Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 12:45 PM EDT

PDB ID	:	6OXI
Title	:	Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (UAA)
Authors	:	Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-05-13
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

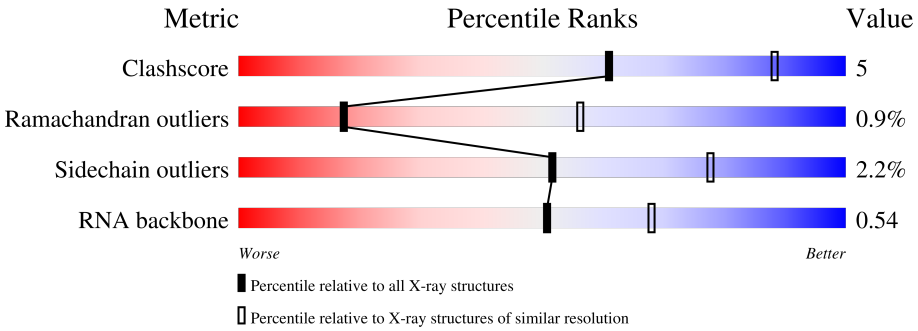
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1521	61% 31% 7%
1	XA	1521	63% 28% 8%
2	QB	256	70% 19% 8%
2	XB	256	76% 15% 8%
3	QC	239	75% 10% 14%
3	XC	239	72% 13% 14%

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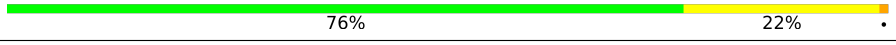
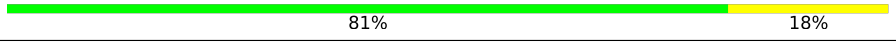
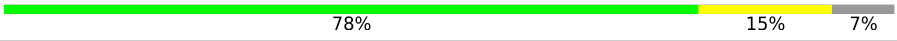
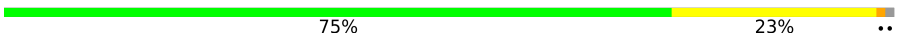
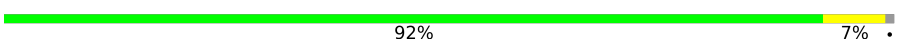
Mol	Chain	Length	Quality of chain
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	

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Mol	Chain	Length	Quality of chain
16	XP	88	85% 8% • 5%
17	QQ	105	84% 10% • 5%
17	XQ	105	78% 16% • 5%
18	QR	88	59% 19% • 20%
18	XR	88	63% 16% • 20%
19	QS	93	68% 18% • • 11%
19	XS	93	73% 16% 11%
20	QT	106	82% 11% 7%
20	XT	106	70% 23% • 7%
21	QU	27	67% 22% • 7%
21	XU	27	70% 22% 7%
22	QV	77	78% 22%
22	XV	77	81% 17% •
23	QX	20	35% 45% 10% 10%
23	XX	20	35% 40% 15% 10%
24	QY	84	77% 23%
24	QZ	84	74% 23% •
24	XY	84	79% 21%
24	XZ	84	81% 18% •
25	R0	85	74% 20% • 5%
25	Y0	85	75% 20% • •
26	R1	98	85% 9% • •
26	Y1	98	77% 22% •
27	R2	72	68% 26% • •
27	Y2	72	85% 11% •

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Mol	Chain	Length	Quality of chain
28	R3	60	82% 17%
28	Y3	60	83% 15%
29	R4	71	59% 30% 6%
29	Y4	71	76% 18%
30	R5	60	72% 27%
30	Y5	60	85% 13%
31	R6	54	72% 22%
31	Y6	54	85% 13%
32	R7	49	88% 8%
32	Y7	49	84% 14%
33	R8	65	74% 17% 6%
33	Y8	65	71% 23% 5%
34	R9	37	70% 30%
34	Y9	37	81% 19%
35	RA	2915	61% 31% 6%
35	YA	2915	64% 29% 6%
36	RB	124	57% 33%
36	YB	124	63% 24% 9%
37	RD	276	76% 20%
37	YD	276	89% 9%
38	RE	206	73% 25%
38	YE	206	81% 18%
39	RF	210	87% 9%
39	YF	210	78% 17%
40	RG	182	80% 18%

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Mol	Chain	Length	Quality of chain
40	YG	182	80% 18%
41	RH	180	78% 17%
41	YH	180	84% 12%
42	RI	148	76% 16%
42	YI	148	86% 9%
43	RN	140	79% 17%
43	YN	140	83% 14%
44	RO	122	78% 22%
44	YO	122	80% 20%
45	RP	150	75% 23%
45	YP	150	81% 19%
46	RQ	141	73% 24%
46	YQ	141	82% 18%
47	RR	118	81% 16%
47	YR	118	81% 16%
48	RS	112	78% 21%
48	YS	112	79% 20%
49	RT	146	69% 23% 6%
49	YT	146	77% 16% 6%
50	RU	118	82% 15%
50	YU	118	84% 14%
51	RV	101	74% 21%
51	YV	101	74% 21% 5%
52	RW	113	88% 11%
52	YW	113	79% 21%

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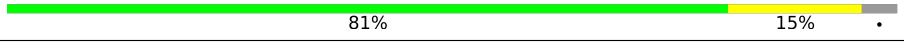
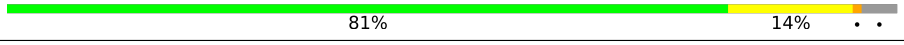
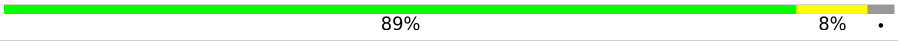
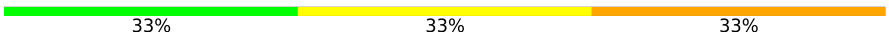
Mol	Chain	Length	Quality of chain
53	RX	96	
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	
56	ZA	3	
56	ZB	3	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 295153 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	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	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 tRNA-fMet.

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 394	C 176	N 79	O 121	P 18	0	0	0
23	XX	18	Total 394	C 176	N 79	O 121	P 18	0	0	0

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	84	Total 723	C 464	N 126	O 131	S 2	0	0	0
24	QZ	84	Total 723	C 464	N 126	O 131	S 2	0	0	0
24	XY	84	Total 723	C 464	N 126	O 131	S 2	0	0	0
24	XZ	84	Total 723	C 464	N 126	O 131	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	81	Total 643	C 398	N 137	O 107	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	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
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	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	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	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	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	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- 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
			2576	1146	476	834	120			
36	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- 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	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	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	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	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	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
41	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
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	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	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	117	Total	C	N	O	0	0	0
			960	599	202	159			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called CCPuro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	93	Total	Mg	0	0
			93	93		
57	QD	1	Total	Mg	0	0
			1	1		
57	QE	1	Total	Mg	0	0
			1	1		
57	QV	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QY	1	Total Mg 1 1	0	0
57	R0	2	Total Mg 2 2	0	0
57	R3	1	Total Mg 1 1	0	0
57	RA	302	Total Mg 302 302	0	0
57	RB	3	Total Mg 3 3	0	0
57	RD	2	Total Mg 2 2	0	0
57	RE	1	Total Mg 1 1	0	0
57	RN	1	Total Mg 1 1	0	0
57	RO	1	Total Mg 1 1	0	0
57	RP	1	Total Mg 1 1	0	0
57	RQ	4	Total Mg 4 4	0	0
57	RR	1	Total Mg 1 1	0	0
57	RY	1	Total Mg 1 1	0	0
57	XA	99	Total Mg 99 99	0	0
57	XE	1	Total Mg 1 1	0	0
57	XF	1	Total Mg 1 1	0	0
57	XL	1	Total Mg 1 1	0	0
57	XM	1	Total Mg 1 1	0	0
57	XV	4	Total Mg 4 4	0	0
57	Y0	2	Total Mg 2 2	0	0
57	Y1	1	Total Mg 1 1	0	0

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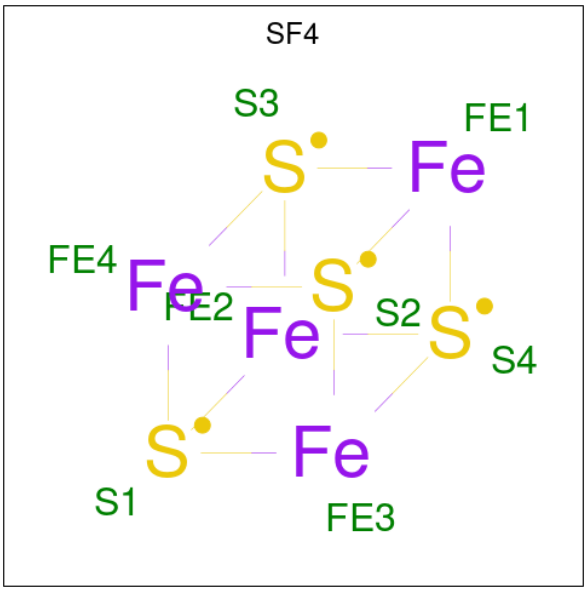
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y3	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0
57	Y9	1	Total Mg 1 1	0	0
57	YA	335	Total Mg 335 335	0	0
57	YB	3	Total Mg 3 3	0	0
57	YD	4	Total Mg 4 4	0	0
57	YE	5	Total Mg 5 5	0	0
57	YF	1	Total Mg 1 1	0	0
57	YG	1	Total Mg 1 1	0	0
57	YO	1	Total Mg 1 1	0	0
57	YP	1	Total Mg 1 1	0	0
57	YQ	5	Total Mg 5 5	0	0
57	YR	1	Total Mg 1 1	0	0
57	YV	1	Total Mg 1 1	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	R4	1	Total Zn 1 1	0	0
59	R5	1	Total Zn 1 1	0	0
59	R6	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	Y4	1	Total Zn 1 1	0	0
59	Y6	1	Total Zn 1 1	0	0

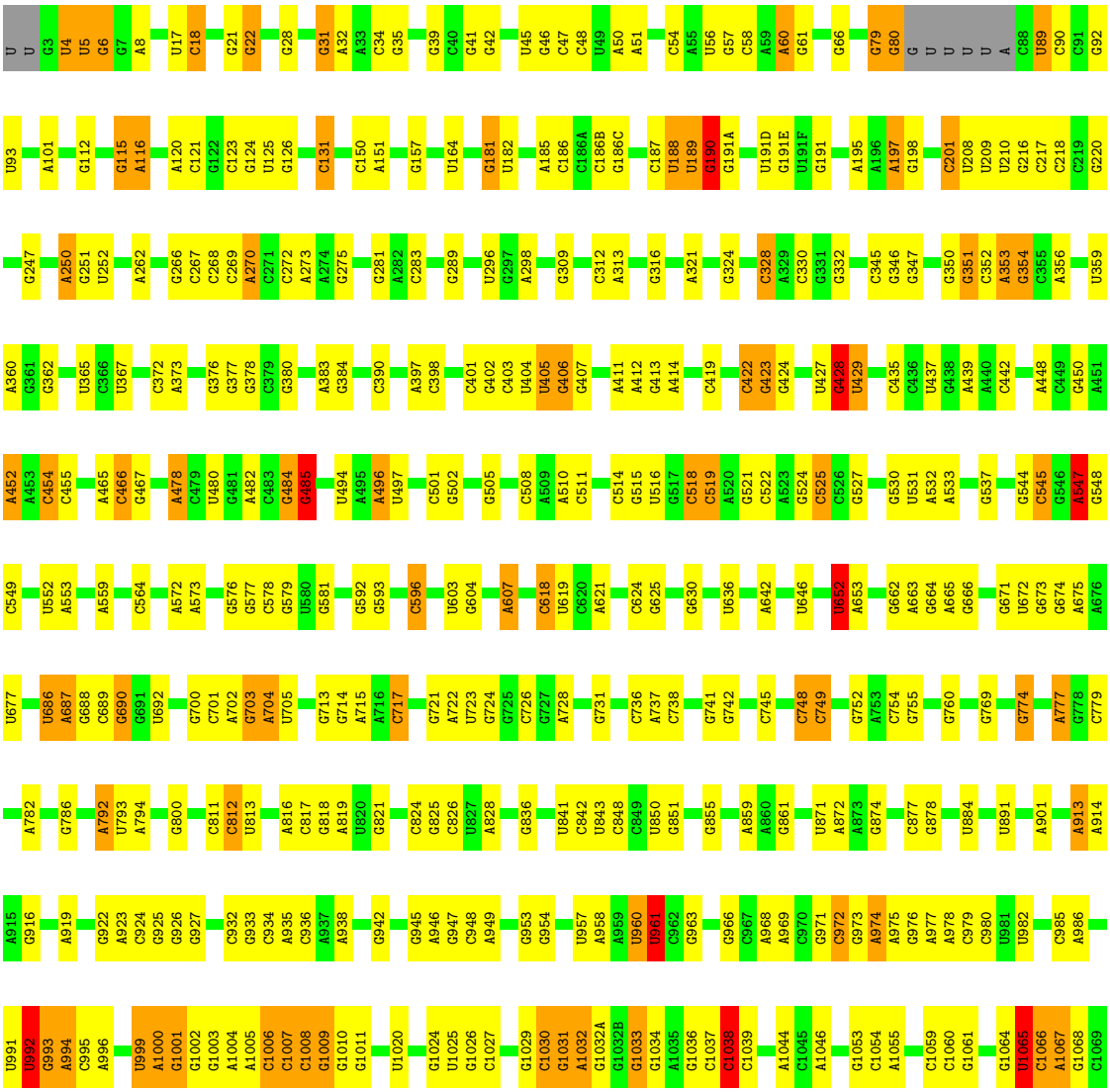
3 Residue-property plots (i)

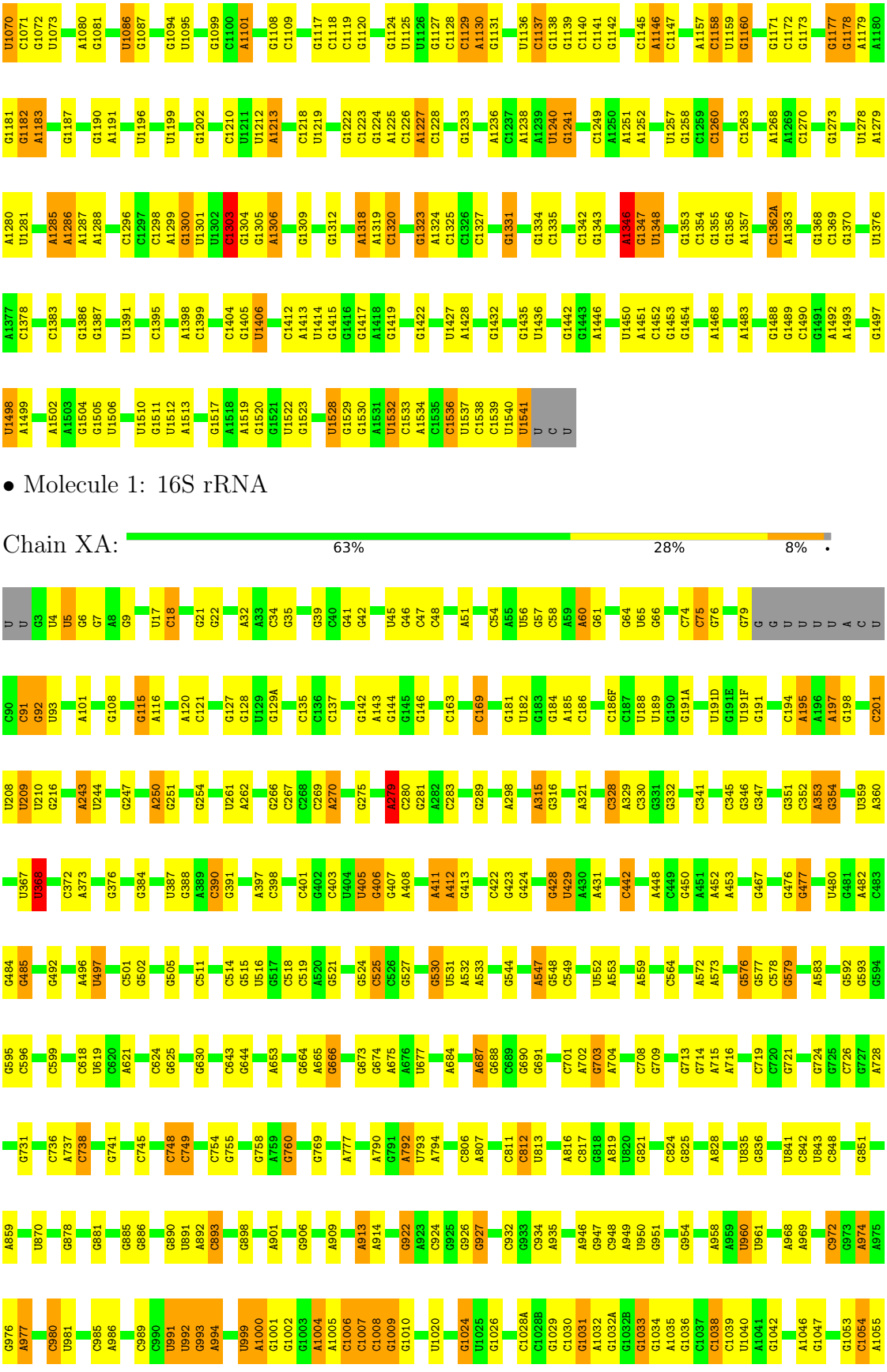
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

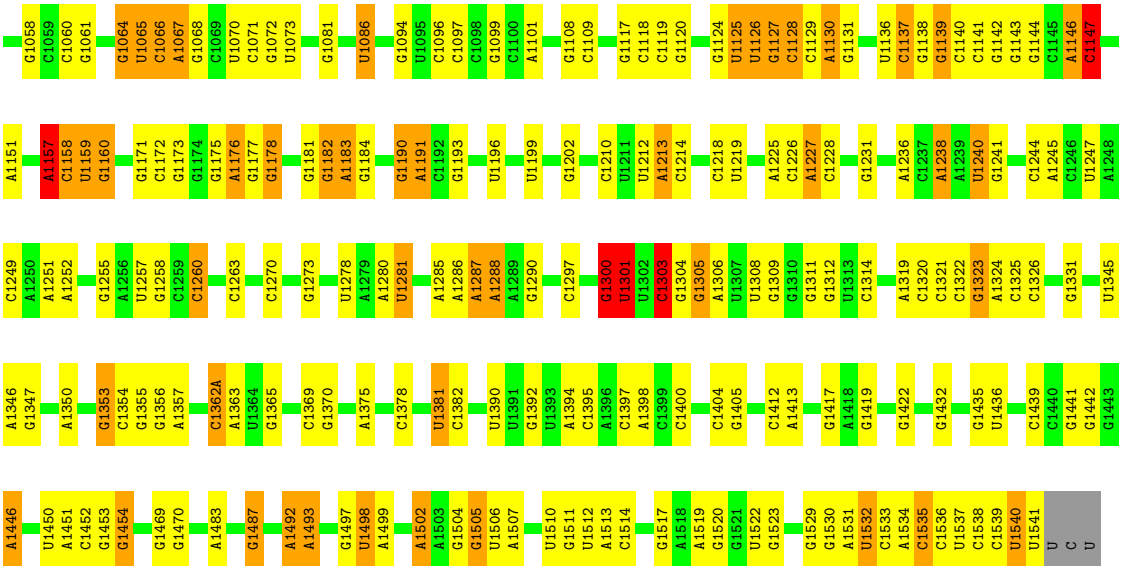
Chain QA:





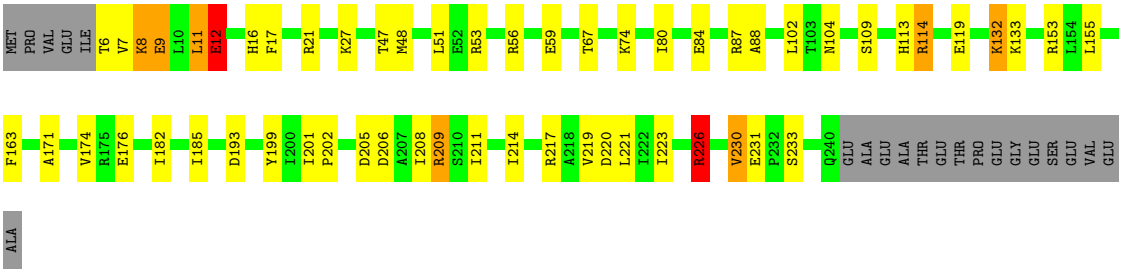
• Molecule 1: 16S rRNA

Chain XA:



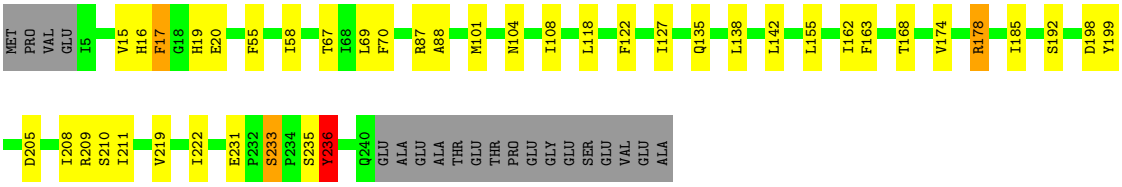
• Molecule 2: 30S ribosomal protein S2

Chain QB:



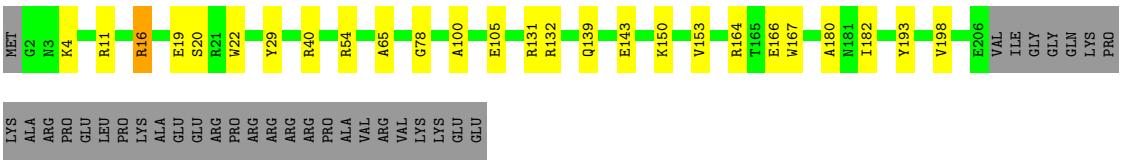
• Molecule 2: 30S ribosomal protein S2

Chain XB:



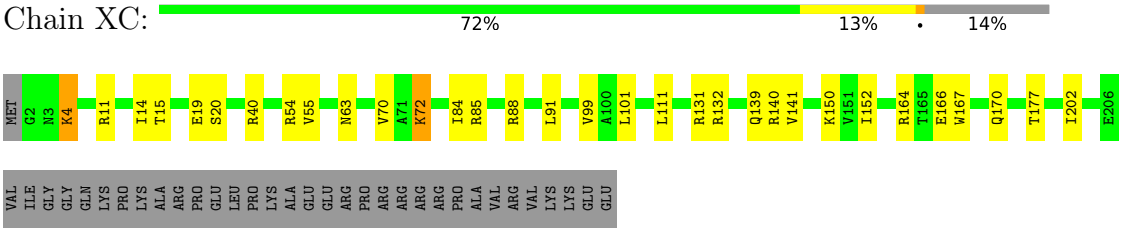
• Molecule 3: 30S ribosomal protein S3

Chain QC:



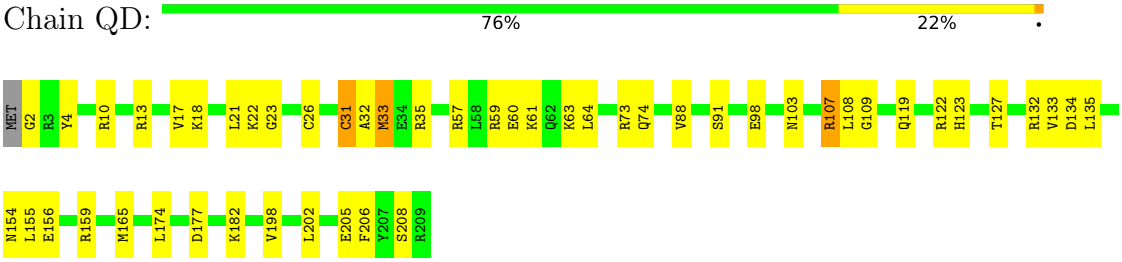
• Molecule 3: 30S ribosomal protein S3

Chain XC:



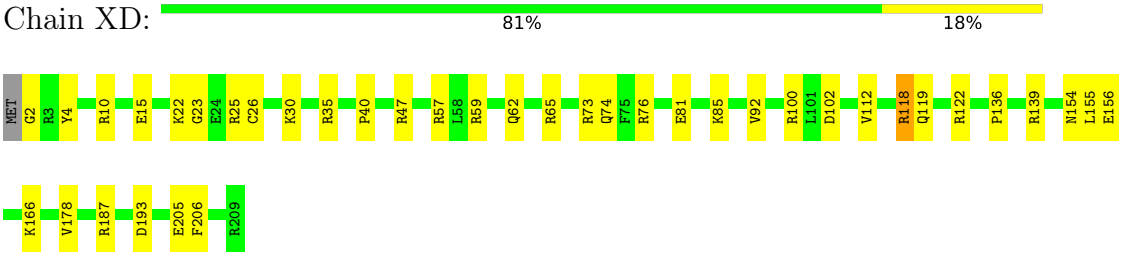
• Molecule 4: 30S ribosomal protein S4

Chain QD:



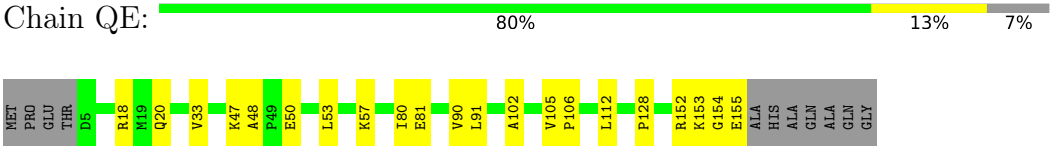
• Molecule 4: 30S ribosomal protein S4

Chain XD:



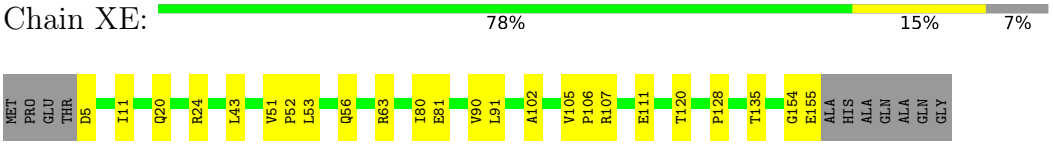
• Molecule 5: 30S ribosomal protein S5

Chain QE:



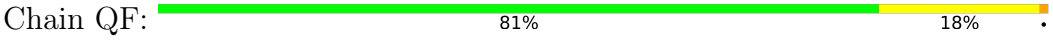
• Molecule 5: 30S ribosomal protein S5

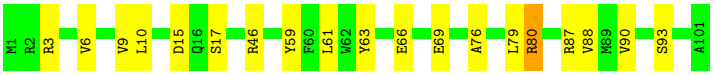
Chain XE:



• Molecule 6: 30S ribosomal protein S6

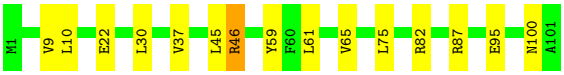
Chain QF:





• 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

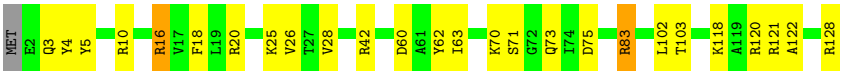
Chain QH:

• Molecule 8: 30S ribosomal protein S8

Chain XH:

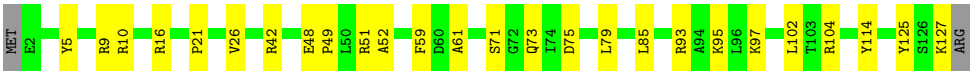
• Molecule 9: 30S ribosomal protein S9

Chain QI:



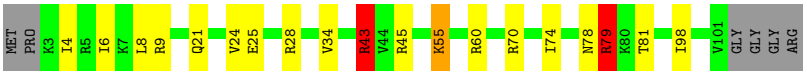
• Molecule 9: 30S ribosomal protein S9

Chain XI:



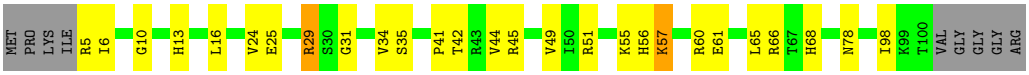
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



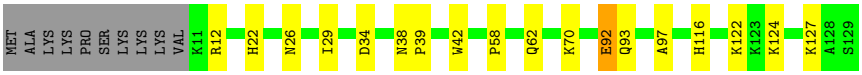
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



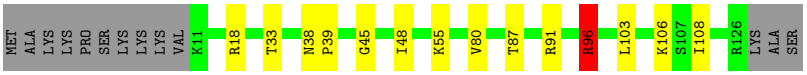
• Molecule 11: 30S ribosomal protein S11

Chain QK:



• Molecule 11: 30S ribosomal protein S11

Chain XK:

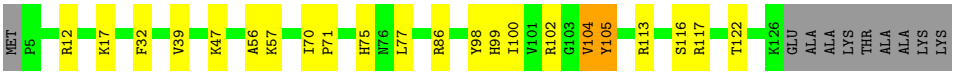


• Molecule 12: 30S ribosomal protein S12

Chain QL:

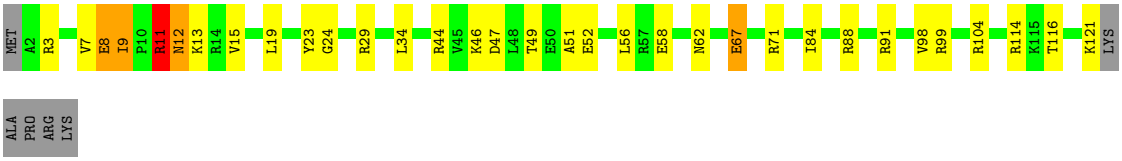
• Molecule 12: 30S ribosomal protein S12

Chain XL:



• Molecule 13: 30S ribosomal protein S13

Chain QM:

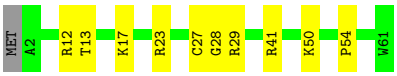


• Molecule 13: 30S ribosomal protein S13

Chain XM:

• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:

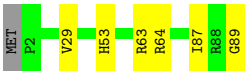


• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:

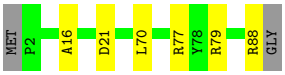
• Molecule 15: 30S ribosomal protein S15

Chain QO:



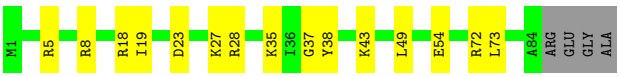
• Molecule 15: 30S ribosomal protein S15

Chain XO:



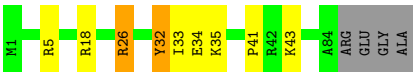
• Molecule 16: 30S ribosomal protein S16

Chain QP:



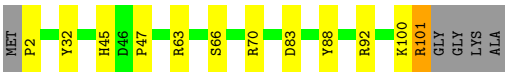
• Molecule 16: 30S ribosomal protein S16

Chain XP:



• Molecule 17: 30S ribosomal protein S17

Chain QQ:

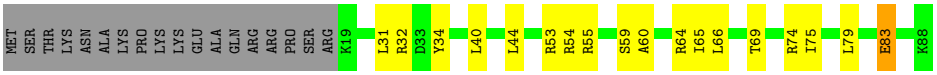


• Molecule 17: 30S ribosomal protein S17

Chain XQ:

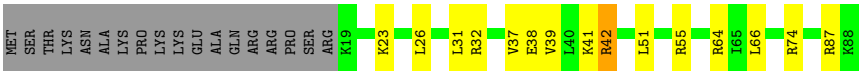
• Molecule 18: 30S ribosomal protein S18

Chain QR:



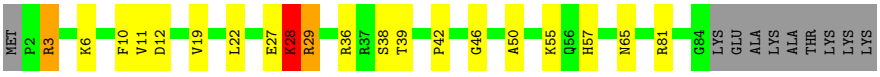
• Molecule 18: 30S ribosomal protein S18

Chain XR:



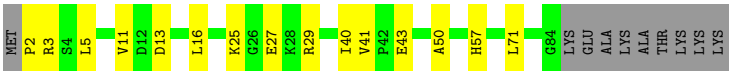
• Molecule 19: 30S ribosomal protein S19

Chain QS:



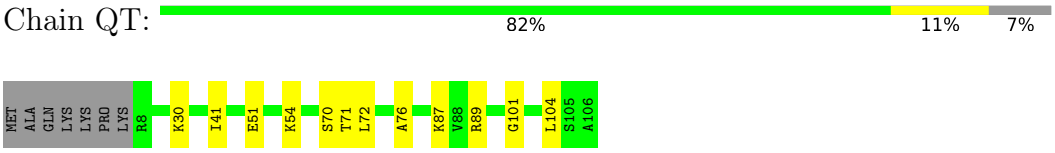
• Molecule 19: 30S ribosomal protein S19

Chain XS:



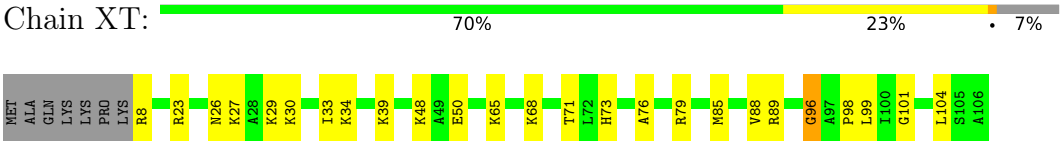
• Molecule 20: 30S ribosomal protein S20

Chain QT:



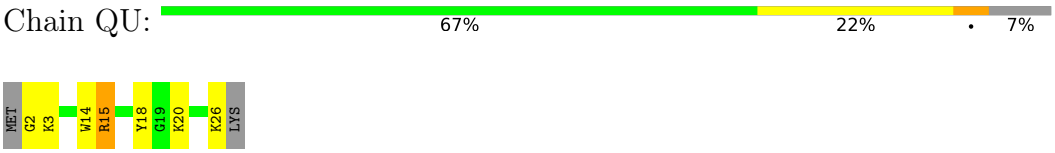
• Molecule 20: 30S ribosomal protein S20

Chain XT:



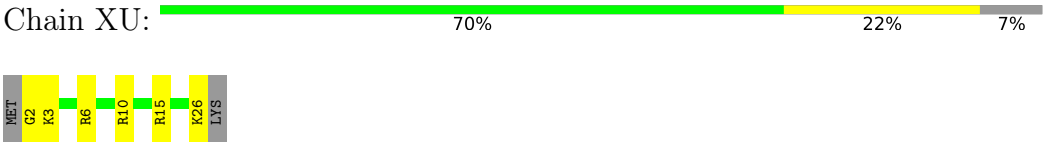
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



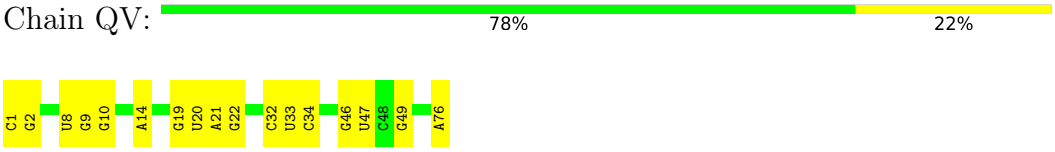
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



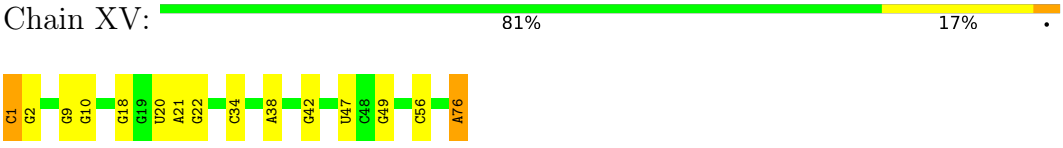
• Molecule 22: P-site tRNA-fMet

Chain QV:



• Molecule 22: P-site tRNA-fMet

Chain XV:



• Molecule 23: mRNA

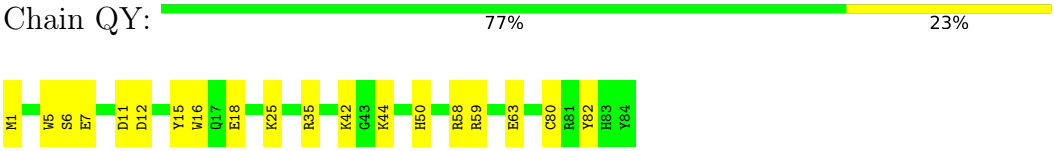
Chain QX:

• Molecule 23: mRNA

Chain XX:

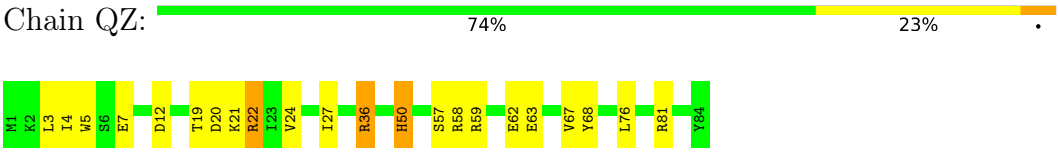
• Molecule 24: Addition module toxin, Txe/YoeB family

Chain QY:



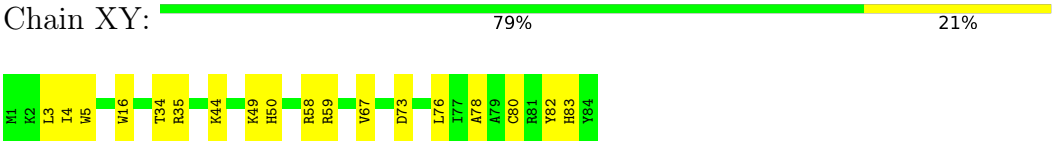
• Molecule 24: Addition module toxin, Txe/YoeB family

Chain QZ:



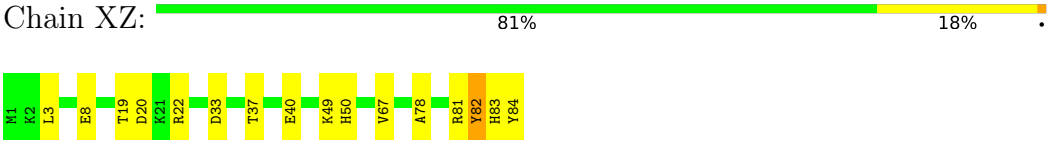
• Molecule 24: Addition module toxin, Txe/YoeB family

Chain XY:



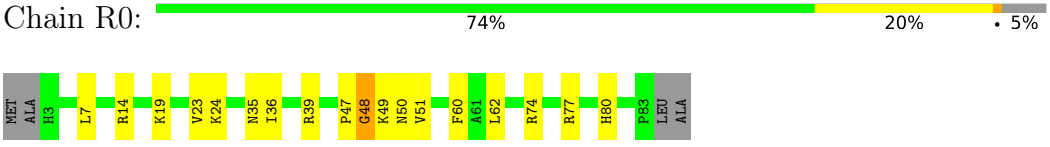
• Molecule 24: Addition module toxin, Txe/YoeB family

Chain XZ:



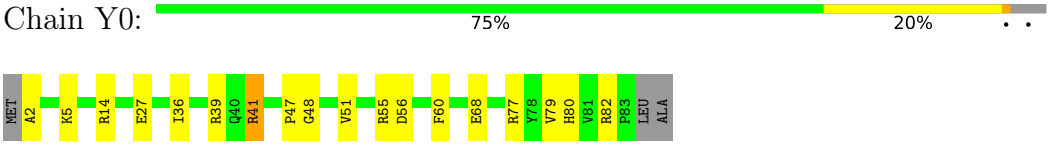
• Molecule 25: 50S ribosomal protein L27

Chain R0:



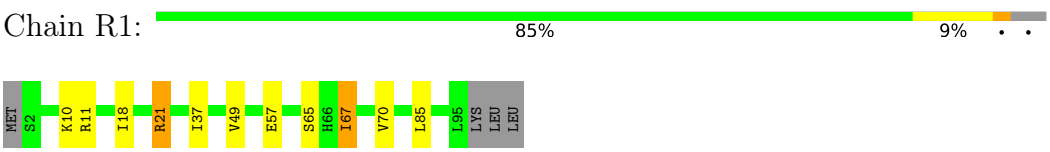
• Molecule 25: 50S ribosomal protein L27

Chain Y0:



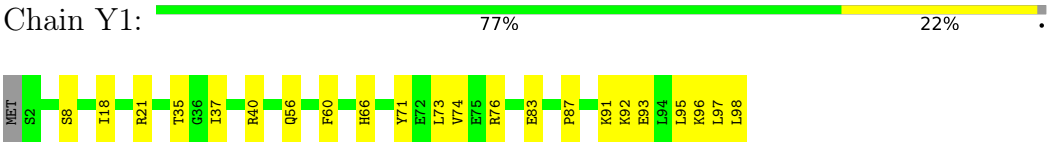
• Molecule 26: 50S ribosomal protein L28

Chain R1:



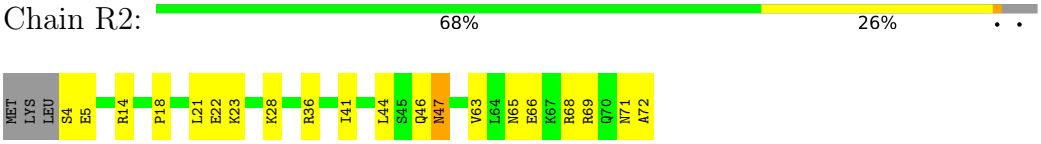
• Molecule 26: 50S ribosomal protein L28

Chain Y1:



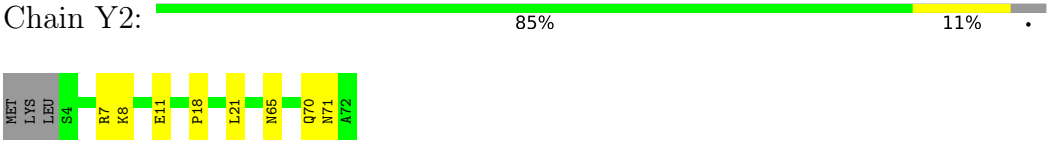
• Molecule 27: 50S ribosomal protein L29

Chain R2:



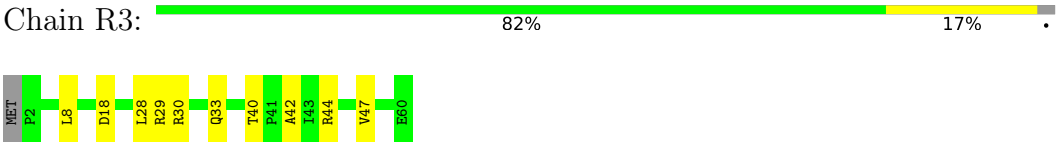
• Molecule 27: 50S ribosomal protein L29

Chain Y2:



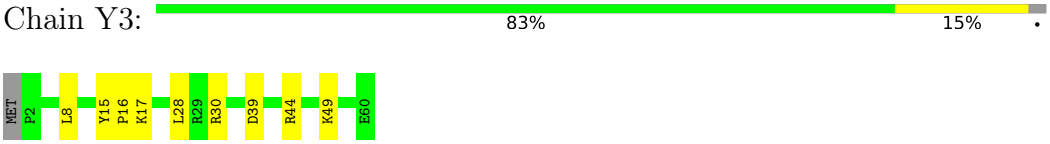
• Molecule 28: 50S ribosomal protein L30

Chain R3:



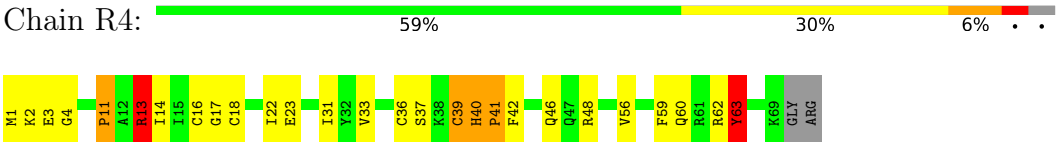
• Molecule 28: 50S ribosomal protein L30

Chain Y3:



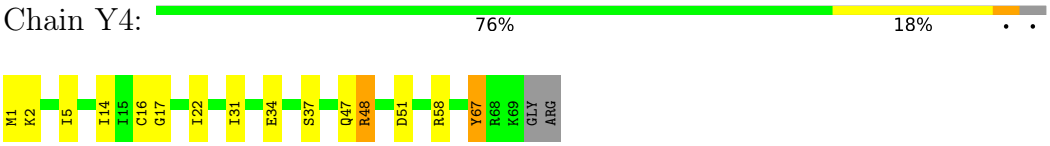
• Molecule 29: 50S ribosomal protein L31

Chain R4:



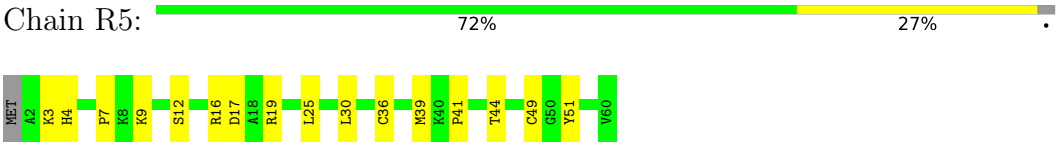
• Molecule 29: 50S ribosomal protein L31

Chain Y4:



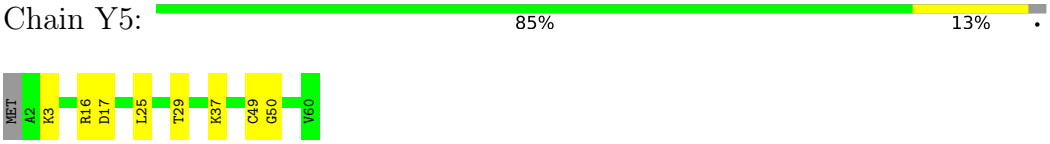
• Molecule 30: 50S ribosomal protein L32

Chain R5:



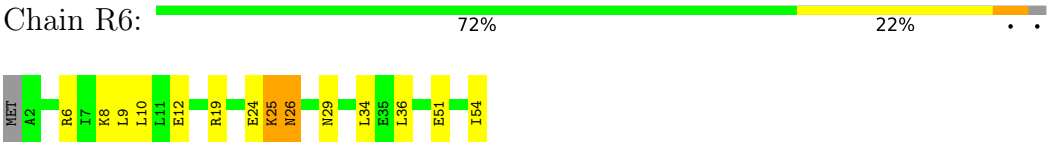
• Molecule 30: 50S ribosomal protein L32

Chain Y5:



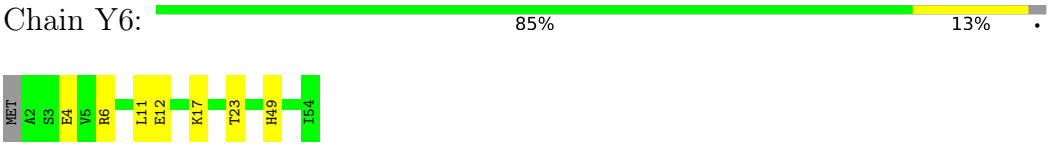
• Molecule 31: 50S ribosomal protein L33

Chain R6:



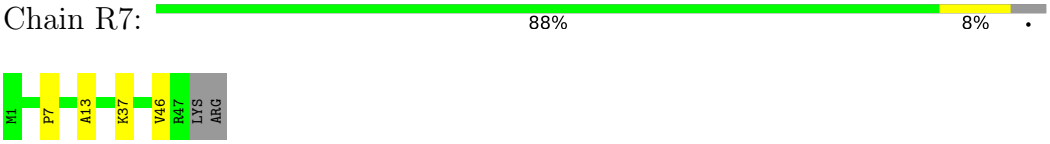
• Molecule 31: 50S ribosomal protein L33

Chain Y6:



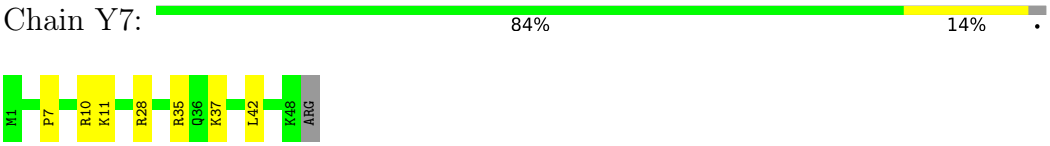
• Molecule 32: 50S ribosomal protein L34

Chain R7:



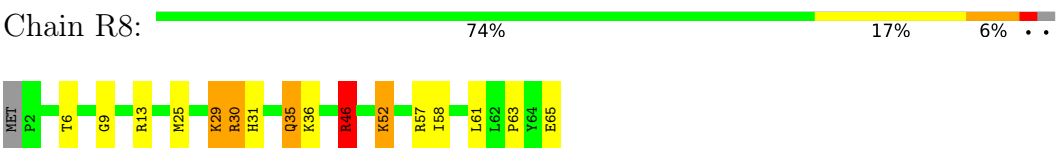
• Molecule 32: 50S ribosomal protein L34

Chain Y7:



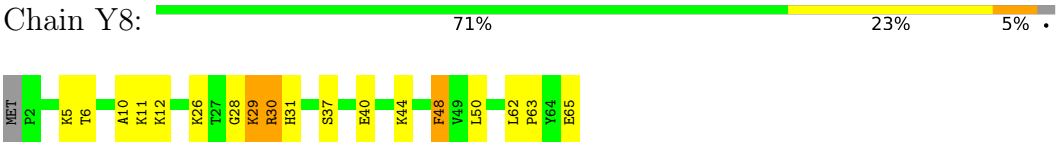
• Molecule 33: 50S ribosomal protein L35

Chain R8:



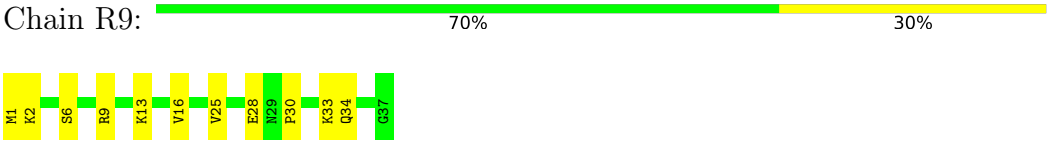
• Molecule 33: 50S ribosomal protein L35

Chain Y8:



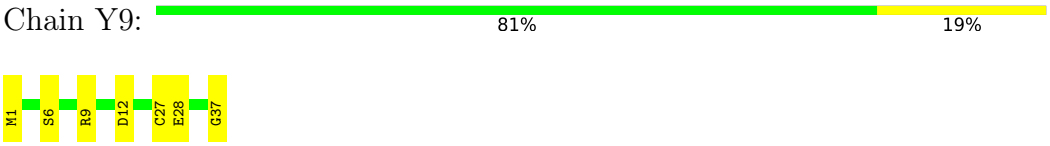
• Molecule 34: 50S ribosomal protein L36

Chain R9:



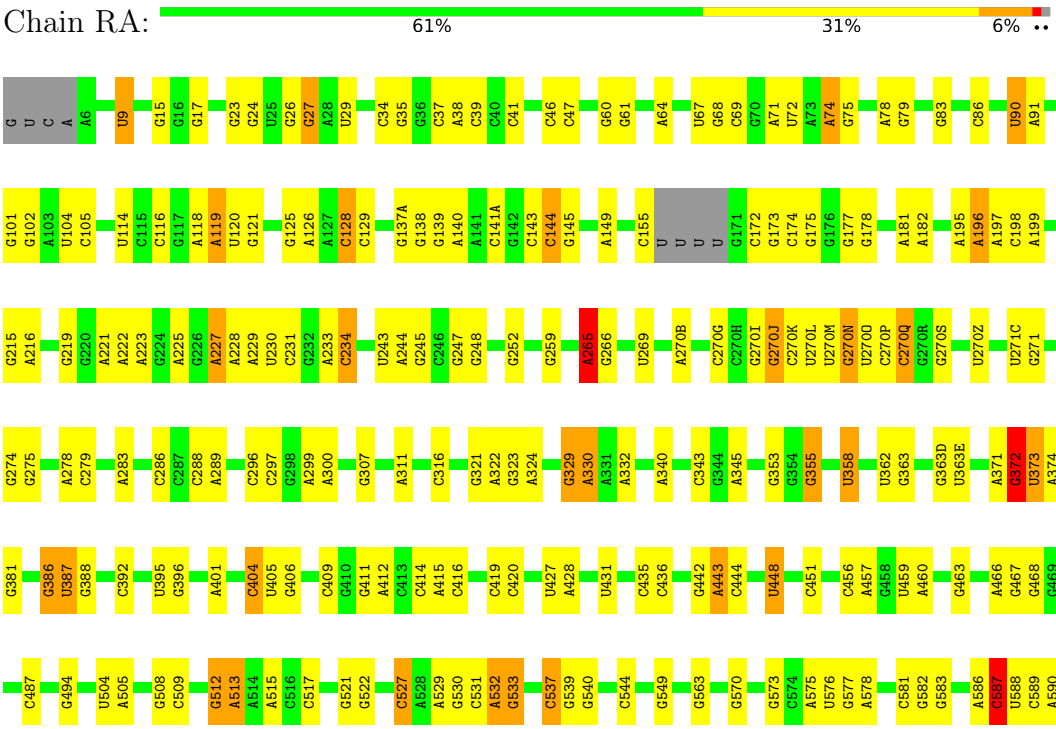
• Molecule 34: 50S ribosomal protein L36

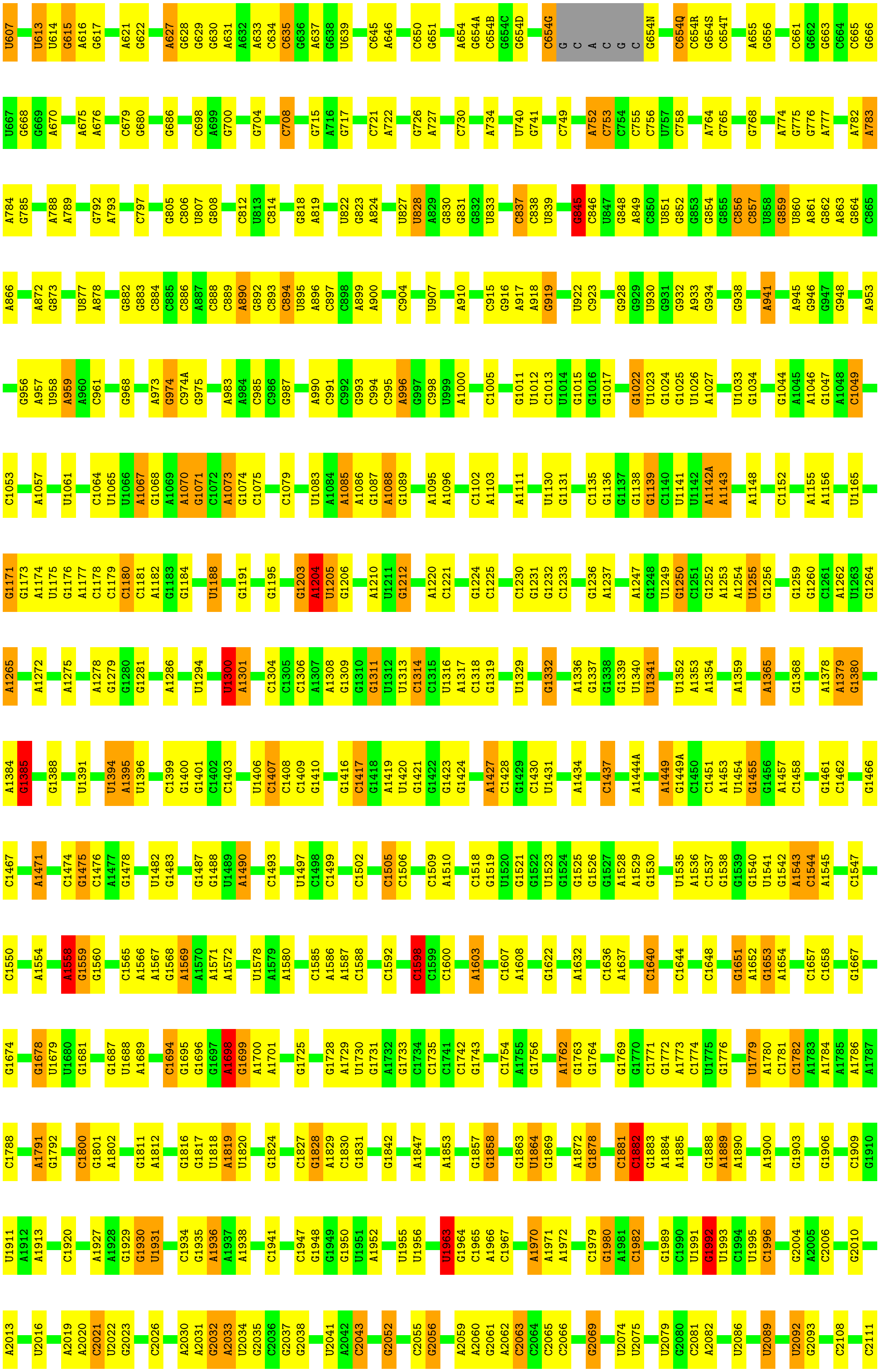
Chain Y9:



