

Electronic Supplementary Information (ESI)

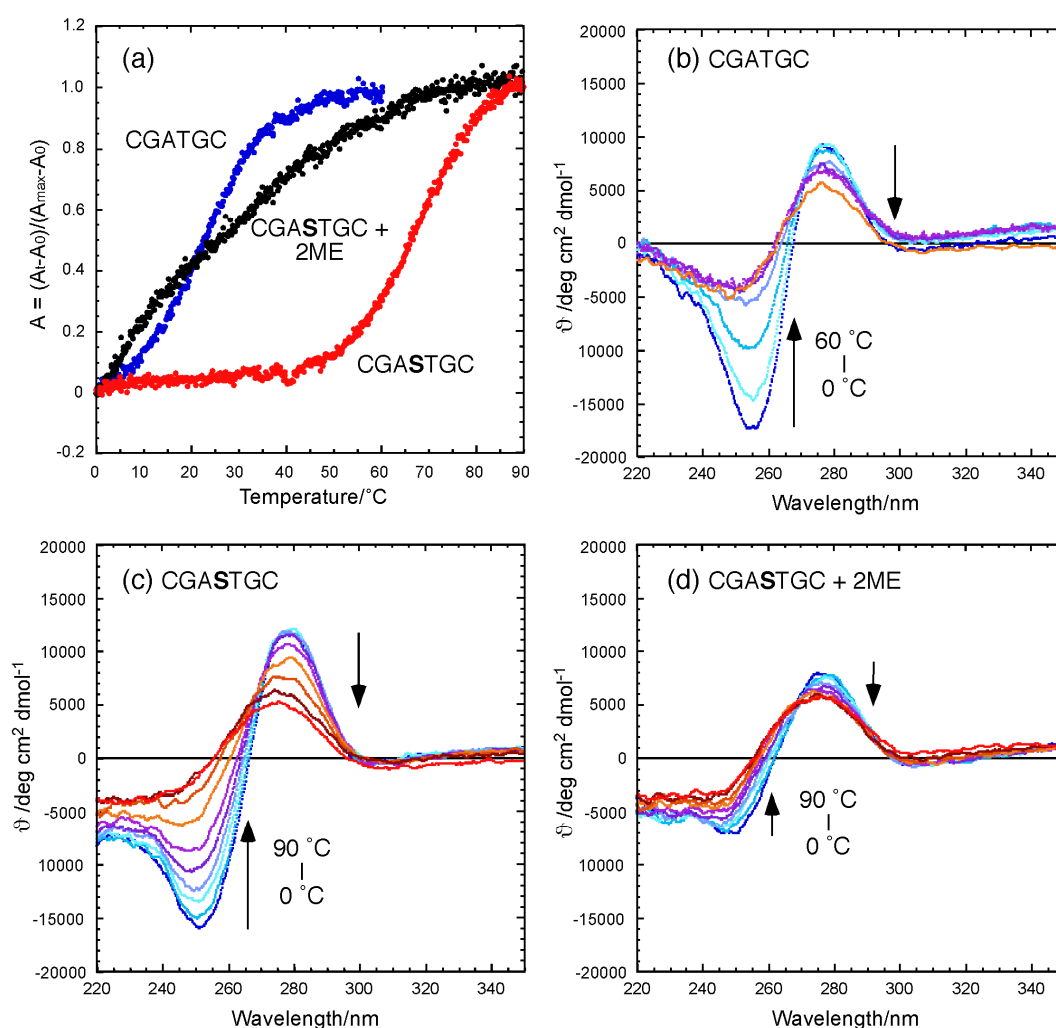
Solution structure of S-DNA formed by covalent base pairing involving a disulfide bond

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- Supplementary Data 1.** Melting curves and CD spectra.
- Supplementary Data 2.** Proton Assignment Table.
- Supplementary Data 3.** NOESY spectrum from 4.5 to 9.0 ppm for C¹G²A³S⁴T⁵C⁶G⁷.
- Supplementary Data 4.** NOESY spectrum from 0 to 4.5 ppm for C¹G²A³S⁴T⁵C⁶G⁷.
- Supplementary Data 5.** NOESY spectrum between the imino protons and the base protons for C¹G²A³S⁴T⁵C⁶G⁷.
- Supplementary Data 6.** Structures of four different base pairs.
- Supplementary Data 7.** The shapes of backbone and the helical axis for B-DNA and S-DNA calculated by Curves+ 1.3.
- Supplementary Data 8.** Comparison of each conformation of S-DNA and B-DNA calculated by Curves+ 1.3.
- Supplementary Data 9.** Parameter file.

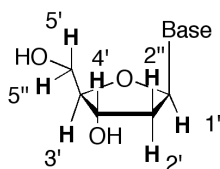


Supplementary Data 1. Melting curves and CD spectra for the duplexes induced by the formation of disulfide bonding. (a) showed UV melting curves (260 nm), Red: CGASTCG, black: CGASTCG in the presence of 100 μ M of 2-mercaptoethanol, blue: CGATCG. (b) CD spectra of CGATCG for temperature, (c) CD spectra of CGASTCG for temperature, (d) CD spectra of CGASTCG for temperature in the presence of 100 μ M of 2-mercaptoethanol.

Supplementary Data 2. Proton Assignment Table for C¹G²A³S⁴T⁵C⁶G⁷ at 280 K in 10 mM sodium phosphate buffer and 200 mM NaCl in D₂O.

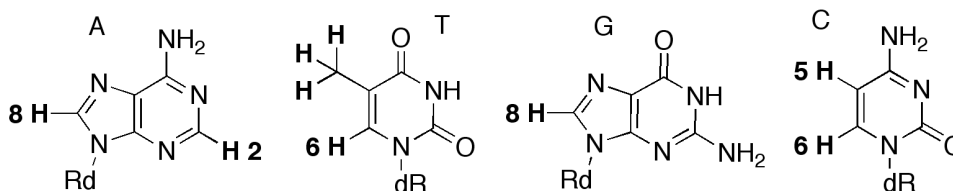
Ribosyl protons

	C ¹	G ²	A ³	S ⁴	T ⁵	C ⁶	G ⁷
H1'	5.38	4.94	5.64	4.66	5.61	5.37	5.93
H2'	1.38	2.29	2.40	1.51	1.85	1.77	2.10
H2''	1.96	2.29	2.50	2.21	2.13	2.08	2.39
H3'	4.36	4.67	4.75	4.42	4.55	4.55	4.42
H4'	3.75	3.98	4.16	3.96	3.85	3.89	3.94
H5'	3.41	3.63	3.72	3.85	3.78	3.49	3.88
H5''	3.44	3.68	3.72	3.85	3.78	3.49	3.88



Base protons

	C ¹	G ²	A ³	S ⁴	T ⁵	C ⁶	G ⁷
H2	-	-	7.46	-	-	-	-
H5	5.42	-	-	6.05	-	5.61	-
H6	7.31	-	-	6.54	7.01	7.26	-
H8	-	7.62	7.94	-	-	-	7.71



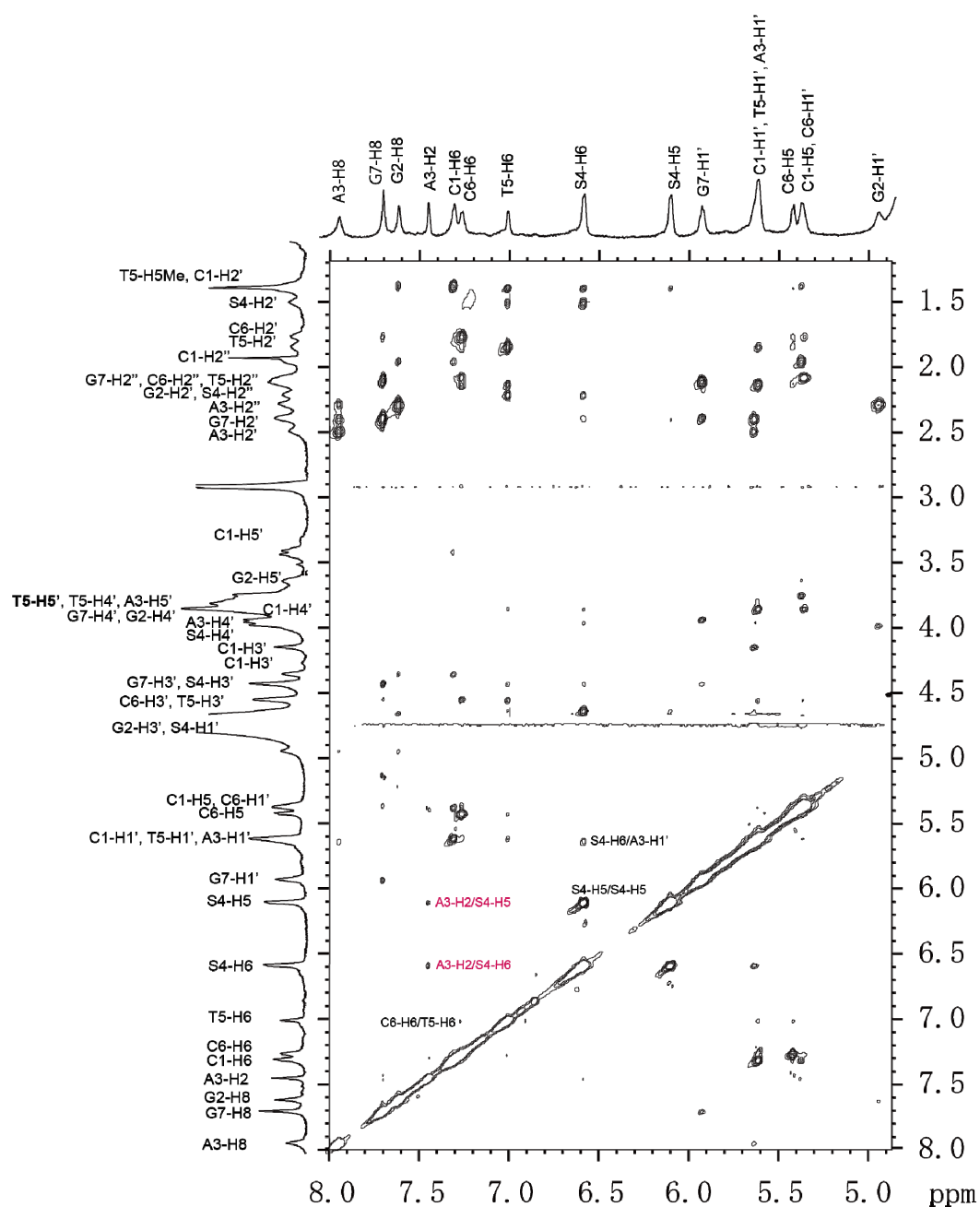
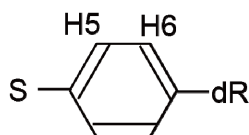
Imino protons (10 mM sodium phosphate buffer and 200 mM NaCl in 10 % D₂O, pH 6.8)

