Table 1. Overview of the tools and motifs and interaction types used to annotate the dataset of long-range nucleotide doublets

Tool	Reference	Link	Version / Access date	Allowed format	Command	Dependencies	Motif / Interaction type	Involving the long-range pair	Involving each residue separately
MC-Annotate	Gendron et al. 2001	https://major.iric.ca/MajorLabEn/MC-Tools.html	standalone 1.6.2	PDB	MC-Annotate inpfile > outpfile	-	base pair	yes	yes
							base stacking	yes	yes
RNAView	Yang et al. 2003	http://ndbserver.rutgers.edu/ndbmodule/services/download/rnaview.html	standalone June 2022	PDB	rnaview inpfile	-	base pair	yes	yes
							base stacking	yes	yes
FR3D	Sarver et al. 2008	http://rna.bgsu.edu/rna3dhub/pdb/1XJR/interactions/fr3d/all/csv	web-database June 2022	-	-	-	base pair	yes	yes
							base stacking	yes	yes
							base phosphate	yes	yes
							base ribose	yes	yes
NASSAM	Hamdani et al. 2012	http://211.25.251.163/nassam/	web-server June 2022	PDB / mmCIF	-	-	-	-	-
ClaRNA	Waleń et al. 2014	http://genesilico.pl/clarna/	standalone July 2022	PDB	python27 clarna.py -i inpfile > outpfile	simplejson networkx scipy biopython==1.76	base pair	yes	yes
							base stacking	yes	yes
							base phosphate	yes	yes
							base ribose	yes	yes
							other (diagonal / sandwich)	yes	yes
DSSR	Lu et al. 2015	http://forum.x3dna.org/rna-structures/	standalone v2.0.0-2020aug01	PDB / mmCIF	x3dna-dssr-2 -i=inpfile --format=mmcif --idstr=long --u-turn --more --non-pair --po4 --a-minor=N -o=outpfile	-	residue conformation (syn/anti + sugar pucker)	-	yes
							base pair	yes	yes
							base stacking	yes	yes
							non-base-pair H-bond	yes	yes
							atom-base capping	yes	yes
							N-minor	yes	yes
							ribose-zipper	yes	yes
							U-turn	-	yes
							kink-turn	-	yes
urslib2	Shalybkova et al. 2021	https://github.com/febos/urslib2	standalone May 2022	PDB / mmCIF	see https://github.com/febos/urslib2/blob/main/playground.ipynb	DSSR	bie/bwe	yes	yes
							coaxial (helical) stacking	-	yes
							dinucleotide platform	-	yes
							UAA/GAN internal loop	-	yes
							TandemGA internal loop	-	yes
							tetraloop (ANYA / CUYG / GNRA / UNAC / UNCG)	-	yes
							Stem / Loop	-	yes