

BIOCHEMISTRY

including biophysical chemistry & molecular biology

Supporting information for *Biochemistry*, **1995**, 34(42), 13871 – 13880, DOI: [10.1021/bi00042a019](https://doi.org/10.1021/bi00042a019)

MCEVOY

13871-13880

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>.



ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1995 American Chemical Society

Supplementary Material

Table S-1 Resonance assignments of CheA124-257 in 50 mM sodium phosphate pH 6.5 at 30°C

residue	H _N	H _α	H _β	others	C-carbonyl
R124					
Q125		4.38(55.02)	2.10, 2.02(29.27)	Hγ2.39, 2.39(33.60)	
L126	8.33(124.60)	4.16(54.58)	1.63(42.19)	1.29,0.93(26.75,23.14,24.71)	177.75
A127	8.26(125.30)	4.36(52.18)	1.41(18.91)		178.20
L128	8.11(121.51)	4.36(55.05)	1.64, 1.64(42.10)	1.64,0.96,0.90(29.24,24.64,23.21)	176.46
E129	8.31(121.55)	4.29(56.23)	2.06, 1.98(30.03)	Hγ2.27, 2.27(35.98)	176.82
A130	8.23(125.53)	4.30(52.08)	1.41(18.94)		173.23
K131	8.25(121.14)	4.36(55.93)	1.90, 1.83(32.76)	Hε3.02(41.88)1.50, 1.42,1.72, 1.70(24.37,28.70)	177.72
G132	8.32(110.08)	3.96(44.90)			174.58
E133	8.26(120.78)	4.37(56.02)	2.07, 1.94(30.51)	Hγ2.27(35.95)	177.18
T134	8.31(118.38)	4.62(59.52)	4.17(69.33)		
P135		4.48(63.68)	2.36, 2.05(31.87)	Hγ2.00(27.04) Hδ3.9, 3.75(50.88)	177.67
S136	8.37(116.37)	4.35(58.02)	3.83(63.68)		175.20
A137	8.54(126.63)	4.38(52.52)	1.43(19.13)		178.48
V138	8.01(118.69)	4.08(62.24)	2.03(32.39)	Hγ0.96(20.70)	177.19
T139	8.12(118.09)	4.22(61.96)	(69.29)	Hγ1.23(21.28)	175.00
R140	8.28(123.74)	4.33(55.79)	1.87, 1.81(30.63)	Hγ1.64, 1.64(26.81) Hδ3.21(42.24)	176.68
L141	8.22(123.33)	4.42(54.97)	1.66, 1.66(42.17)	1.65,0.95, 0.90(24.64,23.10)	177.10
S142	8.26(116.85)	4.50(58.05)	3.87, 3.87(63.41)		173.83
V143	8.05(121.85)	4.21(61.90)	2.12(32.52)	Hγ0.95(20.60)	176.69
V144	8.10(123.85)	4.06(61.88)	1.99(32.50)	Hγ0.85(20.60)	176.35
A145	8.32(128.48)	4.29(52.00)	1.41(19.16)		178.02
K146	8.26(121.29)	4.37(55.58)	1.86, 1.79(33.01)	1.72,1.49, 1.44(24.39,28.75) Hε3.03(41.86)	177.05
S147	8.32(117.73)	4.50(57.76)	3.87, 3.87(63.57)		174.71
E148	8.40(124.18)	4.59(54.06)	1.85(29.48)	Hγ2.21, 2.05	
P149		4.44(63.09)	2.23, 2.07(31.80)	Hγ1.97(27.15) Hδ3.83, 3.75(50.42)	177.76
Q150	8.53(120.54)	4.30(55.46)	1.91(29.40)	Hγ2.32, 2.05(33.54)	
D151	8.32(121.69)	4.33(56.28)	2.73(41.07)		
E152	8.44(121.79)	4.25(57.15)	2.11, 2.00(29.73)	Hγ2.30(35.94)	177.81
Q153	8.39(120.54)	4.33(56.25)	2.18, 2.07(28.86)	2.42(33.68)	177.28
S154	8.23(116.58)	(58.47)	3.92(63.14)		
R155	8.18(122.85)	4.35(55.95)	1.92, 1.82(30.60)	Hγ1.66(26.81) Hδ3.23(43.13)	
S156	8.26(116.85)	4.33(58.04)	3.90(63.41)		
Q157	8.35(122.38)	4.48(55.30)	2.15, 1.96(29.95)	Hγ2.38(33.62)	176.50
S158	8.31(119.76)	(56.44)	63.02		
P159		4.58(62.57)	2.30(32.38)	Hγ2.01(27.09) Hδ3.95, 3.76(50.60)	179.86
R160	8.31(118.71)	5.04(53.85)	1.85, 1.79(33.51)	Hγ1.74, 1.74(26.26) Hδ3.11, 3.04(43.30)	174.38

