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K-4025-M1

Supplementary Material for Microfilm Edition.

Table 1. Chemical shifts (ppm) of the protons of DHD.

	H6/H8	H5/CH3/H2	H1'	H2'	H2''	H3'	H4'	Imino	Amino
1G	7.59		5.48	2.32	2.47	4.58	4.00	12.56	N.A. N.A.
2G	7.51		5.50	2.51	2.51	4.80	4.19	12.45	N.A. N.A.
3A	7.82	7.36	5.80	4.77		4.40	4.24		5.94 8.90
4G	7.29		5.53	4.51		4.43	3.95	12.33	N.A. N.A.
5A	7.57	7.53	5.74	4.32		4.43	N.A.	12.33	N.A. N.A.
6U	7.29	4.87	5.26	4.10		4.25	4.16	13.52	
7G	7.59		5.67	2.29	2.49	4.67	4.17	12.02	N.A. N.A.
8A	7.95	7.71	6.10	2.41	2.70	4.79	4.25		6.55 7.94
9C	7.04	4.92	5.83	1.91	2.00	3.81	4.28		N.A. N.A.
10G	7.67		5.73	2.54	5.54	4.57	3.97	12.56	N.A. N.A.
11T	7.39	1.11	5.97	2.22	2.46	4.73	4.15	13.97	
12C	7.48	5.55	5.74	2.21	2.42	4.70	4.07		6.12 8.91
13A	7.95	7.33	6.01	2.39	2.67	4.69	4.22		7.53 8.42
14T	7.16	1.13	5.77	2.12	2.34	4.67	4.08	13.60	
15C	7.31	5.25	5.79	2.01	2.41	4.48	4.06		6.60 8.03
16T	7.28	1.35	5.86	2.02	2.40	4.70	4.02	13.37	
17C	7.37	5.47	5.86	1.98	2.29	4.65	4.00		6.75 8.25
18C	7.32	5.27	6.00	2.11	2.11	3.80	4.38		N.A. N.A.

N.A.: not assigned.

Table 2. Chemical shifts (ppm) of the protons of DDH.

	H6/H8	H5/CH3/H2	H1'	H2'	H2''	H3'	H4'	Imino	Amino
1G	7.63		5.45	2.28	2.48	4.71	4.60	12.55	N.A. N.A.
2G	7.63		5.28	2.47	2.58	5.00	4.31	12.50	N.A. N.A.
3A	7.91	7.53	5.88	2.49	2.76	5.08	4.42		N.A. N.A.
4G	7.45		5.39	2.39	2.50	5.01	4.38	12.30	N.A. N.A.
5A	7.85	7.55	5.98	2.71	2.71	4.90	4.44		N.A. N.A.
6U	7.24	4.88	5.41	4.32		4.40	4.41	12.85	
7G	7.61		5.52	4.47		4.52	4.50	11.66	N.A. N.A.
8A	7.78	7.75	5.75	4.29		4.59	4.42		N.A. N.A.
9C	7.19	5.10	5.51	3.82		4.03	4.09		N.A. N.A.
10G	7.76		5.80	2.56	2.56	4.80	4.01	12.63	N.A. N.A.
11T	7.47	1.29	6.20	2.25	2.51	4.93	4.33	14.12	
12C	7.43	5.48	5.82	2.17	2.45	4.97	4.53		N.A. N.A.
13A	7.92	7.13	6.03	2.38	2.75	4.97	4.40		N.A. N.A.
14T	7.16	1.21	5.78	1.99	2.35	4.91	4.28	13.15	
15C	7.41	5.37	5.81	1.97	2.37	4.78	4.21		N.A. N.A.
16T	7.31	1.59	5.90	2.04	2.38	4.41	4.23	13.56	
17C	7.41	5.58	5.89	2.03	2.30	4.52	4.13		N.A. N.A.
18C	7.42	5.49	6.02	2.11	2.11	3.85	4.50		N.A. N.A.

N.A.: not assigned.

K-4025-m2

DHD distance constraints from D0
 error 0.3, 0.4Å lower, upper respectively

! Sugar-noes

! H1'-H2'

assign (resid 8 name H1') (resid 8 name H2') 2.9
 assign (resid 15 name H1') (resid 15 name H2') 2.9

assign (resid 1 name H2') (resid 1 name H1') 3.3
 assign (resid 7 name H2') (resid 7 name H1') 3.1
 assign (resid 8 name H2') (resid 8 name H1') 3.0
 assign (resid 9 name H2') (resid 9 name H1') 2.7
 assign (resid 11 name H2') (resid 11 name H1') 2.9
 assign (resid 12 name H2') (resid 12 name H1') 2.9
 assign (resid 13 name H2') (resid 13 name H1') 3.0
 assign (resid 14 name H2') (resid 14 name H1') 3.0
 assign (resid 17 name H2') (resid 17 name H1') 2.5

! H1'-H2''

assign (resid 1 name H1') (resid 1 name H2'') 2.8
 assign (resid 3 name H1') (resid 3 name H2'') 3.1
 assign (resid 5 name H1') (resid 5 name H2'') 2.6
 assign (resid 7 name H1') (resid 7 name H2'') 2.5
 assign (resid 9 name H1') (resid 9 name H2'') 2.5
 assign (resid 12 name H1') (resid 12 name H2'') 2.5
 assign (resid 13 name H1') (resid 13 name H2'') 2.5
 assign (resid 14 name H1') (resid 14 name H2'') 2.5
 assign (resid 15 name H1') (resid 15 name H2'') 2.5
 assign (resid 17 name H1') (resid 17 name H2'') 2.5

assign (resid 4 name H2'') (resid 4 name H1') 2.8
 assign (resid 6 name H2'') (resid 6 name H1') 2.6
 assign (resid 8 name H2'') (resid 8 name H1') 2.5
 assign (resid 11 name H2'') (resid 11 name H1') 2.5
 assign (resid 16 name H2'') (resid 16 name H1') 2.5

! inter sugar noe

assign (resid 5 name H2'') (resid 6 name H1') 4.0

! H1'-H2'*

assign (resid 2 name H1') (resid 2 name H2'*) 2.7
 assign (resid 10 name H1') (resid 10 name H2'*) 2.5
 assign (resid 18 name H1') (resid 18 name H2'*) 2.3

! H1'-H3'

assign (resid 12 name H1') (resid 12 name H3') 3.5

assign (resid 2 name H3') (resid 2 name H1') 3.8
 assign (resid 4 name H3') (resid 4 name H1') 3.6
 assign (resid 6 name H3') (resid 6 name H1') 3.4
 assign (resid 7 name H3') (resid 7 name H1') 3.4
 assign (resid 8 name H3') (resid 8 name H1') 3.6
 assign (resid 9 name H3') (resid 9 name H1') 3.6
 assign (resid 10 name H3') (resid 10 name H1') 3.6
 assign (resid 11 name H3') (resid 11 name H1') 3.6
 assign (resid 13 name H3') (resid 13 name H1') 3.6
 assign (resid 14 name H3') (resid 14 name H1') 3.9
 assign (resid 15 name H3') (resid 15 name H1') 3.6
 assign (resid 16 name H3') (resid 16 name H1') 3.7
 assign (resid 17 name H3') (resid 17 name H1') 3.8
 assign (resid 18 name H3') (resid 18 name H1') 3.8

! H1'-H4'

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```

assign (resid 3 name H1') (resid 3 name H4') 3.7
assign (resid 5 name H1') (resid 5 name H4') 4.0
assign (resid 7 name H1') (resid 7 name H4') 3.5
assign (resid 12 name H1') (resid 12 name H4') 3.0
assign (resid 13 name H1') (resid 13 name H4') 3.4
assign (resid 15 name H1') (resid 15 name H4') 2.8

```

```

assign (resid 2 name H4') (resid 2 name H1') 3.5
assign (resid 4 name H4') (resid 4 name H1') 3.6
assign (resid 6 name H4') (resid 6 name H1') 3.4
assign (resid 8 name H4') (resid 8 name H1') 3.4
assign (resid 9 name H4') (resid 9 name H1') 3.0
assign (resid 10 name H4') (resid 10 name H1') 3.6
assign (resid 11 name H4') (resid 11 name H1') 3.3
assign (resid 16 name H4') (resid 16 name H1') 3.1
assign (resid 17 name H4') (resid 17 name H1') 3.0
assign (resid 18 name H4') (resid 18 name H1') 3.2
! intra residue H6-H1'

```

```

assign (resid 6 name H1') (resid 6 name H6) 3.8
assign (resid 9 name H1') (resid 9 name H6) 3.6
assign (resid 11 name H1') (resid 11 name H6) 3.8
assign (resid 12 name H1') (resid 12 name H6) 3.6
assign (resid 14 name H1') (resid 14 name H6) 3.7
assign (resid 18 name H1') (resid 18 name H6) 3.5
assign (resid 12 name H6) (resid 12 name H1') 3.8
assign (resid 17 name H1') (resid 17 name H6) 3.4

```

```

! inter residue H6-H1'
assign (resid 9 name H6) (resid 8 name H1') 3.4
assign (resid 11 name H6) (resid 10 name H1') 3.6
assign (resid 12 name H6) (resid 11 name H1') 3.4
assign (resid 14 name H6) (resid 13 name H1') 3.7
assign (resid 15 name H6) (resid 14 name H1') 3.3
assign (resid 16 name H6) (resid 15 name H1') 3.7
assign (resid 18 name H6) (resid 17 name H1') 3.7

```

```

assign (resid 5 name H1') (resid 6 name H6) 3.6

```

```

! intra residue H8-H1'
assign (resid 2 name H8) (resid 2 name H1') 3.3
assign (resid 4 name H8) (resid 4 name H1') 3.1
assign (resid 7 name H8) (resid 7 name H1') 3.8

```

```

assign (resid 1 name H1') (resid 1 name H8) 4.0
assign (resid 3 name H1') (resid 3 name H8) 4.0
assign (resid 5 name H1') (resid 5 name H8) 3.9
assign (resid 8 name H1') (resid 8 name H8) 3.6
assign (resid 10 name H1') (resid 10 name H8) 3.6
assign (resid 13 name H1') (resid 13 name H8) 3.6

```

