117.86	120.30
1	XA	137	C	N3-C2-O2	-6.09	117.64	121.90
35	YA	1021	A	N3-C4-N9	-6.09	122.53	127.40
35	RA	231	C	C5-C6-N1	6.09	124.04	121.00
35	YA	268	C	N3-C2-O2	-6.09	117.64	121.90
35	RA	273(F)	C	N1-C2-O2	6.08	122.55	118.90
1	XA	533	A	O5'-P-OP1	-6.08	100.23	105.70
35	RA	1598	C	C5-C6-N1	6.08	124.04	121.00
35	RA	2126	A	P-O3'-C3'	6.08	126.99	119.70
1	XA	1267	C	C5-C6-N1	6.08	124.04	121.00
35	YA	2471	C	N1-C2-O2	6.08	122.55	118.90
35	YA	2814	C	N3-C2-O2	-6.07	117.65	121.90
35	YA	2889	C	N3-C2-O2	-6.07	117.65	121.90
1	QA	442	C	C6-N1-C2	-6.07	117.87	120.30
43	RN	48	MET	CG-SD-CE	-6.07	90.49	100.20
36	YB	70	C	C5-C6-N1	6.07	124.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	752	A	P-O3'-C3'	6.07	126.98	119.70
35	YA	57	C	C6-N1-C2	-6.07	117.87	120.30
24	QY	16	C	C6-N1-C2	-6.06	117.88	120.30
35	YA	2889	C	C2-N1-C1'	6.06	125.47	118.80
35	RA	221	A	P-O3'-C3'	6.06	126.97	119.70
35	RA	523	C	C6-N1-C2	-6.06	117.88	120.30
1	XA	1367	C	N1-C2-O2	6.06	122.53	118.90
35	YA	2855	C	N1-C2-O2	6.05	122.53	118.90
35	RA	2703	C	C2-N1-C1'	6.05	125.45	118.80
35	YA	1881	C	N3-C2-O2	-6.05	117.67	121.90
35	YA	1893	C	N1-C2-O2	6.05	122.53	118.90
35	YA	2856	C	C5-C6-N1	6.05	124.03	121.00
35	RA	912	C	C5-C6-N1	6.04	124.02	121.00
1	XA	1384	C	N3-C2-O2	-6.04	117.67	121.90
35	RA	2889	C	N1-C2-O2	6.03	122.52	118.90
35	RA	1474	C	C6-N1-C2	-6.02	117.89	120.30
1	XA	686	U	N3-C2-O2	-6.02	117.98	122.20
1	QA	244	U	P-O3'-C3'	6.02	126.93	119.70
35	YA	1640	C	C6-N1-C2	-6.02	117.89	120.30
23	QX	18	G	OP2-P-O3'	6.02	118.44	105.20
35	RA	1589	C	N1-C2-O2	6.02	122.51	118.90
35	RA	2889	C	N3-C2-O2	-6.02	117.69	121.90
35	YA	2766	G	C4-N9-C1'	6.01	134.32	126.50
35	YA	2441	C	N3-C2-O2	-6.01	117.69	121.90
1	XA	764	C	C6-N1-C2	-6.01	117.90	120.30
35	RA	2785	C	C6-N1-C2	-6.01	117.90	120.30
1	QA	960	U	N3-C2-O2	-6.01	118.00	122.20
1	XA	137	C	C6-N1-C2	-6.01	117.90	120.30
35	YA	333	G	C8-N9-C1'	-6.00	119.19	127.00
35	YA	580	C	C6-N1-C2	-6.00	117.90	120.30
35	RA	291	C	C6-N1-C2	-6.00	117.90	120.30
35	YA	1396	U	C5-C6-N1	6.00	125.70	122.70
35	RA	2855	C	C6-N1-C2	-5.99	117.90	120.30
1	QA	501	C	C6-N1-C2	-5.99	117.90	120.30
1	XA	346	G	C4-N9-C1'	5.99	134.29	126.50
35	RA	2260	C	N3-C2-O2	-5.99	117.71	121.90
35	YA	2566	A	P-O3'-C3'	5.99	126.88	119.70
35	RA	1178	C	C5-C6-N1	5.98	123.99	121.00
35	YA	517	C	C6-N1-C2	-5.98	117.91	120.30
35	YA	2739	U	N3-C2-O2	-5.98	118.01	122.20
1	QA	1502	A	C5-N7-C8	-5.98	100.91	103.90
35	YA	2776	A	P-O3'-C3'	5.98	126.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	YH	153	LYS	N-CA-C	5.98	127.14	111.00
35	RA	797	C	C6-N1-C2	-5.97	117.91	120.30
35	RA	1725	G	C4-N9-C1'	5.97	134.27	126.50
35	YA	2468	G	C4-N9-C1'	5.97	134.27	126.50
1	QA	369	C	N1-C2-O2	5.97	122.48	118.90
35	RA	2403	C	C6-N1-C2	-5.97	117.91	120.30
35	RA	2648	C	N1-C2-O2	5.97	122.48	118.90
35	RA	2691	C	C6-N1-C2	-5.97	117.91	120.30
1	XA	963	G	C4-N9-C1'	5.97	134.26	126.50
35	RA	783	A	C5-N7-C8	-5.97	100.92	103.90
35	YA	867	C	C5-C6-N1	5.97	123.98	121.00
35	RA	860	U	C6-N1-C2	-5.97	117.42	121.00
42	YI	11	ASN	C-N-CA	5.96	136.61	121.70
35	YA	2439	A	P-O3'-C3'	5.96	126.86	119.70
24	QY	54	U	C2-N3-C4	5.96	130.58	127.00
35	RA	951	C	C6-N1-C2	-5.96	117.92	120.30
35	RA	2880	C	C6-N1-C2	-5.96	117.92	120.30
35	RA	76	C	N3-C2-O2	-5.96	117.73	121.90
35	YA	976	C	C6-N1-C2	-5.96	117.92	120.30
35	YA	1313	U	C5-C6-N1	5.96	125.68	122.70
35	RA	601	C	C6-N1-C2	-5.95	117.92	120.30
35	YA	1549	C	N3-C2-O2	-5.95	117.74	121.90
1	QA	1369	C	N3-C2-O2	-5.94	117.74	121.90
36	RB	66	A	P-O3'-C3'	5.94	126.83	119.70
35	YA	2768	C	C6-N1-C2	-5.94	117.92	120.30
35	YA	485	C	C6-N1-C2	-5.94	117.92	120.30
35	YA	2321	G	C8-N9-C1'	-5.94	119.28	127.00
1	XA	266	G	P-O3'-C3'	5.93	126.82	119.70
35	YA	912	C	N1-C2-O2	5.93	122.46	118.90
35	YA	1535	U	N3-C2-O2	-5.93	118.05	122.20
35	YA	1788	C	C5-C6-N1	5.93	123.97	121.00
1	QA	1163	C	C2-N1-C1'	5.93	125.32	118.80
35	YA	535	C	C6-N1-C2	-5.93	117.93	120.30
35	YA	1675	C	N3-C2-O2	-5.93	117.75	121.90
35	YA	2441	C	N1-C2-O2	5.93	122.46	118.90
24	QY	54	U	N1-C2-O2	5.93	126.95	122.80
1	QA	346	G	C4-N9-C1'	5.93	134.20	126.50
35	RA	1786	A	C4-N9-C1'	5.93	136.97	126.30
35	YA	47	C	C6-N1-C2	-5.93	117.93	120.30
35	YA	1018	C	C6-N1-C2	-5.92	117.93	120.30
3	QC	201	TYR	CA-CB-CG	5.92	124.64	113.40
35	RA	1026	U	P-O3'-C3'	5.92	126.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1827	C	N3-C2-O2	-5.91	117.76	121.90
49	RT	105	LEU	CA-CB-CG	5.91	128.90	115.30
35	RA	517	C	C6-N1-C2	-5.91	117.94	120.30
35	RA	1062	G	C4-N9-C1'	5.91	134.18	126.50
1	QA	435	C	C6-N1-C2	-5.91	117.94	120.30
35	RA	1062	G	N3-C4-N9	5.91	129.54	126.00
1	QA	1066	C	C6-N1-C2	-5.91	117.94	120.30
35	YA	237	C	C6-N1-C2	-5.91	117.94	120.30
1	QA	1024	G	O5'-P-OP2	-5.91	100.39	105.70
35	RA	1899	G	N3-C4-C5	-5.90	125.65	128.60
1	QA	980	C	N1-C2-O2	5.90	122.44	118.90
35	YA	991	C	C6-N1-C2	-5.90	117.94	120.30
1	XA	115	G	P-O3'-C3'	5.90	126.78	119.70
35	RA	1574	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	2656	U	N1-C2-O2	5.89	126.93	122.80
41	RH	82	GLY	N-CA-C	5.89	127.84	113.10
1	XA	963	G	C4-C5-N7	5.89	113.16	110.80
1	QA	412	A	P-O3'-C3'	5.89	126.77	119.70
35	RA	2178	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	1882	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	297	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	1052	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	1549	C	C6-N1-C2	-5.89	117.94	120.30
24	QY	70	U	C2-N1-C1'	5.89	124.77	117.70
35	RA	2610	C	P-O3'-C3'	5.89	126.77	119.70
35	YA	2096	U	C5-C6-N1	5.89	125.64	122.70
35	YA	2773	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	1644	C	N1-C2-O2	5.89	122.43	118.90
1	XA	314	C	C5-C6-N1	5.88	123.94	121.00
35	YA	99	U	P-O3'-C3'	5.88	126.76	119.70
35	YA	544	C	N1-C2-O2	5.88	122.43	118.90
35	RA	898	C	N3-C2-O2	-5.88	117.79	121.90
1	XA	485	G	P-O3'-C3'	5.88	126.75	119.70
1	XA	169	C	N1-C2-O2	5.87	122.42	118.90
1	XA	753	A	P-O3'-C3'	5.87	126.75	119.70
35	YA	1200	C	C6-N1-C2	-5.87	117.95	120.30
1	QA	442	C	C5-C6-N1	5.87	123.94	121.00
1	QA	689	C	N1-C2-O2	5.87	122.42	118.90
35	RA	974(A)	C	C2-N1-C1'	5.87	125.26	118.80
35	RA	1375	C	C6-N1-C2	-5.87	117.95	120.30
29	Y4	40	HIS	N-CA-C	5.87	126.84	111.00
35	YA	1914	C	C6-N1-C1'	-5.87	113.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2205	C	C5-C6-N1	5.87	123.93	121.00
1	QA	115	G	P-O3'-C3'	5.86	126.73	119.70
42	RI	11	ASN	C-N-CA	5.86	136.36	121.70
35	YA	915	C	N3-C2-O2	-5.86	117.80	121.90
35	YA	2420	C	C6-N1-C2	-5.86	117.95	120.30
35	RA	265	A	O4'-C1'-N9	5.86	112.89	108.20
35	RA	523	C	C5-C6-N1	5.86	123.93	121.00
35	YA	1882	C	C2-N1-C1'	5.86	125.25	118.80
35	YA	1931	U	C6-N1-C2	-5.86	117.48	121.00
35	RA	530	G	N1-C6-O6	-5.86	116.39	119.90
35	RA	2063	C	C6-N1-C2	-5.85	117.96	120.30
1	XA	1254	C	C6-N1-C2	-5.85	117.96	120.30
35	RA	1644	C	C5-C6-N1	5.85	123.92	121.00
35	YA	1804	C	N3-C2-O2	-5.85	117.81	121.90
35	RA	1506	C	C6-N1-C2	-5.85	117.96	120.30
35	RA	1567	A	N1-C6-N6	-5.85	115.09	118.60
35	YA	650	C	C5-C6-N1	5.85	123.92	121.00
35	RA	485	C	N1-C2-O2	5.84	122.41	118.90
35	RA	2776	A	P-O3'-C3'	5.84	126.71	119.70
35	YA	812	C	C6-N1-C2	-5.84	117.96	120.30
35	YA	393	C	C6-N1-C2	-5.84	117.96	120.30
1	QA	442	C	N1-C2-O2	5.84	122.40	118.90
35	RA	898	C	C2-N1-C1'	5.84	125.22	118.80
35	RA	2889	C	C2-N1-C1'	5.84	125.22	118.80
1	XA	314	C	N3-C2-O2	-5.84	117.81	121.90
35	RA	1305	C	N3-C2-O2	-5.83	117.82	121.90
35	RA	930	U	N1-C2-O2	5.83	126.88	122.80
35	YA	508	G	N3-C4-N9	5.83	129.50	126.00
35	YA	1653	G	P-O3'-C3'	5.83	126.70	119.70
35	YA	1992	G	P-O3'-C3'	5.83	126.70	119.70
35	YA	97	C	N3-C2-O2	-5.83	117.82	121.90
1	XA	896	C	C5-C6-N1	5.83	123.91	121.00
35	RA	1914	C	C6-N1-C1'	-5.83	113.81	120.80
1	QA	429	U	C5-C6-N1	5.82	125.61	122.70
35	RA	2405	G	P-O3'-C3'	5.82	126.69	119.70
35	RA	2755	C	C2-N1-C1'	5.82	125.20	118.80
55	RZ	3	TYR	CA-CB-CG	5.82	124.46	113.40
35	YA	426	C	N1-C2-O2	5.82	122.39	118.90
35	YA	512	G	O4'-C1'-N9	5.82	112.86	108.20
35	YA	2043	C	C5-C6-N1	5.82	123.91	121.00
35	YA	2723	C	C6-N1-C2	-5.82	117.97	120.30
35	RA	1636	C	C6-N1-C2	-5.82	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2575	C	C6-N1-C2	-5.82	117.97	120.30
35	RA	1930	G	OP2-P-O3'	5.81	117.98	105.20
35	YA	67	U	N3-C4-O4	5.81	123.47	119.40
35	YA	2350	C	N3-C2-O2	-5.81	117.83	121.90
35	YA	898	C	N3-C2-O2	-5.80	117.84	121.90
35	YA	1931	U	N1-C2-O2	5.80	126.86	122.80
35	YA	2841	C	C6-N1-C2	-5.80	117.98	120.30
1	QA	1502	A	N7-C8-N9	5.80	116.70	113.80
35	RA	1616	A	C4-C5-N7	5.80	113.60	110.70
35	YA	613	U	N1-C2-O2	5.80	126.86	122.80
35	YA	1095	A	N3-C4-N9	5.80	132.04	127.40
35	YA	2424	C	N1-C2-O2	5.80	122.38	118.90
36	YB	30	C	N1-C2-O2	5.80	122.38	118.90
1	XA	369	C	C5-C6-N1	5.79	123.90	121.00
1	XA	1203	C	C6-N1-C2	-5.79	117.98	120.30
35	YA	2126	A	P-O3'-C3'	5.79	126.65	119.70
35	RA	1882	C	N1-C2-O2	5.79	122.37	118.90
35	YA	618(A)	C	N3-C2-O2	-5.79	117.85	121.90
1	XA	354	G	C4-N9-C1'	5.79	134.02	126.50
35	YA	1407	C	N1-C2-O2	5.79	122.37	118.90
1	XA	980	C	C5-C6-N1	5.78	123.89	121.00
1	XA	1070	U	N1-C2-O2	5.78	126.85	122.80
1	QA	1192	C	C6-N1-C2	-5.78	117.99	120.30
35	RA	2789	C	N1-C2-O2	5.78	122.37	118.90
1	XA	1070	U	N3-C2-O2	-5.78	118.16	122.20
35	YA	1979	C	C6-N1-C2	-5.78	117.99	120.30
1	XA	1374	A	O4'-C1'-N9	5.77	112.82	108.20
51	YV	91	TYR	CA-CB-CG	5.77	124.37	113.40
35	RA	77	C	C5-C6-N1	5.77	123.89	121.00
35	YA	965	C	C5-C6-N1	5.77	123.89	121.00
35	YA	1396	U	C6-N1-C1'	-5.77	113.12	121.20
35	YA	2321	G	N3-C4-N9	5.77	129.46	126.00
35	YA	2772	C	C6-N1-C2	-5.77	117.99	120.30
35	YA	754	C	C6-N1-C2	-5.77	117.99	120.30
46	YQ	25	ASP	CB-CG-OD1	5.77	123.49	118.30
1	QA	266	G	P-O3'-C3'	5.77	126.62	119.70
35	YA	529	A	N7-C8-N9	5.77	116.68	113.80
1	QA	536	C	N1-C2-O2	5.76	122.36	118.90
55	RZ	8	TYR	CA-CB-CG	5.76	124.35	113.40
1	QA	1230	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	991	U	C2-N1-C1'	5.76	124.61	117.70
35	YA	273(F)	C	N1-C2-O2	5.76	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	808	C	C6-N1-C2	-5.75	118.00	120.30
35	YA	120	U	C6-N1-C1'	-5.75	113.14	121.20
35	YA	2701	C	P-O3'-C3'	5.75	126.61	119.70
36	RB	31	C	N3-C2-O2	-5.75	117.87	121.90
35	RA	512	G	P-O3'-C3'	5.75	126.60	119.70
1	XA	369	C	C6-N1-C2	-5.75	118.00	120.30
35	YA	76	C	C5-C6-N1	5.75	123.88	121.00
1	QA	596	C	N1-C2-O2	5.75	122.35	118.90
26	R1	43	TYR	CA-CB-CG	5.75	124.32	113.40
35	RA	2294	C	N1-C2-O2	5.75	122.35	118.90
35	YA	731	C	C6-N1-C2	-5.74	118.00	120.30
35	RA	1306	C	N3-C2-O2	-5.74	117.88	121.90
35	YA	273(F)	C	C6-N1-C2	-5.74	118.00	120.30
1	QA	1114	C	C6-N1-C2	-5.74	118.00	120.30
35	RA	2321	G	C8-N9-C1'	-5.74	119.54	127.00
35	YA	102	G	P-O3'-C3'	5.74	126.59	119.70
35	YA	1467	C	C6-N1-C2	-5.74	118.00	120.30
35	YA	1686	C	C2-N1-C1'	5.74	125.11	118.80
35	YA	2666	C	N3-C2-O2	-5.74	117.89	121.90
35	YA	1045	A	P-O3'-C3'	5.73	126.58	119.70
1	QA	1225	A	C4-N9-C1'	5.73	136.62	126.30
35	RA	702	G	C4-N9-C1'	5.73	133.95	126.50
35	YA	377	C	C6-N1-C2	-5.73	118.01	120.30
1	QA	754	C	N1-C2-O2	5.73	122.34	118.90
35	RA	749	C	C6-N1-C2	-5.73	118.01	120.30
35	RA	1688	U	N3-C2-O2	-5.73	118.19	122.20
35	YA	1407	C	C6-N1-C2	-5.72	118.01	120.30
17	XQ	42	TYR	CA-CB-CG	5.72	124.27	113.40
35	RA	930	U	N3-C2-O2	-5.72	118.20	122.20
51	RV	35	LEU	CA-CB-CG	5.72	128.45	115.30
1	XA	169	C	C2-N1-C1'	5.72	125.09	118.80
35	YA	1095	A	N3-C4-C5	-5.72	122.80	126.80
35	YA	1222	C	C6-N1-C2	-5.72	118.01	120.30
12	QL	27	LEU	C-N-CA	5.71	135.98	121.70
35	YA	2138	C	C5-C6-N1	5.71	123.86	121.00
36	YB	71	C	N1-C2-O2	5.71	122.33	118.90
35	RA	372	G	OP2-P-O3'	5.71	117.77	105.20
35	RA	587	C	P-O3'-C3'	5.71	126.55	119.70
35	RA	1688	U	C6-N1-C2	-5.71	117.57	121.00
35	RA	1504	C	C6-N1-C2	-5.71	118.02	120.30
35	RA	420	C	N3-C2-O2	-5.71	117.91	121.90
1	XA	932	C	N1-C2-O2	5.71	122.32	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	911	A	C8-N9-C4	-5.70	103.52	105.80
35	YA	1528	A	C8-N9-C4	-5.70	103.52	105.80
35	YA	1332	G	C5-N7-C8	-5.70	101.45	104.30
1	QA	762	C	C6-N1-C2	-5.70	118.02	120.30
35	RA	2703	C	N3-C2-O2	-5.70	117.91	121.90
35	YA	1905	C	C2-N1-C1'	5.69	125.06	118.80
35	RA	611	C	C6-N1-C2	-5.69	118.02	120.30
1	XA	974	A	O4'-C1'-N9	5.69	112.75	108.20
1	QA	1109	C	N3-C2-O2	-5.69	117.92	121.90
35	RA	2112	G	C4-N9-C1'	5.69	133.89	126.50
35	YA	964	C	C6-N1-C2	-5.69	118.03	120.30
35	RA	271(B)	G	P-O3'-C3'	5.68	126.52	119.70
37	YD	63	ARG	N-CA-C	-5.68	95.65	111.00
35	RA	2378	A	N9-C4-C5	-5.68	103.53	105.80
35	YA	1920	C	C5-C6-N1	5.68	123.84	121.00
35	RA	267	C	C6-N1-C2	-5.68	118.03	120.30
35	RA	2363	C	C6-N1-C2	-5.68	118.03	120.30
35	YA	2559	C	N1-C2-O2	5.68	122.31	118.90
35	RA	253	C	C6-N1-C2	-5.68	118.03	120.30
1	XA	186	C	C6-N1-C2	-5.68	118.03	120.30
35	RA	1544	C	N1-C2-O2	5.67	122.31	118.90
35	RA	74	A	P-O3'-C3'	5.67	126.51	119.70
1	QA	243	A	P-O3'-C3'	5.67	126.50	119.70
35	YA	540	G	C4-N9-C1'	5.67	133.87	126.50
35	YA	1691	C	C6-N1-C2	-5.67	118.03	120.30
35	RA	1899	G	C8-N9-C1'	-5.67	119.63	127.00
35	RA	2566	A	P-O3'-C3'	5.67	126.50	119.70
22	QV	32	C	N1-C2-O2	5.67	122.30	118.90
35	YA	992	C	N1-C2-O2	5.67	122.30	118.90
35	RA	1844	C	C6-N1-C2	-5.67	118.03	120.30
24	QY	70	U	N3-C2-O2	-5.66	118.23	122.20
1	QA	175	C	C6-N1-C2	-5.66	118.04	120.30
1	XA	1056	U	N3-C2-O2	-5.66	118.24	122.20
35	RA	1816	G	N7-C8-N9	5.66	115.93	113.10
1	QA	346	G	C2-N3-C4	5.66	114.73	111.90
1	XA	1228	C	N3-C2-O2	-5.66	117.94	121.90
1	QA	1336	C	N3-C2-O2	-5.66	117.94	121.90
35	RA	2211	G	C4-N9-C1'	5.66	133.85	126.50
35	RA	1313	U	C6-N1-C2	-5.65	117.61	121.00
35	YA	184	C	N1-C2-O2	5.65	122.29	118.90
35	YA	1142(A)	A	N3-C4-C5	5.65	130.76	126.80
35	RA	2730	C	C6-N1-C2	-5.65	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	288	C	N1-C2-O2	5.65	122.29	118.90
35	YA	828	U	N1-C2-O2	5.65	126.75	122.80
1	XA	754	C	C6-N1-C2	-5.65	118.04	120.30
35	YA	2646	C	N3-C2-O2	-5.65	117.95	121.90
35	YA	2828	C	C6-N1-C2	-5.65	118.04	120.30
1	XA	1056	U	N1-C2-O2	5.65	126.75	122.80
35	YA	912	C	C2-N1-C1'	5.64	125.00	118.80
1	XA	132	C	N1-C2-O2	5.64	122.28	118.90
35	RA	2836	U	C5-C6-N1	5.63	125.52	122.70
1	XA	266	G	C4-C5-N7	5.63	113.05	110.80
35	YA	2506	U	C6-N1-C2	-5.63	117.62	121.00
1	XA	314	C	C2-N1-C1'	5.63	125.00	118.80
35	YA	1790	C	N1-C2-O2	5.63	122.28	118.90
35	YA	587	C	P-O3'-C3'	5.63	126.45	119.70
35	RA	2320	A	C2-N3-C4	5.63	113.41	110.60
36	RB	3	C	C5-C6-N1	5.63	123.81	121.00
1	XA	754	C	N3-C2-O2	-5.63	117.96	121.90
1	XA	1109	C	N3-C2-O2	-5.62	117.96	121.90
35	YA	2307	G	C4-N9-C1'	5.62	133.81	126.50
35	YA	1528	A	C5-N7-C8	-5.62	101.09	103.90
1	XA	250	A	P-O3'-C3'	5.62	126.44	119.70
35	RA	2896	C	C6-N1-C2	-5.62	118.05	120.30
35	RA	1658	C	C5-C6-N1	5.62	123.81	121.00
35	RA	537	C	N3-C2-O2	-5.61	117.97	121.90
35	YA	2739	U	N1-C2-O2	5.61	126.73	122.80
35	RA	1599	C	C6-N1-C2	-5.61	118.06	120.30
1	XA	1505	G	N9-C4-C5	5.61	107.64	105.40
35	RA	1496	A	C5-N7-C8	-5.61	101.10	103.90
35	YA	898	C	C2-N1-C1'	5.61	124.97	118.80
35	YA	1332	G	C4-C5-N7	5.61	113.04	110.80
35	RA	564	C	C6-N1-C2	-5.60	118.06	120.30
35	YA	1352	U	C6-N1-C2	-5.60	117.64	121.00
1	XA	221	C	N1-C2-O2	5.60	122.26	118.90
1	XA	764	C	C5-C6-N1	5.60	123.80	121.00
35	YA	1376	C	C5-C6-N1	5.60	123.80	121.00
24	QY	55	U	C2-N1-C1'	5.60	124.42	117.70
35	RA	1971	A	C2-N3-C4	5.60	113.40	110.60
1	QA	1038	C	N3-C2-O2	-5.60	117.98	121.90
35	RA	67	U	C5-C6-N1	5.60	125.50	122.70
35	RA	2584	U	N1-C2-O2	5.60	126.72	122.80
35	YA	560	C	C6-N1-C2	-5.59	118.06	120.30
46	YQ	9	TYR	CA-CB-CG	5.59	124.03	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y4	39	CYS	N-CA-C	-5.59	95.90	111.00
1	XA	1439	C	N1-C2-O2	5.59	122.25	118.90
35	YA	2043	C	C6-N1-C2	-5.59	118.06	120.30
35	RA	1644	C	N3-C2-O2	-5.59	117.99	121.90
35	RA	1793	C	N3-C2-O2	-5.59	117.99	121.90
35	YA	1174	A	C4-N9-C1'	5.59	136.36	126.30
35	YA	1174	A	N3-C4-C5	-5.59	122.89	126.80
40	YG	94	LEU	CB-CG-CD2	-5.59	101.50	111.00
37	YD	33	LEU	CA-CB-CG	5.59	128.15	115.30
24	QY	40	C	N1-C2-O2	5.59	122.25	118.90
35	RA	2699	C	C6-N1-C2	-5.59	118.06	120.30
35	YA	860	U	C6-N1-C1'	-5.59	113.38	121.20
35	YA	1506	C	C6-N1-C2	-5.59	118.07	120.30
1	XA	1496	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	697	C	C6-N1-C2	-5.58	118.07	120.30
35	RA	2702	U	C2-N1-C1'	5.58	124.40	117.70
35	YA	1313	U	C6-N1-C2	-5.58	117.65	121.00
1	XA	749	C	C2-N1-C1'	5.58	124.94	118.80
35	RA	2471	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	635	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	74	A	C2-N3-C4	-5.58	107.81	110.60
35	YA	2287	A	N3-C4-C5	5.58	130.70	126.80
35	RA	2112	G	N3-C4-N9	5.57	129.34	126.00
1	XA	435	C	C5-C6-N1	5.57	123.79	121.00
1	XA	971	G	C4-N9-C1'	-5.57	119.25	126.50
35	YA	2814	C	C6-N1-C2	-5.57	118.07	120.30
35	RA	1920	C	C6-N1-C2	-5.57	118.07	120.30
35	YA	783	A	C4-C5-N7	5.57	113.49	110.70
35	YA	2328	A	N7-C8-N9	5.57	116.59	113.80
35	YA	1893	C	N3-C2-O2	-5.57	118.00	121.90
35	YA	2394	C	C6-N1-C2	-5.57	118.07	120.30
35	YA	2321	G	N3-C4-C5	-5.57	125.82	128.60
35	RA	529	A	C2-N3-C4	5.57	113.38	110.60
35	RA	1902	C	C6-N1-C2	-5.57	118.07	120.30
35	RA	2767	C	C6-N1-C2	-5.57	118.07	120.30
36	YB	15	A	OP1-P-O3'	5.57	117.45	105.20
35	RA	1174	A	C4-N9-C1'	5.57	136.32	126.30
35	YA	2689	U	P-O3'-C3'	5.57	126.38	119.70
35	RA	856	C	P-O3'-C3'	5.56	126.38	119.70
35	YA	97	C	C5-C6-N1	5.56	123.78	121.00
35	RA	1686	C	C5-C6-N1	5.56	123.78	121.00
1	XA	1114	C	N3-C2-O2	-5.56	118.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2392	A	N7-C8-N9	5.55	116.58	113.80
35	YA	2855	C	N3-C2-O2	-5.55	118.01	121.90
35	RA	2576	G	N3-C4-C5	-5.55	125.82	128.60
35	YA	134	C	N1-C2-O2	5.55	122.23	118.90
35	RA	1600	C	N3-C2-O2	-5.55	118.02	121.90
1	XA	1321	C	C6-N1-C2	-5.55	118.08	120.30
35	YA	828	U	C6-N1-C2	-5.55	117.67	121.00
35	YA	1135	C	N1-C2-O2	5.55	122.23	118.90
35	YA	242	G	OP2-P-O3'	5.55	117.41	105.20
35	RA	1375	C	C5-C6-N1	5.55	123.77	121.00
35	RA	1686	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	991	U	N1-C2-O2	5.54	126.68	122.80
35	YA	992	C	N3-C2-O2	-5.54	118.02	121.90
36	YB	31	C	N1-C2-O2	5.54	122.23	118.90
35	RA	2468	G	C4-N9-C1'	5.54	133.70	126.50
1	XA	686	U	N1-C2-O2	5.54	126.68	122.80
1	XA	1505	G	N3-C4-N9	-5.54	122.67	126.00
35	YA	172	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	896	C	C6-N1-C2	-5.54	118.08	120.30
1	QA	449	C	N1-C2-O2	5.54	122.22	118.90
35	RA	825	C	C6-N1-C2	-5.54	118.08	120.30
35	RA	915	C	N3-C2-O2	-5.54	118.02	121.90
1	QA	764	C	N1-C2-O2	5.54	122.22	118.90
35	YA	1607	C	C5-C6-N1	5.54	123.77	121.00
35	RA	860	U	N1-C2-O2	5.54	126.67	122.80
35	YA	243	U	C2-N1-C1'	5.54	124.34	117.70
35	YA	302	C	C6-N1-C2	-5.54	118.08	120.30
35	YA	1781	C	N1-C2-O2	5.54	122.22	118.90
35	RA	105	C	C6-N1-C2	-5.53	118.09	120.30
1	XA	449	C	N3-C2-O2	-5.53	118.03	121.90
1	XA	1439	C	C5-C6-N1	5.53	123.77	121.00
1	XA	704	A	O5'-P-OP1	-5.53	100.72	105.70
35	RA	77	C	C6-N1-C2	-5.53	118.09	120.30
35	YA	1786	A	N7-C8-N9	5.53	116.56	113.80
35	YA	2236	C	C6-N1-C2	-5.53	118.09	120.30
35	RA	817	C	C5-C6-N1	5.53	123.76	121.00
35	RA	1510	A	C2-N3-C4	5.53	113.36	110.60
35	RA	1544	C	N3-C2-O2	-5.53	118.03	121.90
35	YA	420	C	N3-C2-O2	-5.53	118.03	121.90
31	R6	34	LEU	CA-CB-CG	5.52	128.00	115.30
35	RA	530	G	C5-C6-O6	5.52	131.91	128.60
35	YA	246	C	N1-C2-O2	5.52	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	1445	C	N3-C2-O2	-5.52	118.03	121.90
1	XA	856	C	C6-N1-C2	-5.52	118.09	120.30
1	XA	1038	C	N3-C2-O2	-5.52	118.04	121.90
35	RA	1786	A	C4-C5-N7	5.52	113.46	110.70
22	XV	34	C	C2-N1-C1'	5.52	124.87	118.80
35	YA	1905	C	N3-C2-O2	-5.52	118.04	121.90
35	YA	2772	C	C5-C6-N1	5.52	123.76	121.00
1	QA	103	C	N3-C2-O2	-5.51	118.04	121.90
35	RA	1394	U	C5-C6-N1	5.51	125.46	122.70
36	RB	7	G	C4-C5-N7	5.51	113.00	110.80
1	XA	634	C	C6-N1-C2	-5.51	118.09	120.30
1	QA	1369	C	N1-C2-O2	5.51	122.21	118.90
35	RA	309	G	O5'-P-OP1	5.51	117.31	110.70
1	QA	1097	C	N3-C2-O2	-5.51	118.04	121.90
35	RA	465	G	C8-N9-C4	-5.51	104.20	106.40
35	RA	1549	C	C5-C6-N1	5.51	123.75	121.00
35	YA	817	C	C5-C6-N1	5.51	123.75	121.00
35	YA	2730	C	C6-N1-C2	-5.51	118.10	120.30
1	XA	810	C	C6-N1-C2	-5.51	118.10	120.30
35	RA	2688	U	N1-C2-O2	5.50	126.65	122.80
35	RA	912	C	C2-N1-C1'	5.50	124.85	118.80
35	RA	1881	C	C5-C6-N1	5.50	123.75	121.00
35	YA	645	C	C6-N1-C2	-5.50	118.10	120.30
35	YA	2524	G	C8-N9-C4	-5.50	104.20	106.40
38	RE	116	VAL	C-N-CA	5.50	135.44	121.70
35	YA	1386	C	C6-N1-C2	-5.50	118.10	120.30
35	YA	2138	C	C6-N1-C2	-5.50	118.10	120.30
1	QA	1277	C	C6-N1-C2	-5.50	118.10	120.30
22	QV	62	C	N3-C2-O2	-5.49	118.06	121.90
35	RA	2161	C	N1-C2-O2	5.49	122.20	118.90
1	XA	255	G	N1-C6-O6	-5.49	116.60	119.90
45	YP	59	LEU	N-CA-C	-5.49	96.17	111.00
1	XA	514	C	C6-N1-C2	-5.49	118.10	120.30
1	XA	826	C	C2-N1-C1'	5.49	124.84	118.80
1	XA	169	C	C5-C6-N1	5.49	123.74	121.00
35	YA	1670	C	C5-C6-N1	5.48	123.74	121.00
35	YA	2506	U	C5-C6-N1	5.48	125.44	122.70
35	RA	2116	G	C8-N9-C4	-5.48	104.21	106.40
37	RD	35	LYS	N-CA-C	5.48	125.80	111.00
1	XA	703	G	P-O3'-C3'	5.48	126.28	119.70
1	XA	346	G	C8-N9-C1'	-5.48	119.88	127.00
35	YA	2771	C	C6-N1-C2	-5.48	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	354	G	C4-N9-C1'	5.47	133.62	126.50
1	QA	882	C	N1-C2-O2	5.47	122.18	118.90
35	YA	27	G	C8-N9-C1'	5.47	134.12	127.00
35	YA	1233	C	C6-N1-C2	-5.47	118.11	120.30
35	RA	530	G	N3-C4-N9	-5.47	122.72	126.00
35	RA	1403	C	N1-C2-O2	5.47	122.18	118.90
35	YA	2210	G	N3-C4-C5	-5.47	125.87	128.60
35	RA	2076	U	C5-C6-N1	5.47	125.43	122.70
35	YA	105	C	C5-C6-N1	5.47	123.73	121.00
35	YA	1333	C	N1-C2-O2	5.47	122.18	118.90
35	RA	971	C	C6-N1-C2	-5.46	118.11	120.30
35	YA	1095	A	C4-N9-C1'	5.46	136.14	126.30
55	YZ	3	TYR	CA-CB-CG	5.46	123.78	113.40
1	QA	764	C	N3-C2-O2	-5.46	118.08	121.90
41	RH	153	LYS	N-CA-C	5.46	125.75	111.00
36	YB	30	C	C6-N1-C2	-5.46	118.11	120.30
1	XA	948	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	882	C	N3-C2-O2	-5.46	118.08	121.90
35	YA	2185	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	58	C	C6-N1-C2	-5.46	118.12	120.30
1	XA	272	C	N3-C2-O2	-5.46	118.08	121.90
35	RA	253	C	C5-C6-N1	5.45	123.73	121.00
35	RA	1899	G	N7-C8-N9	5.45	115.83	113.10
35	YA	74	A	O4'-C1'-N9	-5.45	103.84	108.20
1	XA	169	C	C6-N1-C2	-5.45	118.12	120.30
35	YA	2468	G	O4'-C1'-N9	5.45	112.56	108.20
1	QA	1230	C	C5-C6-N1	5.45	123.72	121.00
35	RA	2787	C	N3-C2-O2	-5.45	118.08	121.90
35	YA	1178	C	P-O3'-C3'	5.45	126.24	119.70
35	RA	914	C	C6-N1-C2	-5.45	118.12	120.30
35	RA	1983	C	C6-N1-C2	-5.45	118.12	120.30
35	YA	871	U	O5'-P-OP1	-5.45	100.80	105.70
1	XA	385	C	C6-N1-C2	-5.44	118.12	120.30
35	YA	284	U	C6-N1-C2	-5.44	117.73	121.00
35	YA	1376	C	C2-N1-C1'	5.44	124.79	118.80
35	RA	1178	C	P-O3'-C3'	5.44	126.23	119.70
35	RA	140	A	C5-N7-C8	-5.44	101.18	103.90
35	RA	692	C	C5-C6-N1	5.44	123.72	121.00
26	Y1	43	TYR	CA-CB-CG	5.44	123.74	113.40
35	YA	1598	C	C6-N1-C2	-5.44	118.12	120.30
35	YA	1295	C	C6-N1-C2	-5.44	118.12	120.30
24	QY	30	G	N3-C4-N9	5.44	129.26	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	120	U	C6-N1-C1'	-5.44	113.59	121.20
35	RA	904	C	N1-C2-O2	5.44	122.16	118.90
1	QA	789	U	N1-C2-O2	5.44	126.61	122.80
35	RA	2321	G	N3-C4-N9	5.44	129.26	126.00
35	YA	2403	C	C2-N1-C1'	5.43	124.78	118.80
35	YA	1804	C	C6-N1-C2	-5.43	118.13	120.30
1	XA	1039	C	N1-C2-O2	5.43	122.16	118.90
35	RA	2321	G	N3-C4-C5	-5.43	125.89	128.60
35	YA	944	G	C4-N9-C1'	5.43	133.56	126.50
35	RA	1827	C	N1-C2-O2	5.43	122.16	118.90
1	QA	1071	C	C6-N1-C2	-5.43	118.13	120.30
17	QQ	42	TYR	CA-CB-CG	5.42	123.70	113.40
35	YA	634	C	N1-C2-O2	5.42	122.15	118.90
35	RA	1578	U	N3-C2-O2	-5.42	118.41	122.20
35	RA	2036	C	N3-C2-O2	-5.42	118.11	121.90
1	XA	827	U	C6-N1-C1'	-5.42	113.62	121.20
35	YA	1433	U	C5-C6-N1	5.42	125.41	122.70
1	XA	991	U	C5-C6-N1	5.42	125.41	122.70
35	YA	1786	A	C5-N7-C8	-5.42	101.19	103.90
35	RA	231	C	C6-N1-C2	-5.41	118.14	120.30
35	RA	1534	G	N3-C4-N9	5.41	129.25	126.00
35	YA	2688	U	C5-C4-O4	5.41	129.15	125.90
1	QA	1502	A	C4-C5-N7	5.41	113.40	110.70
35	RA	1600	C	C6-N1-C2	-5.41	118.14	120.30
35	YA	264	C	N1-C2-O2	5.41	122.14	118.90
35	RA	2210	G	N3-C4-C5	-5.40	125.90	128.60
35	RA	2559	C	C6-N1-C2	-5.40	118.14	120.30
1	XA	652	U	N1-C2-O2	5.40	126.58	122.80
1	QA	181	G	P-O3'-C3'	5.40	126.18	119.70
1	QA	690	G	O4'-C1'-N9	5.40	112.52	108.20
1	QA	960	U	C6-N1-C1'	-5.40	113.64	121.20
35	RA	2689	U	P-O3'-C3'	5.40	126.18	119.70
1	XA	233	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	640	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	1387	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	1879	C	C5-C6-N1	5.39	123.70	121.00
1	XA	1290	G	C4-N9-C1'	5.39	133.51	126.50
35	RA	2471	C	C2-N1-C1'	5.39	124.73	118.80
35	RA	1062	G	C8-N9-C1'	-5.39	120.00	127.00
1	XA	417	C	C6-N1-C2	-5.39	118.15	120.30
1	XA	699	C	C5-C6-N1	5.38	123.69	121.00
35	YA	595	C	C5-C6-N1	5.38	123.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2575	C	C5-C6-N1	5.38	123.69	121.00
35	RA	595	C	C6-N1-C2	-5.38	118.15	120.30
1	XA	739	C	C5-C6-N1	5.38	123.69	121.00
1	XA	810	C	N3-C2-O2	-5.38	118.13	121.90
1	XA	1527	C	C6-N1-C2	-5.38	118.15	120.30
42	RI	126	TYR	CA-CB-CG	5.38	123.61	113.40
49	RT	100	TYR	CA-CB-CG	5.38	123.61	113.40
35	YA	1994	C	C6-N1-C2	-5.37	118.15	120.30
35	RA	702	G	C8-N9-C1'	-5.37	120.02	127.00
35	RA	2559	C	N3-C2-O2	-5.37	118.14	121.90
35	YA	2056	G	N3-C2-N2	-5.37	116.14	119.90
35	RA	196	A	C2-N3-C4	5.37	113.28	110.60
36	RB	60	C	C6-N1-C2	-5.37	118.15	120.30
35	YA	343	C	C6-N1-C2	-5.37	118.15	120.30
35	YA	1506	C	N1-C2-O2	5.37	122.12	118.90
35	YA	1988	C	C5-C6-N1	5.37	123.68	121.00
35	RA	1314	C	N3-C2-O2	-5.37	118.14	121.90
35	YA	503	A	P-O3'-C3'	5.37	126.14	119.70
35	YA	529	A	C2-N3-C4	5.37	113.28	110.60
35	YA	1496	A	C8-N9-C4	-5.36	103.66	105.80
16	QP	17	TYR	CA-CB-CG	5.36	123.59	113.40
35	YA	1411	C	N1-C2-O2	5.36	122.12	118.90
35	YA	595	C	C6-N1-C2	-5.36	118.16	120.30
35	RA	1376	C	N3-C2-O2	-5.36	118.15	121.90
35	RA	1879	C	C6-N1-C2	-5.36	118.16	120.30
35	YA	893	C	C6-N1-C2	-5.36	118.16	120.30
35	YA	1920	C	C6-N1-C2	-5.36	118.16	120.30
36	RB	22	U	C5-C6-N1	5.36	125.38	122.70
1	XA	1505	G	C8-N9-C1'	5.36	133.96	127.00
35	RA	364	C	C5-C6-N1	5.35	123.68	121.00
1	XA	311	C	C6-N1-C2	-5.35	118.16	120.30
1	XA	353	A	OP2-P-O3'	5.35	116.98	105.20
35	YA	1686	C	N1-C2-O2	5.35	122.11	118.90
35	RA	912	C	N3-C2-O2	-5.35	118.15	121.90
1	XA	1384	C	C6-N1-C2	-5.35	118.16	120.30
1	QA	1322	C	C6-N1-C2	-5.35	118.16	120.30
35	YA	2097	C	N1-C2-O2	5.35	122.11	118.90
1	XA	1008	C	N1-C2-O2	5.35	122.11	118.90
35	YA	1535	U	O4'-C1'-N1	5.35	112.48	108.20
49	YT	111	ARG	N-CA-C	-5.35	96.56	111.00
42	RI	133	HIS	N-CA-C	-5.35	96.56	111.00
1	XA	1346	A	C8-N9-C4	5.35	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	271(B)	G	OP2-P-O3'	5.35	116.97	105.20
35	YA	904	C	C6-N1-C2	-5.35	118.16	120.30
35	RA	273(F)	C	N3-C2-O2	-5.35	118.16	121.90
35	YA	1376	C	N3-C2-O2	-5.34	118.16	121.90
35	YA	234	C	C6-N1-C2	-5.34	118.16	120.30
35	YA	1686	C	C5-C6-N1	5.34	123.67	121.00
1	QA	1203	C	C5-C6-N1	5.34	123.67	121.00
35	YA	816	C	N3-C2-O2	-5.34	118.16	121.90
1	QA	369	C	C6-N1-C2	-5.34	118.16	120.30
35	RA	1026	U	OP1-P-O3'	5.34	116.95	105.20
35	RA	1535	U	N3-C2-O2	-5.34	118.46	122.20
1	QA	1336	C	P-O3'-C3'	5.34	126.11	119.70
1	XA	1230	C	C5-C6-N1	5.34	123.67	121.00
35	YA	971	C	C6-N1-C2	-5.34	118.17	120.30
35	YA	140	A	N7-C8-N9	5.33	116.47	113.80
35	YA	1765	C	N3-C2-O2	-5.33	118.17	121.90
35	RA	2559	C	C5-C6-N1	5.33	123.67	121.00
35	YA	2097	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	1496	A	C5-N7-C8	-5.33	101.24	103.90
35	YA	201	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	99	U	C2-N1-C1'	5.32	124.09	117.70
35	YA	1402	C	C5-C6-N1	5.32	123.66	121.00
35	YA	2832	U	OP2-P-O3'	5.32	116.91	105.20
1	QA	1097	C	N1-C2-O2	5.32	122.09	118.90
35	RA	2378	A	C8-N9-C4	5.32	107.93	105.80
1	XA	131	C	N1-C2-O2	5.32	122.09	118.90
35	YA	267	C	C6-N1-C2	-5.32	118.17	120.30
35	YA	269	U	C2-N1-C1'	5.32	124.08	117.70
35	YA	1982	C	C5-C6-N1	5.32	123.66	121.00
35	RA	1332	G	C5-N7-C8	-5.32	101.64	104.30
35	YA	537	C	N3-C2-O2	-5.32	118.18	121.90
35	YA	1105	U	N3-C2-O2	-5.32	118.48	122.20
31	Y6	46	HIS	N-CA-C	5.31	125.34	111.00
35	RA	461	C	N1-C2-O2	5.31	122.09	118.90
1	QA	866	C	C5-C6-N1	5.31	123.65	121.00
35	YA	911	A	N7-C8-N9	5.31	116.45	113.80
1	QA	972	C	C6-N1-C2	-5.31	118.18	120.30
1	XA	596	C	N1-C2-O2	5.31	122.08	118.90
35	YA	253	C	C6-N1-C2	-5.31	118.18	120.30
46	RQ	27	VAL	N-CA-C	-5.31	96.67	111.00
1	QA	970	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1786	A	C6-C5-N7	-5.30	128.59	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1881	C	N3-C2-O2	-5.30	118.19	121.90
1	XA	290	C	N1-C2-O2	5.30	122.08	118.90
35	RA	856	C	C2'-C3'-O3'	5.30	122.19	113.70
35	YA	1087	G	C8-N9-C4	-5.30	104.28	106.40
1	XA	328	C	C5-C6-N1	5.30	123.65	121.00
1	XA	1452	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1180	C	N1-C2-O2	5.30	122.08	118.90
35	RA	776	G	C4-N9-C1'	5.30	133.39	126.50
1	QA	307	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1437	C	C5-C6-N1	5.30	123.65	121.00
35	RA	1691	C	N1-C2-O2	5.30	122.08	118.90
35	RA	271(B)	G	OP2-P-O3'	5.29	116.85	105.20
35	RA	687	C	C2-N1-C1'	5.29	124.62	118.80
35	YA	535	C	C5-C6-N1	5.29	123.65	121.00
1	QA	412	A	OP2-P-O3'	5.29	116.85	105.20
35	RA	269	U	N1-C2-O2	5.29	126.50	122.80
1	XA	243	A	P-O3'-C3'	5.29	126.05	119.70
1	XA	1439	C	N3-C2-O2	-5.29	118.19	121.90
35	RA	914	C	C5-C6-N1	5.29	123.64	121.00
35	YA	114	U	C5-C6-N1	5.29	125.34	122.70
35	RA	2576	G	C8-N9-C1'	-5.29	120.12	127.00
35	YA	1781	C	N3-C2-O2	-5.29	118.20	121.90
12	QL	104	VAL	C-N-CA	5.29	134.92	121.70
36	RB	31	C	C2-N1-C1'	5.29	124.62	118.80
35	YA	702	G	C4-N9-C1'	5.29	133.38	126.50
35	YA	2617	C	N1-C2-O2	5.29	122.07	118.90
35	YA	1438	U	C5-C6-N1	5.29	125.34	122.70
1	XA	792	A	N7-C8-N9	5.28	116.44	113.80
35	YA	856	C	P-O3'-C3'	5.28	126.04	119.70
35	YA	2562	U	N3-C2-O2	-5.28	118.50	122.20
35	RA	409	C	N1-C2-O2	5.28	122.07	118.90
1	XA	221	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	1956	U	C6-N1-C2	-5.28	117.83	121.00
35	RA	588	U	O5'-P-OP1	-5.28	100.95	105.70
1	XA	1429	C	N1-C2-O2	5.28	122.07	118.90
35	YA	1686	C	N3-C2-O2	-5.28	118.20	121.90
35	RA	242	G	OP2-P-O3'	5.28	116.81	105.20
55	RZ	115	GLY	N-CA-C	5.28	126.29	113.10
35	RA	1468	C	C6-N1-C2	-5.28	118.19	120.30
35	RA	2766	G	C4-N9-C1'	5.28	133.36	126.50
35	YA	2441	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	2443	C	N3-C2-O2	-5.28	118.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	YB	22	U	C6-N1-C2	-5.28	117.83	121.00
35	YA	41	C	C6-N1-C2	-5.27	118.19	120.30
35	YA	529	A	C4-N9-C1'	5.27	135.79	126.30
35	YA	974(A)	C	C2-N1-C1'	5.27	124.60	118.80
1	QA	370	C	N1-C2-O2	5.27	122.06	118.90
35	RA	1708	C	C6-N1-C2	-5.27	118.19	120.30
35	RA	2307	G	C4-N9-C1'	5.27	133.35	126.50
35	RA	530	G	C6-C5-N7	5.27	133.56	130.40
35	YA	2559	C	C2-N1-C1'	5.27	124.60	118.80
35	RA	1502	C	N3-C4-N4	5.27	121.69	118.00
35	RA	1774	C	C5-C6-N1	5.27	123.64	121.00
1	XA	1395	C	N1-C2-O2	5.27	122.06	118.90
5	XE	72	GLN	C-N-CA	5.27	134.88	121.70
35	YA	2490	G	C4-C5-N7	5.27	112.91	110.80
35	YA	1053	C	C6-N1-C2	-5.27	118.19	120.30
35	YA	1656	C	C5-C6-N1	5.27	123.63	121.00
1	QA	1234	C	N3-C2-O2	-5.26	118.21	121.90
35	RA	2471	C	C5-C6-N1	5.26	123.63	121.00
42	RI	14	ASP	C-N-CA	5.26	134.86	121.70
30	R5	51	TYR	C-N-CA	5.26	134.85	121.70
35	YA	316	C	C6-N1-C2	-5.26	118.20	120.30
1	QA	792	A	C4-N9-C1'	5.26	135.77	126.30
35	YA	141	A	N7-C8-N9	5.26	116.43	113.80
35	YA	544	C	C6-N1-C2	-5.26	118.20	120.30
41	YH	83	TYR	N-CA-C	5.26	125.20	111.00
35	RA	676	A	O4'-C1'-N9	5.26	112.41	108.20
35	YA	1598	C	C2-N1-C1'	5.26	124.58	118.80
35	YA	2666	C	N1-C2-O2	5.25	122.05	118.90
24	QY	69	C	N1-C2-O2	5.25	122.05	118.90
35	YA	1174	A	N3-C4-N9	5.25	131.60	127.40
35	YA	850	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	1163	C	N1-C2-O2	5.25	122.05	118.90
35	RA	1781	C	N1-C2-O2	5.25	122.05	118.90
35	YA	1315	C	N3-C2-O2	-5.25	118.23	121.90
1	QA	1336	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	1447	G	C4-N9-C1'	5.25	133.32	126.50
35	YA	528	A	C5-N7-C8	-5.25	101.28	103.90
36	YB	27	C	C6-N1-C2	-5.25	118.20	120.30
35	RA	1766	U	C5-C6-N1	5.25	125.32	122.70
35	YA	1223	C	C6-N1-C2	-5.25	118.20	120.30
35	RA	1021	A	C8-N9-C4	-5.24	103.70	105.80
35	RA	1982	C	C5-C4-N4	-5.24	116.53	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	358	U	C5-C6-N1	5.24	125.32	122.70
35	RA	738	G	N3-C4-C5	-5.24	125.98	128.60
1	XA	381	C	N1-C2-O2	5.24	122.04	118.90
35	YA	2238	G	N3-C4-N9	5.24	129.14	126.00
35	YA	1085	A	P-O3'-C3'	5.24	125.99	119.70
35	RA	692	C	C6-N1-C2	-5.24	118.20	120.30
35	RA	2701	C	C6-N1-C2	-5.24	118.20	120.30
35	RA	654(T)	C	N1-C2-O2	5.24	122.04	118.90
35	YA	1992	G	OP2-P-O3'	5.24	116.72	105.20
35	YA	2474	C	C6-N1-C1'	-5.24	114.52	120.80
35	RA	333	G	C4-N9-C1'	5.23	133.30	126.50
35	YA	2391	G	O4'-C1'-N9	5.23	112.39	108.20
35	RA	2506	U	C6-N1-C2	-5.23	117.86	121.00
35	YA	1544	C	N3-C2-O2	-5.23	118.24	121.90
35	RA	2559	C	C2-N1-C1'	5.23	124.55	118.80
35	YA	221	A	P-O3'-C3'	5.23	125.97	119.70
38	YE	37	ARG	C-N-CA	5.23	134.77	121.70
1	QA	449	C	N3-C2-O2	-5.23	118.24	121.90
35	RA	1332	G	C8-N9-C1'	-5.23	120.20	127.00
35	RA	991	C	C6-N1-C2	-5.22	118.21	120.30
35	YA	1568	G	C8-N9-C1'	5.22	133.79	127.00
35	YA	2307	G	C8-N9-C4	-5.22	104.31	106.40
1	QA	1452	C	N1-C2-O2	5.22	122.03	118.90
35	YA	1352	U	N3-C2-O2	-5.22	118.54	122.20
35	RA	1290	C	C6-N1-C2	-5.22	118.21	120.30
35	RA	1920	C	C5-C6-N1	5.22	123.61	121.00
1	QA	565	U	C5-C4-O4	-5.22	122.77	125.90
35	YA	1315	C	C6-N1-C2	-5.22	118.21	120.30
35	YA	2766	G	C8-N9-C1'	-5.22	120.22	127.00
35	YA	1786	A	C4-N9-C1'	5.22	135.69	126.30
35	YA	974(A)	C	N3-C2-O2	-5.22	118.25	121.90
35	YA	2774	C	N3-C2-O2	-5.22	118.25	121.90
1	XA	973	G	C8-N9-C4	-5.21	104.31	106.40
35	RA	1589	C	N3-C2-O2	-5.21	118.25	121.90
35	YA	2403	C	C5-C6-N1	5.21	123.61	121.00
1	QA	726	C	C6-N1-C2	-5.21	118.22	120.30
35	RA	1376	C	C6-N1-C2	-5.21	118.22	120.30
35	RA	893	C	N1-C2-O2	5.21	122.02	118.90
35	RA	1461	G	C4-N9-C1'	5.21	133.27	126.50
35	YA	2443	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1395	C	C2-N1-C1'	5.21	124.53	118.80
35	YA	1950	G	C6-C5-N7	-5.21	127.28	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1982	C	N3-C4-N4	5.20	121.64	118.00
35	RA	74	A	O4'-C1'-N9	-5.20	104.04	108.20
35	RA	1797	C	C5-C6-N1	5.20	123.60	121.00
35	RA	2616	C	C6-N1-C2	-5.20	118.22	120.30
35	YA	1644	C	C6-N1-C2	-5.20	118.22	120.30
1	QA	932	C	C2-N1-C1'	5.20	124.52	118.80
1	XA	43	C	C6-N1-C2	-5.20	118.22	120.30
1	QA	1070	U	N3-C2-O2	-5.20	118.56	122.20
1	XA	963	G	C4-C5-C6	5.20	121.92	118.80
22	XV	34	C	N3-C2-O2	-5.20	118.26	121.90
35	YA	1437	C	C2-N1-C1'	5.20	124.52	118.80
35	YA	393	C	C5-C6-N1	5.19	123.60	121.00
35	YA	141	A	C5-N7-C8	-5.19	101.30	103.90
35	YA	318	C	C6-N1-C2	-5.19	118.22	120.30
35	YA	1827	C	N1-C2-O2	5.19	122.02	118.90
35	RA	1819	A	P-O3'-C3'	5.19	125.93	119.70
35	YA	650	C	N3-C2-O2	-5.19	118.27	121.90
35	YA	2504	U	N1-C2-O2	5.19	126.43	122.80
35	YA	2814	C	N1-C2-O2	5.19	122.01	118.90
1	XA	328	C	OP2-P-O3'	5.19	116.61	105.20
36	RB	30	C	N1-C2-O2	5.18	122.01	118.90
1	XA	174	C	C6-N1-C2	-5.18	118.23	120.30
1	XA	645	C	N3-C2-O2	-5.18	118.27	121.90
1	QA	91	C	N3-C2-O2	-5.18	118.27	121.90
1	QA	680	C	C6-N1-C2	-5.18	118.23	120.30
35	RA	102	G	P-O3'-C3'	5.18	125.92	119.70
35	RA	1187	G	N7-C8-N9	5.18	115.69	113.10
35	RA	1404	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	1005	C	N3-C2-O2	-5.18	118.27	121.90
35	YA	564	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	797	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	2328	A	C8-N9-C4	-5.18	103.73	105.80
35	RA	273(F)	C	C5-C6-N1	5.18	123.59	121.00
35	RA	2616	C	N3-C2-O2	-5.18	118.27	121.90
35	YA	965	C	C6-N1-C2	-5.18	118.23	120.30
42	YI	131	LYS	N-CA-C	5.18	124.97	111.00
1	QA	1163	C	N3-C2-O2	-5.17	118.28	121.90
35	RA	2311	A	C8-N9-C4	-5.17	103.73	105.80
13	QM	13	LYS	N-CA-C	5.17	124.96	111.00
35	RA	409	C	N3-C2-O2	-5.17	118.28	121.90
1	XA	977	A	N7-C8-N9	5.17	116.39	113.80
35	YA	786	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2611	U	C5-C6-N1	5.17	125.29	122.70
36	RB	44	G	C4-N9-C1'	-5.17	119.78	126.50
1	QA	1313	U	C5-C6-N1	5.17	125.28	122.70
1	XA	960	U	N1-C2-O2	5.17	126.42	122.80
35	YA	2726	U	C2-N1-C1'	5.17	123.90	117.70
35	RA	456	C	N3-C2-O2	-5.17	118.28	121.90
35	YA	138	G	O4'-C1'-N9	5.17	112.33	108.20
1	QA	1301	U	C5-C6-N1	5.17	125.28	122.70
35	RA	307	G	N7-C8-N9	5.17	115.68	113.10
1	XA	645	C	N1-C2-O2	5.17	122.00	118.90
35	RA	1930	G	P-O3'-C3'	5.16	125.90	119.70
35	YA	41	C	N1-C2-O2	5.16	122.00	118.90
35	RA	1502	C	C6-N1-C2	-5.16	118.24	120.30
35	RA	1941	C	C5-C6-N1	5.16	123.58	121.00
35	YA	673	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	308	C	C6-N1-C2	-5.16	118.24	120.30
35	RA	2656	U	N3-C2-O2	-5.16	118.59	122.20
35	YA	270(Y)	G	C8-N9-C4	-5.16	104.34	106.40
1	QA	980	C	N3-C2-O2	-5.16	118.29	121.90
1	QA	1158	C	C5-C6-N1	5.16	123.58	121.00
22	QV	34	C	N1-C2-O2	5.16	121.99	118.90
35	RA	2394	C	C6-N1-C2	-5.16	118.24	120.30
44	YO	4	PRO	C-N-CA	5.16	134.59	121.70
35	RA	313	C	C5-C6-N1	5.15	123.58	121.00
1	XA	19	C	N3-C2-O2	-5.15	118.29	121.90
35	RA	480	A	OP1-P-O3'	5.15	116.53	105.20
35	RA	1534	G	C4-N9-C1'	5.15	133.20	126.50
35	RA	1795	C	C5-C6-N1	5.15	123.58	121.00
35	RA	1931	U	N3-C2-O2	-5.15	118.59	122.20
1	XA	413	G	O4'-C1'-N9	5.15	112.32	108.20
35	YA	1836	C	N3-C2-O2	-5.15	118.29	121.90
1	XA	948	C	C5-C6-N1	5.15	123.58	121.00
35	YA	153	C	C6-N1-C2	-5.15	118.24	120.30
35	YA	2667	C	C5-C6-N1	5.15	123.58	121.00
1	XA	1263	C	N1-C2-O2	5.15	121.99	118.90
1	QA	328	C	C2-N3-C4	5.15	122.47	119.90
35	RA	66	C	C5-C6-N1	5.15	123.57	121.00
35	YA	228	A	C8-N9-C4	-5.14	103.74	105.80
35	RA	537	C	C6-N1-C2	-5.14	118.24	120.30
51	RV	45	THR	N-CA-C	5.14	124.89	111.00
1	XA	690	G	C4-N9-C1'	5.14	133.18	126.50
35	YA	1038	C	N1-C2-O2	5.14	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1833	U	N3-C2-O2	-5.14	118.60	122.20
35	YA	268	C	C6-N1-C2	-5.14	118.24	120.30
35	YA	588	U	O5'-P-OP1	-5.14	101.07	105.70
35	YA	2066	C	N1-C2-O2	5.14	121.98	118.90
35	YA	2056	G	C4-N9-C1'	5.14	133.18	126.50
35	YA	591	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	2097	C	C6-N1-C2	-5.13	118.25	120.30
1	QA	369	C	C2-N1-C1'	5.13	124.44	118.80
1	XA	290	C	N3-C2-O2	-5.13	118.31	121.90
35	YA	541	C	C6-N1-C2	-5.13	118.25	120.30
35	YA	1947	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	1514	U	C2-N1-C1'	5.13	123.86	117.70
35	YA	2079	U	C5-C6-N1	5.13	125.27	122.70
1	QA	346	G	C8-N9-C1'	-5.13	120.33	127.00
1	QA	703	G	P-O3'-C3'	5.13	125.85	119.70
35	RA	1502	C	C5-C6-N1	5.13	123.56	121.00
1	XA	991	U	N3-C2-O2	-5.13	118.61	122.20
24	XY	56	C	N1-C2-O2	5.13	121.98	118.90
35	RA	530	G	N9-C4-C5	5.13	107.45	105.40
1	XA	1114	C	C2-N1-C1'	5.13	124.44	118.80
35	YA	316	C	N1-C2-O2	5.13	121.98	118.90
35	YA	1888	G	N3-C4-N9	5.13	129.08	126.00
38	RE	186	GLY	N-CA-C	5.12	125.91	113.10
1	XA	526	C	C5-C6-N1	5.12	123.56	121.00
35	YA	1669	A	C4-N9-C1'	5.12	135.52	126.30
35	YA	1411	C	N3-C2-O2	-5.12	118.32	121.90
35	YA	1779	U	C2-N1-C1'	5.12	123.84	117.70
35	RA	2699	C	C5-C6-N1	5.12	123.56	121.00
1	XA	1260	C	N3-C2-O2	-5.12	118.32	121.90
35	YA	1005	C	C2-N1-C1'	5.12	124.43	118.80
35	YA	1437	C	C6-N1-C2	-5.12	118.25	120.30
1	XA	1086	U	C5-C6-N1	5.12	125.26	122.70
35	YA	18	C	C6-N1-C2	-5.12	118.25	120.30
35	YA	137	C	C6-N1-C2	-5.12	118.25	120.30
35	YA	2039	C	C5-C6-N1	5.12	123.56	121.00
35	YA	2096	U	C6-N1-C2	-5.12	117.93	121.00
35	RA	529	A	C4-N9-C1'	5.11	135.50	126.30
35	RA	1574	C	C5-C6-N1	5.11	123.56	121.00
35	YA	859	G	OP2-P-O3'	5.11	116.45	105.20
35	YA	1509	C	OP1-P-O3'	5.11	116.45	105.20
35	YA	2666	C	C6-N1-C2	-5.11	118.25	120.30
1	QA	1420	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	269	U	N3-C2-O2	-5.11	118.62	122.20
35	RA	752	A	OP2-P-O3'	5.11	116.44	105.20
35	RA	1258	C	C6-N1-C2	-5.11	118.25	120.30
35	RA	1062	G	N3-C4-C5	-5.11	126.05	128.60
35	RA	1406	U	N3-C2-O2	-5.11	118.62	122.20
25	R0	26	TYR	CA-CB-CG	5.11	123.10	113.40
35	RA	828	U	C6-N1-C1'	-5.11	114.05	121.20
1	QA	449	C	C6-N1-C2	-5.11	118.26	120.30
1	QA	1070	U	C6-N1-C2	-5.11	117.94	121.00
35	RA	2702	U	O4'-C1'-N1	5.11	112.28	108.20
35	YA	335	C	C5-C6-N1	5.11	123.55	121.00
35	RA	345	A	P-O3'-C3'	5.10	125.82	119.70
1	XA	1505	G	N3-C2-N2	-5.10	116.33	119.90
35	YA	838	C	C5-C6-N1	5.10	123.55	121.00
35	YA	1979	C	N1-C2-O2	5.10	121.96	118.90
35	YA	2880	C	C5-C6-N1	5.10	123.55	121.00
35	RA	756	C	N3-C2-O2	-5.10	118.33	121.90
35	RA	1776	G	C4-N9-C1'	5.10	133.13	126.50
36	RB	5	C	N1-C2-O2	5.10	121.96	118.90
44	RO	32	TYR	CA-CB-CG	5.10	123.08	113.40
1	XA	792	A	C4-N9-C1'	5.10	135.48	126.30
35	YA	2692	C	N3-C2-O2	-5.10	118.33	121.90
35	YA	404	C	OP2-P-O3'	5.10	116.41	105.20
50	RU	90	VAL	C-N-CA	5.09	134.44	121.70
35	YA	1786	A	C4-C5-N7	5.09	113.25	110.70
35	YA	2473	U	N3-C2-O2	-5.09	118.63	122.20
35	YA	1411	C	C5-C6-N1	5.09	123.55	121.00
36	YB	43	C	C6-N1-C2	-5.09	118.26	120.30
35	RA	2129	C	N1-C2-O2	5.09	121.95	118.90
1	XA	868	C	N3-C2-O2	-5.09	118.34	121.90
35	YA	2317	C	C6-N1-C2	-5.09	118.26	120.30
1	QA	687	A	C2-N3-C4	5.09	113.14	110.60
24	XY	72	C	C6-N1-C2	-5.09	118.26	120.30
35	YA	2726	U	N1-C2-O2	5.09	126.36	122.80
35	RA	1963	U	C5-C6-N1	5.09	125.24	122.70
35	RA	2626	C	C6-N1-C2	-5.09	118.27	120.30
1	XA	932	C	C2-N1-C1'	5.09	124.39	118.80
35	YA	1178	C	N3-C2-O2	-5.09	118.34	121.90
35	YA	1956	U	C2-N1-C1'	5.08	123.80	117.70
1	QA	328	C	C6-N1-C1'	-5.08	114.70	120.80
35	RA	253	C	N3-C2-O2	-5.08	118.34	121.90
35	RA	1691	C	N3-C2-O2	-5.08	118.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	410	G	P-O3'-C3'	5.08	125.80	119.70
1	QA	652	U	N3-C2-O2	-5.08	118.64	122.20
35	RA	1765	C	C6-N1-C2	-5.08	118.27	120.30
42	RI	132	PRO	C-N-CA	5.08	134.40	121.70
35	YA	1534	G	C4-N9-C1'	5.08	133.10	126.50
1	XA	1114	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	2620	C	C5-C6-N1	5.08	123.54	121.00
1	XA	354	G	C8-N9-C1'	-5.08	120.40	127.00
1	XA	963	G	N3-C4-C5	-5.08	126.06	128.60
35	YA	626	U	C6-N1-C2	-5.08	117.95	121.00
1	QA	689	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	1404	C	C2-N1-C1'	5.08	124.38	118.80
35	RA	1575	C	N1-C2-O2	5.08	121.94	118.90
42	RI	13	GLY	N-CA-C	5.08	125.79	113.10
35	YA	756	C	C6-N1-C2	-5.08	118.27	120.30
35	YA	1158	C	C6-N1-C2	-5.08	118.27	120.30
1	XA	497	U	N1-C2-O2	5.07	126.35	122.80
35	RA	964	C	C6-N1-C2	-5.07	118.27	120.30
35	YA	1332	G	C8-N9-C1'	-5.07	120.41	127.00
35	YA	265	A	C5-C6-N1	5.07	120.23	117.70
24	XY	16	C	C6-N1-C2	-5.07	118.27	120.30
35	YA	529	A	C8-N9-C4	-5.07	103.77	105.80
35	YA	661	C	C5-C6-N1	5.07	123.53	121.00
1	QA	812	C	OP2-P-O3'	5.07	116.34	105.20
35	RA	2226	C	N1-C2-O2	5.07	121.94	118.90
1	XA	154	C	N3-C2-O2	-5.07	118.35	121.90
35	YA	565	C	N1-C2-O2	5.07	121.94	118.90
35	RA	945	A	C4-C5-N7	5.06	113.23	110.70
1	QA	103	C	N1-C2-O2	5.06	121.94	118.90
35	YA	838	C	N1-C2-O2	5.06	121.94	118.90
35	YA	1053	C	N1-C2-O2	5.06	121.94	118.90
35	YA	2439	A	N7-C8-N9	5.06	116.33	113.80
1	XA	1297	C	OP2-P-O3'	5.06	116.33	105.20
35	YA	228	A	C2-N3-C4	5.06	113.13	110.60
35	YA	2066	C	C5-C6-N1	5.06	123.53	121.00
1	QA	897	C	N1-C2-O2	5.06	121.94	118.90
1	QA	1019	C	C6-N1-C2	-5.06	118.28	120.30
35	RA	1832	C	C6-N1-C2	-5.06	118.28	120.30
38	RE	82	ARG	C-N-CA	5.06	134.34	121.70
35	YA	537	C	N1-C2-O2	5.06	121.93	118.90
1	QA	1499	A	O5'-P-OP1	-5.06	101.15	105.70
35	RA	29	U	C5-C6-N1	5.05	125.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	YT	99	LEU	CA-CB-CG	5.05	126.92	115.30
35	RA	2060	A	OP2-P-O3'	5.05	116.31	105.20
35	YA	930	U	C6-N1-C1'	-5.05	114.13	121.20
1	XA	789	U	N1-C2-O2	5.05	126.33	122.80
35	RA	613	U	C6-N1-C2	-5.04	117.97	121.00
1	QA	465	A	N1-C6-N6	-5.04	115.57	118.60
1	QA	1238	A	O5'-P-OP1	-5.04	101.16	105.70
35	RA	307	G	C8-N9-C4	-5.04	104.38	106.40
35	RA	373	U	N3-C2-O2	-5.04	118.67	122.20
35	YA	825	C	C6-N1-C2	-5.04	118.28	120.30
36	YB	60	C	C6-N1-C2	-5.04	118.28	120.30
49	RT	99	LEU	CA-CB-CG	5.04	126.90	115.30
22	XV	69	C	N3-C2-O2	-5.04	118.37	121.90
35	RA	2318	G	C4-N9-C1'	5.04	133.05	126.50
36	RB	68	C	C6-N1-C2	-5.04	118.28	120.30
1	XA	754	C	N1-C2-O2	5.04	121.92	118.90
1	XA	1397	C	C6-N1-C2	-5.04	118.28	120.30
1	QA	108	G	C4-N9-C1'	5.04	133.05	126.50
35	RA	104	U	N1-C2-O2	5.04	126.33	122.80
35	YA	1142(A)	A	N3-C4-N9	-5.04	123.37	127.40
35	YA	1514	U	C2-N1-C1'	5.04	123.75	117.70
35	YA	1264	G	N7-C8-N9	5.04	115.62	113.10
35	RA	2651	C	N1-C2-O2	5.04	121.92	118.90
35	YA	1819	A	P-O3'-C3'	5.04	125.74	119.70
29	R4	39	CYS	N-CA-C	-5.03	97.41	111.00
35	RA	1411	C	C5-C6-N1	5.03	123.52	121.00
35	RA	1657	C	C6-N1-C2	-5.03	118.29	120.30
35	RA	270(H)	C	C6-N1-C2	-5.03	118.29	120.30
1	XA	1303	C	C6-N1-C2	-5.03	118.29	120.30
1	XA	1397	C	C2-N1-C1'	5.03	124.33	118.80
35	YA	540	G	C8-N9-C4	-5.03	104.39	106.40
35	YA	1142(A)	A	C2-N3-C4	-5.03	108.08	110.60
35	YA	1343	G	C4-N9-C1'	5.03	133.04	126.50
35	YA	2053	G	O5'-P-OP1	-5.03	101.17	105.70
35	YA	1006	C	C6-N1-C2	-5.03	118.29	120.30
1	QA	406	G	C4-N9-C1'	5.03	133.03	126.50
35	YA	140	A	C8-N9-C4	-5.03	103.79	105.80
35	YA	231	C	C2-N1-C1'	5.03	124.33	118.80
22	QV	1	C	C6-N1-C2	-5.03	118.29	120.30
35	RA	1882	C	N3-C2-O2	-5.03	118.38	121.90
35	RA	2044	C	N1-C2-O2	5.02	121.92	118.90
35	RA	2107	C	C6-N1-C2	-5.02	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	1336	C	OP2-P-O3'	5.02	116.25	105.20
35	RA	588	U	C5-C6-N1	5.02	125.21	122.70
35	RA	2036	C	N1-C2-O2	5.02	121.91	118.90
35	YA	364	C	N3-C2-O2	-5.02	118.39	121.90
35	YA	2368	C	C6-N1-C2	-5.02	118.29	120.30
1	QA	753	A	OP2-P-O3'	5.02	116.24	105.20
35	RA	1474	C	N3-C2-O2	-5.02	118.39	121.90
35	YA	1433	U	C6-N1-C2	-5.02	117.99	121.00
35	YA	2261	C	C6-N1-C2	-5.02	118.29	120.30
50	YU	92	ARG	C-N-CA	5.02	134.24	121.70
1	QA	1336	C	C5-C6-N1	5.02	123.51	121.00
35	RA	697	C	C5-C6-N1	5.01	123.51	121.00
1	XA	545	C	C6-N1-C2	-5.01	118.29	120.30
35	YA	2592	G	N3-C4-N9	5.01	129.01	126.00
1	XA	963	G	N9-C4-C5	-5.01	103.39	105.40
35	YA	2074	U	C6-N1-C2	-5.01	117.99	121.00
35	YA	2891	G	C4-N9-C1'	5.01	133.01	126.50
35	YA	1836	C	N1-C2-O2	5.01	121.91	118.90
35	YA	2768	C	C5-C6-N1	5.01	123.50	121.00
1	QA	435	C	N3-C2-O2	-5.01	118.39	121.90
35	RA	377	C	C6-N1-C2	-5.01	118.30	120.30
35	RA	1461	G	N7-C8-N9	5.01	115.60	113.10
1	XA	1260	C	C5-C6-N1	5.01	123.50	121.00
36	YB	30	C	N3-C2-O2	-5.01	118.40	121.90
7	QG	56	GLN	C-N-CA	5.00	134.21	121.70
35	RA	404	C	OP2-P-O3'	5.00	116.21	105.20
35	YA	1504	C	N1-C2-O2	5.00	121.90	118.90
35	RA	1513	C	C5-C6-N1	5.00	123.50	121.00
35	RA	2238	G	C4-N9-C1'	5.00	133.00	126.50
36	RB	79	C	C6-N1-C2	-5.00	118.30	120.30
35	YA	1805	U	N1-C2-N3	5.00	117.90	114.90
49	YT	105	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