K-13880-M1

R161	9.22(123.64)	5.37(53.86)	1.77, 1.55(33.21)	H γ 1.54, 1.36(27.45)	H δ 3.15, 3.15(43.04)		175.79
I162	9.22(126.14)	4.90(58.05)	1.52(40.84)	H γ 0.73, 0.64(28.14)	H δ 0.86(14.62)	H γ m0.68(16.35)	173.26
I163	8.66(126.17)	4.59(60.78)	1.59(40.52)	H γ 1.29, 0.93(27.67)	H δ 0.73(14.92)	H γ m0.72(18.16)	175.98
L164	9.31(128.85)	5.51(52.13)	2.04, 1.22(43.19)	H γ 1.59(26.75)	H δ 0.86(26.75), H δ 0.84(25.19)		176.71
S165	8.54(116.58)	4.97(56.86)	3.82, 3.7(66.20)				172.62
R166	8.94(116.49)	3.91(56.57)	1.94(27.15)	H γ 1.59, 1.59(28.13)	H δ 3.33, 3.22(43.39)		175.99
L167	8.36(117.29)	4.30(53.88)	1.22(41.66)	H γ 1.49, 1.22(26.97)	H δ 0.66(22.10)		178.72
K168	8.90(122.81)	4.40(54.55)	2.01, 1.51(33.57)	H γ 1.57, 1.52(24.99)	H δ 1.74, 1.74(28.70)	He3.11, 3.11(41.91)	178.20
A169	8.47(124.77)	4.20(54.58)	1.48(17.89)				180.16
G170	8.71(110.00)	4.22, 3.98(45.47)					176.73
E171	8.17(119.63)	4.12(58.37)	2.44, 1.90(30.47)	H γ 2.23, 2.10(37.49)			178.49
V172	7.81(119.61)	3.42(67.08)	2.12(31.29)	H γ 0.98(22.39), H γ 1.04(21.28)			177.44
D173	7.79(117.15)	4.42(56.75)	2.75, 2.55(39.88)				180.01
L174	7.23(121.45)	4.23(57.66)	1.79, 1.79(42.49)	H γ 1.69(26.97)	H δ 0.98(24.42), H δ 0.98(24.42)		179.83
L175	8.52(118.99)	4.02(57.10)	1.93, 1.93(40.24)	H γ 1.13(27.34)	H δ 0.90(27.34), H δ 0.85(22.43)		179.29
E176	7.91(121.03)	3.64(60.11)	2.35, 1.95(29.28)	H γ 2.13, 2.03(35.51)			179.22
E177	7.55(120.01)	3.95(58.83)	2.19, 2.19(29.01)	H γ 2.29, 2.18(35.84)			175.60
E178	8.29(118.75)	4.01(58.78)	2.05(29.33)	H γ 2.42, 2.26(35.03)			181.18
L179	8.60(119.39)	4.03(57.89)	1.98, 1.43(42.40)	H γ 1.80(26.97)	H δ 0.89(24.14), H δ 0.84(24.75)		179.66
G180	7.92(105.32)	4.43, 3.91(45.58)					176.13
H181	7.39(115.67)	4.80(55.83)	3.39, 3.39(28.65)				176.34
L182	7.76(119.00)	4.42(55.73)	1.95, 1.62(43.68)	H γ 1.86(26.74)	H δ 1.00(25.17), H δ 0.94(23.47)		177.07
T183	8.03(113.87)	4.62(59.44)	4.14(67.50)	H γ 1.07(18.09)			172.33
T184	7.98(116.56)	4.47(61.31)	4.05(69.81)	H γ 1.66(21.34)			174.33
L185	8.54(124.82)	4.87(53.82)	1.73, 1.27(43.60)	H γ 1.28(26.85)	H δ 0.86(24.82), H δ 0.72(23.44)		177.25
T186	8.41(114.54)	4.65(60.19)	4.10(71.15)	H γ 1.19(21.23)			173.00
D187	8.78(122.02)	4.14(54.64)	2.92, 2.49(39.47)				174.55
V188	8.02(117.97)	4.40(63.13)	1.98(31.51)	H γ 0.92(22.97), H γ 0.88(21.03)			178.40
V189	9.23(131.22)	4.25(61.89)	2.02(33.49)	H γ 0.83(20.83), H γ 0.85(20.64)			176.43
K190	8.86(129.14)	4.75(55.64)	1.79(33.71)	H γ 1.41, 1.15(25.75)	H δ 1.65, 1.65(28.99)	He2.77, 2.70(41.83)	176.62
G191	8.40(112.95)	4.62, 3.79(42.93)					174.12
A192	8.64(122.25)	4.19(54.47)	1.43(18.26)				179.65
D193	7.93(112.92)	4.56(51.73)	3.33, 2.44(41.50)				175.46
S194	6.96(110.56)	5.25(56.47)	3.86, 3.86(66.46)				
L195	8.43(121.81)	5.11(54.06)	1.57, 1.57(46.49)	H γ 1.41(27.28)	H δ 0.85(25.24), H δ 0.71(25.24)		174.40
S196	8.78(120.48)	5.88(55.25)	3.85, 3.8(66.16)				173.35
A197	8.59(122.53)	4.76(51.36)	1.36(23.73)				175.25
I198	8.90(120.81)	4.76(60.57)	1.85(36.96)	H γ 1.71, 1.04(27.94)	H δ 0.84(12.97)	H γ m1.04(17.74)	176.00
L199	9.13(128.01)	5.13(51.33)	1.81, 1.68(42.56)	H δ 1.03(26.55), H δ 0.91(24.28)			