	C ¹	G ²	A ³	S ⁴	T ⁵	C ⁶	G ⁷
H1 or H3	-	12.8	-	-	13.4	-	13.0

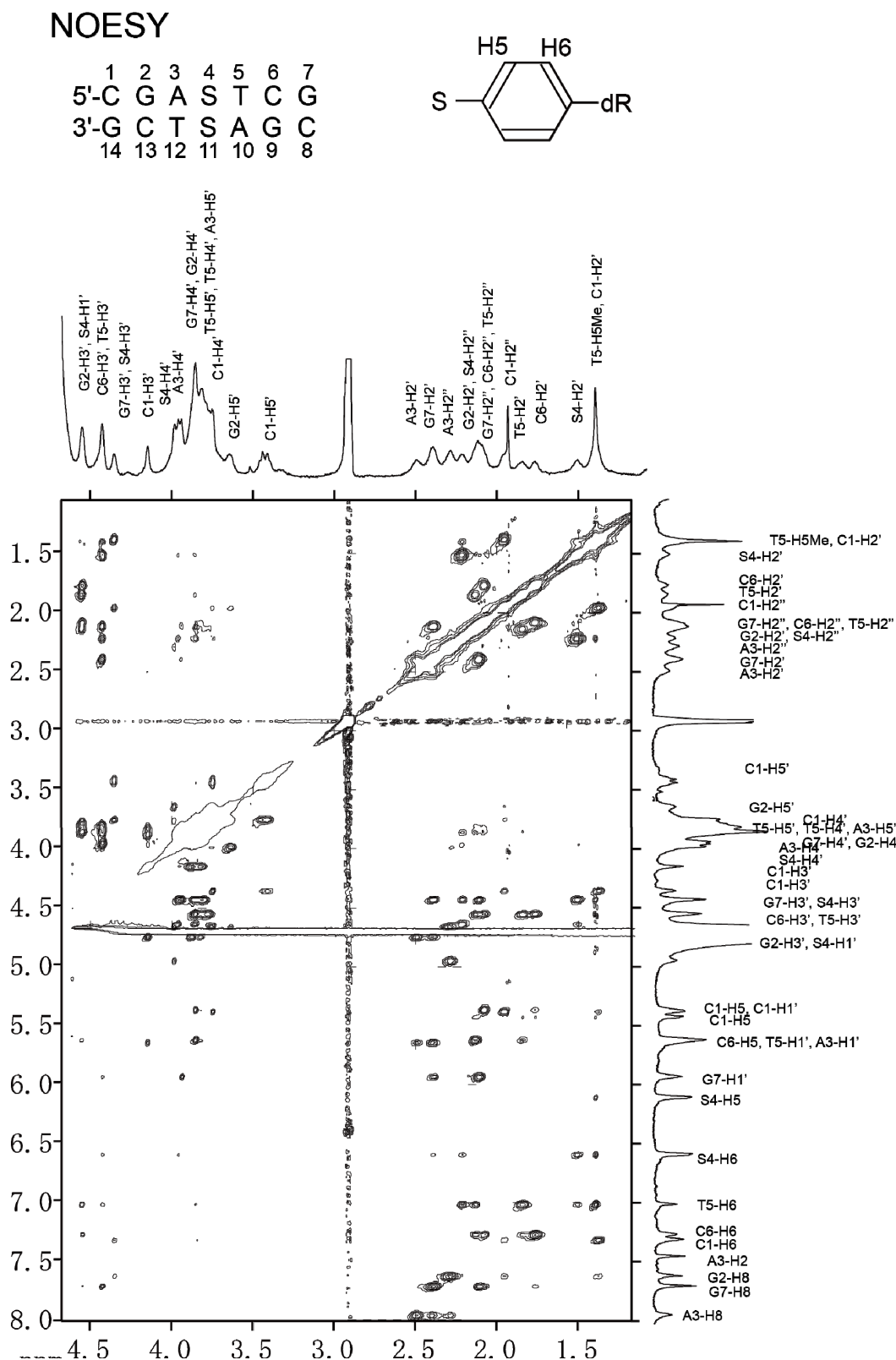
Supplementary Data 3. NOESY spectrum from 4.5 to 9.0 ppm for $C^1G^2A^3S^4T^5C^6G^7$ at 280 K in 10 mM sodium phosphate buffer and 200 mM NaCl in D_2O .

NOESY

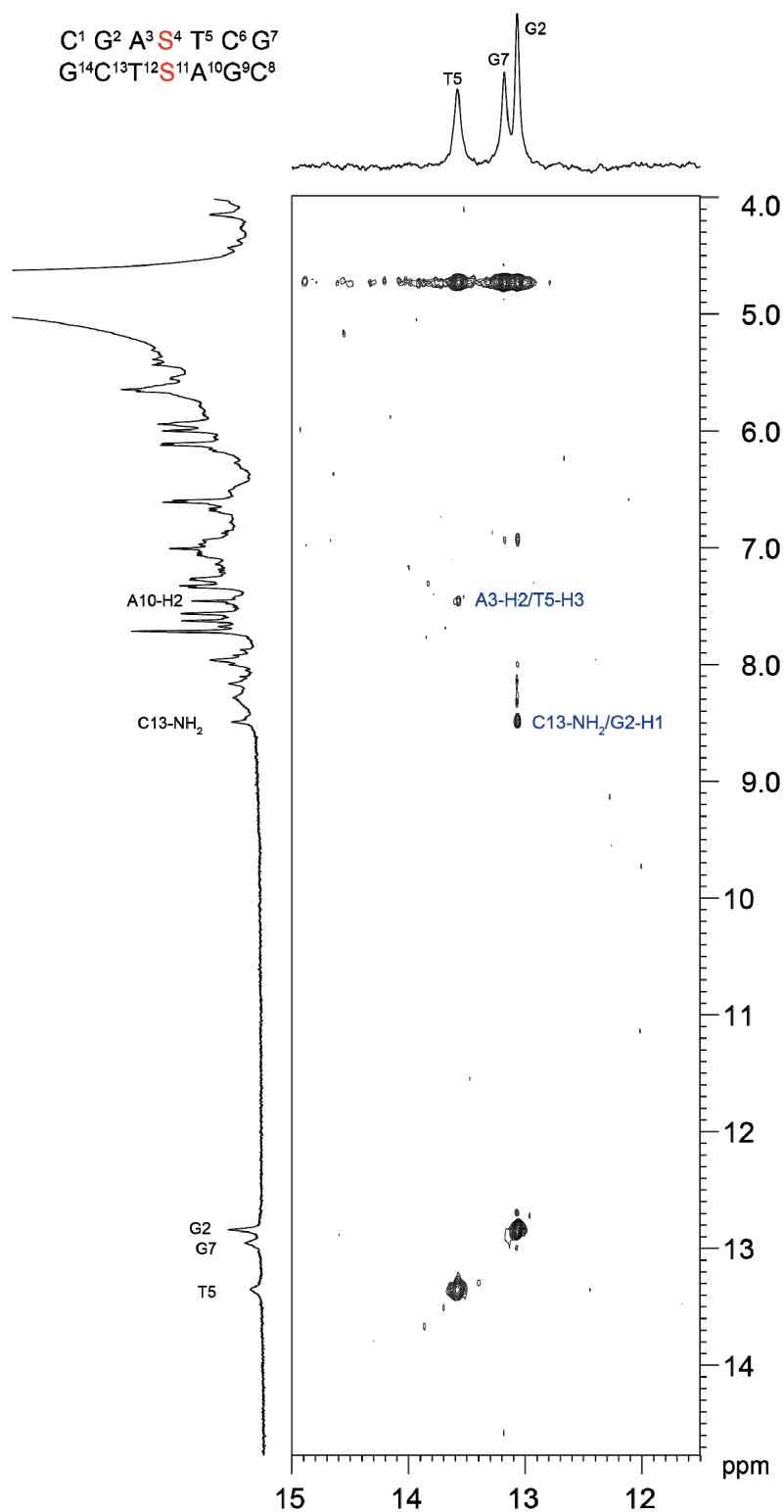
	1	2	3	4	5	6	7
5'-C	G	A	S	T	C	G	
3'-G	C	T	S	A	G	C	
	14	13	12	11	10	9	8

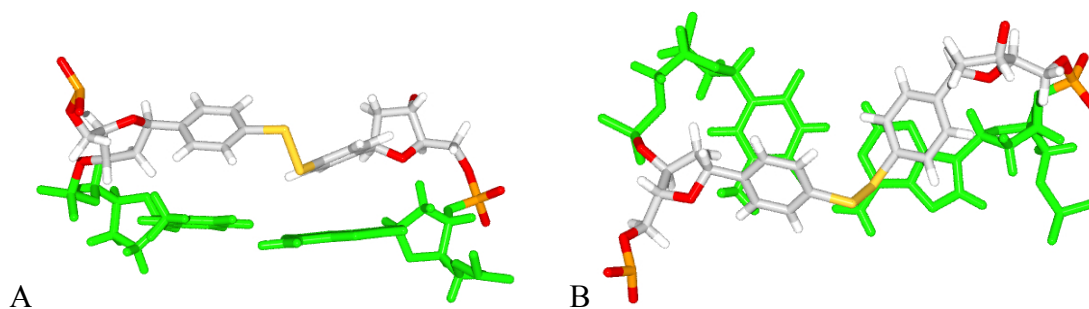


Supplementary Data 4. NOESY spectrum from 0 to 4.5 ppm for C¹G²A³S⁴T⁵C⁶G⁷ at 280 K in 10 mM sodium phosphate buffer and 200 mM NaCl in D₂O.

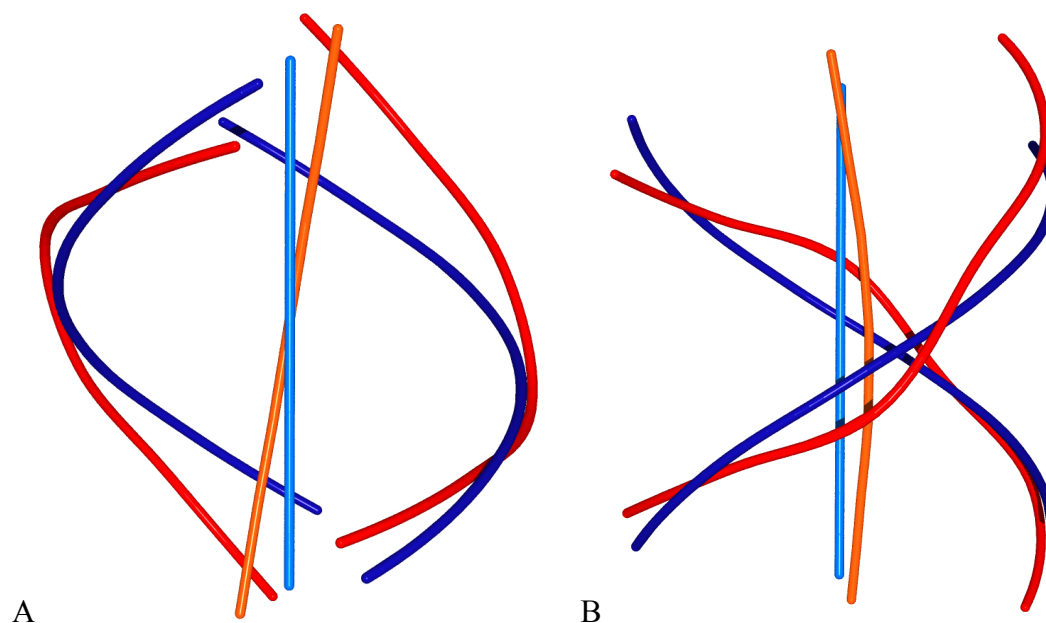


Supplementary Data 5. NOESY spectrum between the imino protons and the base protons for C¹G²A³S⁴T⁵C⁶G⁷ at 280 K in 10 mM sodium phosphate buffer and 200 mM NaCl contained 10 % D₂O (H₂O:D₂O/90:10), pH 6.8.