• Molecule 35: 23S rRNA

Chain RA:

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U667 G668 G669 A670 A675 A676 C679 G680 G686 C698 A699 G700 G704 C708 G715 A716 G717 C721 A722 G726 A727 C730 A734 U740 G741 C749 A752 C753 C754 C755 C756 U757 C758 A764 G765 G768 A774 G775 G776 A777 A782 A783
A784 G785 A788 A789 G792 A793 C797 G805 C806 U807 G808 C812 U813 C814 G818 A819 U822 G823 A824 U827 U828 A829 G830 G831 G832 U833 C837 C838 U839 C845 C846 U847 G848 A849 C850 U851 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865
A866 A872 G873 U877 A878 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 C904 U907 A910 C915 G916 A917 A918 G919 U922 C923 G928 G929 U930 G931 G932 A933 G934 G938 A941 A945 G946 G947 G948 A953
G956 A957 U958 A959 A960 C961 G968 A973 G974 C974A G975 A983 A984 C985 C986 G987 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 C1005 G1011 U1012 C1013 U1014 G1015 G1016 G1017 G1022 U1023 G1024 G1025 U1026 A1027 U1033 G1034 G1044 A1045 A1046 G1047 A1048 C1049
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G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 U1188 G1191 G1195 G1203 A1204 U1205 G1206 A1210 U1211 G1212 A1220 C1221 G1224 C1225 C1230 G1231 G1232 C1233 G1236 A1237 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 G1259 G1260 C1261 A1262 U1263 G1264
A1265 A1272 A1275 A1278 G1279 G1280 G1281 A1286 U1294 U1300 A1301 C1304 C1305 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 U1329 G1332 A1336 G1337 G1338 G1339 U1340 U1341 U1352 A1353 A1354 A1359 A1365 G1368 A1378 A1379 G1380
A1384 G1385 G1388 U1391 U1394 A1395 U1396 C1399 G1400 G1401 C1402 C1403 U1406 C1407 C1408 C1409 G1410 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 G1429 C1430 U1431 A1434 C1437 A1444A A1449 G1449A C1450 C1451 A1453 U1454 G1455 G1456 A1457 C1458 G1461 C1462 G1466
C1467 A1471 C1474 G1475 C1476 A1477 G1478 U1482 G1483 G1487 G1488 U1489 A1490 C1493 U1497 C1498 C1499 C1502 C1505 C1506 C1509 A1510 C1518 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 G1527 A1528 A1529 G1530 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 C1547
C1550 A1554 A1558 G1559 G1560 C1565 A1566 A1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 C1585 A1586 A1587 C1588 C1592 C1598 C1599 C1600 A1603 C1607 A1608 G1622 A1632 C1636 A1637 C1640 C1644 C1648 G1651 A1652 G1653 A1654 C1657 C1658 G1667
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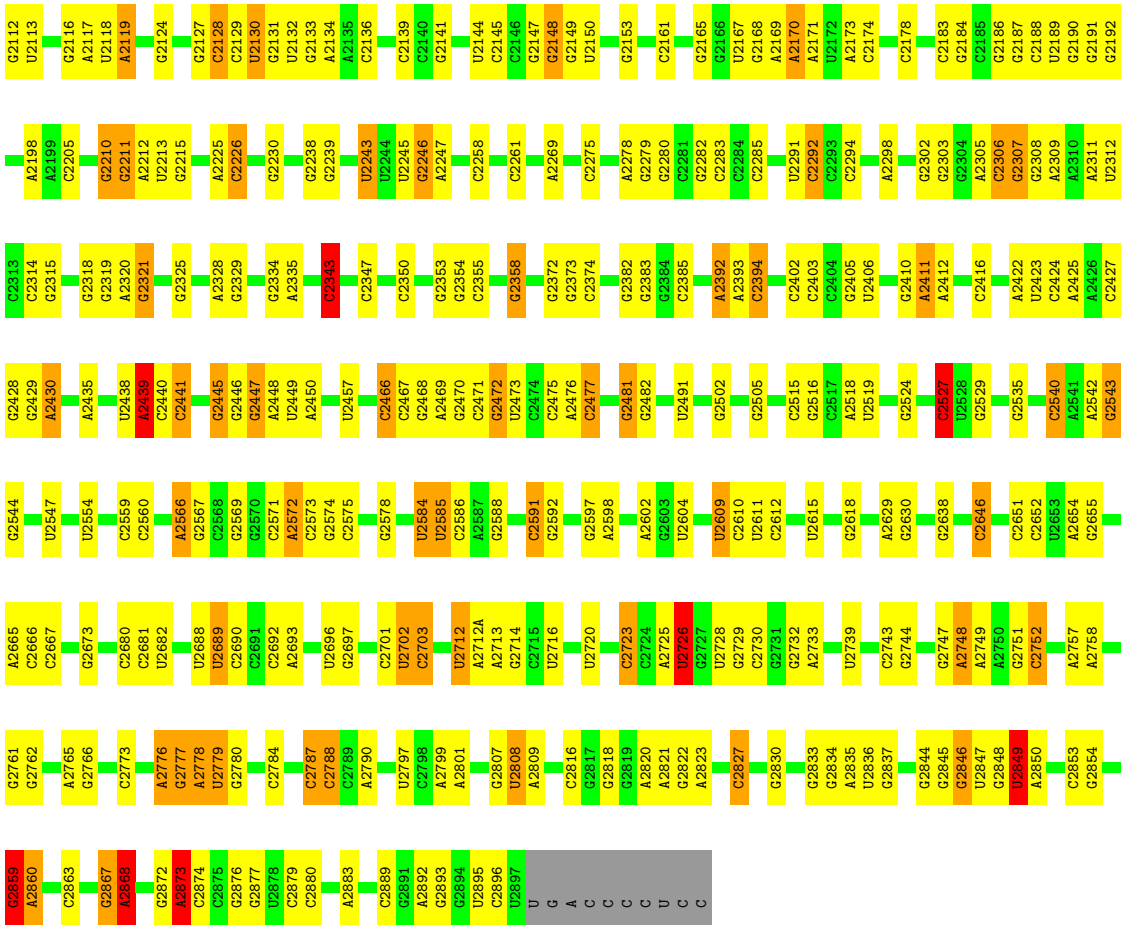
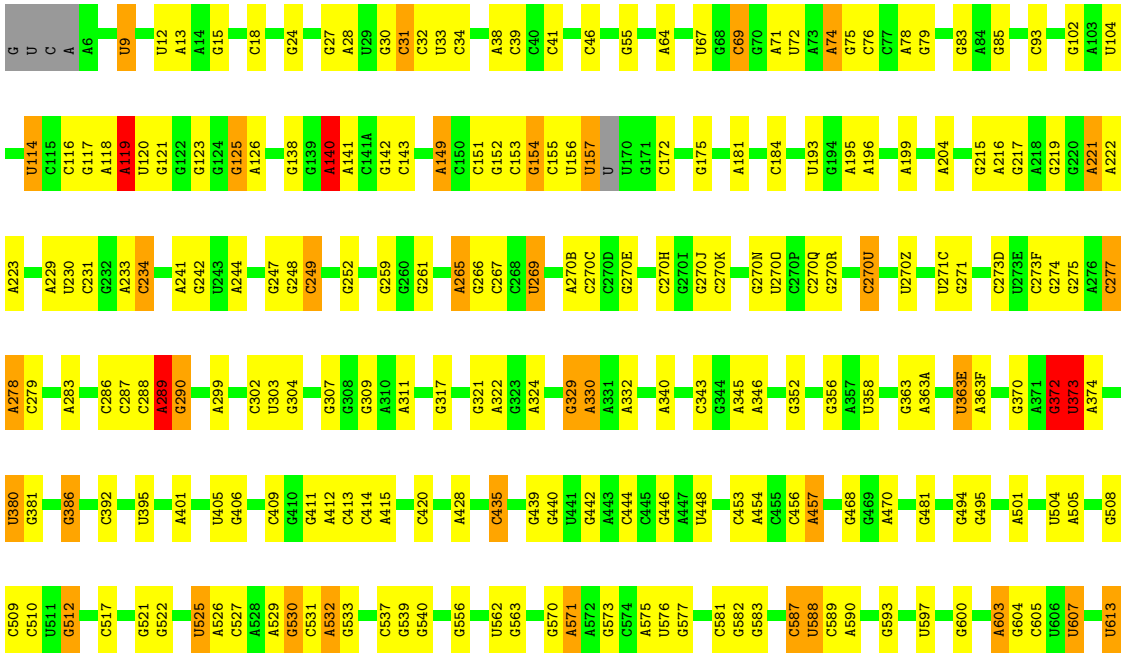
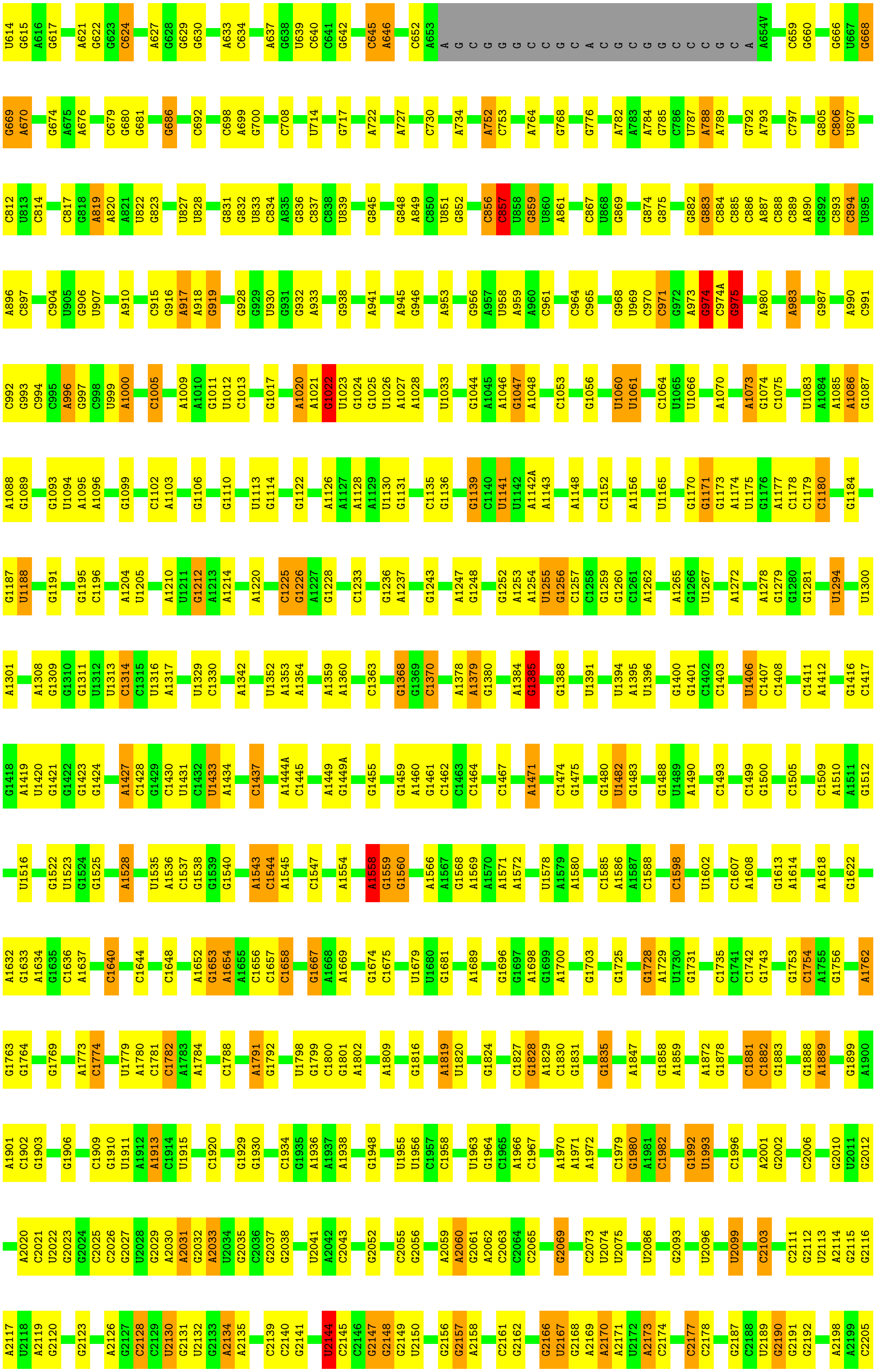
C1788 A1791 G1792 C1800 G1801 A1802 G1811 A1812 G1816 G1817 U1818 A1819 U1820 G1824 C1827 G1828 A1829 C1830 G1831 G1842 A1847 A1853 G1857 G1858 G1863 U1864 G1869 A1872 G1878 C1881 C1882 G1883 A1884 A1885 G1888 A1889 A1890 A1900 G1903 G1906 C1909 G1910
U1911 A1912 A1913 C1920 A1927 A1928 G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 C1941 C1947 G1948 G1949 G1950 U1951 A1952 U1955 U1956 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 C1979 G1980 A1981 C1982 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G2004 A2005 C2006 G2010
A2013 U2016 A2019 A2020 C2021 U2022 G2023 C2026 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 U2041 A2042 C2043 G2052 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 U2074 U2075 U2079 G2080 C2081 A2082 U2086 U2089 U2092 G2093 C2108 C2111

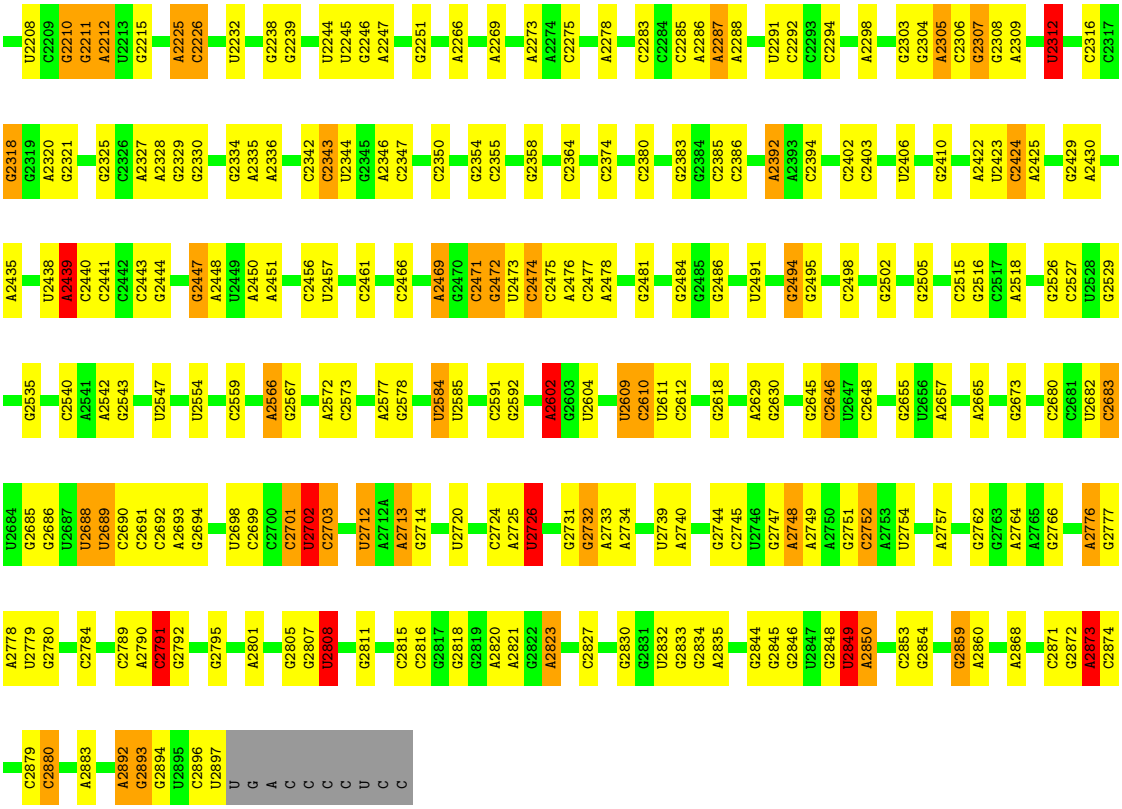


• Molecule 35: 23S rRNA

Chain YA:




U614 G615 A616 G617 A621 G622 G623 C624 A627 G628 G629 G630 A633 C634 A637 G638 U639 C640 C641 G642 C645 A646 C652 A653 A G C G G G C C G C A C G C G G C C C G C A A654V C659 G660 G666 U667 G668
G669 A670 G674 A675 A676 C679 G680 G681 G686 C692 C698 A699 G700 C708 U714 G717 A722 A727 C730 A734 A752 C753 A764 G768 G776 A782 A783 A784 G785 C786 U787 A788 A789 G792 A793 C797 G805 C806 U807
C812 U813 C814 C817 G818 A819 A820 A821 U822 G823 U827 U828 G831 G832 U833 C834 A835 G836 C837 C838 U839 G845 G848 A849 C850 U851 G852 C856 C857 U858 G859 U860 A861 C867 U868 G869 G874 G875 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895
A896 C897 C904 U905 G906 U907 A910 C915 G916 A917 A918 G919 G928 G929 U930 G931 G932 A933 G938 A941 A945 G946 A953 G956 A957 U958 A959 A960 C961 C964 C965 G968 U969 C970 C971 G972 A973 G974 C974A G975 A980 A983 G987 A990 C991
C992 G993 C994 C995 A996 G997 C998 U999 A1000 C1005 A1009 A1010 G1011 U1012 C1013 G1017 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 U1033 G1044 A1045 A1046 G1047 A1048 C1053 G1056 U1060 U1061 C1064 U1065 U1066 A1070 A1073 G1074 C1075 U1083 A1084 A1085 A1086 G1087
A1088 G1089 G1093 U1094 A1095 A1096 G1099 C1102 A1103 G1106 G1110 U1113 G1114 G1122 A1126 A1127 A1128 A1129 U1130 G1131 C1135 G1136 G1139 C1140 U1141 U1142 A1142A A1143 A1148 C1152 A1156 U1165 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1184
G1187 U1188 G1191 G1195 C1196 A1204 U1205 A1210 U1211 G1212 A1213 A1214 A1220 C1225 G1226 A1227 G1228 C1233 G1236 A1237 G1243 A1247 G1248 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 A1265 G1266 U1267 A1272 A1278 G1279 G1280 G1281 U1294 U1300
A1301 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 U1329 C1330 A1342 U1352 A1353 A1354 A1359 A1360 C1363 G1368 G1369 C1370 A1378 A1379 G1380 A1384 G1385 G1388 U1391 U1394 A1395 U1396 G1400 G1401 C1402 C1403 U1406 C1407 C1408 C1411 A1412 G1416 C1417
G1418 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 C1437 A1444A C1445 A1449 G1449A G1455 G1459 A1460 G1461 C1462 C1463 C1464 C1467 A1471 C1474 G1475 G1480 U1482 G1483 G1488 U1489 A1490 C1493 C1499 G1500 C1505 C1509 A1510 A1511 G1512
U1516 G1522 U1523 G1524 G1525 A1528 U1535 A1536 C1537 G1538 G1539 G1540 A1543 C1544 A1545 C1547 A1554 A1558 G1559 G1560 A1566 A1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 C1585 A1586 A1587 C1588 C1598 U1602 C1607 A1608 G1613 A1614 A1618 G1622
A1632 G1633 A1634 G1635 C1636 A1637 C1640 C1644 C1648 A1652 G1653 A1654 A1655 C1656 C1657 C1658 G1667 A1668 A1669 G1674 C1675 U1679 U1680 G1681 A1689 G1696 G1697 A1698 G1699 A1700 G1703 G1725 G1728 A1729 U1730 G1731 C1735 C1741 C1742 G1743 G1753 C1754 A1755 G1756 A1762
G1763 G1764 G1769 A1773 C1774 U1779 A1780 C1781 C1782 A1783 A1784 C1788 A1791 G1792 U1798 G1799 C1800 G1801 A1802 A1809 G1816 A1819 U1820 G1824 C1827 G1828 A1829 C1830 G1831 G1835 A1847 G1858 A1859 A1872 G1878 C1881 C1882 G1883 G1888 A1889 G1899 A1900
A1901 C1902 G1903 G1906 C1909 G1910 U1911 A1912 A1913 C1914 U1915 C1920 G1929 G1930 C1934 G1935 A1936 A1937 A1938 G1948 U1955 U1956 C1957 C1958 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 C1979 G1980 A1981 C1982 G1992 U1993 C1996 A2001 G2002 C2006 G2010 U2011 G2012
A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 U2041 A2042 C2043 G2052 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 G2069 C2073 U2074 U2075 U2086 G2093 U2096 U2099 C2103 C2111 G2112 U2113 A2114 G2115 G2116
A2117 U2118 A2119 G2120 G2123 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2139 C2140 G2141 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2156 G2157 A2158 C2161 G2162 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2177 C2178 G2187 C2188 U2189 G2190 G2191 G2192 A2198 A2199 C2205

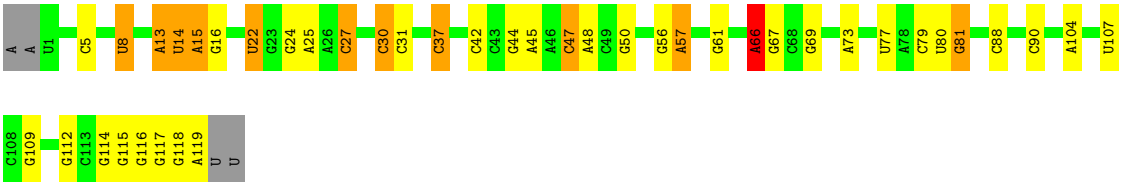


• Molecule 36: 5S rRNA

Chain RB:

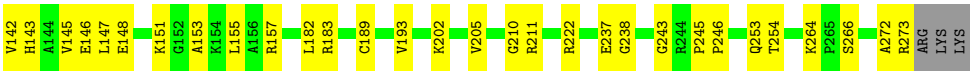
• Molecule 36: 5S rRNA

Chain YB:



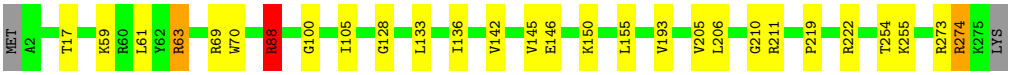
• Molecule 37: 50S ribosomal protein L2

Chain RD:



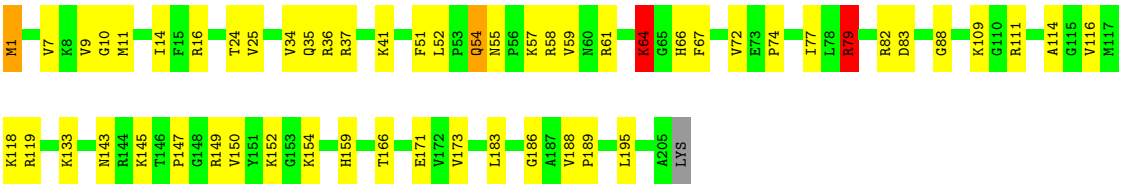
• Molecule 37: 50S ribosomal protein L2

Chain YD:



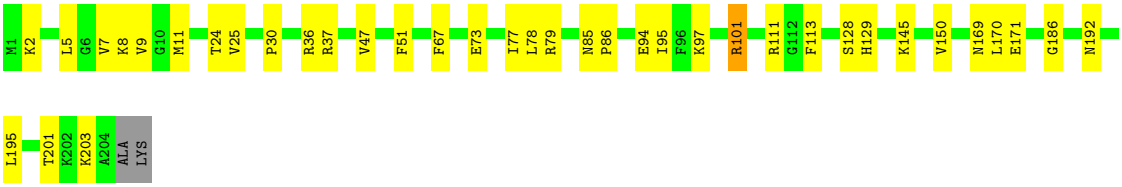
• Molecule 38: 50S ribosomal protein L3

Chain RE:



• Molecule 38: 50S ribosomal protein L3

Chain YE:

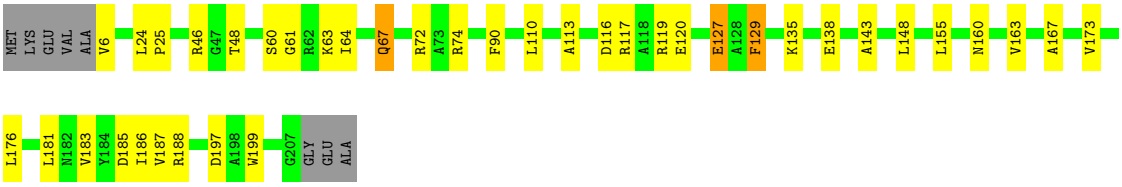


• Molecule 39: 50S ribosomal protein L4

Chain RF:

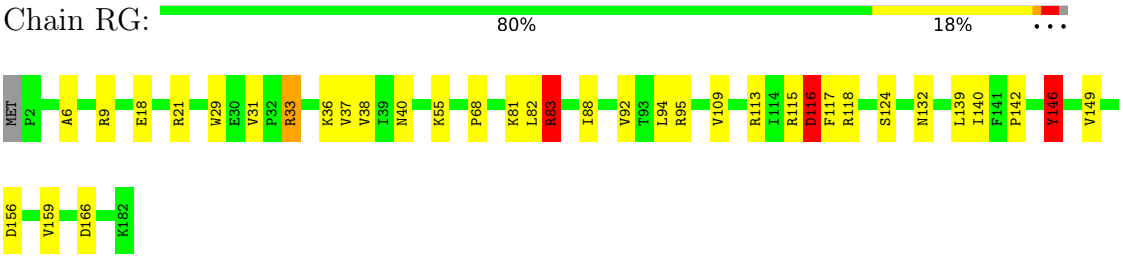
• Molecule 39: 50S ribosomal protein L4

Chain YF:



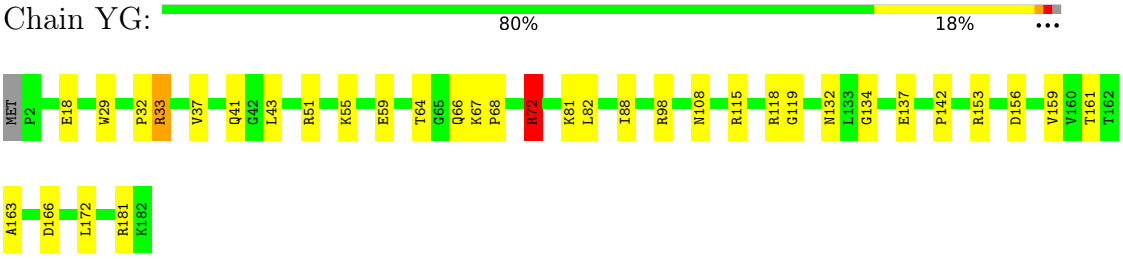
• Molecule 40: 50S ribosomal protein L5

Chain RG:



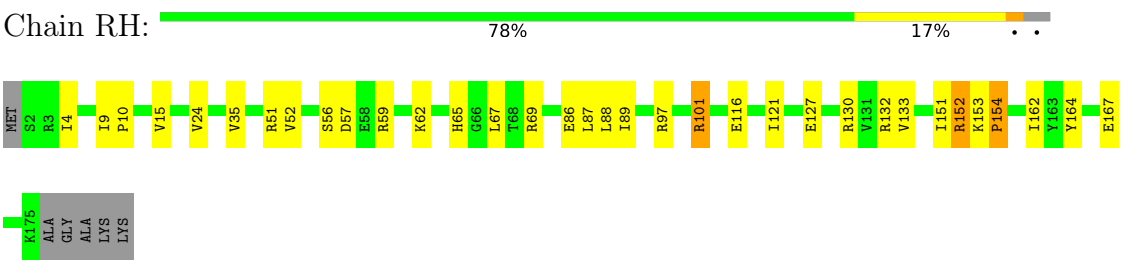
• Molecule 40: 50S ribosomal protein L5

Chain YG:



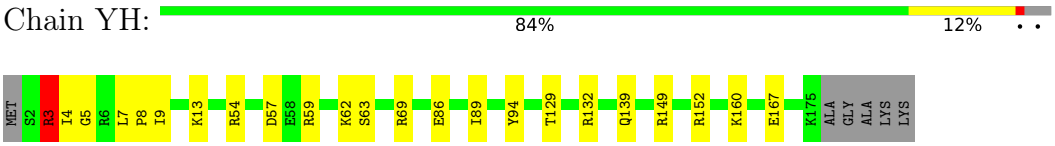
• Molecule 41: 50S ribosomal protein L6

Chain RH:



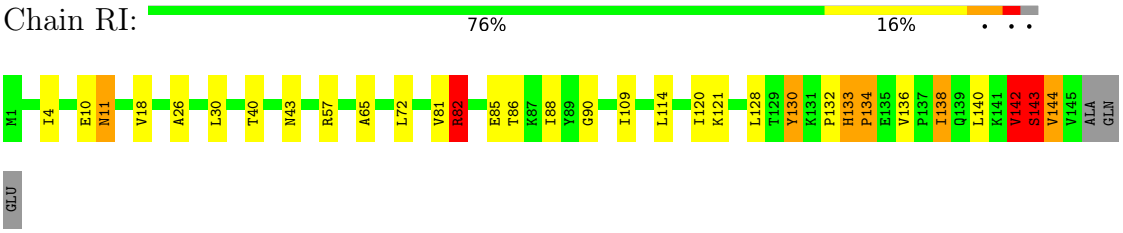
• Molecule 41: 50S ribosomal protein L6

Chain YH:



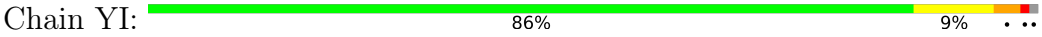
• Molecule 42: 50S ribosomal protein L9

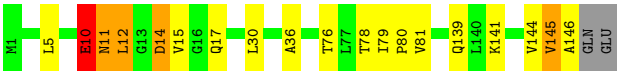
Chain RI:



• Molecule 42: 50S ribosomal protein L9

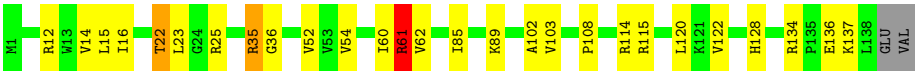
Chain YI:





• Molecule 43: 50S ribosomal protein L13

Chain RN:

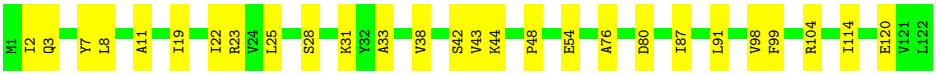


• Molecule 43: 50S ribosomal protein L13

Chain YN:

• Molecule 44: 50S ribosomal protein L14

Chain RO:



• Molecule 44: 50S ribosomal protein L14

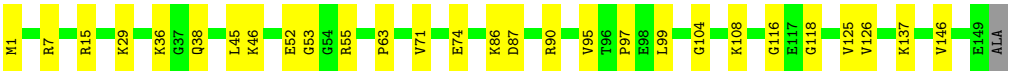
Chain YO:

• Molecule 45: 50S ribosomal protein L15

Chain RP:

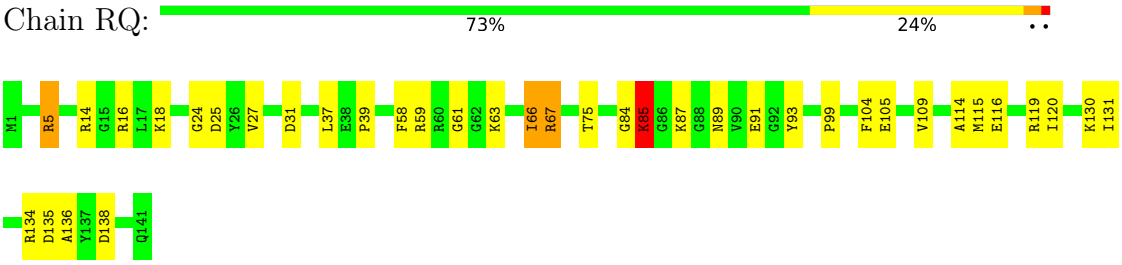
• Molecule 45: 50S ribosomal protein L15

Chain YP:



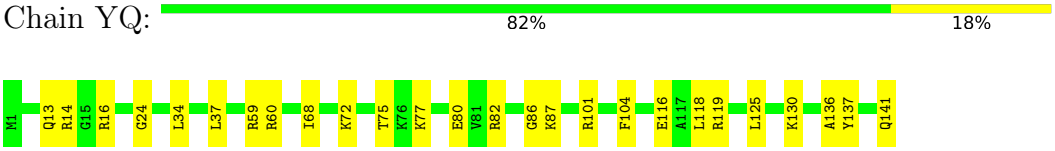
• Molecule 46: 50S ribosomal protein L16

Chain RQ:



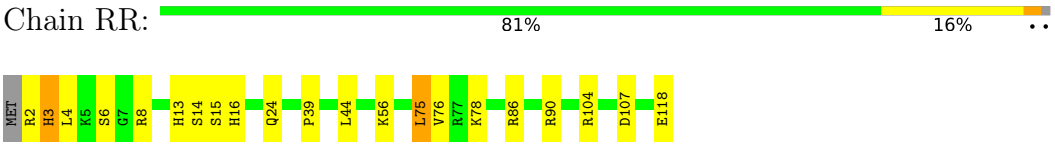
• Molecule 46: 50S ribosomal protein L16

Chain YQ:



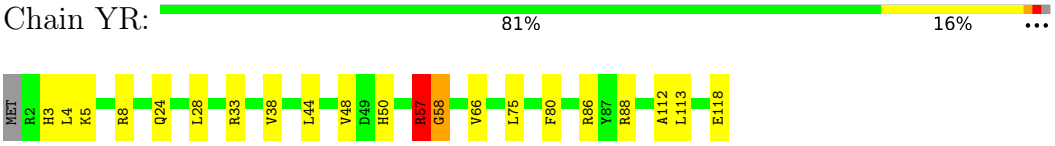
• Molecule 47: 50S ribosomal protein L17

Chain RR:



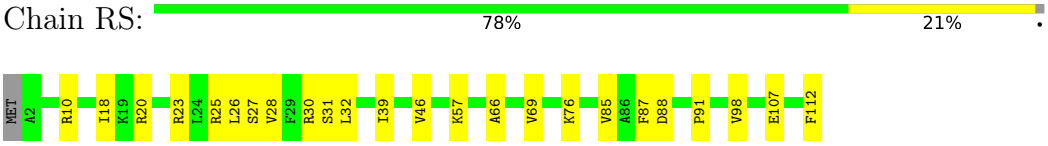
• Molecule 47: 50S ribosomal protein L17

Chain YR:



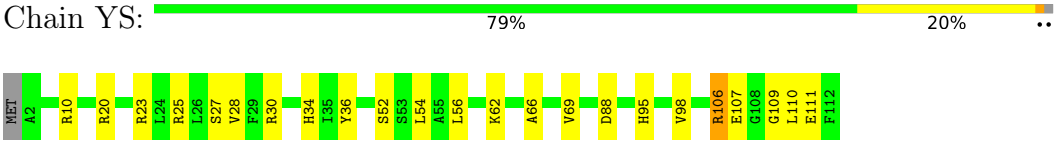
• Molecule 48: 50S ribosomal protein L18

Chain RS:



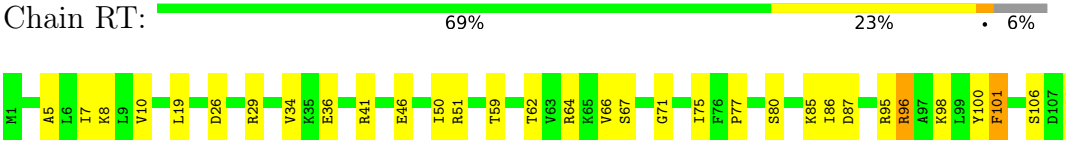
• Molecule 48: 50S ribosomal protein L18

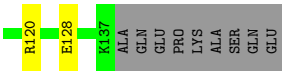
Chain YS:



• Molecule 49: 50S ribosomal protein L19

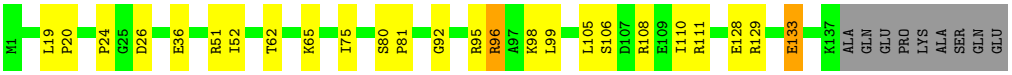
Chain RT:





• Molecule 49: 50S ribosomal protein L19

Chain YT:

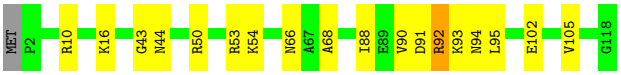


• Molecule 50: 50S ribosomal protein L20

Chain RU:

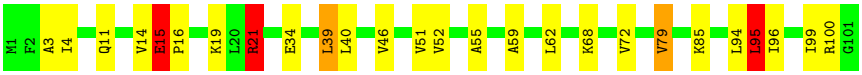
• Molecule 50: 50S ribosomal protein L20

Chain YU:



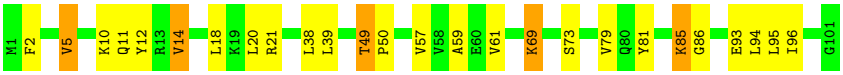
• Molecule 51: 50S ribosomal protein L21

Chain RV:



• Molecule 51: 50S ribosomal protein L21

Chain YV:

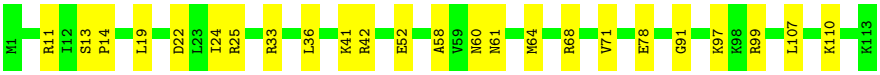


• Molecule 52: 50S ribosomal protein L22

Chain RW:

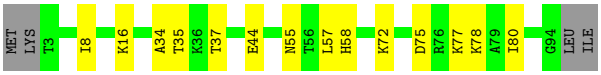
• Molecule 52: 50S ribosomal protein L22

Chain YW:



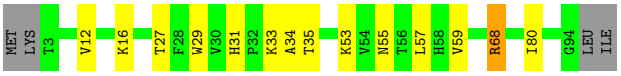
• Molecule 53: 50S ribosomal protein L23

Chain RX:



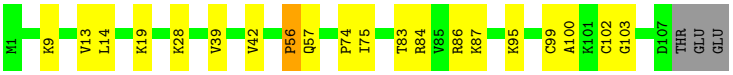
• Molecule 53: 50S ribosomal protein L23

Chain YX:



• Molecule 54: 50S ribosomal protein L24

Chain RY:



• Molecule 54: 50S ribosomal protein L24

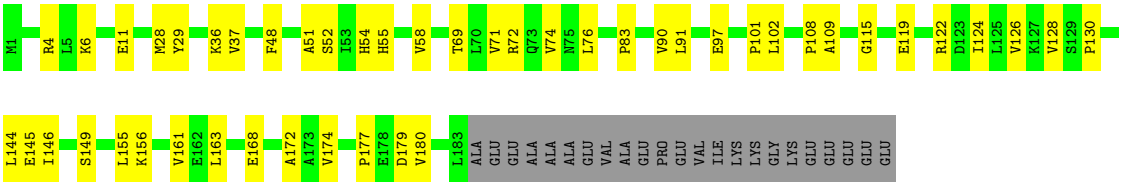
Chain YY:

• Molecule 55: 50S ribosomal protein L25

Chain RZ:

• Molecule 55: 50S ribosomal protein L25

Chain YZ:

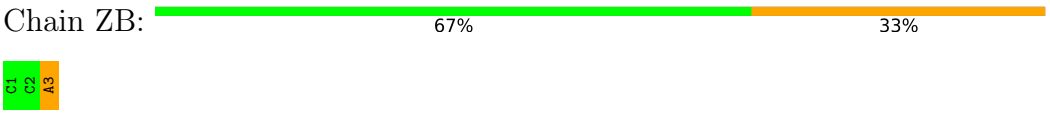


• Molecule 56: CCPuro

Chain ZA:

• Molecule 56: CCPuro

Chain ZB:



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	214.68Å 453.51Å 609.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.72 – 3.50	Depositor
% Data completeness (in resolution range)	98.0 (146.72-3.50)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.216 , 0.246	Depositor
Wilson B-factor (Å^2)	89.9	Xtriage
Anisotropy	0.032	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: PPU, MG, SF4, ZN, A3P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.35	1/36324 (0.0%)	1.07	174/56690 (0.3%)
1	XA	1.32	6/36254 (0.0%)	1.08	179/56581 (0.3%)
2	QB	0.57	4/1942 (0.2%)	0.84	4/2619 (0.2%)
2	XB	0.39	0/1950	0.77	4/2630 (0.2%)
3	QC	0.38	0/1629	0.76	1/2195 (0.0%)
3	XC	0.38	0/1629	0.79	4/2195 (0.2%)
4	QD	0.38	0/1733	0.73	2/2318 (0.1%)
4	XD	0.38	0/1733	0.78	4/2318 (0.2%)
5	QE	0.36	0/1171	0.71	0/1576
5	XE	0.33	0/1171	0.67	0/1576
6	QF	0.32	0/856	0.67	0/1154
6	XF	0.33	0/856	0.70	1/1154 (0.1%)
7	QG	0.38	0/1276	0.75	0/1709
7	XG	0.36	0/1276	0.66	1/1709 (0.1%)
8	QH	0.32	0/1128	0.70	0/1517
8	XH	0.31	0/1128	0.72	3/1517 (0.2%)
9	QI	0.47	0/1029	0.87	2/1379 (0.1%)
9	XI	0.37	0/1017	0.79	2/1365 (0.1%)
10	QJ	0.44	1/814 (0.1%)	0.96	7/1095 (0.6%)
10	XJ	0.41	1/790 (0.1%)	0.81	2/1063 (0.2%)
11	QK	0.40	1/900 (0.1%)	0.71	0/1213
11	XK	0.38	0/879	0.73	2/1187 (0.2%)
12	QL	0.34	0/991	0.81	0/1327
12	XL	0.39	0/972	0.82	1/1301 (0.1%)
13	QM	0.42	0/965	0.92	4/1292 (0.3%)
13	XM	0.40	0/956	0.82	2/1281 (0.2%)
14	QN	0.43	0/501	0.82	1/664 (0.2%)
14	XN	0.32	0/501	0.72	1/664 (0.2%)
15	QO	0.34	0/745	0.66	1/992 (0.1%)
15	XO	0.28	0/740	0.55	0/987
16	QP	0.36	0/721	0.80	2/970 (0.2%)
16	XP	0.34	0/721	0.77	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.37	0/847	0.77	4/1131 (0.4%)
17	XQ	0.33	0/847	0.66	0/1131
18	QR	0.41	1/579 (0.2%)	0.81	0/768
18	XR	0.38	0/579	0.77	1/768 (0.1%)
19	QS	0.45	0/680	0.93	1/915 (0.1%)
19	XS	0.32	0/671	0.78	1/904 (0.1%)
20	QT	0.36	0/765	0.81	0/1007
20	XT	0.35	0/765	0.81	2/1007 (0.2%)
21	QU	0.43	0/221	0.89	1/288 (0.3%)
21	XU	0.31	0/221	0.83	0/288
22	QV	0.33	0/1832	1.01	4/2855 (0.1%)
22	XV	0.33	0/1832	1.02	3/2855 (0.1%)
23	QX	0.33	0/414	0.96	2/645 (0.3%)
23	XX	0.30	0/414	0.92	2/645 (0.3%)
24	QY	0.40	0/743	0.78	1/1002 (0.1%)
24	QZ	0.61	2/743 (0.3%)	0.99	2/1002 (0.2%)
24	XY	0.35	0/743	0.74	1/1002 (0.1%)
24	XZ	0.45	0/743	0.90	2/1002 (0.2%)
25	R0	0.39	0/652	0.87	2/867 (0.2%)
25	Y0	0.35	0/657	0.76	0/874
26	R1	0.43	1/744 (0.1%)	0.78	2/989 (0.2%)
26	Y1	0.36	0/770	0.73	0/1022
27	R2	0.43	0/583	0.90	4/771 (0.5%)
27	Y2	0.31	0/583	0.65	0/771
28	R3	0.31	0/474	0.67	0/635
28	Y3	0.33	0/474	0.73	0/635
29	R4	0.63	0/578	1.13	3/776 (0.4%)
29	Y4	0.40	0/578	0.93	3/776 (0.4%)
30	R5	0.37	0/473	0.72	1/639 (0.2%)
30	Y5	0.46	0/473	0.74	0/639
31	R6	0.38	0/460	0.85	1/613 (0.2%)
31	Y6	0.39	0/460	0.74	0/613
32	R7	0.31	0/417	0.64	0/550
32	Y7	0.33	0/426	0.64	0/561
33	R8	0.48	0/525	0.97	4/691 (0.6%)
33	Y8	0.51	0/525	0.80	0/691
34	R9	0.41	0/310	0.80	0/407
34	Y9	0.38	0/310	0.85	1/407 (0.2%)
35	RA	0.37	0/69739	1.11	428/108870 (0.4%)
35	YA	0.38	0/69419	1.11	379/108369 (0.3%)
36	RB	0.40	0/2881	1.13	17/4494 (0.4%)
36	YB	0.47	1/2881 (0.0%)	1.21	31/4494 (0.7%)
37	RD	0.40	0/2165	0.86	6/2919 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	YD	0.35	0/2185	0.74	4/2944 (0.1%)
38	RE	0.48	0/1601	0.93	4/2160 (0.2%)
38	YE	0.39	0/1592	0.86	4/2149 (0.2%)
39	RF	0.33	0/1620	0.70	2/2194 (0.1%)
39	YF	0.37	1/1620 (0.1%)	0.72	3/2194 (0.1%)
40	RG	0.38	0/1499	0.88	5/2016 (0.2%)
40	YG	0.50	3/1499 (0.2%)	0.82	2/2016 (0.1%)
41	RH	0.47	0/1362	1.04	5/1841 (0.3%)
41	YH	0.39	0/1356	0.77	3/1834 (0.2%)
42	RI	2.84	2/1146 (0.2%)	1.40	9/1551 (0.6%)
42	YI	0.44	0/1151	0.92	4/1558 (0.3%)
43	RN	0.43	0/1131	0.83	3/1525 (0.2%)
43	YN	0.33	0/1131	0.72	3/1525 (0.2%)
44	RO	0.33	0/943	0.70	0/1269
44	YO	0.35	0/943	0.72	0/1269
45	RP	0.45	0/1162	0.96	4/1544 (0.3%)
45	YP	0.36	0/1152	0.86	3/1533 (0.2%)
46	RQ	0.50	2/1143 (0.2%)	0.89	3/1527 (0.2%)
46	YQ	0.34	0/1143	0.73	1/1527 (0.1%)
47	RR	0.32	0/974	0.76	3/1302 (0.2%)
47	YR	0.35	0/974	0.84	4/1302 (0.3%)
48	RS	0.38	0/892	0.83	1/1187 (0.1%)
48	YS	0.43	0/892	0.85	2/1187 (0.2%)
49	RT	0.45	0/1155	0.87	1/1542 (0.1%)
49	YT	0.45	1/1155 (0.1%)	0.83	4/1542 (0.3%)
50	RU	0.38	0/982	0.68	1/1306 (0.1%)
50	YU	0.37	0/982	0.64	0/1306
51	RV	0.72	2/790 (0.3%)	1.15	6/1057 (0.6%)
51	YV	1.42	8/790 (1.0%)	1.02	4/1057 (0.4%)
52	RW	0.33	0/911	0.70	0/1220
52	YW	0.33	0/911	0.69	0/1220
53	RX	0.34	0/739	0.68	0/993
53	YX	0.35	0/739	0.66	0/993
54	RY	0.38	0/831	0.75	1/1108 (0.1%)
54	YY	0.35	0/831	0.76	0/1108
55	RZ	0.39	0/1493	0.84	3/2026 (0.1%)
55	YZ	0.36	0/1493	0.77	0/2026
56	ZA	0.52	0/40	1.41	1/60 (1.7%)
56	ZB	0.58	0/40	1.53	0/60
All	All	0.60	38/319487 (0.0%)	1.03	1407/477274 (0.3%)

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
2	QB	0	1
7	XG	0	1
8	XH	0	1
10	QJ	0	1
11	XK	0	1
24	QZ	0	1
37	RD	0	2
37	YD	0	1
38	RE	0	1
40	RG	0	2
40	YG	0	1
41	RH	0	2
41	YH	0	1
42	RI	0	4
47	RR	0	1
47	YR	0	1
51	RV	0	1
All	All	0	23

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	368	U	C2-N3	131.42	2.29	1.37
1	XA	368	U	N3-C4	105.69	2.33	1.38
42	RI	82	ARG	CZ-NH1	93.68	2.54	1.33
1	XA	368	U	N1-C2	92.50	2.21	1.38
1	XA	368	U	N1-C6	90.74	2.19	1.38
1	XA	368	U	C4-C5	83.89	2.19	1.43
1	XA	368	U	C5-C6	79.02	2.05	1.34
51	YV	85	LYS	CD-CE	23.53	2.10	1.51
51	YV	85	LYS	CE-NZ	15.44	1.87	1.49
51	YV	85	LYS	CB-CG	11.18	1.82	1.52
51	YV	85	LYS	CG-CD	9.90	1.86	1.52
24	QZ	22	ARG	CZ-NH1	8.88	1.44	1.33
2	QB	132	LYS	CD-CE	8.71	1.73	1.51
51	RV	51	VAL	CB-CG2	-8.08	1.35	1.52
40	YG	72	ARG	CG-CD	7.85	1.71	1.51
42	RI	82	ARG	NE-CZ	7.83	1.43	1.33
51	YV	69	LYS	CD-CE	-7.83	1.31	1.51
40	YG	72	ARG	CD-NE	7.36	1.58	1.46
51	RV	51	VAL	CB-CG1	-7.18	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	YV	14	VAL	CB-CG2	-6.71	1.38	1.52
51	YV	5	VAL	CB-CG2	-6.26	1.39	1.52
2	QB	12	GLU	CG-CD	-6.06	1.42	1.51
2	QB	8	LYS	C-N	6.03	1.48	1.34
40	YG	72	ARG	CB-CG	5.85	1.68	1.52
36	YB	116	G	C2'-C1'	-5.80	1.47	1.53
2	QB	8	LYS	N-CA	5.73	1.57	1.46
49	YT	133	GLU	CB-CG	-5.67	1.41	1.52
1	QA	496	A	N9-C4	5.44	1.41	1.37
46	RQ	85	LYS	CD-CE	-5.44	1.37	1.51
24	QZ	22	ARG	CZ-NH2	5.35	1.40	1.33
39	YF	127	GLU	CB-CG	5.33	1.62	1.52
10	XJ	57	LYS	CD-CE	5.21	1.64	1.51
11	QK	92	GLU	CG-CD	5.20	1.59	1.51
18	QR	83	GLU	CB-CG	5.17	1.61	1.52
26	R1	67	ILE	C-N	5.14	1.44	1.34
10	QJ	43	ARG	CG-CD	5.07	1.64	1.51
51	YV	49	THR	CB-CG2	-5.05	1.35	1.52
46	RQ	85	LYS	CE-NZ	-5.03	1.36	1.49

