



Supplementary Data

Web 3DNA 2.0 for the analysis, visualization, and modeling of 3D nucleic acid structures

by

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S1 ‘Simple’ base-pair and step parameters for non-Watson-Crick pairs

The relative position and orientation of the two bases in a base pair (bp) can be rigorously quantified by six rigid-body parameters—three translations (Shear, Stretch, and Stagger) and three rotations (Buckle, Propeller, and Opening) (see Fig. S1). Similarly, taking each bp as a rigid body, a set of six step parameters (Shift, Slide, Rise for translations, Tilt, Roll, and Twist for rotations) can be used to describe the spatial arrangement of neighboring bps. The numerical values of these bp and step parameters depend upon the choice of reference frames. For Watson-Crick (WC) pairs and DNA/RNA duplexes consisting of WC pairs, local 3DNA parameters make ‘intuitive’ sense (e.g., a Rise of around 3.4 Å and a twist of 36°). For non-WC pairs, however, the 3DNA local bp parameters could become cryptic, and the local step parameters may seem to be nonsensical (for example a Rise of 0, as reported on the 3DNA Forum. See also below).

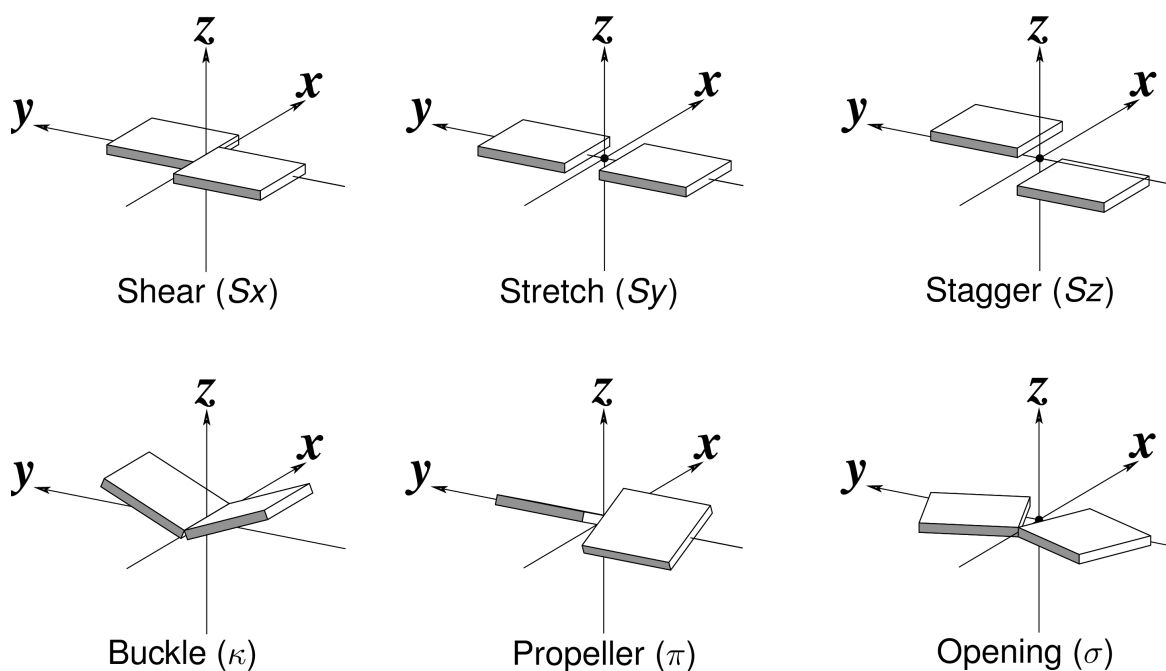


Fig. S1 Schematic diagrams of the six rigid-body parameters commonly used for the characterization of base pair geometry

To address the increasingly common issues on the characterization of DNA/RNA structures with non-WC pairs, 3DNA (as of v2.3-2016jan01) introduced a set of ‘simple’ bp and

step parameters. Shown below are related results using PDB entry [1xvk](#) as an example. This echinomycin-(GCGTACGC)₂ complex has a single DNA strand as the asymmetric unit. The biological unit is contained in an NMR-like MODEL/ENDMDL ensemble of two models, each corresponding to one chain of the duplex. This structure has two A+T Hoogsteen base pairs. In March 2013, questions were asked on the 3DNA Forum about the “zero or negative helical rise?” from a 3DNA analysis on [1xvk](#).

The related 3DNA commands for the analysis of [1xvk](#) are shown below. Note the `-symm` option to include both strands of the duplex in the biological unit. The main output file is named ‘1xvk.out’.

```

1 find_pair -symm 1xvk.pdb1 1xvk.bps
2 analyze -symm 1xvk.bps
3
4 # or the above two commands can be combined:
5 find_pair -symm 1xvk.pdb1 | analyze -symm

```

A comparison of the classic 3DNA local bp parameters and the new ‘simple’ ones is shown below. For the four WC pairs, the two sets are very similar. For non-WC pairs (no. 1, 4, 5, and 8 of M+N type pairs; prefixed with * in the list of ‘simple’ parameters), however, they are obviously different (e.g., in Shear and Stretch).

Local base-pair parameters							
bp	Shear	Stretch	Stagger	Buckle	Propeller	Opening	
1 G+C	0.46	-3.41	-0.35	3.71	-5.92	67.37	
2 C-G	0.27	-0.18	0.35	-22.28	3.73	-2.75	
3 G-C	-0.38	-0.18	0.41	22.84	2.54	-2.67	
4 T+A	-0.69	3.57	0.31	-3.48	7.41	-70.55	
5 A+T	0.69	-3.57	-0.31	3.48	-7.41	70.54	
6 C-G	0.38	-0.18	0.41	-22.84	2.54	-2.67	
7 G-C	-0.27	-0.18	0.35	22.28	3.73	-2.75	
8 C+G	-0.46	3.41	0.35	-3.71	5.93	-67.37	
~~~~~							
ave.	0.00	-0.09	0.19	-0.00	1.57	-1.36	
s.d.	0.51	2.64	0.32	17.27	5.36	52.16	

```

1 The 'simple' parameters are intuitive for non-Watson-Crick base pairs
2 and associated base-pair steps (where the above corresponding 3DNA
3 parameters often appear cryptic). Note that they are for structural
4 *description* only, not to be fed into the 'rebuild' program. See URL
5 http://x3dna.org/highlights/details-on-the-simple-base-pair-parameters
6 and related blogposts on the 3DNA home page for details.
7

```

```

8 This structure contains 4 non-Watson-Crick (with leading *) base pair(s)

```

```

9 -----
10 Simple base-pair parameters based on RC8--YC6 vectors
11      bp      Shear      Stretch      Stagger      Buckle      Propeller      Opening
12 *   1 G+C      -3.07       1.55       -0.35       -6.98        0.29        67.33
13     2 C-G        0.27      -0.17        0.35      -22.34        3.33        -2.80
14     3 G-C      -0.39      -0.17        0.41       22.91        1.81        -2.73
15 *   4 T+A      -3.29       1.56        0.31       -8.03        1.59       -70.46
16 *   5 A+T      -3.29       1.56       -0.31       -8.03        1.59        70.46
17     6 C-G        0.39      -0.17        0.41      -22.91        1.81        -2.72
18     7 G-C      -0.27      -0.17        0.35       22.34        3.32        -2.80
19 *   8 C+G      -3.07       1.55        0.35       -6.98        0.30       -67.33
20 -----
21      ave.      -1.59        0.69        0.19       -3.75        1.75        -1.38
22      s.d.       1.72        0.92        0.32       17.57        1.15        52.11

```

The comparison becomes more pronounced at the step level. The local TA/TA step (no. 4) has a Rise of zero, and a Twist of 180 degrees. A duplex containing Hoogsteen pairs with zero Rise surely does not make ‘intuitive’ sense, especially when visualized in an interactive molecular viewer like Jmol or PyMOL. This zero-Rise result is due to the symmetry of the biological unit of PDB entry [1xvk](#): the z-axes of the T+A (no. 4) and A+T (no. 5) Hoogsteen pairs are perfectly anti-parallel. As a result, the z-axis of the middle reference frame of the step (no. 4) is [0, 0, 0], which leads to zero Rise. On the other hand, the corresponding ‘simple’ parameters for step no. 4 has a Rise of 3.1 Å, and a Twist of 26°, which are more intuitively reasonable.

```

1 Local base-pair step parameters
2      step      Shift      Slide      Rise      Tilt      Roll      Twist
3     1 GC/GC      3.49       6.57      -0.02     -144.30     94.22     26.41
4     2 CG/CG     -0.06       0.87       2.44      -0.59      3.94     -4.56
5     3 GT/AC      0.52       0.32       7.23      -6.90      6.39     69.20
6     4 TA/TA      2.71      -4.96      -0.00     -152.05    81.49    180.00
7     5 AC/GT      3.97       6.04      -0.58     -140.44    96.86    -85.61
8     6 CG/CG      0.06       0.87       2.44       0.59      3.94     -4.56
9     7 GC/GC      0.65       0.18       7.41      -7.46     -1.75     66.30
10 -----
11      ave.       1.62       1.41       2.70     -64.45     40.73     35.31
12      s.d.       1.71       3.92       3.37     76.04     47.20     82.59

```

```

1 Simple base-pair step parameters based on consecutive C1'-C1' vectors
2      step      Shift      Slide      Rise      Tilt      Roll      Twist
3 *   1 GC/GC     -0.55       0.39       7.41       6.40     -4.22     23.36
4     2 CG/CG     -0.05       0.87       2.44      -0.55      3.94     -0.81
5 *   3 GT/AC      0.38       0.47       7.23      -8.62      3.75     25.70
6 *   4 TA/TA     -0.00       4.73       3.09      -0.00      7.49     25.67

```

7	*	5	AC/GT	-0.38	0.47	7.23	8.62	3.75	25.70
8		6	CG/CG	0.05	0.87	2.44	0.55	3.94	-0.82
9	*	7	GC/GC	0.55	0.39	7.41	-6.40	-4.22	23.36
10			-----						
11			ave.	-0.00	1.17	5.32	-0.00	2.06	17.45
12			s.d.	0.39	1.59	2.50	6.21	4.49	12.52

Bizarre as the local 3DNA bp and step parameters may appear for [1xvk](#), these are the parameters needed for *rigorous* reconstruction of the original structure, at the bp level (i.e., without considering the sugar-phosphate backbone). See the following list of commands for details. This `analyze/rebuild` reversibility is a defining feature of 3DNA and can be applied to DNA and RNA.

```

1 # The analysis step generates file 'bp_step.par'
2 find_pair -symm 1xvk.pdb1 | analyze -symm
3 # 'rebuild' using local bp and step parameters
4 rebuild -atomic bp_step.par 1xvk-3dna.pdb
5
6 # 'analyze' of the 3DNA-rebuilt structure (1xvk-3dna.pdb)
7 # Note here the '-symm' option is no longer needed
8 # The main output file is '1xvk-3dna.out' with bp and step
9 # parameters very close to the original output in '1xvk.out'
10 find_pair 1xvk-3dna.pdb | analyze

```

Overall, bp geometry can be described in more than one way. The existing set of six local bp and step parameters in 3DNA is mathematically rigorous, allowing for an unambiguous characterization of any pair of interacting bases and serving as input for exact model building. The new set of six ‘simple’ bp and step parameters provides a more intuitive interpretation of structural variations in non-WC-containing structures. The term ‘simple’ is used to distinguish the new set of parameters from the traditional 3DNA local parameters. It should be emphasized that the ‘simple’ parameters are for structural *description* only, and are not suitable as input for the 3DNA `rebuild` program. The two sets of parameters complement one another and serve different audiences and/or purposes. Numerical values of both are readily obtained with 3DNA.

For more technical details, please see the blog post [“Details on the simple base-pair parameters”](#) and related posts on the [3DNA home page](#).

## S2 Sample input files for the 3DNA rebuild program

The 3DNA rebuild program can be used for building DNA/RNA duplexes or single-stranded nucleic acid structures, given an input file containing base sequence and local bp and step parameters. The input file is most conveniently generated by running the 3DNA analyze program on a starting structure, and then modifying the resultant `bp_step.par` file. Two sample input files, one for a DNA duplex and another for an RNA single helix, are given below.

### S2.1 Rebuilding of a double-helical DNA structure

The following data set is based on PDB entry [355d](#), the classical Dickerson-Drew B-DNA dodecamer with base sequence  $d(\text{CGCGAATTCGCG})_2$ . It can be generated with the following 3DNA command, in a file named `bp_step.par`. The bases or associated parameters can be easily changed to build a customized duplex structure based on the starting one. Alternatively, such an input file can be created on purpose.