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	32247	0	16277	208	0
1	XA	32249	0	16279	169	0
2	QB	1924	0	1975	27	0
2	XB	1924	0	1975	28	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	16	0
4	QD	1674	0	1718	30	0
4	XD	1674	0	1718	21	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	10	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	19	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	18	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	15	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	17	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	9	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	13	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	396	0	197	2	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0
25	Y0	648	0	672	10	0
26	R1	763	0	847	13	0
26	Y1	763	0	848	12	0
27	R2	581	0	629	15	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	16	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	10	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	11	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	6	0
33	R8	517	0	582	17	0
33	Y8	517	0	582	30	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	341	0
35	YA	62091	0	31290	289	0
36	RB	2573	0	1306	15	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	51	0
38	RE	1568	0	1633	45	0
38	YE	1568	0	1634	31	0
39	RF	1585	0	1632	22	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YG	1474	0	1535	18	0
41	RH	1307	0	1382	20	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	11	0
43	RN	1104	0	1180	23	0
43	YN	1104	0	1180	8	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	27	0
46	RQ	1122	0	1179	23	0
46	YQ	1122	0	1177	20	0
47	RR	968	0	1033	17	0
47	YR	968	0	1033	16	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0
49	YT	1141	0	1202	23	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	19	0
51	RV	779	0	852	17	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	17	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	27	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199665	2182	0

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 5.