P200		4.56(63.43)	2.41, 1.76(32.37)	H γ 2.12, 2.03(27.65)	H δ 4.15, 3.70(50.68)	178.21
G201	8.51(106.04)	3.95, 3.78(45.96)				174.77
D202	8.06(116.65)	4.53(53.42)	2.85, 2.60(39.72)			176.22
I203	7.07(118.08)	4.36(58.88)	1.89(39.04)	H γ 1.56, 1.36(27.22)	H δ 0.90(13.38) H γ m1.01(17.45)	175.05
A204	8.75(130.19)	4.37(51.36)	1.48(18.69)			179.06
E205	8.82(124.17)	3.45(60.06)	1.60, 1.50(28.84)	H γ 1.71, 1.27(35.71)		179.60
D206	8.72(116.56)	4.45(56.35)	2.71, 2.53(39.62)			179.05
D207	7.17(120.19)	4.54(56.60)	2.95, 2.72(39.92)			178.86
I208	7.43(118.94)	3.78(63.84)	2.23(37.76)	H γ 1.75, 1.13(28.31)	H δ 0.79 H γ m0.96(17.90)	178.80
T209	8.67(115.10)	3.76(66.55)	4.35(68.06)	H γ 1.40(21.78)		176.64
A210	7.63(122.03)	4.06(54.94)	1.57(18.13)			180.26
V211	7.07(114.50)	3.98(64.56)	2.22, 2.22(32.19)	H γ 1.17(21.44), H γ 1.07(20.69)		179.56
L212	8.09(118.23)	4.14(56.90)	1.90, 1.32(41.34)	H δ 0.85(26.78), H δ 0.62(22.01)		180.19
C213	8.20(115.76)	5.20(61.38)	3.13, 2.91(26.22)			175.60
F214	7.25(117.24)	4.62(59.63)	3.31, 3.15(38.77)	H δ 7.48		176.76
V215	8.10(117.56)	4.26(63.46)	2.07(34.55)	H γ 1.00(21.11), H γ 0.96(21.11)		176.04
I216	7.81(114.03)	4.81(59.13)	1.93(40.45)	H γ 1.13, 0.97(24.51)	H δ 0.70(15.01) H γ m0.88(18.90)	174.92
E217	8.01(116.96)	4.59(54.85)	2.26, 2.18(31.12)	H γ 2.46, 2.34(36.42)		179.08
A218	8.75(122.92)	3.85(55.00)	1.48(17.96)			180.13
D219	8.04(112.93)	4.55(54.66)	2.88, 2.63(39.42)			178.06
Q220	7.89(118.65)	4.14(56.57)	2.87, 2.32(31.06)	H γ 2.18(37.36)		174.52
I221	7.40(119.58)	4.45(60.65)	1.85(39.79)	H γ 0.62(26.86)	H δ 0.83(15.90) H γ m0.46(17.63)	175.78
T222	8.53(122.31)	4.60(60.71)	4.00(71.60)	H γ 1.19(21.44)		172.24
F223	8.58(120.79)	5.75(56.15)	2.85(42.65)	H δ 7.09 H ϵ 6.97		176.67
E224	9.26(120.83)	4.88(54.10)	2.06, 1.88(33.75)	H γ 2.20, 2.14(35.79)		176.39
T225	8.71(119.35)	4.41(62.74)	4.09(69.08)	H γ 1.17(21.78)		174.89
V226	8.24(125.43)	4.11(61.71)	1.96(32.64)	H γ 0.89(21.06)		175.63
E227	8.39(125.42)	4.38(55.71)	2.03, 1.94(30.23)	H γ 2.24, 2.24(35.89)		176.84
V228	8.26(122.29)	4.17(61.78)	2.00(32.65)	H γ 0.95(20.62)		176.81
S229	8.37(120.87)	4.72(55.86)	3.82, 3.82(63.06)			
P230		4.46(62.86)	2.34, 1.98(31.93)	H γ 2.06(26.94)	H δ 3.90, 3.76(50.5)	
K231	8.34(121.89)	4.37(55.83)	1.85, 1.79(32.64)	H ϵ 3.21(41.89)	1.66 (24.48, 28.70)	177.19
I232	8.10(122.36)	4.07(60.60)	1.76(38.59)	1.11, 0.80 (26.80, 12.98, 17.31)		174.77
S233	8.42(120.72)	4.57(57.54)	3.87(63.50)			
T234	8.14(118.90)	4.56(59.34)	4.06(69.30)	H γ 1.17		
P235						
P236		4.48(62.23)	2.30, 2.06(31.68)	H γ 1.91(26.96)	H δ 3.84, 3.70(50.19)	177.39
V237	8.12(120.54)	4.07(62.05)	2.06(32.41)	0.97(20.68)		176.72
L238	8.24(126.67)	4.40(54.67)	1.61(42.19)	0.93(23.55)		177.51