```

1 find_pair 355d.pdb | analyze

```

---

```

1 12 # base-pairs
2 0 # ***local base-pair & step parameters***
3 #      Shear  Stretch  Stagger  Buckle  Prop-Tw  Opening  Shift   Slide  Rise   Tilt   Roll   Twist
4 C-G    0.276   -0.140   0.073   6.930  -17.308  -0.606   0.000   0.000  0.000  0.000  0.000  0.000
5 G-C   -0.236   -0.182   0.491   9.341  -14.302  -2.077   0.087   0.039  3.200 -3.216  8.520  32.731
6 C-G    0.244   -0.171   0.159  -4.433  -5.405   0.434   0.496   0.668  3.691  2.847 -9.055  43.879
7 G-C   -0.255   -0.115   0.008  10.806  -9.449   1.012  -0.138   0.593  3.000  0.967 11.300  25.114
8 A-T   -0.037   -0.107   0.011   4.724 -15.314   1.601  -0.453  -0.139  3.388 -1.585  1.373  37.500
9 A-T    0.051   -0.050   0.065   0.442 -15.001   6.233   0.171  -0.325  3.298 -0.330  0.459  37.520
10 T-A   -0.037   -0.117   0.173  -0.264 -16.744   3.928  -0.011  -0.601  3.219 -0.311 -2.675  32.403
11 T-A   -0.108   -0.120  -0.004  -1.561 -16.364   5.120  -0.082  -0.397  3.216  1.681 -0.974  33.744
12 C-G    0.209   -0.127   0.003 -12.410 -10.274  -1.223  -0.267  -0.226  3.465  0.684 -1.686  42.136
13 G-C   -0.106   -0.053   0.239   4.205  -9.603   3.206   0.700   0.776  3.068 -3.656  4.180  26.581
14 C-G    0.156   -0.130   0.208   0.283 -17.417  -1.755  -1.311   0.360  3.371 -2.853 -9.368  41.601
15 G-C   -0.244   -0.069   0.254   4.671  -4.954  -1.620  -0.309   0.211  3.174 -0.679  6.692  33.310

```

## S2.2 Rebuilding a single-stranded RNA structure

The following data set is based on PDB entry [1fir](#), the crystal structure of HIV reverse-transcription primer tRNA(Lys,3). It can be generated with the following 3DNA command, in a file named `bp_step.par`. The 15 modified bases (in lower cases) have been replaced by their standard counterparts, and the numerical values of the base-step parameters are rounded to two decimal places.

```

1 find_pair -s 1fir.pdb | analyze
2
3 # in file 'bp_step.par', replace modified bases with standard ones
4 # GCCCGgAUAgCUCAGuCGGuAGAGCAPCAGACUtUUaAPCUGAGGguccAGGGtPCAaGUCCUGUUCGGGCGCCA
5 #      *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *
6 # GCCCGGAUAGCUCAGUCGGUAGAGCAUCAGACUUUUAAUCUGAGGGUCCAGGGUUAAGUCCUGUUCGGGCGCCA

```

```

1 76 # bases
2 0 # ***local step parameters***
3 #      Shift   Slide   Rise    Tilt    Roll    Twist
4 G      0.00    0.00    0.00    0.00    0.00    0.00
5 C     -0.07   -1.62    2.99    7.24    3.05   24.71
6 C      0.34   -1.73    3.33    0.06   12.16   33.11
7 C     -0.02   -1.22    3.28    6.35    8.61   29.90
8 G     -0.20   -1.71    3.41   -6.30   18.47   29.24
9 G     -0.30   -2.41    2.90   -4.07    9.63   32.20
10 A      0.30   -2.14    2.92   -1.01   15.53   35.60
11 U     14.78   -2.10    8.45  -137.23  -1.76  153.31
12 A     -7.40   -4.51    4.65   27.02    5.03  -48.56
13 G     -7.48    1.52    5.26  -93.06  111.24  -17.94
14 C     -0.33   -1.80    3.59   -7.88   12.91   29.67
15 U      0.26   -1.42    3.86   -3.52    1.55   39.41
16 C      1.42   -1.85    2.00   20.65   -1.96   31.30
17 A     -1.03   -2.90    3.65   -5.63   10.81   20.03
18 G      3.52   -1.48    3.42   -4.64    7.07   54.61
19 U    -13.45   -3.43    8.03   22.59  -29.43 -140.64
20 C    -12.52   -3.78   -1.72   -6.64  109.92 -161.18
21 G    -16.94   -6.10   -1.94   52.16    8.33 -102.20
22 G      0.20    1.63    7.10  -14.28    5.30   39.90
23 U    -15.14   -3.50    7.80  -81.58    1.91  -75.35
24 A    -18.26   -5.48   -1.30   73.93   31.00 -125.50
25 G     -6.72   -1.93    2.91   12.30    4.21  -34.75
26 A     -1.18   -1.53    2.98    6.38    1.85   26.55
27 G      0.29   -0.74    3.41    0.20    8.64   37.61
28 C      1.28   -1.60    3.40   -3.53   15.25   35.58
29 A      2.37   -2.09    3.28   -2.01    3.76   46.35
30 U      1.92   -2.10    3.81  -13.91   13.53   40.42
31 C      0.72   -2.18    3.41   -8.90    1.29   43.61
32 A     -0.07   -1.84    1.92    7.70   11.30   35.77

```

33	G	-0.40	-1.76	3.24	-4.00	-0.37	24.02
34	A	0.37	-1.93	3.33	-0.44	-2.48	41.11
35	C	0.84	-2.60	4.32	-5.47	9.06	27.18
36	U	4.28	-0.82	3.08	7.15	15.18	58.51
37	U	-8.15	-0.34	-5.54	51.26	141.12	-29.35
38	U	1.22	-1.45	3.48	-0.69	6.93	39.40
39	U	-0.10	-2.65	3.09	3.04	6.64	32.41
40	A	2.74	-1.92	3.28	-1.26	5.37	46.45
41	A	2.45	-1.45	3.14	0.12	7.06	43.88
42	U	3.83	-0.71	3.24	4.70	3.37	54.25
43	C	1.19	-1.18	3.81	-1.94	15.17	46.74
44	U	0.60	-1.74	3.28	-0.86	13.71	31.74
45	G	-0.18	-1.92	3.26	-3.62	7.27	23.71
46	A	0.58	-1.99	3.21	1.41	-3.49	33.78
47	G	-0.80	-1.66	3.05	0.07	1.51	18.85
48	G	2.71	-0.94	3.01	14.03	1.75	60.99
49	G	1.13	0.54	7.24	-1.44	-1.82	11.39
50	U	-17.80	-5.68	5.24	26.35	12.25	-158.08
51	C	-18.87	-3.47	2.25	15.50	-5.53	-169.23
52	C	-16.22	-4.09	-2.69	-74.33	66.26	-146.49
53	A	-0.11	-2.47	1.77	18.47	-8.44	32.95
54	G	-0.76	-1.37	2.93	-1.90	12.59	30.60
55	G	0.64	-1.66	3.78	-9.80	2.35	30.68
56	G	0.68	-2.82	3.09	3.32	-1.95	32.76
57	U	1.10	-1.35	3.21	7.01	-5.34	39.70
58	U	2.61	-1.08	3.25	6.09	26.43	37.98
59	C	-7.49	-0.23	-7.39	58.51	127.22	-7.19
60	A	2.49	-1.17	3.76	-2.03	9.07	49.24
61	A	0.74	-0.38	6.47	8.57	-2.42	16.06
62	G	-7.04	-0.66	-7.40	17.11	101.72	-1.16
63	U	2.89	-0.21	2.50	20.56	4.03	55.18
64	C	6.61	-1.45	10.23	-94.94	52.00	98.74
65	C	-0.56	-1.47	3.99	-2.23	12.46	33.35
66	C	-0.42	-1.12	3.43	0.71	13.49	22.88
67	U	0.74	-1.12	3.61	-4.15	19.65	39.34
68	G	-0.37	-2.01	3.67	-4.48	3.86	25.88
69	U	0.41	-1.88	3.22	-2.18	1.81	36.70
70	U	1.14	-1.56	3.54	-11.12	7.02	36.86
71	C	-1.50	-1.97	3.13	-1.34	2.58	26.12
72	G	0.31	-2.24	2.27	6.92	9.06	29.83
73	G	0.35	-1.82	2.99	5.34	4.32	35.85
74	G	0.14	-2.04	3.03	2.84	9.64	32.93
75	C	0.78	-2.04	3.47	-3.42	7.62	26.84
76	G	1.01	-2.12	3.17	3.03	2.10	29.20
77	C	3.19	-0.30	3.19	9.58	-1.40	60.31
78	C	17.48	2.98	4.32	6.43	-13.77	135.87
79	A	-0.60	0.29	2.84	18.44	5.41	42.16



## S3 Two new backbone parameters

Two new parameters have been added in recent releases of 3DNA. One is a set of *virtual* backbone torsion angles, based on the positions of the phosphorus atom (P) and the origin of the standard base reference frame. The other is ssZp, single-stranded Zp, defined as the z-coordinate of the bridging P atom expressed in the standard reference frame of the preceding base (at 5', see Figure 2 in the main text). Note that ssZp is sensitive to base conformation relative to the sugar moiety: for the *syn* conformation, ssZp is negative, while for the more common *anti* conformation, it is positive.

The following set of backbone torsion angles is based on 1xvk, the echinomycin-(GCGTACGC)₂ complex. The output file is generated with the command listed below.

```
1 analyze -symm -tor=1xvk-torsions.txt 1xvk.pdb1
```

The output list includes three sections, (1) “Main chain and chi torsion angles”, (2) “Pseudo (virtual) eta/theta torsion angles”, and (3) “Sugar conformational parameters”. Note the correspondence between *syn/anti* base conformations in section (1) and negative/positive ssZp values in section (3).

```
1 *****
2 Main chain and chi torsion angles:
3
4 Note: alpha:   03'(i-1)-P-05'-C5'
5       beta:    P-05'-C5'-C4'
6       gamma:   05'-C5'-C4'-C3'
7       delta:   C5'-C4'-C3'-03'
8       epsilon: C4'-C3'-03'-P(i+1)
9       zeta:    C3'-03'-P(i+1)-05'(i+1)
10
11      chi for pyrimidines(Y): 04'-C1'-N1-C2
12      chi for purines(R): 04'-C1'-N9-C4
13
14      chi in [165, -45(315)] for anti conformation
15      chi in [45, 95] for syn conformation
16
17      e-z: epsilon - zeta
18      BI: e-z = [-160, +20]
19      BII: e-z = [+20, +200]
20
21      base      chi A/S      alpha      beta      gamma      delta      epsilon      zeta      e-z BI/BII
22  1 ...1>A:...1_: [.DG]G      74.1 syn      ---      ---      69.9      133.5      -139.7      -74.4      -65.3 BI
23  2 ...1>A:...2_: [.DC]C     -103.9 anti    139.1     160.3     -173.4     71.9      170.0      -72.0     -118.0 BI
24  3 ...1>A:...3_: [.DG]G     -108.4 anti    152.0    -154.8    -178.0    124.7     -84.0     -173.2     89.2 BII
25  4 ...1>A:...4_: [.DT]T     -95.4 anti     -65.4    154.8     38.2     129.7    179.1     -87.5     -93.4 BI
26  5 ...1>A:...5_: [.DA]A      68.3 syn     -66.4    171.3     54.6     107.5    -147.0     -65.4     -81.6 BI
27  6 ...1>A:...6_: [.DC]C     -107.8 anti    168.3    145.7    168.8     79.1    -177.4     -84.9     -92.5 BI
28  7 ...1>A:...7_: [.DG]G     -105.3 anti    154.2    -152.3    -178.3    123.5    -105.8    179.4     74.8 BII
29  8 ...1>A:...8_: [.DC]C     -100.4 anti    -57.3    157.3     50.8     143.2     ---      ---      ---
30  76 ...2>A:...1_: [.DG]G      74.1 syn      ---      ---      69.9     133.5    -139.7     -74.4     -65.3 BI
31  77 ...2>A:...2_: [.DC]C     -103.9 anti    139.1     160.3    -173.4     71.9     170.0     -72.0    -117.9 BI
32  78 ...2>A:...3_: [.DG]G     -108.3 anti    152.0    -154.8    -178.0    124.7     -84.0    -173.2     89.2 BII
33  79 ...2>A:...4_: [.DT]T     -95.4 anti     -65.4    154.8     38.2     129.7    179.1     -87.5     -93.4 BI
34  80 ...2>A:...5_: [.DA]A      68.3 syn     -66.4    171.3     54.6     107.5    -147.0     -65.4     -81.6 BI
```