```

! inter residue H1'-H8
assign (resid 4 name H8) (resid 3 name H1') 4.9
assign (resid 5 name H8) (resid 4 name H1') 3.8
assign (resid 7 name H8) (resid 6 name H1') 4.0
assign (resid 8 name H8) (resid 7 name H1') 3.4
assign (resid 13 name H8) (resid 12 name H1') 3.4

```

```

assign (resid 1 name H1') (resid 2 name H8) 3.7

```

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```
assign (resid 2 name H1') (resid 3 name H8) 3.3
```

```
! H2'-H3'
```

```
assign (resid 13 name H2') (resid 13 name H3') 2.8
```

```
assign (resid 8 name H3') (resid 8 name H2') 2.7
```

```
assign (resid 9 name H3') (resid 9 name H2') 2.7
```

```
assign (resid 11 name H3') (resid 11 name H2') 2.7
```

```
assign (resid 12 name H3') (resid 12 name H2') 2.7
```

```
assign (resid 14 name H3') (resid 14 name H2') 2.8
```

```
assign (resid 15 name H3') (resid 15 name H2') 2.8
```

```
assign (resid 16 name H3') (resid 16 name H2') 2.7
```

```
assign (resid 17 name H3') (resid 17 name H2') 2.7
```

```
! H4'-H2'
```

```
assign (resid 7 name H4') (resid 7 name H2') 3.7
```

```
assign (resid 8 name H4') (resid 8 name H2') 3.8
```

```
assign (resid 9 name H4') (resid 9 name H2') 3.8
```

```
assign (resid 11 name H4') (resid 11 name H2') 3.7
```

```
assign (resid 12 name H4') (resid 12 name H2') 3.3
```

```
assign (resid 13 name H4') (resid 13 name H2') 3.6
```

```
assign (resid 14 name H4') (resid 14 name H2') 3.5
```

```
assign (resid 15 name H4') (resid 15 name H2') 3.4
```

```
assign (resid 16 name H4') (resid 16 name H2') 3.3
```

```
! H5-H2'
```

```
assign (resid 9 name H5) (resid 8 name H2') 3.8
```

```
assign (resid 9 name H5) (resid 9 name H2') 4.1
```

```
assign (resid 15 name H5) (resid 14 name H2') 3.8
```

```
assign (resid 15 name H5) (resid 15 name H2') 4.2
```

```
assign (resid 18 name H5) (resid 17 name H2') 3.7
```

```
assign (resid 11 name H2') (resid 12 name H5) 3.4
```

```
assign (resid 16 name H2') (resid 17 name H5) 3.3
```

```
! H2'-H6
```

```
! inter residue
```

```
assign (resid 9 name H6) (resid 9 name H2') 2.9
```

```
assign (resid 15 name H6) (resid 15 name H2') 2.5
```

```
assign (resid 11 name H2') (resid 11 name H6) 2.7
```

```
assign (resid 14 name H2') (resid 14 name H6) 2.7
```

```
! inter residue H2'-H6
```

```
assign (resid 9 name H6) (resid 8 name H2') 3.2
```

```
assign (resid 12 name H6) (resid 11 name H2') 2.6
```

```
assign (resid 18 name H6) (resid 17 name H2') 2.7
```

```
assign (resid 13 name H2') (resid 14 name H6) 3.0
```

```
! intra residue H2'-H8
```

```
assign (resid 2 name H2') (resid 2 name H8) 3.8
```

```
assign (resid 7 name H2') (resid 7 name H8) 3.0
```

```
! inter residue H2'-H8
```

```
assign (resid 2 name H8) (resid 1 name H2') 3.5
```

```
assign (resid 8 name H8) (resid 7 name H2') 3.3
```

```
assign (resid 13 name H8) (resid 12 name H2') 3.0
```

```
! intra residue H2''-H3'
```

```
assign (resid 7 name H3') (resid 7 name H2'') 3.3
```

```
assign (resid 8 name H3') (resid 8 name H2'') 3.1
```

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```

assign (resid 9 name H3') (resid 9 name H2'') 3.3
assign (resid 11 name H3') (resid 11 name H2'') 3.0
assign (resid 13 name H3') (resid 13 name H2'') 3.3
assign (resid 14 name H3') (resid 14 name H2'') 3.2
assign (resid 15 name H3') (resid 15 name H2'') 3.2
assign (resid 16 name H3') (resid 16 name H2'') 2.5

```

```
! intra residue H2'*-H3'
```

```

assign (resid 2 name H2'*) (resid 2 name H3') 2.7
assign (resid 10 name H2'*) (resid 10 name H3') 2.9
assign (resid 18 name H2'*) (resid 18 name H3') 2.6

```

```
! intra residue H2''-H4'
```

```

assign (resid 11 name H4') (resid 11 name H2'') 3.3
assign (resid 17 name H4') (resid 17 name H2'') 3.2

```

```

assign (resid 8 name H2'') (resid 8 name H4') 3.9
assign (resid 9 name H2'') (resid 9 name H4') 3.6
assign (resid 13 name H2'') (resid 13 name H4') 3.6
assign (resid 14 name H2'') (resid 14 name H4') 3.3
assign (resid 15 name H2'') (resid 15 name H4') 3.3

```

```
! intra residue H2'*-H4'
```

```

assign (resid 2 name H4') (resid 2 name H2'*) 3.2
assign (resid 10 name H4') (resid 10 name H2'*) 3.0
assign (resid 18 name H4') (resid 18 name H2'*) 3.2

```

```
! inter residue H2''-H5
```

```

assign (resid 9 name H5) (resid 8 name H2'') 3.8
assign (resid 12 name H5) (resid 11 name H2'') 3.6
assign (resid 15 name H5) (resid 14 name H2'') 3.6
assign (resid 17 name H5) (resid 16 name H2'') 3.8
assign (resid 18 name H5) (resid 17 name H2'') 3.9
assign (resid 5 name H2'') (resid 6 name H5) 3.6

```

```
! intra residue H2''-H6
```

```

assign (resid 9 name H6) (resid 9 name H2'') 3.8
assign (resid 17 name H6) (resid 17 name H2'') 3.5

```

```

assign (resid 6 name H2'') (resid 6 name H6) 3.6
assign (resid 9 name H2'') (resid 9 name H6) 3.7
assign (resid 11 name H2'') (resid 11 name H6) 3.4
assign (resid 12 name H2'') (resid 12 name H6) 3.3
assign (resid 14 name H2'') (resid 14 name H6) 3.2

```

```
! inter residue H2''-H6
```

```
assign (resid 15 name H6) (resid 14 name H2'') 3.1
```

```

assign (resid 5 name H2'') (resid 6 name H6) 2.6
assign (resid 8 name H2'') (resid 9 name H6) 3.0
assign (resid 11 name H2'') (resid 12 name H6) 2.9
assign (resid 13 name H2'') (resid 14 name H6) 3.1
assign (resid 16 name H2'') (resid 17 name H6) 3.0
assign (resid 17 name H2'') (resid 18 name H6) 3.2

```

```
! intra & inter residue H2'*-H6
```

```
assign (resid 10 name H2'*) (resid 11 name H6) 2.7
```

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! intra residue H2''-H8

assign (resid 3 name H8) (resid 3 name H2'') 3.4
assign (resid 5 name H2'') (resid 5 name H8) 3.5

! inter residue H2''-H8

assign (resid 4 name H8) (resid 3 name H2'') 3.1
assign (resid 5 name H8) (resid 4 name H2'') 2.6
assign (resid 7 name H8) (resid 6 name H2'') 2.7
assign (resid 8 name H8) (resid 7 name H2'') 3.7

! intra residue H2'*-H8

assign (resid 2 name H2'*) (resid 2 name H8) 2.7
assign (resid 10 name H2'*) (resid 10 name H8) 3.1

! inter residue H2'*-H8

assign (resid 3 name H8) (resid 2 name H2'*) 3.0

! intra residue H3'-H4'

assign (resid 2 name H3') (resid 2 name H4') 2.9
assign (resid 9 name H3') (resid 9 name H4') 2.9
assign (resid 10 name H3') (resid 10 name H4') 2.9
assign (resid 11 name H3') (resid 11 name H4') 2.8
assign (resid 15 name H3') (resid 15 name H4') 2.8
assign (resid 16 name H3') (resid 16 name H4') 3.0

assign (resid 7 name H4') (resid 7 name H3') 2.9
assign (resid 8 name H4') (resid 8 name H3') 2.7
assign (resid 13 name H4') (resid 13 name H3') 2.8
assign (resid 18 name H4') (resid 18 name H3') 2.6

! intra residue H3'-H6

assign (resid 6 name H6) (resid 6 name H3') 2.8
assign (resid 15 name H6) (resid 15 name H3') 4.4

assign (resid 9 name H3') (resid 9 name H6) 3.2
assign (resid 11 name H3') (resid 11 name H6) 3.4
assign (resid 12 name H3') (resid 12 name H6) 3.3
assign (resid 14 name H3') (resid 14 name H6) 3.4
assign (resid 17 name H3') (resid 17 name H6) 3.4

! inter residue H3'-H6

assign (resid 11 name H6) (resid 10 name H3') 3.9
assign (resid 18 name H6) (resid 17 name H3') 3.4
assign (resid 8 name H3') (resid 9 name H6) 4.0
assign (resid 11 name H3') (resid 12 name H6) 4.0
assign (resid 13 name H3') (resid 14 name H6) 4.1
assign (resid 14 name H3') (resid 15 name H6) 3.8

! intra residue H3'-H8

assign (resid 2 name H8) (resid 2 name H3') 3.9
assign (resid 7 name H8) (resid 7 name H3') 3.7
assign (resid 10 name H8) (resid 10 name H3') 4.0

assign (resid 8 name H3') (resid 8 name H8) 3.5

! inter residue H3'-H8

assign (resid 3 name H8) (resid 2 name H3') 4.7
assign (resid 7 name H8) (resid 6 name H3') 3.1

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```

assign (resid 13 name H8) (resid 12 name H3') 3.2
assign (resid 4 name H3') (resid 5 name H8) 3.1
assign (resid 6 name H3') (resid 7 name H8) 2.9