K239	8.23(123.33)	4.37(55.23)	1.84, 1.77(32.79)	H ϵ 3.01(41.72) 1.49, 1.42, 1.74(24.41, 28.79)	176.72
L240	8.34(125.28)	4.33(54.92)	1.63(42.24)	1.65, 0.93, 0.89(26.77, 24.62, 23.19)	177.65
A241	8.30(124.89)	4.33(52.07)	1.42(18.89)		178.19
A242	8.20(123.27)	4.37(52.27)	1.41(19.05)		178.52
E243	8.31(119.78)	4.37(56.44)	2.06, 1.99(29.96)	H γ 2.29(36.04)	
Q244	8.26(121.27)	4.36(55.10)	2.13, 2.00(29.46)	H γ 2.39(33.55)	175.94
A245	8.29(126.91)	4.55(50.26)	1.31(17.92)		
P246		4.54(63.02)	2.34, 2.07(31.68)	H γ 1.99(27.05) H δ 3.83, 3.70(50.21)	177.98
T247	8.18(113.72)	4.29(61.65)	3.24(69.52)	H γ 1.27(21.21)	175.96
G248	8.37(111.16)	4.01(45.01)			174.56
R249	8.15(121.23)	4.38(55.93)	1.81, 1.79(30.64)	H γ 1.61(26.72) 3.21(42.98)	176.93
V250	8.23(122.31)	4.11(62.09)	2.07(32.54)	H γ 0.95(20.68)	176.90
E251	8.52(125.33)	4.25(56.28)	1.88, 1.73(30.00)	H γ 2.20, 1.88(35.89)	175.51
R252	8.22(122.96)	4.39(56.05)	1.83, 1.80(30.63)	H γ 1.66(26.73) H δ 3.22(43.05)	176.33
E253	8.57(123.07)	4.28(55.58)	2.06, 1.99(29.36)	H γ 2.30(35.96)	
K254	8.36(122.41)	4.38(56.40)	1.89(32.76)	H ϵ 3.02(41.91) 1.48, 1.72(24.56, 28.80)	177.56
T255	8.12(115.10)	4.35(61.57)	4.22(69.35)	H γ 1.14(21.19)	175.33
T256	8.13(117.10)	4.34(61.60)	4.19(69.28)	H γ 1.17(21.28)	175.15
R257	8.28(123.85)	4.37(55.83)	1.73(30.54)	H γ 1.45(26.79) H δ 3.03(42.95)	176.71
I258	8.09(122.32)	4.16(60.84)	1.86(38.54)	1.49, 1.21, 0.95, 0.88(26.95, 17.25, 12.99)	
K259	8.33(126.14)	4.35(55.78)	1.82, 1.73(32.82)	H ϵ 3.01(41.77) 1.70, 1.50, 1.41(28.79, 24.43)	176.81
L260	8.22(124.35)	4.42(54.86)	1.67(42.14)	0.93(26.74, 24.65, 23.11)	178.33
G261	8.42(110.52)	4.03(45.04)			174.20
T262	7.67(118.73)	4.17(62.74)	4.28(70.30)	H γ 1.18	