All (2182) 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)
55:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.13	1.11
35:RA:2055:C:H5'	35:RA:2056:G:H5"	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06
35:RA:1138:G:H21	43:RN:106:MET:CE	1.72	1.02
26:Y1:4:VAL:HG12	26:Y1:11:ARG:HD3	1.41	1.01
55:YZ:94:GLU:HG3	55:YZ:95:PRO:HD3	1.42	1.00
55:YZ:94:GLU:CB	55:YZ:95:PRO:HD3	1.90	1.00
25:R0:69:PHE:CE2	25:R0:79:VAL:HG22	1.98	0.96
25:R0:69:PHE:CD2	25:R0:79:VAL:HG22	2.00	0.96
3:QC:159:GLY:CA	3:QC:193:TYR:HE2	1.78	0.96
3:QC:159:GLY:CA	3:QC:193:TYR:CE2	2.50	0.95
55:YZ:94:GLU:CB	55:YZ:95:PRO:CD	2.45	0.94
49:RT:54:ARG:HA	49:RT:59:THR:HG23	1.52	0.90
4:QD:68:TYR:HE1	4:QD:103:ASN:ND2	1.70	0.90
24:QY:76:A:H2	35:RA:2583:G:H21	1.17	0.89
38:RE:13:ARG:HH21	49:RT:58:ASN:HB2	1.39	0.88
3:QC:159:GLY:HA2	3:QC:193:TYR:CE2	2.10	0.86
3:QC:159:GLY:HA2	3:QC:193:TYR:CD2	2.12	0.85
3:QC:159:GLY:N	3:QC:193:TYR:HE2	1.75	0.84
33:Y8:4:MET:CE	33:Y8:61:LEU:CD1	2.55	0.84
35:RA:1138:G:N3	43:RN:106:MET:CE	2.42	0.83
35:RA:1138:G:N2	43:RN:106:MET:CE	2.42	0.82
10:XJ:57:LYS:HD2	10:XJ:60:ARG:HH21	1.44	0.82
35:RA:1138:G:N2	43:RN:106:MET:HE1	1.93	0.82
41:YH:103:LEU:HD22	41:YH:123:PHE:CE2	2.16	0.81
55:YZ:94:GLU:HB3	55:YZ:95:PRO:HD3	1.56	0.80
55:YZ:94:GLU:HB3	55:YZ:95:PRO:HD2	1.63	0.80
41:YH:103:LEU:HD22	41:YH:123:PHE:HE2	1.47	0.79
24:QY:76:A:C2	35:RA:2583:G:N2	2.48	0.79
33:Y8:4:MET:SD	33:Y8:61:LEU:HD12	2.23	0.78
3:XC:9:GLY:HA2	3:XC:12:LEU:HD23	1.65	0.78
35:RA:1043:C:H42	35:RA:1112:G:H1	1.30	0.77
18:QR:26:LEU:HD11	18:QR:29:PHE:CE2	2.20	0.77
38:RE:13:ARG:NH2	49:RT:58:ASN:HB2	2.00	0.76
26:Y1:11:ARG:HG3	26:Y1:12:PRO:HD2	1.69	0.75
35:YA:2102:U:H3	35:YA:2187:G:H1	1.35	0.75
26:Y1:4:VAL:CG1	26:Y1:11:ARG:HD3	2.15	0.75
1:XA:659:U:H5"	15:XO:5:LYS:HE3	1.67	0.75
35:RA:676:A:H8	35:RA:2069:G:H21	1.35	0.74
24:XY:5:C:H42	24:XY:68:G:H1	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:QR:26:LEU:HD11	18:QR:29:PHE:HE2	1.53	0.73
33:Y8:4:MET:HE3	33:Y8:61:LEU:CD1	2.18	0.73
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.54	0.72
38:YE:143:ASN:HD22	38:YE:147:PRO:HG2	1.54	0.72
13:QM:84:ILE:HD11	13:QM:86:CYS:HB2	1.72	0.72
32:Y7:9:ARG:NH1	35:YA:1310:G:OP2	2.22	0.72
35:RA:2056:G:H2'	35:RA:2056:G:N3	2.02	0.72
2:QB:178:ARG:HH22	8:QH:74:PRO:HB3	1.54	0.71
13:QM:80:ARG:O	13:QM:84:ILE:HG21	1.90	0.71
30:Y5:4:HIS:O	35:YA:2056:G:N2	2.23	0.71
5:QE:51:VAL:HG23	5:QE:52:PRO:HD3	1.71	0.71
30:Y5:38:ALA:HB3	30:Y5:40:LYS:HZ3	1.54	0.71
33:Y8:62:LEU:HD13	35:YA:242:G:H5"	1.73	0.71
39:YF:107:LYS:HD2	39:YF:207:GLY:H	1.56	0.71
18:QR:54:ARG:HH21	18:QR:55:ARG:HH22	1.38	0.71
35:YA:1693:U:H1'	37:YD:14:ARG:HH22	1.56	0.71
19:XS:10:PHE:HZ	19:XS:16:LEU:HB2	1.58	0.69
37:RD:35:LYS:NZ	37:RD:83:GLU:OE1	2.24	0.69
1:QA:1360:A:OP2	14:QN:35:ARG:NH2	2.26	0.69
31:Y6:14:THR:HG21	31:Y6:19:ARG:HH21	1.58	0.69
50:YU:92:ARG:NH1	51:YV:11:GLN:O	2.25	0.69
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.26	0.69
37:YD:182:LEU:H	37:YD:272:ALA:HB3	1.58	0.69
35:YA:1728:G:H8	35:YA:1732:A:H62	1.41	0.69
41:YH:130:ARG:HH12	41:YH:132:ARG:HH21	1.40	0.69
5:QE:154:GLY:HA2	8:QH:64:LYS:HD2	1.74	0.69
35:RA:1061:U:H5'	35:RA:1070:A:H1'	1.75	0.69
45:RP:58:THR:O	45:RP:61:ARG:NH2	2.26	0.69
54:RY:73:ARG:HD2	54:RY:82:PRO:HB2	1.75	0.69
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.26	0.68
35:RA:2055:C:H5'	35:RA:2056:G:C5'	2.19	0.68
35:RA:2100:G:H1	35:RA:2189:U:H3	1.39	0.68
36:YB:74:U:H1'	55:YZ:34:ASN:HD21	1.57	0.68
1:XA:1295:G:N2	1:XA:1302:U:O4	2.27	0.68
25:R0:69:PHE:CE2	25:R0:79:VAL:CG2	2.76	0.68
50:RU:44:ASN:HD21	51:RV:75:PHE:HB3	1.58	0.68
51:YV:76:LYS:HG3	51:YV:81:TYR:CD1	2.28	0.68
9:QI:10:ARG:HE	9:QI:105:ASP:HB2	1.58	0.68
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.57	0.68
35:RA:1138:G:N3	43:RN:106:MET:HE3	2.07	0.68
33:Y8:4:MET:HE3	33:Y8:61:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.67	0.68
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.27	0.68
35:RA:2055:C:C5'	35:RA:2056:G:H5"	2.19	0.68
44:YO:104:ARG:NH2	49:YT:43:GLN:OE1	2.26	0.68
29:Y4:14:ILE:HG22	29:Y4:31:ILE:HB	1.75	0.68
10:QJ:61:GLU:OE1	14:QN:45:ARG:NH1	2.27	0.67
35:RA:2313:C:H4'	40:RG:91:ARG:HG3	1.76	0.67
35:YA:2068:U:H3	35:YA:2430:A:H2	1.42	0.67
36:RB:7:G:H21	48:RS:38:GLN:HE22	1.40	0.67
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.75	0.67
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.26	0.67
49:YT:51:ARG:HG2	49:YT:98:LYS:HD2	1.75	0.67
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	1.76	0.67
1:QA:1009:G:H1	1:QA:1020:U:H3	1.43	0.67
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.59	0.67
33:Y8:65:GLU:HB2	35:YA:628:G:OP1	1.94	0.67
37:RD:35:LYS:HD2	37:RD:63:ARG:HG3	1.77	0.66
10:XJ:50:ILE:HA	10:XJ:60:ARG:HB3	1.76	0.66
35:RA:1138:G:C2	43:RN:106:MET:CE	2.79	0.66
35:YA:1902:C:OP1	37:YD:242:ARG:NH1	2.28	0.66
54:YY:39:VAL:HG13	54:YY:42:VAL:HB	1.77	0.66
35:RA:1138:G:N3	43:RN:106:MET:HE2	2.11	0.66
1:XA:1316:G:N7	19:XS:7:LYS:NZ	2.43	0.66
35:YA:2483:C:N3	46:YQ:124:LYS:NZ	2.40	0.66
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.78	0.66
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.59	0.66
1:QA:407:G:H5"	4:QD:115:ARG:HG2	1.77	0.66
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.28	0.66
35:RA:2115:G:N2	35:RA:2165:G:N7	2.41	0.66
1:XA:8:A:N6	4:XD:205:GLU:O	2.29	0.66
1:XA:664:G:H22	1:XA:741:G:H1	1.42	0.66
34:R9:27:CYS:SG	34:R9:28:GLU:N	2.69	0.66
35:RA:2032:G:N2	38:RE:146:THR:OG1	2.29	0.66
27:Y2:47:ASN:ND2	35:YA:94:G:N3	2.44	0.66
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.29	0.65
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.30	0.65
35:RA:1112:G:HO2'	41:RH:2:SER:N	1.95	0.65
49:RT:53:ARG:O	49:RT:59:THR:HG23	1.96	0.65
35:YA:2013:A:N3	52:YW:88:ARG:NH2	2.43	0.65
1:QA:1252:A:H61	1:QA:1285:A:H61	1.43	0.65
2:XB:168:THR:HB	2:XB:192:SER:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:159:GLY:N	3:QC:193:TYR:CE2	2.63	0.65
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.29	0.65
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.77	0.65
35:YA:265:A:N6	35:YA:427:U:O2'	2.30	0.65
50:RU:90:VAL:HG22	51:RV:39:LEU:HD12	1.78	0.65
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.62	0.65
10:XJ:57:LYS:HD2	10:XJ:60:ARG:NH2	2.10	0.65
35:YA:919:G:N2	35:YA:2269:A:OP2	2.29	0.65
1:QA:8:A:N6	4:QD:205:GLU:O	2.29	0.65
4:QD:68:TYR:CE1	4:QD:103:ASN:ND2	2.59	0.65
55:YZ:52:SER:O	55:YZ:54:HIS:N	2.30	0.65
15:QO:26:GLU:OE2	15:QO:77:ARG:NH1	2.30	0.65
38:RE:143:ASN:HD22	38:RE:147:PRO:HG2	1.61	0.65
18:XR:86:VAL:HG12	18:XR:87:ARG:HG2	1.78	0.65
33:Y8:65:GLU:H	33:Y8:65:GLU:CD	2.00	0.65
38:YE:78:LEU:HG	38:YE:79:ARG:HG3	1.79	0.65
35:YA:960:A:H61	46:YQ:82:ARG:HH21	1.43	0.64
3:QC:47:LEU:HD11	3:QC:76:VAL:HG12	1.79	0.64
35:RA:27:G:N2	35:RA:513:A:OP2	2.30	0.64
2:XB:212:GLN:NE2	2:XB:216:SER:OG	2.30	0.64
38:RE:176:ILE:HB	38:RE:181:LEU:HB2	1.79	0.64
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.30	0.64
37:RD:13:ARG:NH1	37:RD:16:MET:SD	2.70	0.64
55:RZ:52:SER:O	55:RZ:54:HIS:N	2.31	0.64
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.80	0.64
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.79	0.64
35:RA:2751:G:N7	41:RH:2:SER:OG	2.28	0.64
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.69	0.64
55:RZ:99:TYR:HB3	55:RZ:123:ASP:HB2	1.79	0.64
15:XO:7:GLU:OE2	15:XO:38:ARG:NH2	2.27	0.64
35:YA:1113:U:H5'	41:YH:2:SER:HB3	1.79	0.64
35:RA:2651:C:H42	35:RA:2669:G:H1	1.42	0.64
41:RH:89:ILE:HG22	41:RH:162:ILE:HG12	1.78	0.64
54:YY:55:TYR:HE2	54:YY:61:ILE:HG21	1.61	0.64
39:RF:29:ASN:HD22	39:RF:32:LEU:HD23	1.63	0.64
2:XB:223:ILE:HG23	2:XB:229:VAL:HG22	1.78	0.64
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.30	0.64
19:QS:9:VAL:CG1	19:QS:39:THR:HB	2.28	0.64
37:YD:85:ASP:OD2	37:YD:88:ARG:NH1	2.31	0.64
35:YA:1693:U:O2	37:YD:14:ARG:NH1	2.30	0.63
19:QS:3:ARG:HH12	19:QS:11:VAL:HG11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.61	0.63
36:YB:9:G:OP1	48:YS:15:ARG:NH1	2.28	0.63
35:RA:2303:G:N3	40:RG:132:ASN:ND2	2.47	0.63
8:XH:18:ARG:NH2	8:XH:81:HIS:O	2.32	0.63
35:YA:1068:G:O2'	35:YA:1096:A:N3	2.31	0.63
45:YP:65:ARG:O	45:YP:68:GLN:NE2	2.32	0.63
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.63	0.63
3:QC:7:PRO:O	3:QC:11:ARG:NE	2.31	0.63
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.71	0.63
35:RA:67:U:H3	35:RA:74:A:H2	1.45	0.63
35:RA:321:G:O2'	35:RA:340:A:N3	2.32	0.63
37:YD:17:THR:HB	37:YD:205:VAL:H	1.63	0.63
52:RW:11:ARG:HH21	52:RW:98:LYS:HD2	1.64	0.63
1:QA:406:G:H5'	4:QD:5:ILE:HD11	1.80	0.63
35:RA:2701:C:H3'	35:RA:2702:U:H5"	1.79	0.63
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.32	0.63
44:RO:2:ILE:HG23	44:RO:6:THR:HG21	1.79	0.63
4:XD:18:LYS:NZ	4:XD:31:CYS:SG	2.71	0.63
30:Y5:19:ARG:NH2	35:YA:1264:G:OP1	2.28	0.63
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.81	0.62
1:QA:1086:U:H3	1:QA:1099:G:H22	1.47	0.62
3:QC:64:VAL:HG22	3:QC:99:VAL:HA	1.81	0.62
35:RA:1667:G:H8	35:RA:1667:G:OP2	1.82	0.62
35:YA:2130:U:HO2'	35:YA:2133:G:HO2'	1.47	0.62
45:RP:65:ARG:O	45:RP:68:GLN:NE2	2.28	0.62
35:YA:2392:A:H2	35:YA:2424:C:H42	1.47	0.62
42:RI:90:GLY:O	42:RI:121:LYS:NZ	2.32	0.62
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.32	0.62
1:XA:992:U:H3	1:XA:1044:A:H62	1.46	0.62
35:YA:67:U:H3	35:YA:74:A:H2	1.48	0.62
55:YZ:7:ALA:HB2	55:YZ:59:LEU:HB3	1.80	0.62
3:QC:76:VAL:HG21	3:QC:103:VAL:HG21	1.81	0.62
49:RT:51:ARG:HG2	49:RT:98:LYS:HD2	1.81	0.62
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.33	0.62
13:QM:2:ALA:HA	13:QM:11:ARG:HG2	1.82	0.62
29:R4:39:CYS:SG	29:R4:40:HIS:N	2.72	0.62
34:R9:36:GLN:NE2	35:RA:1124:C:O2	2.32	0.62
35:RA:1991:U:O5'	35:RA:1991:U:H6	1.82	0.62
35:YA:2292:C:OP1	48:YS:17:ARG:NH2	2.32	0.62
41:RH:107:VAL:O	41:RH:153:LYS:NZ	2.33	0.62
35:RA:1056:G:H21	35:RA:1103:A:H62	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:765:G:N2	1:XA:813:U:OP2	2.33	0.62
37:YD:27:THR:HG21	37:YD:81:ALA:HB1	1.80	0.62
1:QA:979:C:OP1	1:QA:1223:C:N4	2.33	0.62
46:RQ:27:VAL:HG21	46:RQ:134:ARG:HA	1.82	0.62
1:XA:406:G:H5'	4:XD:5:ILE:HD11	1.79	0.62
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.33	0.62
42:YI:40:THR:HG23	42:YI:43:ASN:H	1.65	0.62
2:QB:178:ARG:NH1	2:QB:196:LEU:O	2.33	0.61
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.33	0.61
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.82	0.61
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.32	0.61
42:RI:30:LEU:HB3	42:RI:36:ALA:HB3	1.83	0.61
37:YD:148:GLU:HB2	37:YD:151:LYS:HD2	1.82	0.61
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.33	0.61
35:YA:987:G:O2'	35:YA:1000:A:N3	2.33	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.32	0.61
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.65	0.61
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.83	0.61
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.34	0.61
29:Y4:68:ARG:HG2	29:Y4:69:LYS:HG2	1.82	0.61
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.65	0.61
50:YU:44:ASN:HD21	51:YV:75:PHE:HB3	1.65	0.61
37:RD:143:HIS:ND1	37:RD:194:GLY:O	2.32	0.61
51:YV:7:THR:HG23	51:YV:22:VAL:HG11	1.83	0.61
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.82	0.61
19:QS:10:PHE:HB2	19:QS:16:LEU:CD1	2.22	0.61
30:Y5:2:ALA:N	35:YA:2015:A:N3	2.48	0.61
35:YA:573:G:N1	35:YA:2031:A:OP2	2.24	0.61
35:YA:807:U:O2	39:YF:74:ARG:NH2	2.34	0.61
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.83	0.60
9:QI:10:ARG:NH1	9:QI:75:ASP:OD2	2.34	0.60
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.82	0.60
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.33	0.60
35:RA:1059:G:O6	35:RA:1079:C:N4	2.34	0.60
52:YW:18:ARG:HD2	52:YW:76:VAL:HG13	1.82	0.60
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.83	0.60
27:R2:47:ASN:ND2	35:RA:94:G:N3	2.48	0.60
33:R8:58:ILE:HG13	45:RP:49:ARG:HD2	1.83	0.60
9:XI:31:GLN:HE21	9:XI:35:GLU:HG2	1.66	0.60
35:YA:948:G:N2	35:YA:985:C:OP2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1130:U:O2	38:RE:149:ARG:NH2	2.34	0.60
35:RA:1800:C:OP2	37:RD:183:ARG:NH1	2.33	0.60
36:RB:52:A:O2'	36:RB:53:A:N7	2.34	0.60
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.83	0.60
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.66	0.60
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.35	0.60
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.33	0.60
35:YA:2575:C:H5'	38:YE:144:ARG:HG2	1.82	0.60
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.84	0.60
26:R1:51:VAL:HG21	26:R1:74:VAL:HG11	1.84	0.60
33:Y8:62:LEU:N	33:Y8:63:PRO:HD3	2.15	0.60
35:YA:571:A:O2'	51:YV:78:LYS:NZ	2.35	0.60
55:YZ:94:GLU:HG3	55:YZ:95:PRO:CD	2.26	0.60
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.48	0.60
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.20	0.60
38:RE:26:ILE:HG23	38:RE:182:LEU:HB3	1.81	0.60
32:R7:39:ARG:NH2	35:RA:468:G:N7	2.49	0.60
38:RE:117:MET:HA	38:RE:122:PHE:H	1.67	0.60
1:XA:1348:U:H3	1:XA:1374:A:H2	1.48	0.60
21:XU:8:THR:HG23	21:XU:11:GLY:H	1.66	0.60
33:Y8:4:MET:SD	33:Y8:61:LEU:CD1	2.89	0.60
6:QF:3:ARG:NH1	6:QF:38:GLU:OE2	2.34	0.60
35:YA:2727:G:O2'	44:YO:70:LYS:NZ	2.34	0.60
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.35	0.60
1:QA:842:C:O2'	1:QA:848:C:N4	2.34	0.60
35:RA:693:C:O2'	35:RA:1353:A:N3	2.31	0.60
37:RD:85:ASP:OD2	37:RD:88:ARG:NH1	2.32	0.60
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.35	0.60
35:RA:864:G:H1'	35:RA:914:C:H42	1.65	0.60
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.84	0.60
1:XA:1124:G:H1'	10:XJ:38:ILE:HD13	1.84	0.60
27:Y2:7:ARG:NH2	35:YA:102:G:OP1	2.35	0.60
1:XA:842:C:O2'	1:XA:848:C:N4	2.35	0.60
1:XA:970:C:N4	9:XI:128:ARG:OXT	2.35	0.60
35:YA:662:G:OP1	45:YP:15:ARG:NH1	2.35	0.60
35:YA:820:A:N3	35:YA:943:U:O2'	2.33	0.60
55:YZ:119:GLU:HG3	55:YZ:122:ARG:HB3	1.83	0.60
35:RA:309:G:N3	35:RA:329:G:O2'	2.34	0.59
38:RE:128:SER:OG	38:RE:129:HIS:N	2.35	0.59
55:RZ:69:THR:OG1	55:RZ:70:LEU:N	2.35	0.59
33:Y8:14:VAL:HG23	45:YP:61:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:46:ARG:NH1	35:YA:630:G:OP1	2.35	0.59
35:RA:2759:G:N2	41:RH:139:GLN:OE1	2.35	0.59
1:XA:375:U:H5"	16:XP:69:THR:HG21	1.83	0.59
6:XF:35:ALA:HB1	6:XF:65:VAL:HG11	1.84	0.59
35:YA:1689:A:H62	35:YA:1698:A:H2	1.50	0.59
52:YW:78:GLU:OE2	52:YW:99:ARG:NH1	2.34	0.59
1:QA:587:G:N2	1:QA:754:C:OP2	2.35	0.59
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.35	0.59
35:RA:910:A:H62	46:RQ:12:GLN:HA	1.68	0.59
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.36	0.59
28:R3:6:VAL:HG12	28:R3:56:VAL:HG12	1.85	0.59
35:RA:141:A:H8	35:RA:1595:G:H21	1.50	0.59
37:RD:31:LYS:NZ	37:RD:32:SER:OG	2.36	0.59
46:RQ:75:THR:HG21	46:RQ:85:LYS:HE3	1.84	0.59
27:Y2:29:LYS:HE3	27:Y2:57:ILE:HG21	1.84	0.59
33:Y8:13:ARG:HG3	45:YP:61:ARG:NH2	2.16	0.59
1:QA:439:A:OP2	1:QA:493:G:N1	2.34	0.59
1:QA:582:U:OP1	15:QO:68:ARG:NH2	2.33	0.59
1:QA:945:G:N2	1:QA:1334:G:O2'	2.36	0.59
1:QA:1002:G:H1	1:QA:1038:C:H42	1.49	0.59
27:R2:66:GLU:OE2	27:R2:70:GLN:NE2	2.35	0.59
36:RB:44:G:O2'	36:RB:47:C:N4	2.36	0.59
1:XA:587:G:N2	1:XA:754:C:OP2	2.35	0.59
35:YA:309:G:N3	35:YA:329:G:O2'	2.34	0.59
35:YA:662:G:H5"	45:YP:17:LYS:HG2	1.85	0.59
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.20	0.59
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.35	0.59
48:YS:106:ARG:NH1	48:YS:107:GLU:OE2	2.35	0.59
34:R9:22:ARG:HH12	35:RA:2741:A:H5"	1.66	0.59
35:RA:750:A:OP1	35:RA:1615:C:N4	2.35	0.59
46:RQ:12:GLN:HE21	46:RQ:72:LYS:HG3	1.68	0.59
49:RT:16:ARG:NH1	49:RT:80:SER:O	2.35	0.59
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.84	0.59
35:YA:2032:G:N2	38:YE:146:THR:OG1	2.33	0.59
35:YA:2680:C:H5'	38:YE:189:PRO:HA	1.85	0.59
49:YT:16:ARG:HH21	49:YT:19:LEU:HD21	1.66	0.59
24:QY:53:G:O2'	46:RQ:51:ARG:NH2	2.36	0.59
35:YA:184:C:O2'	35:YA:217:G:N3	2.34	0.59
35:YA:517:C:O2'	52:YW:18:ARG:NH2	2.36	0.59
35:YA:2343:C:HO2'	35:YA:2373:G:HO2'	1.48	0.59
1:QA:1259:C:H42	1:QA:1276:G:H1	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:414:C:O2	35:RA:1864:U:O2'	2.21	0.59
40:RG:4:ASP:OD1	40:RG:9:ARG:NH1	2.36	0.59
35:YA:729:G:OP2	37:YD:13:ARG:NH1	2.35	0.59
52:YW:88:ARG:HB2	52:YW:92:ARG:HB3	1.84	0.59
7:QG:152:ALA:O	7:QG:155:ARG:HD2	2.03	0.59
16:QP:15:PRO:HD2	16:QP:42:ARG:HD2	1.85	0.59
1:XA:1510:U:H3	1:XA:1525:G:H1	1.50	0.59
9:XI:25:LYS:N	9:XI:60:ASP:OD1	2.36	0.59
35:YA:2701:C:H3'	35:YA:2702:U:H5"	1.84	0.59
27:R2:51:ARG:HH21	27:R2:55:ARG:HH22	1.51	0.59
1:XA:405:U:O4	4:XD:2:GLY:N	2.36	0.59
35:YA:952:G:OP1	46:YQ:16:ARG:NH1	2.36	0.59
35:YA:1364:G:N2	35:YA:1367:A:OP2	2.29	0.59
1:QA:410:G:N2	1:QA:431:A:N7	2.51	0.58
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.75	0.58
28:R3:12:PRO:O	28:R3:20:LYS:NZ	2.35	0.58
35:RA:960:A:H61	46:RQ:82:ARG:HH21	1.50	0.58
35:RA:1309:G:HO2'	35:RA:1611:C:HO2'	1.46	0.58
44:RO:17:ARG:HE	44:RO:47:ILE:HD13	1.68	0.58
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.36	0.58
35:YA:336:C:HO2'	54:YY:35:TYR:HH	1.49	0.58
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.84	0.58
27:R2:47:ASN:O	27:R2:48:HIS:ND1	2.36	0.58
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.85	0.58
1:XA:1241:G:OP1	7:XG:35:LYS:NZ	2.36	0.58
33:Y8:14:VAL:HG23	45:YP:61:ARG:NH2	2.18	0.58
46:YQ:20:ALA:HB3	55:YZ:79:ARG:HE	1.68	0.58
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.84	0.58
27:R2:4:SER:OG	27:R2:5:GLU:N	2.34	0.58
1:XA:407:G:H5"	4:XD:115:ARG:HB3	1.83	0.58
38:RE:116:VAL:HG23	38:RE:120:TRP:HD1	1.68	0.58
1:XA:1503:A:O2'	23:XX:12:A:N6	2.36	0.58
35:YA:2304:G:H22	35:YA:2312:U:H3	1.51	0.58
35:YA:2787:C:H1'	38:YE:62:PRO:HG3	1.86	0.58
42:YI:12:LEU:HG	42:YI:19:VAL:HG11	1.85	0.58
9:QI:33:PHE:CE1	9:QI:37:PHE:HD2	2.21	0.58
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.36	0.58
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.37	0.58
39:YF:101:LEU:O	39:YF:106:ARG:NH1	2.36	0.58
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.36	0.58
13:XM:77:ASN:OD1	29:Y4:71:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:47:LEU:HB3	3:QC:52:LEU:HD23	1.85	0.58
46:RQ:81:VAL:O	46:RQ:82:ARG:NH1	2.36	0.58
35:YA:10:G:N2	35:YA:2802:G:OP1	2.35	0.58
2:XB:20:GLU:HG3	2:XB:191:ASP:OD1	2.04	0.58
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.85	0.58
35:YA:1454:U:O2'	35:YA:1455:G:N7	2.35	0.58
35:YA:2118:U:H3	35:YA:2147:G:HO2'	1.51	0.58
39:YF:11:VAL:HG22	39:YF:125:LEU:HB2	1.86	0.58
55:YZ:5:LEU:H	55:YZ:59:LEU:HA	1.67	0.58
43:RN:99:LEU:O	43:RN:103:VAL:HG23	2.03	0.58
35:YA:2111:C:N3	35:YA:2118:U:O2'	2.35	0.58
1:QA:189:U:O2	17:QQ:63:ARG:NH2	2.37	0.58
1:QA:593:G:H1	1:QA:646:U:H3	1.51	0.58
1:QA:811:C:O2'	1:QA:901:A:N1	2.37	0.58
31:R6:46:HIS:HD1	35:RA:2371:G:HO2'	1.41	0.58
35:RA:223:A:O2'	35:RA:420:C:O2	2.20	0.58
45:RP:135:LEU:HB3	45:RP:139:LYS:HE2	1.84	0.58
42:YI:68:LEU:HD13	42:YI:71:ILE:HD11	1.85	0.58
1:QA:437:U:H3	1:QA:495:A:H62	1.51	0.57
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.69	0.57
35:RA:486:C:O2'	52:RW:60:ASN:ND2	2.35	0.57
37:RD:17:THR:HB	37:RD:205:VAL:H	1.68	0.57
38:RE:141:ILE:O	38:RE:154:LYS:NZ	2.36	0.57
1:XA:1494:G:N7	57:XA:1670:PAR:N32	2.52	0.57
35:YA:1057:A:N6	35:YA:1087:G:OP2	2.37	0.57
1:QA:1004:A:H1'	1:QA:1036:G:H22	1.70	0.57
35:RA:807:U:OP2	45:RP:41:ARG:NH1	2.37	0.57
35:RA:1791:A:H5'	37:RD:206:LEU:HD12	1.86	0.57
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.37	0.57
35:YA:1266:G:O5'	52:YW:15:ARG:NH2	2.37	0.57
27:R2:66:GLU:OE1	27:R2:69:ARG:NH1	2.37	0.57
35:RA:605:C:O2	35:RA:657:U:O2'	2.21	0.57
35:RA:1140:C:OP2	43:RN:66:LYS:NZ	2.34	0.57
35:RA:1266:G:O5'	52:RW:15:ARG:NH2	2.36	0.57
37:RD:76:PRO:HB2	37:RD:116:GLN:HE21	1.69	0.57
39:RF:101:LEU:O	39:RF:106:ARG:NH1	2.37	0.57
39:RF:200:GLU:O	39:RF:204:ASN:ND2	2.37	0.57
6:XF:80:ARG:NH2	6:XF:88:VAL:O	2.37	0.57
27:Y2:23:LYS:NZ	27:Y2:27:GLU:OE2	2.35	0.57
1:QA:538:G:H5"	12:QL:114:LYS:HB2	1.86	0.57
26:R1:6:GLU:O	26:R1:91:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.21	0.57
1:XA:486:U:H2'	1:XA:487:A:H8	1.68	0.57
35:YA:138:G:N2	53:YX:44:GLU:OE1	2.32	0.57
35:YA:1859:A:N6	35:YA:1883:G:O2'	2.38	0.57
39:YF:31:HIS:NE2	39:YF:35:GLU:OE2	2.37	0.57
1:QA:1074:G:OP1	5:QE:64:ARG:NH2	2.37	0.57
35:RA:900:A:H3'	35:RA:901:A:H8	1.70	0.57
35:RA:2055:C:OP1	35:RA:2056:G:H5"	2.04	0.57
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.86	0.57
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.68	0.57
35:YA:2777:G:OP2	35:YA:2781:A:O2'	2.23	0.57
13:QM:80:ARG:O	13:QM:84:ILE:CG2	2.52	0.57
15:QO:29:VAL:HG21	15:QO:81:LEU:HD21	1.86	0.57
1:XA:532:A:H2	1:XA:1206:G:H21	1.52	0.57
35:YA:918:A:N3	36:YB:80:U:O2'	2.35	0.57
1:QA:1309:G:O2'	13:QM:77:ASN:ND2	2.37	0.57
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.86	0.57
33:R8:28:GLY:O	33:R8:36:LYS:NZ	2.38	0.57
55:RZ:53:ILE:HG22	55:RZ:71:VAL:HG13	1.87	0.57
3:XC:138:VAL:HG13	3:XC:149:ALA:HB3	1.87	0.57
22:XV:50:U:H3	22:XV:64:G:H1	1.53	0.57
3:QC:179:ARG:HD2	3:QC:206:GLU:HG2	1.86	0.57
38:RE:78:LEU:HG	38:RE:79:ARG:HG2	1.85	0.57
4:QD:72:GLU:OE2	4:QD:207:TYR:OH	2.23	0.57
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.85	0.57
24:QY:18:G:N2	24:QY:57:G:N7	2.51	0.57
35:YA:1853:A:N3	35:YA:2233:U:O2'	2.33	0.57
35:YA:2287:A:H62	35:YA:2344:U:H3	1.49	0.57
47:YR:96:ARG:HE	47:YR:117:VAL:HG12	1.70	0.57
35:RA:2396:G:H1	35:RA:2420:C:H42	1.53	0.57
35:YA:612:G:N2	35:YA:616:A:O2'	2.37	0.57
29:R4:56:VAL:HG12	29:R4:61:ARG:HG2	1.87	0.56
55:RZ:97:GLU:HB3	55:RZ:125:LEU:HD11	1.87	0.56
33:Y8:28:GLY:O	33:Y8:44:LYS:NZ	2.29	0.56
43:YN:12:ARG:NH1	43:YN:50:ASP:OD2	2.38	0.56
4:QD:98:GLU:OE2	4:QD:107:ARG:HG3	2.04	0.56
35:RA:2010:G:H5"	52:RW:42:ARG:HB2	1.86	0.56
10:XJ:3:LYS:N	10:XJ:74:ILE:O	2.38	0.56
24:XY:4:G:H1	24:XY:69:C:H42	1.52	0.56
48:YS:106:ARG:HA	48:YS:110:LEU:HD11	1.87	0.56
49:YT:20:PRO:HD2	49:YT:86:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:376:G:H5"	16:QP:5:ARG:HB2	1.86	0.56
2:QB:74:LYS:NZ	2:QB:206:ASP:OD1	2.36	0.56
11:QK:50:TYR:HD2	11:QK:54:ARG:HB3	1.70	0.56
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.38	0.56
43:RN:108:PRO:HG2	43:RN:113:GLY:HA2	1.87	0.56
20:XT:100:ILE:HG12	20:XT:102:GLY:H	1.68	0.56
24:XY:56:C:H5"	35:YA:896:A:H2'	1.87	0.56
38:YE:128:SER:OG	38:YE:129:HIS:N	2.38	0.56
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.38	0.56
35:RA:868:U:O2	46:RQ:8:LYS:NZ	2.38	0.56
26:R1:47:GLN:OE1	35:RA:2228:G:N2	2.39	0.56
55:RZ:126:VAL:HG11	55:RZ:161:VAL:HG13	1.87	0.56
1:XA:937:A:O2'	7:XG:76:ARG:NH2	2.38	0.56
38:YE:8:LYS:HA	38:YE:26:ILE:HG22	1.88	0.56
20:QT:100:ILE:HG22	20:QT:102:GLY:H	1.69	0.56
30:Y5:53:ALA:O	47:YR:96:ARG:NH1	2.34	0.56
39:YF:12:LEU:HB3	39:YF:126:VAL:HG12	1.87	0.56
42:YI:26:ALA:HA	42:YI:30:LEU:HB2	1.87	0.56
55:YZ:72:ARG:NH1	55:YZ:97:GLU:O	2.38	0.56
17:QQ:100:LYS:O	17:QQ:101:ARG:NH2	2.38	0.56
35:RA:1138:G:C2	43:RN:106:MET:HE3	2.41	0.56
57:XA:1670:PAR:N64	57:XA:1670:PAR:O44	2.39	0.56
35:YA:861:A:N3	36:YB:79:C:O2'	2.36	0.56
38:RE:2:LYS:HB2	38:RE:95:ILE:HD12	1.88	0.56
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.56
1:XA:971:G:N2	1:XA:1363:A:OP2	2.39	0.56
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.86	0.56
30:Y5:7:PRO:O	35:YA:2016:U:O2'	2.22	0.56
29:R4:18:CYS:SG	29:R4:19:GLY:N	2.78	0.56
35:RA:2832:U:H4'	35:RA:2833:G:H5"	1.88	0.56
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.88	0.56
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.37	0.56
9:XI:19:LEU:HB3	9:XI:59:PHE:HD2	1.71	0.56
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.38	0.56
1:QA:689:C:OP2	11:QK:55:LYS:NZ	2.39	0.56
1:QA:1422:G:H5"	44:RO:48:PRO:HB3	1.87	0.56
3:QC:159:GLY:CA	3:QC:193:TYR:CD2	2.83	0.56
31:R6:43:CYS:SG	31:R6:44:ARG:NH1	2.78	0.56
35:RA:1138:G:N2	43:RN:106:MET:HE3	2.21	0.56
39:RF:155:LEU:HB2	39:RF:189:THR:HG21	1.88	0.56
1:XA:1305:G:O2'	1:XA:1332:A:N6	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1754:C:H5	49:YT:96:ARG:HH21	1.52	0.56
35:YA:2127:G:H22	35:YA:2162:G:H1'	1.71	0.56
37:YD:134:ARG:HG3	37:YD:135:PHE:HD1	1.71	0.56
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.88	0.55
35:RA:1019:U:H3	35:RA:1142(A):A:H62	1.53	0.55
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.24	0.55
35:YA:1327:C:O2'	47:YR:105:ARG:NH2	2.37	0.55
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.24	0.55
1:QA:1338:G:N3	22:QV:41:C:O2'	2.39	0.55
43:RN:25:ARG:O	43:RN:29:LYS:NZ	2.39	0.55
49:RT:27:THR:HG22	49:RT:48:ILE:HG12	1.88	0.55
1:QA:757:U:O2'	1:QA:879:C:O2	2.24	0.55
9:QI:3:GLN:OE1	9:QI:20:ARG:NH2	2.38	0.55
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.38	0.55
26:R1:87:PRO:O	26:R1:91:LYS:N	2.37	0.55
35:RA:138:G:N2	53:RX:44:GLU:OE2	2.39	0.55
40:RG:63:ILE:HG13	40:RG:64:THR:HG23	1.88	0.55
14:XN:29:ARG:HD3	14:XN:40:CYS:HB2	1.89	0.55
18:XR:48:GLY:O	18:XR:74:ARG:NH2	2.39	0.55
41:YH:156:ALA:O	41:YH:158:HIS:N	2.39	0.55
42:YI:79:ILE:HB	42:YI:142:VAL:HA	1.88	0.55
3:QC:131:ARG:HE	5:QE:50:GLU:HG2	1.71	0.55
35:RA:910:A:N3	35:RA:2264:C:O2'	2.38	0.55
39:YF:155:LEU:HB2	39:YF:189:THR:HG21	1.87	0.55
16:QP:66:PRO:HG2	16:QP:71:ARG:HE	1.71	0.55
47:RR:53:HIS:HA	47:RR:56:LYS:HD3	1.89	0.55
1:XA:1086:U:H3	1:XA:1099:G:H22	1.54	0.55
1:QA:1129:C:OP1	9:QI:62:TYR:OH	2.24	0.55
1:QA:1422:G:O3'	44:RO:49:ARG:NH1	2.40	0.55
13:QM:80:ARG:HH12	19:QS:69:HIS:HE1	1.55	0.55
35:RA:942:G:O2'	35:RA:1189:A:N3	2.38	0.55
35:RA:1638:C:O2	35:RA:2698:U:O2'	2.23	0.55
35:RA:2096:U:H3	35:RA:2193:G:H1	1.55	0.55
35:RA:2406:U:OP1	35:RA:2411:A:N6	2.39	0.55
1:XA:105:G:OP2	20:XT:18:GLN:NE2	2.39	0.55
35:YA:574:C:N3	38:YE:145:LYS:NZ	2.54	0.55
35:YA:2033:A:O2'	35:YA:2035:G:OP2	2.22	0.55
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.71	0.55
50:YU:90:VAL:O	50:YU:92:ARG:N	2.34	0.55
49:RT:30:VAL:HG12	49:RT:86:ILE:HG12	1.89	0.55
1:XA:1498:U:OP2	23:XX:16:A:O2'	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.39	0.55
35:YA:776:G:N7	35:YA:793:A:O2'	2.40	0.55
49:YT:24:PRO:HA	49:YT:49:VAL:HG23	1.89	0.55
1:QA:376:G:H1	1:QA:387:U:H3	1.55	0.55
33:R8:48:PHE:HE2	35:RA:650:C:OP1	1.89	0.55
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.40	0.55
35:RA:307:G:H21	35:RA:330:A:H62	1.53	0.55
36:RB:48:A:OP2	48:RS:30:ARG:NH2	2.40	0.55
38:RE:6:GLY:HA3	38:RE:26:ILE:HD11	1.89	0.55
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.70	0.55
6:XF:81:ILE:HD11	37:YD:125:ILE:HB	1.89	0.55
7:XG:151:TYR:HE1	11:XK:54:ARG:HG2	1.71	0.55
8:XH:73:ASP:OD1	8:XH:75:ARG:NH1	2.40	0.55
37:YD:71:ASP:HB2	37:YD:103:ARG:HH12	1.71	0.55
43:YN:96:GLU:HB2	43:YN:122:VAL:HG12	1.89	0.55
1:QA:642:A:N3	8:QH:113:SER:OG	2.37	0.55
24:QY:30:G:H1	24:QY:40:C:H42	1.55	0.55
33:R8:7:HIS:HD2	45:RP:50:ARG:HH11	1.55	0.55
35:RA:768:G:O2'	35:RA:1379:A:N6	2.40	0.55
42:RI:73:GLU:HG3	42:RI:136:VAL:HG23	1.89	0.55
35:YA:27:G:N2	35:YA:512:G:O2'	2.40	0.55
1:QA:129(A):G:N2	1:QA:188:U:HO2'	2.05	0.54