```

```
! intra residue H6-H4'
```

```

assign (resid 6 name H6) (resid 6 name H4') 4.1
assign (resid 11 name H6) (resid 11 name H4') 4.3

```

```

assign (resid 9 name H4') (resid 9 name H6) 4.4
assign (resid 12 name H4') (resid 12 name H6) 3.8
assign (resid 14 name H4') (resid 14 name H6) 4.1

```

```
! intra residue H8-H4'
```

```
assign (resid 10 name H8) (resid 10 name H4') 4.4
```

```

assign (resid 8 name H4') (resid 8 name H8) 4.4
assign (resid 13 name H4') (resid 13 name H8) 4.5

```

```
! inter residue H8-H6
```

```

assign (resid 6 name H5) (resid 5 name H8) 4.0
assign (resid 9 name H5) (resid 8 name H8) 3.5

```

```
! inter residue H5-H6
```

```

assign (resid 11 name H6) (resid 12 name H5) 4.1
assign (resid 14 name H6) (resid 15 name H5) 3.9
assign (resid 16 name H6) (resid 17 name H5) 3.7
assign (resid 17 name H6) (resid 18 name H5) 4.0

```

```
! inter residue H5-H5#
```

```
assign (resid 12 name H5) (resid 11 name H5#) 3.9
```

```

assign (resid 16 name H5#) (resid 15 name H5) 3.4
assign (resid 14 name H5#) (resid 15 name H5) 4.1
assign (resid 16 name H5#) (resid 17 name H5) 4.2

```

```
! inter residue H6-H5#
```

```
assign (resid 15 name H6) (resid 16 name H5#) 3.1
```

```
! inter residue H8-H5#
```

```

assign (resid 11 name H5#) (resid 10 name H8) 3.5
assign (resid 14 name H5#) (resid 13 name H8) 3.2

```

```
! inter residue H1'-H5#
```

```
! inter residue H2'-H5#
```

```

assign (resid 13 name H2') (resid 14 name H5#) 3.3
assign (resid 15 name H2') (resid 16 name H5#) 3.1

```

```
! inter residue H2''-H5#
```

```

assign (resid 13 name H2'') (resid 14 name H5#) 3.9
assign (resid 15 name H2'') (resid 16 name H5#) 3.5

```

```
! inter residue H2'*-H5#
```

```
assign (resid 10 name H2'*) (resid 11 name H5#) 3.2
```

```
! inter residue H3'-H5#
```

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assign (resid 10 name H3') (resid 11 name H5#) 3.2

assign (resid 14 name H5#) (resid 13 name H3') 3.7

assign (resid 16 name H5#) (resid 15 name H3') 3.7

K-4025-119

DHD distance constraints in H_2O
error estimates were only upper bounds as 0.3Å

```
assign (resid 10 name h1) (resid 11 name h3) 3.4
assign (resid 7 name h1) (resid 11 name h3) 3.4
assign (resid 4 name h1) (resid 14 name h3) 3.3
assign (resid 7 name h1) (resid 6 name h3) 3.8
assign (resid 2 name h1) (resid 16 name h3) 3.2
assign (resid 4 name h1) (resid 16 name h3) 3.1
assign (resid 11 name h3) (resid 7 name h1) 4.6
assign (resid 6 name h3) (resid 7 name h1) 4.6
assign (resid 6 name h3) (resid 12 name hn') 4.6
assign (resid 7 name h1) (resid 12 name hn') 3.1
assign (resid 16 name h3) (resid 17 name hn') 3.8
assign (resid 2 name h1) (resid 17 name hn') 2.8
assign (resid 16 name h3) (resid 15 name hn') 4.2
assign (resid 14 name h3) (resid 15 name hn') 4.3
assign (resid 4 name h1) (resid 15 name hn') 2.8
assign (resid 10 name h1) (resid 9 name hn') 3.5
assign (resid 11 name h3) (resid 8 name h2) 3.4
assign (resid 10 name h1) (resid 8 name h2) 4.1
assign (resid 14 name h3) (resid 5 name h2) 2.8
assign (resid 6 name h3) (resid 5 name h2) 3.5
assign (resid 16 name h3) (resid 3 name h2) 2.6
assign (resid 6 name h3) (resid 13 name h2) 2.7
assign (resid 10 name h1) (resid 9 name hn') 3.8
assign (resid 6 name h3) (resid 13 name hn') 3.1
```

K-4025-M10

DHD NOE peak volumes from 150 msec NOESY
relative 10 % error estimated

! Sugar-noes

! H1'-H2'

assign (resid 8 name H1') (resid 8 name H2') 3.0
assign (resid 15 name H1') (resid 15 name H2') 3.0

assign (resid 1 name H2') (resid 1 name H1') 1.8
assign (resid 7 name H2') (resid 7 name H1') 2.5
assign (resid 8 name H2') (resid 8 name H1') 2.6
assign (resid 9 name H2') (resid 9 name H1') 3.9
assign (resid 11 name H2') (resid 11 name H1') 3.3
assign (resid 12 name H2') (resid 12 name H1') 3.2
assign (resid 13 name H2') (resid 13 name H1') 2.7
assign (resid 14 name H2') (resid 14 name H1') 2.6
assign (resid 17 name H2') (resid 17 name H1') 4.7

! H1'-H2''

assign (resid 1 name H1') (resid 1 name H2'') 2.5
assign (resid 3 name H1') (resid 3 name H2'') 1.7
assign (resid 5 name H1') (resid 5 name H2'') 4.2
assign (resid 7 name H1') (resid 7 name H2'') 4.2
assign (resid 9 name H1') (resid 9 name H2'') 4.7
assign (resid 12 name H1') (resid 12 name H2'') 5.0
assign (resid 13 name H1') (resid 13 name H2'') 4.2
assign (resid 14 name H1') (resid 14 name H2'') 4.2
assign (resid 15 name H1') (resid 15 name H2'') 4.1
assign (resid 17 name H1') (resid 17 name H2'') 4.3

assign (resid 4 name H2'') (resid 4 name H1') 2.5
assign (resid 6 name H2'') (resid 6 name H1') 4.1
assign (resid 8 name H2'') (resid 8 name H1') 4.4
assign (resid 11 name H2'') (resid 11 name H1') 4.7
assign (resid 16 name H2'') (resid 16 name H1') 4.0

! inter sugar noe

assign (resid 5 name H2'') (resid 6 name H1') 0.5

! H1'-H2'*

assign (resid 2 name H1') (resid 2 name H2'*) 3.4
assign (resid 10 name H1') (resid 10 name H2'*) 5.5
assign (resid 18 name H1') (resid 18 name H2'*) 8.7

! H1'-H3'

assign (resid 12 name H1') (resid 12 name H3') 1.3

assign (resid 2 name H3') (resid 2 name H1') 0.9
assign (resid 4 name H3') (resid 4 name H1') 1.0
assign (resid 6 name H3') (resid 6 name H1') 1.7
assign (resid 7 name H3') (resid 7 name H1') 1.2
assign (resid 8 name H3') (resid 8 name H1') 1.2
assign (resid 9 name H3') (resid 9 name H1') 1.5
assign (resid 10 name H3') (resid 10 name H1') 1.0
assign (resid 11 name H3') (resid 11 name H1') 1.3
assign (resid 13 name H3') (resid 13 name H1') 1.1
assign (resid 14 name H3') (resid 14 name H1') 0.9
assign (resid 15 name H3') (resid 15 name H1') 1.3
assign (resid 16 name H3') (resid 16 name H1') 1.3
assign (resid 17 name H3') (resid 17 name H1') 1.2
assign (resid 18 name H3') (resid 18 name H1') 1.3

! H1'-H4'

K-4025-m11

```

assign (resid 3 name H1') (resid 3 name H4') 1.0
assign (resid 5 name H1') (resid 5 name H4') 0.9
assign (resid 7 name H1') (resid 7 name H4') 0.9
assign (resid 12 name H1') (resid 12 name H4') 2.8
assign (resid 13 name H1') (resid 13 name H4') 1.2
assign (resid 15 name H1') (resid 15 name H4') 4.2

```

```

assign (resid 2 name H4') (resid 2 name H1') 1.0
assign (resid 4 name H4') (resid 4 name H1') 1.1
assign (resid 6 name H4') (resid 6 name H1') 1.2
assign (resid 8 name H4') (resid 8 name H1') 1.1
assign (resid 9 name H4') (resid 9 name H1') 2.2
assign (resid 10 name H4') (resid 10 name H1') 1.1
assign (resid 11 name H4') (resid 11 name H1') 1.3
assign (resid 16 name H4') (resid 16 name H1') 2.0
assign (resid 17 name H4') (resid 17 name H1') 2.7
assign (resid 18 name H4') (resid 18 name H1') 1.7

```

! H1'-H5

! intra residue H6-H1'

```

assign (resid 6 name H1') (resid 6 name H6) 0.7
assign (resid 9 name H1') (resid 9 name H6) 1.0
assign (resid 11 name H1') (resid 11 name H6) 0.9
assign (resid 12 name H1') (resid 12 name H6) 1.0
assign (resid 14 name H1') (resid 14 name H6) 0.9
assign (resid 18 name H1') (resid 18 name H6) 1.2
assign (resid 12 name H6) (resid 12 name H1') 0.9
assign (resid 17 name H1') (resid 17 name H6) 1.6

```

! inter residue H6-H1'

```

assign (resid 9 name H6) (resid 8 name H1') 1.4
assign (resid 11 name H6) (resid 10 name H1') 1.0
assign (resid 12 name H6) (resid 11 name H1') 1.4
assign (resid 14 name H6) (resid 13 name H1') 1.0
assign (resid 15 name H6) (resid 14 name H1') 1.6
assign (resid 16 name H6) (resid 15 name H1') 0.9
assign (resid 18 name H6) (resid 17 name H1') 0.9

```

```

assign (resid 5 name H1') (resid 6 name H6) 1.3

```

! intra residue H8-H1'

```

assign (resid 2 name H8) (resid 2 name H1') 1.7
assign (resid 4 name H8) (resid 4 name H1') 1.9
assign (resid 7 name H8) (resid 7 name H1') 0.9