Supplementary Material

Table S-2 Distance and dihedral angle restraints (X-PLOR input file) used in structure calculations

```

assign (resid 2 and name HA ) (resid 2 and name HB1 ) 1.8 0.0 2.2
assign (resid 2 and name HA ) (resid 2 and name HB2 ) 1.8 0.0 3.2
assign (resid 2 and name HA ) (resid 2 and name HD1 ) 1.8 0.0 3.2
assign (resid 2 and name HA ) (resid 2 and name HD2 ) 1.8 0.0 3.2
assign (resid 2 and name HB1 ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HB2 ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HG* ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HD1 ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HD2 ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 3 and name HA ) (resid 3 and name HB1 ) 1.8 0.0 3.2
assign (resid 3 and name HA ) (resid 3 and name HB2 ) 1.8 0.0 3.2
assign (resid 3 and name HA ) (resid 3 and name HG1 ) 1.8 0.0 3.2
assign (resid 3 and name HA ) (resid 3 and name HG2 ) 1.8 0.0 3.2
assign (resid 3 and name HB1 ) (resid 3 and name HN ) 1.8 0.0 2.2
assign (resid 3 and name HB2 ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 3 and name HG1 ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 3 and name HG2 ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 3 and name HG1 ) (resid 3 and name HD* ) 1.8 0.0 3.2
assign (resid 3 and name HG2 ) (resid 3 and name HD* ) 1.8 0.0 3.2
assign (resid 3 and name HD* ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HB ) (resid 4 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HG11) (resid 4 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HG12) (resid 4 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HD* ) (resid 4 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HB ) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG11) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG12) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG2*) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HD* ) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HA ) (resid 6 and name HB1 ) 1.8 0.0 3.2
assign (resid 6 and name HA ) (resid 6 and name HB2 ) 1.8 0.0 3.2
assign (resid 6 and name HA ) (resid 6 and name HG ) 1.8 0.0 3.2
assign (resid 6 and name HB1 ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HB2 ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HG ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HD1*) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HD2*) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 7 and name HB2 ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 8 and name HB* ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 8 and name HG* ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 8 and name HD1 ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 8 and name HD2 ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HB1 ) (resid 9 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HB2 ) (resid 9 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HG ) (resid 9 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HB1 ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HB2 ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HG1 ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HG2 ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HD* ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HE* ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 11 and name HB* ) (resid 11 and name HN ) 1.8 0.0 2.2
assign (resid 13 and name HA ) (resid 13 and name HN ) 1.8 0.0 2.2
assign (resid 13 and name HB1 ) (resid 13 and name HN ) 1.8 0.0 3.2
assign (resid 13 and name HB2 ) (resid 13 and name HN ) 1.8 0.0 3.2
assign (resid 13 and name HG1 ) (resid 13 and name HN ) 1.8 0.0 3.2