All (1407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	RI	82	ARG	NE-CZ-NH2	-27.28	106.66	120.30
42	RI	82	ARG	NE-CZ-NH1	20.23	130.42	120.30
42	RI	82	ARG	CD-NE-CZ	15.62	145.47	123.60
51	YV	85	LYS	CD-CE-NZ	15.45	147.22	111.70
51	RV	21	ARG	NE-CZ-NH1	14.43	127.52	120.30
35	YA	289	A	O5'-P-OP1	-14.36	92.78	105.70
1	QA	1301	U	C2-N1-C1'	11.98	132.08	117.70
1	QA	1301	U	N1-C2-O2	11.52	130.87	122.80
24	QZ	50	HIS	C-N-CA	11.24	149.81	121.70
42	RI	11	ASN	C-N-CA	10.97	149.12	121.70
38	RE	79	ARG	NE-CZ-NH1	-10.95	114.82	120.30
37	RD	33	LEU	C-N-CA	10.74	148.54	121.70
1	QA	999	U	C2-N1-C1'	10.58	130.40	117.70
38	YE	101	ARG	CA-CB-CG	10.50	136.50	113.40
35	RA	2128	C	C2-N1-C1'	10.46	130.31	118.80
1	XA	1301	U	C2-N1-C1'	10.31	130.07	117.70
1	XA	754	C	C2-N1-C1'	10.28	130.11	118.80
1	XA	368	U	N3-C2-O2	10.18	129.32	122.20
1	QA	1301	U	N3-C2-O2	-10.18	115.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	754	C	C2-N1-C1'	10.13	129.95	118.80
36	YB	31	C	C2-N1-C1'	10.05	129.85	118.80
19	QS	29	ARG	CG-CD-NE	-9.98	90.85	111.80
1	XA	368	U	C2-N3-C4	-9.96	121.02	127.00
47	YR	57	ARG	NE-CZ-NH1	-9.91	115.34	120.30
35	YA	624	C	C6-N1-C2	-9.89	116.34	120.30
35	YA	2063	C	N1-C2-O2	9.85	124.81	118.90
10	QJ	79	ARG	NE-CZ-NH1	9.70	125.15	120.30
35	RA	2666	C	N1-C2-O2	9.68	124.71	118.90
42	RI	143	SER	C-N-CA	9.63	145.76	121.70
1	QA	754	C	N1-C2-O2	9.59	124.65	118.90
35	RA	1774	C	N1-C2-O2	9.44	124.56	118.90
35	RA	856	C	C6-N1-C2	-9.38	116.55	120.30
1	XA	328	C	N1-C2-O2	9.36	124.52	118.90
1	XA	328	C	C2-N1-C1'	9.28	129.01	118.80
35	RA	269	U	N1-C2-O2	9.26	129.28	122.80
40	YG	72	ARG	NE-CZ-NH1	-9.24	115.68	120.30
1	QA	1066	C	N1-C2-O2	9.09	124.36	118.90
35	RA	2128	C	N1-C2-O2	9.08	124.35	118.90
35	YA	1225	C	O4'-C1'-N1	9.00	115.40	108.20
35	RA	1640	C	N1-C2-O2	8.97	124.28	118.90
35	YA	1882	C	C2-N1-C1'	8.97	128.67	118.80
1	XA	1301	U	N1-C2-O2	8.93	129.05	122.80
41	RH	101	ARG	CG-CD-NE	-8.92	93.07	111.80
35	YA	828	U	C2-N1-C1'	8.91	128.40	117.70
35	YA	1313	U	N1-C2-O2	8.91	129.04	122.80
35	RA	1774	C	N3-C2-O2	-8.90	115.67	121.90
35	YA	2063	C	N3-C2-O2	-8.88	115.68	121.90
35	RA	2827	C	C2-N1-C1'	8.87	128.56	118.80
13	QM	114	ARG	CG-CD-NE	-8.86	93.20	111.80
35	YA	363(E)	U	N1-C2-O2	8.85	128.99	122.80
51	RV	21	ARG	NE-CZ-NH2	-8.84	115.88	120.30
35	RA	1313	U	N1-C2-O2	8.78	128.95	122.80
35	YA	2474	C	N1-C2-O2	8.77	124.16	118.90
35	RA	1881	C	C2-N1-C1'	8.74	128.41	118.80
36	YB	31	C	N1-C2-O2	8.74	124.14	118.90
35	RA	2584	U	N3-C2-O2	-8.72	116.09	122.20
1	QA	1158	C	C2-N1-C1'	8.71	128.38	118.80
35	RA	607	U	N3-C2-O2	-8.69	116.12	122.20
35	RA	269	U	C2-N1-C1'	8.67	128.10	117.70
1	QA	1147	C	N1-C2-O2	8.66	124.10	118.90
35	RA	1407	C	C2-N1-C1'	8.60	128.26	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1313	U	N3-C2-O2	-8.58	116.19	122.20
35	YA	363(E)	U	C2-N1-C1'	8.56	127.97	117.70
35	RA	1313	U	C2-N1-C1'	8.55	127.96	117.70
35	YA	1406	U	C5-C6-N1	8.54	126.97	122.70
4	XD	118	ARG	CG-CD-NE	8.53	129.72	111.80
3	XC	140	ARG	NE-CZ-NH2	-8.47	116.06	120.30
35	RA	856	C	C5-C6-N1	8.47	125.23	121.00
1	QA	1158	C	N1-C2-O2	8.44	123.97	118.90
35	YA	269	U	N1-C2-O2	8.43	128.70	122.80
37	YD	88	ARG	CD-NE-CZ	8.43	135.40	123.60
35	YA	1313	U	C2-N1-C1'	8.42	127.81	117.70
3	XC	140	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	XA	135	C	C6-N1-C2	-8.38	116.95	120.30
35	RA	269	U	N3-C2-O2	-8.34	116.36	122.20
55	RZ	112	ARG	CG-CD-NE	-8.33	94.30	111.80
35	YA	69	C	N1-C2-O2	8.33	123.90	118.90
35	RA	1180	C	C2-N1-C1'	8.29	127.92	118.80
35	YA	624	C	C2-N1-C1'	8.25	127.87	118.80
43	RN	61	ARG	CG-CD-NE	-8.23	94.51	111.80
35	RA	2788	C	N1-C2-O2	8.22	123.83	118.90
38	YE	101	ARG	CG-CD-NE	8.22	129.06	111.80
35	YA	1313	U	N3-C2-O2	-8.19	116.47	122.20
35	YA	2128	C	C2-N1-C1'	8.17	127.79	118.80
35	RA	613	U	C2-N1-C1'	8.14	127.47	117.70
1	XA	1381	U	N1-C2-O2	8.10	128.47	122.80
2	QB	132	LYS	CD-CE-NZ	8.10	130.32	111.70
35	YA	856	C	C6-N1-C2	-8.08	117.07	120.30
38	YE	101	ARG	CD-NE-CZ	-8.05	112.33	123.60
1	XA	368	U	C2-N1-C1'	-8.04	108.05	117.70
1	QA	999	U	N1-C2-O2	8.00	128.40	122.80
1	XA	754	C	N1-C2-O2	8.00	123.70	118.90
35	YA	193	U	C2-N1-C1'	8.00	127.30	117.70
1	XA	135	C	N1-C2-O2	8.00	123.70	118.90
1	XA	1007	C	C2-N1-C1'	7.99	127.58	118.80
35	YA	93	C	C2-N1-C1'	7.98	127.58	118.80
35	YA	624	C	C5-C6-N1	7.97	124.98	121.00
35	YA	193	U	N1-C2-O2	7.96	128.37	122.80
1	QA	252	U	C2-N1-C1'	7.96	127.25	117.70
1	QA	1006	C	C2-N1-C1'	7.95	127.55	118.80
35	RA	607	U	N1-C2-O2	7.94	128.36	122.80
35	RA	2688	U	N3-C2-O2	-7.94	116.64	122.20
35	YA	1406	U	C2-N1-C1'	7.93	127.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2787	C	C2-N1-C1'	7.90	127.49	118.80
35	YA	2712	U	C2-N1-C1'	7.88	127.16	117.70
35	YA	270(U)	C	N1-C2-O2	7.88	123.63	118.90
1	XA	1301	U	N3-C2-O2	-7.87	116.69	122.20
35	RA	1588	C	C2-N1-C1'	7.87	127.45	118.80
1	XA	91	C	N3-C2-O2	-7.87	116.39	121.90
35	RA	1407	C	C6-N1-C2	-7.86	117.16	120.30
1	XA	368	U	C6-N1-C2	7.85	125.71	121.00
35	YA	828	U	N1-C2-O2	7.83	128.28	122.80
36	YB	47	C	N1-C2-O2	7.82	123.59	118.90
1	XA	1260	C	N3-C2-O2	-7.82	116.43	121.90
35	RA	2788	C	N3-C2-O2	-7.81	116.43	121.90
1	XA	330	C	N1-C2-O2	7.81	123.58	118.90
35	YA	2226	C	N1-C2-O2	7.80	123.58	118.90
1	QA	1066	C	C2-N1-C1'	7.79	127.37	118.80
35	RA	2666	C	N3-C2-O2	-7.79	116.45	121.90
35	YA	1774	C	N1-C2-O2	7.78	123.57	118.90
35	YA	1882	C	C6-N1-C2	-7.77	117.19	120.30
1	QA	1301	U	C6-N1-C1'	-7.77	110.32	121.20
1	XA	1260	C	N1-C2-O2	7.76	123.56	118.90
1	XA	1535	C	N1-C2-O2	7.76	123.56	118.90
1	XA	91	C	N1-C2-O2	7.73	123.54	118.90
35	RA	363(E)	U	N1-C2-O2	7.73	128.21	122.80
35	RA	708	C	C2-N1-C1'	7.73	127.30	118.80
35	YA	277	C	N1-C2-O2	7.71	123.52	118.90
1	QA	328	C	C2-N1-C1'	7.69	127.26	118.80
1	XA	328	C	C6-N1-C2	-7.68	117.23	120.30
1	QA	1158	C	N3-C2-O2	-7.67	116.53	121.90
1	QA	1038	C	P-O3'-C3'	7.64	128.87	119.70
35	YA	363(E)	U	N3-C2-O2	-7.64	116.85	122.20
36	YB	31	C	C6-N1-C2	-7.64	117.25	120.30
1	QA	754	C	N3-C2-O2	-7.63	116.56	121.90
35	YA	193	U	N3-C2-O2	-7.62	116.86	122.20
1	QA	1301	U	C5-C6-N1	7.61	126.51	122.70
15	QO	89	GLY	N-CA-C	-7.61	94.06	113.10
41	RH	153	LYS	N-CA-C	7.61	131.54	111.00
35	RA	2063	C	C6-N1-C2	-7.60	117.26	120.30
1	QA	328	C	C6-N1-C2	-7.60	117.26	120.30
35	YA	1881	C	C2-N1-C1'	7.60	127.16	118.80
35	RA	613	U	N3-C2-O2	-7.60	116.88	122.20
36	RB	27	C	N1-C2-O2	7.59	123.46	118.90
35	YA	2791	C	C2-N3-C4	-7.58	116.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2177	C	N1-C2-O2	7.57	123.44	118.90
35	YA	1314	C	C2-N1-C1'	7.55	127.11	118.80
35	RA	749	C	N1-C2-O2	7.55	123.43	118.90
41	YH	3	ARG	CD-NE-CZ	7.55	134.17	123.60
1	XA	197	A	P-O3'-C3'	7.55	128.76	119.70
1	XA	1381	U	N3-C2-O2	-7.54	116.92	122.20
35	RA	2787	C	C6-N1-C2	-7.53	117.29	120.30
35	YA	527	C	C2-N1-C1'	7.52	127.08	118.80
1	QA	197	A	P-O3'-C3'	7.52	128.72	119.70
35	YA	613	U	C2-N1-C1'	7.48	126.67	117.70
35	RA	613	U	N1-C2-O2	7.47	128.03	122.80
35	RA	2335	A	O4'-C1'-N9	7.47	114.18	108.20
35	YA	269	U	C2-N1-C1'	7.46	126.66	117.70
1	XA	328	C	N3-C2-O2	-7.43	116.70	121.90
35	YA	2312	U	C5-C6-N1	7.43	126.42	122.70
1	XA	1086	U	N1-C2-O2	7.43	128.00	122.80
1	QA	999	U	N3-C2-O2	-7.42	117.00	122.20
1	QA	961	U	N3-C2-O2	-7.42	117.01	122.20
35	YA	1774	C	N3-C2-O2	-7.41	116.71	121.90
35	RA	1956	U	N3-C2-O2	-7.40	117.02	122.20
35	YA	2210	G	N3-C4-C5	-7.40	124.90	128.60
35	YA	2394	C	N1-C2-O2	7.39	123.33	118.90
1	QA	328	C	N1-C2-O2	7.38	123.33	118.90
35	RA	2667	C	N1-C2-O2	7.38	123.33	118.90
35	YA	1882	C	C5-C6-N1	7.37	124.69	121.00
35	RA	2128	C	C6-N1-C1'	-7.37	111.96	120.80
35	RA	1314	C	C2-N1-C1'	7.36	126.90	118.80
1	QA	454	C	N1-C2-O2	7.35	123.31	118.90
1	XA	135	C	N3-C2-O2	-7.35	116.75	121.90
35	YA	2312	U	C2-N1-C1'	7.35	126.52	117.70
35	RA	286	C	C2-N1-C1'	7.35	126.88	118.80
35	RA	856	C	C2-N1-C1'	7.35	126.88	118.80
35	RA	2063	C	C2-N1-C1'	7.33	126.87	118.80
1	XA	754	C	C6-N1-C1'	-7.33	112.00	120.80
35	YA	603	A	P-O3'-C3'	7.33	128.49	119.70
35	YA	1920	C	C5-C6-N1	7.32	124.66	121.00
35	YA	2294	C	C6-N1-C2	-7.32	117.37	120.30
35	YA	2063	C	C2-N1-C1'	7.32	126.85	118.80
17	QQ	100	LYS	C-N-CA	7.30	139.96	121.70
1	QA	754	C	C6-N1-C1'	-7.30	112.04	120.80
35	YA	2474	C	C2-N1-C1'	7.29	126.82	118.80
35	YA	1774	C	C6-N1-C2	-7.28	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2226	C	N1-C2-O2	7.28	123.27	118.90
35	RA	2868	A	C8-N9-C4	-7.28	102.89	105.80
36	YB	116	G	C1'-O4'-C4'	-7.27	104.08	109.90
47	RR	3	HIS	C-N-CA	7.23	139.78	121.70
35	YA	372	G	P-O3'-C3'	7.23	128.38	119.70
45	YP	15	ARG	CG-CD-NE	7.23	126.98	111.80
35	RA	1640	C	C2-N1-C1'	7.23	126.75	118.80
35	YA	613	U	N3-C2-O2	-7.22	117.14	122.20
35	YA	613	U	N1-C2-O2	7.22	127.86	122.80
36	YB	27	C	N1-C2-O2	7.22	123.23	118.90
35	YA	856	C	C5-C6-N1	7.21	124.61	121.00
35	RA	2787	C	N1-C2-O2	7.18	123.21	118.90
35	YA	269	U	N3-C2-O2	-7.18	117.17	122.20
35	YA	1558	A	P-O3'-C3'	7.18	128.32	119.70
35	RA	1558	A	P-O3'-C3'	7.17	128.31	119.70
1	XA	1263	C	C2-N1-C1'	7.17	126.68	118.80
35	YA	837	C	N1-C2-O2	7.16	123.20	118.90
35	RA	363(E)	U	C2-N1-C1'	7.16	126.29	117.70
35	YA	1956	U	N3-C2-O2	-7.15	117.20	122.20
35	YA	856	C	C2-N1-C1'	7.14	126.66	118.80
35	RA	974(A)	C	C2-N1-C1'	7.14	126.66	118.80
6	XF	46	ARG	CG-CD-NE	-7.13	96.82	111.80
35	YA	2827	C	C2-N1-C1'	7.13	126.64	118.80
1	QA	1158	C	C6-N1-C2	-7.12	117.45	120.30
45	RP	97	PRO	C-N-CA	7.12	139.49	121.70
35	YA	1881	C	C5-C6-N1	7.11	124.56	121.00
35	YA	974(A)	C	C6-N1-C2	7.11	123.14	120.30
1	QA	1065	U	P-O3'-C3'	7.11	128.23	119.70
36	YB	8	U	N1-C2-O2	7.11	127.78	122.80
1	QA	999	U	C6-N1-C1'	-7.10	111.26	121.20
35	RA	2063	C	N1-C2-O2	7.10	123.16	118.90
35	YA	828	U	N3-C2-O2	-7.10	117.23	122.20
35	RA	2559	C	C2-N1-C1'	7.09	126.60	118.80
35	RA	1774	C	C6-N1-C2	-7.09	117.46	120.30
35	RA	2128	C	N3-C2-O2	-7.09	116.94	121.90
35	YA	2210	G	C4-N9-C1'	7.08	135.71	126.50
1	QA	717	C	N1-C2-O2	7.08	123.15	118.90
36	YB	117	G	N3-C2-N2	7.07	124.85	119.90
35	RA	1502	C	C2-N1-C1'	7.07	126.58	118.80
1	QA	328	C	N3-C2-O2	-7.07	116.95	121.90
41	RH	151	ILE	N-CA-C	-7.07	91.92	111.00
26	R1	21	ARG	CG-CD-NE	7.06	126.62	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	RI	144	VAL	N-CA-C	-7.06	91.95	111.00
35	YA	652	C	N1-C2-O2	7.05	123.13	118.90
35	RA	2712	U	C2-N1-C1'	7.05	126.16	117.70
40	RG	116	ASP	C-N-CA	7.05	139.32	121.70
38	RE	54	GLN	C-N-CA	7.04	139.31	121.70
1	XA	1147	C	N1-C2-O2	7.04	123.12	118.90
35	RA	1300	U	P-O3'-C3'	7.03	128.14	119.70
1	XA	328	C	P-O3'-C3'	7.03	128.13	119.70
35	YA	2474	C	N3-C2-O2	-7.01	116.99	121.90
35	YA	286	C	C2-N1-C1'	7.01	126.51	118.80
35	YA	1920	C	C6-N1-C2	-7.00	117.50	120.30
35	RA	105	C	C2-N1-C1'	6.99	126.49	118.80
4	XD	73	ARG	CA-CB-CG	6.98	128.76	113.40
35	YA	2321	G	N3-C4-C5	-6.98	125.11	128.60
35	RA	2128	C	C6-N1-C2	-6.97	117.51	120.30
35	YA	2178	C	C6-N1-C2	-6.97	117.51	120.30
10	QJ	43	ARG	CD-NE-CZ	-6.97	113.84	123.60
35	RA	2827	C	C5-C6-N1	6.96	124.48	121.00
35	RA	2688	U	N1-C2-O2	6.96	127.67	122.80
35	RA	2591	C	C6-N1-C2	-6.95	117.52	120.30
37	RD	33	LEU	CA-CB-CG	6.95	131.28	115.30
35	RA	837	C	N1-C2-O2	6.95	123.07	118.90
45	RP	56	SER	C-N-CA	6.94	139.05	121.70
35	YA	1180	C	C2-N1-C1'	6.93	126.43	118.80
1	QA	250	A	P-O3'-C3'	6.93	128.02	119.70
35	YA	1437	C	C2-N1-C1'	6.93	126.42	118.80
1	QA	1006	C	N1-C2-O2	6.92	123.06	118.90
37	RD	35	LYS	N-CA-C	-6.92	92.31	111.00
35	YA	2128	C	N1-C2-O2	6.92	123.06	118.90
35	YA	1022	G	P-O3'-C3'	6.91	128.00	119.70
42	RI	82	ARG	CG-CD-NE	6.91	126.31	111.80
35	RA	1179	C	C2-N1-C1'	6.91	126.40	118.80
1	XA	1301	U	C6-N1-C1'	-6.91	111.53	121.20
35	YA	2585	U	C2-N1-C1'	6.91	125.99	117.70
1	QA	1528	U	P-O3'-C3'	6.90	127.98	119.70
2	QB	226	ARG	CG-CD-NE	6.90	126.28	111.80
48	RS	107	GLU	N-CA-C	-6.89	92.38	111.00
35	RA	90	U	P-O3'-C3'	6.89	127.97	119.70
1	XA	1065	U	P-O3'-C3'	6.89	127.97	119.70
1	XA	1038	C	P-O3'-C3'	6.89	127.97	119.70
35	RA	721	C	C2-N1-C1'	6.89	126.38	118.80
35	RA	288	C	C2-N1-C1'	6.88	126.37	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	RD	237	GLU	N-CA-C	-6.88	92.42	111.00
35	YA	1881	C	C6-N1-C2	-6.88	117.55	120.30
35	YA	904	C	C2-N1-C1'	6.87	126.36	118.80
35	YA	2294	C	C2-N1-C1'	6.86	126.34	118.80
35	YA	2394	C	N3-C2-O2	-6.86	117.10	121.90
1	XA	1054	C	P-O3'-C3'	6.85	127.92	119.70
48	YS	110	LEU	CA-CB-CG	6.84	131.04	115.30
47	YR	58	GLY	N-CA-C	6.84	130.21	113.10
35	RA	1022	G	P-O3'-C3'	6.84	127.91	119.70
35	YA	1640	C	N1-C2-O2	6.84	123.00	118.90
1	QA	992	U	P-O3'-C3'	6.84	127.91	119.70
1	XA	1067	A	P-O3'-C3'	6.84	127.91	119.70
1	QA	1066	C	C5-C6-N1	6.83	124.42	121.00
35	RA	1598	C	N1-C2-O2	6.83	123.00	118.90
42	YI	145	VAL	N-CA-C	6.83	129.45	111.00
51	RV	39	LEU	CB-CG-CD2	6.83	122.61	111.00
35	RA	363(E)	U	N3-C2-O2	-6.83	117.42	122.20
10	QJ	79	ARG	CD-NE-CZ	6.83	133.16	123.60
35	YA	273(F)	C	C6-N1-C2	-6.83	117.57	120.30
1	QA	283	C	N1-C2-O2	6.82	123.00	118.90
35	YA	2177	C	N3-C2-O2	-6.82	117.12	121.90
1	XA	1260	C	C6-N1-C2	-6.82	117.57	120.30
1	QA	687	A	P-O3'-C3'	6.81	127.88	119.70
35	YA	2584	U	N3-C2-O2	-6.81	117.43	122.20
1	XA	1086	U	N3-C2-O2	-6.80	117.44	122.20
1	QA	1067	A	P-O3'-C3'	6.80	127.86	119.70
35	RA	1171	G	P-O3'-C3'	6.80	127.86	119.70
1	QA	186	C	C2-N1-C1'	6.80	126.28	118.80
35	YA	1956	U	N1-C2-O2	6.80	127.56	122.80
1	XA	1000	A	P-O3'-C3'	6.79	127.84	119.70
35	RA	2787	C	C5-C6-N1	6.78	124.39	121.00
35	YA	1225	C	N3-C4-C5	-6.78	119.19	121.90
35	YA	1314	C	C5-C6-N1	6.78	124.39	121.00
35	YA	2210	G	N3-C4-N9	6.78	130.07	126.00
29	Y4	67	TYR	CB-CA-C	6.78	123.95	110.40
17	QQ	101	ARG	CA-CB-CG	-6.77	98.50	113.40
39	RF	133	ASN	N-CA-C	-6.77	92.72	111.00
35	YA	2226	C	C6-N1-C2	-6.77	117.59	120.30
11	XK	96	ARG	CD-NE-CZ	6.77	133.07	123.60
1	XA	58	C	C6-N1-C2	-6.76	117.59	120.30
38	YE	101	ARG	N-CA-CB	-6.76	98.43	110.60
1	QA	181	G	P-O3'-C3'	6.76	127.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	687	A	P-O3'-C3'	6.75	127.80	119.70
35	YA	607	U	N1-C2-O2	6.75	127.52	122.80
2	XB	178	ARG	CA-CB-CG	6.74	128.23	113.40
35	RA	2394	C	N1-C2-O2	6.73	122.94	118.90
35	RA	2808	U	N3-C2-O2	-6.72	117.49	122.20
1	XA	748	C	P-O3'-C3'	6.72	127.77	119.70
35	YA	1171	G	P-O3'-C3'	6.72	127.77	119.70
35	YA	2584	U	C2-N1-C1'	6.72	125.76	117.70
35	YA	607	U	N3-C2-O2	-6.72	117.50	122.20
35	YA	1979	C	C6-N1-C2	-6.72	117.61	120.30
1	QA	932	C	C2-N1-C1'	6.71	126.19	118.80
36	YB	31	C	C6-N1-C1'	-6.71	112.74	120.80
1	QA	748	C	P-O3'-C3'	6.71	127.75	119.70
35	RA	119	A	P-O3'-C3'	6.71	127.75	119.70
1	QA	186	C	N1-C2-O2	6.71	122.92	118.90
1	QA	1224	G	N3-C4-N9	-6.71	121.97	126.00
35	RA	907	U	N3-C2-O2	-6.70	117.51	122.20
42	RI	142	VAL	C-N-CA	6.70	138.44	121.70
1	XA	992	U	P-O3'-C3'	6.69	127.73	119.70
1	XA	1381	U	C2-N1-C1'	6.68	125.72	117.70
35	RA	2063	C	N3-C2-O2	-6.68	117.23	121.90
35	YA	975	G	N3-C4-N9	6.67	130.00	126.00
1	QA	1147	C	N3-C2-O2	-6.67	117.23	121.90
35	RA	2447	G	P-O3'-C3'	6.67	127.71	119.70
1	QA	1066	C	C6-N1-C2	-6.67	117.63	120.30
35	YA	1005	C	C2-N1-C1'	6.67	126.13	118.80
35	RA	273(C)	C	N1-C2-O2	6.66	122.90	118.90
35	RA	2118	U	C2-N1-C1'	6.66	125.70	117.70
35	YA	288	C	C5-C6-N1	6.66	124.33	121.00
35	RA	404	C	P-O3'-C3'	6.66	127.69	119.70
4	XD	47	ARG	CA-CB-CG	-6.65	98.76	113.40
35	YA	119	A	P-O3'-C3'	6.65	127.68	119.70
1	XA	328	C	C5-C6-N1	6.65	124.32	121.00
1	QA	1066	C	N3-C2-O2	-6.64	117.25	121.90
1	XA	1439	C	C2-N1-C1'	6.64	126.10	118.80
35	RA	2439	A	P-O3'-C3'	6.64	127.66	119.70
35	YA	2212	A	OP1-P-OP2	-6.63	109.65	119.60
22	QV	32	C	N1-C2-O2	6.63	122.88	118.90
13	QM	11	ARG	CB-CA-C	6.63	123.65	110.40
29	R4	63	TYR	CA-CB-CG	6.62	125.98	113.40
1	XA	137	C	C2-N1-C1'	6.62	126.08	118.80
35	RA	2808	U	N1-C2-O2	6.62	127.43	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1930	G	P-O3'-C3'	6.62	127.64	119.70
18	XR	42	ARG	CG-CD-NE	-6.62	97.90	111.80
27	R2	71	ASN	C-N-CA	6.61	138.22	121.70
35	RA	2827	C	C6-N1-C2	-6.61	117.66	120.30
35	YA	1588	C	C2-N1-C1'	6.61	126.07	118.80
1	XA	442	C	C2-N1-C1'	6.60	126.06	118.80
48	YS	109	GLY	C-N-CA	6.59	138.19	121.70
16	QP	54	GLU	N-CA-CB	-6.59	98.74	110.60
35	RA	1956	U	N1-C2-O2	6.59	127.41	122.80
1	QA	454	C	N3-C2-O2	-6.59	117.29	121.90
35	RA	2584	U	C2-N1-C1'	6.58	125.60	117.70
35	YA	2321	G	C4-N9-C1'	6.58	135.06	126.50
36	RB	47	C	N1-C2-O2	6.58	122.85	118.90
1	XA	5	U	P-O3'-C3'	6.58	127.59	119.70
35	YA	893	C	C2-N1-C1'	6.57	126.02	118.80
36	YB	77	U	N1-C2-O2	6.57	127.39	122.80
1	QA	913	A	P-O3'-C3'	6.56	127.58	119.70
35	RA	1735	C	C2-N1-C1'	6.56	126.02	118.80
47	RR	76	VAL	N-CA-C	-6.56	93.29	111.00
35	YA	1417	C	C5-C6-N1	6.55	124.27	121.00
35	YA	69	C	N3-C2-O2	-6.54	117.32	121.90
35	RA	1294	U	N3-C2-O2	-6.54	117.62	122.20
35	YA	708	C	C2-N1-C1'	6.54	125.99	118.80
35	RA	2868	A	N7-C8-N9	6.54	117.07	113.80
23	QX	11	U	P-O3'-C3'	6.53	127.54	119.70
1	XA	1137	C	P-O3'-C3'	6.53	127.54	119.70
35	YA	2791	C	N1-C2-N3	6.53	123.77	119.20
1	QA	792	A	P-O3'-C3'	6.53	127.53	119.70
46	RQ	85	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	QA	1263	C	C2-N1-C1'	6.53	125.98	118.80
35	RA	2688	U	C2-N1-C1'	6.53	125.53	117.70
35	RA	1882	C	C2-N1-C1'	6.52	125.97	118.80
1	QA	812	C	P-O3'-C3'	6.52	127.53	119.70
35	RA	1699	G	P-O3'-C3'	6.50	127.51	119.70
1	QA	484	G	P-O3'-C3'	6.50	127.50	119.70
35	RA	435	C	N1-C2-O2	6.49	122.79	118.90
35	YA	32	C	C2-N1-C1'	6.49	125.93	118.80
38	RE	64	LYS	CD-CE-NZ	-6.48	96.80	111.70
35	YA	358	U	C2-N1-C1'	6.48	125.47	117.70
1	QA	442	C	C2-N1-C1'	6.47	125.92	118.80
1	QA	547	A	P-O3'-C3'	6.47	127.47	119.70
35	RA	544	C	C2-N1-C1'	6.47	125.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	93	C	C6-N1-C2	-6.46	117.71	120.30
27	R2	72	ALA	N-CA-C	6.46	128.44	111.00
35	RA	2559	C	C6-N1-C2	-6.46	117.72	120.30
23	XX	13	A	O5'-P-OP1	6.46	118.45	110.70
35	RA	1437	C	C5-C6-N1	6.46	124.23	121.00
35	YA	867	C	N1-C2-O2	6.46	122.77	118.90
40	RG	146	TYR	CA-CB-CG	6.45	125.66	113.40
1	XA	60	A	P-O3'-C3'	6.45	127.44	119.70
35	YA	358	U	N1-C2-O2	6.45	127.31	122.80
33	R8	46	ARG	CG-CD-NE	-6.45	98.26	111.80
49	YT	133	GLU	CB-CA-C	-6.45	97.51	110.40
35	RA	2065	C	C5-C6-N1	6.44	124.22	121.00
4	QD	208	SER	N-CA-C	-6.44	93.62	111.00
1	XA	754	C	N3-C2-O2	-6.44	117.39	121.90
35	YA	1499	C	C2-N1-C1'	6.44	125.88	118.80
35	RA	1640	C	N3-C2-O2	-6.44	117.39	121.90
21	QU	15	ARG	CG-CD-NE	-6.43	98.29	111.80
35	YA	1314	C	C6-N1-C2	-6.43	117.73	120.30
35	RA	227	A	P-O3'-C3'	6.43	127.42	119.70
35	RA	2666	C	C6-N1-C2	-6.43	117.73	120.30
24	QZ	22	ARG	NE-CZ-NH2	6.43	123.51	120.30
36	YB	31	C	C5-C6-N1	6.42	124.21	121.00
35	RA	2294	C	C6-N1-C2	-6.42	117.73	120.30
1	XA	1535	C	C2-N1-C1'	6.42	125.86	118.80
1	XA	547	A	P-O3'-C3'	6.41	127.39	119.70
1	QA	1346	A	P-O3'-C3'	6.40	127.38	119.70
1	XA	1382	C	N1-C2-O2	6.40	122.74	118.90
1	XA	75	C	C2-N1-C1'	6.40	125.84	118.80
35	YA	234	C	N1-C2-O2	6.40	122.74	118.90
35	YA	270(U)	C	N3-C2-O2	-6.39	117.42	121.90
1	XA	893	C	C5-C6-N1	6.39	124.20	121.00
35	RA	2847	U	N1-C2-O2	6.38	127.27	122.80
35	RA	2092	U	P-O3'-C3'	6.38	127.35	119.70
35	RA	234	C	N1-C2-O2	6.37	122.72	118.90
35	RA	1979	C	C6-N1-C2	-6.37	117.75	120.30
1	QA	1260	C	N3-C2-O2	-6.36	117.45	121.90
35	YA	883	G	N1-C6-O6	-6.36	116.08	119.90
35	YA	1640	C	C6-N1-C2	-6.36	117.76	120.30
1	QA	1325	C	C2-N1-C1'	6.36	125.79	118.80
1	XA	368	U	N1-C2-O2	-6.36	118.35	122.80
35	RA	1314	C	C5-C6-N1	6.35	124.17	121.00
35	YA	2712	U	N1-C2-O2	6.35	127.24	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	RZ	62	PRO	C-N-CA	6.34	137.56	121.70
36	RB	77	U	N1-C2-O2	6.34	127.24	122.80
1	QA	1006	C	C5-C6-N1	6.33	124.17	121.00
1	XA	1158	C	C2-N1-C1'	6.33	125.76	118.80
36	YB	118	G	N1-C6-O6	-6.33	116.10	119.90
35	RA	1653	G	P-O3'-C3'	6.33	127.29	119.70
35	YA	2447	G	P-O3'-C3'	6.33	127.29	119.70
35	RA	387	U	P-O3'-C3'	6.32	127.29	119.70
36	RB	3	C	N1-C2-O2	6.32	122.69	118.90
35	YA	2688	U	N3-C2-O2	-6.32	117.78	122.20
35	RA	1644	C	N1-C2-O2	6.31	122.69	118.90
35	RA	2712	U	O4'-C1'-N1	6.31	113.25	108.20
36	YB	31	C	N3-C2-O2	-6.31	117.48	121.90
35	RA	2752	C	N1-C2-O2	6.31	122.69	118.90
35	RA	372	G	P-O3'-C3'	6.31	127.27	119.70
35	RA	1406	U	C2-N1-C1'	6.31	125.27	117.70
1	QA	428	G	P-O3'-C3'	6.31	127.27	119.70
35	YA	2439	A	P-O3'-C3'	6.31	127.27	119.70
1	XA	1498	U	P-O3'-C3'	6.30	127.26	119.70
35	YA	2874	C	C2-N1-C1'	6.30	125.73	118.80
35	YA	2312	U	N1-C2-O2	6.29	127.20	122.80
35	RA	2666	C	C2-N1-C1'	6.29	125.72	118.80
1	XA	1004	A	P-O3'-C3'	6.29	127.25	119.70
24	XZ	83	HIS	C-N-CA	6.29	137.42	121.70
1	XA	913	A	P-O3'-C3'	6.28	127.24	119.70
1	QA	115	G	P-O3'-C3'	6.28	127.23	119.70
35	RA	2863	C	C2-N1-C1'	6.28	125.70	118.80
1	QA	1347	G	P-O3'-C3'	6.27	127.22	119.70
35	RA	974(A)	C	N1-C2-O2	6.27	122.66	118.90
35	RA	2585	U	C2-N1-C1'	6.27	125.22	117.70
13	QM	8	GLU	C-N-CA	6.26	137.35	121.70
35	RA	2477	C	C2-N1-C1'	6.26	125.69	118.80
50	RU	92	ARG	C-N-CA	6.26	137.35	121.70
1	XA	932	C	C2-N1-C1'	6.26	125.69	118.80
35	YA	1882	C	N1-C2-O2	6.26	122.66	118.90
1	QA	1498	U	P-O3'-C3'	6.25	127.21	119.70
35	RA	1417	C	C5-C6-N1	6.25	124.13	121.00
35	RA	2874	C	C2-N1-C1'	6.25	125.68	118.80
35	RA	1318	C	C2-N1-C1'	6.25	125.67	118.80
1	XA	1190	G	P-O3'-C3'	6.25	127.20	119.70
35	YA	2211	G	P-O3'-C3'	6.25	127.20	119.70
35	YA	2312	U	N3-C2-O2	-6.25	117.83	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1644	C	N3-C2-O2	-6.24	117.53	121.90
36	YB	77	U	N3-C2-O2	-6.24	117.83	122.20
1	QA	485	G	OP2-P-O3'	6.24	118.92	105.20
35	YA	2559	C	N1-C2-O2	6.24	122.64	118.90
35	YA	343	C	C6-N1-C2	-6.23	117.81	120.30
35	RA	797	C	C5-C6-N1	6.23	124.11	121.00
35	RA	907	U	N1-C2-O2	6.23	127.16	122.80
1	XA	1535	C	N3-C2-O2	-6.23	117.54	121.90
35	RA	1474	C	N1-C2-O2	6.22	122.64	118.90
35	RA	1992	G	P-O3'-C3'	6.22	127.17	119.70
35	YA	140	A	N7-C8-N9	6.22	116.91	113.80
1	XA	792	A	P-O3'-C3'	6.22	127.17	119.70
35	YA	270(Q)	C	N1-C2-O2	6.22	122.63	118.90
35	RA	105	C	N1-C2-O2	6.22	122.63	118.90
47	RR	75	LEU	CA-CB-CG	6.21	129.59	115.30
8	XH	60	ARG	NE-CZ-NH2	-6.21	117.19	120.30
35	RA	1332	G	N7-C8-N9	6.21	116.21	113.10
35	RA	2188	C	N3-C2-O2	-6.21	117.55	121.90
35	YA	2585	U	N1-C2-O2	6.21	127.15	122.80
35	RA	1588	C	C5-C6-N1	6.21	124.10	121.00
1	QA	60	A	P-O3'-C3'	6.21	127.15	119.70
35	RA	1180	C	N1-C2-O2	6.21	122.62	118.90
35	YA	2474	C	C6-N1-C2	-6.21	117.82	120.30
35	YA	93	C	C5-C6-N1	6.20	124.10	121.00
35	YA	2712	U	O4'-C1'-N1	6.20	113.16	108.20
35	RA	837	C	C6-N1-C2	-6.20	117.82	120.30
35	YA	1658	C	C5-C6-N1	6.20	124.10	121.00
1	QA	960	U	N1-C2-O2	6.20	127.14	122.80
35	RA	837	C	N3-C2-O2	-6.20	117.56	121.90
35	RA	286	C	N1-C2-O2	6.19	122.62	118.90
35	YA	2477	C	C2-N1-C1'	6.19	125.61	118.80
35	YA	2226	C	N3-C2-O2	-6.19	117.57	121.90
1	QA	268	C	C2-N1-C1'	6.19	125.61	118.80
35	YA	1225	C	C4'-C3'-C2'	6.19	108.79	102.60
35	YA	153	C	N1-C2-O2	6.19	122.61	118.90
35	YA	270(U)	C	C2-N1-C1'	6.19	125.61	118.80
35	YA	527	C	N1-C2-O2	6.19	122.61	118.90
35	RA	2481	G	P-O3'-C3'	6.18	127.12	119.70
1	XA	428	G	P-O3'-C3'	6.18	127.12	119.70
1	XA	1301	U	C5-C6-N1	6.18	125.79	122.70
35	RA	2559	C	C5-C6-N1	6.18	124.09	121.00
35	YA	1437	C	C5-C6-N1	6.18	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1505	C	C5-C6-N1	6.18	124.09	121.00
35	YA	1437	C	C6-N1-C2	-6.18	117.83	120.30
1	XA	1128	C	C6-N1-C2	-6.18	117.83	120.30
37	YD	274	ARG	C-N-CA	6.18	137.14	121.70
1	XA	1007	C	C5-C6-N1	6.17	124.09	121.00
35	YA	2226	C	C5-C6-N1	6.17	124.09	121.00
35	RA	1437	C	C6-N1-C2	-6.17	117.83	120.30
1	QA	1224	G	C4-N9-C1'	-6.16	118.49	126.50
35	YA	2063	C	C6-N1-C2	-6.16	117.83	120.30
35	YA	277	C	N3-C2-O2	-6.16	117.59	121.90
35	RA	1881	C	C6-N1-C2	-6.16	117.84	120.30
35	RA	708	C	N1-C2-O2	6.16	122.59	118.90
2	XB	235	SER	C-N-CA	6.16	137.09	121.70
35	YA	1644	C	N1-C2-O2	6.16	122.59	118.90
9	QI	83	ARG	CA-CB-CG	-6.15	99.86	113.40
35	RA	1180	C	C5-C6-N1	6.15	124.08	121.00
35	RA	1407	C	N1-C2-O2	6.15	122.59	118.90
1	QA	1532	U	P-O3'-C3'	6.15	127.08	119.70
42	YI	14	ASP	CB-CG-OD1	6.14	123.83	118.30
22	QV	34	C	C2-N1-C1'	6.14	125.56	118.80
1	QA	1362(A)	C	N3-C2-O2	-6.14	117.60	121.90
35	RA	9	U	N1-C2-O2	6.14	127.10	122.80
35	YA	2752	C	N1-C2-O2	6.14	122.58	118.90
35	YA	2294	C	C5-C6-N1	6.14	124.07	121.00
35	YA	752	A	P-O3'-C3'	6.14	127.06	119.70
37	RD	122	ASP	C-N-CA	6.13	137.02	121.70
1	QA	31	G	P-O3'-C3'	6.12	127.05	119.70
1	XA	1532	U	P-O3'-C3'	6.12	127.05	119.70
35	YA	1505	C	C2-N1-C1'	6.12	125.53	118.80
35	RA	828	U	N1-C2-O2	6.12	127.08	122.80
35	RA	1204	A	O4'-C1'-N9	6.12	113.10	108.20
35	RA	2584	U	C6-N1-C2	-6.12	117.33	121.00
39	RF	99	TYR	CA-CB-CG	6.12	125.02	113.40
49	YT	99	LEU	CA-CB-CG	6.12	129.37	115.30
35	RA	2128	C	C5-C6-N1	6.11	124.06	121.00
24	XZ	84	TYR	N-CA-C	-6.11	94.50	111.00
35	YA	837	C	N3-C2-O2	-6.11	117.62	121.90
56	ZA	1	C	N1-C2-O2	6.11	122.57	118.90
35	YA	974	G	C4-N9-C1'	-6.11	118.56	126.50
35	YA	1653	G	P-O3'-C3'	6.10	127.03	119.70
35	RA	105	C	C5-C6-N1	6.10	124.05	121.00
33	R8	36	LYS	N-CA-C	-6.10	94.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1407	C	C5-C6-N1	6.10	124.05	121.00
1	QA	435	C	C2-N1-C1'	6.10	125.51	118.80
39	YF	197	ASP	N-CA-C	-6.10	94.53	111.00
1	QA	1406	U	N1-C2-O2	6.10	127.07	122.80
1	QA	353	A	OP2-P-O3'	6.09	118.61	105.20
35	RA	2527	C	C2-N1-C1'	6.09	125.50	118.80
36	YB	8	U	N3-C2-O2	-6.09	117.94	122.20
35	RA	2585	U	N1-C2-O2	6.09	127.06	122.80
1	XA	812	C	P-O3'-C3'	6.09	127.01	119.70
35	YA	1226	G	O5'-P-OP1	-6.09	100.22	105.70
1	XA	960	U	P-O3'-C3'	6.09	127.01	119.70
35	YA	1294	U	C5-C6-N1	6.09	125.74	122.70
35	RA	1300	U	OP2-P-O3'	6.09	118.59	105.20
35	YA	358	U	N3-C2-O2	-6.09	117.94	122.20
35	RA	358	U	N1-C2-O2	6.08	127.06	122.80
35	RA	1640	C	C6-N1-C2	-6.08	117.87	120.30
35	YA	2177	C	C6-N1-C2	-6.08	117.87	120.30
35	RA	288	C	N1-C2-O2	6.07	122.55	118.90
35	YA	930	U	N1-C2-O2	6.07	127.05	122.80
36	YB	47	C	C2-N1-C1'	6.07	125.48	118.80
35	YA	856	C	N1-C2-O2	6.07	122.54	118.90
35	RA	1406	U	N1-C2-O2	6.07	127.05	122.80
35	YA	1559	G	P-O3'-C3'	6.06	126.98	119.70
1	XA	115	G	P-O3'-C3'	6.06	126.98	119.70
1	XA	1325	C	C6-N1-C2	-6.06	117.88	120.30
1	XA	186	C	N1-C2-O2	6.05	122.53	118.90
35	RA	1658	C	C5-C6-N1	6.04	124.02	121.00
1	XA	74	C	C2-N1-C1'	6.04	125.45	118.80
35	RA	1474	C	C2-N1-C1'	6.04	125.45	118.80
35	RA	1588	C	N1-C2-O2	6.04	122.53	118.90
1	XA	690	G	O4'-C1'-N9	6.04	113.03	108.20
1	XA	135	C	C5-C6-N1	6.04	124.02	121.00
1	XA	754	C	C6-N1-C2	-6.04	117.89	120.30
35	YA	435	C	N1-C2-O2	6.04	122.52	118.90
35	RA	2129	C	C5-C6-N1	6.03	124.02	121.00
35	RA	2827	C	N1-C2-O2	6.03	122.52	118.90
1	QA	201	C	P-O3'-C3'	6.03	126.94	119.70
35	RA	708	C	C5-C6-N1	6.03	124.01	121.00
35	RA	2889	C	C2-N1-C1'	6.03	125.43	118.80
35	YA	1644	C	N3-C2-O2	-6.03	117.68	121.90
35	YA	2041	U	N1-C2-O2	6.02	127.02	122.80
1	QA	1224	G	C8-N9-C1'	6.02	134.82	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	828	U	C6-N1-C1'	-6.02	112.77	121.20
35	RA	279	C	C6-N1-C2	-6.01	117.89	120.30
40	YG	72	ARG	NE-CZ-NH2	6.01	123.31	120.30
35	YA	2610	C	P-O3'-C3'	6.01	126.91	119.70
35	YA	1152	C	C2-N1-C1'	6.01	125.41	118.80
35	YA	2312	U	C6-N1-C2	-6.01	117.40	121.00
35	RA	1085	A	P-O3'-C3'	6.00	126.91	119.70
1	QA	1395	C	N1-C2-O2	6.00	122.50	118.90
49	RT	59	THR	N-CA-C	-6.00	94.79	111.00
51	YV	50	PRO	CA-N-CD	-6.00	103.10	111.50
35	RA	2651	C	N1-C2-O2	6.00	122.50	118.90
36	RB	88	C	N1-C2-O2	6.00	122.50	118.90
1	QA	1033	G	N3-C4-N9	6.00	129.60	126.00
35	YA	1735	C	C2-N1-C1'	6.00	125.40	118.80
2	QB	12	GLU	CG-CD-OE1	-6.00	106.31	118.30
35	RA	1699	G	OP1-P-O3'	6.00	118.39	105.20
1	QA	972	C	C6-N1-C2	-5.99	117.90	120.30
35	RA	894	C	N1-C2-O2	5.99	122.50	118.90
35	YA	817	C	C6-N1-C2	-5.99	117.91	120.30
35	RA	2776	A	P-O3'-C3'	5.99	126.88	119.70
35	YA	2726	U	N3-C2-O2	-5.99	118.01	122.20
35	RA	512	G	O4'-C1'-N9	5.98	112.99	108.20
35	YA	1152	C	C6-N1-C2	-5.98	117.91	120.30
1	QA	201	C	OP1-P-O3'	5.98	118.36	105.20
35	RA	1598	C	C2-N1-C1'	5.98	125.38	118.80
35	RA	1881	C	C5-C6-N1	5.98	123.99	121.00
35	RA	2394	C	C2-N1-C1'	5.98	125.38	118.80
35	YA	9	U	N1-C2-O2	5.98	126.99	122.80
35	RA	1881	C	C6-N1-C1'	-5.98	113.62	120.80
1	XA	186	C	C2-N1-C1'	5.97	125.37	118.80
35	RA	828	U	N3-C2-O2	-5.97	118.02	122.20
35	YA	2776	A	P-O3'-C3'	5.97	126.86	119.70
1	XA	330	C	C6-N1-C2	-5.97	117.91	120.30
35	YA	2827	C	N1-C2-O2	5.96	122.48	118.90
1	XA	250	A	P-O3'-C3'	5.96	126.85	119.70
1	QA	1260	C	N1-C2-O2	5.96	122.48	118.90
1	QA	749	C	C6-N1-C2	-5.96	117.92	120.30
35	YA	2849	U	P-O3'-C3'	5.96	126.85	119.70
35	RA	1332	G	C4-N9-C1'	5.96	134.24	126.50
35	RA	2896	C	N1-C2-O2	5.96	122.47	118.90
1	XA	1007	C	P-O3'-C3'	5.96	126.85	119.70
35	RA	1882	C	C6-N1-C2	-5.95	117.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	114	U	C2-N1-C1'	5.95	124.84	117.70
35	RA	828	U	C2-N1-C1'	5.95	124.84	117.70
35	RA	2477	C	N1-C2-O2	5.95	122.47	118.90
35	RA	2294	C	C2-N1-C1'	5.94	125.34	118.80
35	YA	930	U	N3-C2-O2	-5.94	118.04	122.20
35	YA	1233	C	C2-N1-C1'	5.94	125.34	118.80
1	QA	496	A	C2-N3-C4	5.94	113.57	110.60
35	RA	2873	A	N7-C8-N9	5.94	116.77	113.80
45	RP	26	GLY	N-CA-C	-5.94	98.26	113.10
14	XN	13	THR	N-CA-C	5.94	127.03	111.00
35	RA	2849	U	P-O3'-C3'	5.93	126.82	119.70
35	RA	1180	C	C6-N1-C2	-5.93	117.93	120.30
1	XA	1000	A	OP1-P-O3'	5.93	118.25	105.20
4	QD	33	MET	CG-SD-CE	-5.93	90.72	100.20
35	RA	2827	C	C6-N1-C1'	-5.93	113.69	120.80
42	RI	120	ILE	N-CA-C	5.93	127.00	111.00
35	YA	2226	C	C2-N1-C1'	5.93	125.32	118.80
35	RA	358	U	N3-C2-O2	-5.92	118.05	122.20
1	XA	1502	A	N7-C8-N9	5.92	116.76	113.80
35	RA	1233	C	C6-N1-C2	-5.92	117.93	120.30
1	XA	328	C	C6-N1-C1'	-5.92	113.69	120.80
35	RA	1437	C	C2-N1-C1'	5.92	125.31	118.80
35	RA	2226	C	N3-C2-O2	-5.91	117.76	121.90
29	R4	13	ARG	CG-CD-NE	5.91	124.21	111.80
35	RA	2689	U	P-O3'-C3'	5.91	126.79	119.70
35	RA	69	C	C2-N1-C1'	5.91	125.30	118.80
35	RA	1694	C	P-O3'-C3'	5.91	126.79	119.70
1	QA	999	U	C5-C6-N1	5.90	125.65	122.70
45	YP	71	VAL	N-CA-C	5.90	126.93	111.00
35	RA	279	C	C2-N1-C1'	5.90	125.29	118.80
10	QJ	28	ARG	NE-CZ-NH1	5.90	123.25	120.30
35	RA	1588	C	C6-N1-C2	-5.90	117.94	120.30
35	YA	857	C	C2-N1-C1'	5.90	125.29	118.80
1	QA	1031	G	C4-N9-C1'	5.89	134.16	126.50
35	RA	2652	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	1506	C	C2-N1-C1'	5.89	125.28	118.80
35	RA	9	U	C2-N1-C1'	5.89	124.77	117.70
35	YA	1474	C	C2-N1-C1'	5.89	125.28	118.80
35	RA	2467	C	C6-N1-C1'	5.88	127.86	120.80
1	QA	1383	C	N1-C2-O2	5.88	122.43	118.90
1	XA	1300	G	P-O3'-C3'	5.88	126.75	119.70
35	YA	1675	C	N3-C2-O2	-5.88	117.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1233	C	C2-N1-C1'	5.88	125.26	118.80
1	QA	1007	C	P-O3'-C3'	5.87	126.75	119.70
1	QA	525	C	C5-C6-N1	5.87	123.93	121.00
1	XA	442	C	C6-N1-C2	-5.87	117.95	120.30
1	QA	419	C	C2-N1-C1'	5.87	125.25	118.80
35	RA	2210	G	C4-N9-C1'	5.86	134.12	126.50
10	QJ	43	ARG	NE-CZ-NH1	-5.86	117.37	120.30
35	YA	2688	U	C2-N1-C1'	5.86	124.73	117.70
35	YA	2178	C	C2-N1-C1'	5.86	125.24	118.80
1	QA	1000	A	P-O3'-C3'	5.85	126.72	119.70
35	RA	1909	C	C2-N1-C1'	5.85	125.24	118.80
1	XA	341	C	C2-N1-C1'	5.85	125.24	118.80
35	YA	1267	U	C2-N1-C1'	5.85	124.72	117.70
35	YA	2128	C	C6-N1-C1'	-5.85	113.78	120.80
35	RA	1911	U	N1-C2-O2	5.85	126.89	122.80
35	YA	797	C	C6-N1-C2	-5.85	117.96	120.30
1	XA	315	A	P-O3'-C3'	5.85	126.72	119.70
1	QA	5	U	P-O3'-C3'	5.84	126.71	119.70
35	YA	277	C	C6-N1-C2	-5.84	117.96	120.30
1	XA	92	G	P-O3'-C3'	5.84	126.71	119.70
1	XA	1190	G	OP2-P-O3'	5.84	118.05	105.20
35	YA	286	C	N1-C2-O2	5.84	122.41	118.90
36	YB	37	C	N1-C2-O2	5.83	122.40	118.90
35	RA	2211	G	P-O3'-C3'	5.83	126.70	119.70
35	RA	416	C	C2-N1-C1'	5.83	125.21	118.80
35	YA	1911	U	N1-C2-O2	5.83	126.88	122.80
35	RA	198	C	C5-C6-N1	5.83	123.91	121.00
1	XA	749	C	C6-N1-C2	-5.82	117.97	120.30
1	XA	283	C	N1-C2-O2	5.82	122.39	118.90
16	XP	32	TYR	CA-CB-CG	5.82	124.45	113.40
35	YA	2343	C	C2-N1-C1'	5.82	125.20	118.80
42	YI	144	VAL	C-N-CA	5.82	136.24	121.70
1	QA	283	C	C5-C6-N1	5.81	123.91	121.00
1	XA	1031	G	N3-C4-C5	-5.81	125.69	128.60
35	RA	1559	G	P-O3'-C3'	5.81	126.68	119.70
1	XA	137	C	N1-C2-O2	5.81	122.39	118.90
51	RV	15	GLU	CB-CA-C	5.81	122.02	110.40
51	YV	85	LYS	CG-CD-CE	5.81	129.33	111.90
1	QA	1301	U	C6-N1-C2	-5.81	117.52	121.00
17	QQ	101	ARG	N-CA-C	-5.81	95.32	111.00
2	QB	230	VAL	C-N-CA	5.80	136.20	121.70
35	RA	783	A	C2-N3-C4	5.80	113.50	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	270(Q)	C	C6-N1-C2	-5.80	117.98	120.30
23	QX	11	U	OP1-P-O3'	5.80	117.96	105.20
35	RA	343	C	C6-N1-C2	-5.80	117.98	120.30
35	YA	289	A	N7-C8-N9	5.80	116.70	113.80
36	YB	27	C	N3-C2-O2	-5.80	117.84	121.90
1	XA	1031	G	C4-N9-C1'	5.80	134.03	126.50
35	YA	2701	C	C6-N1-C2	-5.79	117.98	120.30
35	YA	114	U	C2-N1-C1'	5.79	124.65	117.70
35	YA	1313	U	C6-N1-C1'	-5.79	113.09	121.20
35	RA	343	C	N1-C2-O2	5.79	122.37	118.90
35	RA	2527	C	C6-N1-C2	-5.79	117.99	120.30
35	YA	1656	C	C5-C6-N1	5.78	123.89	121.00
35	YA	537	C	C5-C6-N1	5.78	123.89	121.00
1	QA	405	U	N1-C2-O2	5.77	126.84	122.80
35	RA	1502	C	N1-C2-O2	5.77	122.36	118.90
35	RA	1318	C	C5-C6-N1	5.76	123.88	121.00
1	QA	1007	C	C2-N1-C1'	5.76	125.14	118.80
1	QA	1137	C	P-O3'-C3'	5.76	126.61	119.70
35	RA	708	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	442	C	C5-C6-N1	5.76	123.88	121.00
35	RA	2667	C	N3-C2-O2	-5.75	117.87	121.90
43	YN	35	ARG	N-CA-C	-5.75	95.47	111.00
35	YA	1656	C	C6-N1-C2	-5.75	118.00	120.30
35	RA	2108	C	C2-N1-C1'	5.75	125.12	118.80
1	QA	960	U	P-O3'-C3'	5.75	126.60	119.70
35	RA	2575	C	C5-C6-N1	5.74	123.87	121.00
35	YA	1781	C	N1-C2-O2	5.74	122.34	118.90
1	QA	754	C	C6-N1-C2	-5.74	118.00	120.30
1	QA	1536	C	N1-C2-O2	5.74	122.34	118.90
36	YB	66	A	P-O3'-C3'	5.74	126.59	119.70
35	RA	487	C	N1-C2-O2	5.74	122.34	118.90
35	RA	527	C	N1-C2-O2	5.74	122.34	118.90
35	RA	1640	C	C5-C6-N1	5.74	123.87	121.00
43	RN	114	ARG	N-CA-C	-5.74	95.52	111.00
1	XA	243	A	P-O3'-C3'	5.73	126.58	119.70
35	RA	105	C	C6-N1-C2	-5.73	118.01	120.30
35	YA	1675	C	N1-C2-O2	5.73	122.34	118.90
35	RA	2294	C	C5-C6-N1	5.73	123.86	121.00
1	XA	1303	C	N1-C2-O2	5.73	122.34	118.90
1	QA	960	U	N3-C2-O2	-5.73	118.19	122.20
35	RA	752	A	P-O3'-C3'	5.73	126.57	119.70
1	XA	279	A	P-O3'-C3'	5.73	126.57	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	190	G	P-O3'-C3'	5.72	126.57	119.70
35	RA	1188	U	N1-C2-O2	5.72	126.81	122.80
35	YA	1774	C	C2-N1-C1'	5.72	125.10	118.80
1	XA	1109	C	N1-C2-O2	5.72	122.33	118.90
35	RA	2466	C	N1-C2-O2	5.72	122.33	118.90
35	YA	2342	C	C6-N1-C2	-5.72	118.01	120.30
35	YA	1781	C	C2-N1-C1'	5.72	125.09	118.80
35	RA	1499	C	C2-N1-C1'	5.71	125.09	118.80
35	YA	277	C	C2-N1-C1'	5.71	125.08	118.80
35	YA	12	U	N3-C2-O2	-5.71	118.20	122.20
35	RA	806	C	C6-N1-C2	-5.71	118.02	120.30
35	YA	2128	C	C5-C6-N1	5.71	123.86	121.00
35	RA	2467	C	C6-N1-C2	-5.71	118.02	120.30
35	YA	1370	C	C2-N1-C1'	5.70	125.07	118.80
35	RA	2527	C	C5-C6-N1	5.70	123.85	121.00
37	YD	88	ARG	NE-CZ-NH2	-5.70	117.45	120.30
35	YA	965	C	C6-N1-C2	-5.70	118.02	120.30
35	YA	1640	C	C2-N1-C1'	5.70	125.06	118.80
35	YA	1640	C	C5-C6-N1	5.69	123.85	121.00
35	YA	1915	U	N1-C2-O2	5.69	126.78	122.80
1	XA	442	C	N1-C2-O2	5.69	122.31	118.90
35	YA	172	C	C2-N1-C1'	5.69	125.06	118.80
35	RA	1679	U	N3-C2-O2	-5.69	118.22	122.20
35	YA	2307	G	O4'-C1'-N9	5.69	112.75	108.20
1	XA	330	C	N3-C2-O2	-5.69	117.92	121.90
35	YA	2210	G	C8-N9-C1'	-5.69	119.61	127.00
1	QA	1306	A	C2-N3-C4	5.69	113.44	110.60
36	YB	118	G	N3-C4-C5	-5.69	125.76	128.60
35	YA	2559	C	C5-C6-N1	5.68	123.84	121.00
25	R0	51	VAL	N-CA-C	-5.67	95.68	111.00
35	YA	18	C	C6-N1-C2	-5.67	118.03	120.30
35	YA	1915	U	N3-C2-O2	-5.67	118.23	122.20
35	YA	1505	C	C6-N1-C2	-5.67	118.03	120.30
1	QA	442	C	N1-C2-O2	5.67	122.30	118.90
1	QA	485	G	P-O3'-C3'	5.67	126.50	119.70
10	QJ	79	ARG	NE-CZ-NH2	-5.67	117.47	120.30
35	YA	2394	C	C6-N1-C2	-5.67	118.03	120.30
35	RA	2343	C	N1-C2-O2	5.66	122.30	118.90
1	QA	1006	C	C6-N1-C1'	-5.66	114.01	120.80
1	QA	1325	C	C6-N1-C2	-5.66	118.04	120.30
1	QA	1033	G	C4-N9-C1'	5.65	133.85	126.50
1	XA	1006	C	C2-N1-C1'	5.65	125.02	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	363(E)	U	C6-N1-C1'	-5.65	113.29	121.20
35	YA	2712	U	C6-N1-C1'	-5.65	113.29	121.20
35	RA	753	C	C6-N1-C2	-5.65	118.04	120.30
35	RA	1313	U	C6-N1-C1'	-5.64	113.30	121.20
35	YA	2096	U	N1-C2-O2	5.64	126.75	122.80
55	RZ	112	ARG	CB-CA-C	5.64	121.68	110.40
1	QA	442	C	C6-N1-C2	-5.64	118.04	120.30
35	RA	1064	C	N1-C2-O2	5.64	122.28	118.90
35	YA	270(U)	C	C6-N1-C2	-5.64	118.05	120.30
10	QJ	28	ARG	CG-CD-NE	5.64	123.64	111.80
35	RA	1427	A	P-O3'-C3'	5.64	126.46	119.70
1	QA	1536	C	C6-N1-C2	-5.63	118.05	120.30
35	RA	753	C	C5-C6-N1	5.63	123.82	121.00
35	RA	1502	C	C5-C6-N1	5.63	123.82	121.00
35	YA	1267	U	N3-C2-O2	-5.63	118.26	122.20
35	RA	1909	C	C6-N1-C2	-5.63	118.05	120.30
35	YA	1294	U	N1-C2-O2	5.63	126.74	122.80
36	YB	77	U	C2-N1-C1'	5.63	124.46	117.70
35	YA	1427	A	P-O3'-C3'	5.63	126.45	119.70
35	YA	2604	U	N3-C2-O2	-5.63	118.26	122.20
35	RA	1180	C	C6-N1-C1'	-5.63	114.05	120.80
1	XA	54	C	N1-C2-O2	5.63	122.28	118.90
35	RA	279	C	C5-C6-N1	5.62	123.81	121.00
1	XA	1439	C	N1-C2-O2	5.62	122.28	118.90
36	RB	47	C	C2-N1-C1'	5.62	124.98	118.80
1	XA	738	C	C5-C6-N1	5.62	123.81	121.00
35	RA	128	C	C6-N1-C2	-5.62	118.05	120.30
36	RB	27	C	C5-C6-N1	5.62	123.81	121.00
35	YA	1588	C	C5-C6-N1	5.62	123.81	121.00
35	YA	2103	C	C5-C6-N1	5.61	123.81	121.00
35	RA	2584	U	N1-C2-O2	5.61	126.73	122.80
35	RA	904	C	C2-N1-C1'	5.61	124.97	118.80
1	QA	1031	G	N3-C4-C5	-5.61	125.80	128.60
35	RA	1881	C	N1-C2-O2	5.61	122.26	118.90
35	RA	2739	U	N3-C2-O2	-5.61	118.28	122.20
22	XV	1	C	P-O3'-C3'	5.61	126.43	119.70
1	QA	419	C	C6-N1-C2	-5.61	118.06	120.30
35	RA	635	C	C6-N1-C2	-5.61	118.06	120.30
35	RA	1152	C	N1-C2-O2	5.61	122.26	118.90
35	RA	2559	C	N1-C2-O2	5.61	122.26	118.90
1	XA	525	C	C5-C6-N1	5.61	123.80	121.00
35	YA	556	G	C6-C5-N7	-5.61	127.04	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	1157	A	P-O3'-C3'	5.60	126.42	119.70
35	RA	1233	C	C5-C6-N1	5.60	123.80	121.00
1	XA	1007	C	C6-N1-C2	-5.60	118.06	120.30
35	YA	2225	A	P-O3'-C3'	5.60	126.42	119.70
35	RA	1735	C	C5-C6-N1	5.59	123.80	121.00
35	YA	69	C	C2-N1-C1'	5.59	124.95	118.80
35	YA	140	A	C8-N9-C4	-5.59	103.56	105.80
35	YA	975	G	N3-C4-C5	-5.59	125.80	128.60
35	YA	1406	U	N1-C2-O2	5.59	126.72	122.80
43	YN	114	ARG	N-CA-C	-5.59	95.90	111.00
35	RA	1779	U	C2-N1-C1'	5.59	124.41	117.70
35	RA	2118	U	N1-C2-O2	5.59	126.72	122.80
35	YA	1934	C	C2-N1-C1'	5.59	124.95	118.80
35	RA	1394	U	C6-N1-C2	-5.59	117.65	121.00
35	RA	1505	C	C6-N1-C2	-5.59	118.06	120.30
35	YA	1882	C	C6-N1-C1'	-5.59	114.09	120.80
1	QA	1147	C	C2-N1-C1'	5.58	124.94	118.80
35	RA	2604	U	N1-C2-O2	5.58	126.71	122.80
35	RA	436	C	N1-C2-O2	5.58	122.25	118.90
1	QA	999	U	OP1-P-O3'	5.58	117.47	105.20
35	RA	856	C	N1-C2-O2	5.58	122.25	118.90
35	YA	2477	C	N1-C2-O2	5.58	122.25	118.90
35	RA	2243	U	N3-C2-O2	-5.58	118.30	122.20
1	XA	186	C	C6-N1-C2	-5.57	118.07	120.30
35	YA	530	G	C5-C6-O6	-5.57	125.26	128.60
9	XI	102	LEU	CA-CB-CG	5.57	128.12	115.30
36	YB	47	C	C5-C6-N1	5.57	123.79	121.00
35	RA	1314	C	N1-C2-O2	5.57	122.24	118.90
36	RB	37	C	N1-C2-O2	5.57	122.24	118.90
1	XA	186	C	C5-C6-N1	5.57	123.78	121.00
1	XA	330	C	C5-C6-N1	5.57	123.78	121.00
1	XA	1031	G	N3-C4-N9	5.56	129.34	126.00
35	YA	9	U	C2-N1-C1'	5.56	124.38	117.70
35	RA	2043	C	C6-N1-C2	-5.55	118.08	120.30
35	YA	1979	C	N1-C2-O2	5.55	122.23	118.90
1	QA	1158	C	C6-N1-C1'	-5.54	114.15	120.80
40	RG	83	ARG	CG-CD-NE	5.54	123.44	111.80
35	YA	154	G	N3-C4-N9	5.54	129.33	126.00
1	XA	169	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	1007	C	C6-N1-C1'	-5.54	114.15	120.80
8	XH	60	ARG	CD-NE-CZ	5.54	131.36	123.60
1	QA	252	U	C5-C6-N1	5.54	125.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1332	G	C6-C5-N7	-5.54	127.08	130.40
34	Y9	37	GLY	N-CA-C	-5.54	99.25	113.10
1	XA	690	G	C4-N9-C1'	5.54	133.70	126.50
1	QA	1109	C	N1-C2-O2	5.54	122.22	118.90
35	RA	1644	C	C6-N1-C2	-5.54	118.09	120.30
36	RB	27	C	C2-N1-C1'	5.54	124.89	118.80
1	QA	960	U	C2-N1-C1'	5.53	124.34	117.70
1	QA	652	U	N1-C2-O2	5.53	126.67	122.80
35	RA	544	C	N1-C2-O2	5.53	122.22	118.90
35	YA	1188	U	N1-C2-O2	5.53	126.67	122.80
36	RB	87	G	N1-C6-O6	-5.53	116.58	119.90
35	YA	1180	C	N1-C2-O2	5.53	122.22	118.90
36	YB	8	U	C2-N1-C1'	5.53	124.33	117.70
1	QA	58	C	C5-C6-N1	5.53	123.76	121.00
35	RA	269	U	C5-C6-N1	5.53	125.46	122.70
35	RA	2108	C	C6-N1-C2	-5.52	118.09	120.30
1	QA	1033	G	C8-N9-C1'	-5.52	119.82	127.00
35	RA	1318	C	C6-N1-C2	-5.52	118.09	120.30
35	YA	2559	C	C6-N1-C2	-5.52	118.09	120.30
35	RA	2540	C	C6-N1-C2	-5.52	118.09	120.30
1	QA	1031	G	N3-C4-N9	5.52	129.31	126.00
35	RA	2006	C	N1-C2-O2	5.52	122.21	118.90
35	YA	652	C	C6-N1-C2	-5.51	118.09	120.30
35	RA	286	C	C5-C6-N1	5.51	123.76	121.00
35	RA	1950	G	O4'-C1'-N9	5.51	112.61	108.20
35	YA	752	A	OP2-P-O3'	5.51	117.33	105.20
1	QA	652	U	N3-C2-O2	-5.51	118.34	122.20
35	YA	652	C	C2-N1-C1'	5.51	124.86	118.80
35	YA	2471	C	C2-N1-C1'	5.51	124.86	118.80
35	RA	758	C	N3-C2-O2	-5.51	118.05	121.90
25	R0	48	GLY	N-CA-C	5.50	126.86	113.10
35	RA	1505	C	C2-N1-C1'	5.50	124.85	118.80
1	XA	703	G	P-O3'-C3'	5.50	126.30	119.70
35	RA	1406	U	N3-C2-O2	-5.50	118.35	122.20
35	YA	1180	C	C5-C6-N1	5.50	123.75	121.00
35	YA	652	C	N3-C2-O2	-5.50	118.05	121.90
1	QA	454	C	C6-N1-C2	-5.50	118.10	120.30
1	QA	18	C	C5-C6-N1	5.49	123.75	121.00
1	QA	1260	C	C6-N1-C2	-5.49	118.10	120.30
35	RA	2873	A	C8-N9-C4	-5.49	103.60	105.80
1	XA	1381	U	C5-C6-N1	5.49	125.45	122.70
35	YA	904	C	N1-C2-O2	5.49	122.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2210	G	C2-N3-C4	5.49	114.64	111.90
35	RA	265	A	O4'-C1'-N9	5.49	112.59	108.20
36	RB	27	C	N3-C2-O2	-5.49	118.06	121.90
11	XK	96	ARG	CB-CG-CD	-5.49	97.33	111.60
35	YA	273(D)	C	C2-N1-C1'	5.49	124.84	118.80
46	RQ	5	ARG	CG-CD-NE	5.49	123.32	111.80
1	XA	1260	C	C2-N1-C1'	5.48	124.83	118.80
35	RA	41	C	C6-N1-C2	-5.48	118.11	120.30
13	XM	8	GLU	N-CA-C	-5.48	96.20	111.00
1	QA	1008	C	O5'-P-OP1	5.48	117.28	110.70
35	RA	9	U	N3-C2-O2	-5.48	118.36	122.20
35	RA	431	U	C5-C6-N1	5.48	125.44	122.70
35	YA	270(Q)	C	N3-C2-O2	-5.48	118.06	121.90
35	YA	288	C	C2-N1-C1'	5.48	124.83	118.80
1	XA	1040	U	C2-N1-C1'	5.48	124.27	117.70
35	RA	650	C	C6-N1-C2	-5.47	118.11	120.30
22	XV	56	C	N1-C2-O2	5.47	122.19	118.90
35	YA	2585	U	N3-C2-O2	-5.47	118.37	122.20
1	XA	1325	C	C2-N1-C1'	5.47	124.82	118.80
35	YA	193	U	C5-C6-N1	5.47	125.44	122.70
35	RA	930	U	N1-C2-O2	5.47	126.63	122.80
29	Y4	67	TYR	N-CA-C	-5.47	96.23	111.00
35	RA	436	C	N3-C2-O2	-5.47	118.07	121.90
1	XA	1228	C	N1-C2-O2	5.47	122.18	118.90
35	YA	2604	U	N1-C2-O2	5.47	126.63	122.80
29	Y4	67	TYR	CA-CB-CG	5.46	123.78	113.40
1	XA	1263	C	C6-N1-C2	-5.46	118.12	120.30
35	RA	2394	C	N3-C2-O2	-5.46	118.08	121.90
3	XC	140	ARG	CD-NE-CZ	5.46	131.24	123.60
1	QA	1006	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	1406	U	N3-C2-O2	-5.46	118.38	122.20
1	XA	1362(A)	C	N3-C2-O2	-5.46	118.08	121.90
1	QA	932	C	C6-N1-C2	-5.45	118.12	120.30
24	QY	63	GLU	CB-CA-C	-5.45	99.49	110.40
35	RA	1314	C	C6-N1-C2	-5.45	118.12	120.30
35	RA	2712	U	N1-C2-O2	5.45	126.62	122.80
36	RB	77	U	N3-C2-O2	-5.45	118.39	122.20
1	XA	1126	U	C5-C6-N1	5.45	125.42	122.70
35	YA	2702	U	O5'-P-OP1	5.45	117.24	110.70
35	RA	2041	U	N1-C2-O2	5.45	126.61	122.80
35	YA	2527	C	C2-N1-C1'	5.45	124.79	118.80
24	XY	49	LYS	C-N-CA	5.44	135.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	2808	U	N1-C2-O2	5.44	126.61	122.80
35	YA	288	C	OP1-P-O3'	5.44	117.17	105.20
1	QA	330	C	N1-C2-O2	5.44	122.16	118.90
1	XA	368	U	N3-C4-C5	5.44	117.86	114.60
35	YA	1528	A	N7-C8-N9	5.44	116.52	113.80
35	RA	1698	A	O4'-C1'-N9	5.43	112.55	108.20
1	XA	137	C	C6-N1-C2	-5.43	118.13	120.30
35	YA	2244	U	N3-C4-O4	5.43	123.20	119.40
35	YA	2712	U	N3-C2-O2	-5.43	118.40	122.20
1	QA	1303	C	C2-N1-C1'	5.43	124.78	118.80
1	XA	169	C	C5-C6-N1	5.43	123.72	121.00
35	YA	894	C	C2-N1-C1'	5.43	124.78	118.80
35	YA	1233	C	C6-N1-C2	-5.43	118.13	120.30
35	RA	2066	C	N1-C2-O2	5.43	122.16	118.90
35	RA	69	C	C6-N1-C2	-5.42	118.13	120.30
35	RA	1963	U	N1-C2-O2	5.42	126.60	122.80
35	RA	143	C	C6-N1-C2	-5.42	118.13	120.30
35	RA	2787	C	N3-C2-O2	-5.42	118.11	121.90
35	RA	2847	U	N3-C2-O2	-5.42	118.41	122.20
37	YD	88	ARG	CB-CA-C	-5.42	99.56	110.40
2	XB	236	TYR	N-CA-CB	-5.42	100.85	110.60
35	YA	286	C	C6-N1-C2	-5.42	118.13	120.30
35	YA	1979	C	N3-C2-O2	-5.42	118.11	121.90
35	RA	1506	C	C6-N1-C2	-5.42	118.13	120.30
51	RV	39	LEU	CA-CB-CG	5.42	127.75	115.30
49	YT	105	LEU	CA-CB-CG	5.42	127.75	115.30
10	XJ	31	GLY	N-CA-C	5.41	126.63	113.10
1	QA	518	C	P-O3'-C3'	5.41	126.19	119.70
35	RA	2889	C	C6-N1-C2	-5.41	118.14	120.30
1	XA	353	A	OP2-P-O3'	5.41	117.10	105.20
1	QA	18	C	C6-N1-C2	-5.41	118.14	120.30
17	QQ	101	ARG	CD-NE-CZ	5.41	131.17	123.60
27	R2	47	ASN	C-N-CA	5.41	135.22	121.70
35	RA	1735	C	C6-N1-C2	-5.41	118.14	120.30
38	RE	116	VAL	C-N-CA	5.41	135.22	121.70
35	YA	1256	G	C4-N9-C1'	5.41	133.53	126.50
35	RA	195	A	P-O3'-C3'	5.41	126.19	119.70
35	YA	9	U	N3-C2-O2	-5.41	118.42	122.20
35	YA	1474	C	N1-C2-O2	5.41	122.14	118.90
39	YF	129	PHE	N-CA-C	5.41	125.60	111.00
1	QA	1225	A	C4-N9-C1'	5.40	136.02	126.30
35	RA	143	C	C5-C6-N1	5.40	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1742	C	C6-N1-C2	-5.40	118.14	120.30
35	RA	273(C)	C	C2-N1-C1'	5.39	124.73	118.80
35	RA	530	G	N1-C6-O6	5.39	123.14	119.90
1	QA	442	C	C5-C6-N1	5.39	123.69	121.00
35	RA	47	C	C6-N1-C2	-5.39	118.14	120.30
41	RH	67	LEU	CA-CB-CG	5.39	127.70	115.30
35	RA	269	U	C6-N1-C1'	-5.39	113.65	121.20
35	RA	2571	C	C6-N1-C2	-5.39	118.14	120.30
35	YA	1881	C	N1-C2-O2	5.38	122.13	118.90
35	RA	1920	C	C5-C6-N1	5.38	123.69	121.00
35	YA	2808	U	N3-C2-O2	-5.38	118.43	122.20
1	QA	283	C	C6-N1-C2	-5.38	118.15	120.30
35	RA	1781	C	N1-C2-O2	5.38	122.13	118.90
36	RB	77	U	C2-N1-C1'	5.38	124.16	117.70
35	RA	537	C	C5-C6-N1	5.38	123.69	121.00
1	QA	1008	C	C2-N1-C1'	5.37	124.71	118.80
1	QA	79	G	N3-C4-C5	-5.37	125.92	128.60
1	QA	268	C	C6-N1-C2	-5.37	118.15	120.30
35	RA	2321	G	N3-C4-C5	-5.37	125.92	128.60
1	XA	169	C	N1-C2-O2	5.37	122.12	118.90
14	QN	13	THR	N-CA-C	5.37	125.50	111.00
35	RA	143	C	C2-N1-C1'	5.37	124.70	118.80
35	RA	1992	G	OP2-P-O3'	5.37	117.00	105.20
13	XM	108	ARG	N-CA-C	5.37	125.48	111.00
35	YA	153	C	C2-N1-C1'	5.36	124.69	118.80
35	YA	234	C	N3-C2-O2	-5.36	118.15	121.90
35	YA	2139	C	C2-N1-C1'	5.36	124.69	118.80
35	YA	2144	U	P-O3'-C3'	5.36	126.13	119.70
35	RA	358	U	C5-C6-N1	5.36	125.38	122.70
35	RA	481	G	O4'-C1'-N9	5.36	112.49	108.20
35	RA	1774	C	C2-N1-C1'	5.36	124.69	118.80
35	RA	1911	U	N3-C2-O2	-5.36	118.45	122.20
1	XA	341	C	C6-N1-C2	-5.35	118.16	120.30
35	YA	1934	C	N1-C2-O2	5.35	122.11	118.90
3	QC	78	GLY	N-CA-C	5.35	126.48	113.10
35	YA	1294	U	C2-N1-C1'	5.35	124.12	117.70
29	R4	22	ILE	C-N-CA	5.35	135.07	121.70
1	XA	1535	C	C6-N1-C2	-5.35	118.16	120.30
35	YA	2321	G	N3-C4-N9	5.35	129.21	126.00
39	YF	199	TRP	N-CA-C	-5.35	96.56	111.00
35	RA	1909	C	C5-C6-N1	5.35	123.67	121.00
35	RA	2667	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	137	C	C5-C6-N1	5.35	123.67	121.00
35	RA	1474	C	C5-C6-N1	5.34	123.67	121.00
35	YA	1909	C	C6-N1-C2	-5.34	118.16	120.30
35	YA	2683	C	N1-C2-O2	5.34	122.10	118.90
35	RA	2752	C	C2-N1-C1'	5.34	124.67	118.80
35	YA	1788	C	C6-N1-C2	-5.34	118.17	120.30
35	YA	2096	U	C2-N1-C1'	5.34	124.11	117.70
35	RA	530	G	C5-C6-O6	-5.34	125.40	128.60
7	XG	111	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	QA	717	C	C2-N1-C1'	5.33	124.67	118.80
35	RA	930	U	N3-C2-O2	-5.33	118.47	122.20
1	XA	330	C	C2-N1-C1'	5.33	124.67	118.80
35	YA	2205	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	2604	U	C2-N1-C1'	5.33	124.10	117.70
35	YA	2873	A	N7-C8-N9	5.33	116.47	113.80
35	RA	1417	C	C2-N1-C1'	5.33	124.67	118.80
36	YB	30	C	C6-N1-C2	-5.33	118.17	120.30
1	QA	252	U	N3-C2-O2	-5.33	118.47	122.20
1	QA	749	C	N1-C2-O2	5.33	122.10	118.90
35	RA	1502	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	1675	C	C6-N1-C2	-5.33	118.17	120.30
36	RB	27	C	C6-N1-C2	-5.33	118.17	120.30
40	RG	146	TYR	N-CA-CB	-5.33	101.02	110.60
35	RA	1931	U	C5-C6-N1	5.32	125.36	122.70
2	XB	178	ARG	CG-CD-NE	5.32	122.98	111.80
1	XA	1147	C	C2-N1-C1'	5.32	124.65	118.80
35	YA	930	U	C2-N1-C1'	5.32	124.08	117.70
35	RA	860	U	N1-C2-O2	5.32	126.52	122.80
51	RV	95	LEU	CA-CB-CG	5.31	127.52	115.30
35	RA	934	G	N3-C4-N9	5.31	129.19	126.00
35	RA	1395	A	O4'-C1'-N9	5.31	112.45	108.20
35	RA	587	C	P-O3'-C3'	5.31	126.07	119.70
42	YI	10	GLU	CA-CB-CG	5.31	125.08	113.40
35	RA	2210	G	N3-C4-N9	5.31	129.19	126.00
35	YA	41	C	C2-N1-C1'	5.31	124.64	118.80
35	YA	527	C	C6-N1-C1'	-5.31	114.43	120.80
1	XA	405	U	N1-C2-O2	5.30	126.51	122.80
51	YV	95	LEU	CA-CB-CG	5.30	127.49	115.30
35	RA	1011	G	C4-N9-C1'	-5.30	119.61	126.50
35	RA	721	C	C6-N1-C2	-5.30	118.18	120.30
1	QA	705	U	N3-C2-O2	-5.29	118.49	122.20
1	XA	932	C	C5-C6-N1	5.29	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	YR	75	LEU	CA-CB-CG	5.29	127.48	115.30
35	RA	104	U	N1-C2-O2	5.29	126.51	122.80
35	RA	1735	C	N1-C2-O2	5.29	122.08	118.90
35	YA	797	C	C5-C6-N1	5.29	123.65	121.00
1	XA	1033	G	P-O3'-C3'	5.29	126.05	119.70
35	RA	1474	C	C6-N1-C2	-5.29	118.19	120.30
35	RA	1934	C	N1-C2-O2	5.29	122.07	118.90
1	XA	75	C	C5-C6-N1	5.29	123.64	121.00
35	RA	2205	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	2096	U	N3-C2-O2	-5.28	118.50	122.20
45	YP	104	GLY	N-CA-C	5.28	126.30	113.10
35	YA	587	C	P-O3'-C3'	5.28	126.03	119.70
22	QV	32	C	N3-C2-O2	-5.27	118.21	121.90
35	RA	1475	G	N3-C4-N9	5.27	129.16	126.00
35	RA	2063	C	C5-C6-N1	5.27	123.64	121.00
35	RA	1930	G	OP2-P-O3'	5.27	116.79	105.20
35	RA	2571	C	C5-C6-N1	5.27	123.63	121.00
1	XA	749	C	N3-C2-O2	-5.27	118.21	121.90
35	YA	372	G	OP2-P-O3'	5.27	116.79	105.20
35	YA	556	G	N7-C8-N9	5.27	115.73	113.10
35	YA	1075	C	C5-C6-N1	5.27	123.63	121.00
1	QA	186	C	C6-N1-C2	-5.26	118.19	120.30
35	RA	273(D)	C	C2-N1-C1'	5.26	124.59	118.80
1	QA	435	C	C5-C6-N1	5.26	123.63	121.00
10	XJ	35	SER	N-CA-C	-5.26	96.79	111.00
35	YA	2343	C	N1-C2-O2	5.26	122.06	118.90
35	RA	2703	C	N1-C2-O2	5.26	122.06	118.90
35	YA	1819	A	P-O3'-C3'	5.26	126.01	119.70
30	R5	51	TYR	CA-CB-CG	5.26	123.39	113.40
35	YA	893	C	N1-C2-O2	5.25	122.05	118.90
35	RA	1462	C	N3-C2-O2	-5.25	118.22	121.90
35	RA	2467	C	N3-C2-O2	-5.25	118.22	121.90
35	RA	358	U	C2-N1-C1'	5.25	124.00	117.70
20	XT	96	GLY	C-N-CA	5.25	134.82	121.70
35	RA	1462	C	N1-C2-O2	5.25	122.05	118.90
35	RA	1786	A	C4-N9-C1'	5.25	135.75	126.30
1	XA	169	C	C2-N1-C1'	5.25	124.57	118.80
35	RA	1005	C	C6-N1-C2	-5.25	118.20	120.30
35	RA	1947	C	N1-C2-O2	5.25	122.05	118.90
35	RA	2394	C	C6-N1-C2	-5.25	118.20	120.30
36	YB	47	C	N3-C2-O2	-5.25	118.23	121.90
35	RA	1407	C	C6-N1-C1'	-5.25	114.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	YQ	59	ARG	C-N-CA	5.25	134.81	121.70
43	YN	114	ARG	C-N-CA	5.24	134.81	121.70
35	RA	372	G	OP2-P-O3'	5.24	116.73	105.20
1	XA	1128	C	C5-C6-N1	5.24	123.62	121.00
1	QA	1490	C	C6-N1-C2	-5.24	118.20	120.30
35	YA	2726	U	O4'-C1'-N1	5.24	112.39	108.20
40	RG	9	ARG	CG-CD-NE	5.24	122.80	111.80
9	XI	85	LEU	CA-CB-CG	5.24	127.34	115.30
35	YA	1735	C	C5-C6-N1	5.23	123.62	121.00
1	QA	455	C	C2-N1-C1'	5.23	124.56	118.80
1	QA	932	C	C5-C6-N1	5.23	123.61	121.00
1	XA	1395	C	C2-N1-C1'	5.23	124.55	118.80
35	YA	2584	U	C6-N1-C2	-5.23	117.86	121.00
35	YA	857	C	C5-C6-N1	5.23	123.61	121.00
9	QI	62	TYR	N-CA-C	-5.22	96.90	111.00
1	XA	999	U	OP1-P-O3'	5.22	116.69	105.20
4	XD	154	ASN	C-N-CA	5.22	134.75	121.70
35	RA	104	U	N3-C2-O2	-5.22	118.55	122.20
35	RA	1963	U	N3-C2-O2	-5.22	118.55	122.20
35	RA	2730	C	C6-N1-C2	-5.22	118.21	120.30
35	RA	1588	C	C6-N1-C1'	-5.22	114.54	120.80
35	YA	435	C	N3-C2-O2	-5.22	118.25	121.90
35	YA	708	C	N1-C2-O2	5.22	122.03	118.90
35	RA	41	C	C2-N1-C1'	5.21	124.54	118.80
35	RA	234	C	N3-C2-O2	-5.21	118.25	121.90
35	RA	893	C	N1-C2-O2	5.21	122.03	118.90
35	RA	2585	U	N3-C2-O2	-5.21	118.55	122.20
35	YA	2456	C	C5-C6-N1	5.21	123.61	121.00
35	RA	435	C	N3-C2-O2	-5.21	118.25	121.90
1	XA	209	U	C2-N1-C1'	5.21	123.95	117.70
35	RA	1819	A	P-O3'-C3'	5.21	125.95	119.70
1	XA	1382	C	C6-N1-C2	-5.21	118.22	120.30
49	YT	96	ARG	CA-CB-CG	5.21	124.86	113.40
1	QA	1347	G	OP2-P-O3'	5.21	116.65	105.20
35	RA	288	C	C5-C6-N1	5.21	123.60	121.00
35	RA	1934	C	C2-N1-C1'	5.21	124.53	118.80
35	RA	2540	C	C2-N1-C1'	5.21	124.53	118.80
1	XA	1158	C	N1-C2-O2	5.21	122.02	118.90
35	RA	1430	C	C5-C6-N1	5.20	123.60	121.00
1	QA	1378	C	N1-C2-O2	5.20	122.02	118.90
35	RA	1544	C	C2-N1-C1'	5.20	124.52	118.80
35	YA	2128	C	C6-N1-C2	-5.20	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	315	A	OP2-P-O3'	5.20	116.63	105.20
1	XA	1128	C	N1-C2-O2	5.20	122.02	118.90
35	YA	974	G	C8-N9-C1'	5.20	133.75	127.00
35	YA	2342	C	C2-N1-C1'	5.19	124.51	118.80
35	YA	634	C	C6-N1-C2	-5.19	118.22	120.30
1	QA	1263	C	N1-C2-O2	5.19	122.02	118.90
35	RA	1304	C	C6-N1-C2	-5.19	118.22	120.30
1	XA	341	C	C5-C6-N1	5.19	123.60	121.00
1	QA	312	C	C2-N1-C1'	5.19	124.51	118.80
1	XA	58	C	C5-C6-N1	5.19	123.59	121.00
1	XA	1007	C	OP1-P-O3'	5.18	116.61	105.20
35	RA	1385	G	O4'-C1'-N9	5.18	112.35	108.20
36	YB	117	G	OP1-P-O3'	5.18	116.60	105.20
35	RA	2604	U	N3-C2-O2	-5.18	118.58	122.20
35	RA	2739	U	N1-C2-O2	5.18	126.43	122.80
3	XC	63	ASN	N-CA-C	-5.18	97.02	111.00
35	YA	114	U	N1-C2-O2	5.18	126.43	122.80
47	YR	57	ARG	CB-CA-C	5.18	120.76	110.40
1	XA	1502	A	C4-N9-C1'	5.18	135.62	126.30
1	QA	1000	A	OP1-P-O3'	5.18	116.59	105.20
35	RA	1911	U	C2-N1-C1'	5.18	123.91	117.70
1	XA	1263	C	N1-C2-O2	5.18	122.01	118.90
35	YA	1993	U	N1-C2-O2	5.18	126.42	122.80
36	YB	27	C	C6-N1-C2	-5.18	118.23	120.30
1	XA	1128	C	N3-C2-O2	-5.17	118.28	121.90
1	QA	405	U	N3-C2-O2	-5.17	118.58	122.20
35	RA	2666	C	C5-C6-N1	5.17	123.58	121.00
36	RB	8	U	N1-C2-O2	5.17	126.42	122.80
35	YA	527	C	N3-C2-O2	-5.17	118.28	121.90
35	YA	2461	C	C2-N1-C1'	5.17	124.48	118.80
35	RA	243	U	N1-C2-O2	5.16	126.42	122.80
35	RA	1475	G	C4-N9-C1'	5.16	133.21	126.50
35	RA	708	C	C6-N1-C1'	-5.16	114.61	120.80
1	XA	1382	C	N3-C2-O2	-5.16	118.29	121.90
35	YA	31	C	C5-C6-N1	5.16	123.58	121.00
35	YA	93	C	C6-N1-C1'	-5.16	114.61	120.80
33	R8	46	ARG	N-CA-CB	-5.16	101.31	110.60
35	RA	128	C	P-O3'-C3'	5.16	125.89	119.70
35	RA	2210	G	N3-C4-C5	-5.16	126.02	128.60
1	XA	1086	U	C5-C6-N1	5.16	125.28	122.70
35	YA	157	U	N1-C2-O2	5.16	126.41	122.80
35	RA	273(C)	C	N3-C2-O2	-5.16	118.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	YA	510	C	N1-C2-O2	5.15	121.99	118.90
35	RA	2292	C	C5-C6-N1	5.15	123.58	121.00
35	RA	2294	C	N1-C2-O2	5.15	121.99	118.90
1	QA	961	U	N1-C2-O2	5.15	126.41	122.80
35	YA	273(D)	C	N1-C2-O2	5.15	121.99	118.90
35	YA	1294	U	N3-C2-O2	-5.15	118.59	122.20
35	YA	1754	C	N1-C2-O2	5.15	121.99	118.90
1	QA	328	C	C5-C6-N1	5.15	123.58	121.00
1	QA	1027	C	N1-C2-O2	5.15	121.99	118.90
20	XT	8	ARG	CG-CD-NE	5.15	122.61	111.80
45	RP	116	GLY	N-CA-C	5.15	125.97	113.10
35	RA	1678	G	C4-N9-C1'	5.15	133.19	126.50
1	QA	749	C	C5-C6-N1	5.14	123.57	121.00
31	R6	26	ASN	N-CA-C	-5.14	97.12	111.00
35	RA	1950	G	C4-N9-C1'	5.14	133.18	126.50
37	RD	131	LEU	CA-CB-CG	5.13	127.11	115.30
33	R8	35	GLN	N-CA-CB	5.13	119.84	110.60
35	RA	1920	C	C6-N1-C2	-5.13	118.25	120.30
35	YA	9	U	C5-C6-N1	5.13	125.27	122.70
35	YA	1911	U	N3-C2-O2	-5.13	118.61	122.20
35	RA	273(D)	C	C6-N1-C2	-5.13	118.25	120.30
1	XA	368	U	C5-C4-O4	-5.13	122.82	125.90
27	R2	46	GLN	C-N-CA	5.13	134.52	121.70
35	RA	1079	C	N1-C2-O2	5.13	121.98	118.90
1	QA	1059	C	C6-N1-C2	-5.12	118.25	120.30
35	RA	2108	C	C5-C6-N1	5.12	123.56	121.00
35	YA	2648	C	C2-N1-C1'	5.12	124.43	118.80
35	RA	613	U	C6-N1-C1'	-5.12	114.03	121.20
13	QM	11	ARG	N-CA-C	-5.12	97.18	111.00
1	XA	497	U	N1-C2-O2	5.12	126.38	122.80
1	QA	1008	C	P-O3'-C3'	5.12	125.84	119.70
26	R1	85	LEU	C-N-CA	5.12	134.49	121.70
35	YA	2874	C	C6-N1-C2	-5.12	118.25	120.30
8	XH	60	ARG	CG-CD-NE	5.12	122.54	111.80
36	RB	15	A	OP1-P-O3'	5.11	116.45	105.20
35	RA	1882	C	C5-C6-N1	5.11	123.56	121.00
35	YA	1430	C	C5-C6-N1	5.11	123.56	121.00
35	RA	9	U	C5-C6-N1	5.11	125.25	122.70
41	RH	151	ILE	C-N-CA	5.11	134.48	121.70
1	XA	932	C	C6-N1-C2	-5.11	118.26	120.30
35	YA	289	A	C8-N9-C4	-5.11	103.76	105.80
35	YA	413	C	C5-C6-N1	5.11	123.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1394	U	C5-C6-N1	5.11	125.25	122.70
54	RY	56	PRO	C-N-CA	5.11	134.47	121.70
1	XA	1439	C	C6-N1-C2	-5.11	118.26	120.30
41	YH	3	ARG	NE-CZ-NH1	-5.11	117.75	120.30
12	XL	104	VAL	C-N-CA	5.11	134.46	121.70
1	QA	54	C	N1-C2-O2	5.10	121.96	118.90
43	RN	35	ARG	N-CA-C	-5.10	97.22	111.00
1	XA	75	C	C6-N1-C2	-5.10	118.26	120.30
16	QP	23	ASP	N-CA-C	-5.10	97.23	111.00
1	QA	496	A	N3-C4-N9	5.10	131.48	127.40
35	RA	2726	U	C2-N1-C1'	5.10	123.82	117.70
35	YA	1835	G	N3-C4-C5	-5.10	126.05	128.60
35	YA	2166	G	P-O3'-C3'	5.10	125.82	119.70
35	RA	749	C	N3-C2-O2	-5.10	118.33	121.90
35	RA	1931	U	N1-C2-O2	5.10	126.37	122.80
35	YA	93	C	N1-C2-O2	5.10	121.96	118.90
35	RA	1788	C	C6-N1-C2	-5.10	118.26	120.30
35	RA	1499	C	N1-C2-O2	5.09	121.96	118.90
35	YA	2205	C	C5-C6-N1	5.09	123.55	121.00
23	XX	13	A	OP1-P-OP2	-5.09	111.96	119.60
35	RA	141(A)	C	C6-N1-C2	-5.09	118.26	120.30
1	XA	1009	G	O5'-P-OP1	5.09	116.81	110.70
35	YA	343	C	C5-C6-N1	5.09	123.55	121.00
35	YA	1774	C	C5-C6-N1	5.09	123.55	121.00
35	YA	2827	C	C5-C6-N1	5.09	123.55	121.00
36	YB	27	C	C2-N1-C1'	5.09	124.39	118.80
1	QA	596	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	1079	C	C2-N1-C1'	5.08	124.39	118.80
35	YA	273(D)	C	C6-N1-C2	-5.08	118.27	120.30
35	YA	692	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	2712	U	C6-N1-C1'	-5.08	114.08	121.20
35	YA	12	U	C2-N1-C1'	5.08	123.80	117.70
35	YA	69	C	C6-N1-C2	-5.08	118.27	120.30
19	XS	25	LYS	N-CA-C	-5.08	97.28	111.00
35	RA	2041	U	N3-C2-O2	-5.08	118.64	122.20
1	XA	749	C	N1-C2-O2	5.08	121.95	118.90
35	YA	613	U	C5-C6-N1	5.08	125.24	122.70
35	RA	1528	A	N7-C8-N9	5.08	116.34	113.80
35	RA	527	C	C2-N1-C1'	5.08	124.38	118.80
35	RA	2540	C	C5-C6-N1	5.08	123.54	121.00
35	RA	527	C	N3-C2-O2	-5.07	118.35	121.90
35	YA	2073	C	C6-N1-C2	-5.07	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2467	C	C5-C4-N4	5.07	123.75	120.20
1	XA	1008	C	P-O3'-C3'	5.07	125.78	119.70
35	YA	104	U	N1-C2-O2	5.07	126.35	122.80
36	YB	118	G	C5-C6-O6	5.07	131.64	128.60