1:QA:1372:U:OP1	9:QI:72:GLY:N	2.41	0.54
4:QD:98:GLU:HG2	4:QD:189:PRO:HG2	1.88	0.54
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.25	0.54
1:XA:1152:A:OP1	10:XJ:70:ARG:NH2	2.36	0.54
27:Y2:14:ARG:NH1	27:Y2:66:GLU:OE1	2.40	0.54
47:YR:38:VAL:HG22	47:YR:112:ALA:HB2	1.89	0.54
1:QA:356:A:N3	1:QA:368:U:O2'	2.34	0.54
1:QA:448:A:OP2	1:QA:485:G:N2	2.35	0.54
3:QC:159:GLY:HA3	3:QC:193:TYR:CE2	2.42	0.54
44:RO:23:ARG:NH2	44:RO:28:SER:O	2.40	0.54
1:XA:152:A:H62	1:XA:169:C:H42	1.54	0.54
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.40	0.54
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.79	0.54
40:YG:29:TRP:O	40:YG:33:ARG:NH1	2.40	0.54
45:YP:64:LYS:O	45:YP:66:GLY:N	2.39	0.54
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.40	0.54
35:RA:2119:A:N6	35:RA:2170:A:N7	2.53	0.54
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.35	0.54
35:YA:2683:C:O2	44:YO:70:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YB:5:C:O2'	36:YB:27:C:O2	2.25	0.54
49:YT:27:THR:HA	49:YT:48:ILE:HA	1.87	0.54
16:QP:13:HIS:O	16:QP:42:ARG:NH1	2.40	0.54
35:RA:1093:G:H21	35:RA:1098:A:H62	1.53	0.54
1:XA:1316:G:H4'	14:XN:18:VAL:HG11	1.90	0.54
13:XM:80:ARG:NH1	19:XS:65:ASN:O	2.40	0.54
18:XR:51:LEU:HD22	18:XR:55:ARG:HD2	1.90	0.54
52:YW:69:LEU:HD13	52:YW:107:LEU:HD13	1.89	0.54
1:QA:1321:C:H5"	1:QA:1322:C:H5"	1.89	0.54
10:QJ:33:GLN:HE21	10:QJ:75:ILE:HD13	1.72	0.54
13:QM:37:THR:O	13:QM:55:ARG:NH1	2.40	0.54
35:RA:83:G:N2	35:RA:103:A:OP2	2.41	0.54
35:RA:2692:C:O2	35:RA:2847:U:O2'	2.21	0.54
36:RB:9:G:OP1	48:RS:15:ARG:NH1	2.41	0.54
28:Y3:8:LEU:HB2	28:Y3:28:LEU:HD13	1.89	0.54
35:YA:1651:G:N7	47:YR:11:ASN:ND2	2.55	0.54
35:YA:1800:C:OP2	37:YD:183:ARG:NH1	2.38	0.54
1:QA:377:G:OP1	16:QP:3:LYS:NZ	2.38	0.54
24:QY:76:A:H2'	35:RA:2585:U:H5	1.72	0.54
20:XT:89:ARG:HD2	20:XT:104:LEU:HD11	1.90	0.54
55:YZ:74:VAL:HG22	55:YZ:86:VAL:HG23	1.87	0.54
25:R0:23:VAL:HG13	25:R0:38:VAL:HG22	1.89	0.54
35:RA:637:A:OP1	45:RP:133:SER:OG	2.22	0.54
35:RA:2857:G:N2	35:RA:2860:A:OP2	2.35	0.54
1:XA:508:C:OP1	4:XD:209:ARG:NH2	2.39	0.54
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.72	0.54
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.39	0.54
29:Y4:23:GLU:O	29:Y4:25:TYR:N	2.39	0.54
35:YA:1728:G:N1	35:YA:1730:U:OP2	2.41	0.54
35:YA:2010:G:H5"	52:YW:42:ARG:HB2	1.90	0.54
43:YN:22:THR:OG1	43:YN:23:LEU:N	2.41	0.54
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.90	0.54
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.41	0.54
26:R1:40:ARG:NH2	35:RA:2232:U:OP2	2.41	0.54
29:R4:42:PHE:O	29:R4:44:THR:N	2.41	0.54
35:RA:1815:A:OP2	37:RD:54:ARG:NH2	2.40	0.54
35:RA:2111:C:N3	35:RA:2118:U:O2'	2.40	0.54
37:YD:146:GLU:HB3	37:YD:189:CYS:HB3	1.90	0.54
41:YH:46:GLU:OE1	41:YH:51:ARG:NH1	2.41	0.54
1:QA:11:G:O2'	1:QA:506:G:N2	2.40	0.54
1:QA:573:A:N3	1:QA:883:C:O2'	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:QG:26:PHE:HD2	7:QG:43:PHE:CE2	2.26	0.54
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HD23	1.89	0.54
35:RA:372:G:N2	35:RA:401:A:OP2	2.33	0.54
49:RT:52:ILE:HG12	49:RT:61:PHE:HB3	1.90	0.54
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.41	0.54
35:YA:2065:C:O2	35:YA:2449:U:N3	2.34	0.54
38:YE:81:ILE:HG21	38:YE:84:PHE:HD2	1.73	0.54
45:YP:18:ARG:HH21	45:YP:32:THR:HG21	1.73	0.54
1:QA:444:C:H2'	1:QA:445:G:H8	1.73	0.54
1:QA:1166:G:N2	1:QA:1170:A:OP2	2.40	0.54
3:QC:88:ARG:HE	3:QC:101:LEU:HB2	1.72	0.54
29:R4:5:ILE:HB	40:RG:67:LYS:HD2	1.89	0.54
35:RA:1689:A:H62	35:RA:1698:A:H2	1.56	0.54
1:XA:439:A:OP2	1:XA:493:G:N1	2.37	0.54
2:XB:16:HIS:HD2	2:XB:210:SER:HA	1.72	0.54
3:XC:14:ILE:HG12	3:XC:15:THR:HG23	1.90	0.54
33:R8:34:TRP:O	33:R8:35:GLN:NE2	2.41	0.53
35:RA:1065:U:O2'	35:RA:1074:G:N2	2.41	0.53
35:RA:1342:A:OP1	53:RX:36:LYS:NZ	2.35	0.53
40:YG:38:VAL:HG22	40:YG:93:THR:HG23	1.89	0.53
5:QE:108:ALA:HA	5:QE:111:GLU:HG2	1.89	0.53
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.89	0.53
1:XA:103:C:OP2	20:XT:17:ARG:NH2	2.39	0.53
1:XA:339:C:OP1	44:YO:13:ASN:ND2	2.41	0.53
13:XM:65:LYS:HB3	29:Y4:50:VAL:HG11	1.90	0.53
1:QA:23:C:OP2	1:QA:561:U:N3	2.40	0.53
1:QA:414:A:OP2	1:QA:428:G:N2	2.41	0.53
2:QB:115:LEU:HD12	2:QB:145:LEU:HG	1.89	0.53
31:R6:7:ILE:HG13	31:R6:8:LYS:H	1.72	0.53
35:RA:1652:A:OP1	47:RR:8:ARG:NH1	2.36	0.53
35:RA:2207:C:O2	37:RD:151:LYS:NZ	2.35	0.53
35:RA:2777:G:OP2	35:RA:2781:A:O2'	2.25	0.53
20:XT:73:HIS:HB3	20:XT:74:LYS:HD3	1.90	0.53
35:YA:307:G:H21	35:YA:330:A:H62	1.57	0.53
35:YA:1065:U:O2'	35:YA:1074:G:N2	2.41	0.53
46:YQ:66:ILE:HA	46:YQ:104:PHE:HA	1.90	0.53
35:RA:1901:A:OP2	37:RD:255:LYS:NZ	2.34	0.53
2:XB:126:GLU:OE2	2:XB:130:ARG:NH1	2.41	0.53
8:XH:4:ASP:OD2	8:XH:85:ARG:NE	2.39	0.53
1:QA:582:U:OP2	1:QA:758:G:N1	2.33	0.53
1:QA:689:C:H3'	1:QA:690:G:H21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:50:GLU:HG3	5:QE:52:PRO:HD2	1.89	0.53
8:QH:110:ALA:HB3	8:QH:121:ASP:HB3	1.90	0.53
24:QY:76:A:H2	35:RA:2583:G:N2	1.96	0.53
1:XA:953:G:N7	13:XM:104:ARG:NH2	2.57	0.53
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.41	0.53
35:YA:2469:A:H2	35:YA:2481:G:H21	1.56	0.53
1:QA:544:G:OP2	4:QD:66:ARG:NH2	2.42	0.53
11:QK:33:THR:OG1	11:QK:34:ASP:N	2.41	0.53
35:RA:530:G:O2'	35:RA:532:A:N7	2.41	0.53
1:XA:953:G:H5'	1:XA:965:A:H61	1.73	0.53
10:XJ:26:ALA:O	10:XJ:84:GLN:NE2	2.41	0.53
37:YD:179:SER:O	37:YD:273:ARG:NH2	2.41	0.53
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.91	0.53
10:QJ:45:ARG:HB2	10:QJ:65:LEU:HB3	1.91	0.53
35:RA:918:A:N3	36:RB:80:U:O2'	2.41	0.53
35:YA:486:C:O2'	52:YW:60:ASN:ND2	2.41	0.53
1:QA:571:U:O4	1:QA:864:A:N6	2.42	0.53
24:QY:75:C:O5'	24:QY:75:C:H6	1.92	0.53
40:RG:16:ARG:HH21	40:RG:28:VAL:HG22	1.74	0.53
1:XA:564:C:OP2	12:XL:15:ARG:NH2	2.37	0.53
1:XA:618:C:H5'	1:XA:619:U:H5"	1.89	0.53
35:YA:806:C:O2	35:YA:2444:G:O2'	2.25	0.53
35:YA:1087:G:O4'	35:YA:1103:A:N6	2.42	0.53
1:QA:662:G:H1	1:QA:743:U:H3	1.56	0.53
2:QB:78:GLN:O	2:QB:94:ASN:ND2	2.36	0.53
35:RA:458:G:O2'	35:RA:469:G:O6	2.23	0.53
39:RF:134:GLY:H	39:RF:162:LEU:HD12	1.73	0.53
45:RP:59:LEU:HA	45:RP:61:ARG:HH21	1.73	0.53
1:XA:1316:G:N1	1:XA:1319:A:OP2	2.41	0.53
13:XM:3:ARG:O	13:XM:57:ARG:NH1	2.40	0.53
33:Y8:14:VAL:CG2	45:YP:61:ARG:NH2	2.72	0.53
35:YA:526:A:O2'	35:YA:2043:C:O2	2.23	0.53
37:YD:134:ARG:HG3	37:YD:135:PHE:CD1	2.44	0.53
45:YP:115:LEU:HA	45:YP:134:ALA:HB2	1.90	0.53
1:QA:1348:U:H4'	9:QI:120:ARG:HG3	1.92	0.53
11:QK:87:THR:HA	11:QK:91:ARG:HD2	1.91	0.53
55:RZ:57:ILE:HG23	55:RZ:69:THR:HG23	1.91	0.53
1:XA:573:A:N3	1:XA:883:C:O2'	2.41	0.53
2:XB:87:ARG:NH2	2:XB:220:ASP:OD1	2.38	0.53
48:YS:26:LEU:HB3	48:YS:87:PHE:HA	1.90	0.53
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:819:A:OP2	35:RA:1187:G:N2	2.29	0.52
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.90	0.52
40:RG:75:LYS:HE3	40:RG:77:ILE:HD11	1.91	0.52
53:RX:11:PRO:HA	53:RX:28:PHE:HA	1.91	0.52
40:YG:47:LYS:HD3	40:YG:81:LYS:HB2	1.91	0.52
1:QA:673:G:O3'	6:QF:87:ARG:NH2	2.43	0.52
3:QC:182:ILE:HG12	3:QC:203:PHE:HA	1.92	0.52
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.43	0.52
12:QL:33:ARG:HG2	12:QL:60:LEU:HD12	1.90	0.52
26:R1:92:LYS:HE2	26:R1:96:LYS:HD3	1.91	0.52
35:RA:2787:C:H1'	38:RE:62:PRO:HG3	1.90	0.52
39:RF:113:ALA:HB2	39:RF:183:VAL:HG23	1.92	0.52
1:XA:60:A:OP1	1:XA:111:G:N2	2.42	0.52
1:XA:62:U:O2'	1:XA:379:C:O2	2.25	0.52
13:XM:58:GLU:O	13:XM:62:ASN:ND2	2.42	0.52
35:YA:942:G:O2'	35:YA:1189:A:N3	2.38	0.52
37:RD:146:GLU:HB3	37:RD:189:CYS:HB3	1.90	0.52
1:XA:401:C:O2'	1:XA:621:A:N3	2.38	0.52
31:Y6:43:CYS:SG	31:Y6:44:ARG:N	2.82	0.52
35:YA:1769:G:O2'	35:YA:1958:C:OP1	2.21	0.52
35:YA:2547:U:O2	44:YO:23:ARG:NH1	2.41	0.52
52:YW:18:ARG:NH1	52:YW:76:VAL:O	2.42	0.52
1:QA:866:C:O2'	1:QA:919:A:OP1	2.27	0.52
35:RA:1394:U:H4'	35:RA:1603:A:H4'	1.92	0.52
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.43	0.52
1:XA:67:C:H2'	1:XA:68:G:C8	2.45	0.52
1:XA:1150:U:O4	1:XA:1151:A:N6	2.43	0.52
1:XA:1422:G:H5"	44:YO:48:PRO:HB3	1.92	0.52
2:XB:7:VAL:HG22	2:XB:11:LEU:HD21	1.91	0.52
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.43	0.52
24:XY:9:A:O2'	24:XY:10:G:N7	2.41	0.52
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.42	0.52
35:YA:1113:U:OP1	41:YH:2:SER:N	2.42	0.52
44:YO:68:GLU:OE2	44:YO:78:ARG:NH1	2.42	0.52
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.75	0.52
22:QV:1:C:O3'	46:RQ:87:LYS:NZ	2.42	0.52
35:RA:1999:C:O2	35:RA:2687:U:O2'	2.27	0.52
38:RE:34:VAL:HG21	38:RE:77:ILE:HD11	1.91	0.52
13:XM:14:ARG:NH2	13:XM:41:PRO:O	2.41	0.52
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.43	0.52
35:YA:2115:G:N2	35:YA:2165:G:O6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:176:ILE:HB	38:YE:181:LEU:HB2	1.92	0.52
49:YT:19:LEU:HD22	49:YT:86:ILE:HG22	1.92	0.52
50:YU:50:ARG:HG2	50:YU:53:ARG:HH22	1.74	0.52
52:YW:29:LEU:HD22	52:YW:69:LEU:HD11	1.91	0.52
1:QA:824:C:O2'	8:QH:1:MET:N	2.42	0.52
35:RA:906:G:O2'	46:RQ:67:ARG:NH2	2.39	0.52
35:RA:2308:G:H22	35:RA:2311:A:H2	1.58	0.52
35:RA:2635:C:H5"	38:RE:78:LEU:HA	1.92	0.52
1:XA:191:G:O2'	20:XT:101:GLY:O	2.27	0.52
7:XG:5:ARG:HE	7:XG:6:ARG:H	1.58	0.52
40:YG:59:GLU:OE1	40:YG:153:ARG:NH2	2.35	0.52
31:R6:36:LEU:HD13	31:R6:50:ARG:HE	1.75	0.52
35:RA:1138:G:O2'	43:RN:102:ALA:O	2.27	0.52
35:RA:2666:C:O2	41:RH:152:ARG:NH1	2.42	0.52
41:RH:3:ARG:NH1	41:RH:4:ILE:O	2.43	0.52
1:XA:745:C:OP1	1:XA:851:G:O2'	2.27	0.52
9:XI:17:VAL:HA	9:XI:63:ILE:HG22	1.91	0.52
35:YA:1252:G:N7	50:YU:36:ARG:NH1	2.57	0.52
48:YS:39:ILE:HD12	48:YS:85:VAL:HG11	1.91	0.52
1:QA:1446:A:O2'	49:RT:125:ARG:NH1	2.43	0.52
36:RB:44:G:H1'	36:RB:47:C:H42	1.74	0.52
42:RI:92:VAL:HG23	42:RI:120:ILE:HG23	1.91	0.52
46:RQ:67:ARG:NH1	46:RQ:105:GLU:OE2	2.42	0.52
1:XA:227:G:N2	16:XP:62:VAL:O	2.38	0.52
1:XA:262:A:H5"	20:XT:76:ALA:HB2	1.92	0.52
15:XO:24:SER:OG	15:XO:25:THR:N	2.42	0.52
19:XS:19:VAL:HG21	19:XS:44:MET:HB3	1.92	0.52
35:YA:1291:C:H5'	35:YA:1536:A:H5'	1.92	0.52
41:YH:153:LYS:HB3	41:YH:162:ILE:H	1.74	0.52
1:QA:1382:C:O2'	7:QG:79:ARG:NH1	2.43	0.52
13:QM:57:ARG:NH1	29:R4:34:GLU:O	2.43	0.52
54:RY:39:VAL:HG13	54:RY:42:VAL:HB	1.91	0.52
10:XJ:38:ILE:HD12	10:XJ:39:PRO:HD2	1.92	0.52
12:XL:24:VAL:HG13	12:XL:98:TYR:HE1	1.75	0.52
35:YA:259:G:H21	35:YA:621:A:H8	1.58	0.52
35:YA:1296:G:OP1	35:YA:2709:G:O2'	2.22	0.52
35:YA:1478:G:H2'	35:YA:1479:G:H8	1.74	0.52
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.42	0.52
44:YO:106:LEU:HB3	44:YO:111:PHE:HB2	1.92	0.52
1:QA:1159:U:O2'	1:QA:1160:G:N7	2.40	0.51
30:R5:36:CYS:SG	30:R5:37:LYS:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:180:G:N2	35:YA:215:G:O6	2.43	0.51
35:YA:598:G:H5'	45:YP:11:GLY:HA3	1.92	0.51
35:YA:2597:G:H5'	37:YD:243:GLY:HA3	1.92	0.51
7:QG:20:ASP:HB3	7:QG:23:VAL:HG23	1.92	0.51
16:QP:34:GLU:OE1	16:QP:55:ARG:NH2	2.37	0.51
29:R4:54:GLY:HA3	29:R4:71:ARG:HG2	1.93	0.51
41:RH:153:LYS:HB3	41:RH:162:ILE:H	1.75	0.51
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.39	0.51
55:RZ:137:ILE:HG21	55:RZ:155:LEU:HD23	1.92	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.58	0.51
1:XA:464:G:N2	1:XA:467:G:N7	2.59	0.51
35:YA:2295:C:OP1	48:YS:10:ARG:NH1	2.43	0.51
1:QA:676:A:H1'	11:QK:115:PRO:HB3	1.92	0.51
1:QA:986:A:N3	19:QS:52:TYR:OH	2.32	0.51
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.42	0.51
1:QA:1359:C:O2'	1:QA:1362:C:N4	2.42	0.51
7:XG:27:ILE:HA	7:XG:30:ILE:HD12	1.91	0.51
15:XO:4:THR:HG23	15:XO:7:GLU:H	1.75	0.51
35:YA:958:U:O2	36:YB:89(A):A:O2'	2.26	0.51
36:YB:8:U:O2'	48:YS:25:ARG:NH2	2.43	0.51
49:YT:62:THR:HG22	49:YT:75:ILE:HG12	1.93	0.51
3:QC:127:ARG:HH22	3:QC:192:THR:H	1.58	0.51
35:RA:523:C:O2	35:RA:553:U:O2'	2.29	0.51
1:XA:375:U:O2	16:XP:28:ARG:NH1	2.43	0.51
1:XA:1367:C:H5"	9:XI:114:TYR:HA	1.93	0.51
1:XA:1392:G:H21	1:XA:1502:A:H8	1.58	0.51
33:Y8:62:LEU:CD1	35:YA:242:G:H5"	2.41	0.51
48:YS:15:ARG:NE	48:YS:88:ASP:OD1	2.43	0.51
53:YX:57:LEU:HG	53:YX:78:LYS:HB2	1.91	0.51
1:QA:64:G:H4'	1:QA:65:U:H5'	1.93	0.51
1:QA:375:U:H5"	16:QP:69:THR:HG21	1.92	0.51
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.91	0.51
16:QP:18:ARG:HA	16:QP:38:TYR:HA	1.93	0.51
1:XA:405:U:OP2	4:XD:3:ARG:NH2	2.38	0.51
4:XD:105:VAL:HG13	4:XD:110:PHE:HB2	1.92	0.51
1:QA:130:A:N3	1:QA:263:A:O2'	2.41	0.51
1:QA:559:A:H4'	1:QA:560:U:H3'	1.91	0.51
1:QA:794:A:HO2'	1:QA:1521:G:HO2'	1.57	0.51
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.92	0.51
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.76	0.51
47:RR:70:LEU:HD12	47:RR:76:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:62:ASP:HA	3:XC:97:LYS:HD3	1.93	0.51
33:Y8:14:VAL:HG13	33:Y8:22:VAL:HG13	1.92	0.51
34:Y9:36:GLN:NE2	35:YA:1124:C:O2	2.43	0.51
41:YH:52:VAL:O	41:YH:65:HIS:NE2	2.36	0.51
42:YI:114:LEU:HD13	42:YI:130:TYR:HD1	1.76	0.51
1:QA:7:G:O2'	5:QE:120:THR:O	2.29	0.51
3:QC:14:ILE:HG12	3:QC:15:THR:HG23	1.93	0.51
37:RD:141:VAL:HG13	37:RD:162:SER:HB2	1.91	0.51
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.44	0.51
27:Y2:41:ILE:HG13	27:Y2:44:LEU:HD13	1.92	0.51
35:YA:701:G:O2'	35:YA:1631:A:N1	2.44	0.51
49:YT:54:ARG:HA	49:YT:59:THR:HG23	1.93	0.51
3:QC:184:TYR:CE1	3:QC:201:TYR:HE1	2.29	0.51
11:QK:21:ILE:HB	11:QK:84:VAL:HG12	1.91	0.51
13:QM:66:LEU:HD12	13:QM:68:GLY:H	1.74	0.51
28:R3:9:VAL:HG11	28:R3:55:ARG:HD3	1.93	0.51
28:R3:29:ARG:NH1	35:RA:1183:G:O3'	2.44	0.51
35:RA:259:G:H21	35:RA:621:A:H8	1.58	0.51
35:RA:336:C:O2'	54:RY:35:TYR:OH	2.27	0.51
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.44	0.51
35:RA:1962:C:O2'	35:RA:1964:G:OP2	2.29	0.51
41:RH:18:GLU:HB3	41:RH:25:LYS:HB3	1.93	0.51
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	1.92	0.51
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.92	0.51
35:YA:535:C:O3'	50:YU:53:ARG:NH1	2.44	0.51
35:YA:878:A:N6	35:YA:899:A:O2'	2.38	0.51
36:YB:48:A:OP2	48:YS:30:ARG:NH2	2.44	0.51
39:YF:59:TYR:HD2	39:YF:78:ILE:HG13	1.76	0.51
18:QR:58:LEU:HB3	18:QR:62:GLU:HG3	1.93	0.51
24:QY:55:U:H3	55:RZ:183:LEU:HB3	1.76	0.51
31:R6:6:ARG:HD2	31:R6:7:ILE:H	1.75	0.51
37:RD:108:PRO:HB3	37:RD:143:HIS:CE1	2.46	0.51
10:XJ:3:LYS:NZ	10:XJ:75:ILE:O	2.41	0.51
35:YA:220:G:O2'	35:YA:233:A:N3	2.41	0.51
35:YA:2287:A:N6	35:YA:2344:U:H3	2.08	0.51
38:YE:10:GLY:HA3	49:YT:8:LYS:HD3	1.92	0.51
52:YW:86:LEU:HD22	52:YW:96:ILE:HD11	1.92	0.51
1:QA:335:C:O2'	1:QA:1433:A:N3	2.38	0.51
13:QM:84:ILE:CD1	13:QM:86:CYS:HB2	2.39	0.51
35:RA:1681:G:HO2'	35:RA:1762:A:HO2'	1.54	0.51
39:RF:198:ALA:HA	39:RF:201:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:23:ARG:HA	41:RH:36:PRO:HA	1.91	0.51
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.76	0.51
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.93	0.51
38:YE:52:LEU:HB2	38:YE:75:VAL:HG22	1.93	0.51
1:QA:165:C:H2'	1:QA:166:G:H8	1.77	0.50
24:QY:58:A:N7	55:RZ:183:LEU:HB2	2.26	0.50
25:R0:32:ARG:H	25:R0:35:ASN:ND2	2.09	0.50
35:RA:2055:C:O2	35:RA:2572:A:N6	2.44	0.50
9:XI:10:ARG:NH1	9:XI:75:ASP:OD2	2.45	0.50
17:XQ:28:PRO:HA	17:XQ:35:VAL:HA	1.92	0.50
35:YA:793:A:N6	35:YA:2073:C:OP1	2.43	0.50
50:YU:29:SER:OG	50:YU:30:LYS:NZ	2.40	0.50
50:YU:52:ARG:HD2	50:YU:55:ARG:NH2	2.26	0.50
35:RA:579:G:O2'	35:RA:2019:A:OP1	2.27	0.50
1:XA:1002:G:H2'	1:XA:1003:G:H8	1.76	0.50
8:XH:13:ILE:HG23	8:XH:63:LEU:HD11	1.92	0.50
49:YT:39:ARG:HH22	49:YT:41:ARG:HD3	1.77	0.50
55:YZ:45:ASP:OD1	55:YZ:49:ARG:NE	2.43	0.50
14:QN:45:ARG:O	14:QN:49:HIS:ND1	2.30	0.50
19:QS:32:LYS:HA	19:QS:50:ALA:HB3	1.93	0.50
29:R4:6:HIS:CE1	40:RG:67:LYS:H	2.30	0.50
38:RE:92:THR:OG1	38:RE:93:VAL:N	2.44	0.50
47:RR:3:HIS:O	47:RR:5:LYS:N	2.45	0.50
50:RU:91:ASP:HA	50:RU:95:LEU:HD12	1.94	0.50
14:XN:4:LYS:HA	14:XN:7:ILE:HG12	1.94	0.50
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	1.93	0.50
35:YA:907:U:O2'	46:YQ:101:ARG:NH2	2.44	0.50
1:QA:651:C:N4	1:QA:753:A:OP2	2.44	0.50
38:RE:48:GLN:OE1	38:RE:64:LYS:NZ	2.44	0.50
49:RT:54:ARG:HA	49:RT:59:THR:CG2	2.33	0.50
26:Y1:5:CYS:SG	26:Y1:8:SER:OG	2.69	0.50
35:YA:363(A):A:H2'	35:YA:363(B):G:H8	1.76	0.50
35:YA:1203:G:O6	35:YA:1204:A:N6	2.44	0.50
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.29	0.50
51:YV:52:VAL:HG21	51:YV:55:ALA:HB3	1.93	0.50
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.77	0.50
12:QL:70:ILE:HG13	12:QL:100:ILE:HD12	1.92	0.50
35:RA:458:G:N2	35:RA:470:A:OP2	2.36	0.50
35:RA:2120:G:H2'	35:RA:2121:G:H8	1.76	0.50
51:RV:24:LYS:HA	51:RV:92:THR:HG23	1.92	0.50
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:84:GLU:HG3	2:XB:215:LEU:HB3	1.94	0.50
1:QA:264:U:O2'	17:QQ:64:PRO:O	2.26	0.50
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.44	0.50
31:R6:14:THR:HG1	31:R6:19:ARG:HE	1.56	0.50
35:RA:265:A:N6	35:RA:427:U:O2'	2.45	0.50
35:RA:1213:A:N3	35:RA:1238:G:O2'	2.41	0.50
35:RA:2730:C:O2'	38:RE:168:MET:O	2.23	0.50
44:RO:106:LEU:HB3	44:RO:111:PHE:HB2	1.93	0.50
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.45	0.50
2:XB:192:SER:OG	2:XB:193:ASP:N	2.45	0.50
37:YD:164:GLN:OE1	37:YD:176:ARG:NH2	2.37	0.50
39:YF:60:SER:OG	39:YF:61:GLY:N	2.43	0.50
1:QA:618:C:H5'	1:QA:619:U:H5"	1.94	0.50
2:QB:21:ARG:HB3	2:QB:39:ILE:HG13	1.93	0.50
19:QS:3:ARG:HH12	19:QS:11:VAL:CG1	2.25	0.50
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.93	0.50
35:RA:1990:C:H2'	35:RA:1991:U:C6	2.47	0.50
35:RA:2130:U:O2'	35:RA:2133:G:O2'	2.26	0.50
55:RZ:47:VAL:O	55:RZ:51:ALA:N	2.39	0.50
1:XA:1452:C:H4'	1:XA:1453:G:H5'	1.93	0.50
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.45	0.50
44:YO:120:GLU:OE1	49:YT:67:SER:OG	2.27	0.50
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.76	0.50
35:RA:224:G:O6	35:RA:419:C:O2'	2.27	0.50
35:RA:270(E):G:H1	35:RA:270(U):C:H42	1.59	0.50
52:RW:59:VAL:HG21	52:RW:66:GLU:HB2	1.94	0.50
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.37	0.50
35:YA:2646:C:OP2	35:YA:2732:G:O2'	2.25	0.50
39:YF:179:GLU:HA	39:YF:205:ARG:HH22	1.74	0.50
50:YU:40:PHE:HB3	51:YV:75:PHE:CD2	2.47	0.50
1:QA:1336:C:H1'	1:QA:1337:G:C2	2.47	0.50
19:QS:33:THR:OG1	19:QS:34:TRP:N	2.45	0.50
25:R0:39:ARG:HH21	35:RA:2355:C:H1'	1.77	0.50
35:RA:677:A:O2'	35:RA:2070:G:O2'	2.29	0.50
49:RT:49:VAL:HG12	49:RT:63:VAL:HG22	1.92	0.50
1:XA:352:C:O2'	1:XA:354:G:OP1	2.22	0.50
1:XA:1318:A:H4'	19:XS:11:VAL:HG11	1.94	0.50
29:Y4:33:VAL:HG21	40:YG:109:VAL:HG13	1.94	0.50
1:QA:429:U:OP2	4:QD:36:ARG:NH2	2.43	0.49
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.39	0.49
20:QT:71:THR:HG22	20:QT:72:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2064:C:O2'	35:RA:2251:G:N2	2.41	0.49
35:RA:2773:C:OP1	38:RE:166:THR:OG1	2.26	0.49
39:RF:135:LYS:HB3	39:RF:138:GLU:HG3	1.94	0.49
44:RO:2:ILE:HG23	44:RO:6:THR:CG2	2.42	0.49
1:QA:974:A:OP2	14:QN:29:ARG:NH2	2.35	0.49
2:QB:84:GLU:OE2	2:QB:235:SER:OG	2.30	0.49
25:R0:19:LYS:NZ	35:RA:2387:U:O2'	2.44	0.49
27:R2:32:LEU:O	27:R2:36:ARG:N	2.43	0.49
35:RA:2839:G:H5'	47:RR:46:GLY:HA2	1.94	0.49
1:XA:390:C:O3'	16:XP:28:ARG:NH2	2.41	0.49
3:XC:150:LYS:HG3	3:XC:167:TRP:HE1	1.77	0.49
3:XC:150:LYS:HB3	3:XC:201:TYR:HB2	1.94	0.49
33:Y8:62:LEU:HD13	35:YA:242:G:C5'	2.41	0.49
41:YH:56:SER:OG	41:YH:61:HIS:ND1	2.35	0.49
8:QH:96:GLY:H	8:QH:99:GLU:HG3	1.77	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
1:XA:1028(B):C:N4	1:XA:1032(B):G:O6	2.45	0.49
35:YA:1479:G:OP2	35:YA:1510:A:N6	2.38	0.49
35:YA:2502:G:H5"	35:YA:2503:A:H5"	1.93	0.49
1:QA:578:C:O2'	1:QA:728:A:N3	2.37	0.49
35:RA:1112:G:O3'	41:RH:2:SER:N	2.45	0.49
35:RA:1669:A:N3	35:RA:1669:A:H2'	2.27	0.49
51:RV:23:GLU:OE2	51:RV:89:GLN:NE2	2.45	0.49
31:Y6:47:THR:HG22	31:Y6:48:VAL:H	1.76	0.49
35:YA:1020:A:N6	35:YA:1141:U:O2'	2.45	0.49
44:YO:107:ARG:HG3	44:YO:115:VAL:HG11	1.94	0.49
2:QB:28:PHE:HD1	2:QB:194:PRO:HD3	1.78	0.49
25:R0:27:GLU:HG3	25:R0:68:GLU:HA	1.95	0.49
35:RA:327:G:N2	54:RY:70:SER:OG	2.46	0.49
38:RE:36:ARG:HH12	38:RE:86:PRO:HD2	1.77	0.49
44:RO:64:ARG:HB2	44:RO:83:ALA:HB3	1.94	0.49
50:RU:90:VAL:HG11	51:RV:40:LEU:HG	1.93	0.49
1:XA:110:C:O2'	16:XP:25:ARG:O	2.29	0.49
1:XA:676:A:H1'	11:XK:115:PRO:HB3	1.94	0.49
1:XA:1002:G:H1	1:XA:1038:C:H42	1.60	0.49
1:QA:1147:C:O2	9:QI:16:ARG:NH1	2.46	0.49
2:QB:70:PHE:O	2:QB:93:VAL:N	2.44	0.49
18:QR:34:TYR:CD1	18:QR:35:ARG:HG3	2.48	0.49
26:R1:11:ARG:HD3	26:R1:12:PRO:HD2	1.93	0.49
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.45	0.49
35:RA:1403:C:H5'	35:RA:1471:A:H1'	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1638:C:O3'	35:RA:2709:G:N2	2.46	0.49
35:RA:2115:G:N1	35:RA:2164:C:OP2	2.45	0.49
37:RD:12:SER:HB2	37:RD:208:LYS:HB3	1.93	0.49
45:RP:9:ASN:OD1	45:RP:9:ASN:N	2.44	0.49
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.92	0.49
8:XH:7:ALA:HB2	8:XH:85:ARG:HD3	1.95	0.49
31:Y6:25:LYS:HE2	31:Y6:27:LYS:NZ	2.28	0.49
35:YA:380:U:H2'	35:YA:381:G:H8	1.77	0.49
1:QA:1325:C:H4'	21:QU:17:THR:HG21	1.95	0.49
35:RA:2392:A:OP2	35:RA:2422:A:N6	2.46	0.49
48:RS:15:ARG:HD2	48:RS:25:ARG:HH11	1.78	0.49
1:XA:452:A:H62	1:XA:480:U:H3	1.59	0.49
9:XI:9:ARG:HG2	9:XI:14:VAL:HG22	1.94	0.49
31:Y6:25:LYS:HE2	31:Y6:27:LYS:HZ3	1.78	0.49
35:YA:833:U:O2	45:YP:55:ARG:NH1	2.46	0.49
18:QR:44:LEU:HD11	18:QR:79:LEU:HD23	1.95	0.49
35:RA:238:C:O2'	35:RA:608:A:N3	2.43	0.49
35:RA:807:U:O2'	35:RA:2060:A:N1	2.40	0.49
35:RA:1190:G:H2'	35:RA:1191:G:H8	1.77	0.49
1:XA:1128:C:N3	1:XA:1144:G:N2	2.60	0.49
35:YA:243:U:OP2	35:YA:254:G:N1	2.44	0.49
35:YA:900:A:H3'	35:YA:901:A:H8	1.77	0.49
35:YA:2656:U:H3	35:YA:2665:A:H2	1.61	0.49
26:R1:42:GLN:OE1	35:RA:379:G:N2	2.39	0.49
26:R1:45:ASN:HB2	35:RA:397:G:H5"	1.94	0.49
2:XB:184:VAL:HG13	2:XB:198:ASP:H	1.78	0.49
26:Y1:65:SER:HG	26:Y1:66:HIS:HD1	1.60	0.49
28:Y3:15:TYR:O	28:Y3:20:LYS:NZ	2.46	0.49
35:YA:1490:A:O2'	37:YD:99:ASP:OD1	2.31	0.49
49:YT:64:ARG:HG3	49:YT:73:GLU:HG2	1.94	0.49
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.56	0.49
13:QM:37:THR:OG1	13:QM:55:ARG:NH1	2.46	0.49
31:R6:27:LYS:HE2	35:RA:2284:C:H3'	1.94	0.49
35:RA:2470:G:OP1	46:RQ:56:ARG:NH2	2.46	0.49
49:RT:24:PRO:HD3	49:RT:52:ILE:HD12	1.94	0.49
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.46	0.49
55:RZ:5:LEU:HD22	55:RZ:43:GLU:HB3	1.95	0.49
4:XD:98:GLU:HG2	4:XD:189:PRO:HG2	1.95	0.49
35:YA:1530:G:O6	35:YA:1542:G:N2	2.45	0.49
51:YV:76:LYS:HG3	51:YV:81:TYR:HD1	1.75	0.49
55:YZ:61:LEU:HB3	55:YZ:65:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2865:U:OP2	49:RT:119:LYS:NZ	2.39	0.48
42:RI:64:GLU:HG3	42:RI:67:ARG:HH21	1.78	0.48
1:XA:642:A:N3	8:XH:113:SER:OG	2.38	0.48
2:XB:164:VAL:HG12	2:XB:166:ASP:H	1.77	0.48
5:XE:75:THR:OG1	5:XE:76:ILE:N	2.46	0.48
24:XY:75:C:H2'	24:XY:76:A:C8	2.48	0.48
35:YA:868:U:O2	46:YQ:8:LYS:NZ	2.45	0.48
35:YA:996:A:H4'	50:YU:92:ARG:HE	1.77	0.48
1:QA:545:C:OP2	4:QD:65:ARG:NH2	2.41	0.48
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.46	0.48
35:RA:984:A:H5"	35:RA:985:C:H5	1.77	0.48
35:RA:2295:C:H5	48:RS:13:ARG:HH12	1.59	0.48
46:RQ:24:GLY:H	46:RQ:101:ARG:HD2	1.79	0.48
35:YA:807:U:OP2	45:YP:41:ARG:NH1	2.46	0.48
35:YA:1342:A:O2'	35:YA:1344:G:OP2	2.27	0.48
35:YA:2125:G:N1	35:YA:2172:U:OP1	2.43	0.48
51:YV:60:GLU:OE1	51:YV:97:LYS:NZ	2.38	0.48
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.72	0.48
6:QF:36:ARG:NH1	6:QF:66:GLU:OE1	2.46	0.48
7:QG:105:VAL:O	7:QG:109:ASN:ND2	2.46	0.48
35:RA:335:C:H4'	54:RY:73:ARG:HE	1.78	0.48
50:RU:92:ARG:HE	50:RU:94:ASN:HB3	1.77	0.48
35:YA:300:A:OP2	54:YY:84:ARG:NH1	2.47	0.48
35:YA:335:C:H4'	54:YY:73:ARG:HE	1.76	0.48
35:YA:1246:A:OP1	45:YP:15:ARG:NH2	2.37	0.48
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.46	0.48
1:QA:662:G:O2'	1:QA:836:G:OP1	2.32	0.48
1:QA:1392:G:H21	1:QA:1502:A:H8	1.60	0.48
2:QB:178:ARG:NH2	8:QH:71:GLY:O	2.46	0.48
13:QM:82:MET:CE	13:QM:92:HIS:HB3	2.42	0.48
35:RA:1666:G:O2'	44:RO:6:THR:OG1	2.28	0.48
37:RD:25:THR:O	37:RD:27:THR:N	2.46	0.48
43:RN:22:THR:OG1	43:RN:23:LEU:N	2.45	0.48
55:RZ:5:LEU:H	55:RZ:59:LEU:HA	1.79	0.48
25:Y0:18:ALA:O	25:Y0:20:ARG:NH1	2.46	0.48
35:YA:1338:G:N7	53:YX:62:LYS:NZ	2.54	0.48
40:YG:12:TYR:HA	40:YG:16:ARG:HD3	1.94	0.48
1:QA:129(A):G:N2	1:QA:188:U:O2'	2.46	0.48
1:QA:1213:A:N6	1:QA:1215:G:N3	2.61	0.48
35:RA:363:G:H2'	35:RA:363(A):A:H8	1.78	0.48
35:RA:476:G:N1	35:RA:479:A:OP2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1651:G:H4'	47:RR:39:PRO:HG2	1.96	0.48
37:RD:31:LYS:HB3	37:RD:35:LYS:HG2	1.94	0.48
1:XA:413:G:O2'	1:XA:428:G:N2	2.46	0.48
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.95	0.48
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.95	0.48
22:XV:63:G:H4'	25:Y0:11:ARG:HH22	1.79	0.48
37:YD:108:PRO:HB3	37:YD:143:HIS:CE1	2.49	0.48
1:QA:297:G:N2	1:QA:300:A:OP2	2.45	0.48
1:QA:976:G:P	14:QN:32:SER:H	2.36	0.48
4:QD:59:ARG:HA	4:QD:59:ARG:HE	1.78	0.48
35:RA:281:G:H21	35:RA:359:A:H62	1.61	0.48
35:RA:1568:G:OP2	37:RD:63:ARG:NH2	2.42	0.48
37:RD:231:HIS:CD2	37:RD:249:PRO:HG3	2.48	0.48
55:RZ:48:PHE:HA	55:RZ:51:ALA:HB3	1.95	0.48
9:XI:26:VAL:HG22	9:XI:61:ALA:HB3	1.96	0.48
1:QA:532:A:H2	1:QA:1206:G:H21	1.61	0.48
28:R3:8:LEU:HA	28:R3:54:VAL:HG12	1.96	0.48
35:RA:1296:G:OP1	35:RA:2709:G:O2'	2.22	0.48
52:RW:29:LEU:HD22	52:RW:69:LEU:HD11	1.95	0.48
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.96	0.48
19:XS:68:GLY:HA2	29:Y4:68:ARG:HB2	1.95	0.48
35:YA:2470:G:H5'	46:YQ:56:ARG:HH21	1.79	0.48
55:YZ:130:PRO:HA	55:YZ:133:ILE:HD11	1.95	0.48
1:QA:1080:A:H5"	5:QE:16:THR:HG21	1.94	0.48
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.94	0.48
35:RA:1479:G:OP2	35:RA:1510:A:N6	2.39	0.48
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.95	0.48
48:RS:26:LEU:HB3	48:RS:87:PHE:HA	1.95	0.48
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.96	0.48
27:Y2:41:ILE:HD11	27:Y2:44:LEU:HD22	1.95	0.48
35:YA:1780:A:O2'	35:YA:1781:C:O2	2.27	0.48
35:YA:1858:G:H2'	35:YA:1883:G:H22	1.78	0.48
41:YH:41:MET:HE1	41:YH:64:LEU:HB3	1.95	0.48
35:RA:2415:G:H4'	45:RP:67:MET:H	1.79	0.48
47:RR:42:LYS:HG2	47:RR:45:ARG:HH12	1.79	0.48
25:Y0:23:VAL:HG22	25:Y0:38:VAL:HG22	1.96	0.48
37:YD:35:LYS:NZ	37:YD:102:LYS:O	2.47	0.48
37:YD:95:LEU:HD22	37:YD:117:VAL:HG21	1.96	0.48
1:QA:970:C:N4	9:QI:128:ARG:OXT	2.46	0.48
27:R2:31:GLU:O	27:R2:35:LEU:N	2.45	0.48
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RO:19:ILE:HG22	44:RO:43:VAL:HA	1.94	0.48
49:RT:73:GLU:OE2	49:RT:103:ARG:NE	2.41	0.48
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.78	0.48
29:Y4:55:ARG:HG3	29:Y4:56:VAL:HG23	1.95	0.48
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.96	0.48
35:YA:414:C:H2'	35:YA:415:A:C8	2.48	0.48
35:YA:1638:C:O2	35:YA:2698:U:O2'	2.31	0.48
35:YA:1682:G:OP1	35:YA:1699:G:N1	2.45	0.48
35:YA:2258:C:O2'	35:YA:2427:C:OP2	2.32	0.48
35:YA:2446:G:N2	35:YA:2449:U:O2	2.38	0.48
38:YE:25:VAL:HG12	38:YE:183:LEU:HG	1.96	0.48
41:YH:103:LEU:HD13	41:YH:131:VAL:HG21	1.96	0.48
1:QA:924:C:O2'	1:QA:1502:A:N6	2.47	0.47
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.96	0.47
33:R8:30:ARG:HH21	45:RP:62:LEU:HD13	1.79	0.47
42:RI:128:LEU:O	42:RI:138:ILE:N	2.40	0.47