```

```

assign (resid 1 name H1') (resid 1 name H8) 0.5
assign (resid 3 name H1') (resid 3 name H8) 0.5
assign (resid 5 name H1') (resid 5 name H8) 0.7
assign (resid 8 name H1') (resid 8 name H8) 1.2
assign (resid 10 name H1') (resid 10 name H8) 0.9
assign (resid 13 name H1') (resid 13 name H8) 1.0

```

! inter residue H1'-H8

```

assign (resid 4 name H8) (resid 3 name H1') 0.1
assign (resid 5 name H8) (resid 4 name H1') 1.1
assign (resid 7 name H8) (resid 6 name H1') 1.1
assign (resid 8 name H8) (resid 7 name H1') 1.4
assign (resid 13 name H8) (resid 12 name H1') 1.3

```

K-4025-M12

```
assign (resid 1 name H1') (resid 2 name H8) 0.7
assign (resid 2 name H1') (resid 3 name H8) 1.2
```

```
! H2'-H3'
```

```
assign (resid 13 name H2') (resid 13 name H3') 2.2
```

```
assign (resid 8 name H3') (resid 8 name H2') 2.9
assign (resid 9 name H3') (resid 9 name H2') 3.0
assign (resid 11 name H3') (resid 11 name H2') 2.6
assign (resid 12 name H3') (resid 12 name H2') 3.4
assign (resid 14 name H3') (resid 14 name H2') 2.3
assign (resid 15 name H3') (resid 15 name H2') 2.4
assign (resid 16 name H3') (resid 16 name H2') 3.0
assign (resid 17 name H3') (resid 17 name H2') 3.0
```

```
! H4'-H2'
```

```
assign (resid 7 name H4') (resid 7 name H2') 0.9
assign (resid 8 name H4') (resid 8 name H2') 0.8
assign (resid 9 name H4') (resid 9 name H2') 0.8
assign (resid 11 name H4') (resid 11 name H2') 0.9
assign (resid 12 name H4') (resid 12 name H2') 1.7
assign (resid 13 name H4') (resid 13 name H2') 1.1
assign (resid 14 name H4') (resid 14 name H2') 1.1
assign (resid 15 name H4') (resid 15 name H2') 1.4
assign (resid 16 name H4') (resid 16 name H2') 1.8
```

```
! H5-H2'
```

```
assign (resid 9 name H5) (resid 8 name H2') 0.8
assign (resid 9 name H5) (resid 9 name H2') 0.6
assign (resid 15 name H5) (resid 14 name H2') 0.7
assign (resid 15 name H5) (resid 15 name H2') 0.6
assign (resid 18 name H5) (resid 17 name H2') 0.8
```

```
assign (resid 11 name H2') (resid 12 name H5) 1.7
assign (resid 16 name H2') (resid 17 name H5) 2.0
```

```
! H2'-H6
```

```
! inter residue
```

```
assign (resid 9 name H6) (resid 9 name H2') 1.9
assign (resid 15 name H6) (resid 15 name H2') 3.5
assign (resid 11 name H2') (resid 11 name H6) 2.0
assign (resid 14 name H2') (resid 14 name H6) 2.3
```

```
! inter residue H2'-H6
```

```
assign (resid 9 name H6) (resid 8 name H2') 1.3
assign (resid 12 name H6) (resid 11 name H2') 3.7
assign (resid 18 name H6) (resid 17 name H2') 3.1
assign (resid 13 name H2') (resid 14 name H6) 1.5
```

```
! intra residue H2'-H8
```

```
assign (resid 2 name H2') (resid 2 name H8) 0.5
assign (resid 7 name H2') (resid 7 name H8) 2.0
```

```
! inter residue H2'-H8
```

```
assign (resid 2 name H8) (resid 1 name H2') 0.7
assign (resid 8 name H8) (resid 7 name H2') 1.1
assign (resid 13 name H8) (resid 12 name H2') 1.7
```

```
! intra residue H2''-H3'
```

```
assign (resid 7 name H3') (resid 7 name H2'') 1.5
```

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```

assign (resid 8 name H3') (resid 8 name H2'') 1.8
assign (resid 9 name H3') (resid 9 name H2'') 1.7
assign (resid 11 name H3') (resid 11 name H2'') 2.2
assign (resid 13 name H3') (resid 13 name H2'') 1.5
assign (resid 14 name H3') (resid 14 name H2'') 1.6
assign (resid 15 name H3') (resid 15 name H2'') 1.7
assign (resid 16 name H3') (resid 16 name H2'') 6.9

```

! intra residue H2'*-H3'

```

assign (resid 2 name H2'*) (resid 2 name H3') 3.4
assign (resid 10 name H2'*) (resid 10 name H3') 2.1
assign (resid 18 name H2'*) (resid 18 name H3') 4.2

```

! intra residue H2''-H4'

```

assign (resid 11 name H4') (resid 11 name H2'') 1.6
assign (resid 17 name H4') (resid 17 name H2'') 1.9

```

```

assign (resid 8 name H2'') (resid 8 name H4') 0.6
assign (resid 9 name H2'') (resid 9 name H4') 1.1
assign (resid 13 name H2'') (resid 13 name H4') 0.7
assign (resid 14 name H2'') (resid 14 name H4') 1.8
assign (resid 15 name H2'') (resid 15 name H4') 1.7

```

! intra residue H2'*-H4'

```

assign (resid 2 name H4') (resid 2 name H2'*) 1.9
assign (resid 10 name H4') (resid 10 name H2'*) 2.2
assign (resid 18 name H4') (resid 18 name H2'*) 2.0

```

! inter residue H2''-H5

```

assign (resid 9 name H5) (resid 8 name H2'') 0.9
assign (resid 12 name H5) (resid 11 name H2'') 1.2
assign (resid 15 name H5) (resid 14 name H2'') 1.0
assign (resid 17 name H5) (resid 16 name H2'') 0.9
assign (resid 18 name H5) (resid 17 name H2'') 0.7
assign (resid 5 name H2'') (resid 6 name H5) 1.4

```

! intra residue H2''-H6

```

assign (resid 9 name H6) (resid 9 name H2'') 0.9
assign (resid 17 name H6) (resid 17 name H2'') 1.1

```

```

assign (resid 6 name H2'') (resid 6 name H6) 1.0
assign (resid 9 name H2'') (resid 9 name H6) 0.9
assign (resid 11 name H2'') (resid 11 name H6) 1.3
assign (resid 12 name H2'') (resid 12 name H6) 1.5
assign (resid 14 name H2'') (resid 14 name H6) 1.4

```

! inter residue H2''-H6

```

assign (resid 15 name H6) (resid 14 name H2'') 1.6

assign (resid 5 name H2'') (resid 6 name H6) 3.1
assign (resid 8 name H2'') (resid 9 name H6) 1.6
assign (resid 11 name H2'') (resid 12 name H6) 2.1
assign (resid 13 name H2'') (resid 14 name H6) 1.5
assign (resid 16 name H2'') (resid 17 name H6) 1.6
assign (resid 17 name H2'') (resid 18 name H6) 1.3

```

K-4025-m14

```
! intra & inter residue H2'*-H6
assign (resid 10 name H2'*) (resid 11 name H6) 3.0
```

```
! intra residue H2''-H8
assign (resid 3 name H8) (resid 3 name H2'') 0.7
assign (resid 5 name H2'') (resid 5 name H8) 1.2
```

```
! inter residue H2''-H8
assign (resid 4 name H8) (resid 3 name H2'') 1.8
assign (resid 5 name H8) (resid 4 name H2'') 3.5
assign (resid 7 name H8) (resid 6 name H2'') 3.9
assign (resid 8 name H8) (resid 7 name H2'') 0.8
```

```
! intra residue H2'*-H8
assign (resid 2 name H2'*) (resid 2 name H8) 3.1
assign (resid 10 name H2'*) (resid 10 name H8) 1.7
```

```
! inter residue H2'*-H8
assign (resid 3 name H8) (resid 2 name H2'*) 1.8
```

```
! intra residue H3'-H4'
assign (resid 2 name H3') (resid 2 name H4') 2.4
assign (resid 9 name H3') (resid 9 name H4') 2.6
assign (resid 10 name H3') (resid 10 name H4') 2.1
assign (resid 11 name H3') (resid 11 name H4') 3.4
assign (resid 15 name H3') (resid 15 name H4') 4.1
assign (resid 16 name H3') (resid 16 name H4') 2.6
```

```
assign (resid 7 name H4') (resid 7 name H3') 3.0
assign (resid 8 name H4') (resid 8 name H3') 3.5
assign (resid 13 name H4') (resid 13 name H3') 3.5
assign (resid 18 name H4') (resid 18 name H3') 3.2
```

```
! intra residue H3'-H6
assign (resid 6 name H6) (resid 6 name H3') 2.9
assign (resid 15 name H6) (resid 15 name H3') 0.4
```

```
assign (resid 9 name H3') (resid 9 name H6) 1.5
assign (resid 11 name H3') (resid 11 name H6) 1.3
assign (resid 12 name H3') (resid 12 name H6) 1.5
assign (resid 14 name H3') (resid 14 name H6) 1.1
assign (resid 17 name H3') (resid 17 name H6) 1.2
```

```
! inter residue H3'-H6
assign (resid 11 name H6) (resid 10 name H3') 0.5
assign (resid 18 name H6) (resid 17 name H3') 1.2
assign (resid 8 name H3') (resid 9 name H6) 0.6
assign (resid 11 name H3') (resid 12 name H6) 0.6
assign (resid 13 name H3') (resid 14 name H6) 0.5
assign (resid 14 name H3') (resid 15 name H6) 0.8
```

```
! intra residue H3'-H8
assign (resid 2 name H8) (resid 2 name H3') 0.8
assign (resid 7 name H8) (resid 7 name H3') 0.9
assign (resid 10 name H8) (resid 10 name H3') 0.5
```

```
assign (resid 8 name H3') (resid 8 name H8) 1.3
```

```
! inter residue H3'-H8
```

K-4025-MLS

```

assign (resid 3 name H8) (resid 2 name H3') 0.4
assign (resid 7 name H8) (resid 6 name H3') 2.3
assign (resid 13 name H8) (resid 12 name H3') 2.1
assign (resid 4 name H3') (resid 5 name H8) 1.8
assign (resid 6 name H3') (resid 7 name H8) 3.5

```

! intra residue H6-H4'