```

```

assign (resid 13 and name HG2 ) (resid 13 and name HN ) 1.8 0.0 3.2
assign (resid 14 and name HA ) (resid 14 and name HN ) 1.8 0.0 1.0
assign (resid 14 and name HA ) (resid 14 and name HB ) 1.8 0.0 2.2
assign (resid 14 and name HA ) (resid 14 and name HG1* ) 1.8 0.0 3.2
assign (resid 14 and name HB ) (resid 14 and name HN ) 1.8 0.0 1.0
assign (resid 14 and name HG1*) (resid 14 and name HN ) 1.8 0.0 3.2
assign (resid 14 and name HG2*) (resid 14 and name HN ) 1.8 0.0 3.2
assign (resid 15 and name HA ) (resid 15 and name HN ) 1.8 0.0 2.2
assign (resid 15 and name HB1 ) (resid 15 and name HN ) 1.8 0.0 2.2
assign (resid 15 and name HB2 ) (resid 15 and name HN ) 1.8 0.0 2.2
assign (resid 16 and name HA ) (resid 16 and name HN ) 1.8 0.0 1.0
assign (resid 16 and name HB* ) (resid 16 and name HN ) 1.8 0.0 3.2
assign (resid 16 and name HG ) (resid 16 and name HN ) 1.8 0.0 3.2
assign (resid 17 and name HA ) (resid 17 and name HN ) 1.8 0.0 2.2
assign (resid 17 and name HB* ) (resid 17 and name HN ) 1.8 0.0 3.2
assign (resid 18 and name HA ) (resid 18 and name HN ) 1.8 0.0 1.0
assign (resid 18 and name HB1 ) (resid 18 and name HN ) 1.8 0.0 3.2
assign (resid 18 and name HB2 ) (resid 18 and name HN ) 1.8 0.0 3.2
assign (resid 18 and name HG1 ) (resid 18 and name HN ) 1.8 0.0 3.2
assign (resid 18 and name HG2 ) (resid 18 and name HN ) 1.8 0.0 3.2
assign (resid 19 and name HA ) (resid 19 and name HN ) 1.8 0.0 1.0
assign (resid 19 and name HB* ) (resid 19 and name HN ) 1.8 0.0 2.2
assign (resid 19 and name HG1 ) (resid 19 and name HN ) 1.8 0.0 2.2
assign (resid 19 and name HG2 ) (resid 19 and name HN ) 1.8 0.0 2.2
assign (resid 20 and name HA ) (resid 20 and name HN ) 1.8 0.0 1.0
assign (resid 20 and name HA ) (resid 20 and name HG1 ) 1.8 0.0 2.2
assign (resid 20 and name HA ) (resid 20 and name HG2 ) 1.8 0.0 2.2
assign (resid 20 and name HG1 ) (resid 20 and name HN ) 1.8 0.0 2.2
assign (resid 20 and name HG2 ) (resid 20 and name HN ) 1.8 0.0 2.2
assign (resid 21 and name HA ) (resid 21 and name HN ) 1.8 0.0 2.2
assign (resid 21 and name HB1 ) (resid 21 and name HN ) 1.8 0.0 2.2
assign (resid 21 and name HB2 ) (resid 21 and name HN ) 1.8 0.0 3.2
assign (resid 21 and name HG ) (resid 21 and name HN ) 1.8 0.0 3.2
assign (resid 22 and name HA1 ) (resid 22 and name HN ) 1.8 0.0 1.0
assign (resid 22 and name HA2 ) (resid 22 and name HN ) 1.8 0.0 1.0
assign (resid 23 and name HB* ) (resid 23 and name HN ) 1.8 0.0 2.2
assign (resid 24 and name HA ) (resid 24 and name HN ) 1.8 0.0 2.2
assign (resid 24 and name HB1 ) (resid 24 and name HN ) 1.8 0.0 2.2
assign (resid 24 and name HB2 ) (resid 24 and name HN ) 1.8 0.0 2.2
assign (resid 24 and name HG ) (resid 24 and name HN ) 1.8 0.0 3.2
assign (resid 24 and name HD1*) (resid 24 and name HN ) 1.8 0.0 3.2
assign (resid 24 and name HD2*) (resid 24 and name HN ) 1.8 0.0 3.2
assign (resid 25 and name HA ) (resid 25 and name HN ) 1.8 0.0 1.0
assign (resid 25 and name HB ) (resid 25 and name HN ) 1.8 0.0 3.2
assign (resid 25 and name HG* ) (resid 25 and name HN ) 1.8 0.0 2.2
assign (resid 26 and name HA ) (resid 26 and name HN ) 1.8 0.0 2.2
assign (resid 26 and name HB ) (resid 26 and name HN ) 1.8 0.0 2.2
assign (resid 26 and name HG* ) (resid 26 and name HN ) 1.8 0.0 3.2
assign (resid 27 and name HA ) (resid 27 and name HN ) 1.8 0.0 2.2
assign (resid 27 and name HB1 ) (resid 27 and name HN ) 1.8 0.0 2.2
assign (resid 27 and name HB2 ) (resid 27 and name HN ) 1.8 0.0 3.2
assign (resid 27 and name HG ) (resid 27 and name HN ) 1.8 0.0 2.2
assign (resid 28 and name HA ) (resid 28 and name HN ) 1.8 0.0 2.2
assign (resid 28 and name HB ) (resid 28 and name HN ) 1.8 0.0 2.2
assign (resid 28 and name HG* ) (resid 28 and name HN ) 1.8 0.0 3.2
assign (resid 29 and name HA ) (resid 29 and name HN ) 1.8 0.0 1.0
assign (resid 29 and name HA ) (resid 29 and name HB1 ) 1.8 0.0 1.0
assign (resid 29 and name HA ) (resid 29 and name HB2 ) 1.8 0.0 2.2
assign (resid 29 and name HB1 ) (resid 29 and name HN ) 1.8 0.0 3.2
assign (resid 29 and name HB2 ) (resid 29 and name HN ) 1.8 0.0 2.2