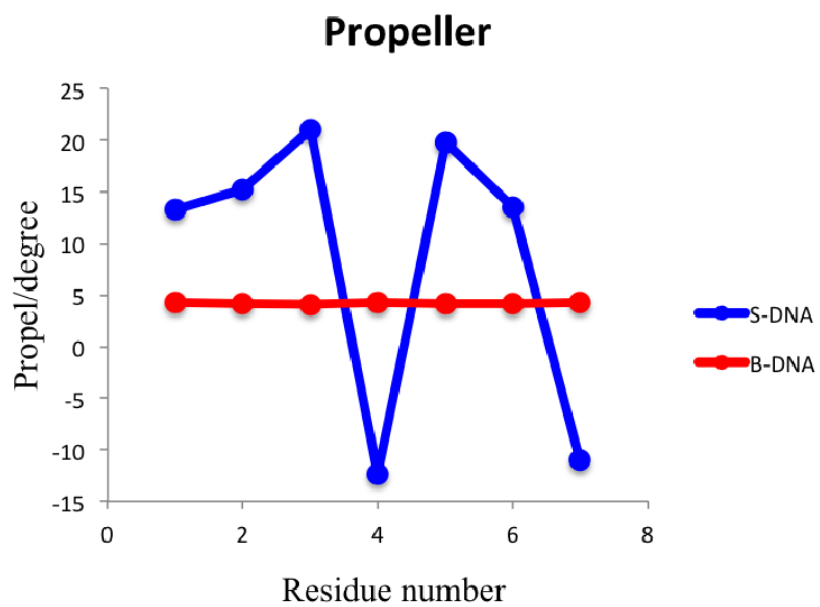
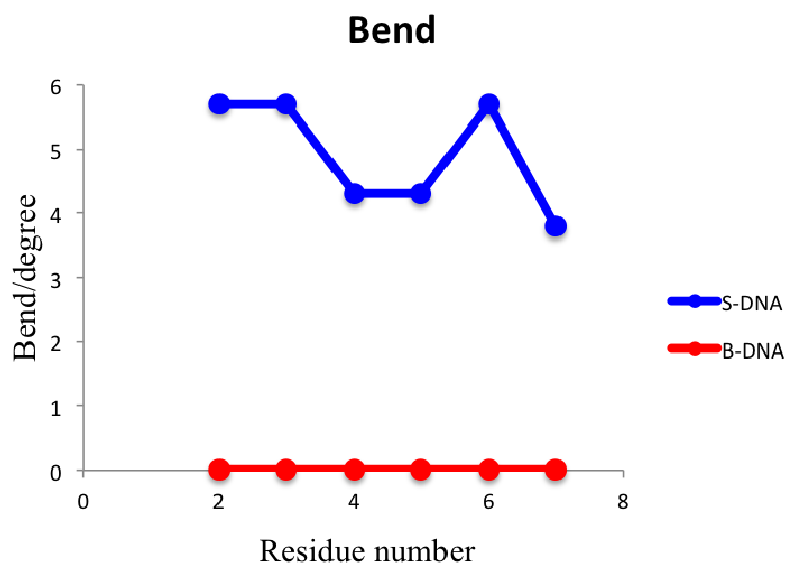
Supplementary Data 6. Structures of four different base pairs ($S^4T^5:A^{10}S^{11}$) in the S-DNA ($C^1G^2A^3S^4T^5C^6G^7$). The adjacent nucleotides were illustrated to realize the base stacking arrangements. A: a side view of $T^5:A^{10}$ (light green) and $S^4:S^{11}$ (bold stick form), B: an upper view of these base pairs.

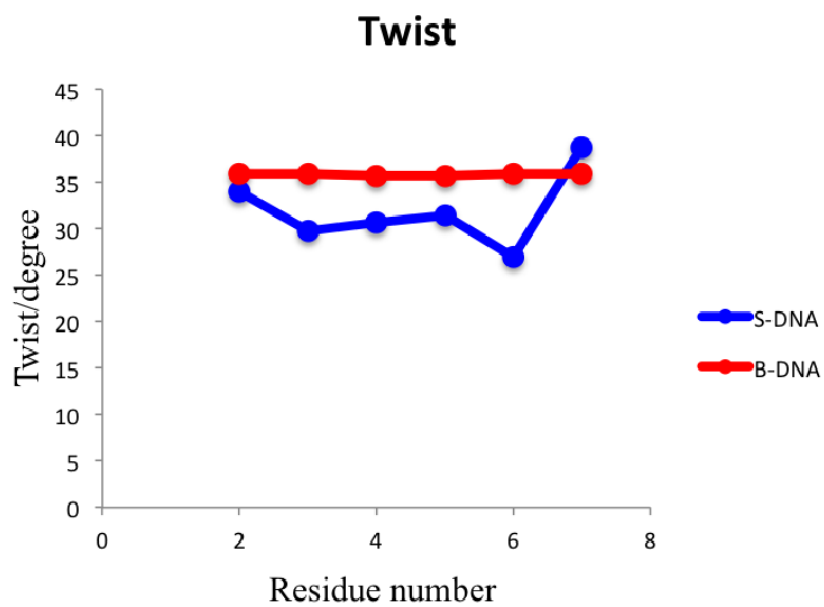
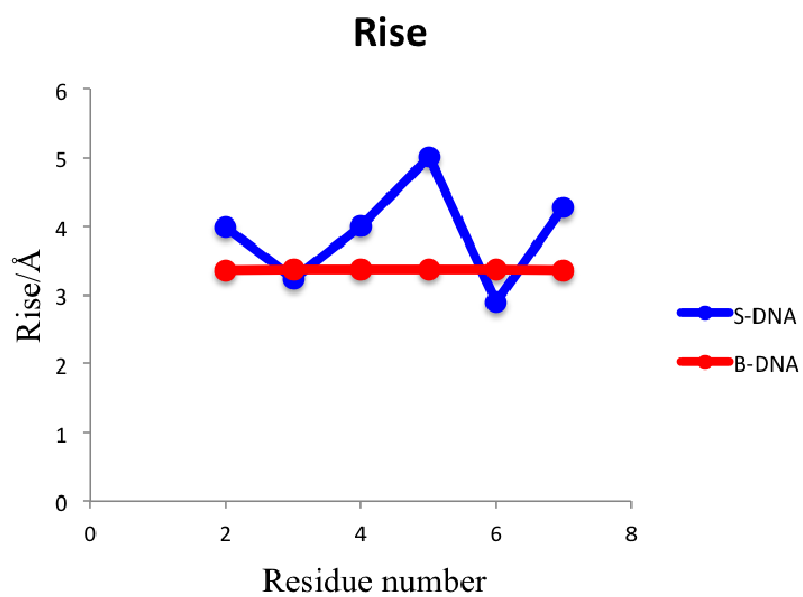


Supplementary Data 7. The shapes of backbone and the helical axis for B-DNA and S-DNA calculated by Curves+ version 1.3.¹ A: the shapes of backbone (blue: B-DNA, red: S-DNA) and the helical axis (light blue: B-DNA, orange: S-DNA), B: the structure rotated by 90° to the left for A on a vertical axis. The total bend of base pair axis of S-DNA was 29°. !

Supplementary Data 8. Comparison of each conformation of S-DNA and B-DNA calculated by Curves+ ver1.3.¹ The numbers on the x axis refer to the base sequence (1 = C, 2 = G, 3 = A, 4 =

S, 5 = T, 6 = C, 7 = G).





Supplementary Data 9. Parameter file.

SD 9-1 Parameter file of dihedral restraints.

!DNA-B helix

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!C2'-endo form

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!DNA-B helix

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!C2'-endo form

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assign (segid B and resid 1 and name O4' )(segid B and resid 1 and name C1' )
    (segid B and resid 1 and name C2' )(segid B and resid 1 and name C3' ) 1.0 29.42 15.00 2
assign (segid B and resid 1 and name C1' )(segid B and resid 1 and name C2' )
    (segid B and resid 1 and name C3' )(segid B and resid 1 and name C4' ) 1.0 -34.92 15.00 2
assign (segid B and resid 1 and name C2' )(segid B and resid 1 and name C3' )
    (segid B and resid 1 and name C4' )(segid B and resid 1 and name O4' ) 1.0 33.25 15.00 2
assign (segid B and resid 1 and name C3' )(segid B and resid 1 and name C4' )
    (segid B and resid 1 and name O4' )(segid B and resid 1 and name C1' ) 1.0 -18.33 15.00 2
assign (segid B and resid 2 and name C4' )(segid B and resid 2 and name O4' )
    (segid B and resid 2 and name C1' )(segid B and resid 2 and name C2' ) 1.0 -4.22 15.00 2
assign (segid B and resid 2 and name O4' )(segid B and resid 2 and name C1' )
    (segid B and resid 2 and name C2' )(segid B and resid 2 and name C3' ) 1.0 29.42 15.00 2
assign (segid B and resid 2 and name C1' )(segid B and resid 2 and name C2' )
    (segid B and resid 2 and name C3' )(segid B and resid 2 and name C4' ) 1.0 -34.92 15.00 2
assign (segid B and resid 2 and name C2' )(segid B and resid 2 and name C3' )
    (segid B and resid 2 and name C4' )(segid B and resid 2 and name O4' ) 1.0 33.25 15.00 2
assign (segid B and resid 2 and name C3' )(segid B and resid 2 and name C4' )
    (segid B and resid 2 and name O4' )(segid B and resid 2 and name C1' ) 1.0 -18.33 15.00 2
assign (segid B and resid 3 and name C4' )(segid B and resid 3 and name O4' )
    (segid B and resid 3 and name C1' )(segid B and resid 3 and name C2' ) 1.0 -4.22 15.00 2
assign (segid B and resid 3 and name O4' )(segid B and resid 3 and name C1' )
    (segid B and resid 3 and name C2' )(segid B and resid 3 and name C3' ) 1.0 29.42 15.00 2
assign (segid B and resid 3 and name C1' )(segid B and resid 3 and name C2' )
    (segid B and resid 3 and name C3' )(segid B and resid 3 and name C4' ) 1.0 -34.92 15.00 2
assign (segid B and resid 3 and name C2' )(segid B and resid 3 and name C3' )
    (segid B and resid 3 and name C4' )(segid B and resid 3 and name O4' ) 1.0 33.25 15.00 2
assign (segid B and resid 3 and name C3' )(segid B and resid 3 and name C4' )
    (segid B and resid 3 and name O4' )(segid B and resid 3 and name C1' ) 1.0 -18.33 15.00 2
assign (segid B and resid 5 and name C4' )(segid B and resid 5 and name O4' )
    (segid B and resid 5 and name C1' )(segid B and resid 5 and name C2' ) 1.0 -4.22 15.00 2
assign (segid B and resid 5 and name O4' )(segid B and resid 5 and name C1' )
    (segid B and resid 5 and name C2' )(segid B and resid 5 and name C3' ) 1.0 29.42 15.00 2
assign (segid B and resid 5 and name C1' )(segid B and resid 5 and name C2' )
    