```

35 81 ...2>A:...6_: [.DC]C -107.8 anti 168.3 145.7 168.8 79.1 -177.4 -84.9 -92.5 BI
36 82 ...2>A:...7_: [.DG]G -105.3 anti 154.2 -152.3 -178.3 123.5 -105.8 179.4 74.8 BII
37 83 ...2>A:...8_: [.DC]C -100.4 anti -57.3 157.3 50.8 143.2 --- --- ---
38 *****
39 Pseudo (virtual) eta/theta torsion angles:
40
41 Note: eta: C4'(i-1)-P(i)-C4'(i)-P(i+1)
42 theta: P(i)-C4'(i)-P(i+1)-C4'(i+1)
43
44 eta': C1'(i-1)-P(i)-C1'(i)-P(i+1)
45 theta': P(i)-C1'(i)-P(i+1)-C1'(i+1)
46
47 eta": Borg(i-1)-P(i)-Borg(i)-P(i+1)
48 theta": P(i)-Borg(i)-P(i+1)-Borg(i+1)
49
50 base eta theta eta' theta' eta" theta"
51 1 ...1>A:...1_: [.DG]G --- --- --- --- --- ---
52 2 ...1>A:...2_: [.DC]C 147.5 152.8 168.2 166.4 143.7 158.9
53 3 ...1>A:...3_: [.DG]G -136.4 135.8 -142.7 168.2 -157.8 -154.2
54 4 ...1>A:...4_: [.DT]T 176.6 -128.8 -163.9 -150.8 -135.9 -73.4
55 5 ...1>A:...5_: [.DA]A 176.4 -101.2 -170.3 -127.0 -88.5 -159.2
56 6 ...1>A:...6_: [.DC]C 158.5 163.0 172.4 173.7 149.5 167.4
57 7 ...1>A:...7_: [.DG]G -151.7 125.6 -152.1 152.4 -163.4 -165.9
58 8 ...1>A:...8_: [.DC]C --- --- --- --- --- ---
59 76 ...2>A:...1_: [.DG]G --- --- --- --- --- ---
60 77 ...2>A:...2_: [.DC]C 147.5 152.8 168.2 166.4 143.7 158.9
61 78 ...2>A:...3_: [.DG]G -136.4 135.8 -142.7 168.2 -157.8 -154.2
62 79 ...2>A:...4_: [.DT]T 176.7 -128.9 -163.9 -150.8 -135.9 -73.4
63 80 ...2>A:...5_: [.DA]A 176.4 -101.2 -170.3 -127.0 -88.5 -159.2
64 81 ...2>A:...6_: [.DC]C 158.5 163.0 172.4 173.7 149.5 167.4
65 82 ...2>A:...7_: [.DG]G -151.7 125.6 -152.1 152.4 -163.4 -165.9
66 83 ...2>A:...8_: [.DC]C --- --- --- --- --- ---
67 *****
68 Sugar conformational parameters:
69
70 Note: v0: C4'-O4'-C1'-C2'
71 v1: O4'-C1'-C2'-C3'
72 v2: C1'-C2'-C3'-C4'
73 v3: C2'-C3'-C4'-O4'
74 v4: C3'-C4'-O4'-C1'
75
76 tm: the amplitude of pucker
77 P: the phase angle of pseudorotation
78
79 ssZp: single-stranded Zp, defined as the z-coordinate of the 3'
80 phosphorus atom (P) expressed in the standard reference
81 frame of preceding base; the value is POSITIVE when P lies
82 on the +z-axis side (base in anti conformation); NEGATIVE
83 if P is on the -z-axis side (base in syn conformation)
84 Dp: perpendicular distance of the 3' P atom to the glycosidic bond
85 [as per the MolProbity paper of Richardson et al. (2010)]
86
87 base v0 v1 v2 v3 v4 tm P Puckering ssZp Dp
88 1 ...1>A:...1_: [.DG]G -29.0 36.2 -32.2 15.5 8.2 37.3 149.7 C2'-endo -1.15 1.32
89 2 ...1>A:...2_: [.DC]C -20.6 -6.4 28.6 -41.4 38.8 41.9 47.0 C4'-exo 1.68 3.80
90 3 ...1>A:...3_: [.DG]G -37.3 35.2 -21.1 1.0 23.2 37.3 124.5 C1'-exo 1.27 1.48
91 4 ...1>A:...4_: [.DT]T -13.3 19.2 -18.3 10.8 1.5 19.7 157.6 C2'-endo 1.53 2.00
92 5 ...1>A:...5_: [.DA]A -41.0 32.8 -12.8 -11.4 32.7 40.4 108.5 C1'-exo -1.84 2.20
93 6 ...1>A:...6_: [.DC]C -24.6 -0.9 24.3 -39.7 39.5 41.4 54.0 C4'-exo 1.78 3.61
94 7 ...1>A:...7_: [.DG]G -39.9 39.3 -23.8 2.2 24.0 40.5 125.9 C1'-exo 1.79 2.11
95 8 ...1>A:...8_: [.DC]C -17.0 31.6 -33.2 24.5 -4.6 33.8 169.1 C2'-endo --- ---
96 76 ...2>A:...1_: [.DG]G -29.0 36.2 -32.2 15.5 8.3 37.3 149.7 C2'-endo -1.15 1.32
97 77 ...2>A:...2_: [.DC]C -20.5 -6.4 28.6 -41.4 38.8 41.9 47.0 C4'-exo 1.68 3.80
98 78 ...2>A:...3_: [.DG]G -37.4 35.3 -21.2 1.1 23.2 37.4 124.5 C1'-exo 1.27 1.48
99 79 ...2>A:...4_: [.DT]T -13.3 19.2 -18.3 10.8 1.5 19.8 157.5 C2'-endo 1.53 2.00
100 80 ...2>A:...5_: [.DA]A -41.0 32.8 -12.9 -11.4 32.7 40.5 108.5 C1'-exo -1.84 2.20
101 81 ...2>A:...6_: [.DC]C -24.6 -0.9 24.3 -39.7 39.5 41.4 54.0 C4'-exo 1.78 3.61
102 82 ...2>A:...7_: [.DG]G -39.8 39.3 -23.8 2.3 24.0 40.5 126.0 C1'-exo 1.79 2.11
103 83 ...2>A:...8_: [.DC]C -17.0 31.6 -33.1 24.4 -4.5 33.7 169.1 C2'-endo --- ---

```

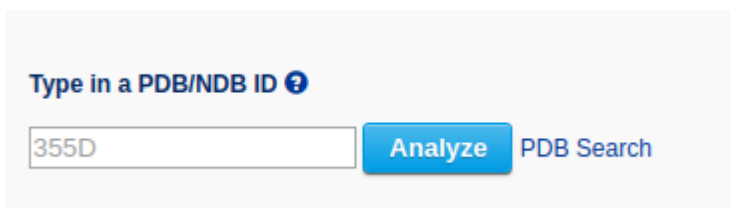
## S4 Tutorials

### S4.1 Analysis module

The **analysis** component of Web 3DNA 2.0 determines a wide range of conformational parameters — such as the rigid-body parameters of interacting nucleic-acid bases, base-pair steps of spatially adjacent base pairs, torsion angles of main chain and side groups, etc. — from a user-provided PDB/NDB ID (the structure identifiers used respectively in the **Protein Data Bank** and the **Nucleic Acid Database**) or a PDB-formatted file. The output files can be downloaded or viewed directly on a results page. Selected base-pairing, base-pair step, and torsion angle data are reported in interactive tables.

#### Example 1-1: Analyze a nucleic-acid-containing structure by using the PDB/NDB ID

Before conducting an analysis on the web server, users are encouraged to verify the PDB/NDB ID of the input structure at the **PDB** or **NDB** website and gain some familiarity with the structure. To use the **analysis** component, the user can enter a valid PDB/NDB ID in the input area, for example “355D”.



Type in a PDB/NDB ID ⓘ

 [Analyze](#) [PDB Search](#)

After clicking the ‘Analyze’ button, the user is directed to a results page containing five sections: **1. Structural summary**, **2. Block Representations**, **3. Interactive 3D view**, **4. Output files of derived structural parameters**, and **5. Interactive tables**.

#### 1. Structural summary

**PDB ID: 355D** Use this structure for Visualization

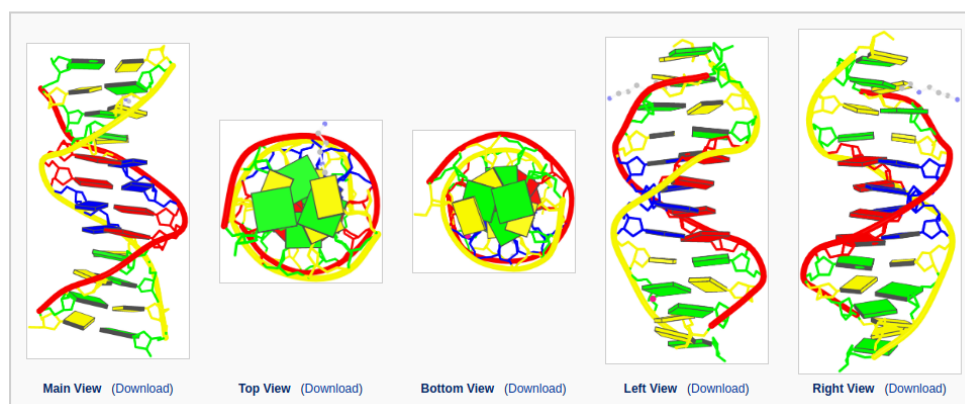
<b>Title:</b>	THE B-DNA DODECAMER AT HIGH RESOLUTION
<b>Author:</b>	Hu, L.D., Shui, X., McFail-Isom, L., Williams, G.G.
<b>Deposit date:</b>	1997-10-07
<b>Experimental methods:</b>	X-ray
<b>Resolution:</b>	1.4
<b>External links:</b>	<a href="#">PDB</a> · <a href="#">NDB</a> · <a href="#">PDBsum</a> · <a href="#">MMDB</a>

This section briefly describes the structure title, the author(s), the deposition date,

the experimental method used to determine the structure, the resolution (for X-ray and EM structures), and any external links related to the structure. If the input file is an NMR structure, the number of models in the structure will be counted and reported (see [Example 1-2](#) for the analysis of a multi-model structure).

## 2. Block Representations

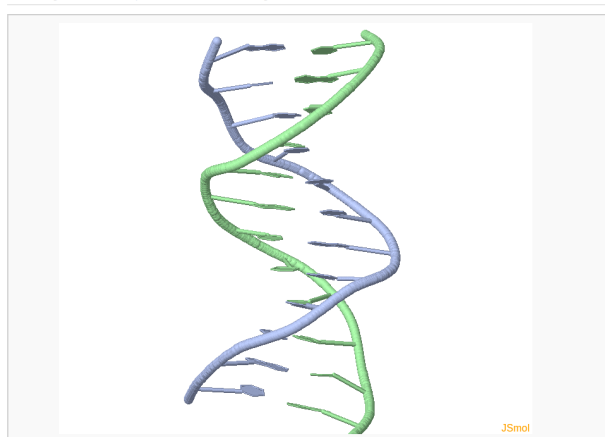
Block representations [\[3D view](#) • [Output files](#) • [Parameter Tables\]](#)



These figures are drawn with schematic block representations of the bases, tube representations of the strands, and atomic representations of the sugar-phosphate-backbones. Proteins (if any) are represented by violet ribbons, and small molecules by ball-and-stick images. The same representations are also used in the [PDB](#) and [NDB](#) websites. The image is enlarged when the mouse is hovered over a specific image.

## 3. Interactive 3D view

3D view [\[Block view](#) • [Output files](#) • [Parameter Tables\]](#)



A 3D interactive visualization of the input structure is presented in this section. The user can click the “JSmol” label on the lower right-hand corner to choose more options provided by [JSmol](#).

## 4. Output files of derived structural parameters

### **Nucleic acid structural parameter summary file.** [View](#) • [Download](#)

This file gives a detailed listing of the DNA structural parameters including but not limited to:

1. H-bonding information
2. Origins and mean base-pair normal vectors in the coordinate system of the given structure
3. Local base-pair parameters [Pictorial definitions]
4. Local base-pair step parameters [Pictorial definitions]
5. Local base-pair helical parameters [Pictorial definitions]
6. 'Simple' base-pair and step parameters [Click for details]
7. Minor- and major-groove widths [Click for details]
8. Structure classification (A, B, Z forms)
9. Main chain and glycosyl ( $\chi$ ) torsion angles [Pictorial definitions]

### **Base-pair and base-pair step parameter file.** [View](#) • [Download](#)

This file contains both base-pair parameters and base-pair step parameters.

1. It can be directly used for reconstruction of a double-stranded nucleic acid structure.
2. It can be modified to reconstruct a variant double-stranded structure.

### **Base step parameter file based on a continuous single-stranded chain.** [View](#) • [Download](#)

This file contains base step parameters based on a continuous single-stranded chain.

1. It can be directly used for reconstruction of a single-stranded nucleic acid structure.
2. It can be modified to reconstruct a variant single-stranded structure.

### **Torsion angle parameter file.** [View](#) • [Download](#)

This file gives a detailed listing of torsion angle parameters including:

1. Main chain and  $\chi$  torsion angles [Pictorial definitions]
2. Pseudo (virtual)  $\eta/\theta$  torsion angles [Pictorial definitions]
3. Sugar conformational parameters [Pictorial definitions]

The list of parameters given above corresponds to the 5' to 3' direction of strand I and the 3' to 5' direction of strand II.

This section includes four derived parameter files: the summary file, the base-pair and base-pair step parameter file, the 'single-stranded' step parameter file and the torsion angle parameter file. Each file can be viewed on the web page or downloaded.

## 5. Interactive tables (one of them shown here)

[Local Base-pair Parameters \[Pictorial definitions\]](#)

Local base-pair parameters							
Pair ID	Pair	Shear	Stretch	Stagger	Buckle	Propeller	Opening
1	C-G	0.28	-0.14	0.07	6.93	-17.31	-0.61
2	G-C	-0.24	-0.18	0.49	9.34	-14.3	-2.08
3	C-G	0.24	-0.17	0.16	-4.43	-5.4	0.43
4	G-C	-0.26	-0.11	0.01	10.81	-9.45	1.01
5	A-T	-0.04	-0.11	0.01	4.72	-15.31	1.6
6	A-T	0.05	-0.05	0.07	0.44	-15	6.23
7	T-A	-0.04	-0.12	0.17	-0.26	-16.74	3.93
8	T-A	-0.11	-0.12	-0	-1.56	-16.36	5.12
9	C-G	0.21	-0.13	0	-12.41	-10.27	-1.22
10	G-C	-0.11	-0.05	0.24	4.21	-9.6	3.21

Page  of 2

Units: Angstroms for Shear, Stretch, and Stagger parameters; Degrees for Buckle, Propeller, and Opening parameters.  
[Download table](#)

This section contains nine interactive tables embracing rigid-body parameters of base pairs and base-pair steps as well as torsion angles. Users can control the number of rows displayed on each page with a limit of 100 entries per page. Data in the table can be sorted by clicking the column headers. Each table can be downloaded in CSV format for further processing. The angles are expressed in degrees and the distances in Angstrom units.

### Example 1-2: Analyze a multi-model structure

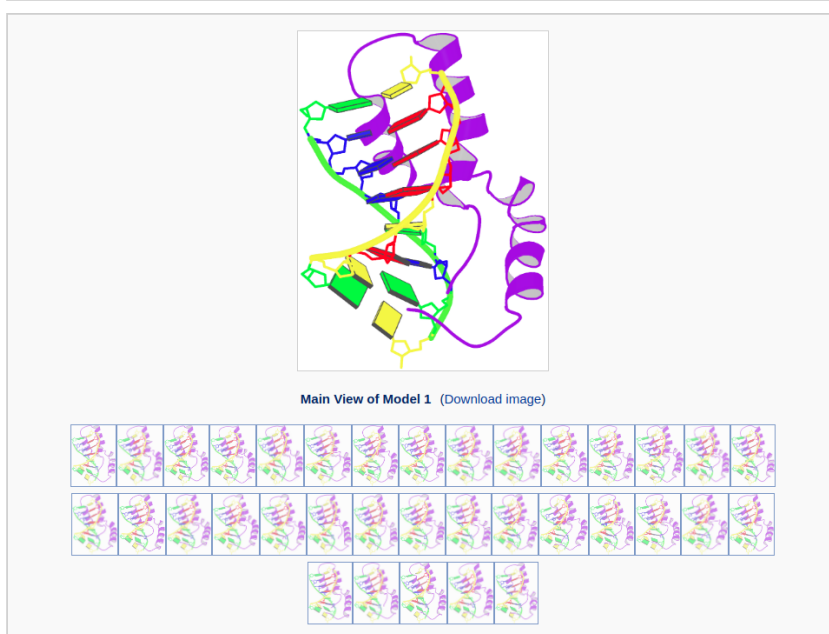
If the input PDB/NDB ID represents a structure with multiple models (for example the NMR structure “1HRZ”), the results page will contain extra information and options in the Structural summary section (see the following figure).