1:XA:79:G:H2'	1:XA:80:G:H8	1.78	0.47
31:Y6:24:GLU:HG3	31:Y6:25:LYS:H	1.79	0.47
35:YA:1568:G:H5"	37:YD:61:LEU:HG	1.97	0.47
51:YV:76:LYS:HG3	51:YV:81:TYR:CE1	2.48	0.47
54:YY:14:LEU:HB2	54:YY:75:ILE:HD11	1.96	0.47
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.47	0.47
1:QA:980:C:O2'	14:QN:9:LYS:NZ	2.46	0.47
35:RA:995:C:O2	43:RN:3:THR:OG1	2.32	0.47
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.39	0.47
35:RA:2012:G:OP1	52:RW:11:ARG:NH2	2.47	0.47
1:XA:826:C:H5'	8:XH:12:ARG:HH21	1.79	0.47
1:XA:1065:U:O2	1:XA:1067:A:N6	2.43	0.47
16:XP:14:ASN:HA	16:XP:42:ARG:HH11	1.79	0.47
20:XT:74:LYS:HD3	20:XT:74:LYS:H	1.80	0.47
35:YA:223:A:O2'	35:YA:420:C:O2	2.27	0.47
35:YA:807:U:O2'	35:YA:2060:A:N1	2.41	0.47
35:YA:2632:A:HO2'	35:YA:2811:G:HO2'	1.52	0.47
55:YZ:125:LEU:HG	55:YZ:164:ALA:HB3	1.95	0.47
1:QA:346:G:OP1	49:RT:41:ARG:NH2	2.40	0.47
24:QY:4:G:H1	24:QY:69:C:H42	1.62	0.47
35:RA:2393:A:H5'	45:RP:62:LEU:HB3	1.96	0.47
35:RA:2495:G:H5"	46:RQ:81:VAL:HG12	1.96	0.47
35:RA:2734:A:H62	35:RA:2770:G:H21	1.61	0.47
35:RA:2791:C:OP1	35:RA:2893:G:N2	2.47	0.47
42:RI:1:MET:N	42:RI:21:VAL:O	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:689:C:H3'	1:XA:690:G:H21	1.79	0.47
1:XA:1321:C:H5"	1:XA:1322:C:H5"	1.97	0.47
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.38	0.47
2:XB:109:SER:O	2:XB:113:HIS:ND1	2.46	0.47
24:XY:55:U:O2'	24:XY:57:G:OP2	2.24	0.47
34:Y9:25:VAL:HB	34:Y9:34:GLN:HB2	1.96	0.47
1:QA:191:G:O2'	20:QT:101:GLY:O	2.32	0.47
1:QA:559:A:OP1	5:QE:126:ARG:NH2	2.48	0.47
1:QA:718:G:H5'	11:QK:117:ASN:HB2	1.96	0.47
1:QA:890:G:O2'	1:QA:906:G:O6	2.27	0.47
4:XD:59:ARG:HA	4:XD:59:ARG:HE	1.79	0.47
24:XY:58:A:O2'	24:XY:61:C:N4	2.46	0.47
25:Y0:32:ARG:H	25:Y0:35:ASN:ND2	2.12	0.47
35:YA:1250:G:OP2	45:YP:21:ARG:NH1	2.47	0.47
35:YA:2402:C:H1'	35:YA:2403:C:H5	1.79	0.47
38:YE:75:VAL:HG23	38:YE:76:ARG:HG2	1.96	0.47
45:YP:90:ARG:NH2	45:YP:105:LEU:HD11	2.29	0.47
1:QA:153:C:N3	1:QA:169:C:N4	2.63	0.47
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.32	0.47
13:QM:84:ILE:O	13:QM:84:ILE:HG13	2.15	0.47
33:R8:16:ILE:HD12	33:R8:57:ARG:HG2	1.95	0.47
35:RA:994:C:OP2	50:RU:54:LYS:NZ	2.34	0.47
41:RH:24:VAL:N	41:RH:35:VAL:O	2.44	0.47
45:RP:4:SER:O	45:RP:7:ARG:NH1	2.48	0.47
47:RR:103:ARG:NH1	47:RR:108:GLY:O	2.47	0.47
35:YA:603:A:H5"	35:YA:655:A:H61	1.78	0.47
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.42	0.47
35:YA:2543:G:H2'	35:YA:2544:G:C8	2.49	0.47
55:YZ:97:GLU:HG2	55:YZ:125:LEU:HD11	1.96	0.47
1:QA:1294:G:H2'	1:QA:1295:G:C8	2.50	0.47
1:QA:1321:C:OP1	13:QM:88:ARG:NH2	2.48	0.47
5:QE:145:LYS:NZ	5:QE:149:GLU:OE2	2.43	0.47
35:RA:2068:U:H3	35:RA:2430:A:H2	1.62	0.47
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.97	0.47
1:XA:1281:U:H5"	1:XA:1282:C:H5	1.79	0.47
7:XG:20:ASP:HB3	7:XG:23:VAL:HG12	1.95	0.47
26:Y1:78:LYS:HG2	35:YA:270(R):G:H21	1.80	0.47
33:Y8:4:MET:CE	33:Y8:61:LEU:HD12	2.35	0.47
37:YD:43:ARG:HB2	37:YD:54:ARG:HB2	1.95	0.47
39:YF:134:GLY:H	39:YF:162:LEU:HD22	1.80	0.47
50:YU:91:ASP:O	50:YU:93:LYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YX:61:GLY:N	53:YX:75:ASP:OD1	2.39	0.47
1:QA:1286:A:N6	1:QA:1354:C:O3'	2.47	0.47
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.48	0.47
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.97	0.47
12:QL:49:ASN:ND2	12:QL:92:ASP:OD2	2.39	0.47
24:QY:19:G:C6	35:RA:881:G:H4'	2.50	0.47
29:R4:38:LYS:HE3	40:RG:112:PRO:HG3	1.97	0.47
30:R5:3:LYS:HB3	30:R5:4:HIS:H	1.41	0.47
35:RA:859:G:O2'	35:RA:916:G:O6	2.23	0.47
35:RA:1860:G:H1	35:RA:1882:C:H42	1.63	0.47
35:RA:2635:C:H5'	38:RE:77:ILE:HG23	1.97	0.47
48:RS:10:ARG:NE	48:RS:91:PRO:O	2.40	0.47
48:RS:38:GLN:HE21	48:RS:47:THR:HG21	1.80	0.47
54:RY:99:CYS:SG	54:RY:100:ALA:N	2.87	0.47
1:XA:1316:G:N2	1:XA:1318:A:H3'	2.29	0.47
26:Y1:8:SER:HB3	26:Y1:66:HIS:CE1	2.50	0.47
26:Y1:80:LEU:HG	26:Y1:81:LYS:HG3	1.97	0.47
35:YA:1130:U:O2	38:YE:149:ARG:NH2	2.42	0.47
35:YA:1826:G:H4'	37:YD:242:ARG:HH21	1.79	0.47
39:YF:157:VAL:HB	39:YF:194:MET:HB3	1.97	0.47
46:YQ:50:ALA:HB1	46:YQ:121:ALA:HB1	1.96	0.47
1:QA:426:G:OP1	4:QD:38:TYR:OH	2.27	0.47
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.79	0.47
3:QC:184:TYR:HE1	3:QC:201:TYR:HE1	1.63	0.47
29:R4:43:TYR:O	29:R4:45:GLY:N	2.47	0.47
35:RA:1217:C:OP1	50:RU:15:LYS:NZ	2.43	0.47
35:RA:2043:C:OP1	35:RA:2777:G:O2'	2.29	0.47
35:RA:2056:G:N3	35:RA:2056:G:C2'	2.77	0.47
44:RO:71:ARG:NH2	44:RO:122:LEU:O	2.48	0.47
46:RQ:29:PHE:N	46:RQ:105:GLU:OE1	2.41	0.47
1:XA:938:A:N3	1:XA:1376:U:O2'	2.44	0.47
34:Y9:22:ARG:HH12	35:YA:2741:A:H5"	1.79	0.47
39:YF:9:ILE:HD11	39:YF:20:LEU:HD22	1.96	0.47
39:YF:63:LYS:NZ	39:YF:75:HIS:O	2.37	0.47
6:QF:97:PHE:HB2	18:QR:32:ARG:HH21	1.80	0.47
15:QO:24:SER:HB3	15:QO:27:VAL:HG23	1.97	0.47
29:R4:25:TYR:HE2	40:RG:3:LEU:HD12	1.80	0.47
32:R7:35:ARG:NH1	35:RA:54:G:O2'	2.46	0.47
35:RA:392:C:H5"	35:RA:409:C:H5"	1.96	0.47
35:RA:535:C:O3'	50:RU:53:ARG:NH1	2.46	0.47
35:RA:2133:G:H1'	35:RA:2158:A:H61	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RW:68:ARG:HH21	52:RW:112:GLY:HA3	1.79	0.47
1:XA:356:A:N3	1:XA:368:U:O2'	2.34	0.47
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.33	0.47
1:QA:941:G:OP1	7:QG:32:ARG:NH1	2.48	0.47
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.47	0.47
24:QY:56:C:H5"	35:RA:897:C:H5'	1.96	0.47
35:RA:1228:G:OP2	50:RU:16:LYS:NZ	2.41	0.47
36:RB:42:C:N4	40:RG:91:ARG:HH12	2.12	0.47
43:RN:133:GLN:HG2	43:RN:135:PRO:HD3	1.97	0.47
1:XA:1129:C:O2'	1:XA:1131:G:N7	2.48	0.47
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.97	0.47
35:YA:2126:A:N6	35:YA:2163:C:O2'	2.47	0.47
35:YA:2788:C:O2'	35:YA:2809:A:N3	2.40	0.47
44:YO:64:ARG:HH12	49:YT:70:VAL:HG21	1.80	0.47
45:YP:29:LYS:HD3	45:YP:30:THR:HG23	1.97	0.47
1:QA:1150:U:O4	1:QA:1151:A:N6	2.48	0.46
13:QM:13:LYS:HG3	13:QM:44:ARG:HD2	1.97	0.46
35:RA:30:G:O2'	35:RA:1214:A:N3	2.47	0.46
35:RA:674:G:H21	39:RF:74:ARG:HH12	1.62	0.46
35:RA:2377:A:H2'	35:RA:2378:A:C8	2.50	0.46
35:RA:2749:A:H5"	41:RH:4:ILE:HD11	1.97	0.46
37:RD:122:ASP:N	37:RD:122:ASP:OD1	2.42	0.46
1:XA:1463:C:OP1	49:YT:111:ARG:NH1	2.48	0.46
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.96	0.46
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.48	0.46
39:YF:133:ASN:H	39:YF:162:LEU:HD13	1.80	0.46
3:QC:184:TYR:CE1	3:QC:201:TYR:CE1	3.03	0.46
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.43	0.46
13:QM:80:ARG:HH12	19:QS:69:HIS:CE1	2.34	0.46
24:QY:54:U:O4	55:RZ:183:LEU:N	2.48	0.46
35:RA:987:G:O2'	35:RA:1000:A:N3	2.43	0.46
35:RA:2008:C:H2'	35:RA:2009:G:H8	1.80	0.46
35:RA:2055:C:OP1	35:RA:2056:G:H4'	2.15	0.46
35:RA:2597:G:H5'	37:RD:243:GLY:HA3	1.97	0.46
36:RB:5:C:OP1	36:RB:61:G:O2'	2.24	0.46
38:RE:52:LEU:O	38:RE:74:PRO:HA	2.15	0.46
55:RZ:115:GLY:H	55:RZ:177:PRO:HD3	1.80	0.46
4:XD:3:ARG:HD3	4:XD:118:ARG:NE	2.30	0.46
35:YA:1077:A:H5'	35:YA:1078:U:H5"	1.96	0.46
37:YD:122:ASP:OD1	37:YD:122:ASP:N	2.48	0.46
29:R4:53:GLU:OE2	29:R4:55:ARG:NE	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1649:G:O2'	47:RR:107:ASP:OD2	2.23	0.46
35:RA:1921:G:H2'	35:RA:1922:G:H8	1.80	0.46
35:RA:2219:G:OP1	37:RD:172:TYR:OH	2.27	0.46
36:RB:5:C:O2'	36:RB:27:C:O2	2.34	0.46
50:RU:102:GLU:OE2	51:RV:13:ARG:NH2	2.48	0.46
54:RY:46:LYS:HG2	54:RY:60:PHE:HD2	1.80	0.46
35:YA:195:A:H61	35:YA:198:C:H3'	1.81	0.46
35:YA:693:C:O2'	35:YA:1353:A:N3	2.43	0.46
35:YA:784:A:O4'	37:YD:227:ASN:ND2	2.48	0.46
35:YA:1858:G:O2'	35:YA:1884:A:N6	2.48	0.46
35:YA:2150:U:H2'	35:YA:2151:G:H8	1.81	0.46
1:QA:62:U:O2'	1:QA:379:C:O2	2.33	0.46
18:QR:58:LEU:HD23	18:QR:62:GLU:HG3	1.97	0.46
30:R5:19:ARG:NH1	35:RA:1264:G:OP1	2.33	0.46
35:RA:323:G:HO2'	35:RA:1205:U:H3	1.64	0.46
35:RA:746:A:HO2'	35:RA:2611:U:HO2'	1.63	0.46
44:RO:71:ARG:NH1	49:RT:74:ARG:HH12	2.14	0.46
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.46	0.46
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.97	0.46
2:XB:178:ARG:NH1	2:XB:196:LEU:O	2.49	0.46
35:YA:676:A:H8	35:YA:2069:G:H21	1.64	0.46
35:YA:2404:C:O3'	45:YP:77:ARG:NH2	2.48	0.46
2:QB:16:HIS:HD2	2:QB:210:SER:HA	1.81	0.46
16:QP:53:VAL:HG13	16:QP:79:VAL:HG22	1.97	0.46
32:R7:49:ARG:NH2	35:RA:128:C:O3'	2.48	0.46
35:RA:1048:A:H2	35:RA:1112:G:H21	1.63	0.46
48:RS:36:TYR:HD2	48:RS:52:SER:OG	1.99	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.49	0.46
26:Y1:87:PRO:HA	26:Y1:90:ILE:HB	1.98	0.46
35:YA:1153:C:H5'	50:YU:76:TYR:HE2	1.81	0.46
1:QA:150:C:H42	1:QA:171:A:H62	1.64	0.46
10:QJ:7:LYS:HB2	10:QJ:97:GLU:HB2	1.98	0.46
11:XK:19:ALA:HA	11:XK:32:ILE:HA	1.98	0.46
35:YA:630:G:N2	35:YA:633:A:OP2	2.38	0.46
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.48	0.46
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.30	0.46
37:YD:12:SER:HB2	37:YD:208:LYS:HB3	1.98	0.46
45:YP:106:LEU:HD13	45:YP:112:LEU:HD13	1.98	0.46
4:QD:8:VAL:HG11	4:QD:22:LYS:HD3	1.98	0.46
29:R4:43:TYR:O	29:R4:46:GLN:N	2.47	0.46
30:R5:4:HIS:HB3	30:R5:5:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RI:79:ILE:HB	42:RI:142:VAL:HG12	1.97	0.46
43:RN:96:GLU:HB2	43:RN:122:VAL:HG12	1.97	0.46
55:YZ:149:SER:OG	55:YZ:150:LEU:N	2.48	0.46
2:QB:60:ASP:O	2:QB:64:ARG:NH1	2.49	0.46
16:QP:14:ASN:HA	16:QP:42:ARG:HH11	1.80	0.46
37:RD:130:ALA:HB2	37:RD:192:THR:HG22	1.97	0.46
38:RE:47:VAL:HG11	38:RE:86:PRO:HD2	1.98	0.46
41:RH:125:VAL:HG22	41:RH:131:VAL:HG23	1.97	0.46
1:XA:1291:G:H4'	9:XI:39:GLY:HA3	1.96	0.46
3:XC:131:ARG:NH1	3:XC:166:GLU:OE1	2.48	0.46
49:YT:27:THR:HB	49:YT:48:ILE:HG13	1.96	0.46
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.51	0.46
2:QB:5:ILE:HG12	2:QB:221:LEU:HB2	1.98	0.46
17:QQ:28:PRO:HA	17:QQ:35:VAL:HA	1.98	0.46
35:RA:630:G:N2	35:RA:633:A:OP2	2.37	0.46
35:RA:1077:A:H5'	35:RA:1078:U:H5"	1.97	0.46
35:RA:2156:G:O6	35:RA:2157:G:N2	2.48	0.46
35:RA:2313:C:O4'	40:RG:40:ASN:ND2	2.49	0.46
35:RA:2795:G:H21	35:RA:2801:A:H62	1.64	0.46
1:XA:909:A:N3	1:XA:1413:A:O2'	2.42	0.46
4:XD:173:TRP:CD1	4:XD:174:LEU:HG	2.50	0.46
35:YA:685:A:OP1	35:YA:686:G:N2	2.49	0.46
35:YA:783:A:H8	35:YA:784:A:H4'	1.80	0.46
35:YA:1204:A:H1'	35:YA:1206:G:C5	2.51	0.46
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.43	0.46
37:YD:35:LYS:HG2	37:YD:104:TYR:CD2	2.51	0.46
37:YD:123:ALA:HB3	37:YD:131:LEU:HG	1.98	0.46
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.64	0.46
1:QA:859:A:OP2	1:QA:869:G:N2	2.41	0.46
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	1.98	0.46
11:QK:16:SER:OG	11:QK:106:LYS:NZ	2.46	0.46
13:QM:82:MET:CE	13:QM:92:HIS:CB	2.93	0.46
35:RA:587:C:OP2	45:RP:21:ARG:NH2	2.31	0.46
35:RA:2146:C:H4'	35:RA:2147:G:C8	2.51	0.46
35:RA:2851:A:O2'	47:RR:64:ARG:NH2	2.49	0.46
35:RA:2851:A:O3'	47:RR:64:ARG:NH2	2.49	0.46
37:RD:35:LYS:HD3	37:RD:104:TYR:CE1	2.50	0.46
1:XA:952:U:H2'	1:XA:953:G:H8	1.80	0.46
35:YA:2118:U:N3	35:YA:2147:G:O2'	2.45	0.46
35:YA:2659:G:N2	35:YA:2662:A:OP2	2.49	0.46
41:YH:103:LEU:HD22	41:YH:123:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:YU:92:ARG:HD3	50:YU:94:ASN:HB3	1.97	0.46
30:R5:56:LYS:HE2	30:R5:58:LEU:HD23	1.98	0.45
34:R9:30:PRO:HB3	35:RA:2527:C:H5"	1.97	0.45
35:RA:483:A:O2'	54:RY:49:VAL:O	2.27	0.45
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.31	0.45
43:RN:10:GLU:HA	43:RN:11:PRO:HD3	1.78	0.45
50:RU:66:ASN:HD21	50:RU:70:ARG:HH21	1.63	0.45
32:Y7:47:ARG:HH22	53:YX:60:ARG:CZ	2.28	0.45
36:YB:80:U:H2'	36:YB:81:G:H21	1.80	0.45
38:YE:16:ARG:HG2	38:YE:21:VAL:HG11	1.98	0.45
38:YE:52:LEU:O	38:YE:74:PRO:HA	2.16	0.45
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.98	0.45
1:QA:1127:G:H21	1:QA:1147:C:H41	1.63	0.45
35:RA:270:A:OP2	35:RA:270(Y):G:N1	2.39	0.45
35:RA:1652:A:N6	47:RR:11:ASN:OD1	2.42	0.45
35:RA:1859:A:N6	35:RA:1883:G:O2'	2.50	0.45
38:RE:8:LYS:O	38:RE:193:GLY:N	2.47	0.45
42:RI:3:VAL:HG12	42:RI:38:LEU:HD23	1.98	0.45
45:RP:7:ARG:HA	45:RP:8:PRO:HD2	1.87	0.45
53:RX:27:THR:HB	53:RX:80:ILE:HG12	1.97	0.45
1:XA:296:U:O2'	1:XA:556:C:O2	2.30	0.45
1:XA:1095:U:P	1:XA:1108:G:H1	2.39	0.45
8:XH:49:GLU:OE2	8:XH:62:TYR:OH	2.23	0.45
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.50	0.45
19:XS:27:GLU:HG3	19:XS:29:ARG:HG2	1.98	0.45
35:YA:141:A:H8	35:YA:1408:C:H1'	1.81	0.45
35:YA:626:U:O4	45:YP:107:LYS:HE2	2.17	0.45
35:YA:870:A:OP1	46:YQ:6:ARG:NH2	2.49	0.45
35:YA:1105:U:H2'	35:YA:1106:G:H8	1.79	0.45
35:YA:2308:G:H22	35:YA:2311:A:H2	1.64	0.45
2:QB:4:GLU:HG2	2:QB:5:ILE:H	1.81	0.45
5:QE:122:GLU:O	5:QE:126:ARG:NH1	2.49	0.45
1:XA:105:G:OP1	20:XT:22:ARG:NH2	2.50	0.45
35:YA:742:G:H2'	35:YA:743:G:H8	1.81	0.45
35:YA:2580:U:H4'	38:YE:130:GLY:HA3	1.98	0.45
35:YA:2781:A:H5"	35:YA:2782:G:H5'	1.99	0.45
39:YF:113:ALA:HB2	39:YF:183:VAL:HG23	1.98	0.45
41:YH:4:ILE:HG22	41:YH:6:ARG:HG2	1.97	0.45
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.47	0.45
35:RA:1155:A:H5"	50:RU:55:ARG:HH11	1.81	0.45
38:RE:117:MET:HA	38:RE:122:PHE:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y2:17:SER:HB3	27:Y2:20:GLU:OE1	2.17	0.45
38:YE:9:VAL:HB	38:YE:25:VAL:HG23	1.98	0.45
1:QA:950:U:H2'	1:QA:951:G:H8	1.82	0.45
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.99	0.45
51:RV:49:THR:HG23	51:RV:50:PRO:CD	2.46	0.45
55:RZ:76:LEU:HA	55:RZ:83:PRO:HA	1.97	0.45
35:YA:1210:A:H5'	35:YA:1210:A:H8	1.80	0.45
40:YG:73:ALA:HB2	40:YG:82:LEU:HD11	1.98	0.45
1:QA:545:C:O2'	1:QA:549:C:OP1	2.35	0.45
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.99	0.45
35:RA:1071:G:H22	35:RA:1091:G:H8	1.65	0.45
35:RA:2392:A:H2	35:RA:2424:C:H42	1.63	0.45
36:RB:45:A:O4'	40:RG:95:ARG:NH1	2.50	0.45
46:RQ:12:GLN:HG2	46:RQ:73:PRO:HD2	1.99	0.45
28:Y3:10:LYS:NZ	28:Y3:15:TYR:OH	2.37	0.45
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.49	0.45
37:YD:44:ASN:OD1	37:YD:44:ASN:N	2.46	0.45
42:YI:30:LEU:HB3	42:YI:36:ALA:HB3	1.97	0.45
46:YQ:39:PRO:HB3	46:YQ:99:PRO:HD3	1.99	0.45
55:YZ:47:VAL:O	55:YZ:51:ALA:N	2.42	0.45
12:QL:56:ALA:O	12:QL:68:ALA:N	2.44	0.45
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.50	0.45
35:RA:2850:A:OP2	35:RA:2866:U:N3	2.44	0.45
50:RU:36:ARG:HG2	50:RU:40:PHE:HE1	1.82	0.45
1:XA:1188:A:OP1	9:XI:114:TYR:OH	2.30	0.45
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.35	0.45
1:XA:1414:U:H3	1:XA:1486:G:H1	1.63	0.45
29:Y4:6:HIS:CE1	40:YG:66:GLN:HA	2.51	0.45
52:YW:73:ALA:HB3	52:YW:106:ILE:HB	1.98	0.45
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.82	0.45
1:QA:1250:A:N3	1:QA:1370:G:O2'	2.44	0.45
2:QB:146:GLN:HG3	2:QB:153:ARG:HH12	1.82	0.45
33:R8:5:LYS:HG2	35:RA:242:G:C8	2.52	0.45
35:RA:1190:G:H2'	35:RA:1191:G:C8	2.52	0.45
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.99	0.45
38:RE:59:VAL:HG11	38:RE:73:GLU:HB2	1.99	0.45
1:XA:23:C:OP2	1:XA:561:U:N3	2.44	0.45
2:XB:178:ARG:HH22	8:XH:74:PRO:HB3	1.80	0.45
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.97	0.45
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.82	0.45
27:Y2:18:PRO:HA	27:Y2:21:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:4:MET:HE1	33:Y8:61:LEU:CD1	2.44	0.45
35:YA:1187:G:N2	35:YA:1188:U:O4	2.49	0.45
35:YA:1434:A:H61	35:YA:1558:A:N6	2.15	0.45
46:YQ:77:LYS:NZ	46:YQ:80:GLU:OE2	2.38	0.45
47:YR:13:HIS:NE2	47:YR:15:SER:OG	2.46	0.45
49:YT:24:PRO:HD3	49:YT:52:ILE:HD12	1.98	0.45
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.52	0.45
26:R1:7:ILE:HD13	26:R1:91:LYS:HZ3	1.81	0.45
27:R2:65:ASN:ND2	35:RA:111:A:O3'	2.49	0.45
31:R6:6:ARG:HD2	31:R6:7:ILE:HG22	1.99	0.45
32:R7:8:ASN:HB3	32:R7:11:LYS:HB3	1.98	0.45
35:RA:627:A:H4'	35:RA:628:G:H5'	1.98	0.45
35:RA:1454:U:O2'	35:RA:1455:G:N7	2.41	0.45
35:RA:2831:G:OP1	38:RE:58:ARG:NH1	2.50	0.45
49:RT:24:PRO:HA	49:RT:49:VAL:HG23	1.98	0.45
1:XA:157:G:H1	1:XA:164:U:H3	1.64	0.45
1:XA:553:A:O2'	12:XL:29:GLY:O	2.32	0.45
1:XA:890:G:O2'	1:XA:906:G:O6	2.28	0.45
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.26	0.45
35:YA:1652:A:N6	47:YR:11:ASN:OD1	2.46	0.45
35:YA:2315:G:OP1	40:YG:36:LYS:NZ	2.43	0.45
42:YI:130:TYR:HB3	42:YI:136:VAL:HG13	1.99	0.45
1:QA:738:C:OP1	6:QF:4:TYR:OH	2.31	0.45
1:QA:954:G:H21	1:QA:1227:A:H62	1.65	0.45
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.46	0.45
4:QD:68:TYR:HE1	4:QD:103:ASN:HD21	1.57	0.45
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.50	0.45
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	1.99	0.45
13:QM:84:ILE:HD11	13:QM:86:CYS:CB	2.45	0.45
35:RA:2319:G:N1	35:RA:2334:G:OP2	2.45	0.45
49:RT:54:ARG:HG3	49:RT:59:THR:HG21	1.99	0.45
51:RV:49:THR:HG23	51:RV:50:PRO:HD3	1.99	0.45
1:XA:522:C:OP2	12:XL:69:TYR:OH	2.30	0.45
35:YA:2150:U:H2'	35:YA:2151:G:C8	2.52	0.45
50:YU:83:LEU:HD12	50:YU:113:ALA:HB2	1.99	0.45
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.34	0.44
25:R0:55:ARG:NH1	35:RA:2364:C:OP1	2.46	0.44
38:RE:32:PRO:HB3	38:RE:90:THR:HG22	1.98	0.44
39:RF:110:LEU:HD11	39:RF:181:LEU:HB3	1.98	0.44
51:RV:28:GLU:HB2	51:RV:31:ALA:HB2	1.99	0.44
24:XY:53:G:N1	55:YZ:183:LEU:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y5:2:ALA:HA	35:YA:2015:A:H1'	1.99	0.44
35:YA:299:A:N3	35:YA:319:C:O2'	2.43	0.44
35:YA:2880:C:O3'	47:YR:90:ARG:NH1	2.49	0.44
39:YF:158:THR:O	39:YF:164:ARG:NH2	2.38	0.44
2:QB:53:ARG:HH22	2:QB:199:TYR:HA	1.83	0.44
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.82	0.44
19:QS:10:PHE:CD1	19:QS:10:PHE:O	2.70	0.44
35:RA:2723:C:OP2	38:RE:109:LYS:NZ	2.50	0.44
20:XT:74:LYS:HB3	20:XT:75:ASN:H	1.68	0.44
29:Y4:37:SER:HB3	40:YG:112:PRO:HB3	2.00	0.44
1:QA:552:U:O2'	12:QL:86:ARG:O	2.35	0.44
1:QA:816:A:OP1	1:QA:1526:G:O2'	2.28	0.44
9:QI:19:LEU:HD22	9:QI:59:PHE:HD2	1.82	0.44
35:RA:2416:C:H5"	45:RP:64:LYS:HE2	1.99	0.44
43:RN:97:ARG:HA	43:RN:100:GLU:HB2	1.98	0.44
1:XA:247:G:OP2	17:XQ:99:SER:OG	2.36	0.44
1:XA:376:G:H5"	16:XP:5:ARG:HD2	1.99	0.44
18:XR:43:PHE:HE2	18:XR:58:LEU:HD11	1.83	0.44
31:Y6:7:ILE:HG13	31:Y6:8:LYS:H	1.81	0.44
31:Y6:14:THR:HG1	31:Y6:19:ARG:HE	1.63	0.44
35:YA:224:G:O6	35:YA:419:C:O2'	2.30	0.44
1:QA:362:G:N2	1:QA:365:U:OP2	2.49	0.44
35:RA:1863:G:O2'	35:RA:2411:A:O2'	2.27	0.44
44:RO:102:VAL:HG23	44:RO:121:VAL:HG23	1.98	0.44
45:RP:126:VAL:HG13	45:RP:145:PRO:HB2	1.98	0.44
51:RV:72:VAL:HG13	51:RV:85:LYS:HB2	2.00	0.44
9:XI:5:TYR:HE1	9:XI:16:ARG:HB3	1.83	0.44
35:YA:617:G:OP1	39:YF:40:GLN:NE2	2.50	0.44
44:YO:122:LEU:HD13	49:YT:72:VAL:HG11	1.99	0.44
55:YZ:76:LEU:HA	55:YZ:83:PRO:HA	2.00	0.44
1:QA:691:G:N7	11:QK:26:ASN:ND2	2.65	0.44
1:QA:950:U:H2'	1:QA:951:G:C8	2.53	0.44
1:QA:1298:C:C4	7:QG:114:ARG:HD2	2.52	0.44
3:QC:24:ALA:HB2	3:QC:32:LEU:HD12	1.99	0.44
6:QF:15:ASP:OD1	6:QF:15:ASP:N	2.48	0.44
24:QY:19:G:H3'	24:QY:20:G:H8	1.82	0.44
33:R8:26:LYS:NZ	35:RA:2361:A:OP2	2.46	0.44
35:RA:33:U:O4	35:RA:446:G:O2'	2.28	0.44
35:RA:2502:G:H5"	35:RA:2503:A:H5"	1.99	0.44
55:RZ:117:LEU:HD11	55:RZ:172:ALA:HB1	1.99	0.44
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:49:THR:HB	13:XM:52:GLU:HG3	1.99	0.44
29:Y4:48:ARG:HH21	29:Y4:51:ASP:HA	1.83	0.44
35:YA:860:U:OP2	35:YA:916:G:N1	2.41	0.44
35:YA:2249:U:N3	35:YA:2253:G:OP2	2.45	0.44
37:YD:231:HIS:CD2	37:YD:249:PRO:HG3	2.53	0.44
49:YT:74:ARG:HG2	49:YT:76:PHE:CE1	2.53	0.44
1:QA:6:G:H4'	1:QA:298:A:H4'	1.99	0.44
1:QA:253:U:OP1	17:QQ:67:LYS:NZ	2.37	0.44
19:QS:9:VAL:CG1	19:QS:39:THR:CB	2.94	0.44
35:RA:407:G:H2'	35:RA:408:G:H8	1.81	0.44
35:RA:1062:G:H2'	35:RA:1063:G:C8	2.52	0.44
35:RA:2880:C:O3'	47:RR:90:ARG:NH1	2.51	0.44
36:RB:111:U:H2'	36:RB:112:G:H8	1.82	0.44
37:RD:123:ALA:HB3	37:RD:131:LEU:HG	1.99	0.44
40:RG:71:THR:N	40:RG:89:GLY:O	2.48	0.44
3:XC:134:ILE:HG23	3:XC:151:VAL:HB	1.99	0.44
5:XE:11:ILE:HD12	5:XE:105:VAL:HG13	1.99	0.44
35:YA:2707:G:H5'	47:YR:68:ARG:HH21	1.83	0.44
55:YZ:94:GLU:CG	55:YZ:95:PRO:CD	2.66	0.44
1:QA:165:C:H2'	1:QA:166:G:C8	2.53	0.44
1:QA:673:G:H2'	1:QA:674:G:C8	2.52	0.44
12:QL:60:LEU:HD21	12:QL:64:TYR:HB2	2.00	0.44
13:QM:91:ARG:HB2	13:QM:98:VAL:HG12	1.99	0.44
35:RA:1568:G:P	37:RD:63:ARG:HH12	2.39	0.44
39:RF:102:PRO:HB2	39:RF:105:VAL:HG23	2.00	0.44
55:RZ:19:ARG:NH1	55:RZ:84:GLU:O	2.51	0.44
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.35	0.44
20:XT:11:SER:HA	20:XT:13:LEU:HD23	1.99	0.44
35:YA:793:A:OP2	35:YA:2071:A:O2'	2.35	0.44
37:YD:143:HIS:ND1	37:YD:194:GLY:O	2.49	0.44
37:YD:254:THR:OG1	37:YD:254:THR:O	2.35	0.44
1:QA:18:C:H5"	5:QE:127:ASN:HD21	1.83	0.44
1:QA:35:G:O2'	12:QL:118:SER:O	2.23	0.44
9:QI:55:ALA:HA	9:QI:58:HIS:HD2	1.83	0.44
14:QN:24:CYS:HB3	14:QN:28:GLY:H	1.83	0.44
24:QY:25:C:H2'	24:QY:26:G:H8	1.82	0.44
35:RA:1444(A):A:O2'	35:RA:1460:A:N3	2.45	0.44
39:RF:167:ALA:HA	39:RF:170:LEU:HD13	2.00	0.44
52:RW:69:LEU:HD13	52:RW:107:LEU:HD13	1.99	0.44
1:XA:632:A:OP1	8:XH:98:LYS:NZ	2.33	0.44
1:XA:1264:C:H2'	1:XA:1265:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:XP:59:TRP:HA	16:XP:62:VAL:HG22	2.00	0.44
42:YI:77:LEU:HD13	42:YI:101:LEU:HD13	2.00	0.44
44:YO:104:ARG:HG3	44:YO:121:VAL:HG12	2.00	0.44
1:QA:1203:C:H5"	14:QN:3:ARG:HH21	1.83	0.44
1:QA:1309:G:N7	13:QM:99:ARG:NH2	2.66	0.44
16:QP:22:THR:HA	16:QP:33:ILE:HG12	2.00	0.44
35:RA:1992:G:OP1	35:RA:1992:G:C8	2.71	0.44
40:RG:38:VAL:HG22	40:RG:93:THR:HG22	2.00	0.44
41:RH:8:PRO:HG2	41:RH:69:ARG:CZ	2.48	0.44
44:RO:71:ARG:NH2	44:RO:122:LEU:OXT	2.39	0.44
44:RO:77:ILE:HD12	49:RT:74:ARG:HD2	2.00	0.44
45:RP:64:LYS:O	45:RP:66:GLY:N	2.51	0.44
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.99	0.44
10:XJ:26:ALA:O	10:XJ:30:SER:OG	2.27	0.44
18:XR:74:ARG:HB3	18:XR:81:PHE:CE1	2.52	0.44
25:Y0:33:ALA:N	25:Y0:64:ASP:OD1	2.50	0.44
35:YA:219:G:N3	35:YA:234:C:O2'	2.50	0.44
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.51	0.44
45:YP:126:VAL:HG23	45:YP:145:PRO:HB2	1.99	0.44
46:YQ:8:LYS:HE3	46:YQ:9:TYR:HE1	1.83	0.44
2:QB:200:ILE:HG22	2:QB:202:PRO:HD3	2.00	0.43
9:QI:33:PHE:HE2	9:QI:47:LEU:HD11	1.83	0.43
33:R8:54:GLU:O	33:R8:58:ILE:HG12	2.18	0.43
35:RA:2151:G:H2'	35:RA:2152:G:H8	1.83	0.43
37:RD:67:PHE:HB3	37:RD:153:ALA:HB3	2.00	0.43
1:XA:1286:A:H2'	1:XA:1287:A:H4'	2.00	0.43
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.53	0.43
4:XD:163:GLU:HA	4:XD:166:LYS:HE3	2.00	0.43
13:XM:86:CYS:SG	13:XM:87:TYR:N	2.91	0.43
14:XN:24:CYS:HB3	14:XN:29:ARG:H	1.83	0.43
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.45	0.43
29:Y4:67:TYR:HB2	29:Y4:68:ARG:H	1.66	0.43
33:Y8:61:LEU:HD23	33:Y8:61:LEU:HA	1.87	0.43
35:YA:392:C:H5"	35:YA:409:C:H5"	1.99	0.43
35:YA:956:G:N2	35:YA:960:A:OP2	2.51	0.43
35:YA:1063:G:H22	35:YA:1076:C:H1'	1.83	0.43
35:YA:2119:A:N1	35:YA:2170:A:N6	2.65	0.43
35:YA:2343:C:O2'	35:YA:2373:G:O2'	2.25	0.43
35:YA:2845:G:H2'	35:YA:2846:G:C8	2.53	0.43
45:YP:90:ARG:HH22	45:YP:105:LEU:HD11	1.83	0.43
48:YS:29:PHE:HB3	48:YS:36:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:76:ASN:OD1	10:QJ:76:ASN:N	2.51	0.43
15:QO:87:ILE:HG22	15:QO:88:ARG:H	1.83	0.43
22:QV:63:G:H4'	25:R0:11:ARG:HH12	1.83	0.43
35:RA:1394:U:O2	53:RX:16:LYS:NZ	2.44	0.43
38:RE:54:GLN:HG3	38:RE:55:ASN:H	1.83	0.43
2:XB:95:GLN:HB3	2:XB:96:ARG:H	1.69	0.43
8:XH:19:VAL:HG13	8:XH:21:LYS:HG3	2.00	0.43
9:XI:3:GLN:OE1	9:XI:20:ARG:NE	2.39	0.43
33:Y8:61:LEU:HD13	35:YA:593:G:H4'	1.99	0.43
35:YA:1407:C:H42	35:YA:1595:G:H1	1.66	0.43
35:YA:2298:A:H62	35:YA:2318:G:H8	1.65	0.43
1:QA:258:G:OP1	20:QT:86:ARG:NH1	2.37	0.43
13:QM:49:THR:OG1	13:QM:50:GLU:N	2.51	0.43
35:RA:229:A:H4'	35:RA:230:U:H5'	2.00	0.43
35:RA:861:A:N3	36:RB:79:C:O2'	2.50	0.43
42:RI:69:LYS:HG3	42:RI:136:VAL:HB	1.99	0.43
44:RO:69:ILE:HD12	44:RO:69:ILE:N	2.32	0.43
19:XS:40:ILE:HD11	19:XS:62:ILE:HG12	2.00	0.43
20:XT:75:ASN:N	20:XT:75:ASN:OD1	2.49	0.43
55:YZ:137:ILE:HG23	55:YZ:156:LYS:HB3	1.99	0.43
1:QA:790:A:OP1	22:QV:38:A:O2'	2.30	0.43
1:QA:1223:C:P	19:QS:78:ARG:HH12	2.41	0.43
13:QM:84:ILE:O	19:QS:74:PHE:CE1	2.72	0.43
33:R8:59:LYS:HG2	45:RP:49:ARG:HE	1.84	0.43
35:RA:1041:C:H2'	35:RA:1042:G:H8	1.84	0.43
35:RA:2006:C:O2'	35:RA:2823:A:N3	2.50	0.43
27:Y2:70:GLN:HG3	27:Y2:71:ASN:H	1.83	0.43
33:Y8:29:LYS:HG2	33:Y8:30:ARG:H	1.83	0.43
35:YA:1005:C:O2	35:YA:1138:G:N2	2.41	0.43
35:YA:2630:G:H2'	35:YA:2631:G:C8	2.53	0.43
48:YS:27:SER:HA	48:YS:88:ASP:HB3	2.00	0.43
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.53	0.43
1:QA:1125:U:O4	10:QJ:5:ARG:NE	2.51	0.43
1:QA:1229:A:OP2	13:QM:114:ARG:NH1	2.50	0.43
19:QS:18:LYS:HD2	19:QS:29:ARG:HH22	1.84	0.43
35:RA:500:G:N1	35:RA:503:A:OP2	2.50	0.43
54:RY:99:CYS:SG	54:RY:101:LYS:N	2.91	0.43
29:Y4:67:TYR:HB2	29:Y4:68:ARG:HD3	2.00	0.43
35:YA:83:G:N2	35:YA:103:A:OP2	2.32	0.43
35:YA:764:A:N3	37:YD:213:ARG:NH1	2.66	0.43
35:YA:1290:C:O2'	35:YA:1536:A:OP2	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YG:43:LEU:HD12	40:YG:90:LEU:HD13	1.99	0.43
41:YH:149:ARG:CZ	41:YH:154:PRO:HG2	2.48	0.43
1:QA:1502:A:H2	1:QA:1505:G:H1	1.66	0.43
10:QJ:27:ALA:HA	10:QJ:30:SER:HB3	1.99	0.43
35:RA:1278:A:H4'	47:RR:34:ILE:HD11	2.00	0.43
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.52	0.43
32:Y7:47:ARG:HH12	53:YX:60:ARG:HH22	1.67	0.43
35:YA:1667:G:O2'	35:YA:1991:U:O4	2.33	0.43
37:YD:33:LEU:HD21	37:YD:102:LYS:HD2	2.00	0.43
41:YH:103:LEU:HD23	41:YH:115:VAL:HB	2.01	0.43
44:YO:8:LEU:HD13	44:YO:82:ASN:HB3	2.00	0.43
47:YR:3:HIS:O	47:YR:5:LYS:N	2.52	0.43
52:YW:6:ILE:HG12	52:YW:104:THR:HG23	1.99	0.43
1:QA:599:C:O2'	8:QH:129:VAL:O	2.27	0.43
2:QB:187:LEU:HA	2:QB:201:ILE:HB	2.01	0.43
4:QD:88:VAL:HG13	5:QE:97:GLY:HA3	1.99	0.43
5:QE:28:PHE:CD2	5:QE:51:VAL:HG13	2.54	0.43
10:QJ:51:ARG:NE	10:QJ:60:ARG:O	2.49	0.43
13:QM:37:THR:HG23	13:QM:39:ILE:HG12	2.00	0.43
35:RA:792:G:N3	35:RA:2072:G:O2'	2.42	0.43
35:RA:2122:U:H2'	35:RA:2123:G:H8	1.83	0.43
35:RA:2503:A:O2'	35:RA:2505:G:OP2	2.25	0.43
44:RO:71:ARG:HH22	44:RO:122:LEU:C	2.17	0.43
51:RV:40:LEU:HD23	51:RV:47:VAL:HA	2.00	0.43
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.66	0.43
1:XA:1437:C:H2'	1:XA:1438:G:H8	1.84	0.43
2:XB:51:LEU:HD23	2:XB:201:ILE:HD12	2.01	0.43
4:XD:111:ALA:HB1	4:XD:116:GLN:HB3	2.01	0.43
35:YA:960:A:H61	46:YQ:82:ARG:NH2	2.15	0.43
35:YA:2445:G:OP1	39:YF:74:ARG:NH1	2.45	0.43
35:YA:2729:G:H1'	38:YE:187:ALA:HB2	2.00	0.43
44:YO:19:ILE:HG22	44:YO:43:VAL:HA	2.00	0.43
47:YR:59:ASP:N	47:YR:59:ASP:OD1	2.51	0.43
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.54	0.43
37:RD:35:LYS:HB2	37:RD:63:ARG:HA	2.00	0.43
16:XP:18:ARG:NH1	16:XP:32:TYR:OH	2.52	0.43
31:Y6:6:ARG:HG3	31:Y6:7:ILE:H	1.84	0.43
35:YA:2572:A:OP1	35:YA:2574:G:O2'	2.36	0.43
35:YA:2619:C:H5"	38:YE:152:LYS:HD3	2.01	0.43
41:YH:6:ARG:HB2	41:YH:65:HIS:CG	2.54	0.43
1:QA:628:G:H2'	1:QA:629:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:QO:76:GLU:HA	15:QO:79:ARG:HH21	1.84	0.43
24:QY:6:U:H2'	24:QY:7:A:H8	1.83	0.43
24:QY:58:A:C6	55:RZ:183:LEU:HD13	2.54	0.43
35:RA:117:G:OP2	35:RA:119:A:O2'	2.28	0.43
1:XA:35:G:N2	12:XL:118:SER:OG	2.37	0.43
1:XA:1376:U:H2'	1:XA:1377:A:C8	2.53	0.43
8:XH:12:ARG:HD3	8:XH:26:VAL:HG22	1.99	0.43
22:XV:15:G:H21	22:XV:21:A:H1'	1.84	0.43
35:YA:1138:G:O2'	43:YN:102:ALA:O	2.34	0.43