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        (segid B and resid 5 and name C3' )(segid B and resid 5 and name C4' ) 1.0 -34.92 15.00 2
assign (segid B and resid 5 and name C2' )(segid B and resid 5 and name C3' )

        (segid B and resid 5 and name C4' )(segid B and resid 5 and name O4' ) 1.0 33.25 15.00 2
assign (segid B and resid 5 and name C3' )(segid B and resid 5 and name C4' )

        (segid B and resid 5 and name O4' )(segid B and resid 5 and name C1' ) 1.0 -18.33 15.00 2
assign (segid B and resid 6 and name C4' )(segid B and resid 6 and name O4' )

        (segid B and resid 6 and name C1' )(segid B and resid 6 and name C2' ) 1.0 -4.22 15.00 2
assign (segid B and resid 6 and name O4' )(segid B and resid 6 and name C1' )

        (segid B and resid 6 and name C2' )(segid B and resid 6 and name C3' ) 1.0 29.42 15.00 2
assign (segid B and resid 6 and name C1' )(segid B and resid 6 and name C2' )

        (segid B and resid 6 and name C3' )(segid B and resid 6 and name C4' ) 1.0 -34.92 15.00 2
assign (segid B and resid 6 and name C2' )(segid B and resid 6 and name C3' )

        (segid B and resid 6 and name C4' )(segid B and resid 6 and name O4' ) 1.0 33.25 15.00 2
assign (segid B and resid 6 and name C3' )(segid B and resid 6 and name C4' )

        (segid B and resid 6 and name O4' )(segid B and resid 6 and name C1' ) 1.0 -18.33 15.00 2
assign (segid B and resid 7 and name C4' )(segid B and resid 7 and name O4' )

        (segid B and resid 7 and name C1' )(segid B and resid 7 and name C2' ) 1.0 -4.22 15.00 2
assign (segid B and resid 7 and name O4' )(segid B and resid 7 and name C1' )

        (segid B and resid 7 and name C2' )(segid B and resid 7 and name C3' ) 1.0 29.42 15.00 2
assign (segid B and resid 7 and name C1' )(segid B and resid 7 and name C2' )

        (segid B and resid 7 and name C3' )(segid B and resid 7 and name C4' ) 1.0 -34.92 15.00 2
assign (segid B and resid 7 and name C2' )(segid B and resid 7 and name C3' )

        (segid B and resid 7 and name C4' )(segid B and resid 7 and name O4' ) 1.0 33.25 15.00 2
assign (segid B and resid 7 and name C3' )(segid B and resid 7 and name C4' )

        (segid B and resid 7 and name O4' )(segid B and resid 7 and name C1' ) 1.0 -18.33 15.00 2

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!anti form

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assign (segid B and resid 1 and name O4' )(segid B and resid 1 and name C1' )

        (segid B and resid 1 and name N1 )(segid B and resid 1 and name C2 ) 1.0 -98.00 30.00 2
assign (segid B and resid 2 and name O4' )(segid B and resid 2 and name C1' )

        (segid B and resid 2 and name N9 )(segid B and resid 2 and name C4 ) 1.0 -98.00 30.00 2
assign (segid B and resid 3 and name O4' )(segid B and resid 3 and name C1' )

        (segid B and resid 3 and name N9 )(segid B and resid 3 and name C4 ) 1.0 -98.00 30.00 2

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assign (segid B and resid 5 and name O4' )(segid B and resid 5 and name C1' )  
      (segid B and resid 5 and name N1 )(segid B and resid 5 and name C2 ) 1.0 -98.00 30.00 2  
assign (segid B and resid 6 and name O4' )(segid B and resid 6 and name C1' )  
      (segid B and resid 6 and name N1 )(segid B and resid 6 and name C2 ) 1.0 -98.00 30.00 2  
assign (segid B and resid 7 and name O4' )(segid B and resid 7 and name C1' )  
      (segid B and resid 7 and name N9 )(segid B and resid 7 and name C4 ) 1.0 -98.00 30.00 2
```

SD 9-2 Parameter file of hydrogen bonds.

!hbond