```

assign (resid 6 name H6) (resid 6 name H4') 0.6
assign (resid 11 name H6) (resid 11 name H4') 0.4

```

```

assign (resid 9 name H4') (resid 9 name H6) 0.4
assign (resid 12 name H4') (resid 12 name H6) 0.9
assign (resid 14 name H4') (resid 14 name H6) 0.7

```

! intra residue H8-H4'

```

assign (resid 10 name H8) (resid 10 name H4') 0.5

```

```

assign (resid 8 name H4') (resid 8 name H8) 0.5
assign (resid 13 name H4') (resid 13 name H8) 0.5

```

! inter residue H8-H6

```

assign (resid 6 name H5) (resid 5 name H8) 0.6
assign (resid 9 name H5) (resid 8 name H8) 1.1

```

! inter residue H5-H6

```

assign (resid 11 name H6) (resid 12 name H5) 0.4
assign (resid 14 name H6) (resid 15 name H5) 0.5
assign (resid 16 name H6) (resid 17 name H5) 0.8
assign (resid 17 name H6) (resid 18 name H5) 0.6

```

! inter residue H5-H5#

```

assign (resid 12 name H5) (resid 11 name H5#) 1.0

```

```

assign (resid 16 name H5#) (resid 15 name H5) 2.1
assign (resid 14 name H5#) (resid 15 name H5) 0.8
assign (resid 16 name H5#) (resid 17 name H5) 0.7

```

! inter residue H6-H5#

```

assign (resid 15 name H6) (resid 16 name H5#) 3.1

```

! inter residue H8-H5#

```

assign (resid 11 name H5#) (resid 10 name H8) 2.0
assign (resid 14 name H5#) (resid 13 name H8) 2.7

```

! inter residue H2'-H5#

```

assign (resid 13 name H2') (resid 14 name H5#) 2.3
assign (resid 15 name H2') (resid 16 name H5#) 2.9

```

! inter residue H2''-H5#

```

assign (resid 13 name H2'') (resid 14 name H5#) 1.2
assign (resid 15 name H2'') (resid 16 name H5#) 1.9

```

! inter residue H2'*-H5#

```

assign (resid 10 name H2'*) (resid 11 name H5#) 2.8

```

K-4025-1116

```
! inter residue H3'-H5#  
assign (resid 10 name H3') (resid 11 name H5#) 2.5
```

```
assign (resid 14 name H5#) (resid 13 name H3') 1.7  
assign (resid 16 name H5#) (resid 15 name H3') 1.5
```

```
! inter residue H4'-H5#
```

```
! intra residue H5-H6 reference
```

```
assign (resid 6 name H5) (resid 6 name H6) 3.5  
assign (resid 9 name H5) (resid 9 name H6) 5.4  
assign (resid 12 name H5) (resid 12 name H6) 5.7  
assign (resid 15 name H5) (resid 15 name H6) 5.1  
assign (resid 17 name H5) (resid 17 name H6) 4.9  
assign (resid 18 name H5) (resid 18 name H6) 5.1
```

```
! intra residue H2'-H2'' reference
```

```
assign (resid 7 name H2') (resid 7 name H2'') 7.0  
assign (resid 14 name H2') (resid 14 name H2'') 4.2  
assign (resid 11 name H2'') (resid 11 name H2') 5.4  
assign (resid 12 name H2'') (resid 12 name H2') 5.4
```

```
! intra residue H6-H5# reference
```

```
assign (resid 11 name H6) (resid 11 name H5#) 3.8  
assign (resid 14 name H6) (resid 14 name H5#) 4.0  
assign (resid 16 name H6) (resid 16 name H5#) 4.0
```

```
! inter residue H1'-H2
```

```
assign (resid 5 name H2) (resid 6 name H1') 1.8  
assign (resid 5 name H2) (resid 6 name H2'') 0.5  
assign (resid 8 name H2) (resid 9 name H1') 0.8  
assign (resid 8 name H2) (resid 12 name H1') 0.8  
assign (resid 5 name H2) (resid 15 name H1') 1.2
```

K-402S-M17

DDH distance constraints in D0
error estimation as 0.3 and 0.4Å lower and upper bounds
respectively.

```
!inter residue H5-H6
  assign (resid 15 name h5) (resid 14 name h6) 3.5
  assign (resid 17 name h5) (resid 16 name h6) 3.9
```

```
!inter residue H5-H8
  assign (resid 6 name h5) (resid 5 name h8) 3.2
  assign (resid 9 name h5) (resid 8 name h8) 3.6
```

```
!inter residue H5-H2'
  assign (resid 11 name h2') (resid 12 name h5) 2.7
  assign (resid 14 name h2') (resid 15 name h5) 3.1
  assign (resid 16 name h2') (resid 17 name h5) 3.3
```

```
!inter residue H5-H3'
  assign (resid 9 name h5) (resid 8 name h3') 3.4
```

```
!inter residue H5-H5#
  assign (resid 15 name h5) (resid 16 name h5#) 3.7
  assign (resid 17 name h5) (resid 16 name h5#) 4.5
  assign (resid 12 name h5) (resid 11 name h5#) 4.6
  assign (resid 15 name h5) (resid 14 name h5#) 5.0
```

```
!inter residue H5-H2''
  assign (resid 15 name h5) (resid 14 name h2'') 2.9
  assign (resid 17 name h5) (resid 16 name h2'') 3.2
  assign (resid 17 name h2'') (resid 18 name h5) 3.3
```

```
!inter residue H5-H2'*
  assign (resid 6 name h5) (resid 5 name h2'*) 2.9
```

```
!inter residue H6-H1'
  assign (resid 5 name h1') (resid 6 name h6) 3.4
  assign (resid 8 name h1') (resid 9 name h6) 4.5
  assign (resid 10 name h1') (resid 11 name h6) 4.1
  assign (resid 11 name h1') (resid 12 name h6) 3.3
  assign (resid 13 name h1') (resid 14 name h6) 3.3
  assign (resid 14 name h1') (resid 15 name h6) 3.3
  assign (resid 15 name h1') (resid 16 name h6) 3.7
  assign (resid 17 name h1') (resid 18 name h6) 3.5
  assign (resid 17 name h6) (resid 16 name h1') 3.5
```

```
!intra residue H6-H1'
  assign (resid 6 name h6) (resid 6 name h1') 3.2
  assign (resid 9 name h1') (resid 9 name h6) 3.5
  assign (resid 11 name h1') (resid 11 name h6) 3.5
  assign (resid 12 name h1') (resid 12 name h6) 3.4
  assign (resid 14 name h1') (resid 14 name h6) 3.6
  assign (resid 16 name h1') (resid 16 name h6) 3.6
  assign (resid 17 name h1') (resid 17 name h6) 3.2
  assign (resid 18 name h1') (resid 18 name h6) 4.0
```

```
!intra residue H6-H2'
  assign (resid 14 name h6) (resid 14 name h2') 2.4
  assign (resid 12 name h6) (resid 12 name h2') 2.4
  assign (resid 11 name h6) (resid 11 name h2') 2.5
```

K-4025-m18

```

assign (resid 17 name h6) (resid 17 name h2') 2.6
assign (resid 16 name h2') (resid 16 name h6) 2.5

```

!inter residue H6-H2'

```

assign (resid 15 name h6) (resid 14 name h2') 2.3
assign (resid 18 name h6) (resid 17 name h2') 2.6
assign (resid 12 name h6) (resid 11 name h2') 3.1
assign (resid 13 name h2') (resid 14 name h6) 3.2
assign (resid 15 name h2') (resid 16 name h6) 2.8

```

!intra residue H6-H3'

```

assign (resid 9 name h6) (resid 9 name h3') 2.5
assign (resid 6 name h6) (resid 6 name h3') 2.9
assign (resid 18 name h6) (resid 18 name h3') 2.9
assign (resid 11 name h6) (resid 11 name h3') 3.1
assign (resid 12 name h6) (resid 12 name h3') 3.3
assign (resid 14 name h3') (resid 14 name h6) 3.6
assign (resid 16 name h3') (resid 16 name h6) 3.5

```

!inter residue H6-H3'

```

assign (resid 11 name h6) (resid 10 name h3') 3.7
assign (resid 18 name h6) (resid 17 name h3') 4.2
assign (resid 14 name h6) (resid 13 name h3') 4.4
assign (resid 12 name h6) (resid 11 name h3') 4.4
assign (resid 5 name h3') (resid 6 name h6) 4.0
assign (resid 8 name h3') (resid 9 name h6) 3.1

```

!inter residue H6-H5#

```

assign (resid 15 name h6) (resid 16 name h5#) 3.2

```

!intra residue H6-H2''

```

assign (resid 6 name h6) (resid 6 name h2'') 2.5

```

!inter residue H6-H2''

```

assign (resid 9 name h6) (resid 8 name h2'') 2.5
assign (resid 15 name h6) (resid 14 name h2'') 2.6
assign (resid 18 name h6) (resid 17 name h2'') 2.7
assign (resid 14 name h6) (resid 13 name h2'') 2.8
assign (resid 17 name h6) (resid 16 name h2'') 3.1
assign (resid 11 name h2'') (resid 12 name h6) 2.8

```

!intra residue H6-H2'*

```

assign (resid 18 name h6) (resid 18 name h2'*) 2.5

```

!inter residue H6-H2'*

```

assign (resid 6 name h6) (resid 5 name h2'*) 2.6
assign (resid 10 name h2'*) (resid 11 name h6) 2.4

```

!inter residue H8-H5

```

assign (resid 6 name h5) (resid 5 name h8) 3.2
assign (resid 9 name h5) (resid 8 name h8) 3.6

```

!intra residue H8-H1'