**PDB ID: 1HRZ** [Use this structure for Visualization](#)

<b>Title:</b>	THE 3D STRUCTURE OF THE HUMAN SRY-DNA COMPLEX SOLVED BY MULTI-DIMENSIONAL HETERONUCLEAR-EDITED AND-FILTERED NMR
<b>Author:</b>	Clore, G.M., Werner, M.H., Huth, J.R., Gronenborn, A.M.
<b>Deposit date:</b>	1995-05-09
<b>Experimental methods:</b>	NMR
<b>External links:</b>	PDB · NDB · PDBsum · MMDB
<b>Model total:</b>	35
<b>Model ID:</b>	1
<b>Further Analysis:</b>	The structural analysis on this page is based on Model 1. To get a full analysis of all models, please click the following button [Note: A maximum of 50 models will be analyzed. You may break the pdb file in parts if it contains over 50 models.]

The user can click the “Analyze multiple models” button to go to a multi-model analysis results page. It should be noted that a maximum of 50 models will be analyzed. If the ensemble has more than 50 models, only the first 50 models will be analyzed. The user should modify the input file to analyze additional models, 50 at a time.

Block representation of all models:



The multi-model results page contains block representations of all models (50 maximum). The user can move the mouse over the small icons at the bottom to display a magnified view of the fluctuations among the models. The user can download each of the images by clicking the corresponding links.

Output of all models:

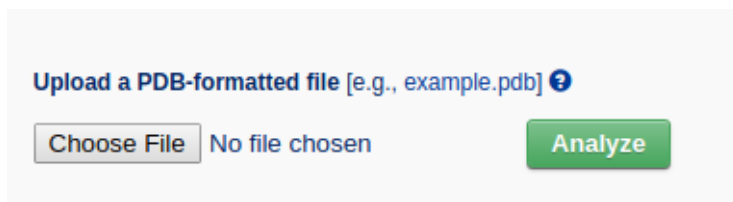


This section includes structural parameter and image files of all the models. The user can directly view the parameter file for each model and a download link is also provided. For the convenience of users, a compressed folder including all the output files in 'tar.gz'

format is offered for downloading.

**Example 1-3: Analyze a nucleic-acid-containing structure by uploading the PDB-formatted file**

The user can also upload a structural file, including a multi-model file, in PDB format for analysis.



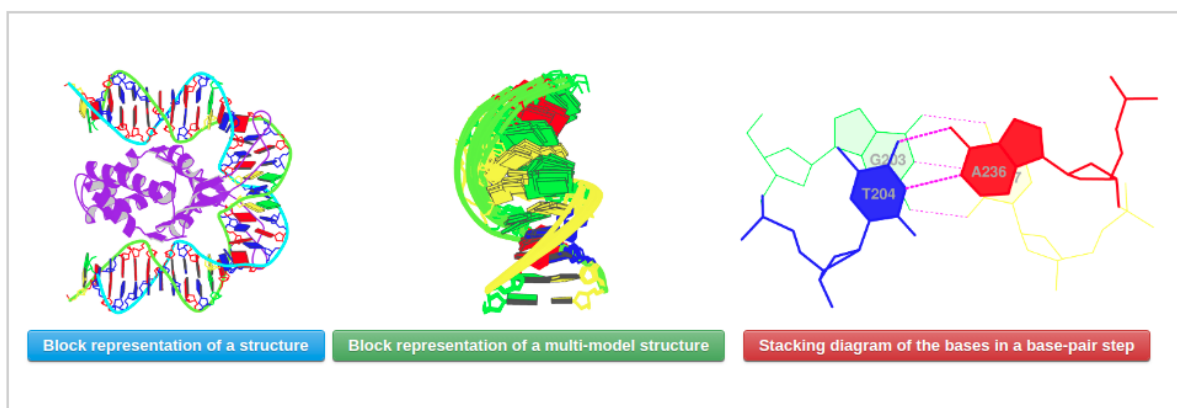
After clicking the 'Analyze' button, the user is redirected to a results page that is similar to [Example 1-1](#), but without the Brief Description section.



## S4.2 Visualization module

The **visualization** component of Web 3DNA 2.0 creates schematic images of molecular presentations. The server takes a PDB/NDB ID or a user-uploaded PDB-formatted file, and returns various representations of the structure or parts of it. In this component, three visualization styles are provided: 1) [Schematic base block representation of a structure](#), 2) [Block representation of a multi-model structure](#), and 3) [Stacking diagram of the bases in a base-pair step](#).


Chose a visualization type: 





### Example 2-1: Block representation of a structure

This module generates composite block/ribbon/backbone representations of a single nucleic-acid-containing structure. The plotted image includes informative color-coding of the nucleic acid. The bases are color-coded by residue type following the **NDB** convention (C, yellow; G, green; A, red; T, blue; U, cyan). Minor-groove edges of the base pairs are shaded.

Clicking the button directs the user to an interface with two options: 1) enter a PDB/NDB ID, or 2) upload a PDB-formatted file.

Current choice: **Block representation of a pdb structure** 

Type in a PDB/NDB ID       —OR—      Upload a PDB-formatted file [e.g., example.pdb] 

PDB Search       No file chosen

After a file is provided (for example “2NP2”) and the ‘Next’ button is clicked, the structure will be analyzed and the user will be directed to an intermediate page, where

various questions will be asked depending on the nature of the structure.

In this page, the user has multiple options to customize the resulting schematic images: 1) whether to display both nucleic acid and protein, if protein is present, or only nucleic acid, or only protein; 2) whether to show only P and base blocks for the nucleic acid structure; 3) whether to show a double-helix ribbon along the nucleic acid structure; and 4) whether to rotate the structure as a whole. The default block view places the structure in a 'best-view' orientation, i.e. the DNA structure is shown in a view perpendicular to the shortest principal axis. The user can specify an arbitrary rotation about the X-, Y-, or Z-axis.

Current choice: **Block representation**

**PDB ID: 2NP2**

This structure contains both nucleic acid and protein. You can specify whether to display both nucleic acid and protein, only nucleic acid, or only protein:

All atoms  Only nucleic acid  Only protein

Nucleic acid representation selection:

All nucleic acid atoms  Show only P and base blocks

Double-helix ribbon selection:

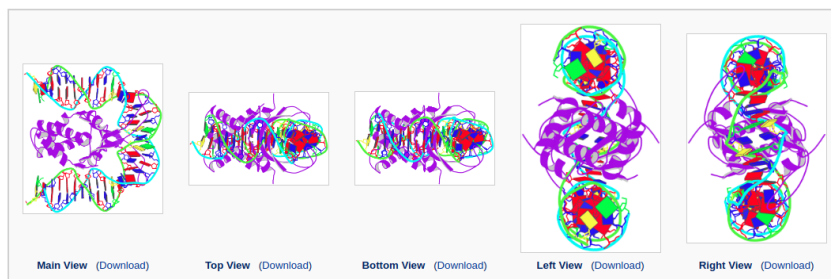
Show double-helix ribbon

Rotating:

Rotate the structure along X-axis 30 degrees

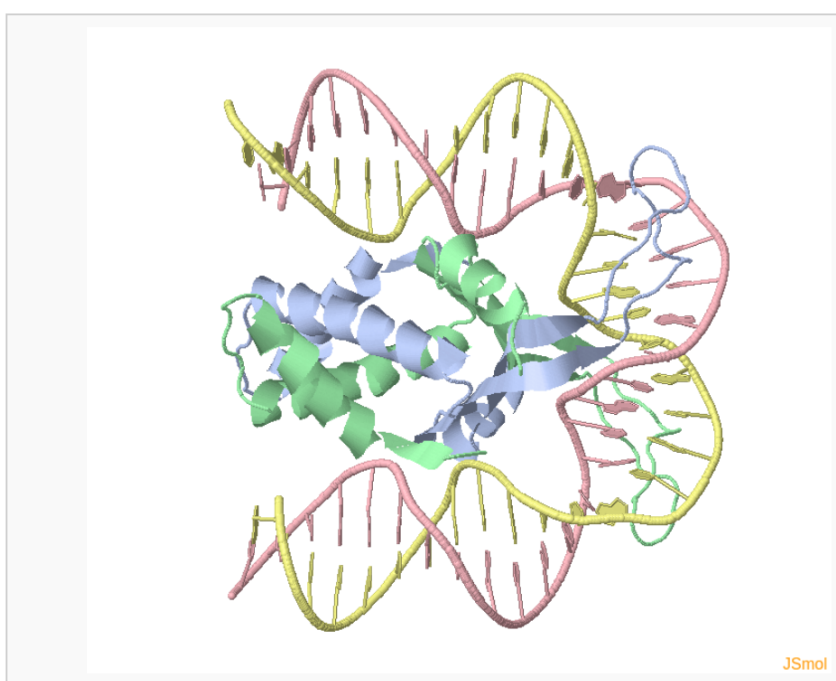
Visualize

After clicking the 'Visualize' button, the user is directed to five generated images with downloadable links.



A 3D interactive visualization of the input structure is also shown.

3D view:



### Example 2-2: Block representation of an ensemble of structures

The ensemble visualization style creates a composite image for a multi-model structure, such as NMR or simulation-generated structures.

Clicking the button directs the user to an interface with two options: 1) enter a PDB/NDB ID, or 2) upload a PDB-formatted file.

**Current choice: Block representation of an ensemble of structures** ⓘ

Type in a PDB/NDB ID ⓘ —OR— Upload a PDB-formatted file [e.g., example.pdb] ⓘ

PDB Search  No file chosen

After a file is provided (for example “2MOE”) and the ‘Next’ button is clicked, the structure will be analyzed and the user will be directed to a control page with the following options: 1) specify an ensemble of models by choosing the starting and ending models, 2) choose a specific base pair from the first model against which all other models will be aligned, or use the original alignment, and 3) indicate whether to display both nucleic acid and protein, if protein is present, or only nucleic acid, or only protein.

Current choice: Ensemble block representation

PDB ID: 2MOE

This structure contains 20 models. Please define an ensemble by choosing a range of models:

Start:  End:

Each model contains 10 base pairs. Please choose a base pair against which all models will be aligned:

—OR—  Use original alignment

This structure contains both nucleic acid and protein. You can specify whether to display both nucleic acid and protein, only nucleic acid, or only protein:

All atoms  Only nucleic acid  Only protein

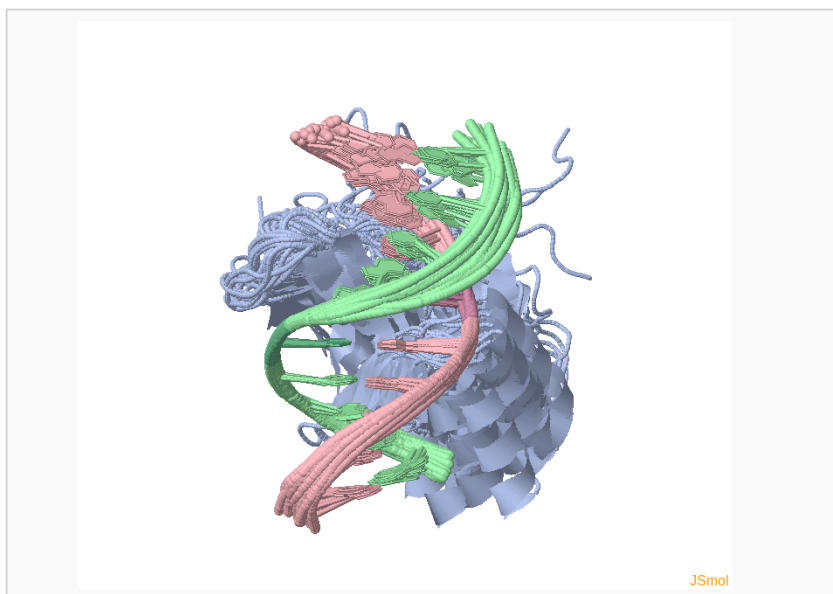
Visualize

Then the user can click the ‘Visualize’ button to view the ensemble image and to download the coordinates of the aligned structures.



The user can also display all of the models in the 3D interactive view (after clicking the “JSmol” label on the lower right-hand corner and selecting “model 1/20” and “All”).

3D view (Note: click the "JSmol" label on the lower right-hand corner for more options, including to show all models)



It should be noted that this module applies only to multi-model structures; otherwise error messages will appear.

### Example 2-3: Stacking diagram of base-pair steps

The 'stacking diagram' component generates images of successive Watson-Crick base pairs in a nucleic-acid-containing structure. The images are plotted with H-bonds and filled base rings; the user has the option to label the bases.

Clicking the button directs the user to an interface with two options: 1) enter a PDB/NDB ID, or 2) upload a PDB-formatted file.

**Current choice: Stacking diagram of base-pair steps** ⓘ

Type in a PDB/NDB ID ⓘ —OR— Upload a PDB-formatted file [e.g., example.pdb] ⓘ

PDB Search
 
 No file chosen

After a file is provided (for example "355D") and the 'Next' button is clicked, the structure will be analyzed and the user will be directed to an intermediate page to choose a base-pair step in the initial plotting. The user can also specify whether to show the labels of base residues and where to place the labels before clicking the 'Visualize' button. The labels can be placed inside the six-membered ring of each base or next to the C8 atom of purine (R) bases and the C6 atom of pyrimidine (Y) bases.

Current choice: Stacking diagram of base-pair steps

PDB ID: 355D

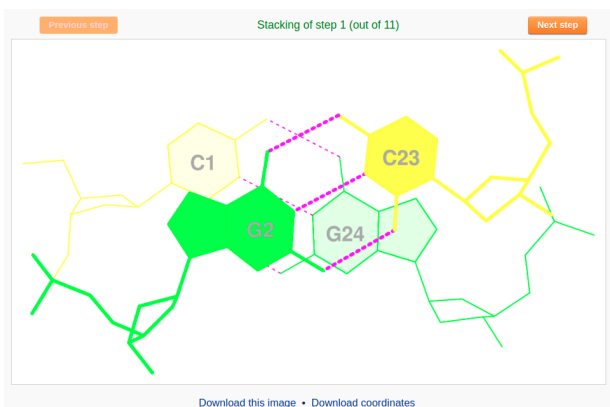
This structure contains 11 base-pair steps. Please choose a step to visualize its stacking:

1: C:G

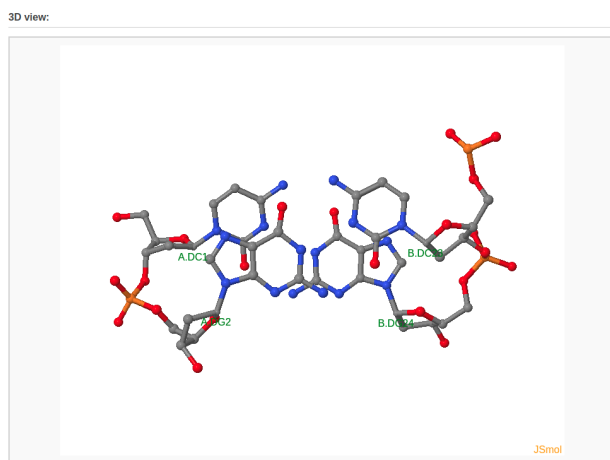
Labels at base ring  Labels at RC8/YC6  No labels

Visualize

The user may need to wait a few minutes for the calculation of all the stacking images of a long piece of DNA, such as that on the nucleosome. After viewing the stacking diagram of the selected base pairs, the user can navigate to other steps along the structure by clicking the “Previous step” and “Next step” buttons.



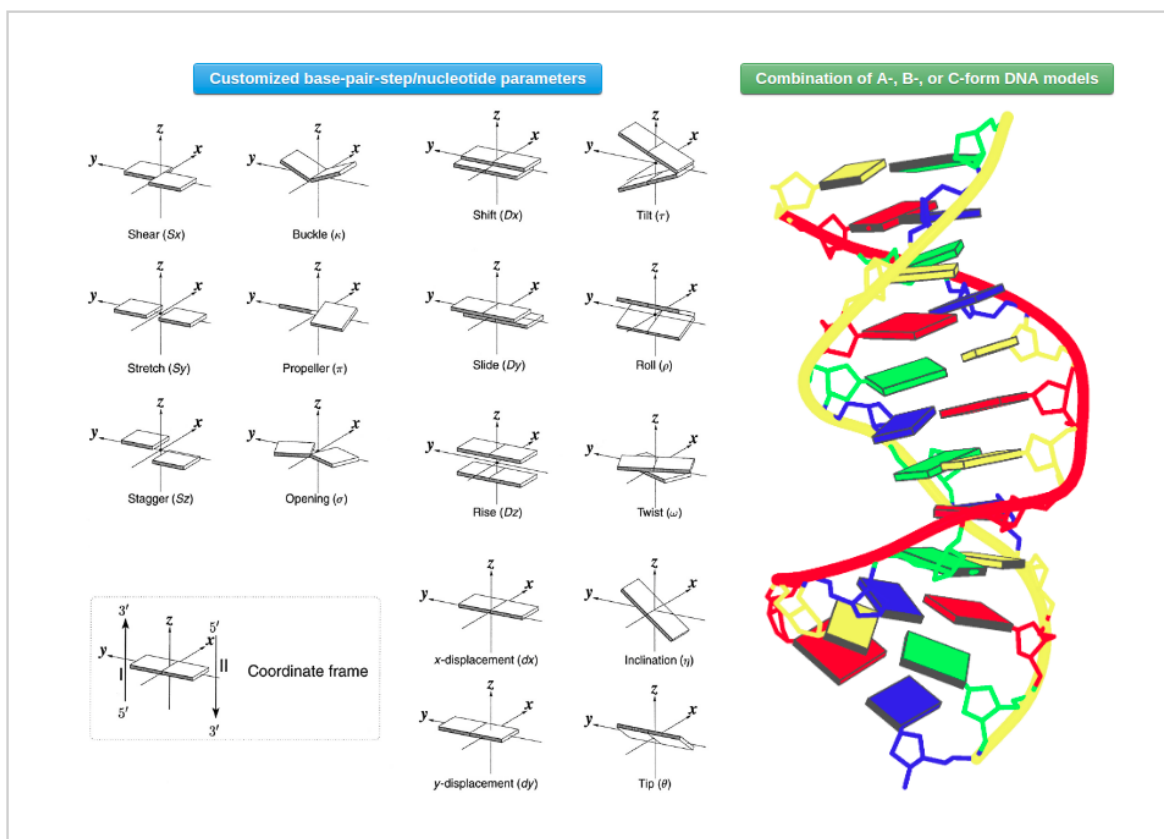
A 3D interactive visualization of the associated base pairs is also shown.



### S4.3 Modeling module: customized rebuilding

The **rebuilding** component of Web 3DNA 2.0 allows the user to build: 1) **3D models of customized double-helical and single-stranded structures** with base pairs and base-pair/nucleotide steps arranged according to user-supplied rigid-body parameters, 2) a **mixed DNA structure** comprised of canonical A-, B-, and C-type DNA fragments. The output webpage includes a schematic representation of the constructed model, a PDB-formatted file with full atomic coordinates and a downloadable link, and a 3D interactive visualization of the constructed model.

**Choose a customized type:** 



#### Example 3-1: Reconstruction of a customized model

Clicking the button directs the user to an interface for building a DNA/RNA model with customized base-pair/nucleotide step parameters.

The user must prepare a file containing the rigid-body parameters for the desired structure. Two example parameter files can be found at the “Test parameters” links. A single click of each button will automatically fill the corresponding content in the text area

(one file for double-stranded DNA, the other one for single-stranded RNA). Note that the base-pair step parameters are null for the first base pair, but the parameter of the first base-pair can have non-zero values.

**Current choice: Customized base-pair-step/nucleotide parameters**

**Test parameters**

---

**Please specify modeling information:**

**Backbone conformation:**

B-DNA (C2'-endo)
  A-DNA (C3'-endo)
  RNA (C3'-endo)

**Copy and paste parameters:**