```

```

assign (resid 30 and name HB ) (resid 30 and name HN ) 1.8 0.0 1.0
assign (resid 30 and name HG1*) (resid 30 and name HN ) 1.8 0.0 2.2
assign (resid 30 and name HG2*) (resid 30 and name HN ) 1.8 0.0 2.2
assign (resid 31 and name HB ) (resid 31 and name HN ) 1.8 0.0 1.0
assign (resid 31 and name HG1*) (resid 31 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HG2*) (resid 31 and name HN ) 1.8 0.0 3.2
assign (resid 32 and name HG1 ) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 32 and name HG2 ) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 32 and name HD* ) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 33 and name HA1 ) (resid 33 and name HN ) 1.8 0.0 2.2
assign (resid 33 and name HA2 ) (resid 33 and name HN ) 1.8 0.0 1.0
assign (resid 34 and name HB* ) (resid 34 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB1 ) (resid 35 and name HB2 ) 1.8 0.0 2.5
assign (resid 35 and name HB1 ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB2 ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 36 and name HA ) (resid 36 and name HB* ) 1.8 0.0 3.2
assign (resid 36 and name HA ) (resid 36 and name HD* ) 1.8 0.0 3.2
assign (resid 36 and name HB* ) (resid 36 and name HN ) 1.8 0.0 3.2
assign (resid 37 and name HA ) (resid 37 and name HB* ) 1.8 0.0 3.2
assign (resid 37 and name HB* ) (resid 37 and name HN ) 1.8 0.0 3.2
assign (resid 37 and name HG ) (resid 37 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HA ) (resid 38 and name HB1 ) 1.8 0.0 3.2
assign (resid 38 and name HA ) (resid 38 and name HB2 ) 1.8 0.0 3.2
assign (resid 38 and name HB1 ) (resid 38 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HB2 ) (resid 38 and name HN ) 1.8 0.0 3.2
assign (resid 39 and name HB* ) (resid 39 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HB* ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HG11) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HG12) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HG2*) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HD* ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 41 and name HA ) (resid 41 and name HB1 ) 1.8 0.0 2.2
assign (resid 41 and name HA ) (resid 41 and name HB2 ) 1.8 0.0 2.2
assign (resid 41 and name HB1 ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 41 and name HB2 ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 41 and name HG ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 43 and name HA1 ) (resid 43 and name HN ) 1.8 0.0 2.2
assign (resid 43 and name HA2 ) (resid 43 and name HN ) 1.8 0.0 2.2
assign (resid 44 and name HA ) (resid 44 and name HN ) 1.8 0.0 1.0
assign (resid 44 and name HA ) (resid 44 and name HB1 ) 1.8 0.0 1.0
assign (resid 44 and name HA ) (resid 44 and name HB2 ) 1.8 0.0 1.0
assign (resid 44 and name HB1 ) (resid 44 and name HN ) 1.8 0.0 2.2
assign (resid 44 and name HB2 ) (resid 44 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HA ) (resid 45 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HB ) (resid 45 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HG11) (resid 45 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HG12) (resid 45 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HG2*) (resid 45 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HD* ) (resid 45 and name HN ) 1.8 0.0 3.2
assign (resid 46 and name HA ) (resid 46 and name HN ) 1.8 0.0 2.2
assign (resid 46 and name HB* ) (resid 46 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HA ) (resid 47 and name HN ) 1.8 0.0 2.2
assign (resid 47 and name HB1 ) (resid 47 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HB2 ) (resid 47 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HG1 ) (resid 47 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HG2 ) (resid 47 and name HN ) 1.8 0.0 3.2
assign (resid 48 and name HA ) (resid 48 and name HN ) 1.8 0.0 1.0
assign (resid 48 and name HB1 ) (resid 48 and name HN ) 1.8 0.0 2.2
assign (resid 48 and name HB2 ) (resid 48 and name HN ) 1.8 0.0 2.2
assign (resid 49 and name HA ) (resid 49 and name HN ) 1.8 0.0 2.2