35:YA:1656:C:P	38:YE:136:ARG:HE	2.41	0.43
37:YD:67:PHE:HB3	37:YD:153:ALA:HB3	2.00	0.43
37:YD:245:PRO:HA	37:YD:246:PRO:HD3	1.93	0.43
39:YF:156:LEU:HD21	39:YF:163:VAL:HG12	2.01	0.43
40:YG:135:LEU:HD13	40:YG:140:ILE:HD11	2.01	0.43
43:YN:47:ALA:HB2	43:YN:112:LEU:HD11	1.99	0.43
48:YS:110:LEU:HB2	48:YS:112:PHE:CE2	2.54	0.43
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	2.00	0.43
1:QA:1286:A:N3	21:QU:18:TYR:OH	2.52	0.43
3:QC:184:TYR:CD1	3:QC:201:TYR:CE1	3.06	0.43
12:QL:70:ILE:HG12	12:QL:77:LEU:HD12	2.01	0.43
19:QS:31:ILE:HB	19:QS:49:ILE:HD13	2.00	0.43
24:QY:6:U:H2'	24:QY:7:A:C8	2.53	0.43
24:QY:76:A:OP2	35:RA:2602:A:C6	2.72	0.43
33:R8:13:ARG:NH1	45:RP:61:ARG:O	2.51	0.43
33:R8:61:LEU:HD13	35:RA:593:G:H4'	2.01	0.43
35:RA:2564:A:OP1	35:RA:2648:C:O2'	2.32	0.43
37:RD:71:ASP:HB2	37:RD:103:ARG:HH12	1.84	0.43
46:RQ:21:THR:HB	46:RQ:22:LYS:H	1.58	0.43
51:RV:62:LEU:HD21	51:RV:95:LEU:HB2	2.00	0.43
35:YA:579:G:O2'	35:YA:2019:A:OP1	2.33	0.43
35:YA:1638:C:OP1	35:YA:2710:C:O2'	2.30	0.43
39:YF:39:TRP:NE1	39:YF:99:TYR:O	2.45	0.43
1:QA:1314:C:N4	19:QS:2:PRO:O	2.50	0.42
27:R2:9:GLN:HE22	27:R2:56:GLN:HG2	1.83	0.42
31:R6:24:GLU:OE2	35:RA:2286:A:N6	2.51	0.42
35:RA:511:U:O4	35:RA:512:G:N1	2.51	0.42
37:RD:145:VAL:HB	37:RD:155:LEU:HB2	2.00	0.42
40:RG:101:ILE:HG22	40:RG:105:LYS:HE2	2.00	0.42
42:RI:131:LYS:HA	42:RI:132:PRO:HD3	1.91	0.42
44:RO:104:ARG:NH2	49:RT:43:GLN:OE1	2.30	0.42
45:RP:122:PRO:HB3	45:RP:141:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:RZ:4:ARG:HD3	55:RZ:60:GLU:OE1	2.19	0.42
55:RZ:74:VAL:HG12	55:RZ:86:VAL:HG23	2.00	0.42
1:XA:1130:A:O5'	9:XI:20:ARG:NH2	2.52	0.42
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	2.01	0.42
26:Y1:19:GLN:HG3	35:YA:2080:G:H5'	1.99	0.42
35:YA:554:U:H2'	35:YA:556:G:C8	2.54	0.42
35:YA:1508:A:O2'	35:YA:1509:C:O4'	2.32	0.42
50:YU:91:ASP:C	50:YU:93:LYS:H	2.22	0.42
1:QA:184:G:H2'	1:QA:185:A:C8	2.55	0.42
1:QA:674:G:H2'	1:QA:675:A:C8	2.53	0.42
1:QA:985:C:H2'	1:QA:986:A:H8	1.84	0.42
1:QA:1095:U:P	1:QA:1108:G:H1	2.42	0.42
1:QA:1129:C:N4	1:QA:1133:G:O6	2.48	0.42
9:QI:92:TYR:HB3	9:QI:96:LEU:HD23	2.00	0.42
10:QJ:55:LYS:HB3	10:QJ:55:LYS:HE3	1.69	0.42
18:QR:34:TYR:HD1	18:QR:35:ARG:HG3	1.83	0.42
35:RA:224:G:OP2	35:RA:408:G:N2	2.48	0.42
35:RA:581:C:H2'	35:RA:582:G:C8	2.53	0.42
1:XA:1405:G:OP2	57:XA:1670:PAR:O34	2.29	0.42
2:XB:220:ASP:HA	2:XB:223:ILE:HG22	2.01	0.42
33:Y8:4:MET:CE	33:Y8:61:LEU:HD13	2.37	0.42
35:YA:639:U:H3	35:YA:649:G:H1	1.67	0.42
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.38	0.42
37:YD:36:PRO:HA	37:YD:62:TYR:O	2.19	0.42
43:YN:116:LEU:HD23	43:YN:116:LEU:HA	1.88	0.42
47:YR:79:LEU:HA	47:YR:83:ILE:HD12	2.00	0.42
49:YT:60:THR:HG22	49:YT:77:PRO:HA	2.00	0.42
55:YZ:48:PHE:O	55:YZ:52:SER:N	2.50	0.42
1:QA:738:C:OP1	6:QF:2:ARG:NH1	2.53	0.42
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.84	0.42
2:QB:95:GLN:HG3	2:QB:96:ARG:H	1.84	0.42
13:QM:57:ARG:NH2	29:R4:32:TYR:OH	2.47	0.42
25:R0:69:PHE:HE2	25:R0:79:VAL:CG2	2.26	0.42
35:RA:1651:G:OP1	47:RR:40:LYS:NZ	2.37	0.42
35:RA:2210:G:OP1	37:RD:68:LYS:NZ	2.50	0.42
35:RA:2745:C:O2	41:RH:139:GLN:NE2	2.48	0.42
37:RD:35:LYS:HD3	37:RD:104:TYR:CZ	2.53	0.42
37:RD:69:ARG:HH11	37:RD:105:ILE:HG12	1.84	0.42
47:RR:83:ILE:HG23	47:RR:86:ARG:HH21	1.85	0.42
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.40	0.42
7:XG:16:LEU:HD11	9:XI:45:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:38:THR:HG23	12:XL:39:VAL:HG23	2.00	0.42
12:XL:124:LYS:HD2	12:XL:125:PRO:HD2	2.00	0.42
35:YA:582:G:OP1	50:YU:14:HIS:ND1	2.50	0.42
35:YA:747:U:H5"	35:YA:748:G:H5'	2.00	0.42
35:YA:2293:C:OP1	48:YS:89:ARG:NH2	2.53	0.42
35:YA:2308:G:H1	35:YA:2311:A:H2	1.67	0.42
1:QA:902:G:H2'	1:QA:903:G:H8	1.85	0.42
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.85	0.42
35:RA:1067:A:H5"	35:RA:1068:G:C8	2.54	0.42
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.49	0.42
36:RB:80:U:H2'	36:RB:81:G:H21	1.84	0.42
1:XA:542:G:OP1	4:XD:10:ARG:NH2	2.46	0.42
1:XA:812:C:H4'	1:XA:813:U:H5'	2.01	0.42
30:Y5:55:ARG:HD2	30:Y5:55:ARG:HA	1.76	0.42
35:YA:742:G:H2'	35:YA:743:G:C8	2.54	0.42
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.47	0.42
38:YE:134:ILE:HA	38:YE:137:HIS:CD2	2.54	0.42
40:YG:107:LEU:HD23	40:YG:111:LEU:HD12	2.01	0.42
1:QA:67:C:H2'	1:QA:68:G:C8	2.55	0.42
1:QA:272:C:H2'	1:QA:273:A:H8	1.84	0.42
1:QA:429:U:H5'	4:QD:9:CYS:HB2	2.01	0.42
1:QA:444:C:H2'	1:QA:445:G:C8	2.52	0.42
1:QA:765:G:N2	1:QA:813:U:OP2	2.40	0.42
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.83	0.42
4:QD:31:CYS:SG	4:QD:32:ALA:N	2.92	0.42
26:R1:47:GLN:NE2	35:RA:2229:C:O2	2.53	0.42
35:RA:1262:A:OP1	52:RW:99:ARG:NH1	2.48	0.42
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	2.01	0.42
1:XA:395:C:N4	1:XA:396:G:O6	2.52	0.42
1:XA:940:C:H1'	1:XA:1374:A:H62	1.85	0.42
10:XJ:34:VAL:HG23	10:XJ:74:ILE:HG22	2.02	0.42
35:YA:639:U:H2'	35:YA:640:C:C6	2.55	0.42
35:YA:2405:G:H5'	45:YP:75:ILE:HD13	2.01	0.42
39:YF:127:GLU:OE1	39:YF:196:LEU:HB2	2.20	0.42
43:YN:130:HIS:HB3	43:YN:134:ARG:NH2	2.34	0.42
45:YP:98:GLU:HA	45:YP:101:VAL:HG22	2.02	0.42
46:YQ:111:GLU:OE2	46:YQ:133:ARG:NH2	2.52	0.42
48:YS:83:LYS:HG3	48:YS:109:GLY:HA3	2.02	0.42
53:YX:53:LYS:H	53:YX:82:GLN:HB3	1.83	0.42
1:QA:254:G:H2'	1:QA:255:G:H8	1.84	0.42
4:QD:31:CYS:SG	4:QD:33:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:QU:10:ARG:HA	21:QU:13:ILE:HD12	2.01	0.42
35:RA:807:U:O2	39:RF:74:ARG:NH2	2.51	0.42
35:RA:2102:U:H3	35:RA:2187:G:H1	1.68	0.42
37:RD:3:VAL:HG23	37:RD:19:ALA:HA	2.00	0.42
53:RX:21:PHE:CE2	53:RX:92:LEU:HB3	2.55	0.42
1:XA:1408:A:N1	57:XA:1670:PAR:O61	2.50	0.42
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	2.01	0.42
8:XH:86:ILE:HG22	8:XH:93:VAL:HG21	2.01	0.42
35:YA:1105:U:H2'	35:YA:1106:G:C8	2.53	0.42
38:YE:144:ARG:HB3	38:YE:145:LYS:H	1.65	0.42
39:YF:24:LEU:HD23	39:YF:115:ALA:HA	2.00	0.42
44:YO:8:LEU:HB2	44:YO:19:ILE:HG13	2.01	0.42
1:QA:701:C:O2	1:QA:703:G:N1	2.53	0.42
5:QE:12:LEU:HB3	5:QE:31:LEU:HB3	2.01	0.42
12:QL:27:LEU:O	12:QL:33:ARG:NH2	2.52	0.42
17:QQ:4:LYS:HE3	17:QQ:6:LEU:HD21	2.02	0.42
26:R1:50:ARG:NH2	35:RA:2199:A:OP1	2.53	0.42
35:RA:574:C:N3	38:RE:145:LYS:NZ	2.68	0.42
35:RA:1666:G:OP1	44:RO:66:LYS:HD3	2.19	0.42
35:RA:2133:G:H2'	35:RA:2157:G:N2	2.34	0.42
35:RA:2306:C:H3'	35:RA:2307:G:H5"	2.02	0.42
40:RG:122:PRO:HB3	40:RG:180:PHE:HD2	1.84	0.42
50:RU:66:ASN:OD1	50:RU:70:ARG:NE	2.50	0.42
52:RW:88:ARG:NH1	52:RW:94:ASP:OD2	2.52	0.42
13:XM:16:ASP:HB3	13:XM:41:PRO:HB3	2.01	0.42
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.55	0.42
55:YZ:80:ARG:HH11	55:YZ:82:ARG:HH12	1.68	0.42
1:QA:464:G:N2	1:QA:467:G:N7	2.68	0.42
2:QB:93:VAL:HG11	2:QB:97:TRP:HD1	1.84	0.42
6:QF:45:LEU:HD12	6:QF:59:TYR:HD1	1.85	0.42
35:RA:307:G:N1	35:RA:310:A:OP2	2.49	0.42
35:RA:363:G:H2'	35:RA:363(A):A:C8	2.54	0.42
35:RA:1005:C:O2'	43:RN:28:THR:HG21	2.20	0.42
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.01	0.42
39:RF:167:ALA:HB1	39:RF:173:VAL:HG11	2.02	0.42
51:RV:2:PHE:HB2	51:RV:3:ALA:H	1.72	0.42
55:RZ:89:PHE:HE2	55:RZ:96:VAL:HG11	1.85	0.42
1:XA:79:G:H2'	1:XA:80:G:C8	2.54	0.42
1:XA:781:A:O2'	1:XA:1522:U:O2	2.32	0.42
6:XF:5:GLU:HB3	6:XF:62:TRP:HE1	1.85	0.42
37:YD:25:THR:HG22	37:YD:82:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:134:ILE:HA	38:YE:137:HIS:HD2	1.85	0.42
40:YG:126:ASP:OD2	40:YG:130:ASN:ND2	2.50	0.42
49:YT:3:ARG:HG3	49:YT:7:ILE:HG12	2.02	0.42
1:QA:1299:A:C8	1:QA:1301:U:H1'	2.54	0.42
13:QM:82:MET:HE3	13:QM:92:HIS:HB3	2.02	0.42
25:R0:26:TYR:HA	25:R0:69:PHE:HE1	1.85	0.42
53:RX:53:LYS:HB2	53:RX:82:GLN:HB3	2.02	0.42
13:XM:47:ASP:OD1	13:XM:47:ASP:N	2.53	0.42
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.20	0.42
31:Y6:44:ARG:HB2	31:Y6:45:LYS:H	1.67	0.42
40:YG:86:MET:HA	40:YG:87:PRO:HD2	1.97	0.42
40:YG:101:ILE:HG22	40:YG:105:LYS:HE2	2.01	0.42
1:QA:730:G:C5	1:QA:731:G:H1'	2.55	0.42
13:QM:14:ARG:H	13:QM:44:ARG:HA	1.84	0.42
18:QR:35:ARG:HH11	18:QR:35:ARG:HD2	1.70	0.42
35:RA:1902:C:H5'	37:RD:246:PRO:HD3	2.02	0.42
35:YA:297:C:H5"	54:YY:87:LYS:HG3	2.02	0.42
35:YA:363:G:H2'	35:YA:363(A):A:H8	1.85	0.42
35:YA:500:G:N1	35:YA:503:A:OP2	2.50	0.42
35:YA:1817:G:OP1	37:YD:88:ARG:NH2	2.53	0.42
35:YA:2233:U:H2'	35:YA:2234:G:C8	2.55	0.42
36:YB:8:U:H3	36:YB:112:G:H1	1.68	0.42
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	2.01	0.42
45:YP:91:PHE:CE2	45:YP:95:VAL:HG22	2.55	0.42
1:QA:1004:A:P	1:QA:1025:U:H3	2.43	0.41
3:QC:37:GLN:NE2	14:QN:52:GLN:OE1	2.38	0.41
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	2.01	0.41
10:QJ:61:GLU:OE2	14:QN:58:LYS:HE2	2.20	0.41
27:R2:50:ILE:H	27:R2:50:ILE:HG12	1.70	0.41
35:RA:2618:G:H21	38:RE:150:VAL:HG21	1.85	0.41
38:RE:37:ARG:HB2	38:RE:46:ALA:H	1.85	0.41
50:RU:17:ILE:HG23	50:RU:39:LEU:HD12	2.02	0.41
1:XA:1238:A:H62	1:XA:1301:U:H3	1.68	0.41
2:XB:166:ASP:HB3	2:XB:169:LYS:HB3	2.02	0.41
12:XL:105:TYR:O	12:XL:107:ALA:N	2.53	0.41
18:XR:45:SER:OG	18:XR:47:THR:OG1	2.29	0.41
35:YA:1827:C:O2'	35:YA:1970:A:N3	2.46	0.41
35:YA:2503:A:O2'	35:YA:2505:G:OP2	2.29	0.41
37:YD:31:LYS:HD3	37:YD:94:LEU:HD11	2.02	0.41
41:YH:103:LEU:CD2	41:YH:123:PHE:HE2	2.26	0.41
2:QB:102:LEU:HB3	2:QB:180:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:32:GLU:O	13:QM:36:LYS:HG2	2.20	0.41
31:R6:30:THR:HG23	31:R6:31:PRO:HD3	2.02	0.41
35:RA:1043:C:N3	35:RA:1112:G:N2	2.47	0.41
35:RA:1062:G:H2'	35:RA:1063:G:H8	1.85	0.41
35:RA:2777:G:H5"	35:RA:2778:A:H3'	2.01	0.41
35:RA:2847:U:OP1	49:RT:98:LYS:NZ	2.34	0.41
41:RH:126:PRO:HG2	41:RH:130:ARG:HE	1.85	0.41
46:RQ:56:ARG:HA	46:RQ:56:ARG:HD2	1.89	0.41
50:RU:92:ARG:HD2	51:RV:11:GLN:HB2	2.02	0.41
52:RW:45:TYR:CZ	52:RW:49:LYS:HD2	2.54	0.41
1:XA:7:G:O2'	5:XE:120:THR:O	2.38	0.41
1:XA:824:C:H2'	1:XA:825:G:H8	1.82	0.41
29:Y4:18:CYS:SG	29:Y4:19:GLY:N	2.93	0.41
33:Y8:54:GLU:O	33:Y8:58:ILE:HG12	2.19	0.41
35:YA:363(A):A:H2'	35:YA:363(B):G:C8	2.53	0.41
35:YA:2468:G:O2'	35:YA:2481:G:N2	2.54	0.41
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.85	0.41
24:QY:20:G:OP2	24:QY:60:C:N4	2.54	0.41
25:R0:26:TYR:HA	25:R0:69:PHE:CE1	2.56	0.41
27:R2:4:SER:OG	27:R2:5:GLU:OE1	2.33	0.41
32:R7:49:ARG:HH12	35:RA:1600:C:H4'	1.85	0.41
44:RO:78:ARG:HH12	49:RT:75:ILE:HD11	1.85	0.41
54:RY:46:LYS:HG2	54:RY:60:PHE:CD2	2.56	0.41
55:RZ:75:ASN:HB2	55:RZ:85:HIS:HB3	2.02	0.41
55:RZ:91:LEU:HD23	55:RZ:130:PRO:HG3	2.02	0.41
1:XA:445:G:H2'	1:XA:446:G:C8	2.55	0.41
3:XC:23:TYR:HE1	10:XJ:67:THR:HG23	1.84	0.41
35:YA:1266:G:O2'	35:YA:2012:G:O6	2.32	0.41
52:YW:45:TYR:CZ	52:YW:49:LYS:HD2	2.55	0.41
53:YX:26:TYR:HD2	53:YX:92:LEU:HD22	1.85	0.41
1:QA:581:G:OP1	15:QO:65:ARG:NH1	2.53	0.41
1:QA:855:G:OP2	1:QA:871:U:N3	2.44	0.41
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.85	0.41
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	2.02	0.41
4:QD:116:GLN:HE21	4:QD:157:LEU:HD11	1.85	0.41
10:QJ:79:ARG:HD3	10:QJ:79:ARG:HA	1.91	0.41
19:QS:63:THR:OG1	19:QS:64:GLU:OE1	2.38	0.41
35:RA:1254:A:H5"	35:RA:1255:U:H5"	2.02	0.41
38:RE:30:PRO:HA	38:RE:92:THR:HA	2.02	0.41
39:RF:11:VAL:HG22	39:RF:125:LEU:HB2	2.02	0.41
41:RH:85:LYS:HB3	41:RH:86:GLU:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RR:57:ARG:HE	47:RR:62:ALA:HB2	1.85	0.41
54:RY:10:GLY:H	54:RY:27:VAL:HG23	1.85	0.41
1:XA:152:A:H62	1:XA:169:C:N4	2.16	0.41
1:XA:243:A:H4'	1:XA:244:U:H3'	2.01	0.41
1:XA:411:A:C4	1:XA:413:G:H1'	2.55	0.41
1:XA:562:C:H1'	12:XL:15:ARG:HD2	2.02	0.41
1:XA:711:G:H2'	1:XA:712:A:C8	2.55	0.41
1:XA:1130:A:N6	1:XA:1131:G:O6	2.53	0.41
26:Y1:97:LEU:HD13	35:YA:270(T):G:H5"	2.02	0.41
35:YA:729:G:H5'	35:YA:730:C:H5"	2.01	0.41
35:YA:1056:G:H4'	35:YA:1086:A:H8	1.85	0.41
2:QB:115:LEU:HD22	2:QB:153:ARG:HD3	2.02	0.41
9:QI:33:PHE:CD1	9:QI:37:PHE:HD2	2.37	0.41
12:QL:85:ILE:HG23	12:QL:98:TYR:HB3	2.02	0.41
13:QM:84:ILE:CG1	13:QM:86:CYS:HB2	2.50	0.41
19:QS:63:THR:OG1	19:QS:64:GLU:N	2.52	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:NH1	2.18	0.41
25:R0:38:VAL:HG21	25:R0:45:PHE:CD2	2.55	0.41
35:RA:195:A:H61	35:RA:198:C:H3'	1.85	0.41
35:RA:332:A:O2'	35:RA:334:C:OP2	2.32	0.41
35:RA:2579:C:O2'	38:RE:131:ALA:O	2.34	0.41
35:RA:2630:G:H2'	35:RA:2631:G:H8	1.86	0.41
35:RA:2849:U:O4	49:RT:23:ARG:NH2	2.38	0.41
40:RG:12:TYR:HA	40:RG:16:ARG:HD3	2.03	0.41
45:RP:121:LYS:O	45:RP:123:LEU:N	2.54	0.41
53:RX:12:VAL:HG12	53:RX:29:TRP:CD2	2.56	0.41
1:XA:861:G:O2'	1:XA:874:G:O2'	2.38	0.41
33:Y8:16:ILE:HD12	33:Y8:63:PRO:HB2	2.02	0.41
35:YA:566:U:P	51:YV:80:GLN:HE21	2.43	0.41
35:YA:1657:C:H4'	38:YE:133:LYS:HB3	2.03	0.41
39:YF:185:ASP:HA	39:YF:188:ARG:HD3	2.03	0.41
1:QA:419:C:OP1	1:QA:513:C:O2'	2.34	0.41
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.37	0.41
4:QD:57:ARG:HH12	5:QE:107:ARG:NH1	2.19	0.41
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	2.03	0.41
13:QM:106:ASN:OD1	13:QM:106:ASN:N	2.52	0.41
27:R2:41:ILE:HD11	27:R2:44:LEU:HD22	2.03	0.41
35:RA:629:G:N3	35:RA:639:U:O2'	2.52	0.41
41:RH:103:LEU:HD22	41:RH:123:PHE:HD2	1.85	0.41
45:RP:99:LEU:HA	45:RP:102:ARG:NE	2.35	0.41
46:RQ:24:GLY:HA2	46:RQ:67:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:437:U:H2'	1:XA:438:G:O4'	2.21	0.41
1:XA:1345:U:OP1	9:XI:120:ARG:NH1	2.53	0.41
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.53	0.41
37:YD:241:PRO:O	37:YD:242:ARG:HG2	2.20	0.41
54:YY:90:LEU:HB3	54:YY:91:GLU:H	1.71	0.41
1:QA:243:A:H4'	1:QA:244:U:H3'	2.03	0.41
1:QA:769:G:OP2	1:QA:803:G:O2'	2.36	0.41
1:QA:1512:U:H3	1:QA:1523:G:H1	1.69	0.41
10:QJ:13:HIS:HB3	10:QJ:68:HIS:CD2	2.55	0.41
11:QK:80:VAL:HG13	11:QK:103:LEU:HD12	2.02	0.41
35:RA:494:G:H4'	52:RW:6:ILE:HB	2.03	0.41
35:RA:919:G:N2	35:RA:2269:A:OP2	2.54	0.41
35:RA:1441:G:H2'	35:RA:1442:G:H8	1.84	0.41
35:RA:1588:C:H2'	35:RA:1589:C:H6	1.85	0.41
35:RA:2345:G:O2'	35:RA:2381:C:O2	2.33	0.41
38:RE:21:VAL:HA	38:RE:22:PRO:HD3	1.93	0.41
40:RG:52:ILE:HG23	40:RG:55:LYS:HB3	2.03	0.41
45:RP:99:LEU:HA	45:RP:102:ARG:HE	1.85	0.41
1:XA:1022:G:H2'	1:XA:1023:G:C8	2.56	0.41
9:XI:46:ALA:HA	9:XI:78:LYS:HB2	2.02	0.41
24:XY:19:G:H4'	24:XY:57:G:H22	1.85	0.41
25:Y0:68:GLU:HG3	25:Y0:80:HIS:HB2	2.01	0.41
33:Y8:62:LEU:N	33:Y8:63:PRO:CD	2.83	0.41
55:YZ:59:LEU:HD11	55:YZ:88:PHE:HD2	1.86	0.41
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.56	0.41
9:QI:77:ILE:O	9:QI:81:ILE:HG12	2.20	0.41
16:QP:5:ARG:NH2	16:QP:27:LYS:O	2.53	0.41
29:R4:7:PRO:HG2	40:RG:65:GLY:HA2	2.03	0.41
30:R5:25:LEU:HD11	52:RW:41:LYS:HE3	2.03	0.41
31:R6:46:HIS:ND1	35:RA:2371:G:O2'	2.35	0.41
35:RA:259:G:H2'	35:RA:260:G:H8	1.86	0.41
35:RA:593:G:H2'	35:RA:594:U:C6	2.55	0.41
35:RA:672:C:H5	45:RP:42:SER:HB2	1.86	0.41
35:RA:1467:C:C5	35:RA:1546:C:H2'	2.56	0.41
35:RA:1991:U:H6	35:RA:1991:U:C5'	2.32	0.41
35:RA:2630:G:H2'	35:RA:2631:G:C8	2.55	0.41
51:RV:2:PHE:CD1	51:RV:13:ARG:NH2	2.89	0.41
1:XA:973:G:H3'	1:XA:974:A:H5"	2.03	0.41
26:Y1:7:ILE:HD12	26:Y1:62:VAL:HG21	2.02	0.41
35:YA:458:G:O2'	35:YA:469:G:O6	2.28	0.41
35:YA:2076:U:OP2	35:YA:2238:G:N2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2661:G:H2'	35:YA:2662:A:C8	2.56	0.41
35:YA:2702:U:H5	47:YR:73:VAL:HG21	1.86	0.41
37:YD:232:PRO:HB3	37:YD:244:ARG:NH1	2.36	0.41
40:YG:10:LYS:NZ	40:YG:175:LEU:O	2.54	0.41
1:QA:34:C:H2'	1:QA:35:G:H8	1.85	0.41
3:QC:6:HIS:HB3	14:QN:49:HIS:CD2	2.55	0.41
5:QE:144:THR:N	5:QE:147:ASP:OD1	2.48	0.41
9:QI:24:GLY:N	9:QI:60:ASP:OD1	2.44	0.41
10:QJ:47:PHE:CE1	10:QJ:63:PHE:HB2	2.56	0.41
16:QP:20:VAL:HG23	16:QP:35:LYS:HA	2.03	0.41
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.53	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:HH11	1.69	0.41
23:QX:15:A:HO2'	23:QX:16:A:H8	1.66	0.41
27:R2:52:ASP:O	27:R2:56:GLN:HG3	2.20	0.41
29:R4:68:ARG:HB3	29:R4:69:LYS:H	1.56	0.41
32:R7:5:TRP:NE1	32:R7:7:PRO:HG3	2.36	0.41
33:R8:34:TRP:CD1	33:R8:35:GLN:HG2	2.56	0.41
35:RA:907:U:O2'	46:RQ:101:ARG:NH2	2.40	0.41
35:RA:971:C:O2'	35:RA:983:A:N3	2.38	0.41
35:RA:1142(A):A:H4'	43:RN:25:ARG:HH22	1.86	0.41
35:RA:1817:G:OP1	37:RD:62:TYR:OH	2.27	0.41
35:RA:2032:G:H21	38:RE:146:THR:HG1	1.61	0.41
35:RA:2036:C:H2'	35:RA:2037:G:H8	1.86	0.41
35:RA:2055:C:H1'	38:RE:145:LYS:HE3	2.03	0.41
35:RA:2375:G:N2	35:RA:2378:A:OP2	2.49	0.41
35:RA:2656:U:H3	35:RA:2665:A:H2	1.69	0.41
1:XA:884:U:H4'	1:XA:885:G:H5"	2.02	0.41
1:XA:1022:G:H2'	1:XA:1023:G:H8	1.86	0.41
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.34	0.41
1:XA:1237:C:HO2'	1:XA:1300:G:H1	1.69	0.41
10:XJ:57:LYS:CD	10:XJ:60:ARG:HH21	2.23	0.41
11:XK:25:TYR:HD1	11:XK:88:GLY:HA2	1.85	0.41
11:XK:127:LYS:HE3	23:XX:10:G:H5'	2.03	0.41
13:XM:108:ARG:HD2	13:XM:114:ARG:HG3	2.03	0.41
28:Y3:26:LEU:O	28:Y3:35:ARG:NE	2.53	0.41
31:Y6:39:TYR:HB3	31:Y6:40:CYS:H	1.76	0.41
35:YA:1568:G:P	37:YD:63:ARG:HH22	2.42	0.41
35:YA:2100:G:H1	35:YA:2189:U:H3	1.68	0.41
36:YB:111:U:H2'	36:YB:112:G:H8	1.85	0.41
38:YE:12:THR:OG1	38:YE:13:ARG:N	2.53	0.41
39:YF:198:ALA:HA	39:YF:201:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YH:126:PRO:HB3	41:YH:131:VAL:HA	2.02	0.41
44:YO:64:ARG:HB2	44:YO:83:ALA:HB3	2.03	0.41
1:QA:67:C:O2'	1:QA:171:A:N3	2.46	0.41
1:QA:346:G:H1'	1:QA:347:G:H5'	2.03	0.41
1:QA:553:A:O2'	12:QL:29:GLY:O	2.34	0.41
26:R1:91:LYS:HB3	26:R1:92:LYS:H	1.58	0.41
33:R8:29:LYS:O	33:R8:33:ASN:ND2	2.38	0.41
35:RA:1012:U:OP1	50:RU:75:ASN:ND2	2.51	0.41
35:RA:2470:G:H5'	46:RQ:56:ARG:HH21	1.86	0.41
39:RF:24:LEU:HB3	39:RF:115:ALA:HB2	2.02	0.41
39:RF:157:VAL:HB	39:RF:194:MET:HG2	2.03	0.41
42:RI:14:ASP:OD1	42:RI:14:ASP:N	2.54	0.41
44:RO:85:VAL:HG11	44:RO:114:ILE:HD12	2.02	0.41
55:RZ:10:ARG:HE	55:RZ:36:LYS:HB3	1.85	0.41
1:XA:25:C:H2'	1:XA:26:A:C8	2.56	0.41
27:Y2:50:ILE:HD12	35:YA:61:G:H5'	2.01	0.41
29:Y4:37:SER:HB2	29:Y4:42:PHE:HB3	2.02	0.41
30:Y5:38:ALA:HB3	30:Y5:40:LYS:NZ	2.31	0.41
33:Y8:29:LYS:HE3	33:Y8:44:LYS:HB2	2.02	0.41
34:Y9:2:LYS:HB2	34:Y9:34:GLN:HG2	2.02	0.41
34:Y9:14:CYS:HA	34:Y9:27:CYS:HB2	2.02	0.41
47:YR:56:LYS:NZ	47:YR:90:ARG:O	2.54	0.41
1:QA:501:C:H2'	1:QA:502:G:H8	1.86	0.40
3:QC:159:GLY:HA2	3:QC:193:TYR:HD2	1.74	0.40
4:QD:165:MET:SD	4:QD:168:ARG:NH1	2.94	0.40
8:QH:49:GLU:HG3	8:QH:51:VAL:HG13	2.03	0.40
18:QR:74:ARG:HB3	18:QR:81:PHE:CE1	2.55	0.40
33:R8:59:LYS:HZ1	45:RP:50:ARG:NE	2.19	0.40
35:RA:571:A:N6	35:RA:2499:C:O3'	2.54	0.40
35:RA:2212:A:H1'	35:RA:2215:G:C4	2.56	0.40
38:RE:101:ARG:NH1	38:RE:171:GLU:HB2	2.36	0.40
39:RF:29:ASN:ND2	39:RF:32:LEU:HD23	2.33	0.40
39:RF:65:TRP:HZ3	39:RF:75:HIS:HD1	1.69	0.40
40:RG:97:ASP:HA	40:RG:100:TRP:HD1	1.86	0.40
50:RU:40:PHE:HB3	51:RV:75:PHE:CD2	2.55	0.40
1:XA:277:C:OP1	17:XQ:68:ARG:NH1	2.54	0.40
1:XA:662:G:H2'	1:XA:663:A:C8	2.56	0.40
33:Y8:26:LYS:HD3	33:Y8:47:LYS:HB3	2.03	0.40
35:YA:1190:G:H5'	45:YP:32:THR:HA	2.03	0.40
35:YA:1266:G:O6	52:YW:13:SER:OG	2.30	0.40
35:YA:1565:C:H5"	37:YD:18:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1662:C:O2'	35:YA:2687:U:OP1	2.34	0.40
36:YB:44:G:H1'	36:YB:47:C:N4	2.36	0.40
47:YR:86:ARG:HH21	47:YR:118:GLU:HB2	1.85	0.40
1:QA:1256:A:OP1	3:QC:26:LYS:NZ	2.39	0.40
5:QE:110:LEU:HD13	5:QE:118:ILE:HG21	2.03	0.40
24:QY:3:G:H22	24:QY:70:U:H3	1.68	0.40
41:RH:41:MET:HG2	41:RH:55:PRO:HD2	2.03	0.40
49:RT:19:LEU:HA	49:RT:20:PRO:HD3	1.97	0.40
50:RU:90:VAL:HG12	50:RU:91:ASP:H	1.86	0.40
1:XA:1302:U:H1'	13:XM:17:VAL:HG11	2.02	0.40
19:XS:64:GLU:O	29:Y4:60:GLN:NE2	2.54	0.40
42:YI:4:ILE:HG12	42:YI:18:VAL:HG22	2.02	0.40
46:YQ:75:THR:HG21	46:YQ:85:LYS:HE3	2.03	0.40
46:YQ:81:VAL:O	46:YQ:82:ARG:NH1	2.45	0.40
47:YR:58:GLY:HA2	47:YR:80:PHE:HE2	1.86	0.40
1:QA:1111:A:H61	3:QC:177:THR:HG22	1.85	0.40
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.56	0.40
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	2.02	0.40
12:QL:11:VAL:HG11	17:QQ:36:ILE:HG21	2.03	0.40
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	2.03	0.40
20:QT:37:SER:O	20:QT:41:ILE:HG12	2.22	0.40
30:R5:51:TYR:HB3	30:R5:52:TYR:H	1.48	0.40
35:RA:620:G:H4'	35:RA:621:A:H5"	2.04	0.40
35:RA:1193:G:OP1	45:RP:14:LYS:NZ	2.51	0.40
35:RA:1657:C:OP1	38:RE:136:ARG:N	2.54	0.40
35:RA:2577:A:H5"	35:RA:2578:G:H5'	2.03	0.40
49:RT:73:GLU:OE1	49:RT:103:ARG:NH2	2.52	0.40
1:XA:170:U:H2'	1:XA:171:A:H8	1.86	0.40
1:XA:979:C:O2	14:XN:19:ARG:NE	2.55	0.40
2:XB:31:TYR:HD2	2:XB:202:PRO:HB3	1.86	0.40
3:XC:71:ALA:HA	3:XC:106:VAL:HG22	2.03	0.40
8:XH:39:LEU:HB3	8:XH:45:ILE:HG12	2.03	0.40
24:XY:19:G:C6	35:YA:881:G:H4'	2.57	0.40
25:Y0:46:LYS:HB2	25:Y0:78:TYR:CD1	2.56	0.40
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.40
35:YA:33:U:O4	35:YA:446:G:O2'	2.31	0.40
35:YA:530:G:C5	35:YA:2022:U:H5"	2.55	0.40
35:YA:1045:A:O2'	35:YA:1046:A:OP2	2.34	0.40
35:YA:2576:G:O2'	35:YA:2579:C:OP2	2.39	0.40
43:YN:16:ILE:HG21	43:YN:26:LEU:HD11	2.02	0.40
46:YQ:21:THR:HB	46:YQ:22:LYS:H	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:YZ:155:LEU:HD21	55:YZ:163:LEU:HD22	2.03	0.40
1:QA:392:G:H5'	16:QP:12:LYS:HG3	2.04	0.40
1:QA:427:U:OP2	1:QA:428:G:O2'	2.36	0.40
1:QA:877:C:O2'	8:QH:3:THR:OG1	2.33	0.40
1:QA:985:C:H2'	1:QA:986:A:C8	2.56	0.40
1:QA:1292:U:H5'	9:QI:38:GLN:HE22	1.86	0.40
1:QA:1318:A:OP1	19:QS:3:ARG:NH2	2.54	0.40
24:QY:55:U:H5	24:QY:57:G:H8	1.69	0.40
30:R5:51:TYR:HB2	30:R5:56:LYS:HG2	2.03	0.40
33:R8:46:ARG:NH1	35:RA:630:G:OP1	2.55	0.40
35:RA:514:A:N3	35:RA:581:C:O2'	2.42	0.40
35:RA:818:G:N1	35:RA:1188:U:OP2	2.42	0.40
35:RA:845:G:O2'	35:RA:847:U:O4	2.40	0.40
35:RA:1024:G:H5"	35:RA:1025:G:H5"	2.03	0.40
45:RP:115:LEU:HA	45:RP:134:ALA:HB2	2.02	0.40
1:XA:19:C:H5"	5:XE:86:ALA:HB3	2.02	0.40
1:XA:130:A:H5'	17:XQ:63:ARG:NH2	2.37	0.40
1:XA:1292:U:H2'	1:XA:1293:G:C8	2.57	0.40
17:XQ:66:SER:OG	17:XQ:67:LYS:N	2.55	0.40
32:Y7:19:ARG:HD3	35:YA:125:G:H5"	2.03	0.40
35:YA:49:A:N7	35:YA:120:U:H5	2.20	0.40
35:YA:483:A:O2'	54:YY:49:VAL:O	2.27	0.40
35:YA:729:G:P	37:YD:13:ARG:HD3	2.61	0.40
37:YD:159:ALA:HB1	37:YD:198:ASN:HB3	2.03	0.40
42:YI:6:LEU:HD13	42:YI:36:ALA:HA	2.02	0.40
1:QA:627:G:H2'	1:QA:628:G:C8	2.57	0.40
3:QC:134:ILE:HG23	3:QC:151:VAL:HB	2.04	0.40
4:QD:53:ASP:HB3	4:QD:57:ARG:HH12	1.86	0.40
11:QK:43:SER:HB3	11:QK:68:ALA:HB2	2.03	0.40
23:QX:20:C:H2'	23:QX:21:A:C8	2.57	0.40
35:RA:227:A:H5"	45:RP:76:LYS:HD3	2.04	0.40
35:RA:446:G:OP1	50:RU:3:ARG:NH1	2.54	0.40
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.56	0.40
38:RE:201:THR:HG22	38:RE:203:LYS:H	1.87	0.40
39:RF:150:GLY:HA2	39:RF:172:TRP:CD2	2.57	0.40
45:RP:88:LEU:HD12	45:RP:95:VAL:HG11	2.04	0.40
1:XA:170:U:H2'	1:XA:171:A:C8	2.56	0.40
1:XA:468:A:H5"	16:XP:80:PHE:HB3	2.03	0.40
1:XA:626:U:H4'	16:XP:38:TYR:CE2	2.55	0.40
3:XC:8:ILE:HD12	3:XC:16:ARG:NE	2.36	0.40
4:XD:191:ARG:NH2	4:XD:200:GLU:OE1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:16:ASP:N	13:XM:16:ASP:OD1	2.54	0.40
32:Y7:12:ARG:NH2	32:Y7:44:PRO:HB3	2.37	0.40
33:Y8:63:PRO:CD	33:Y8:63:PRO:O	2.70	0.40
39:YF:82:ILE:HG13	39:YF:83:PHE:HD1	1.86	0.40
39:YF:178:PRO:HB3	39:YF:198:ALA:HB2	2.04	0.40
41:YH:54:ARG:NH2	41:YH:57:ASP:OD1	2.55	0.40
44:YO:120:GLU:HB2	49:YT:68:TYR:HE2	1.86	0.40
45:YP:46:LYS:HE3	45:YP:46:LYS:HB3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	27 (12%)	2 (1%)	17	52
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	57
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	57
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	54
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	19	54
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	3	16
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	19	54
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	36
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	36
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	3	19
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	23
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	4	22
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	10 39
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100 100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0 3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	4 24
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100 100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100 100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1 8
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1 8
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100 100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100 100
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4 22
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	9 37
34	R9	35/37 (95%)	35 (100%)	0	0	100 100
34	Y9	35/37 (95%)	35 (100%)	0	0	100 100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	8 33
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	34 69
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	10 39
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	5 27
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	10 39
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15 49
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100 100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	25 59
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	6 27
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	13 44
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	2 11
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	3 16
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22 57
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22 57
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19 54
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	5 25
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	11 40
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22 57
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	4 24
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9 36
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9 36
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	5 25
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	17 52
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100 100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	22 57
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17 52
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	5 26
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	7 31
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15 49
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100 100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100 100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100 100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	14 46
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100 100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100 100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	5 25
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	6 29
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	14 46