```

assign (resid 2 name h8) (resid 2 name h1') 3.5
assign (resid 8 name h8) (resid 8 name h1') 3.6
assign (resid 7 name h8) (resid 7 name h1') 3.7
assign (resid 4 name h8) (resid 4 name h1') 3.8
assign (resid 3 name h1') (resid 3 name h8) 3.6
assign (resid 5 name h1') (resid 5 name h8) 3.7
assign (resid 10 name h1') (resid 10 name h8) 3.5

```

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```

assign (resid 13 name h1') (resid 13 name h8) 3.5

!inter residue H8-H1'
assign (resid 7 name h8) (resid 6 name h1') 2.8
assign (resid 5 name h8) (resid 4 name h1') 2.8
assign (resid 2 name h8) (resid 1 name h1') 3.0
assign (resid 8 name h8) (resid 7 name h1') 3.2
assign (resid 3 name h1') (resid 4 name h8) 3.3
assign (resid 12 name h1') (resid 13 name h8) 3.1
assign (resid 3 name h8) (resid 2 name h1') 3.0

!intra residue H8-H2'
assign (resid 1 name h8) (resid 1 name h2') 2.5
assign (resid 3 name h2') (resid 3 name h8) 2.5
assign (resid 4 name h2') (resid 4 name h8) 2.4
assign (resid 13 name h2') (resid 13 name h8) 2.4

!inter residue H8-H2'
assign (resid 4 name h2') (resid 5 name h8) 3.5
assign (resid 13 name h8) (resid 12 name h2') 2.9
assign (resid 8 name h8) (resid 7 name h2') 2.3

!intra residue H8-H3'
assign (resid 8 name h8) (resid 8 name h3') 2.8
assign (resid 3 name h8) (resid 3 name h3') 3.4
assign (resid 5 name h8) (resid 5 name h3') 3.5
assign (resid 2 name h8) (resid 2 name h3') 3.5
assign (resid 10 name h8) (resid 10 name h3') 3.7
assign (resid 4 name h8) (resid 4 name h3') 3.7
assign (resid 1 name h3') (resid 1 name h8) 3.6
assign (resid 13 name h3') (resid 13 name h8) 3.4

!inter residue H8-H3'
assign (resid 3 name h3') (resid 4 name h8) 3.9
assign (resid 7 name h3') (resid 8 name h8) 2.9
assign (resid 12 name h3') (resid 13 name h8) 4.5

!intra residue H8-H4'

!inter residue H8-H5#
assign (resid 11 name h5#) (resid 10 name h8) 4.1
assign (resid 14 name h5#) (resid 13 name h8) 3.5

!intra residue H8-H2''
assign (resid 2 name h8) (resid 2 name h2'') 3.4
assign (resid 8 name h8) (resid 8 name h2'') 3.7
assign (resid 7 name h2'') (resid 7 name h8) 3.2

!inter residue H8-H2''
assign (resid 4 name h8) (resid 3 name h2'') 3.0
assign (resid 13 name h8) (resid 12 name h2'') 3.1
assign (resid 3 name h8) (resid 2 name h2'') 3.8
assign (resid 4 name h2'') (resid 5 name h8) 2.6
assign (resid 6 name h2'') (resid 7 name h8) 2.5
assign (resid 7 name h2'') (resid 8 name h8) 2.3

!intra residue H8-H2'*
assign (resid 10 name h8) (resid 10 name h2'*) 3.2

```

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```
assign (resid 5 name h2'*) (resid 5 name h8) 2.8
```

```
!intra residue H1'-H2'
```

```
assign (resid 2 name h1') (resid 2 name h2') 2.6
assign (resid 14 name h1') (resid 14 name h2') 2.7
assign (resid 3 name h1') (resid 3 name h2') 2.7
assign (resid 17 name h1') (resid 17 name h2') 2.8
assign (resid 11 name h1') (resid 11 name h2') 2.9
assign (resid 4 name h1') (resid 4 name h2') 2.9
assign (resid 13 name h1') (resid 13 name h2') 3.0
assign (resid 1 name h1') (resid 1 name h2') 3.0
assign (resid 12 name h2') (resid 12 name h1') 2.7
assign (resid 15 name h2') (resid 15 name h1') 2.8
assign (resid 16 name h2') (resid 16 name h1') 2.7
```

```
!intra residue H1'-H3'
```

```
assign (resid 11 name h1') (resid 11 name h3') 3.2
assign (resid 3 name h1') (resid 3 name h3') 3.4
assign (resid 14 name h1') (resid 14 name h3') 3.5
assign (resid 5 name h1') (resid 5 name h3') 3.5
assign (resid 9 name h1') (resid 9 name h3') 3.5
assign (resid 18 name h1') (resid 18 name h3') 3.6
assign (resid 8 name h1') (resid 8 name h3') 3.7
assign (resid 16 name h1') (resid 16 name h3') 3.8
assign (resid 6 name h3') (resid 6 name h1') 3.1
assign (resid 13 name h3') (resid 13 name h1') 3.6
```

```
!intra residue H1'-H4'
```

```
assign (resid 15 name h1') (resid 15 name h4') 2.7
assign (resid 17 name h1') (resid 17 name h4') 2.8
assign (resid 13 name h1') (resid 13 name h4') 3.0
assign (resid 18 name h1') (resid 18 name h4') 3.0
assign (resid 3 name h1') (resid 3 name h4') 3.2
assign (resid 4 name h1') (resid 4 name h4') 3.3
assign (resid 5 name h1') (resid 5 name h4') 3.4
assign (resid 2 name h1') (resid 2 name h4') 3.5
assign (resid 6 name h4') (resid 6 name h1') 2.8
assign (resid 8 name h4') (resid 8 name h1') 3.7
assign (resid 11 name h4') (resid 11 name h1') 3.3
assign (resid 12 name h4') (resid 12 name h1') 3.4
assign (resid 14 name h4') (resid 14 name h1') 3.2
assign (resid 16 name h4') (resid 16 name h1') 3.3
```

```
!intra residue H1'-H2''
```

```
assign (resid 14 name h1') (resid 14 name h2'') 2.2
assign (resid 11 name h1') (resid 11 name h2'') 2.3
assign (resid 7 name h1') (resid 7 name h2'') 2.4
assign (resid 13 name h1') (resid 13 name h2'') 2.4
assign (resid 12 name h1') (resid 12 name h2'') 2.4
assign (resid 4 name h1') (resid 4 name h2'') 2.4
assign (resid 3 name h1') (resid 3 name h2'') 2.4
assign (resid 9 name h1') (resid 9 name h2'') 2.5
assign (resid 2 name h1') (resid 2 name h2'') 2.5
assign (resid 1 name h1') (resid 1 name h2'') 2.5
assign (resid 6 name h2'') (resid 6 name h1') 2.7
assign (resid 7 name h2'') (resid 7 name h1') 2.4
assign (resid 8 name h2'') (resid 8 name h1') 2.5
assign (resid 15 name h2'') (resid 15 name h1') 2.3
```

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```
assign (resid 16 name h2'') (resid 16 name h1') 2.4
assign (resid 17 name h2'') (resid 17 name h1') 2.3
```

!intra residue H1'-H2'*

```
assign (resid 18 name h1') (resid 18 name h2'*) 2.2
assign (resid 5 name h1') (resid 5 name h2'*) 2.3
assign (resid 10 name h1') (resid 10 name h2'*) 2.3
```

!intra residue H2'-H3'

```
assign (resid 4 name h2') (resid 4 name h3') 2.3
assign (resid 1 name h3') (resid 1 name h2') 2.8
assign (resid 3 name h3') (resid 3 name h2') 2.4
assign (resid 11 name h3') (resid 11 name h2') 2.6
assign (resid 12 name h3') (resid 12 name h2') 2.7
assign (resid 13 name h3') (resid 13 name h2') 2.4
assign (resid 14 name h3') (resid 14 name h2') 2.4
assign (resid 15 name h3') (resid 15 name h2') 3.0
assign (resid 16 name h3') (resid 16 name h2') 2.5
assign (resid 17 name h3') (resid 17 name h2') 2.5
```

!intra residue H2'-H4'

```
assign (resid 17 name h2') (resid 17 name h4') 3.4
assign (resid 2 name h4') (resid 2 name h2') 3.5
assign (resid 3 name h4') (resid 3 name h2') 3.4
assign (resid 4 name h4') (resid 4 name h2') 3.9
assign (resid 11 name h4') (resid 11 name h2') 3.7
assign (resid 12 name h4') (resid 12 name h2') 3.5
assign (resid 13 name h4') (resid 13 name h2') 3.8
assign (resid 14 name h4') (resid 14 name h2') 3.5
assign (resid 15 name h4') (resid 15 name h2') 3.4
```

!inter residue H2'-H5#

```
assign (resid 13 name h2') (resid 14 name h5#) 3.1
assign (resid 15 name h2') (resid 16 name h5#) 3.3
```

!intra residue H3'-H4'

```
assign (resid 3 name h3') (resid 3 name h4') 2.7
assign (resid 13 name h3') (resid 13 name h4') 2.8
assign (resid 2 name h3') (resid 2 name h4') 2.8
assign (resid 18 name h3') (resid 18 name h4') 2.8
assign (resid 4 name h3') (resid 4 name h4') 2.9
```

!inter residue H3'-H5#

```
assign (resid 10 name h3') (resid 11 name h5#) 3.2
assign (resid 15 name h3') (resid 16 name h5#) 4.1
assign (resid 13 name h3') (resid 14 name h5#) 4.5
```

!intra residue H3'-H2''

```
assign (resid 11 name h3') (resid 11 name h2'') 2.5
assign (resid 14 name h3') (resid 14 name h2'') 2.6
assign (resid 16 name h3') (resid 16 name h2'') 2.6
assign (resid 9 name h3') (resid 9 name h2'') 2.6
assign (resid 2 name h3') (resid 2 name h2'') 2.8
assign (resid 1 name h3') (resid 1 name h2'') 2.9
assign (resid 13 name h3') (resid 13 name h2'') 2.9
assign (resid 12 name h3') (resid 12 name h2'') 2.9
assign (resid 3 name h2'') (resid 3 name h3') 2.7
```

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```
!intra residue H3'-H2'*
  assign (resid 10 name h3') (resid 10 name h2'*) 2.5
  assign (resid 18 name h3') (resid 18 name h2'*) 2.5
  assign (resid 5 name h3') (resid 5 name h2'*) 2.6
```

