

Table 3. Overview of the tools and motifs and interaction types used to annotate the dataset of long-range residue-residue pairs

Tool	Year	Reference	Link	Version / Access date	Allowed format	Command	Dependencies	Motif / Interaction type	Involving the long-range pair	Involving each residue separately
MC-Annotate	2001	10.1006/jmbi.2001.4626	https://major.tic.ca/MajorLabEn/MC-Tools.html	standalone 1.6.2	PDB	MC-Annotate ininfile > outfile	-	base pair	yes	yes
								base stacking	yes	yes
RNAView	2003	10.1093/nar/gkg529	http://ndbserver.rutgers.edu/ndbmodule/services/download/rnaview.html	standalone June 2022	PDB	rnview ininfile	-	base pair	yes	yes
								base stacking	yes	yes
NASSAM	2012	10.1093/nar/gks513	http://211.25.251.163/nassam/	web-server June 2022	PDB / mmCIF	-	-	-	-	-
FR3D	2013	10.1261/rna.039438.113	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
ClARNA	2014	10.1093/nar/gku765	http://genesilico.pl/clarna/	standalone version-2014	PDB	python27 clarna.py -i ininfile > outfile	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	2015	10.1093/nar/gkv716	http://forum.x3dna.org/rna-structures/	standalone v2.0.0-2020aug01	PDB / mmCIF	x3dna-dssr-2 -i=ininfile --format=mmcif --idstr=long --u-turn --more --non-pair --po4 --a-minor=N -o=outfile	-	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	2021	10.1261/rna.078535.120	https://github.com/febos/urslib2	standalone May 2022	PDB / mmCIF	see https://github.com/febos/urslib2/blob/main/playground.ipynb	DSSR	BIE/BWE [10.1093/nar/gkaa610]	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