1	XA	1007	C	N1-C2-O2	5.07	121.94	118.90
36	YB	22	U	N1-C2-O2	5.07	126.35	122.80
41	YH	3	ARG	CB-CA-C	-5.07	100.27	110.40
1	QA	754	C	C5-C6-N1	5.06	123.53	121.00
35	RA	2726	U	N3-C2-O2	-5.06	118.66	122.20
1	QA	936	C	N1-C2-O2	5.06	121.94	118.90
35	RA	845	G	P-O3'-C3'	5.06	125.77	119.70
35	RA	2723	C	C6-N1-C2	-5.06	118.28	120.30
1	QA	812	C	OP2-P-O3'	5.06	116.33	105.20
1	QA	891	U	N1-C2-O2	5.06	126.34	122.80
1	QA	1395	C	N3-C2-O2	-5.06	118.36	121.90
35	RA	2089	U	C5-C6-N1	5.06	125.23	122.70
46	RQ	84	GLY	C-N-CA	5.06	134.34	121.70
1	XA	431	A	N1-C6-N6	-5.06	115.57	118.60
1	XA	1086	U	C2-N1-C1'	5.06	123.77	117.70
35	YA	343	C	N1-C2-O2	5.06	121.93	118.90
35	YA	2791	C	C6-N1-C1'	5.06	126.87	120.80
1	QA	1325	C	C5-C6-N1	5.05	123.53	121.00
35	YA	104	U	N3-C2-O2	-5.05	118.66	122.20
35	RA	2859	G	P-O3'-C3'	5.05	125.76	119.70
35	RA	286	C	C6-N1-C1'	-5.05	114.74	120.80
35	YA	373	U	N3-C2-O2	-5.05	118.66	122.20
35	YA	2602	A	C4-N9-C1'	5.05	135.39	126.30
35	RA	1024	G	N3-C4-N9	5.05	129.03	126.00
1	XA	1305	G	P-O3'-C3'	5.05	125.76	119.70
35	YA	2689	U	P-O3'-C3'	5.05	125.76	119.70
1	XA	354	G	C4-N9-C1'	5.05	133.06	126.50
35	YA	669	G	N3-C4-N9	5.05	129.03	126.00
36	YB	117	G	N1-C2-N2	-5.05	111.66	116.20
1	QA	1160	G	N3-C4-N9	5.04	129.03	126.00
35	YA	1588	C	C6-N1-C2	-5.04	118.28	120.30
1	QA	690	G	O4'-C1'-N9	5.04	112.23	108.20
22	QV	32	C	C2-N1-C1'	5.04	124.35	118.80
35	RA	1011	G	C8-N9-C1'	5.04	133.55	127.00
35	RA	2210	G	C8-N9-C1'	-5.04	120.45	127.00
35	RA	86	C	C2-N1-C1'	5.04	124.34	118.80
35	RA	544	C	C6-N1-C2	-5.04	118.28	120.30
35	RA	355	G	C6-C5-N7	-5.04	127.38	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	1882	C	N1-C2-O2	5.04	121.92	118.90
35	YA	867	C	N3-C2-O2	-5.04	118.37	121.90
35	YA	971	C	C6-N1-C2	-5.04	118.28	120.30
35	YA	2859	G	P-O3'-C3'	5.04	125.75	119.70
35	RA	2321	G	C4-N9-C1'	5.04	133.05	126.50
1	XA	18	C	C5-C6-N1	5.04	123.52	121.00
1	XA	1024	G	N3-C4-C5	-5.04	126.08	128.60
35	YA	1658	C	C6-N1-C2	-5.04	118.29	120.30
35	RA	2896	C	N3-C2-O2	-5.03	118.38	121.90
1	XA	201	C	P-O3'-C3'	5.03	125.74	119.70
35	YA	2752	C	N3-C2-O2	-5.03	118.38	121.90
35	RA	2730	C	C2-N1-C1'	5.03	124.33	118.80
22	XV	34	C	C2-N1-C1'	5.03	124.33	118.80
35	YA	1385	G	O4'-C1'-N9	5.03	112.22	108.20
36	RB	77	U	C5-C6-N1	5.03	125.21	122.70
35	YA	1433	U	N1-C2-O2	5.03	126.32	122.80
35	YA	154	G	C4-N9-C1'	5.03	133.03	126.50
35	YA	1679	U	N3-C2-O2	-5.03	118.68	122.20
35	YA	2065	C	C5-C6-N1	5.03	123.51	121.00
35	YA	834	C	C6-N1-C2	-5.02	118.29	120.30
35	YA	1406	U	C6-N1-C2	-5.02	117.98	121.00
35	YA	2880	C	C6-N1-C2	-5.02	118.29	120.30
35	YA	817	C	C5-C6-N1	5.02	123.51	121.00
35	YA	527	C	O4'-C1'-N1	5.02	112.21	108.20
35	YA	806	C	C6-N1-C2	-5.01	118.30	120.30
35	RA	837	C	C5-C6-N1	5.01	123.51	121.00
35	RA	1306	C	C6-N1-C2	-5.01	118.30	120.30
1	XA	1065	U	OP2-P-O3'	5.01	116.23	105.20
35	YA	76	C	C6-N1-C2	-5.01	118.30	120.30
1	XA	1024	G	N3-C4-N9	5.01	129.01	126.00
35	RA	758	C	N1-C2-O2	5.01	121.91	118.90
35	RA	1979	C	N1-C2-O2	5.01	121.91	118.90
35	YA	12	U	N1-C2-O2	5.01	126.31	122.80
1	QA	283	C	C2-N3-C4	5.01	122.40	119.90
35	YA	837	C	C6-N1-C2	-5.01	118.30	120.30
35	YA	1640	C	N3-C2-O2	-5.01	118.39	121.90
35	YA	1742	C	C6-N1-C2	-5.01	118.30	120.30
35	RA	279	C	N1-C2-O2	5.00	121.90	118.90
1	XA	1024	G	C4-N9-C1'	5.00	133.01	126.50
35	YA	1993	U	N3-C2-O2	-5.00	118.70	122.20
35	RA	907	U	C2-N1-C1'	5.00	123.70	117.70
35	YA	2177	C	C2-N1-C1'	5.00	124.30	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RA	2889	C	N1-C2-O2	5.00	121.90	118.90
35	YA	363(E)	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Sidechain
10	QJ	79	ARG	Sidechain
24	QZ	50	HIS	Peptide
37	RD	33	LEU	Peptide
37	RD	35	LYS	Peptide
38	RE	79	ARG	Sidechain
40	RG	116	ASP	Peptide
40	RG	83	ARG	Sidechain
41	RH	116	GLU	Sidechain
41	RH	9	ILE	Peptide
42	RI	11	ASN	Peptide
42	RI	142	VAL	Peptide
42	RI	143	SER	Peptide
42	RI	82	ARG	Sidechain
47	RR	3	HIS	Peptide
51	RV	15	GLU	Sidechain
7	XG	111	ARG	Sidechain
8	XH	60	ARG	Sidechain
11	XK	96	ARG	Sidechain
37	YD	88	ARG	Sidechain
40	YG	72	ARG	Sidechain
41	YH	3	ARG	Sidechain
47	YR	57	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	32452	0	16383	236	0
1	XA	32389	0	16350	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	QB	1907	0	1958	31	0
2	XB	1915	0	1969	26	0
3	QC	1605	0	1668	13	0
3	XC	1605	0	1668	16	0
4	QD	1703	0	1767	31	0
4	XD	1703	0	1767	23	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	13	0
6	QF	843	0	857	13	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	7	0
7	XG	1257	0	1296	17	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	13	0
9	QI	1010	0	1037	16	0
9	XI	998	0	1024	18	0
10	QJ	801	0	849	11	0
10	XJ	777	0	816	18	0
11	QK	885	0	904	12	0
11	XK	864	0	881	9	0
12	QL	975	0	1062	11	0
12	XL	956	0	1046	13	0
13	QM	955	0	1021	26	0
13	XM	946	0	1008	15	0
14	QN	492	0	529	5	0
14	XN	492	0	529	11	0
15	QO	734	0	771	4	0
15	XO	729	0	768	3	0
16	QP	705	0	725	12	0
16	XP	705	0	725	6	0
17	QQ	834	0	904	7	0
17	XQ	834	0	904	11	0
18	QR	574	0	644	9	0
18	XR	574	0	644	12	0
19	QS	665	0	686	15	0
19	XS	656	0	666	9	0
20	QT	763	0	861	8	0
20	XT	763	0	861	15	0
21	QU	217	0	234	5	0
21	XU	217	0	234	6	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	QX	394	0	196	2	0
23	XX	394	0	196	4	0
24	QY	723	0	713	10	0
24	QZ	723	0	712	11	0
24	XY	723	0	713	9	0
24	XZ	723	0	713	7	0
25	R0	643	0	667	13	0
25	Y0	648	0	672	15	0
26	R1	737	0	813	6	0
26	Y1	763	0	848	18	0
27	R2	581	0	629	9	0
27	Y2	581	0	629	3	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	5	0
29	R4	565	0	561	24	0
29	Y4	565	0	559	10	0
30	R5	459	0	476	12	0
30	Y5	459	0	480	6	0
31	R6	453	0	474	10	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	3	0
32	Y7	418	0	467	6	0
33	R8	517	0	582	10	0
33	Y8	517	0	582	12	0
34	R9	307	0	337	9	0
34	Y9	307	0	336	4	0
35	RA	62266	0	31392	344	0
35	YA	61981	0	31243	331	0
36	RB	2576	0	1303	27	0
36	YB	2576	0	1305	19	0
37	RD	2115	0	2194	39	0
37	YD	2135	0	2221	20	0
38	RE	1568	0	1634	40	0
38	YE	1559	0	1617	23	0
39	RF	1585	0	1632	14	0
39	YF	1585	0	1632	26	0
40	RG	1474	0	1535	23	0
40	YG	1474	0	1535	20	0
41	RH	1336	0	1418	12	0
41	YH	1330	0	1407	18	0
42	RI	1131	0	1216	16	0
42	YI	1136	0	1223	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	RN	1104	0	1180	16	0
43	YN	1104	0	1180	14	0
44	RO	933	0	996	17	0
44	YO	933	0	996	16	0
45	RP	1145	0	1228	28	0
45	YP	1135	0	1212	16	0
46	RQ	1122	0	1179	26	0
46	YQ	1122	0	1179	20	0
47	RR	960	0	1021	12	0
47	YR	960	0	1021	11	0
48	RS	882	0	943	14	0
48	YS	882	0	943	15	0
49	RT	1141	0	1202	21	0
49	YT	1141	0	1202	13	0
50	RU	964	0	1022	19	0
50	YU	964	0	1022	22	0
51	RV	779	0	852	16	0
51	YV	779	0	852	25	0
52	RW	900	0	964	8	0
52	YW	900	0	964	16	0
53	RX	725	0	778	11	0
53	YX	725	0	778	8	0
54	RY	818	0	913	12	0
54	YY	818	0	913	5	0
55	RZ	1461	0	1493	17	0
55	YZ	1461	0	1493	28	0
56	ZA	74	0	51	2	0
56	ZB	74	0	51	7	0
57	QA	93	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	2	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RQ	4	0	0	0	0
57	RR	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	99	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	335	0	0	0	0
57	YB	3	0	0	0	0
57	YD	4	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	5	0	0	0	0
57	YR	1	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y6	1	0	0	0	0
All	All	295153	0	201053	2175	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 (2175) 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)
51:YV:85:LYS:CG	51:YV:85:LYS:CD	1.86	1.53
51:YV:85:LYS:CG	51:YV:85:LYS:CB	1.82	1.50
1:XA:368:U:C5	1:XA:368:U:C6	2.05	1.45
51:YV:85:LYS:NZ	51:YV:85:LYS:CE	1.87	1.36
51:YV:85:LYS:CD	51:YV:85:LYS:CE	2.10	1.30
1:XA:368:U:C5	1:XA:368:U:C4	2.19	1.29
23:QX:20:A3P:C1'	23:QX:20:A3P:O4'	1.67	1.27
29:R4:39:CYS:C	29:R4:41:PRO:HD3	1.58	1.22
23:XX:20:A3P:C1'	23:XX:20:A3P:O4'	1.66	1.15
1:XA:368:U:C6	1:XA:368:U:N1	2.19	1.10
1:XA:368:U:N1	1:XA:368:U:C2	2.21	1.08
29:R4:39:CYS:O	29:R4:41:PRO:HD3	1.54	1.04
35:RA:1311:G:N2	35:RA:1603:A:H62	1.57	1.03
1:XA:368:U:C2	1:XA:368:U:N3	2.29	1.00
35:RA:1311:G:H21	35:RA:1603:A:N6	1.61	0.98
1:XA:368:U:C4	1:XA:368:U:N3	2.33	0.95
29:R4:18:CYS:HB3	29:R4:39:CYS:SG	2.07	0.94
29:R4:39:CYS:O	29:R4:39:CYS:SG	2.28	0.91
29:R4:39:CYS:O	29:R4:41:PRO:CD	2.18	0.90
35:YA:2141:G:H1	35:YA:2150:U:H3	1.20	0.87
35:RA:1311:G:H21	35:RA:1603:A:H62	0.87	0.84
35:YA:2808:U:H3	35:YA:2892:A:H62	1.22	0.83
6:XF:46:ARG:HH22	18:XR:37:VAL:HG11	1.43	0.83
29:R4:36:CYS:HB3	29:R4:39:CYS:HB3	1.63	0.80
29:R4:18:CYS:CB	29:R4:39:CYS:SG	2.71	0.78
51:RV:16:PRO:HD3	51:RV:99:ILE:HD11	1.64	0.78
35:RA:676:A:H8	35:RA:2069:G:H21	1.31	0.77
29:R4:39:CYS:C	29:R4:41:PRO:CD	2.50	0.76
33:Y8:26:LYS:HG2	33:Y8:48:PHE:HD2	1.52	0.74
51:RV:40:LEU:HB2	51:RV:46:VAL:HG12	1.70	0.73
35:YA:676:A:H8	35:YA:2069:G:H21	1.35	0.73
1:QA:663:A:H61	1:QA:742:G:H1	1.37	0.73
35:RA:2141:G:H1	35:RA:2150:U:H3	1.35	0.73
51:RV:15:GLU:HG3	51:RV:16:PRO:HD2	1.72	0.70
35:RA:2584:U:H5'	56:ZA:3:PPU:H103	1.73	0.70
24:QY:7:GLU:OE1	24:QY:7:GLU:N	2.18	0.70
35:RA:1857:G:H21	35:RA:1885:A:H62	1.39	0.70
13:XM:94:ARG:HH12	35:YA:887:A:H5'	1.57	0.69
42:RI:82:ARG:CZ	42:RI:82:ARG:NH1	2.54	0.69
1:XA:1357:A:H61	1:XA:1365:G:H1	1.38	0.69
56:ZA:3:PPU:H93	56:ZA:3:PPU:N7	2.06	0.69
29:R4:36:CYS:HB3	29:R4:39:CYS:CB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y7:11:LYS:HE2	35:YA:686:G:H5"	1.73	0.69
56:ZB:3:PPU:H93	56:ZB:3:PPU:N7	2.07	0.69
46:RQ:24:GLY:HA2	46:RQ:67:ARG:HH21	1.58	0.69
29:Y4:16:CYS:SG	29:Y4:17:GLY:N	2.66	0.68
46:RQ:75:THR:HA	46:RQ:89:ASN:HA	1.75	0.68
33:R8:25:MET:HG3	45:RP:64:LYS:HB3	1.75	0.68
1:XA:1086:U:H3	1:XA:1099:G:H22	1.39	0.68
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.75	0.68
35:YA:67:U:H3	35:YA:74:A:H2	1.42	0.68
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.74	0.68
36:RB:118:G:HO2'	36:RB:119:A:C4'	2.07	0.68
49:RT:36:GLU:HG3	49:RT:41:ARG:HE	1.58	0.68
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.57	0.67
4:QD:154:ASN:HA	4:QD:159:ARG:HH21	1.59	0.67
1:XA:452:A:H62	1:XA:480:U:H3	1.42	0.67
9:QI:25:LYS:N	9:QI:60:ASP:OD1	2.28	0.67
36:RB:3:C:N4	36:RB:118:G:H1	1.93	0.67
35:YA:1053:C:H42	35:YA:1106:G:H1	1.40	0.67
35:RA:259:G:H21	35:RA:621:A:H8	1.41	0.67
38:RE:11:MET:HG2	38:RE:24:THR:HG22	1.76	0.67
1:XA:677:U:H3	1:XA:713:G:H22	1.42	0.67
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.60	0.67
36:YB:22:U:H3	36:YB:61:G:H1	1.42	0.66
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.61	0.66
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.78	0.66
33:Y8:6:THR:HG22	33:Y8:63:PRO:HD2	1.77	0.66
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.60	0.65
45:YP:126:VAL:HG12	45:YP:146:VAL:HB	1.75	0.65
35:YA:845:G:H21	35:YA:933:A:H61	1.43	0.65
38:YE:9:VAL:HB	38:YE:25:VAL:HG23	1.78	0.65
35:RA:68:G:H21	35:RA:74:A:H5'	1.62	0.65
38:RE:25:VAL:HG12	38:RE:183:LEU:HD22	1.77	0.65
43:RN:22:THR:OG1	43:RN:23:LEU:N	2.30	0.65
35:YA:994:C:O2	51:YV:10:LYS:NZ	2.30	0.65
35:RA:845:G:H21	35:RA:933:A:H61	1.44	0.65
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.79	0.65
2:QB:9:GLU:HA	2:QB:12:GLU:HG2	1.79	0.65
1:XA:1157:A:C2	1:XA:1178:G:N2	2.64	0.65
41:YH:4:ILE:HG22	41:YH:69:ARG:HD2	1.78	0.65
41:YH:54:ARG:HH21	41:YH:57:ASP:HA	1.62	0.64
1:XA:1030:C:N4	1:XA:1032:A:N7	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.45	0.64
14:QN:23:ARG:NH1	14:QN:28:GLY:O	2.30	0.64
34:R9:13:LYS:HE3	34:R9:28:GLU:HG2	1.79	0.64
55:YZ:91:LEU:HD23	55:YZ:130:PRO:HB3	1.78	0.64
24:QY:7:GLU:H	24:QY:7:GLU:CD	2.01	0.64
1:XA:991:U:H3	1:XA:1213:A:H62	1.45	0.64
1:XA:1238:A:H62	1:XA:1301:U:H3	1.46	0.64
45:YP:86:LYS:HB3	45:YP:118:GLY:HA3	1.77	0.64
35:RA:2777:G:H5"	35:RA:2778:A:H5'	1.80	0.64
5:QE:81:GLU:HG3	5:QE:90:VAL:HG12	1.80	0.64
35:YA:1464:C:HO2'	35:YA:1528:A:H8	1.46	0.64
35:YA:1899:G:H21	35:YA:1902:C:H41	1.46	0.64
35:RA:2303:G:N3	40:RG:132:ASN:ND2	2.46	0.64
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.79	0.64
1:QA:782:A:H62	1:QA:800:G:H21	1.46	0.64
38:RE:16:ARG:NH2	38:RE:171:GLU:OE2	2.31	0.64
1:QA:1422:G:H5"	44:RO:48:PRO:HB3	1.80	0.63
36:RB:3:C:C4	36:RB:118:G:N1	2.57	0.63
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	1.80	0.63
38:RE:24:THR:HG23	38:RE:186:GLY:HA2	1.79	0.63
44:YO:104:ARG:NH1	49:YT:36:GLU:OE1	2.32	0.63
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.79	0.63
33:Y8:30:ARG:HH21	45:YP:63:PRO:HB2	1.64	0.63
35:YA:974:G:O2'	35:YA:975:G:N7	2.29	0.63
35:YA:1009:A:OP2	43:YN:37:LYS:NZ	2.30	0.63
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.64	0.63
50:YU:92:ARG:NH1	51:YV:11:GLN:O	2.32	0.63
41:RH:101:ARG:NH2	41:RH:121:ILE:O	2.30	0.63
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.81	0.63
2:XB:87:ARG:HH21	2:XB:219:VAL:HB	1.63	0.62
4:XD:166:LYS:HB2	4:XD:178:VAL:HG11	1.81	0.62
1:QA:4:U:O2	8:QH:105:ARG:NH1	2.31	0.62
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.32	0.62
24:QY:5:TRP:HB2	24:QZ:3:LEU:HB2	1.81	0.62
36:RB:30:C:H1'	36:RB:57:A:H61	1.64	0.62
36:RB:118:G:O2'	36:RB:119:A:O4'	2.18	0.62
46:YQ:136:ALA:HB1	55:YZ:52:SER:HB3	1.80	0.62
1:QA:692:U:OP2	11:QK:26:ASN:ND2	2.33	0.62
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.32	0.62
20:QT:30:LYS:HZ3	20:QT:72:LEU:HD21	1.64	0.62
26:R1:49:VAL:HG11	26:R1:70:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RV:62:LEU:HD11	51:RV:95:LEU:HB2	1.82	0.62
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.65	0.62
35:RA:17:G:H4'	50:RU:25:TRP:HE1	1.65	0.62
29:Y4:1:MET:SD	40:YG:98:ARG:NH1	2.72	0.62
39:RF:153:SER:HB2	39:RF:190:GLU:H	1.65	0.62
49:RT:51:ARG:HG2	49:RT:98:LYS:HD2	1.81	0.62
35:YA:345:A:O2'	35:YA:346:A:N7	2.33	0.62
26:R1:21:ARG:NH2	35:RA:2079:U:OP1	2.33	0.62
55:RZ:52:SER:O	55:RZ:54:HIS:N	2.31	0.62
7:XG:79:ARG:HE	7:XG:84:ASN:HB2	1.64	0.62
35:YA:727:A:OP1	35:YA:1431:U:O2'	2.18	0.62
12:QL:114:LYS:O	12:QL:117:ARG:NH1	2.33	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
42:RI:88:ILE:HG22	42:RI:90:GLY:H	1.64	0.61
1:XA:674:G:H2'	1:XA:675:A:H8	1.65	0.61
35:RA:67:U:H3	35:RA:74:A:H2	1.47	0.61
31:R6:25:LYS:NZ	31:R6:51:GLU:OE2	2.34	0.61
35:RA:956:G:OP2	46:RQ:14:ARG:NH2	2.33	0.61
19:XS:41:VAL:HG12	19:XS:43:GLU:H	1.66	0.61
35:YA:2304:G:H22	35:YA:2312:U:H3	1.47	0.61
2:QB:16:HIS:HE1	2:QB:209:ARG:HG2	1.65	0.61
35:RA:2618:G:H21	38:RE:150:VAL:HG21	1.65	0.61
54:RY:102:CYS:SG	54:RY:103:GLY:N	2.74	0.61
47:YR:38:VAL:HG12	47:YR:112:ALA:HB2	1.83	0.61
25:Y0:55:ARG:NH1	35:YA:2364:C:OP1	2.34	0.61
35:YA:2010:G:H5"	52:YW:42:ARG:HB2	1.83	0.61
38:YE:2:LYS:HB2	38:YE:95:ILE:HD12	1.83	0.61
13:XM:6:GLY:O	40:YG:115:ARG:NH1	2.34	0.61
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.34	0.60
44:RO:104:ARG:HH21	49:RT:34:VAL:HG11	1.66	0.60
50:RU:92:ARG:HD2	51:RV:11:GLN:HB2	1.82	0.60
12:XL:117:ARG:HB2	12:XL:122:THR:HB	1.82	0.60
11:QK:124:LYS:O	11:QK:127:LYS:NZ	2.34	0.60
55:RZ:135:GLU:HG2	55:RZ:136:PHE:HD1	1.66	0.60
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.35	0.60
40:YG:37:VAL:HG22	40:YG:159:VAL:HG12	1.84	0.60
55:YZ:119:GLU:O	55:YZ:122:ARG:NH1	2.34	0.60
18:QR:31:LEU:HD12	18:QR:66:LEU:HB2	1.82	0.60
29:R4:59:PHE:HA	29:R4:62:ARG:HG2	1.82	0.60
35:RA:1451:C:O2'	35:RA:1457:A:N6	2.34	0.60
9:QI:28:VAL:HB	9:QI:63:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:XJ:10:GLY:HA3	10:XJ:16:LEU:HD21	1.84	0.60
1:QA:217:C:O2'	1:QA:466:C:N4	2.34	0.60
35:RA:1139:G:O2'	35:RA:1143:A:N6	2.32	0.60
33:Y8:11:LYS:NZ	33:Y8:65:GLU:OE2	2.33	0.60
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.35	0.60
41:RH:164:TYR:HB2	41:RH:167:GLU:HB2	1.82	0.60
1:QA:1252:A:H61	1:QA:1285:A:H61	1.48	0.60
6:QF:10:LEU:HB2	6:QF:59:TYR:HB3	1.84	0.60
40:RG:29:TRP:O	40:RG:33:ARG:NH1	2.35	0.60
39:YF:120:GLU:OE2	45:YP:1:MET:N	2.34	0.60
35:RA:265:A:N6	35:RA:427:U:O2'	2.34	0.60
35:RA:2393:A:H4'	45:RP:62:LEU:H	1.67	0.60
49:RT:19:LEU:HD22	49:RT:86:ILE:HG22	1.84	0.60
3:XC:84:ILE:HG12	3:XC:88:ARG:HE	1.67	0.60
9:XI:48:GLU:OE1	9:XI:51:ARG:NH2	2.35	0.60
1:QA:674:G:H2'	1:QA:675:A:H8	1.67	0.60
30:R5:19:ARG:NH2	35:RA:1264:G:OP1	2.35	0.60
36:RB:118:G:H2'	36:RB:119:A:O4'	2.02	0.60
35:YA:1482:U:H3	35:YA:1512:G:H1	1.48	0.60
35:YA:2135:A:H62	35:YA:2156:G:H21	1.50	0.60
37:YD:17:THR:HB	37:YD:205:VAL:H	1.66	0.60
35:RA:959:A:N3	35:RA:2457:U:O2'	2.33	0.59
22:XV:76:A:O3'	35:YA:2602:A:N6	2.35	0.59
35:RA:587:C:OP2	45:RP:21:ARG:NH1	2.32	0.59
35:RA:1265:A:H61	35:RA:2013:A:H5"	1.67	0.59
50:RU:95:LEU:HD13	51:RV:4:ILE:HD13	1.82	0.59
24:XY:16:TRP:NE1	24:XY:80:CYS:O	2.34	0.59
35:RA:1900:A:H1'	35:RA:1970:A:H2'	1.83	0.59
12:XL:39:VAL:HB	12:XL:57:LYS:HB3	1.83	0.59
35:YA:2305:A:H5"	40:YG:134:GLY:HA3	1.84	0.59
1:QA:1086:U:H3	1:QA:1099:G:H22	1.51	0.59
3:QC:153:VAL:HG22	3:QC:198:VAL:HG12	1.85	0.59
35:RA:2010:G:H5"	52:RW:42:ARG:HB2	1.84	0.59
37:RD:25:THR:HG21	37:RD:81:ALA:HA	1.84	0.59
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.35	0.59
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.36	0.59
15:XO:16:ALA:HB1	15:XO:21:ASP:HB3	1.83	0.59
48:YS:106:ARG:NH1	48:YS:107:GLU:OE2	2.35	0.59
36:RB:118:G:O2'	36:RB:119:A:C4'	2.51	0.59
1:QA:422:C:O2'	1:QA:423:G:N2	2.35	0.59
1:QA:664:G:H22	1:QA:741:G:H1	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:768:G:O2'	35:RA:1379:A:N6	2.33	0.59
1:XA:452:A:OP1	16:XP:43:LYS:NZ	2.36	0.59
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.85	0.59
35:YA:2789:C:O2'	35:YA:2893:G:N2	2.33	0.59
31:R6:26:ASN:ND2	31:R6:29:ASN:OD1	2.34	0.59
38:RE:14:ILE:HG21	38:RE:173:VAL:HG11	1.84	0.59
46:RQ:75:THR:HG22	46:RQ:89:ASN:HB2	1.83	0.59
43:YN:73:THR:HB	43:YN:82:LEU:HD11	1.84	0.59
50:YU:92:ARG:HD3	50:YU:94:ASN:HB3	1.85	0.59
5:QE:80:ILE:HG22	5:QE:91:LEU:HB2	1.85	0.58
1:XA:413:G:N2	1:XA:429:U:OP2	2.35	0.58
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.84	0.58
26:Y1:73:LEU:HD21	26:Y1:98:LEU:HD23	1.83	0.58
35:YA:495:G:N3	52:YW:61:ASN:ND2	2.51	0.58
51:YV:69:LYS:HE2	51:YV:86:GLY:HA3	1.85	0.58
1:XA:1191:A:OP1	3:XC:4:LYS:NZ	2.37	0.58
1:XA:1540:U:O2'	18:XR:55:ARG:NH2	2.36	0.58
27:Y2:65:ASN:ND2	35:YA:72:U:O4	2.36	0.58
35:YA:1689:A:H62	35:YA:1698:A:H2	1.52	0.58
35:YA:2134:A:N7	35:YA:2157:G:O2'	2.37	0.58
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.86	0.58
35:RA:2032:G:H22	35:RA:2572:A:H5'	1.68	0.58
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.36	0.58
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.76	0.58
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.36	0.58
40:YG:118:ARG:HG3	40:YG:181:ARG:HD3	1.84	0.58
1:QA:1191:A:H5"	3:QC:4:LYS:HE3	1.84	0.58
1:QA:1318:A:H4'	19:QS:11:VAL:HG11	1.85	0.58
25:R0:48:GLY:O	25:R0:80:HIS:ND1	2.37	0.58
43:RN:54:VAL:HB	43:RN:122:VAL:HG12	1.85	0.58
45:RP:19:VAL:HG23	45:RP:27:HIS:HB3	1.86	0.58
35:RA:1812:A:H4'	37:RD:46:GLN:HE22	1.67	0.58
37:RD:43:ARG:HB2	37:RD:54:ARG:HB2	1.85	0.58
25:R0:23:VAL:HG21	35:RA:857:C:H4'	1.85	0.58
2:XB:118:LEU:HB3	2:XB:142:LEU:HD13	1.86	0.58
17:XQ:88:TYR:OH	17:XQ:92:ARG:NH1	2.36	0.58
35:YA:1667:G:O2'	35:YA:1669:A:N6	2.36	0.58
55:YZ:109:ALA:HB3	55:YZ:145:GLU:HG2	1.86	0.58
24:XY:4:ILE:HB	24:XY:76:LEU:HA	1.85	0.58
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.86	0.58
1:QA:958:A:OP1	24:QZ:36:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R4:16:CYS:SG	29:R4:36:CYS:HB2	2.44	0.57
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.84	0.57
31:R6:6:ARG:NH2	35:RA:2285:C:OP2	2.37	0.57
35:RA:586:A:H5'	39:RF:89:VAL:HG11	1.86	0.57
36:YB:30:C:H1'	36:YB:57:A:H61	1.69	0.57
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.57
17:QQ:88:TYR:OH	17:QQ:92:ARG:NH2	2.37	0.57
35:YA:583:G:OP2	50:YU:10:ARG:NH1	2.37	0.57
53:YX:53:LYS:NZ	53:YX:55:ASN:OD1	2.36	0.57
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.86	0.57
29:R4:23:GLU:OE2	40:RG:6:ALA:N	2.32	0.57
49:YT:51:ARG:HG2	49:YT:98:LYS:HD2	1.86	0.57
25:R0:36:ILE:HA	25:R0:60:PHE:HA	1.87	0.57
38:RE:34:VAL:HG12	38:RE:72:VAL:HG21	1.86	0.57
1:XA:4:U:O2	8:XH:105:ARG:NH1	2.37	0.57
36:YB:50:G:OP2	48:YS:62:LYS:NZ	2.37	0.57
42:YI:80:PRO:HB2	42:YI:146:ALA:HB2	1.87	0.57
1:QA:1030:C:N4	35:YA:2167:U:O2'	2.38	0.57
34:R9:6:SER:HB3	35:RA:2466:C:H5"	1.86	0.57
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.57
1:XA:951:G:OP2	13:XM:102:ARG:NH1	2.37	0.57
35:YA:269:U:H3	35:YA:370:G:H1	1.52	0.57
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.87	0.57
22:QV:19:G:O6	40:RG:83:ARG:NH2	2.37	0.57
31:R6:8:LYS:HG3	31:R6:54:ILE:HD13	1.87	0.57
47:RR:75:LEU:HA	47:RR:78:LYS:HB3	1.86	0.57
1:XA:972:C:H1'	10:XJ:55:LYS:HE2	1.87	0.57
13:XM:3:ARG:NH1	13:XM:8:GLU:OE2	2.37	0.57
38:YE:67:PHE:HZ	38:YE:78:LEU:HD11	1.70	0.57
46:YQ:13:GLN:O	46:YQ:72:LYS:NZ	2.37	0.57
1:QA:974:A:OP2	14:QN:41:ARG:NH1	2.38	0.57
35:RA:727:A:OP1	35:RA:1431:U:O2'	2.21	0.57
35:RA:1992:G:N2	35:RA:1996:C:O2'	2.37	0.57
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.86	0.57
35:YA:987:G:O2'	35:YA:1000:A:N3	2.34	0.57
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.37	0.57
44:RO:2:ILE:HB	44:RO:33:ALA:HB3	1.85	0.57
4:XD:57:ARG:NH2	4:XD:205:GLU:OE2	2.38	0.57
1:QA:1304:G:OP1	21:QU:2:GLY:N	2.38	0.57
34:R9:1:MET:HG2	35:RA:2477:C:H2'	1.86	0.57
35:RA:995:C:H5"	50:RU:54:LYS:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2848:G:O2'	35:RA:2867:G:N2	2.34	0.57
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.38	0.57
40:RG:82:LEU:HD12	40:RG:88:ILE:HG21	1.86	0.57
1:QA:672:U:H2'	1:QA:673:G:H8	1.69	0.56
4:QD:60:GLU:HG3	4:QD:202:LEU:HD12	1.87	0.56
45:YP:38:GLN:HB3	45:YP:45:LEU:HB3	1.86	0.56
1:QA:774:G:OP1	37:RD:202:LYS:NZ	2.38	0.56
8:XH:51:VAL:HG11	8:XH:60:ARG:HG3	1.87	0.56
30:Y5:49:CYS:SG	30:Y5:50:GLY:N	2.78	0.56
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.38	0.56
38:YE:8:LYS:NZ	38:YE:192:ASN:OD1	2.38	0.56
35:RA:1102:C:H2'	35:RA:1103:A:H8	1.70	0.56
35:RA:1138:G:O2'	43:RN:102:ALA:O	2.23	0.56
1:XA:664:G:H22	1:XA:741:G:H1	1.51	0.56
35:YA:674:G:H1'	39:YF:74:ARG:HD3	1.88	0.56
49:YT:106:SER:HA	49:YT:110:ILE:HD11	1.87	0.56
55:YZ:126:VAL:HG12	55:YZ:163:LEU:HA	1.86	0.56
47:RR:86:ARG:NH2	47:RR:118:GLU:OXT	2.39	0.56
52:RW:18:ARG:HD2	52:RW:76:VAL:HB	1.87	0.56
4:XD:10:ARG:HG3	4:XD:40:PRO:HG3	1.86	0.56
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.88	0.56
9:XI:10:ARG:NH1	9:XI:75:ASP:OD2	2.38	0.56
35:YA:15:G:H1	35:YA:525:U:H3	1.53	0.56
35:YA:807:U:O2'	35:YA:2060:A:N1	2.38	0.56
50:YU:90:VAL:HG22	51:YV:38:LEU:HB3	1.85	0.56
13:QM:23:TYR:HD2	13:QM:67:GLU:HA	1.71	0.56
35:RA:818:G:HO2'	35:RA:838:C:HO2'	1.53	0.56
35:RA:2148:G:H2'	35:RA:2149:G:H8	1.69	0.56
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.38	0.56
26:Y1:91:LYS:O	26:Y1:95:LEU:HG	2.05	0.56
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.39	0.56
35:YA:1388:G:HO2'	35:YA:1525:G:HO2'	1.54	0.56
51:YV:85:LYS:CG	51:YV:85:LYS:CA	2.79	0.56
55:YZ:102:LEU:HD21	55:YZ:155:LEU:HD11	1.87	0.56
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.39	0.56
25:R0:19:LYS:NZ	35:RA:2261:C:OP1	2.35	0.56
36:RB:9:G:H1	36:RB:111:U:H3	1.52	0.56
38:RE:119:ARG:NH1	38:RE:159:HIS:O	2.39	0.56
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.38	0.56
52:YW:24:ILE:HD13	52:YW:36:LEU:HD11	1.88	0.56
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1247:U:H3	1:XA:1290:G:H1	1.53	0.56
10:XJ:45:ARG:HB3	10:XJ:65:LEU:HB3	1.87	0.56
35:YA:141:A:HO2'	35:YA:1407:C:HO2'	1.52	0.56
48:YS:27:SER:HA	48:YS:88:ASP:HB3	1.87	0.56
49:YT:128:GLU:HG3	49:YT:129:ARG:HG3	1.88	0.56
1:QA:1236:A:H4'	1:QA:1304:G:H4'	1.86	0.56
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.39	0.56
35:RA:1388:G:HO2'	35:RA:1525:G:HO2'	1.54	0.56
35:RA:2445:G:OP1	39:RF:74:ARG:NH1	2.39	0.56
1:XA:405:U:O4	4:XD:2:GLY:N	2.39	0.56
7:XG:78:ARG:NH1	7:XG:154:TYR:O	2.38	0.56
41:YH:9:ILE:HD11	41:YH:69:ARG:HG2	1.88	0.56
24:QZ:57:SER:HB2	24:QZ:67:VAL:HG12	1.88	0.56
35:RA:629:G:N3	35:RA:639:U:O2'	2.39	0.56
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.39	0.56
35:RA:1782:C:H1'	35:RA:2609:U:H5"	1.87	0.56
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.39	0.56
9:XI:26:VAL:HG12	9:XI:61:ALA:HB3	1.87	0.56
35:YA:768:G:O2'	35:YA:1379:A:N6	2.39	0.56
1:QA:811:C:O2'	1:QA:901:A:N1	2.38	0.55
13:QM:58:GLU:O	13:QM:62:ASN:HB2	2.06	0.55
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.87	0.55
9:QI:25:LYS:NZ	9:QI:60:ASP:OD2	2.39	0.55
33:R8:52:LYS:H	33:R8:52:LYS:HD3	1.70	0.55
35:RA:2751:G:OP1	35:RA:2751:G:N2	2.37	0.55
26:Y1:92:LYS:NZ	26:Y1:96:LYS:NZ	2.55	0.55
32:Y7:35:ARG:HG3	32:Y7:42:LEU:HD21	1.88	0.55
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.40	0.55
1:QA:957:U:OP1	19:QS:81:ARG:NH2	2.39	0.55
44:RO:80:ASP:OD2	49:RT:64:ARG:NH2	2.40	0.55
55:YZ:108:PRO:HB3	55:YZ:144:LEU:HB2	1.87	0.55
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.80	0.55
35:RA:987:G:O2'	35:RA:1000:A:N3	2.37	0.55
35:RA:1858:G:O2'	35:RA:1884:A:N6	2.39	0.55
35:RA:2472:G:H5'	35:RA:2473:U:H5"	1.89	0.55
35:YA:1139:G:O2'	35:YA:1143:A:N6	2.40	0.55
35:YA:2495:G:H5"	46:YQ:82:ARG:HG2	1.88	0.55
52:YW:22:ASP:OD1	52:YW:25:ARG:NH1	2.39	0.55
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.39	0.55
42:RI:4:ILE:HG12	42:RI:18:VAL:HG12	1.88	0.55
1:QA:186(B):C:H2'	1:QA:186(C):G:H8	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:521:G:H2'	35:RA:522:G:H8	1.72	0.55
35:RA:1250:G:OP2	45:RP:18:ARG:NH2	2.40	0.55
48:RS:18:ILE:HG13	48:RS:88:ASP:HA	1.88	0.55
26:Y1:93:GLU:O	26:Y1:97:LEU:HD13	2.06	0.55
35:YA:270(E):G:H1	35:YA:270(U):C:H42	1.54	0.55
35:RA:1565:C:OP1	37:RD:4:LYS:NZ	2.37	0.55
35:YA:2749:A:H5"	41:YH:3:ARG:HE	1.72	0.55
53:YX:55:ASN:HB2	53:YX:80:ILE:HG23	1.87	0.55
1:QA:112:G:OP2	16:QP:27:LYS:NZ	2.39	0.55
35:RA:665:C:H2'	35:RA:666:G:H8	1.71	0.55
35:RA:1339:G:H5"	53:RX:16:LYS:HD3	1.88	0.55
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.89	0.55
24:XY:73:ASP:OD1	24:XY:73:ASP:N	2.40	0.55
35:YA:2130:U:H3	35:YA:2158:A:H1'	1.71	0.55
1:QA:547:A:OP1	4:QD:73:ARG:NH2	2.40	0.55
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.71	0.55
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.40	0.55
35:YA:1102:C:H2'	35:YA:1103:A:H8	1.72	0.55
35:YA:2245:U:H5"	35:YA:2246:G:H5'	1.89	0.55
48:YS:56:LEU:HD12	48:YS:69:VAL:HG23	1.88	0.55
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.25	0.55
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.25	0.55
41:RH:56:SER:OG	41:RH:57:ASP:N	2.39	0.55
20:XT:85:MET:HA	20:XT:88:VAL:HG22	1.89	0.55
25:Y0:51:VAL:HG21	25:Y0:79:VAL:HG23	1.89	0.55
1:QA:405:U:O4	4:QD:2:GLY:N	2.40	0.54
20:QT:89:ARG:HD2	20:QT:104:LEU:HD11	1.89	0.54
19:XS:11:VAL:HG12	19:XS:13:ASP:H	1.72	0.54
35:YA:859:G:N2	35:YA:917:A:OP2	2.40	0.54
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.38	0.54
44:RO:25:LEU:HB2	44:RO:38:VAL:HG13	1.88	0.54
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.40	0.54
29:Y4:48:ARG:NH2	29:Y4:51:ASP:OD2	2.37	0.54
47:YR:28:LEU:HD23	47:YR:48:VAL:HG21	1.88	0.54
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.40	0.54
35:RA:392:C:H5"	35:RA:409:C:H5"	1.89	0.54
46:RQ:27:VAL:N	46:RQ:138:ASP:OD2	2.40	0.54
1:XA:1357:A:N6	1:XA:1365:G:H1	2.04	0.54
10:XJ:61:GLU:HB2	14:XN:58:LYS:HE2	1.88	0.54
38:YE:101:ARG:HH21	38:YE:171:GLU:HB2	1.72	0.54
1:QA:552:U:H2'	1:QA:553:A:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:963:G:H21	10:QJ:55:LYS:HG2	1.72	0.54
2:QB:16:HIS:CE1	2:QB:209:ARG:HG2	2.42	0.54
6:QF:3:ARG:NH1	6:QF:66:GLU:OE1	2.39	0.54
13:QM:88:ARG:HG2	13:QM:98:VAL:HB	1.89	0.54
26:R1:18:ILE:HG12	26:R1:37:ILE:HG12	1.89	0.54
1:XA:1304:G:OP1	21:XU:2:GLY:N	2.40	0.54
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.72	0.54
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.41	0.54
35:YA:2303:G:N3	40:YG:132:ASN:ND2	2.55	0.54
1:QA:452:A:H62	1:QA:480:U:H3	1.55	0.54
1:QA:1119:C:OP1	9:QI:83:ARG:NH2	2.40	0.54
29:R4:56:VAL:O	29:R4:60:GLN:NE2	2.40	0.54
37:RD:18:VAL:HA	37:RD:211:ARG:HH22	1.73	0.54
10:XJ:51:ARG:HB2	10:XJ:60:ARG:HA	1.89	0.54
26:Y1:76:ARG:HH22	26:Y1:97:LEU:HB3	1.72	0.54
35:YA:997:G:H5'	50:YU:93:LYS:HD2	1.89	0.54
45:YP:95:VAL:HB	45:YP:125:VAL:HG12	1.89	0.54
1:QA:218:C:H5'	1:QA:466:C:H42	1.73	0.54
1:QA:262:A:H5"	20:QT:76:ALA:HB2	1.88	0.54
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.40	0.54
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.89	0.54
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.37	0.54
35:YA:219:G:N3	35:YA:234:C:O2'	2.40	0.54
1:QA:701:C:O2'	1:QA:703:G:N3	2.41	0.54
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.41	0.54
35:RA:2547:U:O2	44:RO:23:ARG:NH2	2.41	0.54
1:XA:1502:A:H2	1:XA:1505:G:H1	1.54	0.54
2:XB:70:PHE:HD1	2:XB:163:PHE:HB3	1.73	0.54
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.22	0.54
39:YF:135:LYS:HB2	39:YF:138:GLU:HG3	1.90	0.54
41:YH:5:GLY:HA2	41:YH:69:ARG:HG3	1.88	0.54
47:YR:24:GLN:HG3	47:YR:44:LEU:HD13	1.89	0.54
1:QA:380:G:N2	1:QA:383:A:OP2	2.34	0.54
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.41	0.54
46:YQ:116:GLU:OE2	46:YQ:119:ARG:NH1	2.41	0.54
24:QZ:59:ARG:NH2	24:QZ:62:GLU:OE1	2.41	0.54
30:R5:36:CYS:HB3	30:R5:49:CYS:HB3	1.90	0.54
36:RB:8:U:O2'	48:RS:25:ARG:NH2	2.41	0.54
1:XA:1219:U:OP1	14:XN:19:ARG:NH2	2.41	0.54
1:XA:1297:C:O2'	7:XG:114:ARG:NH1	2.41	0.54
37:YD:69:ARG:NH2	37:YD:128:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:YS:28:VAL:HG11	48:YS:98:VAL:HG12	1.89	0.54
1:QA:437:U:O2'	4:QD:123:HIS:ND1	2.39	0.54
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.90	0.54
10:QJ:34:VAL:HG22	10:QJ:74:ILE:HG23	1.90	0.54
40:RG:68:PRO:HB3	40:RG:92:VAL:HB	1.90	0.54
45:RP:101:VAL:HB	45:RP:106:LEU:HB3	1.90	0.54
1:QA:401:C:O2'	1:QA:621:A:N3	2.39	0.53
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.56	0.53
1:QA:992:U:H3	1:QA:1044:A:H62	1.55	0.53
35:RA:974:G:O2'	35:RA:975:G:N7	2.34	0.53
53:RX:72:LYS:NZ	53:RX:75:ASP:OD1	2.38	0.53
2:XB:118:LEU:HD11	2:XB:138:LEU:HD12	1.88	0.53
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.89	0.53
46:YQ:137:TYR:HB3	55:YZ:76:LEU:HD21	1.90	0.53
1:QA:1032:A:N6	35:YA:2167:U:O3'	2.42	0.53
20:QT:41:ILE:HD13	20:QT:87:LYS:HD3	1.90	0.53
35:RA:372:G:N2	35:RA:401:A:OP2	2.37	0.53
35:RA:2701:C:H3'	35:RA:2702:U:H5"	1.91	0.53
46:RQ:58:PHE:HD2	46:RQ:61:GLY:HA3	1.72	0.53
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.89	0.53
35:YA:700:G:O2'	35:YA:1632:A:N3	2.37	0.53
35:YA:1859:A:N6	35:YA:1883:G:O2'	2.41	0.53
15:QO:29:VAL:HG23	15:QO:63:ARG:HG3	1.89	0.53
35:RA:1300:U:H4'	35:RA:1301:A:H5'	1.90	0.53
1:XA:958:A:N3	1:XA:985:C:O2'	2.37	0.53
15:XO:70:LEU:HD11	15:XO:77:ARG:HE	1.73	0.53
35:YA:259:G:H21	35:YA:621:A:H8	1.57	0.53
38:YE:77:ILE:HD13	38:YE:195:LEU:HD13	1.89	0.53
38:YE:101:ARG:NH1	38:YE:169:ASN:O	2.42	0.53
32:R7:37:LYS:NZ	35:RA:468:G:OP2	2.40	0.53
55:RZ:7:ALA:HB3	55:RZ:61:LEU:HB3	1.89	0.53
1:XA:1288:A:O3'	21:XU:10:ARG:NH1	2.39	0.53
35:YA:2748:A:H8	41:YH:63:SER:HB2	1.73	0.53
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.41	0.53
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.41	0.53
46:RQ:138:ASP:OD1	55:RZ:81:ARG:NH2	2.41	0.53
35:YA:2547:U:O2	44:YO:23:ARG:NH2	2.41	0.53
36:YB:47:C:OP1	48:YS:10:ARG:NH2	2.41	0.53
1:QA:973:G:O6	1:QA:974:A:N6	2.42	0.53
25:Y0:2:ALA:N	35:YA:2494:G:OP1	2.41	0.53
35:YA:1433:U:H3	35:YA:1560:G:H1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2451:A:C2	56:ZB:3:PPU:HD2	2.43	0.53
2:QB:7:VAL:HG12	2:QB:12:GLU:OE1	2.09	0.53
9:QI:128:ARG:NH2	22:QV:33:U:OP2	2.38	0.53
33:R8:29:LYS:O	33:R8:31:HIS:N	2.32	0.53
35:RA:631:A:OP1	45:RP:64:LYS:NZ	2.41	0.53
35:RA:996:A:OP2	50:RU:92:ARG:NH2	2.42	0.53
38:RE:24:THR:HG21	38:RE:188:VAL:HG12	1.90	0.53
1:XA:191:G:O2'	20:XT:101:GLY:O	2.26	0.53
1:XA:1210:C:O2'	1:XA:1213:A:O2'	2.26	0.53
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.74	0.53
35:YA:2646:C:OP2	35:YA:2732:G:O2'	2.26	0.53
38:YE:128:SER:OG	38:YE:129:HIS:N	2.40	0.53
43:YN:21:LYS:HB3	43:YN:26:LEU:HB2	1.90	0.53
5:QE:153:LYS:HE2	5:QE:155:GLU:HB3	1.89	0.53
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.24	0.53
53:RX:57:LEU:HG	53:RX:78:LYS:HB2	1.89	0.53
1:XA:673:G:H2'	1:XA:674:G:C8	2.44	0.53
35:YA:114:U:O2'	53:YX:33:LYS:NZ	2.41	0.53
35:YA:116:C:O2'	35:YA:126:A:N3	2.36	0.53
35:YA:181:A:H1'	35:YA:435:C:H5'	1.90	0.53
35:YA:392:C:H5"	35:YA:409:C:H5"	1.91	0.53
35:YA:2287:A:H62	35:YA:2344:U:H3	1.56	0.53
44:YO:47:ILE:O	44:YO:53:LYS:NZ	2.42	0.53
42:RI:40:THR:HG23	42:RI:43:ASN:H	1.73	0.53
42:RI:140:LEU:HD12	42:RI:142:VAL:HG12	1.90	0.53
35:YA:833:U:O2	45:YP:55:ARG:NH2	2.41	0.53
44:YO:43:VAL:HG23	44:YO:54:GLU:HA	1.89	0.53
1:QA:1286:A:H4'	21:QU:26:LYS:HD2	1.91	0.53
40:RG:37:VAL:HB	40:RG:94:LEU:HB2	1.90	0.53
43:RN:15:LEU:HD22	43:RN:134:ARG:HD3	1.90	0.53
48:RS:27:SER:HA	48:RS:88:ASP:HB3	1.90	0.53
49:RT:66:VAL:HA	49:RT:71:GLY:HA2	1.91	0.53
1:XA:1492:A:H2'	35:YA:1913:A:H61	1.73	0.53
38:YE:94:GLU:O	38:YE:97:LYS:NZ	2.42	0.53
4:QD:57:ARG:NH2	4:QD:205:GLU:OE2	2.35	0.52
35:YA:1196:C:HO2'	35:YA:1228:G:HO2'	1.57	0.52
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.43	0.52
5:QE:48:ALA:HB2	5:QE:57:LYS:HE3	1.90	0.52
35:RA:998:C:OP2	50:RU:58:ARG:NH1	2.42	0.52
48:RS:26:LEU:HB3	48:RS:87:PHE:HA	1.90	0.52
52:RW:22:ASP:OD1	52:RW:25:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.41	0.52
35:YA:1543:A:H2'	35:YA:1544:C:H3'	1.92	0.52
35:YA:1728:G:N7	35:YA:1731:G:N2	2.50	0.52
35:YA:2251:G:OP2	46:YQ:82:ARG:NH2	2.41	0.52
1:QA:450:G:OP1	16:QP:43:LYS:NZ	2.35	0.52
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.39	0.52
2:QB:87:ARG:NH1	2:QB:220:ASP:OD1	2.26	0.52
35:RA:270(J):G:N2	35:RA:270(Q):C:O2	2.42	0.52
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.42	0.52
35:YA:1889:A:N3	35:YA:2086:U:O2'	2.43	0.52
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	1.90	0.52
1:QA:1296:C:O3'	13:QM:13:LYS:NZ	2.42	0.52
2:QB:67:THR:HG21	2:QB:155:LEU:HG	1.91	0.52
35:RA:299:A:N1	35:RA:322:A:O2'	2.37	0.52
38:RE:36:ARG:NH2	38:RE:88:GLY:O	2.42	0.52
1:XA:514:C:H2'	1:XA:515:G:H8	1.74	0.52
2:XB:174:VAL:O	2:XB:178:ARG:HB3	2.09	0.52
5:XE:80:ILE:HG22	5:XE:91:LEU:HB2	1.90	0.52
35:YA:1654:A:O2'	38:YE:113:PHE:O	2.24	0.52
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.75	0.52
29:R4:14:ILE:HG13	29:R4:31:ILE:HG13	1.92	0.52
35:RA:26:G:H1'	35:RA:515:A:H61	1.73	0.52
39:RF:116:ASP:OD2	45:RP:1:MET:N	2.36	0.52
6:XF:95:GLU:O	18:XR:32:ARG:NH1	2.42	0.52
35:YA:1827:C:OP2	37:YD:222:ARG:NH1	2.43	0.52
39:YF:160:ASN:HB3	39:YF:163:VAL:HG12	1.91	0.52
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.73	0.52
1:QA:501:C:H1'	1:QA:549:C:H1'	1.91	0.52
25:R0:24:LYS:NZ	35:RA:2355:C:O2'	2.42	0.52
35:RA:442:G:H1'	39:RF:48:THR:HG21	1.90	0.52
35:RA:581:C:H2'	35:RA:582:G:H8	1.74	0.52
35:RA:1864:U:H3	35:RA:1878:G:H1	1.56	0.52
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.24	0.52
35:RA:2725:A:O2'	35:RA:2726:U:O2	2.27	0.52
51:RV:59:ALA:HB1	51:RV:94:LEU:HB3	1.91	0.52
10:XJ:13:HIS:HA	10:XJ:16:LEU:HB2	1.90	0.52
24:XY:67:VAL:HG23	24:XY:78:ALA:HB3	1.92	0.52
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.38	0.52
51:YV:59:ALA:HB2	51:YV:96:ILE:HD13	1.91	0.52
56:ZB:3:PPU:N7	56:ZB:3:PPU:C9	2.73	0.52
1:QA:1128:C:O2	1:QA:1146:A:N6	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1279:A:OP2	10:QJ:9:ARG:NH1	2.42	0.52
3:QC:139:GLN:O	3:QC:143:GLU:HB2	2.10	0.52
35:RA:1952:A:N3	35:RA:2560:C:O2'	2.39	0.52
44:RO:87:ILE:HD12	44:RO:91:LEU:HD13	1.92	0.52
35:YA:2849:U:OP1	49:YT:95:ARG:NH1	2.42	0.52
1:QA:1145:C:H4'	1:QA:1146:A:H8	1.75	0.52
1:QA:1241:G:H1	1:QA:1296:C:H42	1.57	0.52
4:QD:32:ALA:HA	4:QD:35:ARG:HB2	1.92	0.52
35:RA:833:U:O2	45:RP:55:ARG:NH1	2.40	0.52
9:XI:93:ARG:HH21	9:XI:97:LYS:HD2	1.75	0.52
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.43	0.52
35:YA:1798:U:OP2	37:YD:274:ARG:NH2	2.43	0.52
41:YH:54:ARG:HH22	41:YH:62:LYS:HE2	1.74	0.52
1:QA:979:C:OP1	1:QA:1223:C:N4	2.43	0.52
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.74	0.52
35:RA:1689:A:H62	35:RA:1698:A:H2	1.58	0.52
1:XA:406:G:N3	4:XD:119:GLN:NE2	2.54	0.52
33:Y8:29:LYS:O	33:Y8:31:HIS:N	2.32	0.52
35:YA:1011:G:OP2	50:YU:66:ASN:ND2	2.42	0.52
35:YA:1047:G:O2'	35:YA:1110:G:N2	2.43	0.52
38:YE:36:ARG:HG2	38:YE:47:VAL:HG12	1.90	0.52
1:QA:861:G:HO2'	1:QA:874:G:HO2'	1.58	0.52
44:RO:120:GLU:OE1	49:RT:67:SER:OG	2.26	0.52
48:RS:31:SER:OG	48:RS:32:LEU:N	2.42	0.52
49:RT:64:ARG:NH1	49:RT:106:SER:OG	2.41	0.52
1:XA:1350:A:O2'	7:XG:33:ASP:OD1	2.28	0.52
35:YA:13:A:O2'	35:YA:15:G:N7	2.41	0.52
35:YA:1131:G:C2	43:YN:75:TYR:HB2	2.45	0.52
1:QA:427:U:OP1	4:QD:13:ARG:NH2	2.42	0.51
1:QA:855:G:OP2	1:QA:871:U:N3	2.43	0.51
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.83	0.51
35:RA:2638:G:OP1	38:RE:82:ARG:NH2	2.43	0.51
36:RB:48:A:OP2	48:RS:30:ARG:NH2	2.43	0.51
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.91	0.51
45:RP:39:LYS:HE2	45:RP:45:LEU:HD11	1.91	0.51
49:RT:29:ARG:NH1	49:RT:46:GLU:OE1	2.44	0.51
1:XA:714:G:H2'	1:XA:715:A:C8	2.45	0.51
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.73	0.51
35:YA:442:G:H1'	39:YF:48:THR:HG21	1.91	0.51
35:YA:2148:G:H2'	35:YA:2149:G:H8	1.75	0.51
35:YA:2795:G:H21	35:YA:2801:A:H62	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:YO:3:GLN:HG2	44:YO:4:PRO:HD2	1.92	0.51
1:QA:80:G:N2	1:QA:89:U:O2	2.40	0.51
1:QA:925:G:H1	1:QA:1391:U:H3	1.56	0.51
25:R0:74:ARG:NH1	36:RB:12:C:O2	2.42	0.51
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.43	0.51
1:XA:1417:G:O2'	1:XA:1483:A:N6	2.42	0.51
35:YA:309:G:N3	35:YA:329:G:O2'	2.42	0.51
35:YA:2115:G:N2	35:YA:2170:A:N7	2.58	0.51
43:YN:133:GLN:HG2	43:YN:135:PRO:HD3	1.92	0.51
46:YQ:34:LEU:HB2	46:YQ:118:LEU:HD22	1.92	0.51
55:YZ:28:MET:HG3	55:YZ:37:VAL:HG21	1.92	0.51
1:QA:501:C:H2'	1:QA:502:G:H8	1.75	0.51
1:QA:581:G:O3'	15:QO:64:ARG:NH2	2.43	0.51
35:RA:1165:U:H3	35:RA:1184:G:H1	1.58	0.51
35:RA:1550:C:H5'	35:RA:1733:G:H22	1.76	0.51
35:RA:1889:A:N3	35:RA:2086:U:O2'	2.43	0.51
48:RS:10:ARG:NH1	48:RS:91:PRO:O	2.44	0.51
2:XB:127:ILE:O	2:XB:135:GLN:NE2	2.43	0.51
32:Y7:37:LYS:NZ	35:YA:468:G:OP2	2.38	0.51
35:YA:289:A:H3'	35:YA:290:G:H8	1.76	0.51
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.40	0.51
33:R8:52:LYS:HD3	33:R8:52:LYS:N	2.25	0.51
35:RA:1142(A):A:O2'	43:RN:25:ARG:NH2	2.43	0.51
35:RA:1385:G:O2'	35:RA:1396:U:O2	2.27	0.51
1:XA:501:C:H1'	1:XA:549:C:H1'	1.93	0.51
33:Y8:29:LYS:HG3	33:Y8:30:ARG:H	1.75	0.51
36:YB:104:A:OP1	55:YZ:72:ARG:NH1	2.43	0.51
46:YQ:104:PHE:HE2	46:YQ:125:LEU:HD11	1.76	0.51
51:YV:14:VAL:HG11	51:YV:57:VAL:HG11	1.93	0.51
16:QP:5:ARG:NH2	16:QP:27:LYS:O	2.43	0.51
31:R6:6:ARG:HH12	35:RA:2285:C:H5	1.58	0.51
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.43	0.51
40:RG:83:ARG:HH11	40:RG:83:ARG:HG3	1.75	0.51
2:XB:178:ARG:NH2	2:XB:198:ASP:OD1	2.44	0.51
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.92	0.51
24:XZ:67:VAL:HG13	24:XZ:78:ALA:HB3	1.93	0.51
35:YA:2584:U:H5'	56:ZB:3:PPU:H103	1.91	0.51
50:YU:92:ARG:CZ	51:YV:11:GLN:H	2.24	0.51
1:QA:537:G:H5"	12:QL:113:ARG:HH12	1.76	0.51
1:QA:1129:C:N4	1:QA:1142:G:O6	2.44	0.51
27:R2:18:PRO:HA	27:R2:21:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:146:GLU:HB2	37:RD:189:CYS:HB3	1.92	0.51
1:XA:501:C:H2'	1:XA:502:G:H8	1.76	0.51
1:XA:1125:U:O4	10:XJ:5:ARG:NH1	2.43	0.51
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.43	0.51
13:XM:45:VAL:HA	13:XM:48:LEU:HD22	1.92	0.51
35:YA:993:G:OP1	50:YU:50:ARG:NH2	2.44	0.51
35:YA:1681:G:O2'	35:YA:1762:A:O2'	2.28	0.51
36:YB:24:G:H1'	36:YB:27:C:H41	1.74	0.51
1:QA:34:C:H2'	1:QA:35:G:H8	1.76	0.51
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	1.93	0.51
1:XA:448:A:OP2	1:XA:485:G:N2	2.42	0.51
1:XA:618:C:H5'	1:XA:619:U:H5"	1.92	0.51
1:XA:1139:G:N2	1:XA:1143:G:O6	2.44	0.51
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.45	0.51
35:RA:862:G:OP1	46:RQ:18:LYS:NZ	2.38	0.51
41:RH:127:GLU:HG2	41:RH:130:ARG:HE	1.75	0.51
43:RN:14:VAL:HB	43:RN:52:VAL:HG13	1.93	0.51
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.44	0.51
35:YA:532:A:N1	35:YA:2035:G:N2	2.58	0.51
35:YA:2566:A:N1	44:YO:28:SER:OG	2.43	0.51
19:QS:10:PHE:CE1	19:QS:38:SER:HB2	2.46	0.51
42:RI:81:VAL:HG21	42:RI:88:ILE:HD13	1.91	0.51
47:RR:56:LYS:NZ	47:RR:90:ARG:O	2.44	0.51
50:RU:74:LEU:HD11	50:RU:114:LYS:HE3	1.93	0.51
11:XK:45:GLY:HA2	11:XK:48:ILE:HD12	1.93	0.51
24:QZ:12:ASP:OD1	24:QZ:81:ARG:NH1	2.44	0.51
35:RA:307:G:H21	35:RA:330:A:H62	1.58	0.51
35:RA:2468:G:OP1	46:RQ:119:ARG:NH2	2.38	0.51
1:XA:954:G:H21	1:XA:1227:A:H62	1.58	0.51
9:XI:9:ARG:HB3	9:XI:104:ARG:HE	1.74	0.51
33:Y8:63:PRO:HB2	35:YA:593:G:H4'	1.92	0.51
35:YA:642:G:H21	35:YA:646:A:H2	1.59	0.51
35:YA:1799:G:OP2	37:YD:273:ARG:NH2	2.44	0.51
1:QA:782:A:H62	1:QA:800:G:N2	2.09	0.50
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.46	0.50
13:QM:15:VAL:HG23	13:QM:34:LEU:HD21	1.92	0.50
35:RA:116:C:O2'	35:RA:126:A:N3	2.40	0.50
42:RI:133:HIS:HB3	42:RI:134:PRO:HD3	1.93	0.50
4:XD:4:TYR:OH	4:XD:10:ARG:NH2	2.43	0.50
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.44	0.50
35:YA:2099:U:O2	35:YA:2190:G:O6	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:6:ILE:HG22	10:QJ:98:ILE:HG22	1.92	0.50
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.91	0.50
35:RA:1818:U:H2'	37:RD:157:ARG:HG2	1.93	0.50
44:RO:43:VAL:HG13	44:RO:54:GLU:HA	1.92	0.50
1:XA:578:C:O2'	1:XA:728:A:N3	2.40	0.50
1:XA:891:U:H2'	1:XA:892:A:H8	1.75	0.50
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.76	0.50
1:XA:1375:A:H4'	7:XG:29:LYS:HD3	1.92	0.50
35:YA:1434:A:H61	35:YA:1558:A:H62	1.59	0.50
35:YA:2515:C:H2'	35:YA:2516:G:H8	1.75	0.50
42:YI:30:LEU:HB3	42:YI:36:ALA:HB3	1.93	0.50
45:YP:97:PRO:HD3	45:YP:126:VAL:HG23	1.93	0.50
1:QA:945:G:N2	1:QA:1334:G:O2'	2.44	0.50
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.44	0.50
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.94	0.50
35:RA:1681:G:O2'	35:RA:1762:A:O2'	2.29	0.50
37:RD:8:PRO:HB3	37:RD:14:ARG:HB3	1.93	0.50
1:XA:924:C:O2'	1:XA:1502:A:N6	2.41	0.50
26:Y1:92:LYS:NZ	26:Y1:96:LYS:HZ2	2.09	0.50
35:YA:302:C:OP2	54:YY:73:ARG:NH1	2.43	0.50
35:YA:571:A:H5'	35:YA:2030:A:H62	1.76	0.50
35:YA:1188:U:H4'	51:YV:79:VAL:HG22	1.92	0.50
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.28	0.50
35:YA:2618:G:H21	38:YE:150:VAL:HG21	1.76	0.50
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.45	0.50
43:YN:34:LEU:HD11	43:YN:120:LEU:HB2	1.93	0.50
54:RY:99:CYS:SG	54:RY:100:ALA:N	2.84	0.50
1:XA:1454:G:OP1	20:XT:39:LYS:NZ	2.34	0.50
5:XE:11:ILE:HD12	5:XE:105:VAL:HG13	1.94	0.50
5:XE:81:GLU:HG2	5:XE:90:VAL:HG12	1.92	0.50
35:YA:668:G:H2'	35:YA:670:A:H62	1.76	0.50
35:YA:1462:C:H4'	35:YA:2703:C:H5'	1.93	0.50
35:YA:2808:U:O4	35:YA:2892:A:N7	2.45	0.50
1:QA:978:A:OP2	1:QA:1362(A):C:N4	2.45	0.50
22:QV:8:U:H3	22:QV:14:A:H62	1.59	0.50
35:YA:2298:A:H62	35:YA:2318:G:H8	1.59	0.50
1:QA:995:C:H2'	1:QA:996:A:H8	1.77	0.50
1:QA:1202:G:O4'	14:QN:29:ARG:NH1	2.44	0.50
2:QB:163:PHE:HD1	2:QB:185:ILE:HG13	1.77	0.50
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.76	0.50
33:R8:6:THR:HG22	33:R8:63:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:373:U:H2'	35:RA:374:A:H8	1.77	0.50
35:RA:459:U:H2'	35:RA:460:A:H8	1.77	0.50
35:RA:1657:C:H4'	38:RE:133:LYS:HB3	1.93	0.50
35:RA:2646:C:OP2	35:RA:2732:G:O2'	2.23	0.50
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.94	0.50
35:YA:372:G:N2	35:YA:401:A:OP2	2.41	0.50
1:QA:924:C:O2'	1:QA:1502:A:N6	2.44	0.50
35:RA:783:A:H4'	35:RA:2588:G:H4'	1.94	0.50
2:XB:19:HIS:ND1	2:XB:20:GLU:OE2	2.45	0.50
18:XR:38:GLU:OE1	18:XR:41:LYS:NZ	2.44	0.50
20:XT:30:LYS:HG3	20:XT:34:LYS:HE2	1.93	0.50
45:YP:52:GLU:OE1	45:YP:55:ARG:NH1	2.45	0.50
35:RA:1863:G:HO2'	35:RA:2411:A:HO2'	1.55	0.50
35:RA:2328:A:H2'	35:RA:2329:G:C8	2.47	0.50
36:RB:44:G:H1'	36:RB:47:C:H42	1.77	0.50
49:RT:26:ASP:OD1	49:RT:120:ARG:NH2	2.40	0.50
50:YU:105:VAL:HG11	51:YV:39:LEU:HD21	1.94	0.50
2:QB:113:HIS:HB3	2:QB:114:ARG:HH21	1.76	0.50
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.38	0.50
34:R9:30:PRO:HB2	35:RA:2527:C:H4'	1.94	0.50
35:RA:1857:G:N2	35:RA:1885:A:H62	2.07	0.50
37:RD:21:PHE:HB3	37:RD:24:ILE:HG12	1.93	0.50
1:XA:835:U:OP1	18:XR:64:ARG:NH2	2.41	0.50
13:XM:91:ARG:HB2	13:XM:98:VAL:HG12	1.93	0.50
35:YA:581:C:H2'	35:YA:582:G:H8	1.76	0.50
35:YA:764:A:H5'	37:YD:210:GLY:HA2	1.94	0.50
55:YZ:115:GLY:HA2	55:YZ:177:PRO:HD3	1.94	0.50
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.47	0.49
35:RA:1340:U:OP2	53:RX:78:LYS:NZ	2.44	0.49
35:RA:1678:G:N2	35:RA:1989:G:H22	2.10	0.49
55:RZ:23:LYS:HD2	55:RZ:38:TYR:HE2	1.76	0.49
1:XA:643:C:H2'	1:XA:644:G:H8	1.76	0.49
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.45	0.49
5:XE:154:GLY:HA2	8:XH:64:LYS:HD3	1.93	0.49
35:YA:1598:C:O3'	53:YX:35:THR:OG1	2.29	0.49
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.34	0.49
46:YQ:37:LEU:HD11	46:YQ:130:LYS:HB2	1.93	0.49
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.45	0.49
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.45	0.49
35:RA:2343:C:O2'	35:RA:2373:G:O2'	2.27	0.49
54:RY:14:LEU:HB2	54:RY:75:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:34:C:H2'	1:XA:35:G:H8	1.77	0.49
1:XA:715:A:H2'	1:XA:716:A:C8	2.47	0.49
11:XK:18:ARG:HB3	11:XK:33:THR:HG23	1.94	0.49
22:XV:9:G:O2'	22:XV:10:G:N7	2.41	0.49
26:Y1:56:GLN:HG3	26:Y1:87:PRO:HD3	1.95	0.49
31:Y6:23:THR:HG21	35:YA:2286:A:H61	1.76	0.49
35:YA:1022:G:N7	43:YN:66:LYS:NZ	2.60	0.49
1:QA:191:G:O2'	20:QT:101:GLY:O	2.26	0.49
1:QA:516:U:O2'	1:QA:519:C:N3	2.41	0.49
2:QB:8:LYS:O	2:QB:11:LEU:N	2.34	0.49
2:QB:223:ILE:HD12	2:QB:226:ARG:HG2	1.94	0.49
35:RA:527:C:N4	35:RA:2779:U:OP2	2.46	0.49
39:RF:185:ASP:OD1	39:RF:188:ARG:NH2	2.45	0.49
1:XA:412:A:OP2	4:XD:35:ARG:NH2	2.44	0.49
1:XA:530:G:N7	24:XY:59:ARG:NH1	2.59	0.49
1:XA:1249:C:O2'	9:XI:73:GLN:OE1	2.30	0.49
35:YA:1254:A:H5"	35:YA:1255:U:H5'	1.94	0.49
36:YB:13:A:N1	36:YB:69:G:O2'	2.41	0.49
38:YE:11:MET:HG2	38:YE:24:THR:HG22	1.95	0.49
1:QA:677:U:O2	1:QA:777:A:O2'	2.27	0.49
15:QO:53:HIS:NE2	35:RA:715:G:O6	2.42	0.49
21:QU:14:TRP:HZ3	21:QU:15:ARG:HH21	1.61	0.49
35:RA:679:C:H2'	35:RA:680:G:H8	1.76	0.49
35:RA:814:C:O2'	35:RA:1225:C:N3	2.44	0.49
35:RA:2749:A:H5"	41:RH:4:ILE:HD12	1.95	0.49
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.45	0.49
3:XC:14:ILE:HG13	3:XC:15:THR:HG23	1.94	0.49
3:XC:141:VAL:HG11	3:XC:202:ILE:HG12	1.95	0.49
16:XP:33:ILE:HG22	16:XP:34:GLU:HG3	1.94	0.49
34:Y9:9:ARG:HH21	34:Y9:12:ASP:HA	1.78	0.49
35:YA:1228:G:OP2	50:YU:16:LYS:NZ	2.46	0.49
35:YA:2731:G:OP1	38:YE:169:ASN:ND2	2.44	0.49
36:YB:90:C:OP2	46:YQ:16:ARG:NH1	2.45	0.49
40:YG:82:LEU:HD11	40:YG:88:ILE:HD13	1.94	0.49
55:YZ:149:SER:OG	55:YZ:172:ALA:O	2.26	0.49
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.77	0.49
1:QA:1541:U:OP2	18:QR:55:ARG:NH1	2.44	0.49
3:QC:19:GLU:HG2	3:QC:54:ARG:HE	1.77	0.49
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.94	0.49
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.45	0.49
25:R0:7:LEU:HD13	46:RQ:85:LYS:HZ1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.46	0.49
46:RQ:37:LEU:HD11	46:RQ:130:LYS:HB2	1.95	0.49
54:RY:56:PRO:HG2	54:RY:57:GLN:HE22	1.78	0.49
1:XA:824:C:H2'	1:XA:825:G:H8	1.78	0.49
35:YA:629:G:N3	35:YA:639:U:O2'	2.43	0.49
35:YA:659:C:H2'	35:YA:660:G:H8	1.77	0.49
35:YA:1257:C:OP1	39:YF:72:ARG:NH2	2.44	0.49
1:QA:1312:G:OP2	29:R4:62:ARG:NH2	2.45	0.49
2:QB:74:LYS:NZ	2:QB:206:ASP:OD1	2.40	0.49
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.95	0.49
35:RA:1454:U:O2'	35:RA:1455:G:N7	2.43	0.49
35:RA:1678:G:H21	35:RA:1989:G:H22	1.59	0.49
35:RA:2844:G:H3'	35:RA:2845:G:H8	1.77	0.49
10:XJ:25:GLU:O	10:XJ:29:ARG:HB3	2.13	0.49
35:YA:1165:U:H3	35:YA:1184:G:H1	1.61	0.49
49:YT:24:PRO:HG3	49:YT:52:ILE:HG22	1.95	0.49
52:YW:58:ALA:HB1	52:YW:64:MET:HB2	1.95	0.49
1:QA:677:U:H3	1:QA:713:G:H22	1.60	0.49
9:QI:118:LYS:H	9:QI:121:ARG:HB3	1.77	0.49
35:RA:1230:C:H2'	35:RA:1231:G:H8	1.76	0.49
35:RA:2720:U:H3	35:RA:2873:A:H2	1.58	0.49
1:XA:1353:G:OP1	21:XU:10:ARG:NH2	2.43	0.49
2:XB:219:VAL:HA	2:XB:222:ILE:HD12	1.95	0.49
35:YA:2472:G:H5'	35:YA:2473:U:H5"	1.93	0.49
44:YO:25:LEU:HB2	44:YO:38:VAL:HG13	1.94	0.49
45:YP:95:VAL:HA	45:YP:99:LEU:HD23	1.95	0.49
46:YQ:68:ILE:HG22	46:YQ:101:ARG:HE	1.77	0.49
46:YQ:141:GLN:NE2	55:YZ:74:VAL:O	2.45	0.49
51:YV:21:ARG:HA	51:YV:93:GLU:HA	1.95	0.49
1:QA:673:G:H1'	18:QR:75:ILE:HD12	1.95	0.49
35:RA:379:G:H1	35:RA:395:U:H3	1.60	0.49
42:RI:88:ILE:HB	42:RI:121:LYS:HG2	1.93	0.49
46:RQ:115:MET:HG2	46:RQ:131:ILE:HG21	1.95	0.49
46:RQ:134:ARG:HH22	55:RZ:122:ARG:HG3	1.78	0.49
35:YA:2443:C:H2'	35:YA:2444:G:H8	1.77	0.49
41:YH:7:LEU:HD12	41:YH:8:PRO:HD2	1.95	0.49
29:R4:36:CYS:SG	29:R4:37:SER:N	2.84	0.49
32:R7:13:ALA:HB2	32:R7:46:VAL:HG11	1.94	0.49
35:RA:270(N):G:H5"	42:RI:57:ARG:HH12	1.77	0.49
36:RB:39:A:O2'	36:RB:46:A:N1	2.43	0.49
1:XA:583:A:N6	1:XA:758:G:O2'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XF:100:ASN:ND2	18:XR:23:LYS:O	2.45	0.49
12:XL:71:PRO:HG3	12:XL:99:HIS:HD2	1.78	0.49
39:YF:117:ARG:HH21	39:YF:187:VAL:HA	1.77	0.49
1:QA:593:G:H1	1:QA:646:U:H3	1.61	0.49
1:QA:663:A:N6	1:QA:742:G:H1	2.07	0.49
6:QF:61:LEU:HD23	6:QF:63:TYR:HE2	1.77	0.49
8:QH:34:GLU:HB3	8:QH:118:VAL:HG11	1.94	0.49
30:R5:25:LEU:HD11	52:RW:41:LYS:HE2	1.94	0.49
35:RA:698:C:O2'	35:RA:734:A:N6	2.45	0.49
1:XA:1151:A:H5"	10:XJ:42:THR:HG23	1.95	0.49
1:XA:1321:C:H5"	1:XA:1322:C:H2'	1.94	0.49
3:XC:139:GLN:OE1	3:XC:170:GLN:NE2	2.45	0.49
1:QA:429:U:O2'	4:QD:22:LYS:NZ	2.45	0.48
35:RA:2747:G:N2	35:RA:2748:A:N1	2.61	0.48
53:RX:55:ASN:HB2	53:RX:80:ILE:HB	1.94	0.48
1:XA:666:G:H5'	1:XA:726:C:H1'	1.95	0.48
35:YA:321:G:O2'	35:YA:340:A:N3	2.44	0.48
35:YA:380:U:H2'	35:YA:381:G:H8	1.78	0.48
1:QA:673:G:H2'	1:QA:674:G:C8	2.48	0.48
1:QA:971:G:N2	1:QA:1363:A:OP2	2.43	0.48
2:QB:223:ILE:HG12	2:QB:230:VAL:HG22	1.95	0.48
25:R0:7:LEU:HB3	46:RQ:85:LYS:NZ	2.28	0.48
29:R4:39:CYS:O	29:R4:41:PRO:CG	2.60	0.48
1:XA:191(F):U:H2'	1:XA:191:G:H8	1.78	0.48
4:XD:23:GLY:HA3	4:XD:112:VAL:HG22	1.96	0.48
27:Y2:18:PRO:HA	27:Y2:21:LEU:HB2	1.95	0.48
35:YA:117:G:OP2	35:YA:119:A:O2'	2.30	0.48
36:YB:15:A:OP2	36:YB:107:U:O2'	2.31	0.48
50:YU:50:ARG:O	50:YU:54:LYS:NZ	2.46	0.48
1:QA:713:G:H2'	1:QA:714:G:C8	2.48	0.48
34:R9:16:VAL:HG22	34:R9:25:VAL:HG22	1.95	0.48
40:RG:18:GLU:OE2	40:RG:21:ARG:NH2	2.38	0.48
43:RN:128:HIS:CE1	43:RN:134:ARG:HG3	2.48	0.48
50:RU:34:LYS:NZ	50:RU:37:GLU:OE1	2.39	0.48
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.43	0.48
3:XC:131:ARG:NH1	3:XC:167:TRP:O	2.46	0.48
4:XD:57:ARG:HB3	4:XD:206:PHE:HB2	1.95	0.48
12:XL:47:LYS:O	24:XY:44:LYS:NZ	2.37	0.48
35:YA:184:C:O2'	35:YA:217:G:N3	2.38	0.48
35:YA:581:C:H2'	35:YA:582:G:C8	2.48	0.48
45:YP:116:GLY:O	45:YP:137:LYS:NZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	1.96	0.48
35:RA:2470:G:OP1	46:RQ:59:ARG:NH2	2.45	0.48
38:RE:7:VAL:HG13	38:RE:51:PHE:HE2	1.78	0.48
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	1.95	0.48
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.94	0.48
12:XL:75:HIS:HA	12:XL:102:ARG:HH22	1.78	0.48
25:Y0:41:ARG:HA	25:Y0:41:ARG:HE	1.77	0.48
35:YA:270(H):C:H42	35:YA:270(R):G:H1	1.60	0.48
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.26	0.48
37:YD:206:LEU:HA	37:YD:211:ARG:HD2	1.94	0.48
51:YV:61:VAL:HA	51:YV:94:LEU:HD23	1.95	0.48
1:QA:501:C:H2'	1:QA:502:G:C8	2.48	0.48
8:QH:119:LEU:HD22	8:QH:123:GLU:HB3	1.96	0.48
27:R2:66:GLU:OE1	27:R2:69:ARG:NH2	2.47	0.48
35:RA:654(G):C:N3	35:RA:654(N):G:N1	2.61	0.48
35:RA:1824:G:N3	37:RD:254:THR:OG1	2.46	0.48
35:RA:2081:C:H2'	35:RA:2082:A:H8	1.79	0.48
38:RE:1:MET:SD	38:RE:1:MET:N	2.70	0.48
38:RE:35:GLN:HB2	38:RE:66:HIS:HE1	1.78	0.48
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.30	0.48
35:YA:307:G:H21	35:YA:330:A:H62	1.60	0.48
35:YA:851:U:H2'	35:YA:852:G:H8	1.79	0.48
30:R5:3:LYS:HG2	35:RA:2611:U:C4	2.49	0.48
35:RA:24:G:O2'	52:RW:78:GLU:O	2.27	0.48
35:RA:270(G):C:H42	35:RA:270(S):G:H1	1.62	0.48
35:RA:296:C:O3'	54:RY:95:LYS:NZ	2.46	0.48
35:RA:521:G:H2'	35:RA:522:G:C8	2.49	0.48
35:RA:2441:C:OP2	35:RA:2586:C:O2'	2.30	0.48
41:RH:88:LEU:HA	41:RH:130:ARG:HA	1.96	0.48
13:XM:58:GLU:O	13:XM:62:ASN:HB2	2.14	0.48
45:YP:87:ASP:O	45:YP:90:ARG:NH1	2.47	0.48
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.78	0.48
4:QD:18:LYS:HB3	4:QD:18:LYS:HE3	1.66	0.48
35:RA:1067:A:N6	35:RA:1068:G:O6	2.47	0.48
35:RA:1598:C:O3'	53:RX:35:THR:OG1	2.29	0.48
40:RG:113:ARG:HB2	40:RG:140:ILE:HB	1.96	0.48
1:XA:501:C:H2'	1:XA:502:G:C8	2.48	0.48
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.79	0.48
25:Y0:47:PRO:HB2	48:YS:20:ARG:HH12	1.79	0.48
35:YA:28:A:N6	35:YA:512:G:O2'	2.47	0.48
35:YA:1385:G:O2'	35:YA:1396:U:O2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R3:44:ARG:HA	28:R3:47:VAL:HG12	1.96	0.48
38:RE:77:ILE:HG21	38:RE:195:LEU:HD22	1.95	0.48
46:RQ:135:ASP:OD2	55:RZ:81:ARG:NH1	2.43	0.48
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.95	0.48
35:YA:2685:G:H1'	35:YA:2726:U:H5	1.79	0.48
44:YO:112:MET:HA	44:YO:115:VAL:HG22	1.95	0.48
47:YR:3:HIS:O	47:YR:5:LYS:N	2.46	0.48
1:QA:738:C:H5"	6:QF:69:GLU:HB2	1.96	0.48
35:RA:1652:A:OP1	47:RR:8:ARG:NH1	2.41	0.48
36:RB:44:G:O2'	36:RB:47:C:N4	2.47	0.48
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.79	0.48
12:XL:56:ALA:HB2	12:XL:70:ILE:HD11	1.95	0.48
26:Y1:71:TYR:HA	26:Y1:74:VAL:HG12	1.95	0.48
35:YA:918:A:N3	36:YB:80:U:O2'	2.41	0.48
31:R6:6:ARG:HD2	31:R6:24:GLU:HB2	1.96	0.48
35:RA:577:G:O2'	35:RA:1254:A:OP1	2.32	0.48
35:RA:1842:G:O2'	37:RD:253:GLN:NE2	2.45	0.48
35:RA:2405:G:O2'	35:RA:2412:A:N6	2.47	0.48
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.79	0.48
46:RQ:63:LYS:HD2	55:RZ:175:VAL:HG21	1.96	0.48
49:RT:106:SER:HA	49:RT:110:ILE:HD11	1.96	0.48
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.96	0.48
1:XA:1175:G:H2'	1:XA:1176:A:C8	2.49	0.48
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.96	0.48
13:XM:105:THR:HG22	13:XM:106:ASN:H	1.78	0.48
1:QA:28:G:O2'	1:QA:296:U:OP1	2.27	0.47
1:QA:269:C:H2'	1:QA:270:A:C8	2.48	0.47
1:QA:745:C:OP1	1:QA:851:G:O2'	2.31	0.47
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.96	0.47
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.45	0.47
5:QE:50:GLU:HB3	5:QE:53:LEU:HD13	1.94	0.47
10:QJ:34:VAL:HG13	10:QJ:74:ILE:HG12	1.96	0.47
19:QS:27:GLU:HB3	19:QS:29:ARG:HH21	1.79	0.47
35:RA:27:G:N2	35:RA:513:A:OP2	2.45	0.47
35:RA:581:C:H2'	35:RA:582:G:C8	2.49	0.47
35:RA:851:U:H2'	35:RA:852:G:H8	1.78	0.47
1:XA:21:G:H2'	1:XA:22:G:C8	2.49	0.47
1:XA:1047:G:H5"	14:XN:4:LYS:HD2	1.95	0.47
1:XA:1413:A:H2	1:XA:1487:G:H22	1.60	0.47
12:XL:32:PHE:HE1	12:XL:86:ARG:HG3	1.79	0.47
12:XL:70:ILE:HG12	12:XL:77:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:577:G:O2'	35:YA:1254:A:OP1	2.32	0.47
35:YA:2747:G:N2	35:YA:2748:A:N1	2.62	0.47
41:YH:89:ILE:O	41:YH:129:THR:OG1	2.33	0.47
1:QA:21:G:H2'	1:QA:22:G:C8	2.49	0.47
1:QA:624:C:H2'	1:QA:625:G:H8	1.79	0.47
1:QA:1009:G:O6	1:QA:1020:U:O2	2.31	0.47
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.95	0.47
8:QH:91:ARG:NH1	17:QQ:32:TYR:O	2.46	0.47
19:QS:3:ARG:HH12	19:QS:11:VAL:HG12	1.78	0.47
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.43	0.47
35:RA:655:A:H4'	35:RA:656:G:H5'	1.96	0.47
35:RA:1139:G:H21	35:RA:1143:A:H8	1.60	0.47
41:RH:52:VAL:O	41:RH:65:HIS:NE2	2.42	0.47
55:RZ:54:HIS:HB3	55:RZ:101:PRO:HD3	1.96	0.47
1:XA:1355:G:H2'	1:XA:1356:G:H8	1.79	0.47
25:Y0:51:VAL:O	48:YS:20:ARG:NH2	2.48	0.47
37:YD:142:VAL:HG23	37:YD:193:VAL:HA	1.96	0.47
40:YG:67:LYS:HD2	40:YG:68:PRO:HD2	1.96	0.47
50:YU:102:GLU:HG3	51:YV:2:PHE:HE1	1.78	0.47
56:ZB:3:PPU:N	56:ZB:3:PPU:CD1	2.73	0.47
1:QA:545:C:OP1	4:QD:61:LYS:NZ	2.48	0.47
37:RD:153:ALA:O	37:RD:157:ARG:NH1	2.47	0.47
43:RN:103:VAL:HG21	43:RN:120:LEU:HD13	1.96	0.47
35:YA:839:U:H1'	35:YA:1191:G:H1'	1.96	0.47
35:YA:2304:G:N2	40:YG:156:ASP:OD2	2.46	0.47
38:YE:170:LEU:HD23	38:YE:186:GLY:HA3	1.96	0.47
49:YT:26:ASP:HB3	49:YT:92:GLY:H	1.79	0.47
10:QJ:21:GLN:HA	10:QJ:24:VAL:HG22	1.96	0.47
18:XR:51:LEU:HD22	18:XR:55:ARG:HD2	1.95	0.47
41:YH:3:ARG:HH21	41:YH:54:ARG:HH12	1.63	0.47
50:YU:102:GLU:HG3	51:YV:2:PHE:CE1	2.49	0.47
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.30	0.47
1:QA:1323:G:H2'	1:QA:1324:A:C8	2.49	0.47
3:QC:19:GLU:O	3:QC:40:ARG:NH2	2.47	0.47
3:QC:131:ARG:NH1	3:QC:167:TRP:O	2.43	0.47
35:RA:1212:G:O2'	35:RA:1237:A:N6	2.48	0.47
35:RA:1388:G:O2'	35:RA:1525:G:O2'	2.30	0.47
35:RA:2306:C:H5'	35:RA:2307:G:H5"	1.96	0.47
35:RA:2853:C:H2'	35:RA:2854:G:H8	1.79	0.47
47:RR:104:ARG:HG3	47:RR:107:ASP:HB3	1.96	0.47
1:XA:1026:G:H22	1:XA:1035:A:H2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:164:ARG:NH1	3:XC:166:GLU:OE2	2.47	0.47
20:XT:48:LYS:HA	20:XT:48:LYS:HD3	1.56	0.47
29:Y4:31:ILE:HG21	40:YG:142:PRO:HB2	1.97	0.47
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.44	0.47
1:QA:56:U:H2'	1:QA:57:G:H8	1.79	0.47
1:QA:187:C:H2'	1:QA:188:U:H4'	1.96	0.47
1:QA:578:C:O2'	1:QA:728:A:N3	2.39	0.47
1:QA:958:A:C5	19:QS:55:LYS:HG3	2.49	0.47
1:QA:961:U:OP2	1:QA:1222:G:O2'	2.33	0.47
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.79	0.47
30:R5:9:LYS:NZ	35:RA:2019:A:N7	2.55	0.47
33:R8:9:GLY:O	33:R8:13:ARG:NE	2.41	0.47
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.95	0.47
3:XC:88:ARG:NH2	3:XC:101:LEU:O	2.48	0.47
10:XJ:6:ILE:HD12	10:XJ:98:ILE:HG22	1.97	0.47
35:YA:2144:U:H1'	35:YA:2147:G:H22	1.79	0.47
36:YB:5:C:O2'	36:YB:27:C:O2	2.30	0.47
38:YE:47:VAL:HG11	38:YE:86:PRO:HD2	1.96	0.47
40:YG:119:GLY:HA3	40:YG:181:ARG:HG3	1.97	0.47
55:YZ:4:ARG:HG2	55:YZ:58:VAL:HB	1.97	0.47
1:QA:157:G:H1	1:QA:164:U:H3	1.62	0.47
1:QA:714:G:H2'	1:QA:715:A:C8	2.50	0.47
1:QA:826:C:O2	8:QH:15:ASN:ND2	2.48	0.47
1:QA:1286:A:N1	21:QU:18:TYR:OH	2.37	0.47
1:QA:1417:G:O2'	1:QA:1483:A:N6	2.46	0.47
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.79	0.47
24:QY:1:MET:HB2	24:QY:35:ARG:HG3	1.97	0.47
35:RA:837:C:N3	35:RA:941:A:N6	2.62	0.47
35:RA:2822:G:OP1	38:RE:159:HIS:NE2	2.48	0.47
46:RQ:136:ALA:HB1	55:RZ:52:SER:HB2	1.96	0.47
