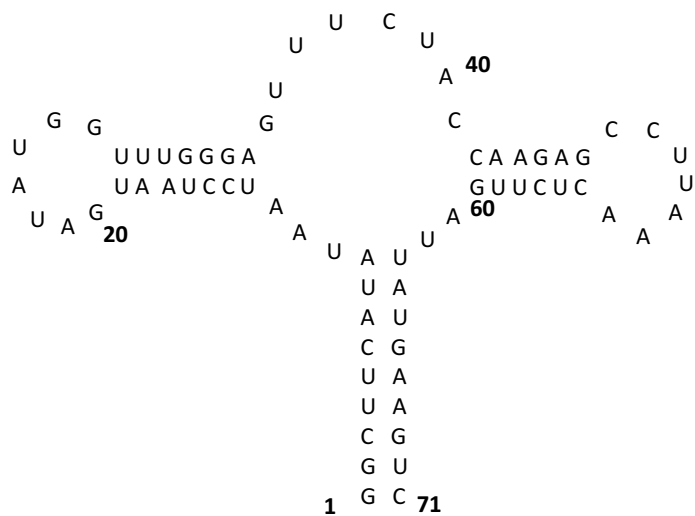
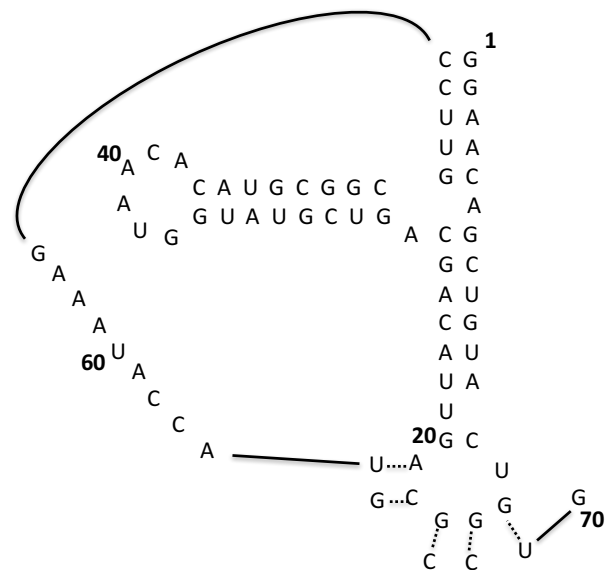


2M58



1Y26



2N8V

RLariat RNA (2M58)

#Configuration file
[GENERAL_DESCRIPTION]

SEQUENCE =
G G A A G A A A G G G C U
U C G G C C A C U C A A A
C U A C A G A G A C G C C
A G U C A C U C A G A U A
U C C U G G U

RNA = 2M58
NPDBS = 5000
SAXS_FILE = saxs_data.dat
DMAX = 93
JUNCTION_TYPE = 2

GENERAL_PROPERTIES =
PROPERTY
PDBFILE rna_ini.pdb
NRESIDUES 59
VDWEXPT 0
VDW 1
CHI 1
MOVESCALE 1
ITERATIONS 20000
CYCLES 60
TEMP 50.0
Qmax 0.3
NGrids 60

NONPAIRED=
INTERIOR_LOOP
UNIT HUNIT_1
9
INTERIOR_LOOP
UNIT HUNIT_2
28 29 30 31 32 33 34 35 36 37
INTERIOR_LOOP
UNIT HUNIT_3
59
TERMINAL_LOOP
NAME TLOOP1
UNIT HUNIT_1
13 14 15 16
TERMINAL_LOOP
NAME TLOOP2
UNIT HUNIT_3
42 43 44 45 46 47 48 49 50 51 52 53 54

PAIRED=

HELICAL_SEGMENT

NAME HSEGMENT_1

UNIT HUNIT_1

1 27

2 26

3 25

4 24

5 23

6 22

7 21

8 20

HELICAL_SEGMENT

NAME HSEGMENT_2

UNIT HUNIT_1

10 19

11 18

12 17

HELICAL_SEGMENT

NAME HSEGMENT_3

UNIT HUNIT_3

38 58

39 57

40 56

41 55

[PSEUDO_DUP]

PSEUDO_DUP1=

32 47

33 46

34 45

35 44

[HELICAL_STACKS]

##Maximum of 6

##Helical stacks names must match the regex HELICAL_STACK_[0-9]+

##It is OK to put every thing under helical stack separated by a line

HELICAL_STACK_1=

6 7 8 9 10 11 12

56 57 58 59 # Helical stack at the end

Adenine Riboswitch RNA (PDB CODE 1Y26)