```

12 # base-pairs
0 # ***local base-pair & step parameters***
#      Shear  Stretch  Stagger  Buckle  Prop-Tw  Opening  Shift  Slide  Rise  Tilt  Roll  Twist
C-G    0.276  -0.140  0.673   6.930  -17.308  -0.606  0.000  0.000  0.000  0.000  0.000  0.000
G-C   -0.236  -0.182  0.491   9.341  -14.302  -2.077  0.087  0.039  3.200  -3.216  8.520  32.731
C-G    0.244  -0.171  0.159  -4.433  -5.405   0.434  0.496  0.668  3.691  2.847  -9.055  43.879
G-C   -0.255  -0.115  0.008  10.806  -9.449   1.012  -0.138  0.593  3.000  0.967  11.300  25.114
A-T   -0.037  -0.107  0.011   4.724  -15.314  1.601  -0.453  -0.139  3.388  -1.585  1.373  37.500
A-T    0.051  -0.050  0.065   0.442  -15.001  6.233  0.171  -0.325  3.298  -0.330  0.459  37.520
T-A   -0.037  -0.117  0.173  -0.264  -16.744  3.928  -0.011  -0.601  3.219  -0.311  -2.675  32.403
T-A   -0.108  -0.120  -0.004  -1.561  -16.364  5.120  -0.082  -0.397  3.216  1.681  -0.974  33.744
C-G    0.209  -0.127  0.003  -12.410  -10.274  -1.223  -0.267  -0.226  3.465  0.684  -1.686  42.136
G-C   -0.106  -0.053  0.239   4.205  -9.603  3.206  0.700  0.776  3.068  -3.656  4.180  26.581
C-G    0.156  -0.130  0.208   0.283  -17.417  -1.755  -1.311  0.360  3.371  -2.853  -9.368  41.601
G-C   -0.244  -0.069  0.254   4.671  -4.954  -1.620  -0.309  0.211  3.174  -0.679  6.692  33.310