1:XA:909:A:N3	1:XA:1413:A:O2'	2.44	0.47
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.95	0.47
12:XL:113:ARG:NH2	12:XL:116:SER:OG	2.43	0.47
21:XU:6:ARG:HH21	21:XU:15:ARG:HH21	1.61	0.47
28:Y3:39:ASP:OD1	28:Y3:44:ARG:NH2	2.47	0.47
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.48	0.47
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.42	0.47
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.47	0.47
37:YD:70:TRP:NE1	37:YD:146:GLU:OE2	2.39	0.47
41:YH:149:ARG:NH2	41:YH:167:GLU:OE2	2.47	0.47
1:QA:131:C:OP1	1:QA:190:G:N2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.32	0.47
29:R4:40:HIS:N	29:R4:41:PRO:HD3	2.24	0.47
35:RA:839:U:H1'	35:RA:1191:G:H1'	1.97	0.47
35:RA:919:G:N2	35:RA:2269:A:OP2	2.44	0.47
37:RD:142:VAL:HG23	37:RD:193:VAL:HA	1.97	0.47
1:XA:45:U:H2'	1:XA:46:G:C8	2.50	0.47
3:XC:19:GLU:HG2	3:XC:54:ARG:HE	1.80	0.47
30:Y5:16:ARG:NH1	30:Y5:17:ASP:OD1	2.47	0.47
35:YA:2844:G:H3'	35:YA:2845:G:H8	1.80	0.47
1:QA:592:G:H2'	1:QA:593:G:H8	1.80	0.47
1:QA:618:C:H5'	1:QA:619:U:H5"	1.96	0.47
2:QB:171:ALA:HA	2:QB:174:VAL:HG22	1.97	0.47
12:QL:83:VAL:HG12	12:QL:107:ALA:HB2	1.95	0.47
36:RB:118:G:C2'	36:RB:119:A:O4'	2.63	0.47
40:RG:139:LEU:HD21	40:RG:149:VAL:HG21	1.96	0.47
46:RQ:39:PRO:HB3	46:RQ:99:PRO:HD3	1.97	0.47
55:RZ:181:GLU:HB2	55:RZ:183:LEU:HG	1.97	0.47
1:XA:624:C:H2'	1:XA:625:G:H8	1.79	0.47
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.79	0.47
4:XD:25:ARG:NE	4:XD:30:LYS:O	2.42	0.47
35:YA:140:A:H8	35:YA:1408:C:HO2'	1.63	0.47
35:YA:1791:A:H3'	35:YA:1792:G:H8	1.80	0.47
35:YA:2692:C:H2'	35:YA:2693:A:H8	1.80	0.47
38:YE:77:ILE:HD11	38:YE:79:ARG:HH21	1.79	0.47
55:YZ:11:GLU:HA	55:YZ:36:LYS:HE2	1.97	0.47
1:QA:674:G:H2'	1:QA:675:A:C8	2.49	0.47
13:QM:19:LEU:HD11	13:QM:56:LEU:HD21	1.97	0.47
35:RA:2845:G:H2'	35:RA:2846:G:H8	1.80	0.47
37:RD:36:PRO:HG3	37:RD:63:ARG:HG3	1.98	0.47
1:XA:429:U:O2'	4:XD:22:LYS:NZ	2.48	0.47
9:XI:125:TYR:HE1	9:XI:127:LYS:HE3	1.80	0.47
13:XM:47:ASP:OD1	13:XM:47:ASP:N	2.48	0.47
26:Y1:92:LYS:HZ1	26:Y1:96:LYS:NZ	2.13	0.47
35:YA:699:A:N3	35:YA:1633:G:O2'	2.40	0.47
35:YA:1139:G:HO2'	35:YA:1143:A:H62	1.63	0.47
37:YD:69:ARG:HH11	37:YD:105:ILE:HG21	1.79	0.47
56:ZB:3:PPU:CD1	56:ZB:3:PPU:HN2	2.26	0.47
1:QA:150:C:H2'	1:QA:151:A:H8	1.80	0.46
1:QA:186(B):C:H2'	1:QA:186(C):G:C8	2.49	0.46
1:QA:390:C:O3'	16:QP:28:ARG:NH2	2.49	0.46
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:27:LYS:HD2	2:QB:193:ASP:HB2	1.96	0.46
13:QM:11:ARG:NH2	40:RG:146:TYR:OH	2.41	0.46
18:QR:32:ARG:HE	18:QR:65:ILE:HD11	1.79	0.46
35:RA:1049:C:N4	35:RA:2751:G:O6	2.48	0.46
35:RA:1230:C:H2'	35:RA:1231:G:C8	2.50	0.46
37:RD:9:TYR:HD1	37:RD:10:THR:HG23	1.80	0.46
38:RE:57:LYS:HD3	38:RE:57:LYS:HA	1.37	0.46
45:RP:115:LEU:HA	45:RP:134:ALA:HB2	1.97	0.46
55:RZ:110:GLY:O	55:RZ:115:GLY:N	2.48	0.46
1:XA:576:G:N2	1:XA:760:G:OP2	2.48	0.46
1:XA:1512:U:H2'	1:XA:1513:A:C8	2.50	0.46
35:YA:2030:A:H4'	35:YA:2031:A:H8	1.79	0.46
1:QA:779:C:H5"	11:QK:122:LYS:HG2	1.97	0.46
1:QA:923:A:O2'	1:QA:1399:C:OP2	2.27	0.46
2:QB:47:THR:HA	2:QB:202:PRO:HG2	1.97	0.46
27:R2:36:ARG:NH2	53:RX:8:ILE:O	2.48	0.46
35:RA:225:A:N6	35:RA:419:C:O2'	2.47	0.46
35:RA:578:A:OP1	35:RA:1255:U:O2'	2.27	0.46
35:RA:1057:A:N6	35:RA:1088:A:OP2	2.49	0.46
35:RA:1530:G:H1	35:RA:1541:U:H3	1.62	0.46
35:RA:1667:G:O2'	35:RA:1991:U:O4	2.32	0.46
35:RA:1830:C:H2'	35:RA:1831:G:H8	1.80	0.46
37:RD:147:LEU:HD21	37:RD:183:ARG:HH22	1.80	0.46
39:RF:115:ALA:O	39:RF:119:ARG:HB2	2.15	0.46
48:RS:66:ALA:HA	48:RS:69:VAL:HG12	1.98	0.46
49:RT:96:ARG:HD2	49:RT:101:PHE:HE2	1.79	0.46
1:XA:376:G:H1	1:XA:387:U:H3	1.64	0.46
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.51	0.46
31:Y6:11:LEU:HG	31:Y6:49:HIS:HB3	1.96	0.46
35:YA:1243:G:O2'	45:YP:7:ARG:NH2	2.49	0.46
52:YW:33:ARG:NE	52:YW:52:GLU:OE2	2.46	0.46
1:QA:1435:G:H2'	1:QA:1436:U:C6	2.50	0.46
24:QY:12:ASP:O	24:QY:15:TYR:N	2.48	0.46
25:R0:50:ASN:HA	25:R0:62:LEU:HD12	1.97	0.46
30:R5:4:HIS:O	35:RA:2056:G:N2	2.48	0.46
35:RA:1434:A:H61	35:RA:1558:A:N6	2.14	0.46
45:RP:148:LEU:HD23	45:RP:148:LEU:HA	1.74	0.46
7:XG:20:ASP:HB3	7:XG:23:VAL:HG23	1.97	0.46
28:Y3:17:LYS:NZ	35:YA:968:G:OP1	2.47	0.46
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.46
35:YA:907:U:OP1	46:YQ:24:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	1.97	0.46
46:YQ:75:THR:HG21	46:YQ:87:LYS:HG2	1.96	0.46
10:QJ:43:ARG:HH11	10:QJ:43:ARG:HD2	1.47	0.46
35:RA:2849:U:H3	35:RA:2867:G:H1'	1.80	0.46
36:RB:47:C:H5'	48:RS:10:ARG:HH12	1.79	0.46
37:RD:245:PRO:HA	37:RD:246:PRO:HD3	1.85	0.46
41:RH:24:VAL:HB	41:RH:35:VAL:HG13	1.98	0.46
44:RO:98:VAL:HG11	44:RO:114:ILE:HG23	1.98	0.46
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.79	0.46
1:XA:1126:U:N3	1:XA:1281:U:O4'	2.45	0.46
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.80	0.46
35:YA:24:G:O2'	52:YW:78:GLU:O	2.32	0.46
35:YA:247:G:OP2	35:YA:249:C:N4	2.49	0.46
39:YF:60:SER:OG	39:YF:61:GLY:N	2.48	0.46
4:QD:177:ASP:HB3	4:QD:182:LYS:HG2	1.98	0.46
16:QP:49:LEU:HD11	16:QP:73:LEU:HG	1.98	0.46
1:XA:579:G:H5'	1:XA:728:A:H1'	1.98	0.46
1:XA:972:C:OP2	10:XJ:57:LYS:NZ	2.46	0.46
11:XK:106:LYS:O	18:XR:87:ARG:NH1	2.48	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.81	0.46
4:QD:133:VAL:HG12	4:QD:135:LEU:H	1.80	0.46
8:QH:104:ARG:HG3	8:QH:107:LEU:HB2	1.98	0.46
13:QM:24:GLY:O	13:QM:29:ARG:NH1	2.49	0.46
30:R5:16:ARG:NH1	30:R5:17:ASP:OD1	2.48	0.46
35:RA:197:A:H62	35:RA:2430:A:H2'	1.79	0.46
35:RA:668:G:H2'	35:RA:670:A:H62	1.81	0.46
35:RA:2037:G:H2'	35:RA:2038:G:C8	2.51	0.46
37:RD:79:VAL:O	37:RD:114:GLY:N	2.46	0.46
1:XA:376:G:O3'	16:XP:5:ARG:NH1	2.42	0.46
26:Y1:18:ILE:HG12	26:Y1:37:ILE:HG12	1.98	0.46
35:YA:2148:G:H2'	35:YA:2149:G:C8	2.51	0.46
35:YA:2693:A:H2'	35:YA:2694:G:H8	1.80	0.46
30:R5:41:PRO:O	30:R5:44:THR:OG1	2.28	0.46
4:XD:85:LYS:HD2	4:XD:92:VAL:HG11	1.98	0.46
47:YR:33:ARG:HE	47:YR:113:LEU:HD11	1.80	0.46
1:QA:662:G:H2'	1:QA:663:A:C8	2.51	0.46
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.48	0.46
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.37	0.46
35:RA:2089:U:H3	35:RA:2230:G:H1	1.63	0.46
35:RA:2298:A:H62	35:RA:2318:G:H8	1.64	0.46
1:XA:1130:A:H62	1:XA:1144:G:H21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:XY:3:LEU:HB2	24:XY:35:ARG:HH21	1.81	0.46
35:YA:1056:G:H4'	35:YA:1086:A:H1'	1.98	0.46
35:YA:2029:G:N1	35:YA:2033:A:OP1	2.32	0.46
55:YZ:146:ILE:HA	55:YZ:174:VAL:HG23	1.97	0.46
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.48	0.46
16:QP:18:ARG:HA	16:QP:38:TYR:HA	1.98	0.46
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.98	0.46
19:QS:28:LYS:NZ	19:QS:46:GLY:O	2.31	0.46
26:R1:67:ILE:O	26:R1:70:VAL:HG12	2.15	0.46
35:RA:589:C:H2'	35:RA:590:A:C8	2.51	0.46
35:RA:661:C:HO2'	45:RP:14:LYS:H	1.63	0.46
35:RA:2124:G:H22	35:RA:2174:C:H42	1.64	0.46
40:RG:124:SER:O	40:RG:124:SER:OG	2.34	0.46
40:RG:166:ASP:OD1	40:RG:166:ASP:N	2.49	0.46
35:YA:831:G:N2	45:YP:53:GLY:O	2.47	0.46
35:YA:1830:C:H2'	35:YA:1831:G:H8	1.79	0.46
1:QA:948:C:H2'	1:QA:949:A:H8	1.80	0.46
1:QA:1346:A:OP1	9:QI:120:ARG:NH1	2.48	0.46
2:QB:53:ARG:HG2	2:QB:56:ARG:HH21	1.80	0.46
4:QD:4:TYR:OH	4:QD:10:ARG:NH2	2.49	0.46
9:QI:10:ARG:NH1	9:QI:75:ASP:OD2	2.49	0.46
35:RA:29:U:H5"	50:RU:7:GLY:HA2	1.98	0.46
35:RA:138:G:N1	53:RX:44:GLU:OE1	2.38	0.46
35:RA:1598:C:H5'	53:RX:37:THR:HG23	1.98	0.46
35:RA:2130:U:O2	35:RA:2133:G:O2'	2.29	0.46
41:RH:130:ARG:HH11	41:RH:132:ARG:HB2	1.81	0.46
48:RS:28:VAL:HG11	48:RS:98:VAL:HG12	1.98	0.46
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.49	0.46
1:XA:552:U:H2'	1:XA:553:A:H8	1.81	0.46
1:XA:592:G:H2'	1:XA:593:G:H8	1.81	0.46
1:XA:806:C:H2'	1:XA:807:A:H8	1.80	0.46
1:XA:885:G:H2'	1:XA:886:G:H8	1.81	0.46
1:XA:948:C:H2'	1:XA:949:A:H8	1.81	0.46
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.51	0.46
4:XD:100:ARG:NH2	4:XD:136:PRO:O	2.49	0.46
7:XG:16:LEU:HD13	9:XI:42:ARG:HA	1.98	0.46
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.98	0.46
35:YA:600:G:N2	35:YA:605:C:O3'	2.49	0.46
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.40	0.46
44:YO:19:ILE:HG22	44:YO:43:VAL:HG12	1.96	0.46
1:QA:671:G:O2'	6:QF:80:ARG:NH2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1354:C:H2'	1:QA:1355:G:H8	1.79	0.45
24:QY:16:TRP:NE1	24:QY:80:CYS:O	2.48	0.45
35:RA:443:A:OP2	35:RA:615:G:N2	2.35	0.45
35:RA:1249:U:H2'	45:RP:18:ARG:HH22	1.81	0.45
43:RN:35:ARG:HH11	43:RN:108:PRO:HG3	1.81	0.45
43:RN:61:ARG:O	43:RN:61:ARG:HG2	2.14	0.45
45:RP:95:VAL:HB	45:RP:125:VAL:HA	1.97	0.45
1:XA:599:C:O2'	8:XH:129:VAL:O	2.25	0.45
1:XA:1312:G:H5'	19:XS:5:LEU:HD11	1.98	0.45
14:XN:26:ARG:HD3	14:XN:43:CYS:HB3	1.98	0.45
35:YA:1262:A:OP1	52:YW:99:ARG:NH1	2.49	0.45
10:QJ:43:ARG:HH12	10:QJ:45:ARG:HB2	1.82	0.45
19:QS:6:LYS:HB2	19:QS:6:LYS:HE3	1.74	0.45
28:R3:40:THR:HG22	28:R3:42:ALA:H	1.81	0.45
35:RA:918:A:N3	36:RB:80:U:O2'	2.47	0.45
35:RA:1262:A:OP2	52:RW:97:LYS:NZ	2.48	0.45
35:RA:2186:G:H2'	35:RA:2187:G:H8	1.81	0.45
35:RA:2566:A:N1	44:RO:28:SER:OG	2.42	0.45
38:RE:10:GLY:HA3	49:RT:7:ILE:HD11	1.98	0.45
43:RN:23:LEU:HB2	43:RN:62:VAL:HG12	1.98	0.45
1:XA:684:A:O2'	11:XK:39:PRO:O	2.34	0.45
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.81	0.45
32:Y7:28:ARG:NH2	35:YA:1368:G:OP1	2.46	0.45
35:YA:2135:A:N6	35:YA:2156:G:H21	2.14	0.45
35:YA:2784:C:H1'	38:YE:37:ARG:HH12	1.81	0.45
1:QA:553:A:H5"	12:QL:24:VAL:HG21	1.98	0.45
4:QD:109:GLY:HA3	4:QD:165:MET:HG3	1.98	0.45
24:QZ:58:ARG:HG3	24:QZ:68:TYR:HE1	1.81	0.45
29:R4:17:GLY:N	29:R4:33:VAL:O	2.49	0.45
35:RA:704:G:O2'	35:RA:726:G:N2	2.49	0.45
35:RA:1827:C:OP2	37:RD:222:ARG:NH1	2.45	0.45
35:RA:2773:C:OP1	38:RE:166:THR:OG1	2.33	0.45
40:RG:37:VAL:HG22	40:RG:159:VAL:HG12	1.97	0.45
47:RR:2:ARG:HD2	47:RR:2:ARG:HA	1.71	0.45
1:XA:713:G:H2'	1:XA:714:G:C8	2.52	0.45
8:XH:25:ASP:HB3	8:XH:58:TYR:HD2	1.82	0.45
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.98	0.45
35:YA:2392:A:H2	35:YA:2424:C:H42	1.64	0.45
35:YA:2540:C:O2'	35:YA:2740:A:N3	2.41	0.45
36:YB:48:A:OP2	48:YS:30:ARG:NH2	2.49	0.45
1:QA:1177:G:H2'	1:QA:1178:G:C4	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:740:U:H2'	35:RA:741:G:C8	2.51	0.45
35:RA:1341:U:OP2	35:RA:1394:U:O2'	2.28	0.45
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.52	0.45
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.38	0.45
35:RA:2591:C:H2'	35:RA:2592:G:C8	2.51	0.45
35:YA:814:C:O2'	35:YA:1225:C:N3	2.48	0.45
35:YA:1028:A:N3	35:YA:2486:G:O2'	2.44	0.45
42:YI:76:THR:OG1	42:YI:139:GLN:NE2	2.49	0.45
54:YY:11:ASP:OD1	54:YY:11:ASP:N	2.49	0.45
1:QA:985:C:H2'	1:QA:986:A:H8	1.81	0.45
1:QA:1432:G:O2'	1:QA:1468:A:N6	2.49	0.45
20:QT:51:GLU:HA	20:QT:54:LYS:HG2	1.99	0.45
35:RA:1423:G:H2'	35:RA:1424:G:H8	1.81	0.45
35:RA:2801:A:OP1	35:RA:2895:U:O2'	2.35	0.45
40:RG:109:VAL:HG11	40:RG:142:PRO:HB3	1.98	0.45
50:RU:34:LYS:HA	50:RU:34:LYS:HD2	1.71	0.45
1:XA:17:U:H2'	1:XA:18:C:C6	2.52	0.45
1:XA:452:A:O2'	1:XA:453:A:O4'	2.33	0.45
1:XA:890:G:O2'	1:XA:906:G:O6	2.29	0.45
4:XD:81:GLU:OE1	4:XD:139:ARG:NH2	2.49	0.45
35:YA:277:C:H3'	35:YA:278:A:H8	1.81	0.45
35:YA:2701:C:H3'	35:YA:2702:U:H5"	1.97	0.45
43:YN:22:THR:OG1	43:YN:23:LEU:N	2.46	0.45
50:YU:88:ILE:HG23	50:YU:90:VAL:HG23	1.98	0.45
1:QA:377:G:H2'	1:QA:378:G:H8	1.82	0.45
37:RD:79:VAL:HG21	37:RD:111:LEU:HD11	1.98	0.45
38:RE:147:PRO:HB2	38:RE:149:ARG:HG2	1.99	0.45
42:RI:109:ILE:HD11	42:RI:130:TYR:CZ	2.52	0.45
51:RV:3:ALA:HB2	51:RV:40:LEU:HD23	1.99	0.45
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.34	0.45
5:XE:107:ARG:O	5:XE:111:GLU:HB2	2.17	0.45
21:XU:26:LYS:HA	21:XU:26:LYS:HD2	1.78	0.45
35:YA:2246:G:H2'	35:YA:2247:A:H8	1.81	0.45
1:QA:309:G:O2'	1:QA:607:A:N1	2.50	0.45
29:R4:2:LYS:HD3	29:R4:2:LYS:HA	1.60	0.45
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.98	0.45
36:RB:60:C:H2'	36:RB:61:G:H8	1.82	0.45
41:RH:121:ILE:HD11	41:RH:133:VAL:HG22	1.99	0.45
49:RT:77:PRO:HB2	49:RT:80:SER:HB2	1.99	0.45
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	1.97	0.45
35:YA:1500:G:O2'	37:YD:100:GLY:O	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1782:C:H1'	35:YA:2609:U:H5"	1.97	0.45
35:YA:2246:G:H2'	35:YA:2247:A:C8	2.51	0.45
42:YI:78:THR:HG22	42:YI:141:LYS:HB2	1.98	0.45
43:YN:1:MET:HG2	51:YV:12:TYR:HD1	1.81	0.45
1:QA:359:U:H2'	1:QA:360:A:H8	1.82	0.45
1:QA:1327:C:H5"	21:QU:20:LYS:HE2	1.99	0.45
31:R6:34:LEU:HG	31:R6:36:LEU:HD13	1.97	0.45
35:RA:230:U:H2'	35:RA:231:C:H6	1.82	0.45
51:RV:68:LYS:H	51:RV:68:LYS:HD2	1.82	0.45
54:RY:9:LYS:NZ	54:RY:28:LYS:O	2.34	0.45
1:XA:1469:G:H2'	1:XA:1470:G:H8	1.81	0.45
35:YA:582:G:H2'	35:YA:583:G:H8	1.82	0.45
35:YA:1636:C:H2'	35:YA:1637:A:C8	2.52	0.45
52:YW:71:VAL:HA	52:YW:107:LEU:HD23	1.99	0.45
1:QA:666:G:H5'	1:QA:726:C:H1'	1.99	0.45
2:QB:201:ILE:HG21	2:QB:214:ILE:HG21	1.99	0.45
5:QE:154:GLY:HA2	8:QH:64:LYS:HE3	1.99	0.45
8:QH:104:ARG:HB3	8:QH:108:GLY:H	1.82	0.45
24:QZ:24:VAL:HA	24:QZ:27:ILE:HD12	1.99	0.45
34:R9:33:LYS:NZ	35:RA:2743:C:OP1	2.38	0.45
35:RA:1600:C:OP1	53:RX:58:HIS:NE2	2.45	0.45
1:XA:411:A:H62	1:XA:413:G:H21	1.65	0.45
16:XP:18:ARG:HH11	16:XP:35:LYS:HD2	1.82	0.45
26:Y1:40:ARG:NH2	35:YA:2232:U:OP2	2.50	0.45
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.89	0.45
44:YO:120:GLU:OE2	49:YT:65:LYS:NZ	2.49	0.45
50:YU:91:ASP:HA	50:YU:95:LEU:HB2	1.97	0.45
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.99	0.45
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.52	0.45
24:QZ:4:ILE:HB	24:QZ:76:LEU:HA	1.99	0.45
35:RA:2867:G:O2'	35:RA:2868:A:O4'	2.35	0.45
45:RP:121:LYS:HB3	45:RP:123:LEU:HD22	1.98	0.45
45:RP:134:ALA:O	45:RP:138:LEU:HB2	2.17	0.45
51:RV:21:ARG:HG3	51:RV:21:ARG:HH11	1.82	0.45
55:RZ:48:PHE:HE1	55:RZ:71:VAL:HG21	1.82	0.45
2:XB:67:THR:HG21	2:XB:155:LEU:HD11	1.98	0.45
35:YA:78:A:H2'	35:YA:79:G:H8	1.81	0.45
35:YA:521:G:H2'	35:YA:522:G:H8	1.82	0.45
35:YA:848:G:H2'	35:YA:849:A:C8	2.52	0.45
35:YA:919:G:N2	35:YA:2269:A:OP2	2.51	0.45
35:YA:971:C:O2'	35:YA:983:A:N3	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YF:113:ALA:HB2	39:YF:183:VAL:HG23	1.99	0.45
1:QA:112:G:O2'	1:QA:354:G:O2'	2.33	0.44
24:QY:42:LYS:O	24:QY:58:ARG:NH1	2.48	0.44
30:R5:12:SER:OG	35:RA:2021:C:OP1	2.34	0.44
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.97	0.44
1:XA:401:C:O2'	1:XA:621:A:N3	2.47	0.44
1:XA:407:G:H2'	1:XA:408:A:H8	1.82	0.44
26:Y1:76:ARG:NH2	26:Y1:97:LEU:HB3	2.32	0.44
35:YA:539:G:H2'	35:YA:540:G:H8	1.82	0.44
35:YA:589:C:H2'	35:YA:590:A:H8	1.82	0.44
35:YA:2720:U:H3	35:YA:2873:A:H2	1.65	0.44
7:QG:20:ASP:HB3	7:QG:23:VAL:HG12	2.00	0.44
35:RA:1399:C:H2'	35:RA:1400:G:H8	1.81	0.44
1:XA:950:U:H3	1:XA:1231:G:H1	1.66	0.44
1:XA:1128:C:H1'	1:XA:1146:A:H61	1.83	0.44
25:Y0:56:ASP:HA	35:YA:2386:C:H4'	1.98	0.44
38:YE:5:LEU:HD11	38:YE:79:ARG:HB2	1.98	0.44
1:QA:17:U:H2'	1:QA:18:C:C6	2.52	0.44
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.99	0.44
6:QF:6:VAL:HB	6:QF:63:TYR:HB2	1.99	0.44
13:QM:98:VAL:HG23	13:QM:99:ARG:HG3	1.99	0.44
31:R6:9:LEU:HA	31:R6:54:ILE:HB	1.99	0.44
35:RA:1188:U:H4'	51:RV:79:VAL:HG22	1.98	0.44
35:RA:1651:G:H4'	47:RR:39:PRO:HG2	2.00	0.44
3:XC:150:LYS:HE3	3:XC:167:TRP:HE1	1.82	0.44
7:XG:26:PHE:HD1	7:XG:101:LEU:HG	1.82	0.44
9:XI:9:ARG:H	9:XI:79:LEU:HD23	1.82	0.44
25:Y0:48:GLY:O	48:YS:20:ARG:NH1	2.50	0.44
33:Y8:12:LYS:NZ	35:YA:249:C:O2	2.40	0.44
34:Y9:6:SER:HB3	35:YA:2466:C:H5"	2.00	0.44
35:YA:121:G:H4'	35:YA:149:A:H5'	1.99	0.44
43:YN:54:VAL:HB	43:YN:122:VAL:HG12	2.00	0.44
53:YX:29:TRP:HZ3	53:YX:59:VAL:HG11	1.82	0.44
1:QA:993:G:O2'	1:QA:994:A:N7	2.50	0.44
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.83	0.44
1:QA:1404:C:H2'	1:QA:1405:G:C8	2.53	0.44
35:RA:321:G:O2'	35:RA:340:A:N3	2.47	0.44
35:RA:627:A:H4'	35:RA:628:G:H5'	1.99	0.44
35:RA:995:C:H5'	50:RU:53:ARG:HG2	1.99	0.44
35:RA:1568:G:OP1	37:RD:63:ARG:NH1	2.41	0.44
35:RA:1936:A:N6	35:RA:1963:U:O2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2246:G:H2'	35:RA:2247:A:C8	2.53	0.44
47:RR:14:SER:OG	47:RR:15:SER:N	2.50	0.44
55:RZ:70:LEU:HG	55:RZ:91:LEU:HD11	1.98	0.44
4:XD:57:ARG:HE	4:XD:205:GLU:HG3	1.82	0.44
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.97	0.44
35:YA:2451:A:C4	56:ZB:3:PPU:HD2	2.51	0.44
35:YA:2692:C:H2'	35:YA:2693:A:C8	2.52	0.44
41:YH:86:GLU:OE2	41:YH:132:ARG:NH2	2.50	0.44
48:YS:25:ARG:HG2	48:YS:88:ASP:HB2	1.99	0.44
1:QA:6:G:H4'	1:QA:298:A:H4'	1.99	0.44
1:QA:1179:A:H4'	9:QI:103:THR:HA	1.99	0.44
8:QH:86:ILE:HG22	8:QH:93:VAL:HG11	1.98	0.44
13:QM:13:LYS:HD2	13:QM:13:LYS:HA	1.72	0.44
24:QY:5:TRP:CD1	24:QZ:5:TRP:HD1	2.36	0.44
26:R1:10:LYS:NZ	26:R1:65:SER:OG	2.50	0.44
35:RA:700:G:O2'	35:RA:1632:A:N3	2.49	0.44
35:RA:2859:G:H2'	35:RA:2860:A:C8	2.52	0.44
37:RD:145:VAL:O	37:RD:155:LEU:N	2.49	0.44
38:RE:58:ARG:HA	38:RE:58:ARG:HD2	1.50	0.44
40:RG:31:VAL:O	40:RG:33:ARG:NH1	2.48	0.44
45:RP:29:LYS:HE3	45:RP:29:LYS:HB3	1.80	0.44
5:XE:51:VAL:HG23	5:XE:52:PRO:HD3	1.99	0.44
34:Y9:1:MET:HB2	35:YA:2526:G:H1'	1.98	0.44
35:YA:247:G:H4'	35:YA:386:G:C5	2.52	0.44
55:YZ:69:THR:HG22	55:YZ:90:VAL:HG12	1.98	0.44
15:QO:87:ILE:HD12	15:QO:87:ILE:HA	1.92	0.44
27:R2:4:SER:OG	27:R2:5:GLU:N	2.47	0.44
35:RA:539:G:H2'	35:RA:540:G:H8	1.83	0.44
35:RA:675:A:H4'	39:RF:67:GLN:HE22	1.83	0.44
35:RA:1571:A:H2'	35:RA:1572:A:C8	2.53	0.44
37:RD:147:LEU:HD11	37:RD:183:ARG:HH12	1.83	0.44
1:XA:450:G:H4'	16:XP:41:PRO:HB2	1.99	0.44
1:XA:745:C:OP1	1:XA:851:G:O2'	2.35	0.44
8:XH:116:LYS:HG2	8:XH:129:VAL:HG11	1.99	0.44
27:Y2:8:LYS:HA	27:Y2:11:GLU:HG2	1.98	0.44
35:YA:630:G:N2	35:YA:633:A:OP2	2.38	0.44
35:YA:2208:U:O2'	37:YD:150:LYS:O	2.35	0.44
35:YA:2329:G:H2'	35:YA:2330:G:C8	2.53	0.44
55:YZ:76:LEU:HA	55:YZ:83:PRO:HA	2.00	0.44
2:QB:80:ILE:HD13	2:QB:211:ILE:HG22	1.98	0.44
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RI:26:ALA:HA	42:RI:30:LEU:HB2	1.98	0.44
50:RU:88:ILE:HG23	50:RU:90:VAL:HG23	2.00	0.44
51:RV:85:LYS:HE2	51:RV:85:LYS:HB2	1.66	0.44
1:XA:1355:G:H2'	1:XA:1356:G:C8	2.52	0.44
1:XA:1483:A:H1'	35:YA:1948:G:H1'	1.99	0.44
2:XB:19:HIS:ND1	2:XB:205:ASP:OD1	2.50	0.44
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.51	0.44
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.99	0.44
35:YA:959:A:N3	35:YA:2457:U:O2'	2.46	0.44
35:YA:2328:A:H2'	35:YA:2329:G:C8	2.52	0.44
35:YA:2469:A:H2	35:YA:2481:G:H21	1.64	0.44
1:QA:736:C:O2'	6:QF:90:VAL:O	2.31	0.44
1:QA:836:G:H1	1:QA:850:U:H3	1.65	0.44
1:QA:1348:U:H4'	9:QI:120:ARG:HD2	1.99	0.44
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.82	0.44
13:QM:91:ARG:HB2	13:QM:98:VAL:HG12	1.97	0.44
25:R0:35:ASN:ND2	35:RA:2353:G:O2'	2.51	0.44
33:R8:57:ARG:NH1	45:RP:52:GLU:OE2	2.48	0.44
35:RA:144:C:H2'	35:RA:145:G:H8	1.82	0.44
35:RA:247:G:H4'	35:RA:386:G:C5	2.53	0.44
35:RA:1204:A:H1'	35:RA:1206:G:C5	2.52	0.44
35:RA:2074:U:H2'	35:RA:2075:U:C6	2.53	0.44
35:RA:2183:C:H2'	35:RA:2184:G:H8	1.82	0.44
38:RE:154:LYS:HA	38:RE:154:LYS:HD2	1.82	0.44
42:RI:128:LEU:O	42:RI:138:ILE:N	2.51	0.44
44:RO:11:ALA:O	44:RO:99:PHE:N	2.40	0.44
54:RY:13:VAL:HG12	54:RY:74:PRO:HA	2.00	0.44
1:XA:691:G:O6	11:XK:55:LYS:NZ	2.47	0.44
1:XA:1300:G:O2'	1:XA:1303:C:N4	2.51	0.44
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.98	0.44
24:XZ:37:THR:OG1	24:XZ:37:THR:O	2.35	0.44
28:Y3:49:LYS:HE2	35:YA:851:U:H5'	1.98	0.44
35:YA:819:A:OP2	35:YA:1187:G:N2	2.40	0.44
39:YF:110:LEU:HD11	39:YF:181:LEU:HG	1.99	0.44
48:YS:36:TYR:CD1	48:YS:52:SER:HB2	2.53	0.44
1:QA:552:U:H2'	1:QA:553:A:C8	2.52	0.44
1:QA:877:C:H2'	1:QA:878:G:H8	1.83	0.44
1:QA:1001:G:H2'	1:QA:1002:G:C8	2.53	0.44
1:QA:1300:G:O2'	1:QA:1303:C:N4	2.44	0.44
2:QB:59:GLU:HG3	2:QB:221:LEU:HD21	1.99	0.44
16:QP:19:ILE:N	16:QP:37:GLY:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R6:12:GLU:HB3	31:R6:19:ARG:HG3	2.00	0.44
35:RA:654(D):G:H1	35:RA:654(Q):C:H42	1.65	0.44
35:RA:1181:C:H2'	35:RA:1182:A:C8	2.53	0.44
35:RA:1518:C:H2'	35:RA:1519:G:H8	1.83	0.44
1:XA:946:A:H2'	1:XA:947:G:C8	2.52	0.44
1:XA:985:C:H2'	1:XA:986:A:C8	2.53	0.44
30:Y5:25:LEU:HD12	52:YW:19:LEU:HB3	1.98	0.44
35:YA:2135:A:H62	35:YA:2156:G:N2	2.16	0.44
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.39	0.43
1:QA:717:C:O2'	11:QK:116:HIS:O	2.32	0.43
4:QD:103:ASN:O	4:QD:107:ARG:HB2	2.18	0.43
4:QD:127:THR:HA	4:QD:132:ARG:HA	2.00	0.43
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.99	0.43
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.49	0.43
35:RA:1542:G:O6	35:RA:1543:A:N6	2.51	0.43
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.28	0.43
1:XA:476:G:H2'	1:XA:477:G:C8	2.53	0.43
29:Y4:2:LYS:HB3	29:Y4:5:ILE:HG12	2.00	0.43
29:Y4:51:ASP:OD1	29:Y4:51:ASP:N	2.50	0.43
33:Y8:28:GLY:HA3	33:Y8:44:LYS:HD3	2.00	0.43
35:YA:142:G:H2'	35:YA:143:C:C6	2.53	0.43
35:YA:589:C:H2'	35:YA:590:A:C8	2.53	0.43
35:YA:2443:C:H2'	35:YA:2444:G:C8	2.53	0.43
53:YX:12:VAL:HB	53:YX:27:THR:HG23	1.99	0.43
1:QA:603:U:H2'	1:QA:604:G:H8	1.83	0.43
1:QA:736:C:H2'	1:QA:737:A:H8	1.83	0.43
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.53	0.43
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	1.99	0.43
35:RA:774:A:O2'	35:RA:777:A:N3	2.51	0.43
35:RA:1403:C:H5"	35:RA:1471:A:H1'	2.00	0.43
35:RA:2446:G:N2	35:RA:2449:U:O2	2.51	0.43
35:RA:2696:U:H2'	35:RA:2697:G:C8	2.53	0.43
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.47	0.43
1:XA:991:U:O4	1:XA:1213:A:N7	2.51	0.43
19:XS:11:VAL:HG11	19:XS:16:LEU:HB2	2.00	0.43
35:YA:1259:G:H2'	35:YA:1260:G:C8	2.52	0.43
46:YQ:60:ARG:HA	55:YZ:179:ASP:HA	2.00	0.43
46:YQ:77:LYS:NZ	46:YQ:86:GLY:O	2.49	0.43
1:QA:985:C:H2'	1:QA:986:A:C8	2.52	0.43
1:QA:1502:A:H2	1:QA:1505:G:H1	1.65	0.43
24:QY:5:TRP:CD1	24:QZ:5:TRP:CD1	3.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:244:A:H4'	45:RP:74:GLU:HB2	2.00	0.43
35:RA:859:G:O2'	35:RA:916:G:O6	2.35	0.43
35:RA:1995:U:O2	44:RO:3:GLN:NE2	2.51	0.43
35:RA:2723:C:OP2	38:RE:109:LYS:NZ	2.46	0.43
35:RA:2853:C:H2'	35:RA:2854:G:C8	2.53	0.43
38:RE:25:VAL:HG21	49:RT:7:ILE:HG12	2.00	0.43
50:RU:75:ASN:HB2	50:RU:78:THR:HG23	2.01	0.43
55:RZ:10:ARG:NH1	55:RZ:26:GLY:O	2.51	0.43
1:XA:878:G:H5'	8:XH:89:PRO:HG2	2.00	0.43
1:XA:1323:G:H2'	1:XA:1324:A:C8	2.53	0.43
1:XA:1422:G:H5"	44:YO:48:PRO:HB3	1.98	0.43
30:Y5:16:ARG:NH2	35:YA:517:C:OP1	2.41	0.43
33:Y8:5:LYS:HG2	35:YA:242:G:C8	2.52	0.43
35:YA:570:G:H2'	35:YA:2030:A:C5	2.53	0.43
35:YA:861:A:N3	36:YB:79:C:O2'	2.49	0.43
35:YA:1571:A:H2'	35:YA:1572:A:C8	2.53	0.43
36:YB:24:G:O6	36:YB:56:G:O2'	2.37	0.43
39:YF:113:ALA:HB1	39:YF:186:ILE:HG21	1.99	0.43
39:YF:143:ALA:O	39:YF:148:LEU:N	2.51	0.43
42:YI:5:LEU:HD21	42:YI:12:LEU:HB3	2.01	0.43
1:QA:514:C:H2'	1:QA:515:G:H8	1.84	0.43
1:QA:689:C:H3'	1:QA:690:G:H21	1.84	0.43
4:QD:60:GLU:OE2	4:QD:63:LYS:NZ	2.36	0.43
13:QM:12:ASN:HB3	13:QM:46:LYS:HB3	2.00	0.43
35:RA:1073:A:H2'	35:RA:1074:G:H8	1.82	0.43
35:RA:2119:A:N6	35:RA:2170:A:N7	2.66	0.43
35:RA:2438:U:O3'	35:RA:2439:A:H3'	2.18	0.43
35:RA:2873:A:H8	47:RR:6:SER:H	1.64	0.43
37:RD:147:LEU:HD12	37:RD:155:LEU:HD11	1.99	0.43
42:RI:88:ILE:HG13	42:RI:121:LYS:HA	2.00	0.43
1:XA:262:A:H5"	20:XT:76:ALA:HB2	2.00	0.43
42:YI:14:ASP:H	42:YI:17:GLN:HB3	1.84	0.43
44:YO:63:VAL:HB	44:YO:102:VAL:HG12	2.00	0.43
1:QA:390:C:H4'	16:QP:28:ARG:HH21	1.83	0.43
1:QA:452:A:O2'	16:QP:72:ARG:NH1	2.51	0.43
1:QA:1086:U:H2'	1:QA:1087:G:H8	1.84	0.43
1:QA:1309:G:OP1	13:QM:88:ARG:NH2	2.51	0.43
2:QB:102:LEU:HD23	2:QB:182:ILE:HD12	2.01	0.43
2:QB:119:GLU:OE2	2:QB:153:ARG:NH2	2.51	0.43
35:RA:2291:U:H2'	35:RA:2292:C:C6	2.54	0.43
38:RE:52:LEU:HB3	38:RE:54:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RO:7:TYR:HE1	44:RO:44:LYS:HG3	1.83	0.43
54:RY:39:VAL:HG13	54:RY:42:VAL:HB	2.00	0.43
1:XA:1127:G:H2'	1:XA:1128:C:C6	2.53	0.43
2:XB:15:VAL:HG11	2:XB:209:ARG:HB2	2.01	0.43
2:XB:55:PHE:HA	2:XB:58:ILE:HB	2.00	0.43
2:XB:168:THR:HB	2:XB:192:SER:HB2	2.00	0.43
35:YA:303:U:H2'	35:YA:304:G:H8	1.83	0.43
35:YA:414:C:H2'	35:YA:415:A:C8	2.54	0.43
35:YA:2291:U:OP1	35:YA:2380:C:O2'	2.36	0.43
43:YN:116:LEU:HD23	43:YN:116:LEU:HA	1.89	0.43
47:YR:86:ARG:NH2	47:YR:118:GLU:OXT	2.44	0.43
55:YZ:128:VAL:HG22	55:YZ:161:VAL:HA	2.01	0.43
1:QA:324:G:OP1	20:QT:70:SER:OG	2.34	0.43
1:QA:736:C:H2'	1:QA:737:A:C8	2.53	0.43
2:QB:48:MET:HA	2:QB:51:LEU:HD12	2.00	0.43
24:QZ:19:THR:OG1	24:QZ:20:ASP:N	2.51	0.43
35:RA:380:U:H2'	35:RA:381:G:H8	1.83	0.43
35:RA:755:C:H2'	35:RA:756:C:C6	2.53	0.43
35:RA:1070:A:H5'	35:RA:1071:G:H5"	2.00	0.43
35:RA:1332:G:H8	35:RA:1332:G:H2'	1.74	0.43
35:RA:2845:G:H2'	35:RA:2846:G:C8	2.53	0.43
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.54	0.43
4:XD:122:ARG:HD2	4:XD:122:ARG:HA	1.80	0.43
24:XY:5:TRP:HB2	24:XZ:3:LEU:HB2	2.01	0.43
35:YA:221:A:H61	35:YA:265:A:H8	1.65	0.43
35:YA:874:G:H2'	35:YA:875:G:H8	1.84	0.43
35:YA:2657:A:O3'	41:YH:160:LYS:NZ	2.49	0.43
35:YA:2871:C:OP1	47:YR:50:HIS:NE2	2.50	0.43
42:YI:10:GLU:O	42:YI:11:ASN:ND2	2.51	0.43
1:QA:216:G:H2'	1:QA:217:C:C6	2.54	0.43
1:QA:946:A:H2'	1:QA:947:G:C8	2.53	0.43
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.84	0.43
8:QH:23:SER:OG	8:QH:24:THR:N	2.52	0.43
20:QT:71:THR:HG22	20:QT:72:LEU:HG	2.00	0.43
43:RN:15:LEU:HD23	43:RN:136:GLU:HG2	1.99	0.43
45:RP:64:LYS:O	45:RP:66:GLY:N	2.52	0.43
28:Y3:8:LEU:HG	28:Y3:28:LEU:HD13	2.01	0.43
35:YA:221:A:N1	35:YA:265:A:O2'	2.52	0.43
35:YA:1614:A:C6	52:YW:91:GLY:HA2	2.54	0.43
35:YA:2591:C:H2'	35:YA:2592:G:C8	2.54	0.43
1:QA:8:A:N6	4:QD:205:GLU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:413:G:O2'	1:QA:428:G:N2	2.52	0.43
4:QD:108:LEU:HD12	4:QD:174:LEU:HD13	2.00	0.43
11:QK:62:GLN:HG3	11:QK:97:ALA:HB2	2.01	0.43
35:RA:589:C:H2'	35:RA:590:A:H8	1.84	0.43
35:RA:630:G:N2	35:RA:633:A:OP2	2.47	0.43
35:RA:1203:G:O6	35:RA:1204:A:N6	2.52	0.43
35:RA:1380:G:O2'	35:RA:1569:A:N6	2.52	0.43
35:RA:1792:G:H5'	37:RD:205:VAL:HG13	2.00	0.43
35:RA:1800:C:H42	35:RA:1817:G:N2	2.17	0.43
36:RB:24:G:H1'	36:RB:27:C:H41	1.83	0.43
43:RN:23:LEU:HD13	43:RN:60:ILE:HD12	2.01	0.43
51:RV:14:VAL:HB	51:RV:96:ILE:HG12	2.00	0.43
1:XA:56:U:H2'	1:XA:57:G:H8	1.82	0.43
1:XA:677:U:O2	1:XA:777:A:O2'	2.34	0.43
8:XH:26:VAL:O	8:XH:59:LEU:N	2.46	0.43
25:Y0:68:GLU:HG3	25:Y0:80:HIS:HB2	2.01	0.43
29:Y4:14:ILE:HB	29:Y4:22:ILE:HB	1.99	0.43
35:YA:373:U:H2'	35:YA:374:A:H8	1.84	0.43
35:YA:1073:A:H2'	35:YA:1074:G:C8	2.54	0.43
35:YA:1434:A:H61	35:YA:1558:A:N6	2.16	0.43
41:YH:3:ARG:HA	41:YH:3:ARG:HD3	1.46	0.43
50:YU:43:GLY:HA3	51:YV:73:SER:OG	2.18	0.43
1:QA:376:G:H5"	16:QP:5:ARG:HB2	2.01	0.43
1:QA:1065:U:O5'	1:QA:1190:G:N2	2.51	0.43
9:QI:5:TYR:HE1	9:QI:16:ARG:HB2	1.84	0.43
12:QL:59:ARG:HA	12:QL:65:GLU:HA	2.01	0.43
35:RA:1568:G:H5"	37:RD:61:LEU:HD23	2.01	0.43
35:RA:2784:C:O2	38:RE:37:ARG:NH2	2.52	0.43
36:RB:90:C:OP2	46:RQ:16:ARG:NH2	2.34	0.43
41:RH:59:ARG:HA	41:RH:62:LYS:HD2	1.99	0.43
46:RQ:109:VAL:HB	46:RQ:114:ALA:HB2	2.01	0.43
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.28	0.43
1:XA:368:U:C2	1:XA:368:U:C1'	3.02	0.43
1:XA:1202:G:O4'	14:XN:29:ARG:NH1	2.52	0.43
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.54	0.43
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	2.00	0.43
15:XO:88:ARG:NH2	35:YA:714:U:OP2	2.49	0.43
26:Y1:8:SER:HB3	26:Y1:66:HIS:CD2	2.53	0.43
35:YA:244:A:H4'	45:YP:74:GLU:HB2	2.01	0.43
35:YA:822:U:H2'	35:YA:823:G:H8	1.83	0.43
35:YA:1899:G:H21	35:YA:1902:C:N4	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YG:41:GLN:HG2	40:YG:43:LEU:HD21	1.99	0.43
8:QH:109:ILE:HG22	8:QH:137:VAL:HB	2.01	0.43
12:QL:32:PHE:HE1	12:QL:86:ARG:HG3	1.84	0.43
30:R5:7:PRO:O	35:RA:2016:U:O2'	2.32	0.43
33:R8:29:LYS:HG3	33:R8:30:ARG:H	1.83	0.43
35:RA:443:A:C8	39:RF:45:ARG:HG3	2.54	0.43
35:RA:2543:G:H2'	35:RA:2544:G:C8	2.54	0.43
36:RB:113:C:H4'	48:RS:46:VAL:HG22	2.01	0.43
45:RP:97:PRO:O	45:RP:98:GLU:HG3	2.18	0.43
50:RU:92:ARG:NH1	51:RV:11:GLN:O	2.52	0.43
1:XA:974:A:OP2	14:XN:41:ARG:NH1	2.45	0.43
1:XA:1308:U:H2'	1:XA:1309:G:C8	2.54	0.43
5:XE:5:ASP:N	5:XE:5:ASP:OD1	2.52	0.43
35:YA:230:U:H2'	35:YA:231:C:H6	1.84	0.43
35:YA:642:G:N2	35:YA:645:C:OP2	2.51	0.43
35:YA:1278:A:H2'	35:YA:1279:G:C8	2.53	0.43
36:YB:14:U:O2'	36:YB:107:U:O2'	2.35	0.43
1:QA:45:U:H2'	1:QA:46:G:C8	2.54	0.42
1:QA:636:U:H5'	17:QQ:2:PRO:HG3	2.00	0.42
7:QG:62:PHE:HD1	7:QG:124:LEU:HD21	1.84	0.42
19:QS:19:VAL:HA	19:QS:22:LEU:HB2	2.00	0.42
35:RA:1316:U:H2'	35:RA:1317:A:C8	2.54	0.42
37:RD:60:ARG:NH1	37:RD:86:PRO:O	2.52	0.42
38:RE:111:ARG:HA	47:RR:2:ARG:HH12	1.83	0.42
1:XA:1326:C:OP2	21:XU:6:ARG:NH1	2.51	0.42
10:XJ:24:VAL:HG13	10:XJ:34:VAL:HG21	2.01	0.42
35:YA:223:A:O2'	35:YA:420:C:O2	2.32	0.42
35:YA:1113:U:H2'	35:YA:1114:G:C8	2.54	0.42
35:YA:1316:U:H2'	35:YA:1317:A:H8	1.82	0.42
36:YB:80:U:H2'	36:YB:81:G:H21	1.82	0.42
1:QA:448:A:OP2	1:QA:485:G:N2	2.39	0.42
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.54	0.42
6:QF:79:LEU:HB3	6:QF:88:VAL:HG21	2.00	0.42
35:RA:873:G:O3'	46:RQ:63:LYS:NZ	2.50	0.42
35:RA:2314:C:H2'	35:RA:2315:G:H8	1.84	0.42
35:RA:2779:U:H6	35:RA:2779:U:H2'	1.73	0.42
36:RB:49:C:OP2	48:RS:30:ARG:NH1	2.52	0.42
37:RD:264:LYS:HD3	37:RD:266:SER:HB3	2.00	0.42
1:XA:516:U:O2'	1:XA:519:C:N3	2.43	0.42
1:XA:1030:C:H42	1:XA:1032:A:H62	1.67	0.42
1:XA:1244:C:H2'	1:XA:1245:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1392:G:N2	1:XA:1502:A:H8	2.17	0.42
9:XI:95:LYS:HE2	9:XI:95:LYS:HB2	1.88	0.42
13:XM:25:ILE:HD11	13:XM:64:TRP:HE1	1.84	0.42
24:XZ:33:ASP:OD1	24:XZ:37:THR:OG1	2.28	0.42
25:Y0:36:ILE:HD13	25:Y0:60:PHE:HB3	2.02	0.42
35:YA:859:G:O2'	35:YA:916:G:O6	2.34	0.42
35:YA:964:C:O2'	35:YA:2273:A:N3	2.38	0.42
35:YA:1278:A:H2'	35:YA:1279:G:H8	1.84	0.42
35:YA:1342:A:H2	35:YA:1602:U:H3	1.66	0.42
35:YA:2074:U:H2'	35:YA:2075:U:C6	2.54	0.42
40:YG:32:PRO:HB2	40:YG:172:LEU:HD22	2.01	0.42
1:QA:1342:C:H2'	1:QA:1343:G:H8	1.85	0.42
3:QC:180:ALA:HB1	3:QC:182:ILE:HG23	2.01	0.42
8:QH:21:LYS:O	8:QH:65:TYR:OH	2.30	0.42
12:QL:60:LEU:HD22	12:QL:85:ILE:HG21	2.01	0.42
13:QM:49:THR:HB	13:QM:52:GLU:HG3	2.02	0.42
24:QY:44:LYS:CE	24:QY:59:ARG:HE	2.32	0.42
37:RD:108:PRO:HB3	37:RD:143:HIS:CE1	2.53	0.42
37:RD:108:PRO:HD2	37:RD:111:LEU:HD22	2.02	0.42
1:XA:407:G:H2'	1:XA:408:A:C8	2.54	0.42
1:XA:922:G:OP1	5:XE:20:GLN:NE2	2.48	0.42
12:XL:104:VAL:HG12	12:XL:105:TYR:H	1.84	0.42
17:XQ:44:ALA:HB1	17:XQ:73:VAL:HG22	2.01	0.42
24:XY:34:THR:OG1	24:XY:58:ARG:NH1	2.51	0.42
24:XZ:19:THR:OG1	24:XZ:20:ASP:N	2.52	0.42
28:Y3:15:TYR:HA	28:Y3:16:PRO:HD3	1.92	0.42
35:YA:1020:A:N1	35:YA:1141:U:H2'	2.34	0.42
35:YA:1353:A:H2'	35:YA:1354:A:C8	2.53	0.42
35:YA:1568:G:H4'	37:YD:59:LYS:HB3	2.01	0.42
35:YA:2438:U:O3'	35:YA:2439:A:H3'	2.19	0.42
35:YA:2693:A:H2'	35:YA:2694:G:C8	2.54	0.42
35:YA:2853:C:H2'	35:YA:2854:G:H8	1.85	0.42
1:QA:508:C:O2	1:QA:510:A:N6	2.52	0.42
1:QA:938:A:N3	1:QA:1376:U:O2'	2.44	0.42
1:QA:1218:C:H2'	1:QA:1219:U:C6	2.54	0.42
6:QF:76:ALA:O	6:QF:80:ARG:NE	2.50	0.42
35:RA:1353:A:H2'	35:RA:1354:A:C8	2.55	0.42
1:XA:41:G:H2'	1:XA:42:G:H8	1.84	0.42
1:XA:1129:C:H4'	1:XA:1130:A:H5'	2.01	0.42
1:XA:1539:C:H42	23:XX:7:G:H1	1.65	0.42
2:XB:70:PHE:CD1	2:XB:163:PHE:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y0:48:GLY:HA3	25:Y0:80:HIS:CE1	2.54	0.42
26:Y1:21:ARG:HD3	26:Y1:35:THR:HG21	2.01	0.42
35:YA:439:G:H2'	35:YA:440:G:C8	2.55	0.42
43:YN:40:PRO:HB3	50:YU:68:ALA:HB2	2.00	0.42
3:QC:65:ALA:HA	3:QC:100:ALA:HB3	2.01	0.42
18:QR:44:LEU:HD21	18:QR:74:ARG:HH21	1.85	0.42
27:R2:41:ILE:HG21	27:R2:44:LEU:HD22	2.02	0.42
35:RA:23:G:OP1	35:RA:504:U:N3	2.43	0.42
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.34	0.42
35:RA:2416:C:H5"	45:RP:64:LYS:HE2	2.00	0.42
42:RI:114:LEU:HD12	42:RI:130:TYR:HB2	2.01	0.42
43:RN:85:ILE:HD11	43:RN:89:LYS:HG2	2.01	0.42
1:XA:1432:G:OP1	49:YT:108:ARG:N	2.53	0.42
2:XB:208:ILE:HA	2:XB:211:ILE:HD12	2.00	0.42
6:XF:22:GLU:OE2	6:XF:82:ARG:NH2	2.45	0.42
11:XK:38:ASN:HA	11:XK:39:PRO:HD3	1.88	0.42
14:XN:12:ARG:HH21	14:XN:14:PRO:HD3	1.85	0.42
26:Y1:73:LEU:HD12	26:Y1:97:LEU:HB2	2.01	0.42
35:YA:2469:A:N6	35:YA:2481:G:O2'	2.53	0.42
35:YA:2683:C:O2	44:YO:70:LYS:NZ	2.43	0.42
35:YA:2791:C:O2	35:YA:2805:G:N2	2.51	0.42
44:YO:68:GLU:HG3	44:YO:78:ARG:HD3	2.01	0.42
48:YS:66:ALA:HA	48:YS:69:VAL:HG12	2.01	0.42
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.18	0.42
8:QH:36:LEU:HD12	8:QH:59:LEU:HD23	2.01	0.42
16:QP:8:ARG:HB3	16:QP:28:ARG:NH1	2.35	0.42
18:QR:60:ALA:O	18:QR:64:ARG:NH1	2.53	0.42
35:RA:679:C:H2'	35:RA:680:G:C8	2.54	0.42
35:RA:807:U:OP2	45:RP:41:ARG:NH1	2.53	0.42
35:RA:948:G:N2	35:RA:985:C:OP2	2.51	0.42
35:RA:1858:G:H2'	35:RA:1883:G:H22	1.84	0.42
35:RA:1882:C:H3'	35:RA:1883:G:H8	1.84	0.42
35:RA:2328:A:H2'	35:RA:2329:G:H8	1.85	0.42
35:RA:2515:C:H2'	35:RA:2516:G:H8	1.84	0.42
35:RA:2692:C:H2'	35:RA:2693:A:H8	1.84	0.42
43:RN:137:LYS:HD3	43:RN:137:LYS:HA	1.77	0.42
52:RW:13:SER:HA	52:RW:14:PRO:HD3	1.92	0.42
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.47	0.42
35:YA:1400:G:H2'	35:YA:1401:G:C8	2.55	0.42
35:YA:1568:G:H5"	37:YD:61:LEU:HG	2.01	0.42
35:YA:2745:C:O2	41:YH:139:GLN:NE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YB:66:A:H61	36:YB:107:U:H2'	1.85	0.42
44:YO:78:ARG:HH12	49:YT:75:ILE:HD11	1.84	0.42
47:YR:58:GLY:HA2	47:YR:80:PHE:HE2	1.84	0.42
1:QA:123:C:H2'	1:QA:124:G:H8	1.84	0.42
1:QA:406:G:H2'	1:QA:407:G:H8	1.85	0.42
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.68	0.42
13:QM:7:VAL:HB	13:QM:9:ILE:HG12	2.01	0.42
35:RA:1205:U:C4	39:RF:171:PRO:HA	2.55	0.42
35:RA:2052:G:O2'	38:RE:143:ASN:O	2.30	0.42
35:RA:2392:A:H2	35:RA:2424:C:H42	1.67	0.42
1:XA:985:C:H2'	1:XA:986:A:H8	1.83	0.42
1:XA:1058:G:H1	1:XA:1199:U:H3	1.67	0.42
1:XA:1172:C:H2'	1:XA:1173:G:H8	1.84	0.42
16:XP:26:ARG:HD3	16:XP:26:ARG:HA	1.91	0.42
24:XZ:49:LYS:HA	24:XZ:49:LYS:HD3	1.81	0.42
35:YA:38:A:H2'	35:YA:39:C:C6	2.55	0.42
35:YA:380:U:H2'	35:YA:381:G:C8	2.54	0.42
35:YA:597:U:H3	35:YA:660:G:H1	1.67	0.42
35:YA:2162:G:O2'	35:YA:2173:A:OP2	2.27	0.42
54:YY:83:THR:OG1	54:YY:84:ARG:N	2.52	0.42
1:QA:700:G:H4'	1:QA:704:A:H1'	2.00	0.42
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.84	0.42
1:QA:1298:C:H4'	1:QA:1299:A:C4	2.54	0.42
1:QA:1512:U:H2'	1:QA:1513:A:H8	1.84	0.42
2:QB:74:LYS:NZ	2:QB:205:ASP:O	2.44	0.42
13:QM:13:LYS:HA	13:QM:44:ARG:HH11	1.84	0.42
35:RA:576:U:H2'	35:RA:577:G:C8	2.55	0.42
35:RA:822:U:H2'	35:RA:823:G:H8	1.84	0.42
35:RA:890:A:H2'	35:RA:892:G:C8	2.55	0.42
35:RA:1259:G:H2'	35:RA:1260:G:C8	2.55	0.42
38:RE:41:LYS:HE2	38:RE:41:LYS:HB3	1.87	0.42
40:RG:109:VAL:O	40:RG:113:ARG:HG2	2.19	0.42
1:XA:1378:C:O2	7:XG:76:ARG:NH2	2.49	0.42
11:XK:80:VAL:HG13	11:XK:103:LEU:HD12	2.01	0.42
13:XM:51:ALA:HA	13:XM:54:VAL:HG12	2.02	0.42
33:Y8:37:SER:HB3	33:Y8:40:GLU:HG3	2.01	0.42
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.52	0.42
35:YA:1021:A:OP2	43:YN:65:LYS:NZ	2.42	0.42
35:YA:1225:C:H2'	35:YA:1226:G:C8	2.54	0.42
35:YA:1363:C:O2'	35:YA:1809:A:N3	2.44	0.42
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:133:LEU:HD23	37:YD:136:ILE:HD12	2.02	0.42
52:YW:110:LYS:HA	52:YW:110:LYS:HD3	1.90	0.42
55:YZ:6:LYS:HD2	55:YZ:6:LYS:HA	1.83	0.42
55:YZ:51:ALA:HB1	55:YZ:55:HIS:HB2	2.02	0.42
1:QA:413:G:N2	1:QA:429:U:OP2	2.44	0.42
1:QA:1356:G:H2'	1:QA:1357:A:H8	1.85	0.42
4:QD:119:GLN:O	4:QD:123:HIS:N	2.49	0.42
35:RA:137(A):G:O2'	35:RA:138:G:N2	2.53	0.42
35:RA:863:A:H2'	35:RA:864:G:C8	2.55	0.42
40:RG:36:LYS:HE2	40:RG:95:ARG:HH12	1.85	0.42
1:XA:1151:A:H5'	10:XJ:41:PRO:HA	2.01	0.42
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	2.00	0.42
2:XB:208:ILE:H	2:XB:208:ILE:HG13	1.65	0.42
5:XE:53:LEU:HA	5:XE:56:GLN:HG2	2.02	0.42
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.53	0.42
35:YA:1212:G:O2'	35:YA:1237:A:N6	2.52	0.42
35:YA:1482:U:O4	35:YA:1512:G:O6	2.37	0.42
39:YF:63:LYS:HE2	39:YF:67:GLN:HB2	2.02	0.42
39:YF:64:ILE:H	39:YF:64:ILE:HG13	1.71	0.42
54:YY:14:LEU:HD22	54:YY:82:PRO:HG3	2.00	0.42
1:QA:1060:C:H2'	1:QA:1061:G:H8	1.84	0.42
1:QA:1226:C:OP1	13:QM:91:ARG:NH1	2.53	0.42
8:QH:19:VAL:HG13	8:QH:21:LYS:HG3	2.02	0.42
13:QM:47:ASP:N	13:QM:47:ASP:OD1	2.52	0.42
40:RG:82:LEU:HD11	40:RG:88:ILE:HD13	2.01	0.42
45:RP:91:PHE:HE2	45:RP:95:VAL:HG22	1.85	0.42
1:XA:41:G:H2'	1:XA:42:G:C8	2.55	0.42
10:XJ:42:THR:HG22	10:XJ:68:HIS:HA	2.01	0.42
13:XM:94:ARG:NH2	35:YA:887:A:OP1	2.46	0.42
20:XT:89:ARG:HG3	20:XT:104:LEU:HD21	2.01	0.42
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.84	0.42
35:YA:78:A:H2'	35:YA:79:G:C8	2.55	0.42
35:YA:151:C:H2'	35:YA:152:G:H8	1.83	0.42
35:YA:530:G:N2	35:YA:2022:U:OP1	2.53	0.42
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.52	0.42
41:YH:94:TYR:OH	41:YH:152:ARG:NH1	2.53	0.42
52:YW:13:SER:HA	52:YW:14:PRO:HD3	1.94	0.42
1:QA:404:U:H2'	1:QA:405:U:H6	1.84	0.41
6:QF:15:ASP:OD2	6:QF:17:SER:OG	2.38	0.41
6:QF:46:ARG:HA	6:QF:46:ARG:HD2	1.88	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R2:28:LYS:HA	27:R2:28:LYS:HD3	1.90	0.41
35:RA:532:A:H4'	35:RA:533:G:C8	2.55	0.41
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.02	0.41
35:RA:1569:A:H5'	37:RD:61:LEU:HD21	2.02	0.41
35:RA:1754:C:N3	35:RA:2716:U:O2'	2.48	0.41
1:XA:891:U:H2'	1:XA:892:A:C8	2.54	0.41
1:XA:980:C:H1'	14:XN:19:ARG:HA	2.02	0.41
7:XG:29:LYS:HA	7:XG:29:LYS:HD2	1.90	0.41
11:XK:108:ILE:O	18:XR:87:ARG:N	2.51	0.41
19:XS:2:PRO:HB2	19:XS:3:ARG:H	1.61	0.41
35:YA:299:A:N1	35:YA:322:A:O2'	2.42	0.41
35:YA:414:C:H2'	35:YA:415:A:H8	1.84	0.41
35:YA:820:A:H4'	35:YA:836:G:N2	2.35	0.41
35:YA:2329:G:H2'	35:YA:2330:G:H8	1.84	0.41
40:YG:166:ASP:OD1	40:YG:166:ASP:N	2.53	0.41
49:YT:19:LEU:HA	49:YT:20:PRO:HD3	1.90	0.41
55:YZ:124:ILE:HG22	55:YZ:126:VAL:HG13	2.01	0.41
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.53	0.41
5:QE:105:VAL:HG11	5:QE:128:PRO:HB3	2.01	0.41
5:QE:152:ARG:NH2	8:QH:107:LEU:O	2.53	0.41
35:RA:2591:C:H2'	35:RA:2592:G:H8	1.84	0.41
35:RA:2681:C:OP2	38:RE:109:LYS:NZ	2.42	0.41
41:RH:89:ILE:HG23	41:RH:162:ILE:HG22	2.01	0.41
1:XA:56:U:H2'	1:XA:57:G:C8	2.55	0.41
1:XA:194:C:H5"	20:XT:65:LYS:HG3	2.02	0.41
1:XA:977:A:O2'	1:XA:981:U:O4	2.38	0.41
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.53	0.41
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.55	0.41
1:XA:1493:A:O2'	23:XX:20:A3P:H8	2.20	0.41
25:Y0:5:LYS:HD3	46:YQ:80:GLU:HG3	2.02	0.41
35:YA:30:G:H2'	35:YA:31:C:C6	2.55	0.41
39:YF:46:ARG:HA	39:YF:46:ARG:HD2	1.86	0.41
40:YG:72:ARG:HH11	40:YG:72:ARG:HG2	1.85	0.41
55:YZ:179:ASP:OD1	55:YZ:180:VAL:N	2.53	0.41
1:QA:1182:G:H5"	1:QA:1183:A:H5'	2.02	0.41
35:RA:219:G:N3	35:RA:234:C:O2'	2.48	0.41
35:RA:223:A:O2'	35:RA:420:C:O2	2.36	0.41
35:RA:329:G:O6	54:RY:19:LYS:N	2.54	0.41
35:RA:2033:A:O2'	35:RA:2035:G:OP2	2.34	0.41
35:RA:2836:U:H2'	35:RA:2837:G:C8	2.55	0.41
51:RV:34:GLU:OE2	51:RV:100:ARG:NH2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:269:C:H2'	1:XA:270:A:C8	2.55	0.41
18:XR:26:LEU:HD11	18:XR:39:VAL:HG13	2.03	0.41
19:XS:27:GLU:HG2	19:XS:29:ARG:NH1	2.35	0.41
24:XZ:81:ARG:HG2	24:XZ:82:TYR:H	1.85	0.41
32:Y7:10:ARG:HD2	35:YA:125:G:C6	2.55	0.41
36:YB:114:G:H2'	36:YB:115:G:H8	1.85	0.41
47:YR:66:VAL:HG21	47:YR:80:PHE:HE1	1.85	0.41
55:YZ:119:GLU:HB2	55:YZ:122:ARG:HH11	1.85	0.41
1:QA:359:U:H2'	1:QA:360:A:C8	2.56	0.41
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.53	0.41
3:QC:16:ARG:HD2	3:QC:16:ARG:HA	1.68	0.41
8:QH:69:ARG:NH2	8:QH:75:ARG:O	2.53	0.41
10:QJ:4:ILE:HG23	10:QJ:74:ILE:HB	2.01	0.41
31:R6:25:LYS:HB2	31:R6:25:LYS:HE2	1.67	0.41
35:RA:196:A:O5'	45:RP:46:LYS:NZ	2.53	0.41
35:RA:1687:G:O2'	35:RA:1701:A:N6	2.47	0.41
35:RA:2314:C:H5'	40:RG:38:VAL:HG11	2.02	0.41
45:RP:46:LYS:HD2	45:RP:46:LYS:HA	1.96	0.41
47:RR:13:HIS:CE1	47:RR:16:HIS:HB2	2.55	0.41
50:RU:90:VAL:C	50:RU:92:ARG:H	2.23	0.41
1:XA:1096:C:H2'	1:XA:1097:C:H6	1.86	0.41
5:XE:106:PRO:HB3	5:XE:135:THR:HG21	2.01	0.41
7:XG:13:GLN:HA	7:XG:14:PRO:HD3	1.91	0.41
18:XR:31:LEU:HD12	18:XR:66:LEU:HB2	2.03	0.41
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.21	0.41
33:Y8:10:ALA:HB3	33:Y8:62:LEU:HD21	2.02	0.41
35:YA:1769:G:O2'	35:YA:1958:C:OP1	2.32	0.41
35:YA:2471:C:H3'	35:YA:2472:G:H8	1.84	0.41
48:YS:34:HIS:CD2	48:YS:54:LEU:HD12	2.56	0.41
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.55	0.41
18:QR:53:ARG:HH21	18:QR:59:SER:HA	1.86	0.41
35:RA:177:G:H3'	35:RA:178:G:H8	1.84	0.41
35:RA:2788:C:H5'	38:RE:61:ARG:HH12	1.86	0.41
40:RG:40:ASN:HB3	40:RG:156:ASP:HB2	2.02	0.41
49:RT:5:ALA:HA	49:RT:8:LYS:HB3	2.03	0.41
1:XA:390:C:H2'	1:XA:391:G:C8	2.55	0.41
3:XC:40:ARG:HG2	3:XC:55:VAL:HG21	2.01	0.41
8:XH:29:SER:HB3	8:XH:32:LYS:HG3	2.03	0.41
17:XQ:53:LEU:HD23	17:XQ:85:VAL:HG11	2.02	0.41
35:YA:806:C:O2	35:YA:2444:G:O2'	2.36	0.41
35:YA:970:C:H2'	35:YA:971:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1187:G:H5”	51:YV:81:TYR:CE1	2.55	0.41
35:YA:1403:C:H5”	35:YA:1471:A:H1’	2.02	0.41
35:YA:2850:A:N7	35:YA:2868:A:O2’	2.42	0.41
41:YH:54:ARG:NH2	41:YH:57:ASP:OD1	2.54	0.41
49:YT:62:THR:HG22	49:YT:75:ILE:HG12	2.02	0.41
50:YU:92:ARG:NH2	51:YV:11:GLN:H	2.18	0.41
1:QA:454:C:H41	1:QA:478:A:H61	1.68	0.41
1:QA:524:G:H2’	1:QA:525:C:C6	2.56	0.41
1:QA:1354:C:H2’	1:QA:1355:G:C8	2.56	0.41
27:R2:14:ARG:HG2	27:R2:63:VAL:HG21	2.03	0.41
28:R3:8:LEU:HG	28:R3:28:LEU:HD12	2.01	0.41
30:R5:30:LEU:HD12	30:R5:39:MET:HB3	2.02	0.41
33:R8:58:ILE:HA	33:R8:61:LEU:HD12	2.03	0.41
35:RA:414:C:H2’	35:RA:415:A:C8	2.55	0.41
35:RA:1771:C:H2’	35:RA:1772:G:C8	2.56	0.41
47:RR:24:GLN:HG3	47:RR:44:LEU:HD13	2.02	0.41
1:XA:45:U:H2’	1:XA:46:G:H8	1.85	0.41
1:XA:359:U:H2’	1:XA:360:A:C8	2.56	0.41
1:XA:524:G:H2’	1:XA:525:C:C6	2.55	0.41
1:XA:736:C:H2’	1:XA:737:A:C8	2.55	0.41
1:XA:1251:A:H2’	1:XA:1252:A:C8	2.56	0.41
1:XA:1436:U:OP1	20:XT:23:ARG:NH2	2.53	0.41
9:XI:49:PRO:HA	9:XI:52:ALA:HB3	2.03	0.41
14:XN:37:PHE:HB3	14:XN:39:LEU:HD13	2.03	0.41
17:XQ:18:THR:OG1	17:XQ:69:LYS:NZ	2.39	0.41
26:Y1:60:PHE:HE1	26:Y1:91:LYS:HG3	1.86	0.41
35:YA:2291:U:H2’	35:YA:2292:C:C6	2.55	0.41
1:QA:919:A:O2’	1:QA:1080:A:N1	2.43	0.41
8:QH:41:ARG:NH2	8:QH:123:GLU:OE1	2.53	0.41
10:QJ:8:LEU:HB3	10:QJ:70:ARG:HB2	2.02	0.41
35:RA:121:G:H4’	35:RA:149:A:H5’	2.02	0.41
35:RA:570:G:H2’	35:RA:2030:A:C5	2.55	0.41
35:RA:1231:G:H2’	35:RA:1232:G:H8	1.85	0.41
38:RE:64:LYS:HA	38:RE:64:LYS:HD3	1.73	0.41
49:RT:85:LYS:NZ	49:RT:87:ASP:OD2	2.46	0.41
1:XA:1127:G:H21	1:XA:1147:C:H42	1.67	0.41
1:XA:1182:G:H4’	1:XA:1183:A:H5’	2.03	0.41
3:XC:91:LEU:HB3	3:XC:99:VAL:HG11	2.03	0.41
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	2.03	0.41
30:Y5:3:LYS:H	35:YA:2577:A:H4’	1.85	0.41
35:YA:33:U:O4	35:YA:446:G:O2’	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:679:C:H2'	35:YA:680:G:H8	1.86	0.41
35:YA:1423:G:H2'	35:YA:1424:G:H8	1.85	0.41
39:YF:155:LEU:HD11	39:YF:176:LEU:HB2	2.03	0.41
1:QA:116:A:H61	1:QA:313:A:H1'	1.85	0.41
1:QA:362:G:N2	1:QA:365:U:OP2	2.52	0.41
1:QA:377:G:H2'	1:QA:378:G:C8	2.56	0.41
1:QA:652:U:O3'	8:QH:56:LYS:NZ	2.54	0.41
1:QA:652:U:O4	1:QA:752:G:O2'	2.32	0.41
13:QM:23:TYR:CE2	13:QM:71:ARG:HG3	2.55	0.41
29:R4:2:LYS:O	29:R4:4:GLY:N	2.53	0.41
44:RO:22:ILE:HD11	44:RO:42:SER:HB2	2.02	0.41
46:RQ:116:GLU:O	46:RQ:120:ILE:HG12	2.20	0.41
1:XA:142:G:H2'	1:XA:143:A:C8	2.56	0.41
1:XA:195:A:H4'	20:XT:68:LYS:HE3	2.03	0.41
1:XA:898:G:N2	1:XA:901:A:OP2	2.48	0.41
1:XA:1127:G:N2	1:XA:1147:C:H42	2.19	0.41
10:XJ:66:ARG:HD2	14:XN:57:ARG:HH22	1.85	0.41
23:XX:14:A:H2'	23:XX:15:A:H8	1.86	0.41
35:YA:764:A:H2	37:YD:219:PRO:HG3	1.85	0.41
35:YA:2001:A:H2'	35:YA:2002:G:C8	2.56	0.41
35:YA:2103:C:N4	35:YA:2187:G:O6	2.54	0.41
35:YA:2749:A:O2'	41:YH:59:ARG:NE	2.48	0.41
1:QA:80:G:H1	1:QA:89:U:H3	1.68	0.41
1:QA:189:U:O4	17:QQ:63:ARG:N	2.53	0.41
1:QA:1228:C:H4'	13:QM:116:THR:HA	2.02	0.41
1:QA:1427:U:H2'	1:QA:1428:A:C8	2.56	0.41
7:QG:88:PRO:HG2	7:QG:152:ALA:HB2	2.03	0.41
8:QH:36:LEU:HD23	8:QH:36:LEU:HA	1.92	0.41
8:QH:86:ILE:HD12	8:QH:133:LEU:HD22	2.03	0.41
9:QI:102:LEU:HD23	9:QI:102:LEU:HA	1.81	0.41
13:QM:3:ARG:HA	13:QM:8:GLU:HA	2.03	0.41
13:QM:121:LYS:HD2	13:QM:121:LYS:HA	1.81	0.41
22:QV:9:G:O2'	22:QV:10:G:N7	2.46	0.41
28:R3:29:ARG:N	28:R3:33:GLN:OE1	2.50	0.41
29:R4:13:ARG:HA	29:R4:13:ARG:HD3	1.94	0.41
35:RA:824:A:H1'	35:RA:2358:G:N7	2.36	0.41
35:RA:922:U:H2'	35:RA:923:C:C6	2.56	0.41
35:RA:1278:A:H2'	35:RA:1279:G:C8	2.56	0.41
35:RA:1336:A:H2'	35:RA:1337:G:C8	2.56	0.41
35:RA:2186:G:H2'	35:RA:2187:G:C8	2.56	0.41
35:RA:2597:G:H2'	35:RA:2598:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2723:C:P	38:RE:109:LYS:HZ3	2.44	0.41
37:RD:77:ALA:HA	37:RD:97:TYR:HA	2.02	0.41
38:RE:25:VAL:HG11	49:RT:10:VAL:HG11	2.03	0.41
42:RI:72:LEU:HG	42:RI:138:ILE:HG13	2.01	0.41
1:XA:708:C:H2'	1:XA:709:G:H8	1.86	0.41
1:XA:790:A:OP1	22:XV:38:A:O2'	2.34	0.41
1:XA:806:C:H2'	1:XA:807:A:C8	2.56	0.41
1:XA:892:A:H2'	1:XA:893:C:C6	2.56	0.41
2:XB:15:VAL:HG11	2:XB:210:SER:N	2.35	0.41
3:XC:152:ILE:HG12	3:XC:167:TRP:HD1	1.85	0.41
6:XF:45:LEU:HD12	6:XF:59:TYR:HD1	1.86	0.41
10:XJ:78:ASN:OD1	10:XJ:78:ASN:N	2.50	0.41
35:YA:195:A:H5"	45:YP:46:LYS:NZ	2.36	0.41
35:YA:453:C:O2	35:YA:457:A:O2'	2.35	0.41
35:YA:1657:C:H2'	35:YA:1658:C:C6	2.55	0.41
35:YA:2853:C:H2'	35:YA:2854:G:C8	2.56	0.41
38:YE:7:VAL:HG13	38:YE:51:PHE:HE2	1.86	0.41
39:YF:24:LEU:HA	39:YF:25:PRO:HD3	1.94	0.41
40:YG:64:THR:HG23	40:YG:66:GLN:H	1.86	0.41
42:YI:14:ASP:H	42:YI:17:GLN:CB	2.34	0.41
1:QA:41:G:H2'	1:QA:42:G:H8	1.85	0.41
1:QA:1119:C:H2'	1:QA:1120:G:C8	2.55	0.41
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.35	0.41
13:QM:84:ILE:HD13	19:QS:65:ASN:HD21	1.86	0.41
19:QS:42:PRO:HD3	29:R4:63:TYR:OH	2.20	0.41
25:R0:39:ARG:HD3	25:R0:39:ARG:HA	1.88	0.41
35:RA:635:C:O2'	35:RA:639:U:OP1	2.37	0.41
35:RA:861:A:N3	36:RB:79:C:O2'	2.53	0.41
35:RA:1400:G:H2'	35:RA:1401:G:C8	2.55	0.41
36:RB:60:C:H2'	36:RB:61:G:C8	2.56	0.41
38:RE:34:VAL:HG12	38:RE:72:VAL:HG11	2.02	0.41
46:RQ:31:ASP:OD1	55:RZ:122:ARG:NH2	2.47	0.41
50:RU:32:PHE:CZ	50:RU:36:ARG:HD2	2.56	0.41
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.56	0.41
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.55	0.41
35:YA:680:G:H2'	35:YA:681:G:C8	2.55	0.41
35:YA:992:C:H2'	35:YA:993:G:H8	1.85	0.41
35:YA:1262:A:OP2	52:YW:97:LYS:NZ	2.54	0.41
35:YA:2698:U:H2'	35:YA:2699:C:C6	2.56	0.41
52:YW:68:ARG:NE	52:YW:110:LYS:O	2.48	0.41
1:QA:125:U:H2'	1:QA:126:G:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1037:C:H2'	1:QA:1038:C:C6	2.56	0.40
4:QD:122:ARG:HA	4:QD:122:ARG:HD2	1.94	0.40
16:QP:18:ARG:HH11	16:QP:35:LYS:HD2	1.86	0.40
18:QR:40:LEU:HB3	18:QR:79:LEU:HD21	2.02	0.40
26:R1:11:ARG:NH2	35:RA:1365:A:O2'	2.52	0.40
35:RA:463:G:N2	35:RA:466:A:OP2	2.42	0.40
35:RA:764:A:H5'	37:RD:210:GLY:HA2	2.02	0.40
35:RA:1316:U:H2'	35:RA:1317:A:H8	1.86	0.40
35:RA:1399:C:H2'	35:RA:1400:G:C8	2.56	0.40
35:RA:1409:C:H2'	35:RA:1410:G:H8	1.86	0.40
35:RA:1449:A:C4	35:RA:1529:A:H2	2.39	0.40
35:RA:1889:A:H2'	35:RA:1890:A:C8	2.56	0.40
48:RS:39:ILE:HD12	48:RS:85:VAL:HG11	2.02	0.40
1:XA:269:C:H2'	1:XA:270:A:H8	1.86	0.40
1:XA:1311:G:OP1	29:Y4:58:ARG:NH2	2.54	0.40
1:XA:1441:G:O2'	1:XA:1446:A:N6	2.49	0.40
7:XG:94:ARG:NH1	7:XG:98:SER:OG	2.54	0.40
9:XI:42:ARG:NH2	9:XI:75:ASP:OD1	2.52	0.40
35:YA:141:A:C8	35:YA:1408:C:H1'	2.56	0.40
35:YA:2037:G:H2'	35:YA:2038:G:C8	2.56	0.40
39:YF:48:THR:O	39:YF:48:THR:OG1	2.39	0.40
40:YG:29:TRP:O	40:YG:33:ARG:NH1	2.54	0.40
46:YQ:116:GLU:HA	46:YQ:119:ARG:HG2	2.03	0.40
49:YT:80:SER:HA	49:YT:81:PRO:HD3	1.92	0.40
50:YU:90:VAL:HG11	51:YV:39:LEU:HB2	2.04	0.40
54:YY:81:LYS:HD2	54:YY:82:PRO:HD2	2.03	0.40
1:QA:401:C:H2'	1:QA:402:G:H8	1.86	0.40
1:QA:1101:A:N6	2:QB:176:GLU:OE2	2.54	0.40
3:QC:164:ARG:NH1	3:QC:166:GLU:OE2	2.37	0.40
6:QF:3:ARG:HB3	6:QF:93:SER:HB2	2.03	0.40
19:QS:10:PHE:HE1	19:QS:38:SER:HB2	1.85	0.40
25:R0:49:LYS:HB3	25:R0:80:HIS:HD1	1.85	0.40
27:R2:65:ASN:ND2	35:RA:72:U:O4	2.54	0.40
35:RA:582:G:H2'	35:RA:583:G:C8	2.56	0.40
38:RE:114:ALA:HB1	38:RE:118:LYS:HD2	2.02	0.40
1:XA:881:G:OP2	12:XL:12:ARG:NH2	2.54	0.40
1:XA:927:G:H1	1:XA:1390:U:H3	1.68	0.40
1:XA:993:G:O2'	1:XA:994:A:N7	2.54	0.40
1:XA:1159:U:O2'	1:XA:1160:G:N7	2.53	0.40
2:XB:16:HIS:ND1	2:XB:17:PHE:O	2.54	0.40
2:XB:178:ARG:NH1	8:XH:74:PRO:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:102:ASP:N	4:XD:102:ASP:OD1	2.53	0.40
7:XG:15:ASP:OD1	7:XG:44:TYR:OH	2.38	0.40
20:XT:27:LYS:HA	20:XT:27:LYS:HD3	1.92	0.40
20:XT:50:GLU:HB3	20:XT:99:LEU:HD21	2.04	0.40
35:YA:698:C:O2'	35:YA:734:A:N6	2.55	0.40
35:YA:969:U:H2'	35:YA:970:C:C6	2.56	0.40
35:YA:1652:A:OP1	47:YR:8:ARG:NH1	2.44	0.40
35:YA:2327:A:H2'	35:YA:2328:A:C8	2.56	0.40
39:YF:155:LEU:HD23	39:YF:186:ILE:HD13	2.02	0.40
42:YI:79:ILE:HG22	42:YI:81:VAL:HG13	2.03	0.40
47:YR:58:GLY:HA2	47:YR:80:PHE:CE2	2.56	0.40
53:YX:31:HIS:HB3	53:YX:34:ALA:HB2	2.03	0.40
55:YZ:48:PHE:HE1	55:YZ:71:VAL:HG21	1.86	0.40
1:QA:954:G:H21	1:QA:1227:A:N6	2.19	0.40
1:QA:1488:G:H2'	1:QA:1489:G:C8	2.56	0.40
2:QB:133:LYS:HA	2:QB:133:LYS:HD2	1.91	0.40
11:QK:70:LYS:HD3	11:QK:70:LYS:HA	1.87	0.40
23:QX:6:G:H2'	23:QX:7:G:C8	2.57	0.40
33:R8:46:ARG:HD2	33:R8:46:ARG:HA	1.83	0.40
35:RA:270(I):G:H2'	35:RA:270(J):G:C8	2.57	0.40
35:RA:663:G:H5"	45:RP:17:LYS:HD3	2.04	0.40
35:RA:807:U:H2'	35:RA:808:G:H8	1.85	0.40
35:RA:1529:A:H62	35:RA:1542:G:N2	2.19	0.40
35:RA:2728:U:H2'	35:RA:2729:G:C8	2.56	0.40
36:RB:9:G:H5'	48:RS:25:ARG:HH22	1.86	0.40
38:RE:67:PHE:HD1	38:RE:67:PHE:HA	1.75	0.40
43:RN:16:ILE:HB	43:RN:54:VAL:HG22	2.03	0.40
1:XA:7:G:O2'	5:XE:120:THR:O	2.40	0.40
1:XA:1314:C:N4	19:XS:2:PRO:O	2.55	0.40
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.86	0.40
7:XG:78:ARG:HE	7:XG:80:VAL:HG23	1.87	0.40
13:XM:3:ARG:NH1	29:Y4:34:GLU:OE2	2.54	0.40
26:Y1:73:LEU:HD13	26:Y1:73:LEU:HA	1.82	0.40
31:Y6:6:ARG:NH1	35:YA:2285:C:OP2	2.53	0.40
35:YA:576:U:H2'	35:YA:577:G:C8	2.56	0.40
35:YA:787:U:H5"	35:YA:788:A:H5'	2.04	0.40
35:YA:1411:C:H2'	35:YA:1412:A:H8	1.86	0.40
43:YN:96:GLU:HG3	43:YN:122:VAL:HG23	2.04	0.40
1:QA:603:U:H2'	1:QA:604:G:C8	2.57	0.40
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.86	0.40
4:QD:88:VAL:HG13	4:QD:91:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R3:18:ASP:OD1	28:R3:18:ASP:N	2.54	0.40
34:R9:6:SER:O	34:R9:6:SER:OG	2.40	0.40
35:RA:37:C:H2'	35:RA:38:A:C8	2.57	0.40
35:RA:78:A:H2'	35:RA:79:G:H8	1.85	0.40
35:RA:323:G:H2'	39:RF:169:ASN:ND2	2.37	0.40
35:RA:616:A:C4	39:RF:180:GLY:HA3	2.56	0.40
35:RA:1935:G:H1'	35:RA:1964:G:N2	2.37	0.40
36:RB:105:G:H2'	36:RB:106:G:H8	1.85	0.40
40:RG:124:SER:OG	40:RG:132:ASN:O	2.38	0.40
42:RI:65:ALA:HB1	42:RI:134:PRO:HD2	2.03	0.40
50:RU:61:TRP:HB3	50:RU:93:LYS:O	2.22	0.40
1:XA:719:C:N3	18:XR:74:ARG:NH1	2.49	0.40
1:XA:1064:G:H1'	1:XA:1066:C:C6	2.56	0.40
1:XA:1064:G:O6	1:XA:1193:G:N1	2.54	0.40
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.86	0.40
19:XS:40:ILE:HG12	19:XS:71:LEU:HG	2.03	0.40
26:Y1:92:LYS:HZ3	26:Y1:96:LYS:NZ	2.19	0.40
29:Y4:37:SER:HB3	40:YG:108:ASN:HA	2.04	0.40
31:Y6:17:LYS:HA	31:Y6:17:LYS:HD3	1.85	0.40
35:YA:588:U:H1'	39:YF:90:PHE:HB3	2.04	0.40
35:YA:1060:U:H5'	35:YA:1061:U:H5	1.86	0.40
40:YG:59:GLU:OE1	40:YG:153:ARG:NH2	2.55	0.40
51:YV:12:TYR:CD1	51:YV:20:LEU:HD11	2.56	0.40
55:YZ:72:ARG:NH2	55:YZ:97:GLU:O	2.54	0.40
1:QA:272:C:H2'	1:QA:273:A:H8	1.87	0.40
1:QA:411:A:H62	1:QA:413:G:H21	1.70	0.40
1:QA:1070:U:OP1	5:QE:18:ARG:NH2	2.45	0.40
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.94	0.40
19:QS:10:PHE:HB2	19:QS:39:THR:HB	2.02	0.40
34:R9:2:LYS:HE2	34:R9:33:LYS:HG2	2.04	0.40
35:RA:448:U:C4	35:RA:583:G:H1'	2.57	0.40
35:RA:848:G:H2'	35:RA:849:A:C8	2.57	0.40
1:XA:674:G:H2'	1:XA:675:A:C8	2.51	0.40
1:XA:737:A:H2'	1:XA:738:C:C6	2.56	0.40
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	2.03	0.40
13:XM:15:VAL:HA	13:XM:18:ALA:HB3	2.02	0.40
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	2.03	0.40
35:YA:639:U:H2'	35:YA:640:C:C6	2.57	0.40
35:YA:1901:A:OP2	37:YD:255:LYS:NZ	2.37	0.40
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.51	0.40
35:YA:2025:C:H2'	35:YA:2026:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YF:6:VAL:HB	39:YF:24:LEU:HB2	2.03	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	233/256 (91%)	202 (87%)	27 (12%)	4 (2%)	9 42
2	XB	234/256 (91%)	211 (90%)	21 (9%)	2 (1%)	17 56
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100 100
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	29 68
4	QD	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	15 54
4	XD	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	15 54
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100 100
5	XE	149/162 (92%)	142 (95%)	7 (5%)	0	100 100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100 100
6	XF	99/101 (98%)	99 (100%)	0	0	100 100
7	QG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22 61
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100 100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100 100
9	XI	124/128 (97%)	113 (91%)	11 (9%)	0	100 100
10	QJ	97/105 (92%)	85 (88%)	12 (12%)	0	100 100
10	XJ	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	14 52
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	XK	114/129 (88%)	105 (92%)	9 (8%)	0	100 100
12	QL	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	9 43
12	XL	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19 58
13	QM	118/126 (94%)	102 (86%)	13 (11%)	3 (2%)	5 34
13	XM	117/126 (93%)	96 (82%)	21 (18%)	0	100 100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9 42
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9 42
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100 100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100 100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100 100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100 100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100 100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100 100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100 100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100 100
19	QS	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	13 50
19	XS	81/93 (87%)	75 (93%)	6 (7%)	0	100 100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100 100
20	XT	97/106 (92%)	88 (91%)	6 (6%)	3 (3%)	4 30
21	QU	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2 22
21	XU	23/27 (85%)	22 (96%)	0	1 (4%)	2 22
24	QY	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	6 35
24	QZ	82/84 (98%)	72 (88%)	10 (12%)	0	100 100
24	XY	82/84 (98%)	71 (87%)	8 (10%)	3 (4%)	3 26
24	XZ	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	13 50
25	R0	79/85 (93%)	72 (91%)	6 (8%)	1 (1%)	12 48
25	Y0	80/85 (94%)	72 (90%)	8 (10%)	0	100 100
26	R1	92/98 (94%)	82 (89%)	10 (11%)	0	100 100
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14 52
27	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10 45
27	Y2	67/72 (93%)	63 (94%)	2 (3%)	2 (3%)	4 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
29	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1 15
29	Y4	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	10 45
30	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
30	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
31	R6	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
31	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
32	R7	45/49 (92%)	45 (100%)	0	0	100 100
32	Y7	46/49 (94%)	46 (100%)	0	0	100 100
33	R8	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	4 29
33	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4 29
34	R9	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
34	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
37	RD	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	10 45
37	YD	272/276 (99%)	263 (97%)	9 (3%)	0	100 100
38	RE	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	7 39
38	YE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15 54
39	RF	200/210 (95%)	195 (98%)	5 (2%)	0	100 100
39	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	15 54
40	RG	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	9 42
40	YG	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	14 52
41	RH	172/180 (96%)	137 (80%)	29 (17%)	6 (4%)	3 27
41	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100 100
42	RI	143/148 (97%)	117 (82%)	20 (14%)	6 (4%)	3 23
42	YI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11 46
43	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	10 45
43	YN	136/140 (97%)	118 (87%)	16 (12%)	2 (2%)	10 45
44	RO	120/122 (98%)	118 (98%)	2 (2%)	0	100 100
44	YO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19 58
45	RP	148/150 (99%)	125 (84%)	19 (13%)	4 (3%)	5 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	YP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11 46
46	RQ	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	3 26
46	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
47	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17 56
47	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17 56
48	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	17 56
48	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100 100
49	RT	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	22 61
49	YT	135/146 (92%)	119 (88%)	16 (12%)	0	100 100
50	RU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17 56
50	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17 56
51	RV	99/101 (98%)	90 (91%)	9 (9%)	0	100 100
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15 54
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100 100
52	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100 100
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100 100
53	YX	90/96 (94%)	86 (96%)	3 (3%)	1 (1%)	14 52
54	RY	105/110 (96%)	94 (90%)	11 (10%)	0	100 100
54	YY	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15 54
55	RZ	181/206 (88%)	166 (92%)	13 (7%)	2 (1%)	14 52
55	YZ	181/206 (88%)	168 (93%)	13 (7%)	0	100 100
All	All	11789/12464 (95%)	10734 (91%)	950 (8%)	105 (1%)	17 56