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS
33	R8	62	LEU

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Mol	Chain	Res	Type
37	RD	33	LEU
41	RH	168	PRO
42	RI	15	VAL
45	RP	108	LYS
47	RR	4	LEU
48	RS	88	ASP
48	RS	89	ARG
50	RU	92	ARG
55	RZ	53	ILE
4	XD	5	ILE
12	XL	105	TYR
12	XL	106	ASP
20	XT	74	LYS
26	Y1	92	LYS
29	Y4	24	THR
38	YE	72	VAL
41	YH	157	TYR
41	YH	168	PRO
42	YI	12	LEU
45	YP	108	LYS
47	YR	4	LEU
50	YU	91	ASP
50	YU	92	ARG
55	YZ	53	ILE
55	YZ	94	GLU
2	QB	208	ILE
14	QN	17	LYS
37	RD	243	GLY
38	RE	83	ASP
42	RI	12	LEU
42	RI	13	GLY
45	RP	15	ARG
47	RR	3	HIS
51	RV	45	THR
51	RV	100	ARG
12	XL	104	VAL
12	XL	116	SER
14	XN	17	LYS
19	XS	27	GLU
20	XT	73	HIS
20	XT	75	ASN
31	Y6	8	LYS

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Mol	Chain	Res	Type
38	YE	132	HIS
39	YF	129	PHE
39	YF	134	GLY
42	YI	15	VAL
43	YN	22	THR
47	YR	3	HIS
48	YS	110	LEU
53	YX	68	ARG
2	QB	238	LEU
13	QM	12	ASN
27	R2	70	GLN
29	R4	23	GLU
31	R6	45	LYS
33	R8	63	PRO
37	RD	32	SER
39	RF	129	PHE
41	RH	40	GLU
42	RI	86	THR
45	RP	6	LEU
19	XS	3	ARG
26	Y1	91	LYS
33	Y8	30	ARG
38	YE	83	ASP
38	YE	129	HIS
42	YI	14	ASP
45	YP	65	ARG
46	YQ	22	LYS
46	YQ	25	ASP
26	R1	91	LYS
29	R4	41	PRO
39	RF	67	GLN
39	RF	130	ALA
41	RH	155	SER
42	RI	134	PRO
48	RS	87	PHE
55	RZ	52	SER
55	RZ	61	LEU
12	XL	115	LYS
31	Y6	7	ILE
40	YG	81	LYS
46	YQ	78	PRO
49	YT	108	ARG

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Mol	Chain	Res	Type
50	YU	90	VAL
29	R4	40	HIS
29	R4	42	PHE
29	R4	44	THR
43	RN	96	GLU
46	RQ	22	LYS
7	XG	8	GLU
19	XS	10	PHE
31	Y6	45	LYS
42	YI	10	GLU
42	YI	16	GLY
51	YV	50	PRO
12	QL	27	LEU
26	R1	54	ALA
38	RE	92	THR
38	RE	93	VAL
45	RP	7	ARG
5	XE	74	GLY
38	YE	131	ALA
44	YO	49	ARG
46	YQ	105	GLU
55	YZ	52	SER
37	RD	123	ALA
55	RZ	180	VAL
37	YD	123	ALA
41	RH	169	VAL
42	RI	16	GLY
42	RI	132	PRO
42	YI	13	GLY
31	R6	7	ILE
42	RI	118	LYS
9	XI	90	PRO
29	Y4	40	HIS
37	RD	36	PRO
55	RZ	111	VAL
55	YZ	61	LEU

5.3.2 Protein sidechains (i)

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	205/220 (93%)	203 (99%)	2 (1%)	76 90
2	XB	205/220 (93%)	204 (100%)	1 (0%)	88 94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69 87
3	XC	159/188 (85%)	159 (100%)	0	100 100
4	QD	173/181 (96%)	171 (99%)	2 (1%)	71 88
4	XD	173/181 (96%)	172 (99%)	1 (1%)	86 94
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78 91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78 91
6	QF	90/90 (100%)	90 (100%)	0	100 100
6	XF	90/90 (100%)	90 (100%)	0	100 100
7	QG	126/127 (99%)	126 (100%)	0	100 100
7	XG	126/127 (99%)	126 (100%)	0	100 100
8	QH	119/119 (100%)	119 (100%)	0	100 100
8	XH	119/119 (100%)	118 (99%)	1 (1%)	81 92
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40 70
9	XI	98/99 (99%)	97 (99%)	1 (1%)	76 90
10	QJ	89/92 (97%)	89 (100%)	0	100 100
10	XJ	89/92 (97%)	88 (99%)	1 (1%)	73 89
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73 89
11	XK	90/99 (91%)	89 (99%)	1 (1%)	73 89
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76 90
12	XL	104/108 (96%)	104 (100%)	0	100 100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76 90
13	XM	97/101 (96%)	97 (100%)	0	100 100
14	QN	49/50 (98%)	49 (100%)	0	100 100
14	XN	49/50 (98%)	49 (100%)	0	100 100
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%)	71 (99%)	1 (1%)	67 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73 89
17	XQ	95/97 (98%)	95 (100%)	0	100 100
18	QR	61/77 (79%)	59 (97%)	2 (3%)	38 69
18	XR	61/77 (79%)	61 (100%)	0	100 100
19	QS	73/80 (91%)	70 (96%)	3 (4%)	30 64
19	XS	73/80 (91%)	71 (97%)	2 (3%)	44 74
20	QT	76/82 (93%)	76 (100%)	0	100 100
20	XT	76/82 (93%)	76 (100%)	0	100 100
21	QU	20/22 (91%)	20 (100%)	0	100 100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24 57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65 85
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27 59
26	R1	82/83 (99%)	82 (100%)	0	100 100
26	Y1	82/83 (99%)	82 (100%)	0	100 100
27	R2	64/67 (96%)	64 (100%)	0	100 100
27	Y2	64/67 (96%)	62 (97%)	2 (3%)	40 70
28	R3	51/52 (98%)	51 (100%)	0	100 100
28	Y3	51/52 (98%)	51 (100%)	0	100 100
29	R4	63/63 (100%)	59 (94%)	4 (6%)	18 48
29	Y4	63/63 (100%)	62 (98%)	1 (2%)	62 84
30	R5	51/52 (98%)	51 (100%)	0	100 100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55 80
31	R6	48/52 (92%)	47 (98%)	1 (2%)	53 79
31	Y6	48/52 (92%)	48 (100%)	0	100 100
32	R7	42/42 (100%)	42 (100%)	0	100 100
32	Y7	42/42 (100%)	41 (98%)	1 (2%)	49 76
33	R8	54/55 (98%)	53 (98%)	1 (2%)	57 81
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34 66
34	R9	34/34 (100%)	34 (100%)	0	100 100
34	Y9	34/34 (100%)	34 (100%)	0	100 100
37	RD	214/218 (98%)	212 (99%)	2 (1%)	78 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	YD	214/218 (98%)	211 (99%)	3 (1%)	67	86
38	RE	165/166 (99%)	163 (99%)	2 (1%)	71	88
38	YE	165/166 (99%)	163 (99%)	2 (1%)	71	88
39	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
40	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
41	RH	142/148 (96%)	141 (99%)	1 (1%)	84	93
41	YH	142/148 (96%)	141 (99%)	1 (1%)	84	93
42	RI	122/124 (98%)	121 (99%)	1 (1%)	81	92
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	98 (98%)	2 (2%)	55	80
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55	80
45	RP	116/116 (100%)	113 (97%)	3 (3%)	46	74
45	YP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	RQ	111/111 (100%)	109 (98%)	2 (2%)	59	82
46	YQ	111/111 (100%)	108 (97%)	3 (3%)	44	74
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	100 (99%)	1 (1%)	76	90
48	RS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37	69
49	RT	120/127 (94%)	118 (98%)	2 (2%)	60	83
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73	89
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73	89
51	RV	82/82 (100%)	81 (99%)	1 (1%)	71	88
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
52	RW	92/92 (100%)	91 (99%)	1 (1%)	73	89
52	YW	92/92 (100%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	RX	74/78 (95%)	74 (100%)	0	100 100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	67 86
54	RY	85/91 (93%)	84 (99%)	1 (1%)	71 88
54	YY	85/91 (93%)	85 (100%)	0	100 100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	86 94
55	YZ	162/179 (90%)	160 (99%)	2 (1%)	71 88
All	All	9688/10064 (96%)	9587 (99%)	101 (1%)	76 90

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	94	ASN
2	QB	226	ARG
3	QC	11	ARG
3	QC	23	TYR
4	QD	59	ARG
4	QD	209	ARG
5	QE	40	ARG
9	QI	33	PHE
9	QI	104	ARG
9	QI	121	ARG
11	QK	12	ARG
12	QL	105	TYR
13	QM	83	ASP
15	QO	18	PHE
15	QO	79	ARG
17	QQ	68	ARG
18	QR	29	PHE
18	QR	34	TYR
19	QS	9	VAL
19	QS	11	VAL
19	QS	44	MET
25	R0	14	ARG
29	R4	16	CYS
29	R4	43	TYR
29	R4	55	ARG
29	R4	67	TYR
31	R6	6	ARG
33	R8	48	PHE
37	RD	6	PHE

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Mol	Chain	Res	Type
37	RD	43	ARG
38	RE	51	PHE
38	RE	84	PHE
39	RF	44	ARG
40	RG	115	ARG
41	RH	152	ARG
42	RI	33	ARG
43	RN	106	MET
44	RO	32	TYR
44	RO	49	ARG
45	RP	7	ARG
45	RP	61	ARG
45	RP	102	ARG
46	RQ	60	ARG
46	RQ	82	ARG
48	RS	17	ARG
48	RS	29	PHE
49	RT	85	LYS
49	RT	115	ARG
50	RU	92	ARG
51	RV	81	TYR
52	RW	92	ARG
54	RY	101	LYS
55	RZ	34	ASN
2	XB	94	ASN
4	XD	47	ARG
5	XE	10	MET
8	XH	104	ARG
9	XI	18	PHE
10	XJ	28	ARG
11	XK	54	ARG
16	XP	38	TYR
19	XS	10	PHE
19	XS	78	ARG
21	XU	24	ARG
25	Y0	14	ARG
25	Y0	45	PHE
25	Y0	74	ARG
27	Y2	59	ARG
27	Y2	65	ASN
29	Y4	68	ARG
30	Y5	37	LYS

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Mol	Chain	Res	Type
32	Y7	49	ARG
33	Y8	62	LEU
33	Y8	65	GLU
37	YD	15	PHE
37	YD	43	ARG
37	YD	62	TYR
38	YE	51	PHE
38	YE	84	PHE
39	YF	38	ARG
40	YG	118	ARG
41	YH	101	ARG
44	YO	64	ARG
44	YO	104	ARG
45	YP	61	ARG
46	YQ	5	ARG
46	YQ	60	ARG
46	YQ	82	ARG
47	YR	94	TYR
48	YS	20	ARG
48	YS	29	PHE
48	YS	106	ARG
49	YT	38	ASN
49	YT	65	LYS
49	YT	100	TYR
50	YU	52	ARG
51	YV	81	TYR
51	YV	91	TYR
53	YX	26	TYR
55	YZ	93	ASP
55	YZ	154	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	40	HIS
4	QD	77	ASN
6	QF	84	ASN
7	QG	84	ASN
7	QG	109	ASN
9	QI	58	HIS
10	QJ	33	GLN
13	QM	77	ASN

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Mol	Chain	Res	Type
19	QS	69	HIS
27	R2	9	GLN
29	R4	6	HIS
33	R8	35	GLN
37	RD	116	GLN
39	RF	40	GLN
41	RH	147	ASN
44	RO	5	GLN
46	RQ	12	GLN
47	RR	24	GLN
48	RS	38	GLN
49	RT	58	ASN
50	RU	44	ASN
52	RW	60	ASN
55	RZ	121	HIS
2	XB	16	HIS
2	XB	94	ASN
2	XB	212	GLN
4	XD	161	ASN
7	XG	109	ASN
8	XH	78	GLN
9	XI	31	GLN
9	XI	73	GLN
9	XI	124	GLN
10	XJ	84	GLN
13	XM	101	GLN
15	XO	62	GLN
19	XS	23	ASN
38	YE	143	ASN
39	YF	40	GLN
47	YR	71	GLN
49	YT	38	ASN
52	YW	60	ASN
55	YZ	34	ASN
55	YZ	55	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	270 (18%)	29 (1%)
1	XA	1498/1522 (98%)	279 (18%)	27 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	7 (41%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	587 (20%)	47 (1%)
35	YA	2880/2915 (98%)	587 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1859 (19%)	150 (1%)

All (1859) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	54	C
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	78	G
1	QA	79	G
1	QA	90	C
1	QA	91	C
1	QA	95	G
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	121	C
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C

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Mol	Chain	Res	Type
1	QA	182	U
1	QA	187	C
1	QA	191(A)	G
1	QA	195	A
1	QA	197	A
1	QA	209	U
1	QA	210	U
1	QA	216	G
1	QA	244	U
1	QA	245	C
1	QA	247	G
1	QA	251	G
1	QA	267	C
1	QA	270	A
1	QA	281	G
1	QA	289	G
1	QA	306	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	344	A
1	QA	346	G
1	QA	347	G
1	QA	348	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
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A
1	QA	412	A
1	QA	413	G
1	QA	421	U

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Mol	Chain	Res	Type
1	QA	422	C
1	QA	423	G
1	QA	429	U
1	QA	440	A
1	QA	452	A
1	QA	466	C
1	QA	467	G
1	QA	484	G
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	508	C
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
1	QA	521	G
1	QA	527	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
1	QA	564	C
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	607	A
1	QA	618	C
1	QA	620	C
1	QA	630	G
1	QA	631	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	671	G
1	QA	688	G
1	QA	693	G

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Mol	Chain	Res	Type
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	723	U
1	QA	724	G
1	QA	731	G
1	QA	748	C
1	QA	753	A
1	QA	754	C
1	QA	755	G
1	QA	773	G
1	QA	777	A
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	815	A
1	QA	817	C
1	QA	819	A
1	QA	820	U
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	872	A
1	QA	889	A
1	QA	902	G
1	QA	914	A
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	948	C
1	QA	960	U
1	QA	966	G
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	972	C
1	QA	974	A

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Mol	Chain	Res	Type
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1004	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1032(A)	G
1	QA	1040	U
1	QA	1054	C
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	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1132	C
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1163	C
1	QA	1171	G

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Mol	Chain	Res	Type
1	QA	1178	G
1	QA	1181	G
1	QA	1183	A
1	QA	1187	G
1	QA	1190	G
1	QA	1196	U
1	QA	1197	G
1	QA	1201	A
1	QA	1202	G
1	QA	1211	U
1	QA	1212	U
1	QA	1213	A
1	QA	1225	A
1	QA	1227	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
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	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1301	U
1	QA	1302	U
1	QA	1305	G
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1326	C
1	QA	1331	G
1	QA	1335	C