# the first column lists the base pairs for double-stranded DNA
  
```

As an alternative, the user can also upload a parameter file in a valid format (please refer to the example parameter files: [double-helix DNA](#) and [single-stranded RNA](#)).

—OR—

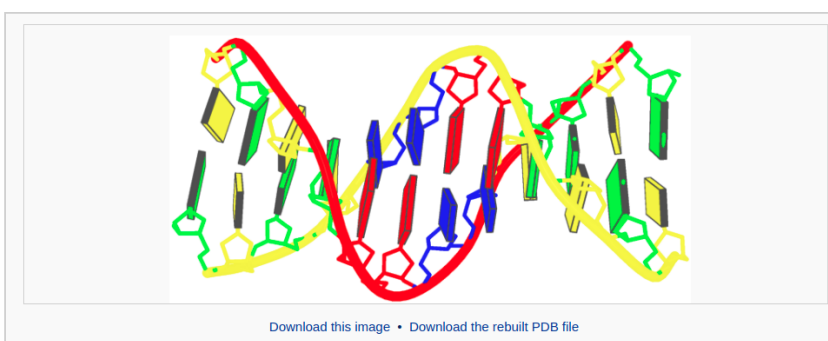
**Upload a base-pair parameter file (.txt or .par format):**  No file chosen

Next, the user needs to specify whether to construct a full atomic model and to select a sugar type: B-DNA (C2'-endo), A-DNA (C3'-endo), or RNA (C3'-endo). The user can also specify whether to optimize the backbone geometry.

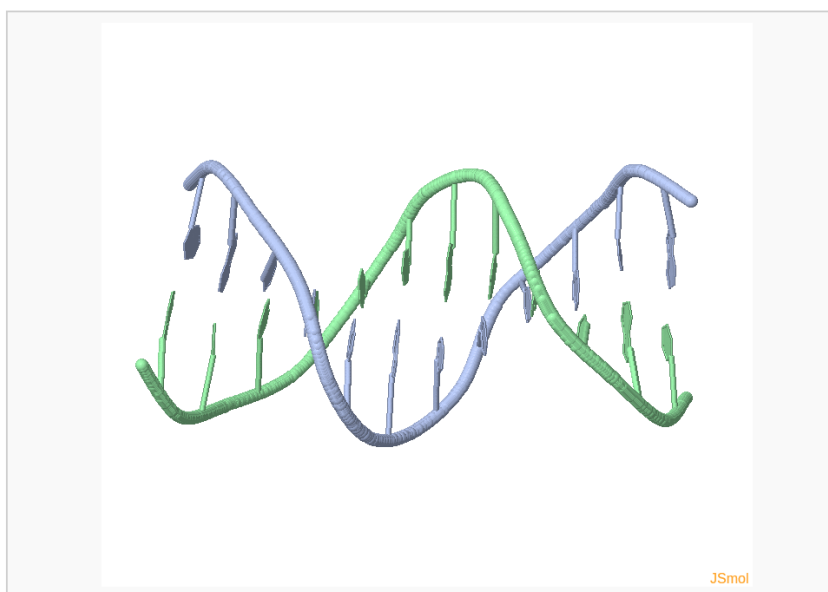
After clicking the “Build Model” button, the user will be directed to a results page shown below.



The structure constructed by 3DNA: [\[Use this structure for mutation\]](#)



3D view:



### Example 3-2: Construction of a model that combines of A-, B-, and C-DNA conformational segments

The user can also construct a DNA model with a combination of A, B, and C double-helical components. Clicking the button directs the user to the following interface:

**Current choice: Combination of A-, B-, or C-form DNA** [↗](#)

Please choose the number of segments:

3

Next

The user then can choose the desired number of segments in the model from a dropdown list (for example “3”). Clicking the “Next” button leads to an intermediate page where the

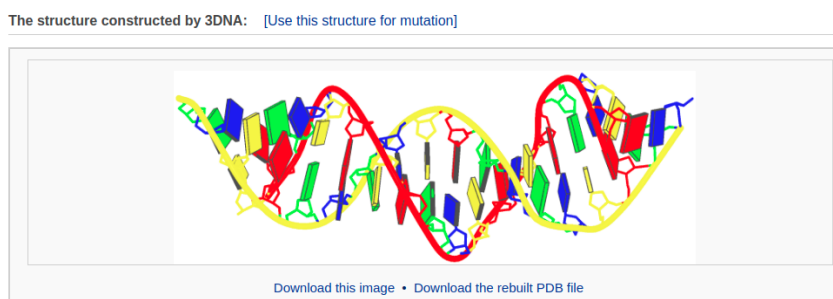
user can select the sequence and conformational form (A-, B-, or C-DNA) of each segment. Note that the input sequence is that of the leading strand.

**Current choice: Combination of A-, B-, or C-form DNA**

Sequence (ACGT only):	Repeating #:	DNA form:
ACTGAC	1	<input type="radio"/> A-form <input type="radio"/> B-form <input type="radio"/> C-form
ACTGAC	1	<input type="radio"/> A-form <input checked="" type="radio"/> B-form <input type="radio"/> C-form
ACTGAC	1	<input type="radio"/> A-form <input type="radio"/> B-form <input checked="" type="radio"/> C-form

Backbone geometry optimization

After clicking the 'Build' button, the user will be directed to a results page shown below.



3D view:



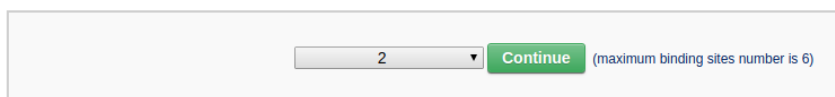
## S4.4 Modeling module: DNA ‘decorated’ with proteins

The **composite** component of Web 3DNA 2.0 allows the user to construct models of DNA ‘decorated’ with proteins and other molecules by providing the requisite DNA-ligand structural templates and the locations of the binding sites. The output webpage includes a schematic representation of the constructed nucleic-acid protein/ligand complex, a PDB-formatted file with full atomic coordinates of the constructed model, and a 3D interactive visualization.

### Example 4-1: Construction of a protein-bound DNA model

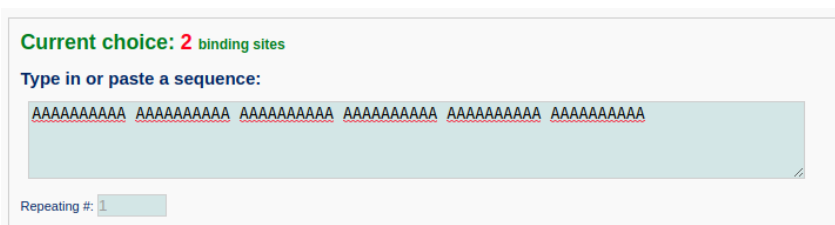
First the user needs to select the number of bound ligands from a dropdown list (for example “2”), and then clicks the ‘Continue’ button.

Choose a binding site number to build a protein-decorated DNA model: ⓘ



2 Continue (maximum binding sites number is 6)

Next, the user is asked to type in the DNA sequence bound by the proteins of interest. Here, we enter a test DNA sequence of 60 base pairs with poly dA:poly dT. Note that the input sequence is that of the leading strand.



Current choice: 2 binding sites

Type in or paste a sequence:

AAAAAAAAAA AAAAAAAAAA AAAAAAAAAA AAAAAAAAAA AAAAAAAAAA AAAAAAAAAA

Repeating #: 1

Then, the user needs to specify the conformation of the unbound DNA (A- or B-form) and to supply, for each binding site, the binding position. The binding position corresponds to the location of the central base or base-pair step of the specified protein-bound DNA segment. Here, two DNA-protein complexes (PDB ID: 1LMB and 5Z2T) serve as templates for binding DNA at positions 20 and 40.

**Choose a form of DNA (unbounded)**

B-form  A-form

**Binding position:**

**Template PDB ID:**

(note: only simple double-stranded DNA-containing structures can be used here)

**Continue**

Clicking the ‘Continue’ button directs the user to a confirmation page, where the binding information can be verified. Warnings are given on this page if the binding input is inappropriate.

**Please confirm following binding information:**

Sequence:[red: binding site]

AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA

**The form of unbounded DNA:**

B-form

**Binding sites:**

**Site 1**

Binding position: 20  
Binding template: 1LMB.pdb  
Template DNA length:19  
Template structural analysis: [\[Base-pair Step Info\]](#) • [\[Comprehensive output file\]](#)

**Site 2**

Binding position: 40  
Binding template: 5Z2T.pdb  
Template DNA length:13  
Template structural analysis: [\[Base-pair Step Info\]](#) • [\[Comprehensive output file\]](#)

Please go back if need any modification. Or please forward to build the structure.

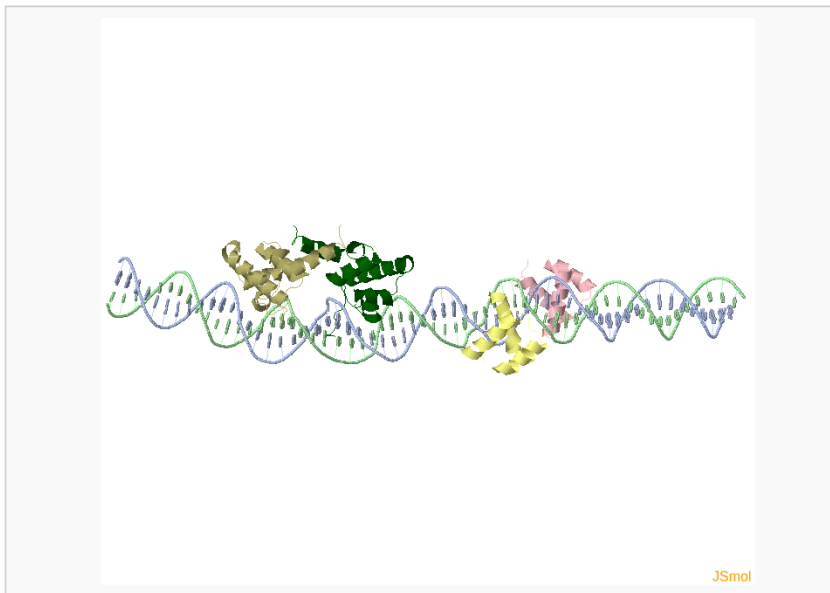
**Build**  Backbone geometry optimization

The user can choose whether to optimize the backbone geometry. After clicking the ‘Build’ button, the user will be directed to a results page that contains: 1) a ribbon-like representation of the DNA-protein complex, 2) downloadable links to the image and the atomic coordinate file, and 3) a 3D interactive visualization of the constructed DNA-protein complex.

The structure constructed by 3DNA: [\[Use this structure for mutation\]](#)



3D view:



### Example 4-2: Construction of a chromatin-like model

The **composite** component also enables the user to build complicated protein-decorated DNA structures, such as a chromatin-like model. Here, we use a three-nucleosome model as an example.

First the user assigns the number of nucleosomes in the final model to 3.

**Choose a binding site number to build a protein-decorated DNA model:** [e](#)

(maximum binding sites number is 6)

Next, the user enter a DNA sequence of poly dA:poly dT with the length of 520 base pairs. The user can just type in an “A” in the sequence text area and assign the repeating number to 520. Note that the input sequence is that of the leading strand.

**Current choice: 3 binding sites**

**Type in or paste a sequence:**

A

Repeating #:

Then, the user specifies the conformation of the unbound DNA to B-form and provides nucleosome structures (for example PDB ID: 4XZQ) as templates to bind DNA at positions 85, 260 and 435.

**Choose a form of DNA (unbounded)**

B-form  A-form

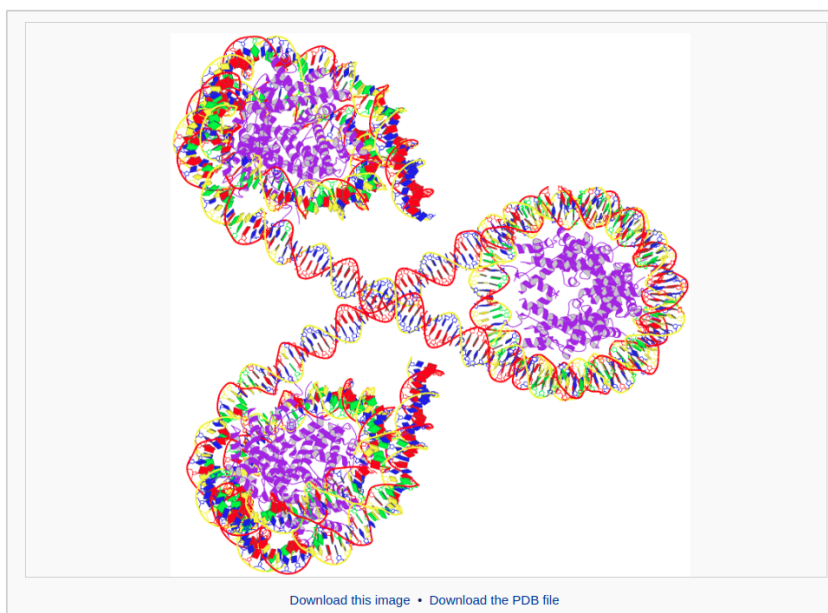
Binding position:	Template PDB ID:
<input type="text" value="85"/>	<input type="text" value="4XZQ"/>
<input type="text" value="260"/>	<input type="text" value="4XZQ"/>
<input type="text" value="435"/>	<input type="text" value="4XZQ"/>

(note: only simple double-stranded DNA-containing structures can be used here)

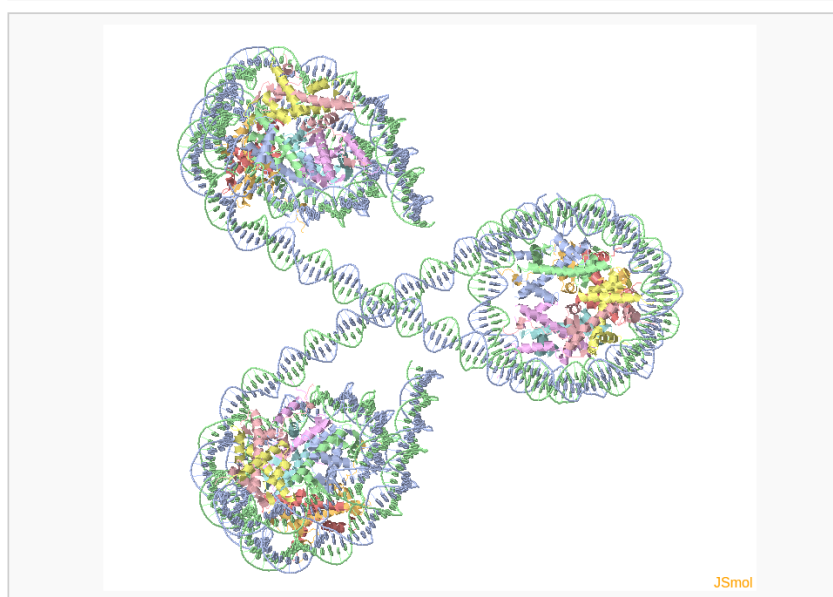
In the confirmation page, the user can verify all the binding information and then click the 'Build' button.



The structure constructed by 3DNA: [Use this structure for mutation]



3D view:





## S4.5 Modeling module: 56 fiber models

The **fiber** component of Web 3DNA 2.0 allows the user to build fiber-diffraction models of nucleic acids with arbitrary sequence and helical types. A total of **56 fiber models** is available in the current web server, with **six commonly used ones** (RNA, A-DNA, B-DNA, C-DNA, Pauling triplex, and poly(I) quadruplex models) placed at the top of the list.

After selecting a fiber model from the list, the user can specify a sequence and/or a repeating unit number. The output webpage includes a schematic representation of the constructed model, a PDB-formatted file with full atomic coordinates of base and sugar-phosphate atoms, and a 3D interactive visualization.

### Commonly used fiber models

Short description	Twist (°)	Rise (Å)	
RNA (generic sequence: A, C, G, U)	32.7	2.548	<input type="button" value="use this model"/>
A-DNA (generic sequence: A, C, G, T)	32.7	2.548	<input type="button" value="use this model"/>
B-DNA (generic sequence: A, C, G, T)	36.0	3.375	<input type="button" value="use this model"/>
C-DNA (generic sequence: A, C, G, T)	40.0	3.32	<input type="button" value="use this model"/>
Pauling triplex model (generic sequence: A, C, G, T, U)	105.0	3.40	<input type="button" value="use this model"/>
poly(I) : poly(I) : poly(I) : poly(I)	31.3	3.410	<input type="button" value="use this model"/>

### Full list of available fiber models

Index	Short description	Twist (°)	Rise (Å)	
1	A-DNA (calf thymus; generic sequence: A, C, G and T)	32.7	2.548	<input type="button" value="use this model"/>