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	208	ILE
14	QN	17	LYS
21	QU	3	LYS
24	QY	82	TYR
27	R2	47	ASN
29	R4	40	HIS
33	R8	29	LYS
33	R8	30	ARG
41	RH	152	ARG

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Mol	Chain	Res	Type
42	RI	132	PRO
42	RI	143	SER
42	RI	144	VAL
43	RN	22	THR
45	RP	27	HIS
45	RP	57	THR
45	RP	108	LYS
46	RQ	85	LYS
55	RZ	53	ILE
2	XB	236	TYR
12	XL	105	TYR
14	XN	17	LYS
20	XT	73	HIS
21	XU	3	LYS
24	XY	82	TYR
33	Y8	30	ARG
42	YI	145	VAL
43	YN	22	THR
47	YR	4	LEU
51	YV	49	THR
4	QD	155	LEU
12	QL	105	TYR
12	QL	128	ALA
29	R4	3	GLU
29	R4	11	PRO
29	R4	41	PRO
37	RD	238	GLY
37	RD	243	GLY
38	RE	145	LYS
41	RH	10	PRO
41	RH	86	GLU
50	RU	92	ARG
4	XD	155	LEU
24	XZ	50	HIS
26	Y1	83	GLU
27	Y2	71	ASN
33	Y8	29	LYS
39	YF	129	PHE
40	YG	137	GLU
42	YI	15	VAL
45	YP	36	LYS
50	YU	92	ARG