```
assign (segid A and resid 1 and name O2 )(segid B and resid 7 and name H22 ) 1.900 0.100 0.100
assign (segid A and resid 1 and name N3 )(segid B and resid 7 and name H1 ) 1.900 0.100 0.100
assign (segid A and resid 1 and name H42 )(segid B and resid 7 and name O6 ) 1.900 0.100 0.100
assign (segid A and resid 2 and name H22 )(segid B and resid 6 and name O2 ) 1.900 0.100 0.100
assign (segid A and resid 2 and name H1 )(segid B and resid 6 and name N3 ) 1.900 0.100 0.100
assign (segid A and resid 2 and name O6 )(segid B and resid 6 and name H42 ) 1.900 0.100 0.100
assign (segid A and resid 3 and name H62 )(segid B and resid 5 and name O4 ) 1.900 0.100 0.100
assign (segid A and resid 3 and name N1 )(segid B and resid 5 and name H3 ) 1.900 0.100 0.100
assign (segid A and resid 5 and name O4 )(segid B and resid 3 and name H62 ) 1.900 0.100 0.100
assign (segid A and resid 5 and name H3 )(segid B and resid 3 and name N1 ) 1.900 0.100 0.100
assign (segid A and resid 6 and name O2 )(segid B and resid 2 and name H22 ) 1.900 0.100 0.100
assign (segid A and resid 6 and name N3 )(segid B and resid 2 and name H1 ) 1.900 0.100 0.100
assign (segid A and resid 6 and name H42 )(segid B and resid 2 and name O6 ) 1.900 0.100 0.100
assign (segid A and resid 7 and name H22 )(segid B and resid 1 and name O2 ) 1.900 0.100 0.100
assign (segid A and resid 7 and name H1 )(segid B and resid 1 and name N3 ) 1.900 0.100 0.100
assign (segid A and resid 7 and name O6 )(segid B and resid 1 and name H42 ) 1.900 0.100 0.100
```

set message=on echo=on end

9-3 Parameter file of NOE restrains.

!"-PLOR restraint NOE modified by CNS_noeEdit

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assign (segid A and resi 6 and name H5) (segid A and resi 5 and name H7*) 3.60 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H7*) (segid A and resi 6 and name H5) 4.02 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 6 and name H5) 3.55 0.50 1.00 !!modified:
assign (segid A and resi 4 and (name H5 or name H3)) (segid A and resi 3 and name H2) 3.56 0.50
1.00 !!modified:
assign (segid A and resi 6 and name H1') (segid A and resi 6 and name H6) 3.50 0.50 1.00 !!modified:
assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 5 and name H6) 3.96 0.50
1.00 !!modified:
assign (segid A and resi 6 and name H5) (segid A and resi 5 and name H6) 3.51 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H1') (segid A and resi 4 and (name H5 or name H3)) 3.66 0.50
1.00 !!modified:
assign (segid A and resi 6 and name H3') (segid A and resi 7 and name H8) 3.62 0.50 1.00 !!modified:

assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 3 and name H2') 3.33 0.50
1.00 !!modified:
assign (segid A and resi 4 and (name H5 or name H3)) (segid A and resi 3 and name H2'') 3.31 0.50
1.00 !!modified:
assign (segid A and resi 3 and name H8) (segid A and resi 3 and name H2'') 2.51 0.50 1.00 !!modified:
assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 3 and name H2'') 3.06 0.50
1.00 !!modified:
assign (segid A and resi 7 and name H1') (segid A and resi 7 and name H2') 2.64 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H8) (segid A and resi 2 and name H2') 2.66 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 4 and name H2'') 2.60 0.50 1.00 !!modified:
assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 4 and name H2'') 2.91 0.50
1.00 !!modified:
assign (segid A and resi 6 and name H6) (segid A and resi 5 and name H2'') 2.66 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 5 and name H2'') 2.72 0.50 1.00 !!modified:
assign (segid A and resi 6 and name H5) (segid A and resi 5 and name H2'') 2.73 0.50 1.00 !!modified:
assign (segid A and resi 6 and name H6) (segid A and resi 6 and name H2'') 2.59 0.50 1.00 !!modified:
    
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assign (segid A and resi 2 and name H8) (segid A and resi 1 and name H2") 2.94 0.50 1.00 !!modified:
 assign (segid A and resi 1 and name H6) (segid A and resi 1 and name H2") 2.95 0.50 1.00 !!modified:
 assign (segid A and resi 6 and name H6) (segid A and resi 5 and name H2') 2.93 0.50 1.00 !!modified:
 assign (segid A and resi 5 and name H1') (segid A and resi 5 and name H2') 2.75 0.50 1.00 !!modified:
 assign (segid A and resi 6 and name H5) (segid A and resi 5 and name H2') 3.02 0.50 1.00 !!modified:
 assign (segid A and resi 7 and name H8) (segid A and resi 6 and name H2') 2.99 0.50 1.00 !!modified:
 assign (segid A and resi 6 and name H5) (segid A and resi 6 and name H2') 3.06 0.50 1.00 !!modified:
 assign (segid A and resi 6 and name H1') (segid A and resi 6 and name H2') 2.83 0.50 1.00 !!modified:
 assign (segid A and resi 5 and name H6) (segid A and resi 4 and name H2") 2.87 0.50 1.00 !!modified:
 assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 4 and name H2') 2.58 0.50
 1.00 !!modified:
 assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 5 and name H7*) 2.85 0.50
 1.00 !!modified:
 assign (segid A and resi 4 and (name H5 or name H3)) (segid A and resi 5 and name H7*) 3.24 0.50
 1.00 !!modified:
 assign (segid A and resi 6 and name H5) (segid A and resi 5 and name H7*) 3.43 0.50 1.00 !!modified:
 assign (segid A and resi 2 and name H8) (segid A and resi 1 and name H2') 2.90 0.50 1.00 !!modified:
 assign (segid A and resi 1 and name H1') (segid A and resi 1 and name H2') 2.99 0.50 1.00 !!modified:
 assign (segid A and resi 3 and name H2") (segid A and resi 3 and name H8) 2.56 0.50 1.00 !!modified:
 assign (segid A and resi 2 and name H2*) (segid A and resi 3 and name H8) 2.73 0.50 1.00 !!modified:
 assign (segid A and resi 6 and name H2') (segid A and resi 7 and name H8) 3.12 0.50 1.00 !!modified:
 assign (segid A and resi 1 and name H2") (segid A and resi 2 and name H8) 2.97 0.50 1.00 !!modified:
 assign (segid A and resi 1 and name H2') (segid A and resi 2 and name H8) 2.91 0.50 1.00 !!modified:
 assign (segid A and resi 1 and name H2") (segid A and resi 1 and name H6) 2.96 0.50 1.00 !!modified:
 assign (segid A and resi 5 and name H2') (segid A and resi 6 and name H6) 2.89 0.50 1.00 !!modified:
 assign (segid A and resi 5 and name H2") (segid A and resi 6 and name H6) 2.69 0.50 1.00 !!modified:
 assign (segid A and resi 6 and name H2") (segid A and resi 6 and name H6) 2.64 0.50 1.00 !!modified:
 assign (segid A and resi 5 and name H2") (segid A and resi 5 and name H6) 2.76 0.50 1.00 !!modified:
 assign (segid A and resi 4 and name H2') (segid A and resi 5 and name H6) 2.90 0.50 1.00 !!modified:
 assign (segid A and resi 4 and name H2") (segid A and resi 4 and (name H6 or name H2)) 2.99 0.50
 1.00 !!modified:
 assign (segid A and resi 4 and name H2') (segid A and resi 4 and (name H6 or name H2)) 2.65 0.50
 1.00 !!modified:

assign (segid A and resi 5 and name H7*) (segid A and resi 4 and (name H6 or name H2)) 2.86 0.50
1.00 !!modified:
assign (segid A and resi 3 and name H2") (segid A and resi 4 and (name H5 or name H3)) 3.32 0.50
1.00 !!modified:
assign (segid A and resi 5 and name H7*) (segid A and resi 4 and (name H5 or name H3)) 3.16 0.50
1.00 !!modified:
assign (segid A and resi 7 and name H2') (segid A and resi 7 and name H1') 2.63 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H2') (segid A and resi 3 and name H1') 2.67 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H2') (segid A and resi 5 and name H1') 2.74 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H2") (segid A and resi 6 and name H5) 2.91 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H2') (segid A and resi 6 and name H5) 3.05 0.50 1.00 !!modified:
assign (segid A and resi 6 and name H2') (segid A and resi 6 and name H5) 3.20 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H7*) (segid A and resi 6 and name H5) 3.50 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H2') (segid A and resi 1 and name H1') 2.95 0.50 1.00 !!modified:
assign (segid A and resi 6 and name H2') (segid A and resi 6 and name H1') 2.85 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H2) (segid A and resi 4 and (name H6 or name H2)) 3.25 0.50
1.00 !!modified:
assign (segid A and resi 3 and name H2) (segid A and resi 4 and (name H5 or name H3)) 3.26 0.50
1.00 !!modified:
assign (segid A and resi 7 and name H8) (segid A and resi 7 and name H1') 3.05 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H8) (segid A and resi 3 and name H1') 3.20 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 5 and name H1') 3.24 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H6) (segid A and resi 1 and name H1') 2.91 0.50 1.00 !!modified:
assign (segid A and resi 7 and name H8) (segid A and resi 6 and name H1') 3.34 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H8) (segid A and resi 2 and name H1') 3.03 0.50 1.00 !!modified:
assign (segid A and resi 7 and name H8) (segid A and resi 7 and name H3') 2.82 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 4 and name H3') 3.05 0.50 1.00 !!modified:
assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 4 and name H3') 2.96 0.50
1.00 !!modified:
assign (segid A and resi 2 and name H8) (segid A and resi 1 and name H3') 3.12 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H6) (segid A and resi 1 and name H3') 3.00 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H1') (segid A and resi 3 and name H8) 3.14 0.50 1.00 !!modified:
assign (segid A and resi 2 and name H1') (segid A and resi 3 and name H8) 3.37 0.50 1.00 !!modified:

assign (segid A and resi 6 and name H1') (segid A and resi 7 and name H8) 3.43 0.50 1.00 !!modified:
assign (segid A and resi 7 and name H1') (segid A and resi 7 and name H8) 3.04 0.50 1.00 !!modified:
assign (segid A and resi 2 and name H1') (segid A and resi 2 and name H8) 3.20 0.50 1.00 !!modified:
assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 3 and name H2) 3.49 0.50
1.00 !!modified:
assign (segid A and resi 1 and name H1') (segid A and resi 1 and name H6) 2.95 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H1') (segid A and resi 5 and name H6) 3.28 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H1') (segid A and resi 4 and (name H6 or name H2)) 2.98 0.50
1.00 !!modified:
assign (segid A and resi 4 and name H3') (segid A and resi 4 and name H2'') 2.78 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H3') (segid A and resi 5 and name H2'') 2.59 0.50 1.00 !!modified:
assign (segid A and resi 7 and name H3') (segid A and resi 7 and name H2'') 2.57 0.50 1.00 !!modified:
assign (segid A and resi 6 and name H3') (segid A and resi 6 and name H2'') 2.62 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H3') (segid A and resi 1 and name H2'') 2.85 0.50 1.00 !!modified:
assign (segid A and resi 4 and name H3') (segid A and resi 5 and name H7*) 3.09 0.50 1.00 !!modified:
assign (segid A and resi 7 and name H3') (segid A and resi 7 and name H8) 2.92 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H3') (segid A and resi 2 and name H8) 3.37 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H3') (segid A and resi 1 and name H6) 3.14 0.50 1.00 !!modified:
assign (segid A and resi 4 and name H3') (segid A and resi 5 and name H6) 3.37 0.50 1.00 !!modified:
assign (segid A and resi 4 and name H3') (segid A and resi 4 and (name H6 or name H2)) 3.42 0.50
1.00 !!modified:
assign (segid A and resi 7 and name H3') (segid A and resi 7 and name H1') 3.26 0.50 1.00 !!modified:
assign (segid A and resi 3 and name H4') (segid A and resi 3 and name H1') 2.86 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H3') (segid A and resi 1 and name H1') 3.03 0.50 1.00 !!modified:
assign (segid A and resi 6 and name H3') (segid A and resi 6 and name H6) 2.86 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H3') (segid A and resi 5 and name H6) 3.10 0.50 1.00 !!modified:
assign (segid A and resi 4 and name H2'') (segid A and resi 4 and name H3') 2.65 0.50 1.00 !!modified:
assign (segid A and resi 7 and name H2'') (segid A and resi 7 and name H3') 2.53 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H7*) (segid A and resi 4 and name H3') 2.94 0.50 1.00 !!modified:
assign (segid A and resi 1 and name H2'') (segid A and resi 1 and name H3') 2.79 0.50 1.00 !!modified:
assign (segid A and resi 5 and name H7*) (segid A and resi 4 and name H2'') 3.04 0.50 1.00 !!modified:
assign (segid A and resi 4 and name H2'') (segid A and resi 5 and name H7*) 3.11 0.50 1.00 !!modified:

assign (segid A and resi 3 and name H8) (segid A and resi 3 and name H2') 2.28 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H8) (segid A and resi 7 and name H2') 2.15 0.50 1.50 !!modified:
assign (segid A and resi 3 and name H1') (segid A and resi 3 and name H2'') 2.44 0.50 1.50 !!modified:
assign (segid A and resi 2 and name H8) (segid A and resi 2 and name H2') 2.13 0.50 1.50 !!modified:
assign (segid A and resi 2 and name H1') (segid A and resi 2 and name H2') 2.25 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H1') (segid A and resi 5 and name H2'') 2.34 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H1') (segid A and resi 7 and name H2'') 2.21 0.50 1.50 !!modified:
!assign (segid A and resi 7 and name H8) ((segid A and resi 7 and name H2'') or (resi 6 and name H2'')) 2.42 0.50
1.50 !!modified:
assign (segid A and resi 6 and name H1') (segid A and resi 6 and name H2'') 2.38 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H1') (segid A and resi 1 and name H2'') 2.37 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 5 and name H2') 2.23 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H6) (segid A and resi 6 and name H2') 2.16 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H6) (segid A and resi 5 and name H7*) 2.41 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H6) (segid A and resi 1 and name H2') 2.42 0.50 1.50 !!modified:
assign (segid A and resi 3 and name H2') (segid A and resi 3 and name H8) 2.30 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H2') (segid A and resi 7 and name H8) 2.16 0.50 1.50 !!modified:
!assign ((segid A and resi 7 and name H2'') or (segid A and resi 6 and name H2'')) (resi 7 and name H8) 2.43 0.50
1.50 !!modified:
assign (segid A and resi 2 and name H2*) (segid A and resi 2 and name H8) 2.13 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H2') (segid A and resi 1 and name H6) 2.46 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H2') (segid A and resi 6 and name H6) 2.19 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H2') (segid A and resi 5 and name H6) 2.25 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H7*) (segid A and resi 5 and name H6) 2.38 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H2'') (segid A and resi 7 and name H1') 2.24 0.50 1.50 !!modified:
assign (segid A and resi 3 and name H2'') (segid A and resi 3 and name H1') 2.47 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H2'') (segid A and resi 5 and name H1') 2.34 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H2'') (segid A and resi 1 and name H1') 2.43 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H2'') (segid A and resi 6 and name H1') 2.38 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H6) (segid A and resi 1 and name H5) 2.27 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H6) (segid A and resi 6 and name H5) 2.32 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H5) (segid A and resi 1 and name H6) 2.21 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H5) (segid A and resi 6 and name H6) 2.28 0.50 1.50 !!modified:

assign (segid A and resi 7 and name H3') (segid A and resi 7 and name H2') 2.41 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H3') (segid A and resi 5 and name H2') 2.35 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H3') (segid A and resi 6 and name H2') 2.39 0.50 1.50 !!modified:
assign (segid A and resi 4 and name H3') (segid A and resi 4 and name H2') 2.41 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H3') (segid A and resi 1 and name H2') 2.49 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H2') (segid A and resi 7 and name H3') 2.39 0.50 1.50 !!modified:
assign (segid A and resi 4 and name H2') (segid A and resi 4 and name H3') 2.38 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H2') (segid A and resi 1 and name H3') 2.45 0.50 1.50 !!modified:
assign (segid A and resi 4 and (name H6 or name H2)) (segid A and resi 4 and (name H5 or name H3)) 2.01 0.50
1.50 !!modified:
assign (segid A and resi 4 and (name H5 or name H3)) (segid A and resi 4 and (name H6 or name H2)) 1.99 0.50
1.50 !!modified:
assign (segid A and resi 3 and name H2'') (segid A and resi 3 and name H2') 1.97 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H2'') (segid A and resi 7 and name H2') 1.93 0.50 1.50 !!modified:
assign (segid A and resi 4 and name H2') (segid A and resi 4 and name H2'') 2.02 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H2') (segid A and resi 5 and name H2'') 1.97 0.50 1.50 !!modified:
assign (segid A and resi 7 and name H2') (segid A and resi 7 and name H2'') 1.92 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H2') (segid A and resi 6 and name H2'') 1.97 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H2') (segid A and resi 1 and name H2'') 2.08 0.50 1.50 !!modified:
assign (segid A and resi 5 and name H2'') (segid A and resi 5 and name H2') 2.00 0.50 1.50 !!modified:
assign (segid A and resi 6 and name H2'') (segid A and resi 6 and name H2') 1.98 0.50 1.50 !!modified:
assign (segid A and resi 4 and name H2'') (segid A and resi 4 and name H2') 2.01 0.50 1.50 !!modified:
assign (segid A and resi 1 and name H2'') (segid A and resi 1 and name H2') 2.09 0.50 1.50 !!modified:

!"-PLOR restraint NOE modified by CNS_noeEdit

assign (segid B and resi 6 and name H5) (segid B and resi 5 and name H7*) 3.60 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H7*) (segid B and resi 6 and name H5) 4.02 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H6) (segid B and resi 6 and name H5) 3.55 0.50 1.00 !!modified:
assign (segid B and resi 4 and (name H5 or name H3)) (segid B and resi 3 and name H2) 3.56 0.50
1.00 !!modified:
assign (segid B and resi 6 and name H1') (segid B and resi 6 and name H6) 3.50 0.50 1.00 !!modified:


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assign (segid B and resi    4  and (name H6 or name H2)) (segid B and resi    5  and name    H6) 3.96 0.50
1.00  !!modified:

assign (segid B and resi    6  and name    H5) (segid B and resi    5  and name    H6) 3.51 0.50 1.00  !!modified:

assign (segid B and resi    3  and name    H1') (segid B and resi    4  and (name H5 or name H3)) 3.66 0.50
1.00  !!modified:

assign (segid B and resi    6  and name    H3') (segid B and resi    7  and name    H8) 3.62 0.50 1.00  !!modified:


assign (segid B and resi    4  and (name H6 or name H2)) (segid B and resi    3  and name    H2') 3.33 0.50
1.00  !!modified:

assign (segid B and resi    4  and (name H5 or name H3)) (segid B and resi    3  and name    H2'') 3.31 0.50
1.00  !!modified:

assign (segid B and resi    3  and name    H8) (segid B and resi    3  and name    H2'') 2.51 0.50 1.00  !!modified:
assign (segid B and resi    4  and (name H6 or name H2)) (segid B and resi    3  and name    H2'') 3.06 0.50
1.00  !!modified:

assign (segid B and resi    7  and name    H1') (segid B and resi    7  and name    H2') 2.64 0.50 1.00  !!modified:
assign (segid B and resi    3  and name    H8) (segid B and resi    2  and name    H2') 2.66 0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H6) (segid B and resi    4  and name    H2'') 2.60 0.50 1.00  !!modified:
assign (segid B and resi    4  and (name H6 or name H2)) (segid B and resi    4  and name    H2'') 2.91 0.50
1.00  !!modified:

assign (segid B and resi    6  and name    H6) (segid B and resi    5  and name    H2'') 2.66 0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H6) (segid B and resi    5  and name    H2'') 2.72 0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H5) (segid B and resi    5  and name    H2'') 2.73 0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H6) (segid B and resi    6  and name    H2'') 2.59 0.50 1.00  !!modified:
assign (segid B and resi    2  and name    H8) (segid B and resi    1  and name    H2'') 2.94 0.50 1.00  !!modified:
assign (segid B and resi    1  and name    H6) (segid B and resi    1  and name    H2'') 2.95 0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H6) (segid B and resi    5  and name    H2') 2.93 0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H1') (segid B and resi    5  and name    H2') 2.75 0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H5) (segid B and resi    5  and name    H2') 3.02 0.50 1.00  !!modified:
assign (segid B and resi    7  and name    H8) (segid B and resi    6  and name    H2') 2.99 0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H5) (segid B and resi    6  and name    H2') 3.06 0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H1') (segid B and resi    6  and name    H2') 2.83 0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H6) (segid B and resi    4  and name    H2'') 2.87 0.50 1.00  !!modified:
    
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assign (segid B and resi    4  and (name H6 or name H2)) (segid B and resi    4  and name    H2') 2.58  0.50
1.00  !!modified:
assign (segid B and resi    4  and (name H6 or name H2)) (segid B and resi    5  and    name H7*) 2.85  0.50
1.00  !!modified:
assign (segid B and resi    4  and (name H5 or name H3)) (segid B and resi    5  and    name H7*) 3.24  0.50
1.00  !!modified:
assign (segid B and resi    6  and name    H5) (segid B and resi    5  and    name H7*) 3.43  0.50 1.00  !!modified:
assign (segid B and resi    2  and name    H8) (segid B and resi    1  and name    H2') 2.90  0.50 1.00  !!modified:
assign (segid B and resi    1  and name    H1') (segid B and resi    1  and name    H2') 2.99  0.50 1.00  !!modified:
assign (segid B and resi    3  and name    H2'') (segid B and resi    3  and name    H8) 2.56  0.50 1.00  !!modified:
assign (segid B and resi    2  and name    H2*) (segid B and resi    3  and name    H8) 2.73  0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H2') (segid B and resi    7  and name    H8) 3.12  0.50 1.00  !!modified:
assign (segid B and resi    1  and name    H2'') (segid B and resi    2  and name    H8) 2.97  0.50 1.00  !!modified:
assign (segid B and resi    1  and name    H2') (segid B and resi    2  and name    H8) 2.91  0.50 1.00  !!modified:
assign (segid B and resi    1  and name    H2'') (segid B and resi    1  and name    H6) 2.96  0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H2') (segid B and resi    6  and name    H6) 2.89  0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H2'') (segid B and resi    6  and name    H6) 2.69  0.50 1.00  !!modified:
assign (segid B and resi    6  and name    H2'') (segid B and resi    6  and name    H6) 2.64  0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H2'') (segid B and resi    5  and name    H6) 2.76  0.50 1.00  !!modified:
assign (segid B and resi    4  and name    H2') (segid B and resi    5  and name    H6) 2.90  0.50 1.00  !!modified:
assign (segid B and resi    4  and name    H2'') (segid B and resi    4  and (name H6 or name H2)) 2.99  0.50
1.00  !!modified:
assign (segid B and resi    4  and name    H2') (segid B and resi    4  and (name H6 or name H2)) 2.65  0.50
1.00  !!modified:
assign (segid B and resi    5  and    name H7*) (segid B and resi    4  and (name H6 or name H2)) 2.86  0.50
1.00  !!modified:
assign (segid B and resi    3  and name    H2'') (segid B and resi    4  and (name H5 or name H3)) 3.32  0.50
1.00  !!modified:
assign (segid B and resi    5  and    name H7*) (segid B and resi    4  and (name H5 or name H3)) 3.16  0.50
1.00  !!modified:
assign (segid B and resi    7  and name    H2') (segid B and resi    7  and name    H1') 2.63  0.50 1.00  !!modified:
assign (segid B and resi    3  and name    H2') (segid B and resi    3  and name    H1') 2.67  0.50 1.00  !!modified:
assign (segid B and resi    5  and name    H2') (segid B and resi    5  and name    H1') 2.74  0.50 1.00  !!modified:
    
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assign (segid B and resi 5 and name H2") (segid B and resi 6 and name H5) 2.91 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H2') (segid B and resi 6 and name H5) 3.05 0.50 1.00 !!modified:
assign (segid B and resi 6 and name H2') (segid B and resi 6 and name H5) 3.20 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H7*) (segid B and resi 6 and name H5) 3.50 0.50 1.00 !!modified:
assign (segid B and resi 1 and name H2') (segid B and resi 1 and name H1') 2.95 0.50 1.00 !!modified:
assign (segid B and resi 6 and name H2') (segid B and resi 6 and name H1') 2.85 0.50 1.00 !!modified:
assign (segid B and resi 3 and name H2) (segid B and resi 4 and (name H6 or name H2)) 3.25 0.50
1.00 !!modified:
assign (segid B and resi 3 and name H2) (segid B and resi 4 and (name H5 or name H3)) 3.26 0.50
1.00 !!modified:
assign (segid B and resi 7 and name H8) (segid B and resi 7 and name H1') 3.05 0.50 1.00 !!modified:
assign (segid B and resi 3 and name H8) (segid B and resi 3 and name H1') 3.20 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H6) (segid B and resi 5 and name H1') 3.24 0.50 1.00 !!modified:
assign (segid B and resi 1 and name H6) (segid B and resi 1 and name H1') 2.91 0.50 1.00 !!modified:
assign (segid B and resi 7 and name H8) (segid B and resi 6 and name H1') 3.34 0.50 1.00 !!modified:
assign (segid B and resi 3 and name H8) (segid B and resi 2 and name H1') 3.03 0.50 1.00 !!modified:
assign (segid B and resi 7 and name H8) (segid B and resi 7 and name H3') 2.82 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H6) (segid B and resi 4 and name H3') 3.05 0.50 1.00 !!modified:
assign (segid B and resi 4 and (name H6 or name H2)) (segid B and resi 4 and name H3') 2.96 0.50
1.00 !!modified:
assign (segid B and resi 2 and name H8) (segid B and resi 1 and name H3') 3.12 0.50 1.00 !!modified:
assign (segid B and resi 1 and name H6) (segid B and resi 1 and name H3') 3.00 0.50 1.00 !!modified:
assign (segid B and resi 3 and name H1') (segid B and resi 3 and name H8) 3.14 0.50 1.00 !!modified:
assign (segid B and resi 2 and name H1') (segid B and resi 3 and name H8) 3.37 0.50 1.00 !!modified:
assign (segid B and resi 6 and name H1') (segid B and resi 7 and name H8) 3.43 0.50 1.00 !!modified:
assign (segid B and resi 7 and name H1') (segid B and resi 7 and name H8) 3.04 0.50 1.00 !!modified:
assign (segid B and resi 2 and name H1') (segid B and resi 2 and name H8) 3.20 0.50 1.00 !!modified:
assign (segid B and resi 4 and (name H6 or name H2)) (segid B and resi 3 and name H2) 3.49 0.50
1.00 !!modified:
assign (segid B and resi 1 and name H1') (segid B and resi 1 and name H6) 2.95 0.50 1.00 !!modified:
assign (segid B and resi 5 and name H1') (segid B and resi 5 and name H6) 3.28 0.50 1.00 !!modified:
assign (segid B and resi 3 and name H1') (segid B and resi 4 and (name H6 or name H2)) 2.98 0.50
1.00 !!modified:

assign (segid B and resi	4	and name	H3')	(segid B and resi	4	and name	H2'')	2.78	0.50	1.00	!!modified:
assign (segid B and resi	5	and name	H3')	(segid B and resi	5	and name	H2'')	2.59	0.50	1.00	!!modified:
assign (segid B and resi	7	and name	H3')	(segid B and resi	7	and name	H2'')	2.57	0.50	1.00	!!modified:
assign (segid B and resi	6	and name	H3')	(segid B and resi	6	and name	H2'')	2.62	0.50	1.00	!!modified:
assign (segid B and resi	1	and name	H3')	(segid B and resi	1	and name	H2'')	2.85	0.50	1.00	!!modified:
assign (segid B and resi	4	and name	H3')	(segid B and resi	5	and name	H7*)	3.09	0.50	1.00	!!modified:
assign (segid B and resi	7	and name	H3')	(segid B and resi	7	and name	H8)	2.92	0.50	1.00	!!modified:
assign (segid B and resi	1	and name	H3')	(segid B and resi	2	and name	H8)	3.37	0.50	1.00	!!modified:
assign (segid B and resi	1	and name	H3')	(segid B and resi	1	and name	H6)	3.14	0.50	1.00	!!modified:
assign (segid B and resi	4	and name	H3')	(segid B and resi	5	and name	H6)	3.37	0.50	1.00	!!modified:
assign (segid B and resi	4	and name	H3')	(segid B and resi	4	and (name H6 or name H2))		3.42	0.50		
1.00 !!modified:											
assign (segid B and resi	7	and name	H3')	(segid B and resi	7	and name	H1')	3.26	0.50	1.00	!!modified:
assign (segid B and resi	3	and name	H4')	(segid B and resi	3	and name	H1')	2.86	0.50	1.00	!!modified:
assign (segid B and resi	1	and name	H3')	(segid B and resi	1	and name	H1')	3.03	0.50	1.00	!!modified:
assign (segid B and resi	6	and name	H3')	(segid B and resi	6	and name	H6)	2.86	0.50	1.00	!!modified:
assign (segid B and resi	5	and name	H3')	(segid B and resi	5	and name	H6)	3.10	0.50	1.00	!!modified:
assign (segid B and resi	4	and name	H2'')	(segid B and resi	4	and name	H3')	2.65	0.50	1.00	!!modified:
assign (segid B and resi	7	and name	H2'')	(segid B and resi	7	and name	H3')	2.53	0.50	1.00	!!modified:
assign (segid B and resi	5	and name	H7*)	(segid B and resi	4	and name	H3')	2.94	0.50	1.00	!!modified:
assign (segid B and resi	1	and name	H2'')	(segid B and resi	1	and name	H3')	2.79	0.50	1.00	!!modified:
assign (segid B and resi	5	and name	H7*)	(segid B and resi	4	and name	H2'')	3.04	0.50	1.00	!!modified:
assign (segid B and resi	4	and name	H2'')	(segid B and resi	5	and name	H7*)	3.11	0.50	1.00	!!modified:
assign (segid B and resi	3	and name	H8)	(segid B and resi	3	and name	H2')	2.28	0.50	1.50	!!modified:
assign (segid B and resi	7	and name	H8)	(segid B and resi	7	and name	H2')	2.15	0.50	1.50	!!modified:
assign (segid B and resi	3	and name	H1')	(segid B and resi	3	and name	H2'')	2.44	0.50	1.50	!!modified:
assign (segid B and resi	2	and name	H8)	(segid B and resi	2	and name	H2')	2.13	0.50	1.50	!!modified:
assign (segid B and resi	2	and name	H1')	(segid B and resi	2	and name	H2')	2.25	0.50	1.50	!!modified:
assign (segid B and resi	5	and name	H1')	(segid B and resi	5	and name	H2'')	2.34	0.50	1.50	!!modified:
assign (segid B and resi	7	and name	H1')	(segid B and resi	7	and name	H2'')	2.21	0.50	1.50	!!modified:
!assign (segid B and resi	7	and name H8)	((segid B and resi	7	and name H2'')	or (resi	6 and name H2''))	2.42	0.50		
1.50 !!modified:											

assign (segid B and resi 6 and name H1') (segid B and resi 6 and name H2'') 2.38 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H1') (segid B and resi 1 and name H2'') 2.37 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H6) (segid B and resi 5 and name H2') 2.23 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H6) (segid B and resi 6 and name H2') 2.16 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H6) (segid B and resi 5 and name H7*) 2.41 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H6) (segid B and resi 1 and name H2') 2.42 0.50 1.50 !!modified:
assign (segid B and resi 3 and name H2') (segid B and resi 3 and name H8) 2.30 0.50 1.50 !!modified:
assign (segid B and resi 7 and name H2') (segid B and resi 7 and name H8) 2.16 0.50 1.50 !!modified:
!assign ((segid B and resi 7 and name H2'') or (segid B and resi 6 and name H2'')) (resi 7 and name H8) 2.43 0.50
1.50 !!modified:
assign (segid B and resi 2 and name H2*) (segid B and resi 2 and name H8) 2.13 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H2') (segid B and resi 1 and name H6) 2.46 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H2') (segid B and resi 6 and name H6) 2.19 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H2') (segid B and resi 5 and name H6) 2.25 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H7*) (segid B and resi 5 and name H6) 2.38 0.50 1.50 !!modified:
assign (segid B and resi 7 and name H2'') (segid B and resi 7 and name H1') 2.24 0.50 1.50 !!modified:
assign (segid B and resi 3 and name H2'') (segid B and resi 3 and name H1') 2.47 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H2'') (segid B and resi 5 and name H1') 2.34 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H2'') (segid B and resi 1 and name H1') 2.43 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H2'') (segid B and resi 6 and name H1') 2.38 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H6) (segid B and resi 1 and name H5) 2.27 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H6) (segid B and resi 6 and name H5) 2.32 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H5) (segid B and resi 1 and name H6) 2.21 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H5) (segid B and resi 6 and name H6) 2.28 0.50 1.50 !!modified:
assign (segid B and resi 7 and name H3') (segid B and resi 7 and name H2') 2.41 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H3') (segid B and resi 5 and name H2') 2.35 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H3') (segid B and resi 6 and name H2') 2.39 0.50 1.50 !!modified:
assign (segid B and resi 4 and name H3') (segid B and resi 4 and name H2') 2.41 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H3') (segid B and resi 1 and name H2') 2.49 0.50 1.50 !!modified:
assign (segid B and resi 7 and name H2') (segid B and resi 7 and name H3') 2.39 0.50 1.50 !!modified:
assign (segid B and resi 4 and name H2') (segid B and resi 4 and name H3') 2.38 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H2') (segid B and resi 1 and name H3') 2.45 0.50 1.50 !!modified:

assign (segid B and resi 4 and (name H6 or name H2)) (segid B and resi 4 and (name H5 or name H3)) 2.01 0.50
1.50 !!modified:
assign (segid B and resi 4 and (name H5 or name H3)) (segid B and resi 4 and (name H6 or name H2)) 1.99 0.50
1.50 !!modified:
assign (segid B and resi 3 and name H2") (segid B and resi 3 and name H2') 1.97 0.50 1.50 !!modified:
assign (segid B and resi 7 and name H2") (segid B and resi 7 and name H2') 1.93 0.50 1.50 !!modified:
assign (segid B and resi 4 and name H2') (segid B and resi 4 and name H2") 2.02 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H2') (segid B and resi 5 and name H2") 1.97 0.50 1.50 !!modified:
assign (segid B and resi 7 and name H2') (segid B and resi 7 and name H2") 1.92 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H2') (segid B and resi 6 and name H2") 1.97 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H2') (segid B and resi 1 and name H2") 2.08 0.50 1.50 !!modified:
assign (segid B and resi 5 and name H2") (segid B and resi 5 and name H2') 2.00 0.50 1.50 !!modified:
assign (segid B and resi 6 and name H2") (segid B and resi 6 and name H2') 1.98 0.50 1.50 !!modified:
assign (segid B and resi 4 and name H2") (segid B and resi 4 and name H2') 2.01 0.50 1.50 !!modified:
assign (segid B and resi 1 and name H2") (segid B and resi 1 and name H2') 2.09 0.50 1.50 !!modified:

SD 9-4 Parameter file of planarity restrains.