```
!intra residue H4'-H2''
  assign (resid 12 name h4') (resid 12 name h2'') 3.1
  assign (resid 14 name h4') (resid 14 name h2'') 3.3
  assign (resid 4 name h4') (resid 4 name h2'') 3.4
  assign (resid 13 name h4') (resid 13 name h2'') 3.5
  assign (resid 2 name h4') (resid 2 name h2'') 3.6
  assign (resid 11 name h4') (resid 11 name h2'') 3.6
  assign (resid 3 name h4') (resid 3 name h2'') 3.7
```

```
!intra residue H4'-H2'*
  assign (resid 5 name h4') (resid 5 name h2'*) 2.9
  assign (resid 18 name h2'*) (resid 18 name h4') 3.1
```

```
!inter residue H2''-H5#
  assign (resid 13 name h2'') (resid 14 name h5#) 3.2
  assign (resid 15 name h2'') (resid 16 name h5#) 3.4
!inter residue H2'*-H5#
  assign (resid 10 name h2'*) (resid 11 name h5#) 2.7
```

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DDH NOE volume from 150 msec NOESY spectrum in 2D.

10 % relative error was estimated.

!intra residue H5-H6 reference

assign (resid 17 name	h5)	(resid 17 name	h6)	6.8
assign (resid 6 name	h5)	(resid 6 name	h6)	5.3
assign (resid 12 name	h6)	(resid 12 name	h5)	8.8
assign (resid 15 name	h6)	(resid 15 name	h5)	7.2

!intra residue H2''-H2'' reference

assign (resid 13 name	h2'')	(resid 13 name	h2'')	6.0
assign (resid 11 name	h2'')	(resid 11 name	h2'')	7.8

!intra residue H6-H5# reference

assign (resid 11 name	h6)	(resid 11 name	h5#)	7.1
assign (resid 16 name	h6)	(resid 16 name	h5#)	6.3
assign (resid 14 name	h6)	(resid 14 name	h5#)	6.4

!inter residue H5-H6

assign (resid 15 name	h5)	(resid 14 name	h6)	1.1
assign (resid 17 name	h5)	(resid 16 name	h6)	0.8

!inter residue H5-H8

assign (resid 6 name	h5)	(resid 5 name	h8)	1.6
assign (resid 9 name	h5)	(resid 8 name	h8)	0.7

!inter residue H5-H2'

assign (resid 11 name	h2')	(resid 12 name	h5)	6.3
assign (resid 14 name	h2')	(resid 15 name	h5)	3.6
assign (resid 16 name	h2')	(resid 17 name	h5)	2.5

!inter residue H5-H3'

assign (resid 9 name	h5)	(resid 8 name	h3')	1.5
----------------------	-----	---------------	------	-----

!inter residue H5-H5#

assign (resid 15 name	h5)	(resid 16 name	h5#)	2.5
assign (resid 17 name	h5)	(resid 16 name	h5#)	0.6
assign (resid 12 name	h5)	(resid 11 name	h5#)	1.0
assign (resid 15 name	h5)	(resid 14 name	h5#)	0.9

!inter residue H5-H2''

assign (resid 15 name	h5)	(resid 14 name	h2'')	4.0
assign (resid 17 name	h5)	(resid 16 name	h2'')	1.4
assign (resid 17 name	h2'')	(resid 18 name	h5)	2.3

!inter residue H5-H2''*

assign (resid 6 name	h5)	(resid 5 name	h2''*)	2.9
----------------------	-----	---------------	--------	-----

!inter residue H6-H1'

assign (resid 5 name	h1')	(resid 6 name	h6)	1.4
assign (resid 8 name	h1')	(resid 9 name	h6)	1.2
assign (resid 10 name	h1')	(resid 11 name	h6)	0.9
assign (resid 11 name	h1')	(resid 12 name	h6)	1.9
assign (resid 13 name	h1')	(resid 14 name	h6)	1.3
assign (resid 14 name	h1')	(resid 15 name	h6)	1.8
assign (resid 15 name	h1')	(resid 16 name	h6)	1.0

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```

assign (resid 17 name h1') (resid 18 name h6) 1.8
assign (resid 17 name h6) (resid 16 name h1') 1.0

```

!intra residue H6-H1'

```

assign (resid 6 name h6) (resid 6 name h1') 1.7
assign (resid 9 name h1') (resid 9 name h6) 1.1
assign (resid 11 name h1') (resid 11 name h6) 1.1
assign (resid 12 name h1') (resid 12 name h6) 1.9
assign (resid 14 name h1') (resid 14 name h6) 1.3
assign (resid 16 name h1') (resid 16 name h6) 1.1
assign (resid 17 name h1') (resid 17 name h6) 2.6
assign (resid 18 name h1') (resid 18 name h6) 1.1

```

!intra residue H6-H2'

```

assign (resid 14 name h6) (resid 14 name h2') 5.4
assign (resid 12 name h6) (resid 12 name h2') 6.7
assign (resid 11 name h6) (resid 11 name h2') 5.2
assign (resid 17 name h6) (resid 17 name h2') 3.8
assign (resid 16 name h2') (resid 16 name h6) 4.6

```

!inter residue H6-H2'

```

assign (resid 15 name h6) (resid 14 name h2') 9.1
assign (resid 18 name h6) (resid 17 name h2') 4.2
assign (resid 12 name h6) (resid 11 name h2') 1.6
assign (resid 13 name h2') (resid 14 name h6) 2.0
assign (resid 15 name h2') (resid 16 name h6) 3.0

```

!intra residue H6-H3'

```

assign (resid 9 name h6) (resid 9 name h3') 5.4
assign (resid 6 name h6) (resid 6 name h3') 2.2
assign (resid 18 name h6) (resid 18 name h3') 3.0
assign (resid 11 name h6) (resid 11 name h3') 2.3
assign (resid 12 name h6) (resid 12 name h3') 2.1
assign (resid 14 name h3') (resid 14 name h6) 1.7
assign (resid 16 name h3') (resid 16 name h6) 1.4

```

!inter residue H6-H3'

```

assign (resid 11 name h6) (resid 10 name h3') 0.8
assign (resid 18 name h6) (resid 17 name h3') 0.5
assign (resid 14 name h6) (resid 13 name h3') 0.3
assign (resid 12 name h6) (resid 11 name h3') 0.3
assign (resid 5 name h3') (resid 6 name h6) 0.6
assign (resid 8 name h3') (resid 9 name h6) 1.8

```

!inter residue H6-H5#

```

assign (resid 15 name h6) (resid 16 name h5#) 4.1

```

!intra residue H6-H2''

```

assign (resid 6 name h6) (resid 6 name h2'') 4.5
assign (resid 11 name h6) (resid 11 name h2'') 4.4
assign (resid 17 name h6) (resid 17 name h2'') 2.9
assign (resid 14 name h2'') (resid 14 name h6) 3.7

```

!inter residue H6-H2''

```

assign (resid 9 name h6) (resid 8 name h2'') 4.8
assign (resid 15 name h6) (resid 14 name h2'') 4.8
assign (resid 18 name h6) (resid 17 name h2'') 5.5
assign (resid 14 name h6) (resid 13 name h2'') 2.1
assign (resid 17 name h6) (resid 16 name h2'') 1.5

```

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```
assign (resid 11 name h2'') (resid 12 name h6) 5.8
```

```
!intra residue H6-H2''
```

```
assign (resid 18 name h6) (resid 18 name h2'*) 5.8
```

```
!inter residue H6-H2''
```

```
assign (resid 6 name h6) (resid 5 name h2'*) 4.6
```

```
assign (resid 10 name h2'*) (resid 11 name h6) 8.3
```

```
!inter residue H8-H5
```

```
assign (resid 6 name h5) (resid 5 name h8) 1.6
```

```
assign (resid 9 name h5) (resid 8 name h8) 0.7
```

```
!intra residue H8-H1'
```

```
assign (resid 2 name h8) (resid 2 name h1') 1.6
```

```
assign (resid 8 name h8) (resid 8 name h1') 0.7
```

```
assign (resid 7 name h8) (resid 7 name h1') 0.6
```

```
assign (resid 4 name h8) (resid 4 name h1') 1.2
```

```
assign (resid 3 name h1') (resid 3 name h8) 1.4
```

```
assign (resid 5 name h1') (resid 5 name h8) 1.3
```

```
assign (resid 10 name h1') (resid 10 name h8) 1.2
```

```
assign (resid 13 name h1') (resid 13 name h8) 1.2
```

```
!inter residue H8-H1'
```

```
assign (resid 7 name h8) (resid 6 name h1') 3.1
```

```
assign (resid 5 name h8) (resid 4 name h1') 3.2
```

```
assign (resid 2 name h8) (resid 1 name h1') 2.3
```

```
assign (resid 8 name h8) (resid 7 name h1') 2.2
```

```
assign (resid 3 name h1') (resid 4 name h8) 1.7
```

```
assign (resid 12 name h1') (resid 13 name h8) 2.0
```

```
assign (resid 3 name h8) (resid 2 name h1') 2.4
```

```
!intra residue H8-H2'
```

```
assign (resid 1 name h8) (resid 1 name h2') 6.9
```

```
assign (resid 3 name h2') (resid 3 name h8) 5.4
```

```
assign (resid 4 name h2') (resid 4 name h8) 8.6
```

```
assign (resid 13 name h2') (resid 13 name h8) 5.8
```

```
!inter residue H8-H2'
```

```
assign (resid 4 name h2') (resid 5 name h8) 2.0
```

```
assign (resid 13 name h8) (resid 12 name h2') 2.8
```

```
assign (resid 8 name h8) (resid 7 name h2'') 8.1
```

```
!intra residue H8-H3'
```

```
assign (resid 8 name h8) (resid 8 name h3') 2.3
```

```
assign (resid 3 name h8) (resid 3 name h3') 1.8
```

```
assign (resid 5 name h8) (resid 5 name h3') 1.2
```

```
assign (resid 2 name h8) (resid 2 name h3') 1.6
```

```
assign (resid 10 name h8) (resid 10 name h3') 0.8
```

```
assign (resid 4 name h8) (resid 4 name h3') 1.2
```

```
assign (resid 1 name h3') (resid 1 name h8) 1.5
```

```
assign (resid 13 name h3') (resid 13 name h8) 1.5
```

```
!inter residue H8-H3'
```

```
assign (resid 3 name h3') (resid 4 name h8) 0.6
```

```
assign (resid 7 name h3') (resid 8 name h8) 2.9
```

```
assign (resid 12 name h3') (resid 13 name h8) 0.6
```

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!inter residue H8-H5#