2	A-DNA poly d(ABr5U) : poly d(ABr5U)	65.5	5.095	<input type="button" value="use this model"/>
3	A-DNA (calf thymus) poly d(A1T2C3G4G5A6A7T8G9G10T11)	0.0	28.030	<input type="button" value="use this model"/>
4	B-DNA (calf thymus; generic sequence: A, C, G and T)	36.0	3.375	<input type="button" value="use this model"/>
5	B-DNA poly d(CG) : poly d(CG)	72.0	6.720	<input type="button" value="use this model"/>
6	B-DNA (calf thymus) poly d(C1C2C3C4C5) : poly d(G6G7G8G9G10)	180.0	16.864	<input type="button" value="use this model"/>
7	C-DNA (calf thymus; generic sequence: A, C, G and T)	38.6	3.310	<input type="button" value="use this model"/>
8	C-DNA poly d(GGT) : poly d(ACC)	40.0	3.312	<input type="button" value="use this model"/>
9	C-DNA poly d(G1G2T3) : poly d(A4C5C6)	120.0	9.937	<input type="button" value="use this model"/>
10	C-DNA poly d(AG) : poly d(CT)	80.0	6.467	<input type="button" value="use this model"/>

The detailed parameters of 55 fiber models are listed in the following table, taken from the initial **3DNA publication**. For the Pauling triplex model, please check the blogpost

“Pauling triplex model of nucleic acids is available in 3DNA” on the 3DNA homepage for further information.

Structure description	Repeating sequence	ID ^a	$\Omega_h$ (°)	$h$ (Å)	Shift (Å)	Slide (Å)	Rise (Å)	Tilt (°)	Roll (°)	Twist (°)
A DNA (calf thymus)	generic	1	32.7	2.55	0.00	-1.40	3.30	0.0	12.4	30.3
A DNA	generic	54	32.73	2.56	0.01	-1.49	3.26	-0.1	11.4	30.7
A DNA	ABr ⁵ U-ABr ⁵ U	2	65.5	5.10	0.00	-1.34	3.25	0.0	12.1	30.5
A DNA (calf thymus)	ATCGGAATGGT TAGCCTTACCA	3	360.0	28.03	0.01	-1.27	3.32	-0.1	13.2	30.0
A RNA	A-U	20	32.7	2.81	-0.08	-1.48	3.30	-0.4	8.6	31.6
A' RNA	I-C	21	30.0	3.00	0.05	-1.88	3.39	-0.1	5.4	29.5
B DNA (calf thymus)	generic	4	36.0	3.38	0.00	0.45	3.36	0.0	1.7	36.0
B DNA (BI nucleotides)	generic	46	36.0	3.38	0.00	0.29	3.37	0.0	2.2	35.9
B DNA	generic	55	36.0	3.39	0.01	0.03	3.40	0.0	-2.4	35.9
B DNA	CG-CG	5	72.0	6.72	0.00	0.84	3.29	0.0	3.5	35.8
B DNA (calf thymus)	CCCCC GGGGG	6	180.0	16.86	0.31	0.37	3.36	2.9	0.6	35.9
B' DNA $\alpha$ (H DNA)	A-T	18	36.0	3.23	-0.08	-0.22	3.23	-2.7	-2.9	35.8
B' DNA $\beta_2$ (H DNA $\beta$ )	A-T	19	36.0	3.23	0.42	-0.76	3.16	-0.6	-5.7	35.6
B' DNA $\beta_2$	A-U	37	36.0	3.20	-0.07	-0.55	3.17	-0.3	-2.7	35.9
B' DNA $\beta_1$	A-T	38	36.0	3.24	0.13	-0.33	3.22	1.0	-4.3	35.7
B' DNA $\beta_2$	AI-CT	39	72.0	6.48	0.02	-0.92	3.15	2.8	-5.3	35.5
B' DNA $\beta_1$	AI-CT	40	72.0	6.46	-0.37	-0.45	3.21	-5.7	0.4	35.6
B' DNA	AATT-AATT	41	144.0	13.54	0.00	0.20	3.39	0.0	-0.3	36.3
DNA $\beta$	A-U	43	36.0	3.20	-0.02	-0.69	3.15	0.4	-3.1	35.9
B DNA (Ca salt)	A-T	44	36.0	3.23	0.00	-0.81	3.17	0.0	-3.7	35.8
B DNA (Na salt)	A-T	45	36.0	3.23	-0.02	-0.89	3.16	1.9	-4.0	35.7
B* DNA	A-T	51	31.6	3.22	-0.04	-0.51	3.33	0.2	4.8	31.2
C DNA (calf thymus)	Generic	7	38.6	3.31	-0.01	0.08	3.35	0.0	-5.3	38.2
C DNA (BII nucleotides)	Generic	47	40.0	3.32	0.00	1.75	3.96	0.0	-11.5	38.4
C DNA (LH ^b )	Generic	53	-38.7	3.29	-0.01	0.89	3.20	0.0	-5.5	-38.3
C DNA	GGT-ACC	8	40.0	3.31	-0.01	1.88	3.53	0.0	-4.4	39.8
C DNA	GGT-ACC	9	120.0	9.94	-0.15	1.30	3.53	1.1	-5.9	39.6
C DNA	AG-CT	10	80.0	6.47	0.00	0.84	3.42	0.1	-7.5	39.8
C DNA	AG-CT	11	80.0	6.47	-0.59	0.86	3.46	-2.0	-8.9	39.2
D DNA	AAT-ATT	12	45.0	3.01	0.00	0.85	3.26	0.0	-9.9	44.0
D DNA	CI-CI	13	90.0	6.13	0.00	1.01	3.40	0.0	-11.2	43.7
D DNA	ATATAT-ATATAT	14	-90.0	18.50	0.00	1.07	3.48	0.0	-13.0	43.3
D _A DNA	AT-AT	48	87.8	6.02	0.00	-2.44	3.07	0.0	0.8	43.9
D _B DNA	AT-AT	52	90.0	6.06	0.00	1.25	3.42	0.0	-11.2	43.7
L DNA (calf thymus)	GC-GC	17	0.0	10.20	0.00	-0.42	5.08	0.0	0.0	0.0
S DNA (C _B G _A , RH ^b )	CG-CG	49	60.0	7.20	0.00	-0.23	3.61	0.0	1.3	30.0
S DNA (C _A G _B , RH ^b )	GC-GC	50	60.0	7.20	0.00	-0.18	3.61	0.0	1.3	30.0
Z DNA	GC-GC	15	-60.0	7.25	0.00	1.92	3.59	0.0	0.2	-30.0
Z DNA	As ⁵ T-As ⁴ T	16	-51.4	7.57	0.00	1.28	3.79	0.0	0.9	-25.7
DNA-RNA hybrid	A-dT	22	32.7	2.56	0.00	-1.66	3.27	0.0	10.8	30.9
DNA-RNA hybrid	dG-C	23	32.0	2.78	0.05	-1.78	3.38	-0.2	8.8	30.8
DNA-RNA hybrid	dI-C	24	36.0	3.13	-0.25	-0.56	3.36	-3.5	9.0	34.7
DNA-RNA hybrid	dA-U	25	32.7	3.06	0.10	-1.25	3.40	-1.1	7.1	31.9
10-fold (RNA)	X-X	26	36.0	3.01	0.00	-0.67	3.44	0.0	12.6	33.8
11-fold (RNA)	X-X	27	32.7	2.52	0.00	-1.69	3.20	0.0	10.4	31.0
Symmetric (RNA)	s ² U-s ² U	28	32.7	2.60	0.02	-1.49	3.30	-0.1	11.4	30.7
Asymmetric (RNA)	s ² U-s ² U	29	32.7	2.60	-0.30	-1.39	3.26	-7.1	11.2	30.0
DNA triplex	C-I-C	30	32.7	3.16	0.07	-0.97	3.38	2.2	5.9	32.1
DNA triplex	T-A-T	31	30.0	3.26	0.04	-0.99	3.47	1.8	5.0	29.5
RNA triplex (11-fold)	U-A-U	32	32.7	3.04	0.02	-0.85	3.31	2.4	7.3	31.8
RNA triplex	U-A-U	42	32.7	3.04	0.06	-0.84	3.27	2.5	6.4	32.0
RNA triplex (12-fold)	U-A-U	33	30.0	3.04	-0.01	-1.03	3.32	2.0	6.1	29.3
RNA triplex	I-A-I	34	30.0	3.29	-0.15	-0.81	3.40	0.9	3.2	29.8
RNA quadruplex	I-I-I	35	31.3	3.41	-0.57	-0.36	3.39	0.1	-2.4	31.2
Single-stranded RNA	eC (O2' ethyl)	36	60.0	3.16	3.24	-0.70	3.86	-3.2	24.2	55.2

^a3DNA identification numbers: models 1–43 from Arnott and co-workers (43,44); models 44 and 45 from Alexeev *et al.* (45); models 46 and 47 from van Dam and Levitt (46); models 48–55 from Premilat and Albiser (47–52).

^bLH, left-handed helix; RH, right-handed helix.

### Example 5-1: Construction of a generic B-form DNA fiber model

The user first selects the B-DNA (generic sequence: A, C, G, T) fiber model from the list of “Commonly used fiber models”.

B-DNA (generic sequence: A, C, G, T)	36.0	3.375	<a href="#">use this model</a>
--------------------------------------	------	-------	--------------------------------

The generic DNA fiber models accommodate arbitrary base sequences of any length and only A, T, C, and G characters can be accepted in the input sequence. For a generic fiber, the user can type in a sequence and the number of repeating units as shown below. Note that the input sequence is that of the leading strand.

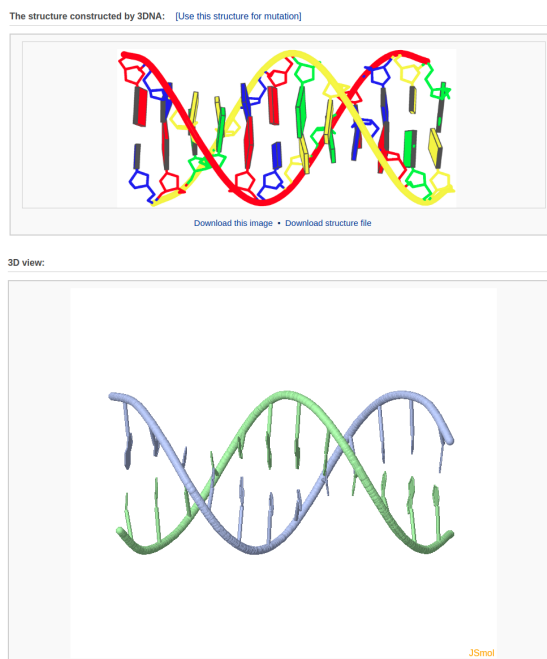
Current choice: B-DNA (generic sequence: A, C, G, T)  
Twist: 36.0° Rise: 3.375 Å

Type in or paste a sequence (ATCG only):  
ATCGATCGATCG

Repeating #:

[Build](#)

After clicking the 'Build' button, the user will be directed to a results page, which contains four sections: 1) a block representation of the constructed model, 2) a link to download a block image of the constructed model, 3) a link to download the coordinates of the constructed model, 4) a 3D interactive visualization of the constructed model.



### Example 5-2: Construction of a Pauling triplex model

The **fiber** component also enables the user to build proposed DNA models. Here, we use the Pauling triplex model as an example.

Pauling triplex model (generic sequence: A, C, G, T, U)

105.0

3.40

use this model

After selecting the Pauling triplex fiber model (generic sequence: A, C, G, T, U) from the list of "Commonly used fiber models", the user can enter a desired sequence, for example "AAAACCCCGGG". The input characters are case-insensitive. Note that the input sequence is the same for all three strands.

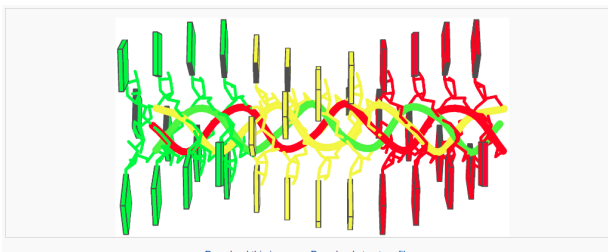
Current choice: Pauling triplex model (generic sequence: A, C, G, T, U)  
Twist: 105.0° Rise: 3.40 Å

Type in or paste a sequence (ACGTU only):  
AAAACCCCGGG

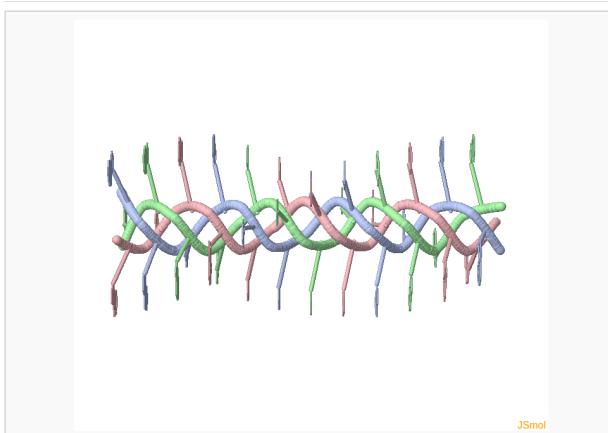
Repeating #: 1

Build

After clicking the 'Build' button, the user is directed to a results page that contains four sections: 1) a block representation of the constructed model, 2) a link to download a block image of the constructed model, 3) a link to download the coordinates of the constructed model, 4) a 3D interactive visualization of the constructed model. The user should notice that the triplex model has phosphates in the center and bases on the outside of the structure.



3D view:



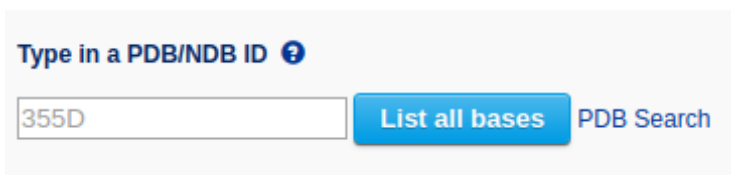
## S4.6 Modeling module: base mutations

The **mutation** component of Web 3DNA 2.0 allows the user to mutate any base(s) of a nucleic acid structure to desired one(s). The user can use a PDB/NDB ID, a user-uploaded PDB-formatted file, or any of the models constructed by the modeling components in the web server. The output includes: 1) schematic representations of the original and mutated structures, 2) a PDB-formatted file with full atomic coordinates of the mutated structure, and 3) 3D interactive visualizations of the original and mutated structures.

It should be noted that both the sugar-phosphate backbone conformation and base reference frame (position and orientation) are preserved in the mutation process. Therefore, the original and mutated structures share the same base-pair/step parameters.