```
set message=off echo=off end
```

```
!restraints plane
```

```
group
```

```
selection=((segid A and resid 1 and name N1 ) or (segid A and resid 1 and name N3 ) or  
(segid A and resid 1 and name C5 ) or (segid B and resid 7 and name N1 ) or  
(segid B and resid 7 and name N3 ) or (segid B and resid 7 and name C5 ))
```

```
weight = 50.000 end
```

```
group
```

```
selection=((segid A and resid 2 and name N1 ) or (segid A and resid 2 and name N3 ) or  
(segid A and resid 2 and name C5 ) or (segid B and resid 6 and name N1 ) or  
(segid B and resid 6 and name N3 ) or (segid B and resid 6 and name C5 ))
```

```
weight = 50.000 end
```

```
group
```

```
selection=((segid A and resid 3 and name N1 ) or (segid A and resid 3 and name N3 ) or  
(segid A and resid 3 and name C5 ) or (segid B and resid 5 and name N1 ) or  
(segid B and resid 5 and name N3 ) or (segid B and resid 5 and name C5 ))
```

```
weight = 50.000 end
```

```
group
```

```
selection=((segid A and resid 5 and name N1 ) or (segid A and resid 5 and name N3 ) or  
(segid A and resid 5 and name C5 ) or (segid B and resid 3 and name N1 ) or  
(segid B and resid 3 and name N3 ) or (segid B and resid 3 and name C5 ))
```

```
weight = 50.000 end
```

```
group
```

```
selection=((segid A and resid 6 and name N1 ) or (segid A and resid 6 and name N3 ) or  
  
(segid A and resid 6 and name C5 ) or (segid B and resid 2 and name N1 ) or  
(segid B and resid 2 and name N3 ) or (segid B and resid 2 and name C5 ))
```

weight = 50.000 end

group

selection=((segid A and resid 7 and name N1) or (segid A and resid 7 and name N3) or
(segid A and resid 7 and name C5) or (segid B and resid 1 and name N1) or
(segid B and resid 1 and name N3) or (segid B and resid 1 and name C5))

weight = 50.000 end

end

set message=on echo=on end

SD 9-5 Parameter file of thionucleoside residue.