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Mol	Chain	Res	Type
2	QB	9	GLU
4	QD	156	GLU
13	QM	12	ASN
19	QS	28	LYS
24	QY	50	HIS
37	RD	36	PRO
38	RE	55	ASN
38	RE	74	PRO
40	RG	117	PHE
46	RQ	25	ASP
47	RR	4	LEU
55	RZ	52	SER
10	XJ	56	HIS
29	Y4	47	GLN
53	YX	68	ARG
25	R0	47	PRO
38	RE	83	ASP
40	RG	81	LYS
40	RG	116	ASP
41	RH	15	VAL
41	RH	87	LEU
42	RI	134	PRO
4	XD	156	GLU
24	XY	50	HIS
24	XY	83	HIS
39	YF	67	GLN
40	YG	81	LYS
7	QG	8	GLU
13	QM	67	GLU
42	RI	10	GLU
42	RI	133	HIS
43	RN	36	GLY
45	RP	36	LYS
46	RQ	105	GLU
27	Y2	70	GLN
38	YE	30	PRO
43	YN	23	LEU
45	YP	29	LYS
2	QB	231	GLU
2	QB	233	SER
13	QM	9	ILE
41	RH	154	PRO

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Mol	Chain	Res	Type
46	RQ	67	ARG
48	RS	57	LYS
49	RT	109	GLU
2	XB	233	SER
3	XC	4	LYS
38	YE	145	LYS
44	YO	97	ARG
46	RQ	66	ILE
54	YY	10	GLY
20	XT	98	PRO
37	RD	123	ALA
20	XT	96	GLY

