

```
#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 = 100
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 8.0
```

```
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

MY_SEGMENT
UNIT HUNIT_4
14 15 16 17 18 19 20

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

#this is a fake pseudoduplex for test
[PSEUDO_DUP]
PSEUDO_DUP1=
1 10
2 11
5 14
PSEUDO_DUP2=
20 60
22 61

23 64

[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

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

HELICAL_STACK_2=

64 65 66 67 68 69 70 71

58 59 60 61 62