```
assign (resid 11 name h5#) (resid 10 name h8) 2.5
assign (resid 14 name h5#) (resid 13 name h8) 3.5
```

!intra residue H8-H2''

```
assign (resid 2 name h8) (resid 2 name h2'') 1.5
assign (resid 8 name h8) (resid 8 name h2'') 1.0
assign (resid 7 name h2'') (resid 7 name h8) 2.2
```

!inter residue H8-H2''

```
assign (resid 4 name h8) (resid 3 name h2'') 1.6
assign (resid 13 name h8) (resid 12 name h2'') 2.8
assign (resid 3 name h8) (resid 2 name h2'') 0.6
assign (resid 4 name h2'') (resid 5 name h8) 5.4
assign (resid 6 name h2'') (resid 7 name h8) 5.0
assign (resid 7 name h2'') (resid 8 name h8) 7.1
```

!intra residue H8-H2'*

```
assign (resid 10 name h8) (resid 10 name h2'*) 2.1
assign (resid 5 name h2'*) (resid 5 name h8) 3.6
```

!intra residue H1'-H2'

```
assign (resid 2 name h1') (resid 2 name h2') 5.4
assign (resid 14 name h1') (resid 14 name h2') 4.6
assign (resid 3 name h1') (resid 3 name h2') 4.4
assign (resid 17 name h1') (resid 17 name h2') 5.0
assign (resid 11 name h1') (resid 11 name h2') 2.4
assign (resid 4 name h1') (resid 4 name h2') 3.4
assign (resid 13 name h1') (resid 13 name h2') 3.1
assign (resid 1 name h1') (resid 1 name h2') 3.5
assign (resid 12 name h2') (resid 12 name h1') 5.4
assign (resid 15 name h2') (resid 15 name h1') 4.3
assign (resid 16 name h2') (resid 16 name h1') 5.4
```

!intra residue H1'-H3'

```
assign (resid 11 name h1') (resid 11 name h3') 2.4
assign (resid 3 name h1') (resid 3 name h3') 1.5
assign (resid 14 name h1') (resid 14 name h3') 1.7
assign (resid 5 name h1') (resid 5 name h3') 1.5
assign (resid 9 name h1') (resid 9 name h3') 1.6
assign (resid 18 name h1') (resid 18 name h3') 1.1
assign (resid 8 name h1') (resid 8 name h3') 1.6
assign (resid 16 name h1') (resid 16 name h3') 1.0
assign (resid 6 name h3') (resid 6 name h1') 2.5
assign (resid 13 name h3') (resid 13 name h1') 1.3
```

!intra residue H1'-H4'

```
assign (resid 15 name h1') (resid 15 name h4') 5.7
assign (resid 17 name h1') (resid 17 name h4') 5.1
assign (resid 13 name h1') (resid 13 name h4') 2.7
assign (resid 18 name h1') (resid 18 name h4') 3.2
assign (resid 3 name h1') (resid 3 name h4') 1.3
assign (resid 4 name h1') (resid 4 name h4') 2.5
assign (resid 5 name h1') (resid 5 name h4') 1.6
assign (resid 2 name h1') (resid 2 name h4') 1.3
assign (resid 6 name h4') (resid 6 name h1') 2.9
assign (resid 8 name h4') (resid 8 name h1') 0.8
assign (resid 11 name h4') (resid 11 name h1') 1.8
assign (resid 12 name h4') (resid 12 name h1') 1.9
```

K-402S-m27

```

assign (resid 14 name h4') (resid 14 name h1') 2.5
assign (resid 16 name h4') (resid 16 name h1') 3.0

!inter residue H1'-H5#
assign (resid 13 name h1') (resid 14 name h5#) 1.3
assign (resid 10 name h1') (resid 11 name h5#) 1.1

!intra residue H1'-H2''
assign (resid 14 name h1') (resid 14 name h2'') 8.3
assign (resid 11 name h1') (resid 11 name h2'') 6.8
assign (resid 7 name h1') (resid 7 name h2'') 7.7
assign (resid 13 name h1') (resid 13 name h2'') 4.5
assign (resid 12 name h1') (resid 12 name h2'') 5.2
assign (resid 4 name h1') (resid 4 name h2'') 5.6
assign (resid 3 name h1') (resid 3 name h2'') 5.4
assign (resid 9 name h1') (resid 9 name h2'') 6.8
assign (resid 2 name h1') (resid 2 name h2'') 4.4
assign (resid 1 name h1') (resid 1 name h2'') 6.8
assign (resid 6 name h2'') (resid 6 name h1') 3.9
assign (resid 7 name h2'') (resid 7 name h1') 8.2
assign (resid 8 name h2'') (resid 8 name h1') 5.7
assign (resid 15 name h2'') (resid 15 name h1') 9.1
assign (resid 16 name h2'') (resid 16 name h1') 7.3
assign (resid 17 name h2'') (resid 17 name h1') 8.7

!intra residue H1'-H2'*
assign (resid 18 name h1') (resid 18 name h2'*) 16.9
assign (resid 5 name h1') (resid 5 name h2'*) 9.4
assign (resid 10 name h1') (resid 10 name h2'*) 9.9

!intra residue H2'-H3'
assign (resid 4 name h2') (resid 4 name h3') 8.8
assign (resid 1 name h3') (resid 1 name h2') 3.3
assign (resid 3 name h3') (resid 3 name h2') 6.2
assign (resid 11 name h3') (resid 11 name h2') 4.8
assign (resid 12 name h3') (resid 12 name h2') 4.4
assign (resid 13 name h3') (resid 13 name h2') 5.7
assign (resid 14 name h3') (resid 14 name h2') 7.2
assign (resid 15 name h3') (resid 15 name h2') 0.9
assign (resid 16 name h3') (resid 16 name h2') 5.4
assign (resid 17 name h3') (resid 17 name h2') 5.9

!intra residue H2'-H4'
assign (resid 17 name h2') (resid 17 name h4') 4.8
assign (resid 2 name h4') (resid 2 name h2') 1.4
assign (resid 3 name h4') (resid 3 name h2') 2.0
assign (resid 4 name h4') (resid 4 name h2') 0.8
assign (resid 11 name h4') (resid 11 name h2') 1.1
assign (resid 12 name h4') (resid 12 name h2') 1.8
assign (resid 13 name h4') (resid 13 name h2') 1.0
assign (resid 14 name h4') (resid 14 name h2') 2.9
assign (resid 15 name h4') (resid 15 name h2') 2.6

!inter residue H2'-H5#
assign (resid 13 name h2') (resid 14 name h5#) 5.8
assign (resid 15 name h2') (resid 16 name h5#) 3.1

!intra residue H3'-H4'

```

K-4025-m28

```

assign (resid 3 name h3') (resid 3 name h4') 5.9
assign (resid 13 name h3') (resid 13 name h4') 4.8
assign (resid 2 name h3') (resid 2 name h4') 5.8
assign (resid 18 name h3') (resid 18 name h4') 7.1
assign (resid 4 name h3') (resid 4 name h4') 3.5

```

!inter residue H3'-H5#

```

assign (resid 10 name h3') (resid 11 name h5#) 4.2
assign (resid 15 name h3') (resid 16 name h5#) 0.5
assign (resid 13 name h3') (resid 14 name h5#) 1.2

```

!intra residue H3'-H2''

```

assign (resid 11 name h3') (resid 11 name h2'') 6.2
assign (resid 14 name h3') (resid 14 name h2'') 6.2
assign (resid 16 name h3') (resid 16 name h2'') 5.9
assign (resid 9 name h3') (resid 9 name h2'') 9.2
assign (resid 2 name h3') (resid 2 name h2'') 2.7
assign (resid 1 name h3') (resid 1 name h2'') 2.4
assign (resid 13 name h3') (resid 13 name h2'') 2.6
assign (resid 12 name h3') (resid 12 name h2'') 3.0
assign (resid 3 name h2'') (resid 3 name h3') 3.8

```

!intra residue H3'-H2'*

```

assign (resid 10 name h3') (resid 10 name h2'*) 4.3
assign (resid 18 name h3') (resid 18 name h2'*) 6.9
assign (resid 5 name h3') (resid 5 name h2'*) 4.9

```

!intra residue H4'-H2''

```

assign (resid 12 name h4') (resid 12 name h2'') 2.6
assign (resid 14 name h4') (resid 14 name h2'') 2.9
assign (resid 4 name h4') (resid 4 name h2'') 1.7
assign (resid 13 name h4') (resid 13 name h2'') 1.3
assign (resid 2 name h4') (resid 2 name h2'') 1.0
assign (resid 11 name h4') (resid 11 name h2'') 1.1
assign (resid 3 name h4') (resid 3 name h2'') 1.2

```

!intra residue H4'-H2'*

```

assign (resid 5 name h4') (resid 5 name h2'*) 3.8
assign (resid 18 name h2'*) (resid 18 name h4') 4.0

```

!inter residue H2''-H5#

```

assign (resid 13 name h2'') (resid 14 name h5#) 2.8
assign (resid 15 name h2'') (resid 16 name h5#) 3.9

```

!inter residue H2'*-H5#

```

assign (resid 10 name h2'*) (resid 11 name h5#) 4.4

```

```

assign (resid 13 name h2) (resid 7 name h1') 1.6
assign (resid 13 name h2) (resid 14 name h1') 0.7
assign (resid 3 name h2) (resid 4 name h1') 0.6
assign (resid 3 name h2) (resid 17 name h1') 1.2
assign (resid 5 name h2) (resid 15 name h1') 1.0
assign (resid 5 name h2) (resid 6 name h1') 1.4
assign (resid 8 name h2) (resid 9 name h1') 2.0
assign (resid 8 name h2) (resid 12 name h1') 1.1

```