#Configuration file

[GENERAL_DESCRIPTION]

SEQUENCE =

```
C G C U U C A U A U A A U
C C U A A U G A U A U G G
U U U G G G A G U U U C U
A C C A A G A G C C U U A
A A C U C U U G A U U A U
G A A G U G
```

RNA = 1y26

NPDBS = 5000

SAXS_FILE = saxs_data.dat

DMAX = 72

JUNCTION_TYPE = 3

GENERAL_PROPERTIES =

PROPERTY

PDBFILE rna_ini.pdb

NRESIDUES 71

VDWEXPT 0

VDW 1

CHI 1

MOVESCALE 1

ITERATIONS 20000

CYCLES 60

TEMP 0.5

Qmax 0.3

NGrids 61

PROXIMITY_CONSTRAINT

GROUPA 20 21 22 23 24 25 26

GROUPB 48 49 50 51 52 53 54

CONSTRAINT_VALUE 10.0

PROXIMITY_CONSTRAINT

GROUPA 36 37 38 39

GROUPB 9 63

CONSTRAINT_VALUE 10.0

NONPAIRED=

TERMINAL_LOOP

UNIT HUNIT_2

20 21 22 23 24 25 26

TERMINAL_LOOP

UNIT HUNIT_3

48 49 50 51 52 53 54

JUNCTION

```
10 11 12
JUNCTION
34 35 36 37 38 39 40 41
JUNCTION
61 62
```

PAIRED=

```
HELICAL_SEGMENT
UNIT HUNIT_1
1 71
2 70
3 69
4 68
5 67
6 66
7 65
8 64
9 63
```

```
HELICAL_SEGMENT
UNIT HUNIT_2
13 33
14 32
15 31
16 30
17 29
18 28
19 27
```

```
HELICAL_SEGMENT
UNIT HUNIT_3
42 60
43 59
44 58
45 57
46 56
47 55
```

[HELICAL_STACKS]

#Maximum of 6

##Helical stacks names must match the regex HELICAL_STACK_[0-9]+

##It is OK to put every thing under helical stack separated by a line

HELICAL_STACK_1=

```
58 59 60 61 62 63 64 65 66 67 68 69 70 71
```

HELICAL_STACK_2=

```
7 8 9 10 11 12 13 14 15 16 17 18 19
```

IRES PK1 RNA (PDB CODE 2N8V)

#Configuration file
[GENERAL_DESCRIPTION]

SEQUENCE =
G G A A C A G C U G U A C
U G G G C A G U U A C A G
C A G U C G U A U G G U A
A C A C A U G C G G C G U
U C C G A A A U A C C A U
G C C U G

RNA = 2n8v
NPDBS = 2000
SAXS_FILE = saxs_data.dat
DMAX = 88
JUNCTION_TYPE = 3

GENERAL_PROPERTIES =
PROPERTY
PDBFILE rna_ini.pdb
NRESIDUES 70
VDWEXPT 0
VDW 1
CHI 1
MOVESCALE 1
ITERATIONS 20000
CYCLES 60
TEMP 0.5
Qmin 0.01
Qmax 0.3
NGrids 60

PAIRED=
HELICAL_SEGMENT
NAME HSEGMENT_1
UNIT HUNIT_1
1 55
2 54
3 53
4 52
5 51
HELICAL_SEGMENT
NAME HSEGMENT_2
UNIT HUNIT_2
7 27
8 26
9 25
10 24
11 23

12 22
HELICAL_SEGMENT
NAME HSEGMENT_3
UNIT HUNIT_3
29 50
30 49
31 48
32 47
33 46
34 45
35 44
36 43

NONPAIRED=

TERMINAL_LOOP
NAME TLOOP1
UNIT HUNIT_2
14 15 16 17 18 19
TERMINAL_LOOP
NAME TLOOP2
UNIT HUNIT_3
37 38 39 40 41 42
INTERIOR_LOOP
UNIT HUNIT_2
13
INTERIOR_LOOP
UNIT HUNIT_2
20 21
INTERIOR_LOOP
UNIT HUNIT_4
56 57 58 59 60 61 62 63 64 65 66 67 68 69 70
JUNCTION
6
JUNCTION
28

[PSEUDO_DUP]

PSEUDO_DUP1=
14 70
15 69
16 68
17 67
18 66
19 65

[HELICAL_STACKS]

HELICAL_STACK_1=
48 49 50 51 52 53 54 55
HELICAL_STACK_2=
3 4 5 6 7 8 9 10 11 12

HELICAL_STACK_3=
25 26 27 28 29 30 31 32 33 34 35 36