## **Programy:**

## **MC-Annotate:**

```
Residue conformations ------
A1: G C2p_endo anti
A2: U C2p_endo anti
A3: G C3p_endo anti
C4: THR
C5: MET
C6: ALA
C7: ILE
C8: LEU
Adjacent stackings ------
A3-A4: adjacent_5p upward
A6-A7: adjacent 5p upward
A7-A8: adjacent_5p upward
Non-Adjacent stackings -----
A1-A470: outward
A3-A105: downward
A5-A2420: upward pairing
Number of stackings = 367
Number of adjacent stackings = 337
Number of non adjacent stackings = 30
Base-pairs ------
A1-A469: G-C Bs/O2P pairing
A4-A5: C-G O2P/Hh adjacent_5p pairing
A5-A386: G-A Ss/C8 pairing parallel cis one hbond
A5-A469: G-C O2P/Ww O2P/Bh pairing
A17-A382: U-A Ww/Ww pairing antiparallel cis XX
A18-A381: G-C Ww/Ww pairing antiparallel cis XIX
A20-A379: U-A Ww/Ww pairing antiparallel cis XX
RNA-View:
   1. NMR
      2n0j.pdb_nmr.pdb.out
      BEGIN_base-pair
                                       XIX
        1_27, A: 1 G-C 27 A: +/+ cis
                                         XXVIII
        2 26, A:
                2 G-U 26 A: W/W cis
        3_25, A: 3 C-G 25 A: +/+ cis
                                       XIX
        4_24, A: 4 U-A 24 A: -/- cis
                                      XX
        13_18, A: 13 U-U 18 A: W/W cis
                                          XVI
        10_21, A: 10 U-U 21 A: W/W cis
                                          !1H(b_b)
        14 16, A: 14 U-A 16 A: S/S tran
                                         !(s s)
     END_base-pair
     The total base pairs = 9 (from 27 bases)
      Standard WW--cis WW-tran HH--cis HH-tran SS--cis SS-tran
                   0
                             0
                        0
                                  0
      WH--cis WH-tran WS--cis WS-tran HS--cis HS-tran
```

## 2. Pozostałe

BEGIN\_base-pair

6\_391, A: 6 C-G 391 A: W/W cis n/a 7\_390, A: 7 C-G 390 A: +/+ cis XIX 685\_687, A: 2485 U-C 2487 A: S/H cis !(b\_s) 1\_690, A: 1 G-C 2490 A: ?/H cis !(s\_s) 24\_36, A: 24 U-A 36 A: S/H tran syn !(s\_s)

Summary of triplets and higher multiplets

BEGIN\_multiplets

23\_373\_376\_| [1 3] A: 23 G + A: 373 A + A: 376 C 172\_358\_362\_| [2 3] A: 172 A + A: 358 A + A: 362 U 401\_403\_455\_| [3 3] A: 401 A + A: 403 C + A: 460 G END\_multiplets

The total base pairs = 128 (from 704 bases)

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Standard WW--cis WW-tran HH--cis HH-tran SS--cis SS-tran 55 54 0 0 0 1 1 WH--cis WH-tran WS--cis WS-tran HS--cis HS-tran 2 3 5 3 2 2

## **ClaRNA:**

"residue1","residue2","n\_type","weight","description","full description"
"A1","A468","GA",0.159591577575,"?W\_345BR","?W\_345BR (O3'-1)"
"A1","A469","GC",0.480961521063,"?W\_345BPh","?W\_345BPh (OP2-5)"
"A1","A470","GG",1.0,"<>","<> (mo)"