### Example 6-1: Mutate a nucleic-acid-containing structure by using the PDB/NDB ID

The user first enters a PDB ID (for example “355D”) and clicks the ‘List all bases’ button.



The screenshot shows a web interface for searching PDB/NDB IDs. At the top, there is a label "Type in a PDB/NDB ID" followed by a question mark icon. Below this is a text input field containing the text "355D". To the right of the input field is a blue button labeled "List all bases". Further to the right, the text "PDB Search" is visible.

Then the user is directed to an intermediate page where an enumeration of all bases is listed.

PDB ID: 355D

Select base(s) you want to mutate: 

Index	Chain	Residue Num	Current Base	Mutate to					<input type="button" value="Clear all"/>
				All: <input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	
1	A	1	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
2	A	2	G	<input checked="" type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
3	A	3	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
4	A	4	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input checked="" type="radio"/> U	<input type="button" value="Clear"/>
5	A	5	A	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
6	A	6	A	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
7	A	7	T	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
8	A	8	T	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
9	A	9	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
10	A	10	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
11	A	11	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
12	A	12	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
13	B	13	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
14	B	14	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
15	B	15	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
16	B	16	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
17	B	17	A	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
18	B	18	A	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
19	B	19	T	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
20	B	20	T	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
21	B	21	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
22	B	22	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
23	B	23	C	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
24	B	24	G	<input type="radio"/> A	<input type="radio"/> C	<input type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>

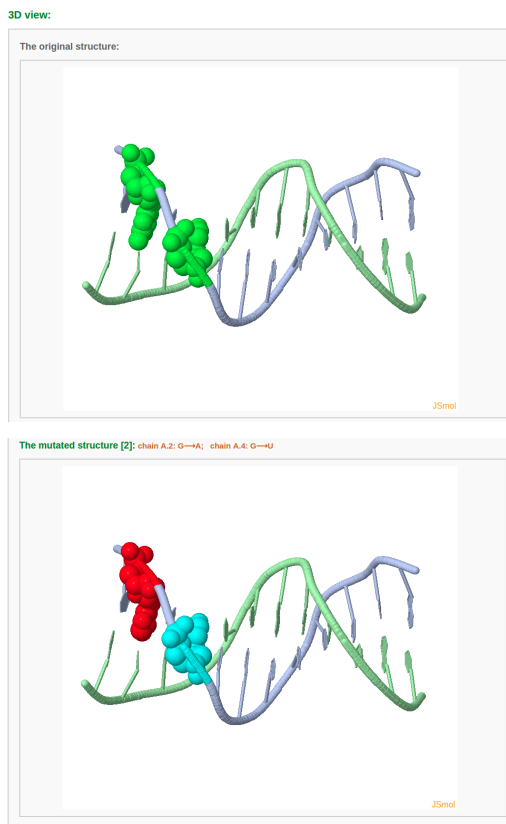
Select base(s) you want to mutate:

After choosing base(s) for mutation (for example here we mutate base G in chain A/residue number 2 to A and base G in chain A/residue number 4 to U) and clicking the “Continue” button, the user will be directed to a results page containing five sections: 1) a block representation of the original structure, 2) a list of mutated bases, 3) a block representation of the mutated structure, 4) a 3D interactive visualization of the original

structure, 5) a 3D interactive visualization of the mutated structure.



The text between the base-block images gives the number and identities of mutated nucleotides.



**Example 6-2: Mutate a structure by uploading a PDB-formatted file**

The user can also upload a PDB-formatted file to conduct base mutation(s). After uploading the structure and clicking the ‘List all bases’ button, the user follows a procedure that is similar to the example of [mutating a structure by using the PDB/NDB ID](#).

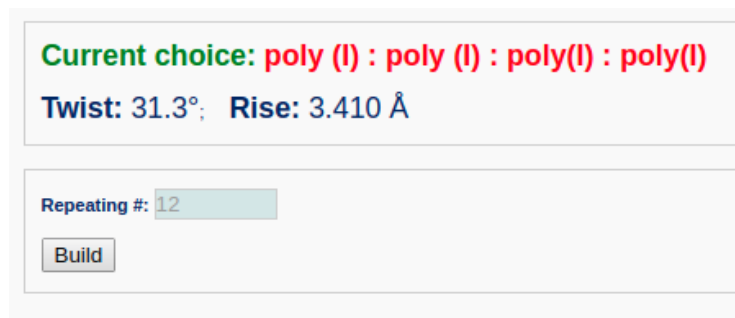
**Example 6-3: Construction of a G-quadruplex DNA model**

The combination of [mutation](#) and [fiber](#) components can be used to build special DNA/RNA models, such as a G-quadruplex DNA model. The steps are as follows:

First, the user selects the poly(I):poly(I):poly(I):poly(I) fiber model from the list of [”Commonly used fiber models”](#).

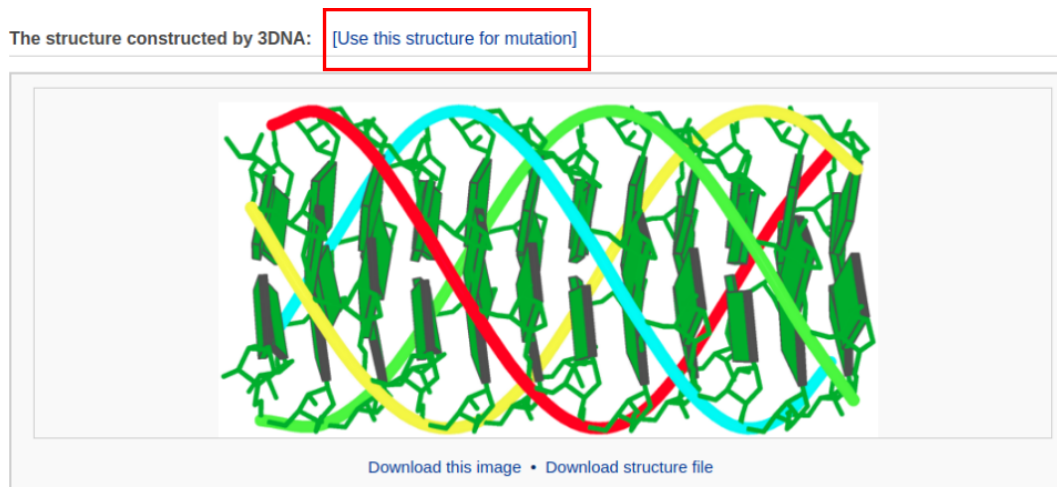


For this non-generic fiber model, the user should enter the number of nucleotide repeating units, for example “12”.

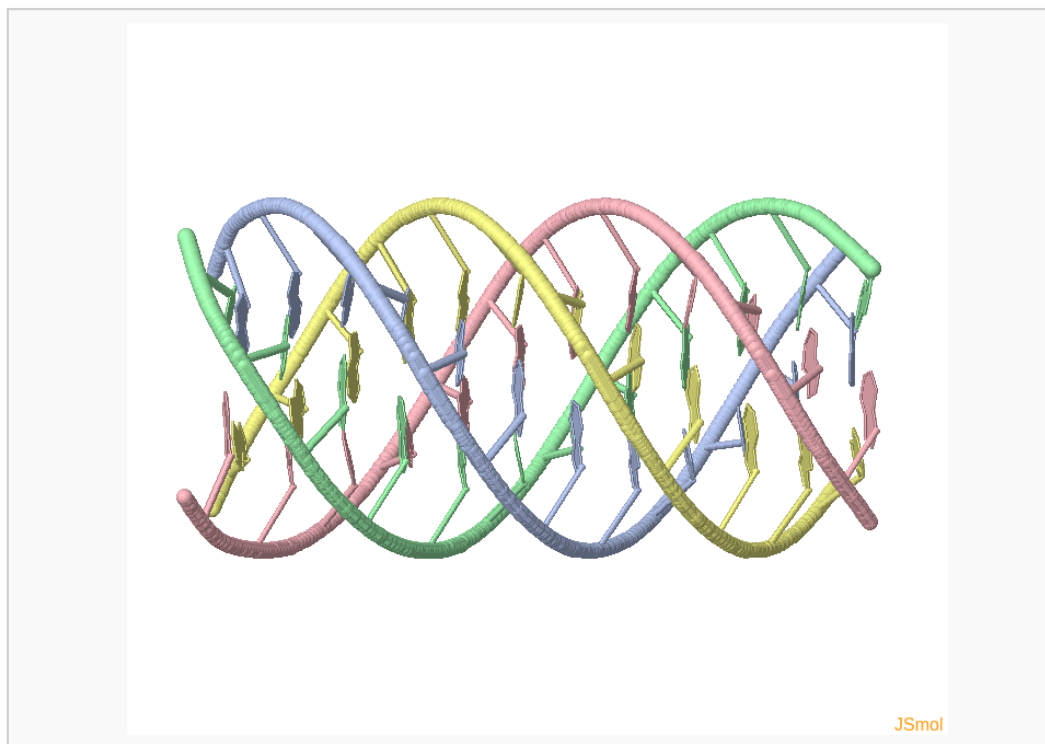


After clicking the ‘Build’ button, the user is directed to a results page containing the constructed model.





3D view:



To build a G-quadruplex DNA model, the user needs to mutate all hypoxanthine bases in the current structure to guanine (G). Clicking the link “Use this structure for mutation” leads the user to a mutation selection interface. The interface contains a list of mutable bases. The user then chooses the option “Mutate to All G” and clicks the “Continue” button. The user will be directed to a results page with the mutated structure: a G-quadruplex DNA model.

Select base(s) you want to mutate:

Index	Chain	Residue Num	Current Base	Mutate to					<input type="button" value="Clear all"/>
				All: <input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	
1	A	1	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
2	A	2	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
3	A	3	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
4	A	4	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
5	A	5	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
6	A	6	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
7	A	7	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
8	A	8	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
9	A	9	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
10	A	10	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
11	A	11	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
12	A	12	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
13	B	13	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
14	B	14	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
15	B	15	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
16	B	16	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
17	B	17	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
18	B	18	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
19	B	19	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>
20	B	20	I	<input type="radio"/> A	<input type="radio"/> C	<input checked="" type="radio"/> G	<input type="radio"/> T	<input type="radio"/> U	<input type="button" value="Clear"/>

The mutated structure [48]: chain A.1: I→G; chain A.2: I→G; chain A.3: I→G; chain A.4: I→G; chain A.5: I→G; chain A.6: I→G; chain A.7: I→G; chain A.8: I→G; chain A.9: I→G; chain A.10: I→G; chain A.11: I→G; chain A.12: I→G; chain B.13: I→G; chain B.14: I→G; chain B.15: I→G; chain B.16: I→G; chain B.17: I→G; chain B.18: I→G; chain B.19: I→G; chain B.20: I→G; chain B.21: I→G; chain B.22: I→G; chain B.23: I→G; chain B.24: I→G; chain C.25: I→G; chain C.26: I→G; chain C.27: I→G; chain C.28: I→G; chain C.29: I→G; chain C.30: I→G; chain C.31: I→G; chain C.32: I→G; chain C.33: I→G; chain C.34: I→G; chain C.35: I→G; chain C.36: I→G; chain D.37: I→G; chain D.38: I→G; chain D.39: I→G; chain D.40: I→G; chain D.41: I→G; chain D.42: I→G; chain D.43: I→G; chain D.44: I→G; chain D.45: I→G; chain D.46: I→G; chain D.47: I→G; chain D.48: I→G;



[Download this image](#) • [Download the mutated PDB file](#)

## S5 Related external resources

- [3DNA Home](#) — the home page of the 3DNA software package
- [3DNA Forum](#) — online discussions of 3DNA-related questions
- [Web DSSR](#) — a webserver for DSSR (Dissecting the Spatial Structure of RNA)
- [do_x3dna](#) — software built on top of 3DNA for the analysis of DNA/RNA molecular dynamics simulations
- [3D-DART \(3DNA-Driven DNA Analysis and Rebuilding Tool\)](#) — a server for generating 3D structural models of double-stranded DNA
- [Phenix](#) — a software suite for the automated determination of molecular structures using X-ray crystallography and other methods. Web 3DNA 2.0 employs the "phenix.geometry_minimization" command to [optimize backbone geometry while keeping base atoms fixed](#)
- [Curves+](#) — a popular approach for analyzing the structures of nucleic acids
- [NAB \(Nucleic Acid Builder\)](#) — a molecular manipulation language for constructing 3D structures of nucleic acids
- [make-na server](#) — a web-based automated tool for making nucleic acid helices powered by NAB
- [NUCGEN-Plus](#) — a web-server for generating sequence-dependent nonuniform nucleic acid structures
- [NUPARM](#) — a program for analyzing sequence-dependent variations in nucleic acid (DNA & RNA) double helices
- [RCSB PDB](#) — a database about 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease
- [Nucleic Acid Database](#) — a database containing information about experimentally-determined nucleic acids and complex assemblies