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Mol	Chain	Res	Type
1	QA	1336	C
1	QA	1337	G
1	QA	1345	U
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1358	U
1	QA	1362(A)	C
1	QA	1370	G
1	QA	1379	G
1	QA	1400	C
1	QA	1419	G
1	QA	1442	G
1	QA	1443	G
1	QA	1446	A
1	QA	1447	G
1	QA	1452	C
1	QA	1453	G
1	QA	1469	G
1	QA	1492	A
1	QA	1497	G
1	QA	1499	A
1	QA	1502	A
1	QA	1503	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1525	G
1	QA	1529	G
1	QA	1530	G
22	QV	7	G
22	QV	8	U
22	QV	9	G
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G
22	QV	19	G
22	QV	20	U

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Mol	Chain	Res	Type
22	QV	21	A
22	QV	47	U
22	QV	48	C
22	QV	49	G
22	QV	65	C
22	QV	76	A
23	QX	7	G
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	G
23	QX	23	A
24	QY	8	U
24	QY	12	U
24	QY	13	C
24	QY	15	G
24	QY	16	C
24	QY	17	U
24	QY	18	G
24	QY	19	G
24	QY	20	G
24	QY	21	A
24	QY	23	A
24	QY	30	G
24	QY	34	G
24	QY	43	G
24	QY	46	G
24	QY	47	U
24	QY	48	C
24	QY	50	G
24	QY	55	U
24	QY	57	G
24	QY	58	A
24	QY	59	U
24	QY	61	C
24	QY	68	G
24	QY	71	C
24	QY	74	C
24	QY	75	C
24	QY	76	A

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Mol	Chain	Res	Type
35	RA	14	A
35	RA	15	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	51	G
35	RA	55	G
35	RA	61	G
35	RA	64	A
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	83	G
35	RA	90	U
35	RA	101	G
35	RA	102	G
35	RA	103	A
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	131	G
35	RA	138	G
35	RA	161	U
35	RA	177	G
35	RA	181	A
35	RA	196	A
35	RA	199	A
35	RA	201	C
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	223	A
35	RA	228	A
35	RA	229	A
35	RA	230	U
35	RA	232	G
35	RA	233	A
35	RA	243	U
35	RA	248	G
35	RA	249	C
35	RA	252	G

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Mol	Chain	Res	Type
35	RA	265	A
35	RA	266	G
35	RA	269	U
35	RA	270(L)	U
35	RA	270(M)	U
35	RA	270(P)	C
35	RA	271(C)	U
35	RA	271	G
35	RA	273(F)	C
35	RA	275	G
35	RA	276	A
35	RA	277	C
35	RA	285	C
35	RA	299	A
35	RA	309	G
35	RA	311	A
35	RA	323	G
35	RA	324	A
35	RA	327	G
35	RA	329	G
35	RA	330	A
35	RA	346	A
35	RA	352	G
35	RA	364	C
35	RA	371	A
35	RA	372	G
35	RA	373	U
35	RA	386	G
35	RA	395	U
35	RA	405	U
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	444	C
35	RA	448	U
35	RA	451	C
35	RA	454	A
35	RA	455	C
35	RA	457	A
35	RA	470	A
35	RA	481	G
35	RA	504	U

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Mol	Chain	Res	Type
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	513	A
35	RA	529	A
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	537	C
35	RA	539	G
35	RA	540	G
35	RA	546	C
35	RA	547	A
35	RA	554	U
35	RA	556	G
35	RA	563	G
35	RA	573	G
35	RA	574	C
35	RA	575	A
35	RA	583	G
35	RA	588	U
35	RA	603	A
35	RA	607	U
35	RA	614	U
35	RA	615	G
35	RA	616	A
35	RA	617	G
35	RA	621	A
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	638	G
35	RA	645	C
35	RA	646	A
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G
35	RA	654(T)	C
35	RA	669	G
35	RA	670	A
35	RA	686	G

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Mol	Chain	Res	Type
35	RA	702	G
35	RA	717	G
35	RA	722	A
35	RA	730	C
35	RA	747	U
35	RA	753	C
35	RA	765	G
35	RA	771	G
35	RA	776	G
35	RA	782	A
35	RA	783	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	790	C
35	RA	793	A
35	RA	800	A
35	RA	805	G
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	847	U
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	869	G
35	RA	880	G
35	RA	881	G
35	RA	884	C
35	RA	885	C
35	RA	886	C
35	RA	888	C
35	RA	889	C
35	RA	893	C
35	RA	896	A
35	RA	897	C
35	RA	898	C
35	RA	900	A
35	RA	901	A
35	RA	904	C
35	RA	907	U

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Mol	Chain	Res	Type
35	RA	910	A
35	RA	917	A
35	RA	932	G
35	RA	938	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	959	A
35	RA	961	C
35	RA	973	A
35	RA	974	G
35	RA	974(A)	C
35	RA	980	A
35	RA	983	A
35	RA	989	G
35	RA	996	A
35	RA	1003	G
35	RA	1005	C
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1022	G
35	RA	1023	U
35	RA	1024	G
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1044	G
35	RA	1045	A
35	RA	1046	A
35	RA	1049	C
35	RA	1050	A
35	RA	1053	C
35	RA	1055	G
35	RA	1057	A
35	RA	1059	G
35	RA	1060	U
35	RA	1061	U
35	RA	1062	G
35	RA	1065	U

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Mol	Chain	Res	Type
35	RA	1066	U
35	RA	1067	A
35	RA	1068	G
35	RA	1071	G
35	RA	1073	A
35	RA	1076	C
35	RA	1077	A
35	RA	1078	U
35	RA	1079	C
35	RA	1080	C
35	RA	1082	U
35	RA	1083	U
35	RA	1084	A
35	RA	1085	A
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1090	U
35	RA	1091	G
35	RA	1093	G
35	RA	1095	A
35	RA	1096	A
35	RA	1104	C
35	RA	1105	U
35	RA	1110	G
35	RA	1111	A
35	RA	1112	G
35	RA	1113	U
35	RA	1122	G
35	RA	1131	G
35	RA	1135	C
35	RA	1136	G
35	RA	1139	G
35	RA	1140	C
35	RA	1142(A)	A
35	RA	1168	G
35	RA	1170	G
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1179	C

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Mol	Chain	Res	Type
35	RA	1195	G
35	RA	1204	A
35	RA	1205	U
35	RA	1206	G
35	RA	1210	A
35	RA	1211	U
35	RA	1220	A
35	RA	1236	G
35	RA	1238	G
35	RA	1240	U
35	RA	1244	G
35	RA	1252	G
35	RA	1253	A
35	RA	1256	G
35	RA	1271	G
35	RA	1272	A
35	RA	1273	U
35	RA	1284	A
35	RA	1300	U
35	RA	1301	A
35	RA	1312	U
35	RA	1313	U
35	RA	1314	C
35	RA	1319	G
35	RA	1329	U
35	RA	1341	U
35	RA	1349	A
35	RA	1352	U
35	RA	1365	A
35	RA	1368	G
35	RA	1370	C
35	RA	1378	A
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1385	G
35	RA	1395	A
35	RA	1403	C
35	RA	1404	C
35	RA	1407	C
35	RA	1411	C
35	RA	1416	G

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Mol	Chain	Res	Type
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1444(A)	A
35	RA	1445	C
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1455	G
35	RA	1458	C
35	RA	1460	A
35	RA	1461	G
35	RA	1467	C
35	RA	1471	A
35	RA	1482	U
35	RA	1483	G
35	RA	1485	G
35	RA	1490	A
35	RA	1493	C
35	RA	1495	A
35	RA	1497	U
35	RA	1507	A
35	RA	1508	A
35	RA	1510	A
35	RA	1511	A
35	RA	1513	C
35	RA	1514	U
35	RA	1525	G
35	RA	1533	C
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1538	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1554	A
35	RA	1558	A
35	RA	1559	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U

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Mol	Chain	Res	Type
35	RA	1586	A
35	RA	1598	C
35	RA	1608	A
35	RA	1609	A
35	RA	1616	A
35	RA	1617	C
35	RA	1618	A
35	RA	1630(A)	C
35	RA	1640	C
35	RA	1648	C
35	RA	1654	A
35	RA	1667	G
35	RA	1668	A
35	RA	1674	G
35	RA	1675	C
35	RA	1688	U
35	RA	1695	G
35	RA	1703	G
35	RA	1725	G
35	RA	1728	G
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1734	C
35	RA	1742	C
35	RA	1743	G
35	RA	1756	G
35	RA	1763	G
35	RA	1764	G
35	RA	1773	A
35	RA	1780	A
35	RA	1782	C
35	RA	1787	A
35	RA	1791	A
35	RA	1799	G
35	RA	1800	C
35	RA	1811	G
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1835	G

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Mol	Chain	Res	Type
35	RA	1847	A
35	RA	1848	A
35	RA	1858	G
35	RA	1860	G
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1882	C
35	RA	1885	A
35	RA	1888	G
35	RA	1889	A
35	RA	1900	A
35	RA	1906	G
35	RA	1913	A
35	RA	1929	G
35	RA	1931	U
35	RA	1936	A
35	RA	1938	A
35	RA	1939	U
35	RA	1955	U
35	RA	1963	U
35	RA	1964	G
35	RA	1967	C
35	RA	1969	A
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1982	C
35	RA	1991	U
35	RA	1992	G
35	RA	1993	U
35	RA	2020	A
35	RA	2023	G
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2039	C
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A

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Mol	Chain	Res	Type
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2069	G
35	RA	2107	C
35	RA	2111	C
35	RA	2113	U
35	RA	2114	A
35	RA	2115	G
35	RA	2116	G
35	RA	2117	A
35	RA	2119	A
35	RA	2126	A
35	RA	2127	G
35	RA	2128	C
35	RA	2131	G
35	RA	2132	U
35	RA	2133	G
35	RA	2135	A
35	RA	2136	C
35	RA	2145	C
35	RA	2146	C
35	RA	2147	G
35	RA	2148	G
35	RA	2158	A
35	RA	2166	G
35	RA	2168	G
35	RA	2169	A
35	RA	2171	A
35	RA	2173	A
35	RA	2176	A
35	RA	2190	G
35	RA	2198	A
35	RA	2199	A
35	RA	2210	G
35	RA	2211	G
35	RA	2212	A
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2238	G
35	RA	2239	G

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Mol	Chain	Res	Type
35	RA	2243	U
35	RA	2249	U
35	RA	2266	A
35	RA	2275	C
35	RA	2283	C
35	RA	2284	C
35	RA	2287	A
35	RA	2288	A
35	RA	2307	G
35	RA	2308	G
35	RA	2311	A
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2335	A
35	RA	2345	G
35	RA	2346	A
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2358	G
35	RA	2372	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2402	C
35	RA	2406	U
35	RA	2410	G
35	RA	2420	C
35	RA	2421	G
35	RA	2423	U
35	RA	2424	C
35	RA	2425	A
35	RA	2429	G
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2440	C
35	RA	2441	C
35	RA	2445	G

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Mol	Chain	Res	Type
35	RA	2448	A
35	RA	2469	A
35	RA	2470	G
35	RA	2475	C
35	RA	2482	G
35	RA	2484	G
35	RA	2494	G
35	RA	2498	C
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2519	U
35	RA	2529	G
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2562	U
35	RA	2564	A
35	RA	2567	G
35	RA	2569	G
35	RA	2573	C
35	RA	2576	G
35	RA	2578	G
35	RA	2582	G
35	RA	2586	C
35	RA	2602	A
35	RA	2609	U
35	RA	2611	U
35	RA	2612	C
35	RA	2615	U
35	RA	2621	A
35	RA	2623	G
35	RA	2629	A
35	RA	2642	G
35	RA	2646	C
35	RA	2654	A
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2689	U
35	RA	2690	C
35	RA	2700	C

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Mol	Chain	Res	Type
35	RA	2702	U
35	RA	2707	G
35	RA	2712	U
35	RA	2712(A)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2718	G
35	RA	2726	U
35	RA	2732	G
35	RA	2733	A
35	RA	2734	A
35	RA	2739	U
35	RA	2744	G
35	RA	2748	A
35	RA	2757	A
35	RA	2761	G
35	RA	2765	A
35	RA	2766	G
35	RA	2777	G
35	RA	2778	A
35	RA	2779	U
35	RA	2780	G
35	RA	2790	A
35	RA	2791	C
35	RA	2797	U
35	RA	2807	G
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2825	C
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2866	U
35	RA	2872	G
35	RA	2879	C
35	RA	2880	C
35	RA	2882	A
35	RA	2892	A
35	RA	2894	G
36	RB	7	G

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Mol	Chain	Res	Type
36	RB	8	U
36	RB	9	G
36	RB	12	C
36	RB	13	A
36	RB	15	A
36	RB	16	G
36	RB	22	U
36	RB	25	A
36	RB	26	A
36	RB	30	C
36	RB	41	U
36	RB	42	C
36	RB	44	G
36	RB	45	A
36	RB	56	G
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	105	G
36	RB	109	G
1	XA	6	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	78	G
1	XA	79	G
1	XA	81	G
1	XA	89	U
1	XA	90	C
1	XA	91	C
1	XA	92	G
1	XA	95	G
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	121	C
1	XA	130	A

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Mol	Chain	Res	Type
1	XA	144	G
1	XA	147	G
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	173	U
1	XA	174	C
1	XA	187	C
1	XA	188	U
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	197	A
1	XA	201	C
1	XA	209	U
1	XA	216	G
1	XA	220	G
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
1	XA	267	C
1	XA	270	A
1	XA	281	G
1	XA	289	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	348	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	372	C
1	XA	382	A
1	XA	384	G

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Mol	Chain	Res	Type
1	XA	388	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	435	C
1	XA	440	A
1	XA	452	A
1	XA	465	A
1	XA	466	C
1	XA	467	G
1	XA	483	C
1	XA	485	G
1	XA	486	U
1	XA	496	A
1	XA	497	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	527	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	546	G
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	565	U
1	XA	568	G
1	XA	572	A

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Mol	Chain	Res	Type
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	596	C
1	XA	614	A
1	XA	618	C
1	XA	630	G
1	XA	631	G
1	XA	652	U
1	XA	653	A
1	XA	661	G
1	XA	665	A
1	XA	688	G
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	724	G
1	XA	731	G
1	XA	748	C
1	XA	749	C
1	XA	754	C
1	XA	755	G
1	XA	774	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	799	G
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	872	A
1	XA	888	G
1	XA	902	G

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Mol	Chain	Res	Type
1	XA	914	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	948	C
1	XA	958	A
1	XA	960	U
1	XA	967	C
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	981	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1009	G
1	XA	1017	G
1	XA	1021	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1042	G
1	XA	1054	C
1	XA	1055	A
1	XA	1066	C
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U

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Mol	Chain	Res	Type
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	1146	A
1	XA	1152	A
1	XA	1154	G
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1184	G
1	XA	1187	G
1	XA	1190	G
1	XA	1196	U
1	XA	1197	G
1	XA	1211	U
1	XA	1212	U
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	1270	C
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	1298	C

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Mol	Chain	Res	Type
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1318	A
1	XA	1320	C
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	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1367	C
1	XA	1368	G
1	XA	1370	G
1	XA	1379	G
1	XA	1397	C
1	XA	1398	A
1	XA	1419	G
1	XA	1442	G
1	XA	1443	G
1	XA	1446	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1469	G
1	XA	1487	G
1	XA	1492	A
1	XA	1497	G
1	XA	1499	A
1	XA	1502	A
1	XA	1503	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G

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Mol	Chain	Res	Type
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
22	XV	3	C
22	XV	16	C
22	XV	17	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	22	G
22	XV	34	C
22	XV	47	U
22	XV	48	C
22	XV	59	A
22	XV	76	A
23	XX	7	G
23	XX	10	G
23	XX	11	U
23	XX	13	A
23	XX	14	A
23	XX	19	G
23	XX	23	A
24	XY	4	G
24	XY	8	U
24	XY	9	A
24	XY	12	U
24	XY	16	C
24	XY	17	U
24	XY	18	G
24	XY	19	G
24	XY	20	G
24	XY	21	A
24	XY	22	G
24	XY	23	A
24	XY	43	G
24	XY	46	G
24	XY	47	U
24	XY	50	G

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Mol	Chain	Res	Type
24	XY	55	U
24	XY	56	C
24	XY	57	G
24	XY	58	A
24	XY	59	U
24	XY	61	C
24	XY	71	C
24	XY	73	A
24	XY	74	C
35	YA	9	U
35	YA	15	G
35	YA	34	C
35	YA	35	G
35	YA	46	C
35	YA	50	U
35	YA	51	G
35	YA	55	G
35	YA	61	G
35	YA	63	U
35	YA	74	A
35	YA	75	G
35	YA	91	A
35	YA	96	G
35	YA	101	G
35	YA	102	G
35	YA	103	A
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	125	G
35	YA	131	G
35	YA	149	A
35	YA	161	U
35	YA	162	U
35	YA	181	A
35	YA	188	G
35	YA	196	A
35	YA	199	A
35	YA	204	A
35	YA	215	G
35	YA	216	A
35	YA	221	A

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Mol	Chain	Res	Type
35	YA	222	A
35	YA	223	A
35	YA	229	A
35	YA	230	U
35	YA	232	G
35	YA	242	G
35	YA	243	U
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	264	C
35	YA	265	A
35	YA	266	G
35	YA	269	U
35	YA	270(L)	U
35	YA	270(M)	U
35	YA	270(N)	G
35	YA	270(P)	C
35	YA	271(A)	C
35	YA	271(B)	G
35	YA	271(C)	U
35	YA	271	G
35	YA	274	G
35	YA	275	G
35	YA	276	A
35	YA	278	A
35	YA	279	C
35	YA	299	A
35	YA	311	A
35	YA	323	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	332	A
35	YA	342	G
35	YA	352	G
35	YA	363	G
35	YA	363(F)	A
35	YA	364	C
35	YA	371	A
35	YA	372	G
35	YA	386	G

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Mol	Chain	Res	Type
35	YA	387	U
35	YA	396	G
35	YA	405	U
35	YA	406	G
35	YA	411	G
35	YA	412	A
35	YA	421	U
35	YA	428	A
35	YA	443	A
35	YA	444	C
35	YA	448	U
35	YA	455	C
35	YA	457	A
35	YA	467	G
35	YA	470	A
35	YA	480	A
35	YA	481	G
35	YA	504	U
35	YA	505	A
35	YA	509	C
35	YA	518	G
35	YA	528	A
35	YA	530	G
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	537	C
35	YA	539	G
35	YA	540	G
35	YA	546	C
35	YA	547	A
35	YA	554	U
35	YA	563	G
35	YA	573	G
35	YA	575	A
35	YA	588	U
35	YA	603	A
35	YA	607	U
35	YA	614	U
35	YA	615	G
35	YA	616	A
35	YA	617	G

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Mol	Chain	Res	Type
35	YA	618	G
35	YA	622	G
35	YA	627	A
35	YA	634	C
35	YA	637	A
35	YA	638	G
35	YA	645	C
35	YA	646	A
35	YA	651	G
35	YA	654	A
35	YA	654(A)	G
35	YA	686	G
35	YA	695	G
35	YA	702	G
35	YA	717	G
35	YA	722	A
35	YA	730	C
35	YA	734	A
35	YA	747	U
35	YA	752	A
35	YA	753	C
35	YA	764	A
35	YA	765	G
35	YA	775	G
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	790	C
35	YA	792	G
35	YA	800	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	828	U
35	YA	829	A
35	YA	846	C
35	YA	847	U
35	YA	856	C

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Mol	Chain	Res	Type
35	YA	857	C
35	YA	859	G
35	YA	860	U
35	YA	866	A
35	YA	880	G
35	YA	881	G
35	YA	882	G
35	YA	884	C
35	YA	885	C
35	YA	886	C
35	YA	888	C
35	YA	889	C
35	YA	890	A
35	YA	896	A
35	YA	897	C
35	YA	900	A
35	YA	901	A
35	YA	907	U
35	YA	910	A
35	YA	917	A
35	YA	918	A
35	YA	932	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	959	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	974(A)	C
35	YA	983	A
35	YA	989	G
35	YA	996	A
35	YA	1003	G
35	YA	1005	C
35	YA	1011	G
35	YA	1012	U
35	YA	1013	C
35	YA	1015	G
35	YA	1022	G
35	YA	1023	U

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Mol	Chain	Res	Type
35	YA	1024	G
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1045	A
35	YA	1046	A
35	YA	1047	G
35	YA	1050	A
35	YA	1054	A
35	YA	1057	A
35	YA	1059	G
35	YA	1060	U
35	YA	1061	U
35	YA	1062	G
35	YA	1065	U
35	YA	1066	U
35	YA	1067	A
35	YA	1068	G
35	YA	1069	A
35	YA	1071	G
35	YA	1076	C
35	YA	1077	A
35	YA	1078	U
35	YA	1079	C
35	YA	1082	U
35	YA	1083	U
35	YA	1084	A
35	YA	1085	A
35	YA	1086	A
35	YA	1088	A
35	YA	1089	G
35	YA	1093	G
35	YA	1095	A
35	YA	1096	A
35	YA	1097	U
35	YA	1103	A
35	YA	1104	C
35	YA	1110	G
35	YA	1111	A
35	YA	1112	G
35	YA	1122	G

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Mol	Chain	Res	Type
35	YA	1126	A
35	YA	1129	A
35	YA	1130	U
35	YA	1131	G
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1142	U
35	YA	1142(A)	A
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1176	G
35	YA	1179	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1211	U
35	YA	1218	C
35	YA	1220	A
35	YA	1238	G
35	YA	1240	U
35	YA	1250	G
35	YA	1252	G
35	YA	1253	A
35	YA	1256	G
35	YA	1265	A
35	YA	1271	G
35	YA	1272	A
35	YA	1300	U
35	YA	1301	A
35	YA	1306	C
35	YA	1309	G
35	YA	1329	U
35	YA	1341	U
35	YA	1349	A
35	YA	1352	U
35	YA	1365	A
35	YA	1368	G
35	YA	1370	C
35	YA	1379	A

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Mol	Chain	Res	Type
35	YA	1384	A
35	YA	1385	G
35	YA	1386	C
35	YA	1391	U
35	YA	1395	A
35	YA	1407	C
35	YA	1411	C
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1427	A
35	YA	1428	C
35	YA	1444(A)	A
35	YA	1449	A
35	YA	1449(A)	G
35	YA	1455	G
35	YA	1458	C
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1483	G
35	YA	1485	G
35	YA	1493	C
35	YA	1497	U
35	YA	1507	A
35	YA	1508	A
35	YA	1510	A
35	YA	1511	A
35	YA	1514	U
35	YA	1523	U
35	YA	1534	G
35	YA	1535	U
35	YA	1536	A
35	YA	1537	C
35	YA	1538	G
35	YA	1540	G
35	YA	1543	A
35	YA	1544	C
35	YA	1545	A
35	YA	1558	A

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Mol	Chain	Res	Type
35	YA	1559	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1579	A
35	YA	1581	G
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1607	C
35	YA	1608	A
35	YA	1609	A
35	YA	1617	C
35	YA	1618	A
35	YA	1640	C
35	YA	1648	C
35	YA	1654	A
35	YA	1668	A
35	YA	1674	G
35	YA	1675	C
35	YA	1693	U
35	YA	1695	G
35	YA	1699	G
35	YA	1700	A
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1730	U
35	YA	1731	G
35	YA	1733	G
35	YA	1742	C
35	YA	1743	G
35	YA	1754	C
35	YA	1756	G
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1773	A
35	YA	1780	A
35	YA	1791	A
35	YA	1799	G
35	YA	1800	C

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Mol	Chain	Res	Type
35	YA	1801	G
35	YA	1808	U
35	YA	1811	G
35	YA	1816	G
35	YA	1820	U
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1858	G
35	YA	1869	G
35	YA	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1896	G
35	YA	1900	A
35	YA	1906	G
35	YA	1919	A
35	YA	1929	G
35	YA	1937	A
35	YA	1938	A
35	YA	1939	U
35	YA	1940	U
35	YA	1955	U
35	YA	1956	U
35	YA	1963	U
35	YA	1964	G
35	YA	1965	C
35	YA	1966	A
35	YA	1967	C
35	YA	1969	A
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1982	C
35	YA	1991	U
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A

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Mol	Chain	Res	Type
35	YA	2021	C
35	YA	2023	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2039	C
35	YA	2043	C
35	YA	2054	A
35	YA	2055	C
35	YA	2056	G
35	YA	2059	A
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2090	G
35	YA	2093	G
35	YA	2099	U
35	YA	2111	C
35	YA	2113	U
35	YA	2114	A
35	YA	2115	G
35	YA	2116	G
35	YA	2119	A
35	YA	2120	G
35	YA	2126	A
35	YA	2127	G
35	YA	2128	C
35	YA	2131	G
35	YA	2132	U
35	YA	2133	G
35	YA	2146	C
35	YA	2147	G
35	YA	2148	G
35	YA	2158	A
35	YA	2165	G
35	YA	2166	G
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2171	A
35	YA	2173	A

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Mol	Chain	Res	Type
35	YA	2176	A
35	YA	2178	C
35	YA	2190	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2213	U
35	YA	2215	G
35	YA	2225	A
35	YA	2234	G
35	YA	2238	G
35	YA	2239	G
35	YA	2243	U
35	YA	2246	G
35	YA	2249	U
35	YA	2269	A
35	YA	2275	C
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2289	G
35	YA	2307	G
35	YA	2308	G
35	YA	2310	A
35	YA	2311	A
35	YA	2318	G
35	YA	2319	G
35	YA	2320	A
35	YA	2325	G
35	YA	2334	G
35	YA	2336	A
35	YA	2342	C
35	YA	2346	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2377	A
35	YA	2383	G
35	YA	2385	C
35	YA	2403	C

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Mol	Chain	Res	Type
35	YA	2406	U
35	YA	2410	G
35	YA	2423	U
35	YA	2425	A
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2440	C
35	YA	2441	C
35	YA	2445	G
35	YA	2448	A
35	YA	2465	C
35	YA	2469	A
35	YA	2470	G
35	YA	2474	C
35	YA	2475	C
35	YA	2478	A
35	YA	2480	C
35	YA	2491	U
35	YA	2494	G
35	YA	2498	C
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2525	G
35	YA	2529	G
35	YA	2542	A
35	YA	2543	G
35	YA	2554	U
35	YA	2562	U
35	YA	2564	A
35	YA	2567	G
35	YA	2573	C
35	YA	2578	G
35	YA	2586	C
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2615	U
35	YA	2629	A

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Mol	Chain	Res	Type
35	YA	2646	C
35	YA	2653	U
35	YA	2654	A
35	YA	2665	A
35	YA	2673	G
35	YA	2679	A
35	YA	2682	U
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2707	G
35	YA	2712	U
35	YA	2712(A)	A
35	YA	2713	A
35	YA	2714	G
35	YA	2718	G
35	YA	2726	U
35	YA	2732	G
35	YA	2733	A
35	YA	2744	G
35	YA	2761	G
35	YA	2765	A
35	YA	2766	G
35	YA	2776	A
35	YA	2777	G
35	YA	2778	A
35	YA	2779	U
35	YA	2780	G
35	YA	2790	A
35	YA	2791	C
35	YA	2797	U
35	YA	2798	C
35	YA	2807	G
35	YA	2808	U
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2823	A
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A

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Mol	Chain	Res	Type
35	YA	2849	U
35	YA	2866	U
35	YA	2872	G
35	YA	2879	C
35	YA	2880	C
35	YA	2891	G
35	YA	2892	A
35	YA	2894	G
36	YB	7	G
36	YB	8	U
36	YB	9	G
36	YB	12	C
36	YB	13	A
36	YB	15	A
36	YB	19	G
36	YB	22	U
36	YB	40	U
36	YB	42	C
36	YB	45	A
36	YB	52	A
36	YB	53	A
36	YB	56	G
36	YB	73	A
36	YB	81	G
36	YB	82	G
36	YB	109	G

All (150) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	115	G
1	QA	181	G
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C
1	QA	410	G
1	QA	412	A
1	QA	484	G
1	QA	485	G
1	QA	509	A

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Mol	Chain	Res	Type
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	992	U
1	QA	1027	C
1	QA	1065	U
1	QA	1285	A
1	QA	1297	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1446	A
1	QA	1498	U
1	QA	1528	U
23	QX	18	G
35	RA	74	A
35	RA	99	U
35	RA	102	G
35	RA	221	A
35	RA	222	A
35	RA	227	A
35	RA	229	A
35	RA	242	G
35	RA	271(B)	G
35	RA	271(C)	U
35	RA	345	A
35	RA	372	G
35	RA	404	C
35	RA	503	A
35	RA	508	G
35	RA	512	G
35	RA	587	C
35	RA	637	A
35	RA	752	A
35	RA	846	C
35	RA	856	C
35	RA	1022	G
35	RA	1026	U
35	RA	1045	A

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Mol	Chain	Res	Type
35	RA	1078	U
35	RA	1085	A
35	RA	1178	C
35	RA	1210	A
35	RA	1312	U
35	RA	1427	A
35	RA	1558	A
35	RA	1653	G
35	RA	1694	C
35	RA	1799	G
35	RA	1819	A
35	RA	1930	G
35	RA	1992	G
35	RA	2060	A
35	RA	2126	A
35	RA	2405	G
35	RA	2439	A
35	RA	2566	A
35	RA	2610	C
35	RA	2689	U
35	RA	2712	U
35	RA	2776	A
35	RA	2832	U
36	RB	66	A
1	XA	60	A
1	XA	78	G
1	XA	89	U
1	XA	115	G
1	XA	243	A
1	XA	244	U
1	XA	250	A
1	XA	266	G
1	XA	328	C
1	XA	345	C
1	XA	410	G
1	XA	412	A
1	XA	484	G
1	XA	485	G
1	XA	509	A
1	XA	560	U
1	XA	687	A
1	XA	703	G

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Mol	Chain	Res	Type
1	XA	753	A
1	XA	793	U
1	XA	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1285	A
1	XA	1297	C
1	XA	1498	U
23	XX	18	G
35	YA	99	U
35	YA	102	G
35	YA	221	A
35	YA	222	A
35	YA	229	A
35	YA	242	G
35	YA	271(B)	G
35	YA	278	A
35	YA	404	C
35	YA	503	A
35	YA	587	C
35	YA	637	A
35	YA	653	A
35	YA	752	A
35	YA	827	U
35	YA	846	C
35	YA	856	C
35	YA	859	G
35	YA	1022	G
35	YA	1026	U
35	YA	1045	A
35	YA	1085	A
35	YA	1178	C
35	YA	1204	A
35	YA	1210	A
35	YA	1427	A
35	YA	1558	A
35	YA	1653	G
35	YA	1694	C
35	YA	1698	A
35	YA	1799	G
35	YA	1819	A

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Mol	Chain	Res	Type
35	YA	1955	U
35	YA	1992	G
35	YA	2126	A
35	YA	2406	U
35	YA	2439	A
35	YA	2566	A
35	YA	2610	C
35	YA	2681	C
35	YA	2689	U
35	YA	2712	U
35	YA	2776	A
35	YA	2832	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 855 ligands modelled in this entry, 851 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PAR	XA	1670	-	45,45,45	0.86	1 (2%)	64,67,67	1.28	7 (10%)
57	PAR	QA	1663	-	45,45,45	0.80	0	64,67,67	1.30	8 (12%)
58	SF4	QD	501	-	0,12,12	-	-	-		
58	SF4	XD	501	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	XA	1670	-	-	3/18/94/94	0/4/4/4
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4
58	SF4	QD	501	-	-	-	0/6/5/5
58	SF4	XD	501	4	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.01	1.44	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	QA	1663	PAR	C13-O52-C52	-3.20	110.03	117.96
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	XA	1670	PAR	C13-O52-C52	-2.87	110.85	117.96
57	QA	1663	PAR	C64-C54-C44	-2.68	107.82	113.10
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.81
57	QA	1663	PAR	O33-C33-C23	-2.57	103.05	111.32
57	QA	1663	PAR	O52-C13-C23	2.55	113.24	107.96
57	XA	1670	PAR	O62-C62-C12	-2.42	105.38	109.81
57	XA	1670	PAR	O33-C33-C23	-2.39	103.62	111.32
57	XA	1670	PAR	O52-C13-C23	2.24	112.60	107.96
57	QA	1663	PAR	O11-C42-C32	-2.18	103.98	109.18
57	QA	1663	PAR	C11-C21-N21	-2.18	106.28	110.20
57	XA	1670	PAR	C31-C41-C51	-2.16	106.39	110.24
57	XA	1670	PAR	O11-C11-C21	-2.10	104.59	108.22
57	QA	1663	PAR	C11-O51-C51	2.04	117.69	113.69

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14

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Mol	Chain	Res	Type	Atoms
57	XA	1670	PAR	C23-C33-O33-C14

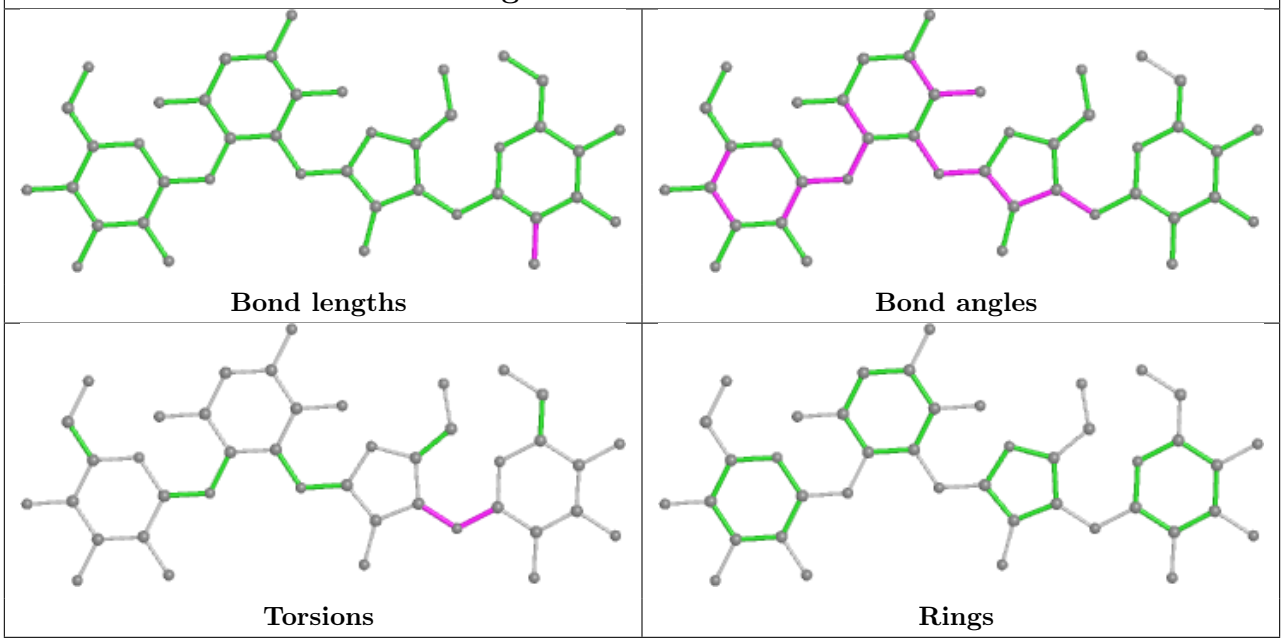
There are no ring outliers.

1 monomer is involved in 4 short contacts:

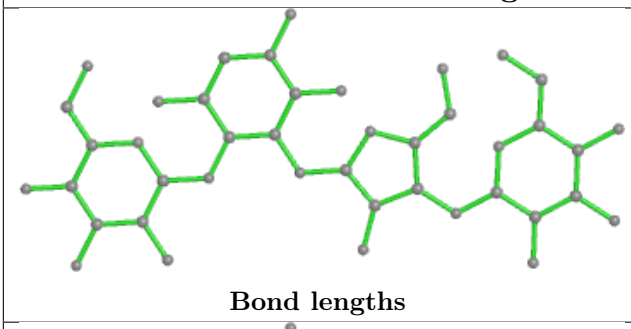
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

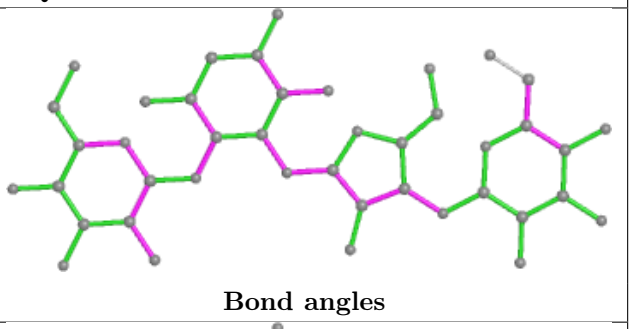
Ligand PAR XA 1670



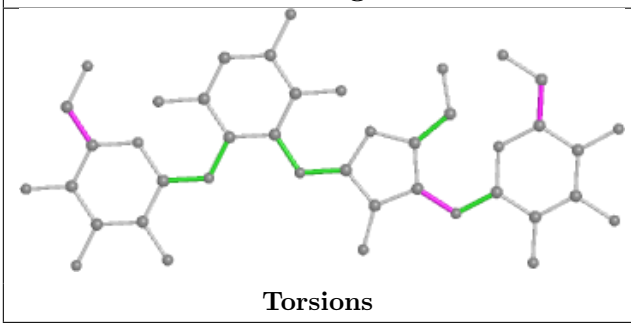
Ligand PAR QA 1663



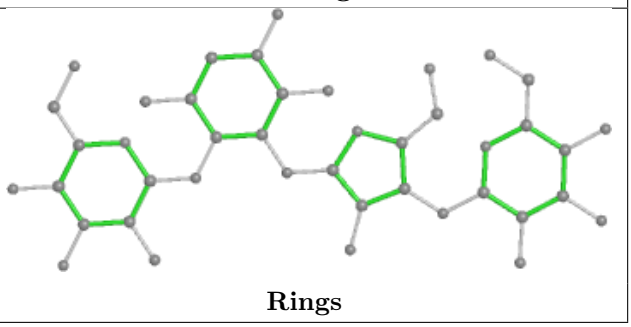
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.