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	203/220 (92%)	196 (97%)	7 (3%)	37	68
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	84
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	70
3	XC	159/188 (85%)	155 (98%)	4 (2%)	47	75
4	QD	180/181 (99%)	175 (97%)	5 (3%)	43	72
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	88
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	90
5	XE	116/123 (94%)	112 (97%)	4 (3%)	37	68
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	88
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	121 (96%)	5 (4%)	31	64
7	XG	126/127 (99%)	121 (96%)	5 (4%)	31	64
8	QH	118/119 (99%)	115 (98%)	3 (2%)	47	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	QI	98/99 (99%)	92 (94%)	6 (6%)	18 51
9	XI	97/99 (98%)	96 (99%)	1 (1%)	76 88
10	QJ	89/92 (97%)	84 (94%)	5 (6%)	21 54
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	71 87
11	QK	90/99 (91%)	88 (98%)	2 (2%)	52 78
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73 88
12	QL	104/109 (95%)	102 (98%)	2 (2%)	57 80
12	XL	103/109 (94%)	101 (98%)	2 (2%)	57 80
13	QM	96/101 (95%)	95 (99%)	1 (1%)	76 88
13	XM	95/101 (94%)	91 (96%)	4 (4%)	30 63
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30 63
14	XN	49/50 (98%)	49 (100%)	0	100 100
15	QO	79/80 (99%)	79 (100%)	0	100 100
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69 86
16	QP	72/74 (97%)	72 (100%)	0	100 100
16	XP	72/74 (97%)	70 (97%)	2 (3%)	43 72
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73 88
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53 79
18	QR	61/77 (79%)	58 (95%)	3 (5%)	25 59
18	XR	61/77 (79%)	60 (98%)	1 (2%)	62 83
19	QS	72/80 (90%)	69 (96%)	3 (4%)	30 63
19	XS	69/80 (86%)	69 (100%)	0	100 100
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%)	20 (100%)	0	100 100
24	QY	78/78 (100%)	74 (95%)	4 (5%)	24 57
24	QZ	78/78 (100%)	73 (94%)	5 (6%)	17 50
24	XY	78/78 (100%)	78 (100%)	0	100 100
24	XZ	78/78 (100%)	74 (95%)	4 (5%)	24 57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27 61
26	R1	79/83 (95%)	78 (99%)	1 (1%)	69 86
26	Y1	82/83 (99%)	82 (100%)	0	100 100
27	R2	64/67 (96%)	63 (98%)	1 (2%)	62 83
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	62 83
28	R3	51/52 (98%)	50 (98%)	1 (2%)	55 79
28	Y3	51/52 (98%)	50 (98%)	1 (2%)	55 79
29	R4	62/63 (98%)	54 (87%)	8 (13%)	4 22
29	Y4	62/63 (98%)	60 (97%)	2 (3%)	39 69
30	R5	51/52 (98%)	51 (100%)	0	100 100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55 79
31	R6	51/52 (98%)	49 (96%)	2 (4%)	32 64
31	Y6	51/52 (98%)	49 (96%)	2 (4%)	32 64
32	R7	40/42 (95%)	40 (100%)	0	100 100
32	Y7	41/42 (98%)	41 (100%)	0	100 100
33	R8	54/55 (98%)	50 (93%)	4 (7%)	13 44
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34 65
34	R9	34/34 (100%)	33 (97%)	1 (3%)	42 71
34	Y9	34/34 (100%)	34 (100%)	0	100 100
37	RD	214/218 (98%)	209 (98%)	5 (2%)	50 77
37	YD	216/218 (99%)	214 (99%)	2 (1%)	78 90
38	RE	165/166 (99%)	160 (97%)	5 (3%)	41 71
38	YE	164/166 (99%)	163 (99%)	1 (1%)	86 94
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%)	149 (96%)	6 (4%)	32 64
40	YG	155/156 (99%)	150 (97%)	5 (3%)	39 69
41	RH	145/148 (98%)	140 (97%)	5 (3%)	37 68
41	YH	144/148 (97%)	142 (99%)	2 (1%)	67 85
42	RI	122/124 (98%)	117 (96%)	5 (4%)	30 63
42	YI	122/124 (98%)	119 (98%)	3 (2%)	47 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	RN	117/119 (98%)	114 (97%)	3 (3%)	46 74
43	YN	117/119 (98%)	117 (100%)	0	100 100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76 88
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55 79
45	RP	116/116 (100%)	114 (98%)	2 (2%)	60 82
45	YP	115/116 (99%)	114 (99%)	1 (1%)	78 90
46	RQ	111/111 (100%)	107 (96%)	4 (4%)	35 66
46	YQ	111/111 (100%)	111 (100%)	0	100 100
47	RR	100/101 (99%)	100 (100%)	0	100 100
47	YR	100/101 (99%)	98 (98%)	2 (2%)	55 79
48	RS	87/88 (99%)	83 (95%)	4 (5%)	27 61
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37 68
49	RT	120/127 (94%)	114 (95%)	6 (5%)	24 58
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47 75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73 88
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73 88
51	RV	82/82 (100%)	76 (93%)	6 (7%)	14 45
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49 76
52	RW	92/92 (100%)	90 (98%)	2 (2%)	52 78
52	YW	92/92 (100%)	90 (98%)	2 (2%)	52 78
53	RX	74/78 (95%)	74 (100%)	0	100 100
53	YX	74/78 (95%)	72 (97%)	2 (3%)	44 73
54	RY	88/91 (97%)	88 (100%)	0	100 100
54	YY	88/91 (97%)	87 (99%)	1 (1%)	73 88
55	RZ	162/179 (90%)	160 (99%)	2 (1%)	71 87
55	YZ	162/179 (90%)	159 (98%)	3 (2%)	57 80
All	All	10001/10378 (96%)	9777 (98%)	224 (2%)	52 78

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	11	LEU
2	QB	17	PHE

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Mol	Chain	Res	Type
2	QB	21	ARG
2	QB	114	ARG
2	QB	132	LYS
2	QB	209	ARG
2	QB	226	ARG
3	QC	11	ARG
3	QC	16	ARG
3	QC	105	GLU
3	QC	132	ARG
3	QC	193	TYR
4	QD	17	VAL
4	QD	21	LEU
4	QD	31	CYS
4	QD	33	MET
4	QD	107	ARG
5	QE	47	LYS
6	QF	80	ARG
7	QG	10	ARG
7	QG	53	LYS
7	QG	79	ARG
7	QG	114	ARG
7	QG	155	ARG
8	QH	29	SER
8	QH	50	ARG
8	QH	104	ARG
9	QI	4	TYR
9	QI	16	ARG
9	QI	18	PHE
9	QI	20	ARG
9	QI	26	VAL
9	QI	70	LYS
10	QJ	25	GLU
10	QJ	43	ARG
10	QJ	55	LYS
10	QJ	60	ARG
10	QJ	79	ARG
11	QK	12	ARG
11	QK	92	GLU
12	QL	59	ARG
12	QL	117	ARG
13	QM	11	ARG
14	QN	12	ARG

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Mol	Chain	Res	Type
14	QN	50	LYS
17	QQ	101	ARG
18	QR	34	TYR
18	QR	54	ARG
18	QR	83	GLU
19	QS	3	ARG
19	QS	12	ASP
19	QS	28	LYS
24	QY	6	SER
24	QY	11	ASP
24	QY	18	GLU
24	QY	25	LYS
24	QZ	7	GLU
24	QZ	21	LYS
24	QZ	22	ARG
24	QZ	36	ARG
24	QZ	63	GLU
25	R0	14	ARG
26	R1	57	GLU
27	R2	23	LYS
28	R3	30	ARG
29	R4	1	MET
29	R4	11	PRO
29	R4	13	ARG
29	R4	39	CYS
29	R4	42	PHE
29	R4	46	GLN
29	R4	48	ARG
29	R4	63	TYR
31	R6	10	LEU
31	R6	25	LYS
33	R8	35	GLN
33	R8	46	ARG
33	R8	52	LYS
33	R8	65	GLU
34	R9	9	ARG
37	RD	7	LYS
37	RD	24	ILE
37	RD	25	THR
37	RD	43	ARG
37	RD	273	ARG
38	RE	1	MET

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Mol	Chain	Res	Type
38	RE	59	VAL
38	RE	64	LYS
38	RE	79	ARG
38	RE	152	LYS
39	RF	99	TYR
40	RG	33	ARG
40	RG	55	LYS
40	RG	83	ARG
40	RG	115	ARG
40	RG	118	ARG
40	RG	146	TYR
41	RH	51	ARG
41	RH	69	ARG
41	RH	97	ARG
41	RH	152	ARG
41	RH	154	PRO
42	RI	85	GLU
42	RI	86	THR
42	RI	130	TYR
42	RI	136	VAL
42	RI	138	ILE
43	RN	12	ARG
43	RN	61	ARG
43	RN	115	ARG
44	RO	31	LYS
45	RP	29	LYS
45	RP	76	LYS
46	RQ	5	ARG
46	RQ	87	LYS
46	RQ	91	GLU
46	RQ	93	TYR
48	RS	20	ARG
48	RS	23	ARG
48	RS	76	LYS
48	RS	112	PHE
49	RT	95	ARG
49	RT	96	ARG
49	RT	101	PHE
49	RT	108	ARG
49	RT	109	GLU
49	RT	128	GLU
50	RU	90	VAL

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Mol	Chain	Res	Type
51	RV	19	LYS
51	RV	21	ARG
51	RV	39	LEU
51	RV	72	VAL
51	RV	79	VAL
51	RV	95	LEU
52	RW	18	ARG
52	RW	113	LYS
55	RZ	80	ARG
55	RZ	135	GLU
2	XB	17	PHE
2	XB	122	PHE
2	XB	236	TYR
3	XC	72	LYS
3	XC	85	ARG
3	XC	111	LEU
3	XC	132	ARG
4	XD	76	ARG
4	XD	118	ARG
5	XE	24	ARG
5	XE	43	LEU
5	XE	63	ARG
5	XE	155	GLU
7	XG	48	LYS
7	XG	57	GLU
7	XG	78	ARG
7	XG	94	ARG
7	XG	111	ARG
8	XH	60	ARG
9	XI	114	TYR
10	XJ	29	ARG
11	XK	96	ARG
12	XL	17	LYS
12	XL	98	TYR
13	XM	13	LYS
13	XM	36	LYS
13	XM	58	GLU
13	XM	102	ARG
15	XO	79	ARG
16	XP	26	ARG
16	XP	32	TYR
17	XQ	52	LYS

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Mol	Chain	Res	Type
17	XQ	92	ARG
18	XR	42	ARG
24	XZ	8	GLU
24	XZ	22	ARG
24	XZ	40	GLU
24	XZ	82	TYR
25	Y0	14	ARG
25	Y0	41	ARG
25	Y0	82	ARG
27	Y2	7	ARG
28	Y3	30	ARG
29	Y4	48	ARG
29	Y4	67	TYR
30	Y5	37	LYS
31	Y6	4	GLU
31	Y6	12	GLU
33	Y8	48	PHE
33	Y8	50	LEU
37	YD	63	ARG
37	YD	88	ARG
38	YE	73	GLU
39	YF	127	GLU
40	YG	18	GLU
40	YG	33	ARG
40	YG	51	ARG
40	YG	55	LYS
40	YG	72	ARG
41	YH	3	ARG
41	YH	13	LYS
42	YI	10	GLU
42	YI	11	ASN
42	YI	12	LEU
44	YO	64	ARG
44	YO	108	GLU
45	YP	108	LYS
47	YR	57	ARG
47	YR	88	ARG
48	YS	23	ARG
48	YS	106	ARG
48	YS	111	GLU
49	YT	96	ARG
49	YT	111	ARG

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Mol	Chain	Res	Type
49	YT	133	GLU
50	YU	44	ASN
51	YV	5	VAL
51	YV	18	LEU
52	YW	41	LYS
52	YW	60	ASN
53	YX	57	LEU
53	YX	68	ARG
54	YY	87	LYS
55	YZ	29	TYR
55	YZ	156	LYS
55	YZ	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	16	HIS
9	QI	3	GLN
37	RD	46	GLN
55	RZ	151	HIS
13	XM	101	GLN
40	YG	132	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	293 (19%)	33 (2%)
1	XA	1505/1521 (98%)	301 (20%)	40 (2%)
22	QV	77/77 (100%)	8 (10%)	1 (1%)
22	XV	77/77 (100%)	9 (11%)	1 (1%)
23	QX	16/20 (80%)	7 (43%)	2 (12%)
23	XX	16/20 (80%)	8 (50%)	0
35	RA	2888/2915 (99%)	623 (21%)	37 (1%)
35	YA	2875/2915 (98%)	578 (20%)	28 (0%)
36	RB	119/124 (95%)	24 (20%)	1 (0%)
36	YB	119/124 (95%)	17 (14%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9202/9320 (98%)	1868 (20%)	144 (1%)

All (1868) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	61	G
1	QA	66	G
1	QA	79	G
1	QA	80	G
1	QA	89	U
1	QA	90	C
1	QA	92	G
1	QA	93	U
1	QA	101	A
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	131	C
1	QA	182	U
1	QA	185	A
1	QA	188	U
1	QA	189	U
1	QA	190	G
1	QA	191(A)	G
1	QA	191(D)	U
1	QA	191(E)	G
1	QA	195	A
1	QA	197	A
1	QA	198	G
1	QA	208	U
1	QA	209	U
1	QA	210	U
1	QA	220	G
1	QA	247	G
1	QA	251	G
1	QA	266	G
1	QA	267	C

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Mol	Chain	Res	Type
1	QA	270	A
1	QA	275	G
1	QA	281	G
1	QA	289	G
1	QA	321	A
1	QA	328	C
1	QA	332	G
1	QA	345	C
1	QA	346	G
1	QA	347	G
1	QA	350	G
1	QA	351	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	373	A
1	QA	384	G
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	412	A
1	QA	414	A
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	439	A
1	QA	452	A
1	QA	465	A
1	QA	466	C
1	QA	467	G
1	QA	478	A
1	QA	482	A
1	QA	484	G
1	QA	485	G
1	QA	494	U
1	QA	497	U
1	QA	505	G
1	QA	511	C

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Mol	Chain	Res	Type
1	QA	518	C
1	QA	519	C
1	QA	521	G
1	QA	527	G
1	QA	530	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	545	C
1	QA	547	A
1	QA	548	G
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	596	C
1	QA	607	A
1	QA	618	C
1	QA	630	G
1	QA	642	A
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	721	G
1	QA	722	A
1	QA	723	U
1	QA	724	G
1	QA	731	G
1	QA	749	C
1	QA	755	G
1	QA	760	G
1	QA	774	G
1	QA	777	A
1	QA	786	G

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Mol	Chain	Res	Type
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	816	A
1	QA	817	C
1	QA	818	G
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	872	A
1	QA	884	U
1	QA	914	A
1	QA	916	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	942	G
1	QA	960	U
1	QA	961	U
1	QA	966	G
1	QA	968	A
1	QA	969	A
1	QA	972	C
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	980	C
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	999	U
1	QA	1000	A
1	QA	1001	G

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Mol	Chain	Res	Type
1	QA	1003	G
1	QA	1004	A
1	QA	1005	A
1	QA	1006	C
1	QA	1007	C
1	QA	1008	C
1	QA	1009	G
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032	A
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1036	G
1	QA	1039	C
1	QA	1046	A
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1068	G
1	QA	1070	U
1	QA	1081	G
1	QA	1086	U
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1117	G
1	QA	1118	C
1	QA	1124	G
1	QA	1125	U
1	QA	1127	G
1	QA	1129	C
1	QA	1130	A
1	QA	1131	G

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Mol	Chain	Res	Type
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1140	C
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1171	G
1	QA	1177	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1187	G
1	QA	1196	U
1	QA	1212	U
1	QA	1213	A
1	QA	1227	A
1	QA	1233	G
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1268	A
1	QA	1270	C
1	QA	1273	G
1	QA	1278	U
1	QA	1280	A
1	QA	1281	U
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1288	A
1	QA	1300	G
1	QA	1303	C
1	QA	1305	G
1	QA	1318	A

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Mol	Chain	Res	Type
1	QA	1319	A
1	QA	1320	C
1	QA	1323	G
1	QA	1331	G
1	QA	1335	C
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1368	G
1	QA	1370	G
1	QA	1398	A
1	QA	1406	U
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1450	U
1	QA	1451	A
1	QA	1452	C
1	QA	1453	G
1	QA	1454	G
1	QA	1492	A
1	QA	1493	A
1	QA	1497	G
1	QA	1499	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
1	QA	1532	U
1	QA	1533	C
1	QA	1534	A
1	QA	1536	C
1	QA	1537	U
1	QA	1538	C
1	QA	1539	C
1	QA	1540	U
1	QA	1541	U
22	QV	2	G

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Mol	Chain	Res	Type
22	QV	20	U
22	QV	21	A
22	QV	22	G
22	QV	46	G
22	QV	47	U
22	QV	49	G
22	QV	76	A
23	QX	8	A
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	U
35	RA	9	U
35	RA	15	G
35	RA	27	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	60	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	91	A
35	RA	95	G
35	RA	99	U
35	RA	101	G
35	RA	102	G
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	125	G
35	RA	129	C
35	RA	139	G
35	RA	140	A
35	RA	144	C
35	RA	155	C
35	RA	172	C

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Mol	Chain	Res	Type
35	RA	173	G
35	RA	174	C
35	RA	175	G
35	RA	181	A
35	RA	182	A
35	RA	196	A
35	RA	199	A
35	RA	204	A
35	RA	205	G
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	228	A
35	RA	229	A
35	RA	233	A
35	RA	245	G
35	RA	248	G
35	RA	252	G
35	RA	265	A
35	RA	266	G
35	RA	270(B)	A
35	RA	270(J)	G
35	RA	270(K)	C
35	RA	270(L)	U
35	RA	270(M)	U
35	RA	270(N)	G
35	RA	270(O)	U
35	RA	270(P)	C
35	RA	270(Q)	C
35	RA	270(Z)	U
35	RA	271(C)	U
35	RA	271	G
35	RA	273(D)	C
35	RA	274	G
35	RA	275	G
35	RA	278	A
35	RA	283	A
35	RA	289	A
35	RA	311	A
35	RA	316	C
35	RA	324	A

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Mol	Chain	Res	Type
35	RA	329	G
35	RA	330	A
35	RA	332	A
35	RA	345	A
35	RA	353	G
35	RA	355	G
35	RA	358	U
35	RA	362	U
35	RA	363	G
35	RA	363(D)	G
35	RA	371	A
35	RA	372	G
35	RA	373	U
35	RA	386	G
35	RA	388	G
35	RA	396	G
35	RA	405	U
35	RA	406	G
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	443	A
35	RA	444	C
35	RA	448	U
35	RA	451	C
35	RA	456	C
35	RA	457	A
35	RA	467	G
35	RA	470	A
35	RA	481	G
35	RA	494	G
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	512	G
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	549	G

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Mol	Chain	Res	Type
35	RA	563	G
35	RA	573	G
35	RA	575	A
35	RA	587	C
35	RA	588	U
35	RA	603	A
35	RA	607	U
35	RA	613	U
35	RA	614	U
35	RA	615	G
35	RA	617	G
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	645	C
35	RA	646	A
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G
35	RA	654(B)	C
35	RA	654(G)	C
35	RA	654(Q)	C
35	RA	654(R)	C
35	RA	654(S)	G
35	RA	654(T)	C
35	RA	686	G
35	RA	708	C
35	RA	717	G
35	RA	722	A
35	RA	730	C
35	RA	753	C
35	RA	765	G
35	RA	775	G
35	RA	776	G
35	RA	782	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	789	A
35	RA	792	G
35	RA	793	A

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Mol	Chain	Res	Type
35	RA	805	G
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	830	G
35	RA	831	G
35	RA	845	G
35	RA	846	C
35	RA	854	G
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	866	A
35	RA	872	A
35	RA	878	A
35	RA	882	G
35	RA	883	G
35	RA	884	C
35	RA	886	C
35	RA	888	C
35	RA	889	C
35	RA	890	A
35	RA	894	C
35	RA	895	U
35	RA	896	A
35	RA	897	C
35	RA	899	A
35	RA	900	A
35	RA	910	A
35	RA	915	C
35	RA	917	A
35	RA	919	G
35	RA	928	G
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	957	A
35	RA	959	A

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Mol	Chain	Res	Type
35	RA	961	C
35	RA	968	G
35	RA	973	A
35	RA	974	G
35	RA	983	A
35	RA	990	A
35	RA	991	C
35	RA	996	A
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1017	G
35	RA	1022	G
35	RA	1023	U
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1034	G
35	RA	1044	G
35	RA	1046	A
35	RA	1047	G
35	RA	1049	C
35	RA	1053	C
35	RA	1061	U
35	RA	1065	U
35	RA	1067	A
35	RA	1070	A
35	RA	1071	G
35	RA	1073	A
35	RA	1075	C
35	RA	1083	U
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1089	G
35	RA	1095	A
35	RA	1096	A
35	RA	1111	A
35	RA	1130	U
35	RA	1131	G
35	RA	1135	C

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Mol	Chain	Res	Type
35	RA	1136	G
35	RA	1139	G
35	RA	1141	U
35	RA	1142(A)	A
35	RA	1143	A
35	RA	1148	A
35	RA	1155	A
35	RA	1156	A
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1177	A
35	RA	1178	C
35	RA	1180	C
35	RA	1195	G
35	RA	1203	G
35	RA	1204	A
35	RA	1205	U
35	RA	1210	A
35	RA	1212	G
35	RA	1220	A
35	RA	1221	C
35	RA	1224	G
35	RA	1236	G
35	RA	1247	A
35	RA	1250	G
35	RA	1252	G
35	RA	1253	A
35	RA	1255	U
35	RA	1256	G
35	RA	1265	A
35	RA	1272	A
35	RA	1275	A
35	RA	1281	G
35	RA	1286	A
35	RA	1300	U
35	RA	1301	A
35	RA	1308	A
35	RA	1311	G
35	RA	1314	C
35	RA	1319	G

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Mol	Chain	Res	Type
35	RA	1329	U
35	RA	1341	U
35	RA	1352	U
35	RA	1359	A
35	RA	1365	A
35	RA	1368	G
35	RA	1378	A
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1385	G
35	RA	1391	U
35	RA	1395	A
35	RA	1407	C
35	RA	1408	C
35	RA	1416	G
35	RA	1417	C
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1437	C
35	RA	1444(A)	A
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1453	A
35	RA	1455	G
35	RA	1458	C
35	RA	1461	G
35	RA	1466	G
35	RA	1467	C
35	RA	1471	A
35	RA	1475	G
35	RA	1476	C
35	RA	1478	G
35	RA	1482	U
35	RA	1483	G
35	RA	1487	G
35	RA	1488	G
35	RA	1490	A
35	RA	1493	C
35	RA	1497	U

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Mol	Chain	Res	Type
35	RA	1505	C
35	RA	1509	C
35	RA	1510	A
35	RA	1521	G
35	RA	1523	U
35	RA	1526	G
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1538	G
35	RA	1540	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1547	C
35	RA	1554	A
35	RA	1558	A
35	RA	1559	G
35	RA	1560	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1580	A
35	RA	1585	C
35	RA	1586	A
35	RA	1587	A
35	RA	1592	C
35	RA	1598	C
35	RA	1603	A
35	RA	1608	A
35	RA	1640	C
35	RA	1648	C
35	RA	1651	G
35	RA	1654	A
35	RA	1674	G
35	RA	1688	U
35	RA	1695	G
35	RA	1696	G
35	RA	1698	A
35	RA	1699	G
35	RA	1700	A
35	RA	1725	G

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Mol	Chain	Res	Type
35	RA	1728	G
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1743	G
35	RA	1756	G
35	RA	1762	A
35	RA	1763	G
35	RA	1764	G
35	RA	1769	G
35	RA	1773	A
35	RA	1776	G
35	RA	1780	A
35	RA	1782	C
35	RA	1791	A
35	RA	1800	C
35	RA	1801	G
35	RA	1802	A
35	RA	1811	G
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1847	A
35	RA	1853	A
35	RA	1858	G
35	RA	1864	U
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1881	C
35	RA	1882	C
35	RA	1888	G
35	RA	1889	A
35	RA	1903	G
35	RA	1906	G
35	RA	1913	A
35	RA	1927	A
35	RA	1929	G
35	RA	1930	G
35	RA	1931	U
35	RA	1936	A

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Mol	Chain	Res	Type
35	RA	1938	A
35	RA	1941	C
35	RA	1948	G
35	RA	1955	U
35	RA	1963	U
35	RA	1965	C
35	RA	1966	A
35	RA	1967	C
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1980	G
35	RA	1982	C
35	RA	1992	G
35	RA	1993	U
35	RA	1996	C
35	RA	2004	G
35	RA	2020	A
35	RA	2021	C
35	RA	2022	U
35	RA	2023	G
35	RA	2026	C
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2034	U
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2063	C
35	RA	2069	G
35	RA	2092	U
35	RA	2093	G
35	RA	2111	C
35	RA	2112	G
35	RA	2113	U
35	RA	2116	G

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Mol	Chain	Res	Type
35	RA	2117	A
35	RA	2119	A
35	RA	2127	G
35	RA	2128	C
35	RA	2130	U
35	RA	2131	G
35	RA	2132	U
35	RA	2134	A
35	RA	2136	C
35	RA	2139	C
35	RA	2145	C
35	RA	2147	G
35	RA	2148	G
35	RA	2153	G
35	RA	2161	C
35	RA	2165	G
35	RA	2167	U
35	RA	2168	G
35	RA	2169	A
35	RA	2170	A
35	RA	2171	A
35	RA	2173	A
35	RA	2178	C
35	RA	2189	U
35	RA	2190	G
35	RA	2192	G
35	RA	2198	A
35	RA	2210	G
35	RA	2212	A
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2226	C
35	RA	2238	G
35	RA	2239	G
35	RA	2243	U
35	RA	2246	G
35	RA	2275	C
35	RA	2278	A
35	RA	2279	G
35	RA	2280	G
35	RA	2282	G

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Mol	Chain	Res	Type
35	RA	2283	C
35	RA	2302	G
35	RA	2305	A
35	RA	2306	C
35	RA	2307	G
35	RA	2308	G
35	RA	2309	A
35	RA	2311	A
35	RA	2312	U
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2343	C
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2358	G
35	RA	2372	G
35	RA	2382	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2394	C
35	RA	2402	C
35	RA	2403	C
35	RA	2406	U
35	RA	2410	G
35	RA	2411	A
35	RA	2422	A
35	RA	2423	U
35	RA	2425	A
35	RA	2428	G
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
35	RA	2448	A

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Mol	Chain	Res	Type
35	RA	2450	A
35	RA	2469	A
35	RA	2471	C
35	RA	2472	G
35	RA	2475	C
35	RA	2476	A
35	RA	2482	G
35	RA	2491	U
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2519	U
35	RA	2524	G
35	RA	2527	C
35	RA	2529	G
35	RA	2535	G
35	RA	2540	C
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2566	A
35	RA	2567	G
35	RA	2569	G
35	RA	2572	A
35	RA	2573	C
35	RA	2578	G
35	RA	2585	U
35	RA	2602	A
35	RA	2609	U
35	RA	2610	C
35	RA	2612	C
35	RA	2615	U
35	RA	2629	A
35	RA	2630	G
35	RA	2646	C
35	RA	2654	A
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2682	U
35	RA	2689	U
35	RA	2690	C

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Mol	Chain	Res	Type
35	RA	2702	U
35	RA	2703	C
35	RA	2712	U
35	RA	2712(A)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2726	U
35	RA	2733	A
35	RA	2744	G
35	RA	2748	A
35	RA	2752	C
35	RA	2757	A
35	RA	2758	A
35	RA	2761	G
35	RA	2762	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	2787	C
35	RA	2790	A
35	RA	2797	U
35	RA	2799	A
35	RA	2807	G
35	RA	2808	U
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2827	C
35	RA	2830	G
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2846	G
35	RA	2850	A
35	RA	2860	A
35	RA	2867	G
35	RA	2868	A
35	RA	2872	G

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Mol	Chain	Res	Type
35	RA	2873	A
35	RA	2876	G
35	RA	2877	G
35	RA	2879	C
35	RA	2880	C
35	RA	2892	A
35	RA	2893	G
36	RB	2	C
36	RB	8	U
36	RB	13	A
36	RB	15	A
36	RB	19	G
36	RB	25	A
36	RB	27	C
36	RB	40	U
36	RB	41	U
36	RB	42	C
36	RB	45	A
36	RB	47	C
36	RB	53	A
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	88	C
36	RB	89	G
36	RB	92	G
36	RB	105	G
36	RB	108	C
36	RB	109	G
36	RB	117	G
36	RB	119	A
1	XA	5	U
1	XA	6	G
1	XA	9	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	64	G
1	XA	65	U

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Mol	Chain	Res	Type
1	XA	66	G
1	XA	75	C
1	XA	76	G
1	XA	79	G
1	XA	91	C
1	XA	93	U
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	120	A
1	XA	121	C
1	XA	129(A)	G
1	XA	144	G
1	XA	146	G
1	XA	163	C
1	XA	169	C
1	XA	182	U
1	XA	184	G
1	XA	185	A
1	XA	186(F)	C
1	XA	188	U
1	XA	189	U
1	XA	191(A)	G
1	XA	191(D)	U
1	XA	195	A
1	XA	197	A
1	XA	198	G
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	244	U
1	XA	247	G
1	XA	251	G
1	XA	266	G
1	XA	267	C
1	XA	270	A
1	XA	275	G
1	XA	279	A
1	XA	280	C
1	XA	281	G
1	XA	289	G

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Mol	Chain	Res	Type
1	XA	298	A
1	XA	316	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	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	367	U
1	XA	368	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
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	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	442	C
1	XA	467	G
1	XA	477	G
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	492	G
1	XA	496	A
1	XA	497	U
1	XA	505	G
1	XA	511	C
1	XA	518	C
1	XA	521	G

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Mol	Chain	Res	Type
1	XA	527	G
1	XA	530	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G
1	XA	595	G
1	XA	596	C
1	XA	630	G
1	XA	653	A
1	XA	665	A
1	XA	666	G
1	XA	688	G
1	XA	701	C
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	749	C
1	XA	755	G
1	XA	760	G
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	812	C
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	819	A
1	XA	821	G
1	XA	828	A
1	XA	836	G

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Mol	Chain	Res	Type
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	870	U
1	XA	914	A
1	XA	922	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	960	U
1	XA	961	U
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	976	G
1	XA	977	A
1	XA	980	C
1	XA	989	C
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	999	U
1	XA	1000	A
1	XA	1001	G
1	XA	1002	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1007	C
1	XA	1008	C
1	XA	1009	G
1	XA	1010	G
1	XA	1020	U
1	XA	1024	G
1	XA	1028(A)	C
1	XA	1029	G
1	XA	1031	G

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Mol	Chain	Res	Type
1	XA	1032(A)	G
1	XA	1033	G
1	XA	1034	G
1	XA	1036	G
1	XA	1038	C
1	XA	1039	C
1	XA	1042	G
1	XA	1046	A
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1064	G
1	XA	1065	U
1	XA	1066	C
1	XA	1068	G
1	XA	1070	U
1	XA	1081	G
1	XA	1094	G
1	XA	1101	A
1	XA	1108	G
1	XA	1117	G
1	XA	1118	C
1	XA	1124	G
1	XA	1125	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1146	A
1	XA	1147	C
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G

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Mol	Chain	Res	Type
1	XA	1181	G
1	XA	1183	A
1	XA	1184	G
1	XA	1191	A
1	XA	1196	U
1	XA	1212	U
1	XA	1213	A
1	XA	1214	C
1	XA	1225	A
1	XA	1226	C
1	XA	1227	A
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1255	G
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1278	U
1	XA	1280	A
1	XA	1281	U
1	XA	1285	A
1	XA	1286	A
1	XA	1287	A
1	XA	1288	A
1	XA	1300	G
1	XA	1301	U
1	XA	1303	C
1	XA	1305	G
1	XA	1306	A
1	XA	1319	A
1	XA	1320	C
1	XA	1323	G
1	XA	1331	G
1	XA	1345	U
1	XA	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A

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Mol	Chain	Res	Type
1	XA	1370	G
1	XA	1381	U
1	XA	1394	A
1	XA	1397	C
1	XA	1398	A
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	A
1	XA	1450	U
1	XA	1451	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1497	G
1	XA	1499	A
1	XA	1504	G
1	XA	1505	G
1	XA	1506	U
1	XA	1507	A
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
1	XA	1532	U
1	XA	1533	C
1	XA	1534	A
1	XA	1535	C
1	XA	1536	C
1	XA	1537	U
1	XA	1538	C
1	XA	1540	U
1	XA	1541	U
22	XV	2	G
22	XV	18	G
22	XV	20	U
22	XV	21	A

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Mol	Chain	Res	Type
22	XV	22	G
22	XV	42	G
22	XV	47	U
22	XV	49	G
22	XV	76	A
23	XX	5	A
23	XX	8	A
23	XX	10	G
23	XX	11	U
23	XX	12	A
23	XX	13	A
23	XX	14	A
23	XX	19	U
35	YA	9	U
35	YA	27	G
35	YA	34	C
35	YA	46	C
35	YA	55	G
35	YA	64	A
35	YA	69	C
35	YA	71	A
35	YA	74	A
35	YA	75	G
35	YA	83	G
35	YA	85	G
35	YA	102	G
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	123	G
35	YA	125	G
35	YA	138	G
35	YA	140	A
35	YA	149	A
35	YA	154	G
35	YA	155	C
35	YA	156	U
35	YA	157	U
35	YA	175	G
35	YA	196	A
35	YA	199	A
35	YA	204	A

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Mol	Chain	Res	Type
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	229	A
35	YA	233	A
35	YA	241	A
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	261	G
35	YA	265	A
35	YA	266	G
35	YA	267	C
35	YA	270(B)	A
35	YA	270(C)	C
35	YA	270(J)	G
35	YA	270(K)	C
35	YA	270(N)	G
35	YA	270(O)	U
35	YA	270(Z)	U
35	YA	271(C)	U
35	YA	271	G
35	YA	274	G
35	YA	275	G
35	YA	278	A
35	YA	279	C
35	YA	283	A
35	YA	287	C
35	YA	289	A
35	YA	290	G
35	YA	311	A
35	YA	317	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	332	A
35	YA	352	G
35	YA	356	G
35	YA	363	G
35	YA	363(A)	A
35	YA	363(E)	U

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Mol	Chain	Res	Type
35	YA	363(F)	A
35	YA	372	G
35	YA	373	U
35	YA	380	U
35	YA	386	G
35	YA	395	U
35	YA	405	U
35	YA	406	G
35	YA	411	G
35	YA	412	A
35	YA	428	A
35	YA	444	C
35	YA	448	U
35	YA	454	A
35	YA	456	C
35	YA	457	A
35	YA	470	A
35	YA	481	G
35	YA	494	G
35	YA	501	A
35	YA	504	U
35	YA	505	A
35	YA	508	G
35	YA	509	C
35	YA	512	G
35	YA	525	U
35	YA	526	A
35	YA	529	A
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	562	U
35	YA	563	G
35	YA	571	A
35	YA	573	G
35	YA	575	A
35	YA	588	U
35	YA	603	A
35	YA	604	G
35	YA	607	U
35	YA	613	U
35	YA	614	U

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Mol	Chain	Res	Type
35	YA	615	G
35	YA	617	G
35	YA	622	G
35	YA	624	C
35	YA	627	A
35	YA	637	A
35	YA	645	C
35	YA	646	A
35	YA	666	G
35	YA	668	G
35	YA	669	G
35	YA	670	A
35	YA	686	G
35	YA	717	G
35	YA	722	A
35	YA	730	C
35	YA	753	C
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	792	G
35	YA	793	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	832	G
35	YA	856	C
35	YA	857	C
35	YA	859	G
35	YA	869	G
35	YA	882	G
35	YA	883	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

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Mol	Chain	Res	Type
35	YA	894	C
35	YA	896	A
35	YA	897	C
35	YA	906	G
35	YA	910	A
35	YA	915	C
35	YA	917	A
35	YA	919	G
35	YA	928	G
35	YA	932	G
35	YA	938	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	975	G
35	YA	980	A
35	YA	983	A
35	YA	990	A
35	YA	991	C
35	YA	996	A
35	YA	999	U
35	YA	1000	A
35	YA	1005	C
35	YA	1012	U
35	YA	1013	C
35	YA	1017	G
35	YA	1020	A
35	YA	1022	G
35	YA	1023	U
35	YA	1024	G
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1044	G
35	YA	1046	A
35	YA	1047	G
35	YA	1048	A

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Mol	Chain	Res	Type
35	YA	1060	U
35	YA	1061	U
35	YA	1064	C
35	YA	1066	U
35	YA	1070	A
35	YA	1073	A
35	YA	1083	U
35	YA	1085	A
35	YA	1086	A
35	YA	1087	G
35	YA	1088	A
35	YA	1089	G
35	YA	1093	G
35	YA	1094	U
35	YA	1095	A
35	YA	1096	A
35	YA	1099	G
35	YA	1122	G
35	YA	1126	A
35	YA	1128	A
35	YA	1130	U
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1141	U
35	YA	1142(A)	A
35	YA	1148	A
35	YA	1156	A
35	YA	1170	G
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1177	A
35	YA	1178	C
35	YA	1179	C
35	YA	1180	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1212	G
35	YA	1220	A

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Mol	Chain	Res	Type
35	YA	1236	G
35	YA	1247	A
35	YA	1248	G
35	YA	1252	G
35	YA	1253	A
35	YA	1255	U
35	YA	1256	G
35	YA	1265	A
35	YA	1272	A
35	YA	1281	G
35	YA	1294	U
35	YA	1300	U
35	YA	1301	A
35	YA	1308	A
35	YA	1311	G
35	YA	1314	C
35	YA	1329	U
35	YA	1330	C
35	YA	1352	U
35	YA	1359	A
35	YA	1360	A
35	YA	1368	G
35	YA	1370	C
35	YA	1378	A
35	YA	1379	A
35	YA	1380	G
35	YA	1384	A
35	YA	1385	G
35	YA	1391	U
35	YA	1395	A
35	YA	1406	U
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1428	C
35	YA	1437	C
35	YA	1444(A)	A
35	YA	1445	C
35	YA	1449	A
35	YA	1449(A)	G
35	YA	1455	G

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Mol	Chain	Res	Type
35	YA	1459	G
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1475	G
35	YA	1480	G
35	YA	1482	U
35	YA	1483	G
35	YA	1488	G
35	YA	1490	A
35	YA	1493	C
35	YA	1509	C
35	YA	1510	A
35	YA	1516	U
35	YA	1522	G
35	YA	1523	U
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	1547	C
35	YA	1554	A
35	YA	1558	A
35	YA	1559	G
35	YA	1560	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1580	A
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1608	A
35	YA	1613	G
35	YA	1618	A
35	YA	1634	A
35	YA	1640	C

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Mol	Chain	Res	Type
35	YA	1648	C
35	YA	1654	A
35	YA	1667	G
35	YA	1674	G
35	YA	1696	G
35	YA	1700	A
35	YA	1703	G
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1743	G
35	YA	1753	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	1774	C
35	YA	1780	A
35	YA	1782	C
35	YA	1791	A
35	YA	1800	C
35	YA	1801	G
35	YA	1802	A
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	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1903	G
35	YA	1906	G
35	YA	1910	G
35	YA	1913	A

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Mol	Chain	Res	Type
35	YA	1929	G
35	YA	1930	G
35	YA	1936	A
35	YA	1938	A
35	YA	1955	U
35	YA	1963	U
35	YA	1964	G
35	YA	1966	A
35	YA	1967	C
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1980	G
35	YA	1982	C
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A
35	YA	2021	C
35	YA	2023	G
35	YA	2027	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2043	C
35	YA	2052	G
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	2093	G
35	YA	2099	U
35	YA	2111	C
35	YA	2112	G
35	YA	2113	U
35	YA	2114	A
35	YA	2116	G
35	YA	2117	A
35	YA	2119	A
35	YA	2120	G

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Mol	Chain	Res	Type
35	YA	2123	G
35	YA	2126	A
35	YA	2128	C
35	YA	2130	U
35	YA	2131	G
35	YA	2132	U
35	YA	2134	A
35	YA	2140	C
35	YA	2145	C
35	YA	2147	G
35	YA	2148	G
35	YA	2157	G
35	YA	2161	C
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2170	A
35	YA	2171	A
35	YA	2173	A
35	YA	2174	C
35	YA	2177	C
35	YA	2189	U
35	YA	2190	G
35	YA	2191	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2215	G
35	YA	2225	A
35	YA	2226	C
35	YA	2238	G
35	YA	2239	G
35	YA	2266	A
35	YA	2275	C
35	YA	2278	A
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2305	A
35	YA	2306	C

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Mol	Chain	Res	Type
35	YA	2307	G
35	YA	2308	G
35	YA	2309	A
35	YA	2312	U
35	YA	2316	C
35	YA	2318	G
35	YA	2320	A
35	YA	2325	G
35	YA	2334	G
35	YA	2335	A
35	YA	2336	A
35	YA	2343	C
35	YA	2346	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2358	G
35	YA	2383	G
35	YA	2385	C
35	YA	2392	A
35	YA	2402	C
35	YA	2403	C
35	YA	2406	U
35	YA	2410	G
35	YA	2422	A
35	YA	2423	U
35	YA	2424	C
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	2448	A
35	YA	2450	A
35	YA	2469	A
35	YA	2472	G
35	YA	2474	C
35	YA	2475	C
35	YA	2476	A
35	YA	2478	A

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Mol	Chain	Res	Type
35	YA	2484	G
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	2529	G
35	YA	2535	G
35	YA	2542	A
35	YA	2543	G
35	YA	2554	U
35	YA	2566	A
35	YA	2567	G
35	YA	2572	A
35	YA	2573	C
35	YA	2578	G
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2629	A
35	YA	2630	G
35	YA	2645	G
35	YA	2646	C
35	YA	2655	G
35	YA	2665	A
35	YA	2673	G
35	YA	2682	U
35	YA	2686	G
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2703	C
35	YA	2712	U
35	YA	2713	A
35	YA	2714	G
35	YA	2724	C
35	YA	2725	A
35	YA	2726	U
35	YA	2732	G

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Mol	Chain	Res	Type
35	YA	2733	A
35	YA	2734	A
35	YA	2739	U
35	YA	2744	G
35	YA	2748	A
35	YA	2751	G
35	YA	2752	C
35	YA	2754	U
35	YA	2757	A
35	YA	2762	G
35	YA	2764	A
35	YA	2766	G
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	2792	G
35	YA	2807	G
35	YA	2808	U
35	YA	2811	G
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2823	A
35	YA	2830	G
35	YA	2832	U
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A
35	YA	2846	G
35	YA	2848	G
35	YA	2849	U
35	YA	2850	A
35	YA	2860	A
35	YA	2872	G
35	YA	2873	A
35	YA	2879	C
35	YA	2880	C
35	YA	2892	A
35	YA	2893	G

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Mol	Chain	Res	Type
35	YA	2894	G
35	YA	2896	C
35	YA	2897	U
36	YB	8	U
36	YB	13	A
36	YB	14	U
36	YB	15	A
36	YB	16	G
36	YB	25	A
36	YB	42	C
36	YB	44	G
36	YB	45	A
36	YB	57	A
36	YB	67	G
36	YB	73	A
36	YB	81	G
36	YB	88	C
36	YB	109	G
36	YB	112	G
36	YB	119	A

All (144) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	31	G
1	QA	60	A
1	QA	115	G
1	QA	181	G
1	QA	190	G
1	QA	197	A
1	QA	201	C
1	QA	208	U
1	QA	250	A
1	QA	428	G
1	QA	484	G
1	QA	496	A
1	QA	518	C
1	QA	547	A
1	QA	687	A
1	QA	748	C
1	QA	792	A

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Mol	Chain	Res	Type
1	QA	812	C
1	QA	841	U
1	QA	913	A
1	QA	960	U
1	QA	992	U
1	QA	1038	C
1	QA	1065	U
1	QA	1067	A
1	QA	1137	C
1	QA	1182	G
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
1	QA	1532	U
22	QV	1	C
23	QX	9	G
23	QX	11	U
35	RA	90	U
35	RA	119	A
35	RA	128	C
35	RA	227	A
35	RA	372	G
35	RA	387	U
35	RA	404	C
35	RA	587	C
35	RA	752	A
35	RA	845	G
35	RA	856	C
35	RA	877	U
35	RA	1022	G
35	RA	1085	A
35	RA	1171	G
35	RA	1204	A
35	RA	1300	U
35	RA	1427	A
35	RA	1558	A
35	RA	1559	G
35	RA	1653	G
35	RA	1694	C
35	RA	1699	G
35	RA	1819	A

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Mol	Chain	Res	Type
35	RA	1930	G
35	RA	1992	G
35	RA	2092	U
35	RA	2144	U
35	RA	2191	G
35	RA	2211	G
35	RA	2439	A
35	RA	2447	G
35	RA	2481	G
35	RA	2689	U
35	RA	2776	A
35	RA	2849	U
35	RA	2859	G
36	RB	66	A
1	XA	5	U
1	XA	60	A
1	XA	92	G
1	XA	115	G
1	XA	181	G
1	XA	197	A
1	XA	201	C
1	XA	243	A
1	XA	250	A
1	XA	279	A
1	XA	315	A
1	XA	328	C
1	XA	428	G
1	XA	547	A
1	XA	595	G
1	XA	687	A
1	XA	703	G
1	XA	748	C
1	XA	792	A
1	XA	812	C
1	XA	913	A
1	XA	960	U
1	XA	992	U
1	XA	1000	A
1	XA	1004	A
1	XA	1033	G
1	XA	1038	C
1	XA	1054	C

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Mol	Chain	Res	Type
1	XA	1065	U
1	XA	1067	A
1	XA	1124	G
1	XA	1137	C
1	XA	1139	G
1	XA	1157	A
1	XA	1182	G
1	XA	1190	G
1	XA	1300	G
1	XA	1305	G
1	XA	1498	U
1	XA	1532	U
22	XV	1	C
35	YA	119	A
35	YA	372	G
35	YA	587	C
35	YA	603	A
35	YA	752	A
35	YA	827	U
35	YA	856	C
35	YA	1022	G
35	YA	1171	G
35	YA	1379	A
35	YA	1427	A
35	YA	1558	A
35	YA	1559	G
35	YA	1653	G
35	YA	1819	A
35	YA	2144	U
35	YA	2166	G
35	YA	2191	G
35	YA	2211	G
35	YA	2225	A
35	YA	2439	A
35	YA	2447	G
35	YA	2610	C
35	YA	2689	U
35	YA	2776	A
35	YA	2848	G
35	YA	2849	U
35	YA	2859	G
36	YB	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	A3P	QX	20	23	23,28,29	5.26	7 (30%)	23,42,45	1.49	4 (17%)
56	PPU	ZA	3	35,56	32,40,41	0.90	0	33,57,60	1.80	7 (21%)
56	PPU	ZB	3	35,56	32,40,41	0.85	2 (6%)	33,57,60	1.87	10 (30%)
23	A3P	XX	20	23	23,28,29	5.22	7 (30%)	23,42,45	1.53	3 (13%)

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
23	A3P	QX	20	23	-	2/8/30/31	0/3/3/3
56	PPU	ZA	3	35,56	-	6/21/43/44	0/4/4/4
56	PPU	ZB	3	35,56	-	14/21/43/44	0/4/4/4
23	A3P	XX	20	23	-	1/8/30/31	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	O4'-C1'	18.93	1.67	1.41
23	XX	20	A3P	O4'-C1'	18.45	1.66	1.41
23	XX	20	A3P	C2'-C1'	-13.73	1.32	1.53
23	QX	20	A3P	C2'-C1'	-13.44	1.33	1.53
23	XX	20	A3P	O4'-C4'	-5.92	1.31	1.45
23	QX	20	A3P	O4'-C4'	-5.91	1.31	1.45
23	QX	20	A3P	P1-O3'	4.79	1.68	1.59
23	XX	20	A3P	P1-O3'	4.10	1.67	1.59
23	XX	20	A3P	O3'-C3'	-3.45	1.31	1.44
23	QX	20	A3P	O3'-C3'	-3.23	1.32	1.44
23	XX	20	A3P	C6-N6	3.22	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	C6-N6	2.85	1.44	1.34
23	XX	20	A3P	C3'-C4'	2.15	1.58	1.52
56	ZB	3	PPU	C2'-C1'	-2.05	1.50	1.53
23	QX	20	A3P	C2'-C3'	2.03	1.57	1.52
56	ZB	3	PPU	C5-C4	2.03	1.46	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	XX	20	A3P	N3-C2-N1	-4.92	120.98	128.68
56	ZA	3	PPU	N1-C6-N6	4.77	122.08	117.06
56	ZB	3	PPU	CG-CB-CA	-4.38	105.02	114.13
23	QX	20	A3P	N3-C2-N1	-4.07	122.32	128.68
56	ZB	3	PPU	N1-C6-N6	3.96	121.22	117.06
56	ZA	3	PPU	C3'-N3'-C	-3.92	117.30	123.21
56	ZA	3	PPU	C9-N6-C6	-3.78	108.08	119.51
56	ZA	3	PPU	CA-C-N3'	3.69	121.27	116.15
56	ZB	3	PPU	C10-N6-C6	-3.49	108.95	119.51
56	ZB	3	PPU	C9-N6-C6	-3.46	109.03	119.51
23	XX	20	A3P	C3'-C2'-C1'	3.24	107.07	99.89
56	ZA	3	PPU	C10-N6-C6	-3.06	110.24	119.51
56	ZA	3	PPU	N3-C2-N1	-3.04	123.92	128.68
23	XX	20	A3P	C4-C5-N7	-2.99	106.28	109.40
56	ZB	3	PPU	N3-C2-N1	-2.96	124.05	128.68
56	ZB	3	PPU	C4-C5-N7	-2.82	106.46	109.40
23	QX	20	A3P	C4-C5-N7	-2.79	106.49	109.40
23	QX	20	A3P	C3'-C2'-C1'	2.67	105.80	99.89
56	ZB	3	PPU	CB-CA-C	2.61	115.07	108.97
56	ZB	3	PPU	CA-C-N3'	-2.58	112.57	116.15
23	QX	20	A3P	C2'-C3'-C4'	2.43	107.53	103.22
56	ZB	3	PPU	C3'-N3'-C	2.39	126.82	123.21
56	ZB	3	PPU	C10-N6-C9	-2.36	108.53	116.12
56	ZA	3	PPU	C4-C5-N7	-2.26	107.04	109.40

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	XX	20	A3P	C3'-O3'-P1-O1P
56	ZA	3	PPU	N-CA-CB-CG
56	ZA	3	PPU	C-CA-CB-CG
56	ZA	3	PPU	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
56	ZB	3	PPU	N3'-C-CA-N
56	ZB	3	PPU	O-C-CA-CB
56	ZB	3	PPU	N3'-C-CA-CB
56	ZB	3	PPU	CA-C-N3'-C3'
56	ZB	3	PPU	C5-C6-N6-C10
56	ZB	3	PPU	O-C-N3'-C3'
56	ZA	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	CE1-CZ-OC-CM
56	ZA	3	PPU	CE2-CZ-OC-CM
56	ZB	3	PPU	CE2-CZ-OC-CM
56	ZB	3	PPU	N1-C6-N6-C10
23	QX	20	A3P	C3'-C4'-C5'-O5'
56	ZA	3	PPU	C5-C6-N6-C10
56	ZB	3	PPU	C5-C6-N6-C9
56	ZB	3	PPU	CA-CB-CG-CD1
56	ZB	3	PPU	CA-CB-CG-CD2
56	ZB	3	PPU	O-C-CA-N
23	QX	20	A3P	O4'-C4'-C5'-O5'
56	ZB	3	PPU	C2'-C3'-N3'-C

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	20	A3P	1	0
56	ZA	3	PPU	2	0
56	ZB	3	PPU	7	0
23	XX	20	A3P	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 900 ligands modelled in this entry, 898 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	QD	302	4	0,12,12	-	-	-		
58	SF4	XD	301	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
58	SF4	QD	302	4	-	-	0/6/5/5
58	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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