```

set echo=off message=off end

checkversion 1.3

evaluate ($kchbond = 2000)
evaluate ($kchangle = 1000)
evaluate ($kchimpr = 1000)

BOND  C1D  C1S  1700.0    1.45
BOND  C1S  C2S  1700.0    1.4
BOND  C1S  C6S  1700.0    1.4
BOND  C2S  C3S  1700.0    1.4
BOND  C3S  C4S  1700.0    1.4
BOND  C4S  C5S  1700.0    1.4
BOND  C5S  C6S  1700.0    1.4
BOND  C2S  HR   1000.0    1.01
BOND  C3S  HR   1000.0    1.01
BOND  C5S  HR   1000.0    1.01
BOND  C6S  HR   1000.0    1.01
BOND  C4S  S4S  1000.0    1.8
BOND  S4S  HR   1000.0    0.96
BOND  C4S  S    1000.0    1.8

bond S    S    2410.110  2.030 ! 0.008

ANGLE  HR    C1D  C1S    $kchangle    108.25
ANGLE  O4D   C1D  C1S    1357.996  107.800 !0.9 S
ANGLE  C1S   C1D  C2D    488.878  114.200 !1.5 S

!Bases

!thiophenol
          kq      x_eq  sigma
ANGLE  C6S   C1S  C2S    2277.447  120.300 !0.40 B
    
```

ANGLE	C1S	C2S	C3S	743.656	119.200	!0.70 B
ANGLE	C2S	C3S	C4S	1457.566	119.900	!0.50 B
ANGLE	C3S	C4S	C5S	2277.447	121.900	!0.40 B
ANGLE	C4S	C5S	C6S	1457.566	117.400	!0.50 B
ANGLE	C5S	C6S	C1S	1457.566	121.000	!0.50 B
ANGLE	C3S	C4S	S4S	743.656	119.500	!0.70 B
ANGLE	C5S	C4S	S4S	743.656	119.500	!0.70 B
ANGLE	C6S	C1S	C1D	763.873	120.800	!1.20 B !DNA
ANGLE	C2S	C1S	C1D	909.071	118.800	!1.10 B
ANGLE	C4S	S4S	HR	105.000	120.000	!from param11.dna, 3*keq
ANGLE	C4S	C5S	HR	\$kchangle	121.54	
ANGLE	C6S	C5S	HR	\$kchangle	121.54	
ANGLE	C1S	C6S	HR	\$kchangle	121.54	
ANGLE	C5S	C6S	HR	\$kchangle	121.54	
ANGLE	C1S	C2S	HR	\$kchangle	121.54	
ANGLE	C3S	C2S	HR	\$kchangle	121.54	
ANGLE	C2S	C3S	HR	\$kchangle	121.54	
ANGLE	C4S	C3S	HR	\$kchangle	121.54	
ANGLE	C3S	C4S	S	743.656	119.500	!0.70 B
ANGLE	C5S	C4S	S	743.656	119.500	!0.70 B
ANGLE	C4S	S	S	500.000	103.800	!0.70 B

!bases

NONBonded	C1S	0.0900	3.2970	0.0900	3.2970
NONBonded	C2S	0.0900	3.2970	0.0900	3.2970
NONBonded	C3S	0.0900	3.2970	0.0900	3.2970
NONBonded	C4S	0.0900	3.2970	0.0900	3.2970
NONBonded	C5S	0.0900	3.2970	0.0900	3.2970
NONBonded	C6S	0.0900	3.2970	0.0900	3.2970
NONBonded	S4S	0.0239	3.7458	0.0239	3.7458
NONBonded	S	0.0430	3.3676	0.0430	3.3676

dihe X C4S S X 1.2 2 0.0

dihe X	S	S	X	1.2	2	0.0		
IMPRoper	C4S	X	X	H2	2400.0	0	0.000	
IMPRoper	C4S	X	X	C1S	250.0	0	0.000	
IMPRoper	C6S	X	X	C3S	250.0	0	0.000	
IMPRoper	C4S	X	X	C2S	2400.0	0	0.000	
IMPRoper	C2S	X	X	H2	2400.0	0	0.000	
IMPRoper	C1D	C2S	C6S	C1S	2400.0	0	0.000	
IMPRoper	C4S	C3S	C5S	C4S	2400.0	0	0.000	
IMPRoper	C2S	C3S	C4S	C5S	250.0	0	0.000	
IMPRoper	C5S	C6S	C1S	C2S	250.0	0	0.000	
IMPRoper	C5S	C4S	S4S	H2	2000.0	0	0.000	
IMPRoper	HR	C4S	C6S	C5S	\$kchimpr	0	0.000	
IMPRoper	HR	C1S	C5S	C6S	\$kchimpr	0	0.000	
IMPRoper	HR	C2S	C4S	C3S	\$kchimpr	0	0.000	
IMPRoper	HR	C1S	C3S	C2S	\$kchimpr	0	0.000	
IMPRoper	HR	C2D	O4D	C1S	\$kchimpr	0	-65.280!C1D	

set echo=on message=on end

set echo=false end

checkversion 1.3

AUTOGENERATE ANGLES=TRUE END

MASS P 30.97400! phosphorus

MASS O1P 15.99940! O in phosphate

MASS O2P 15.99940! O in phosphate

MASS OH 15.99940! corresp. to OH1

MASS C5D 14.02700! corresp. to CH2E

MASS C4D 13.01900! corresp. to CH1E

MASS C3D 13.01900! corresp. to CH1E

MASS C2D 13.01900! corresp. to CH1E

```

MASS  C1D  13.01900! corresp. to CH1E
MASS  O4D  15.99940! ester -P-O-C-
MASS  O5D  15.99940!
MASS  O3D  15.99940!
MASS  C1S  12.01100
MASS  C2S  12.01100! (prev CN)
MASS  C3S  12.01100
MASS  C4S  12.01100! (prev CA)
MASS  C5S  12.011! (prev CF)
MASS  C6S  12.011! (prev CF)
MASS  HR   1.00800! non-exchangeable Hydrogens
MASS  HO   1.00800! hydroxy hydrogen
MASS  S4S  32.060

RESIdue SPH

GROUp

  ATOM P   TYPE=P   CHARGE=0.78   END
  ATOM OP1 TYPE=O1P  CHARGE=-0.66  END
  ATOM OP2 TYPE=O2P  CHARGE=-0.66  END
  ATOM O5' TYPE=O5R  CHARGE=-0.43  END

GROUp

  ATOM C5' TYPE=C5D  CHARGE=0.00   END ! deoxy
  ATOM H5' TYPE=HR   CHARGE=0.10   END
  ATOM H5" TYPE=HR   CHARGE=0.10   END

GROUp

  ATOM C4' TYPE=C4D  CHARGE=0.15   END ! deoxy
  ATOM H4' TYPE=HR   CHARGE=0.10   END
  ATOM O4' TYPE=O4D  CHARGE=-0.50  END ! deoxy
  ATOM C1' TYPE=C1D  CHARGE=0.53   END ! deoxy
  ATOM H1' TYPE=HR   CHARGE=0.10   END

! Insert Base

GROUp

  ATOM C1   TYPE=C1S  CHARGE=-0.19  EXCLUSION=( C4 )  END
    
```

```

    ATOM C6   TYPE=C6S   CHARGE=0.155  EXCLUSION=( C3 )  END
    ATOM H6   TYPE=HR    CHARGE=0.035  END

GROUP
    ATOM C2   TYPE=C2S   CHARGE=0.30   EXCLUSION=( C5 )  END
    ATOM H2   TYPE=HR    CHARGE=-0.30  END

GROUP
    ATOM C3   TYPE=C3S   CHARGE=-0.28  END
    ATOM H3   TYPE=HR    CHARGE=0.0    END

GROUP
    ATOM C4   TYPE=C4S   CHARGE=0.28   END
    ATOM S4   TYPE=S4S   CHARGE=-0.42  END
    ATOM H4   TYPE=HR    CHARGE=0.42   END

GROUP
    ATOM C5   TYPE=C5S   CHARGE=-0.035  END !CHRG
    ATOM H5   TYPE=HR    CHARGE=0.035  END

GROUP
! END

GROUP
    ATOM C2'  TYPE=C2D   CHARGE=-0.20   END ! deoxy
    ATOM H2'  TYPE=HR    CHARGE=0.10    END
    ATOM H2"  TYPE=HR    CHARGE=0.1     END ! deoxy

GROUP
    ATOM C3'  TYPE=C3D   CHARGE=-0.10   END ! deoxy
    ATOM H3'  TYPE=HR    CHARGE=0.10    END

GROUP
    ATOM O3'  TYPE=O3R   CHARGE=-0.43   END

BOND P   OP1          BOND P   OP2          BOND P   O5'
BOND O5'  C5'          BOND C5'  C4'          BOND C4'  O4'
BOND C4'  C3'          BOND O4'  C1'          BOND C1'  C1
BOND C1'  C2'          BOND C1   C2          BOND C1   C6
                BOND C2   C3          BOND C3   C4
    
```

```

BOND C4  S4          BOND S4  H4
BOND C2  H2          BOND C3  H3
BOND C4  C5          BOND C5  C6          BOND C2' C3'
BOND C3' O3'
BOND C6  H6          BOND C5  H5
BOND C5' H5'          BOND C5' H5"          BOND C4' H4'
BOND C3' H3'          BOND C2' H2'          BOND C1' H1'
BOND C2' H2"

```

```

{
  DIHEdral P   O5' C5' C4'          DIHEdral O5' C5' C4' O4'
  DIHEdral O5' C5' C4' C3'
} {
  DIHEdral C3' C4' O4' C1'
  DIHEdral C4' O4' C1' C2'          DIHEdral O4' C1' C2' C3'

  DIHEdral C1' C2' C3' C4'          DIHEdral O4' C4' C3' O3'
  DIHEdral C5' C4' C3' C2'
  DIHEdral O4' C1' N1  C2

! New dihedrals
DIHEdral  C5' C4' C3' O3'          DIHEdral  C4' O4' C1' C1
}

```

```

IMPRoper C1' C2  C6  C1          IMPRoper H3  C2  C4  C3
IMPRoper H2  C1  C3  C2          IMPRoper C4  C3  C5  C4
IMPRoper C1  C2  C3  C4          IMPRoper C2  C3  C4  C5
IMPRoper C3  C4  C5  C6          IMPRoper C4  C5  C6  C1
IMPRoper C5  C6  C1  C2          IMPRoper C6  C1  C2  C3
IMPRoper H5  C4  C6  C5          IMPRoper H6  C1  C5  C6

```

```

IMPRoper  H2' C3' H2" C1"! C2' chirality term ! deoxy

```

!RIBOSE IMPROPER

IMPRoper H1' C2' O4' C1 !C1'

IMPRoper H3' C4' C2' O3' !C3'

IMPRoper H4' C5' C3' O4' !C4'

IMPRoper H5' O5' H5" C4' !C5'

END {SPH}

!disulfide bond

PRESIDUE DISS

group

delete atom 1H4 END

modify atom 1C4 charge=0.19 END

modify atom 1S4 type=S charge=-0.19 END

group

delete atom 2H4 END

modify atom 2C4 charge=0.19 END

modify atom 2S4 type=S charge=-0.19 END

add bond 1S4 2S4

add angle 1C4 1S4 2S4

add angle 1S4 2S4 2C4

add dihedral 1C3 1C4 1S4 2S4

add dihedral 1C5 1C4 1S4 2S4

add dihedral 1C4 1S4 2S4 2C4

add dihedral 1S4 2S4 2C4 2C3

add dihedral 1S4 2S4 2C4 2C5

end {DISS}

set echo=true end

References

- 1) R. Lavery, M. Moakher, J. H. Maddocks, D. Petkeviciute, and K. Zakrzewska, *Nucl. Acids Res.*, 2009, **37**, 5917–5929.