```



```

assign (resid 49 and name HB1 ) (resid 49 and name HN ) 1.8 0.0 2.2
assign (resid 49 and name HB2 ) (resid 49 and name HN ) 1.8 0.0 2.2
assign (resid 50 and name HA ) (resid 50 and name HN ) 1.8 0.0 2.2
assign (resid 50 and name HB ) (resid 50 and name HN ) 1.8 0.0 2.2
assign (resid 50 and name HG11) (resid 50 and name HN ) 1.8 0.0 2.2
assign (resid 50 and name HG12) (resid 50 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HG2*) (resid 50 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HD* ) (resid 50 and name HN ) 1.8 0.0 3.2
assign (resid 51 and name HA ) (resid 51 and name HN ) 1.8 0.0 3.2
assign (resid 51 and name HB ) (resid 51 and name HN ) 1.8 0.0 2.2
assign (resid 51 and name HG* ) (resid 51 and name HN ) 1.8 0.0 3.2
assign (resid 52 and name HA ) (resid 52 and name HN ) 1.8 0.0 1.0
assign (resid 52 and name HB* ) (resid 52 and name HN ) 1.8 0.0 1.0
assign (resid 53 and name HA ) (resid 53 and name HN ) 1.8 0.0 2.2
assign (resid 53 and name HB ) (resid 53 and name HN ) 1.8 0.0 2.2
assign (resid 53 and name HG1*) (resid 53 and name HN ) 1.8 0.0 3.2
assign (resid 53 and name HG2*) (resid 53 and name HN ) 1.8 0.0 2.2
assign (resid 54 and name HA ) (resid 54 and name HN ) 1.8 0.0 2.2
assign (resid 54 and name HB1 ) (resid 54 and name HN ) 1.8 0.0 3.2
assign (resid 54 and name HB2 ) (resid 54 and name HN ) 1.8 0.0 3.2
assign (resid 54 and name HG ) (resid 54 and name HN ) 1.8 0.0 3.2
assign (resid 55 and name HA ) (resid 55 and name HN ) 1.8 0.0 2.2
assign (resid 55 and name HA ) (resid 55 and name HB1 ) 1.8 0.0 2.2
assign (resid 55 and name HA ) (resid 55 and name HB2 ) 1.8 0.0 2.2
assign (resid 55 and name HB1 ) (resid 55 and name HN ) 1.8 0.0 2.2
assign (resid 55 and name HB2 ) (resid 55 and name HN ) 1.8 0.0 2.2
assign (resid 56 and name HA ) (resid 56 and name HN ) 1.8 0.0 1.0
assign (resid 56 and name HB1 ) (resid 56 and name HN ) 1.8 0.0 2.2
assign (resid 56 and name HB2 ) (resid 56 and name HN ) 1.8 0.0 2.2
assign (resid 56 and name HB1 ) (resid 56 and name HD1 ) 1.8 0.0 3.2
assign (resid 56 and name HB2 ) (resid 56 and name HD1 ) 1.8 0.0 3.2
assign (resid 56 and name HB1 ) (resid 56 and name HD2 ) 1.8 0.0 3.2
assign (resid 56 and name HB2 ) (resid 56 and name HD2 ) 1.8 0.0 3.2
assign (resid 57 and name HA ) (resid 57 and name HN ) 1.8 0.0 2.2
assign (resid 57 and name HB ) (resid 57 and name HN ) 1.8 0.0 2.2
assign (resid 57 and name HG1*) (resid 57 and name HN ) 1.8 0.0 3.2
assign (resid 57 and name HG2*) (resid 57 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HA ) (resid 58 and name HN ) 1.8 0.0 2.2
assign (resid 58 and name HB ) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HG11) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HG12) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HG2*) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HD* ) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 59 and name HA ) (resid 59 and name HN ) 1.8 0.0 2.2
assign (resid 59 and name HB1 ) (resid 59 and name HN ) 1.8 0.0 2.2
assign (resid 59 and name HB2 ) (resid 59 and name HN ) 1.8 0.0 2.2
assign (resid 59 and name HG1 ) (resid 59 and name HN ) 1.8 0.0 2.2
assign (resid 59 and name HG2 ) (resid 59 and name HN ) 1.8 0.0 2.2
assign (resid 60 and name HB* ) (resid 60 and name HN ) 1.8 0.0 1.0
assign (resid 61 and name HA ) (resid 61 and name HB1 ) 1.8 0.0 1.0
assign (resid 61 and name HB1 ) (resid 61 and name HB2 ) 1.8 0.0 1.0
assign (resid 61 and name HB1 ) (resid 61 and name HN ) 1.8 0.0 2.2
assign (resid 61 and name HB2 ) (resid 61 and name HN ) 1.8 0.0 2.2
assign (resid 62 and name HB1 ) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HB2 ) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HG* ) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HA ) (resid 63 and name HG1* ) 1.8 0.0 3.2
assign (resid 63 and name HA ) (resid 63 and name HG2* ) 1.8 0.0 3.2
assign (resid 63 and name HB ) (resid 63 and name HN ) 1.8 0.0 2.2
assign (resid 63 and name HG1*) (resid 63 and name HN ) 1.8 0.0 3.2

```

```

assign (resid 63 and name HG2*) (resid 63 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HD* ) (resid 63 and name HN ) 1.8 0.0 3.2
assign (resid 64 and name HB ) (resid 64 and name HN ) 1.8 0.0 2.2
assign (resid 64 and name HG* ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HA ) (resid 65 and name HB* ) 1.8 0.0 2.2
assign (resid 65 and name HA ) (resid 65 and name HD* ) 1.8 0.0 3.2
assign (resid 65 and name HB* ) (resid 65 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HB* ) (resid 65 and name HD* ) 1.8 0.0 3.2
assign (resid 65 and name HD* ) (resid 65 and name HE* ) 1.8 0.0 2.2
assign (resid 66 and name HB1 ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 66 and name HB2 ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 66 and name HG1 ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 66 and name HG2 ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 67 and name HB ) (resid 67 and name HN ) 1.8 0.0 1.0
assign (resid 67 and name HG* ) (resid 67 and name HN ) 1.8 0.0 3.2
assign (resid 68 and name HA ) (resid 68 and name HN ) 1.8 0.0 1.0
assign (resid 68 and name HB ) (resid 68 and name HN ) 1.8 0.0 2.2
assign (resid 68 and name HG* ) (resid 68 and name HN ) 1.8 0.0 3.2
assign (resid 69 and name HA ) (resid 69 and name HN ) 1.8 0.0 2.2
assign (resid 69 and name HB1 ) (resid 69 and name HN ) 1.8 0.0 2.2
assign (resid 69 and name HB2 ) (resid 69 and name HN ) 1.8 0.0 2.2
assign (resid 1 and name HA ) (resid 2 and name HN ) 1.8 0.0 1.0
assign (resid 2 and name HA ) (resid 3 and name HN ) 1.8 0.0 1.0
assign (resid 2 and name HB1 ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HB2 ) (resid 3 and name HN ) 1.8 0.0 2.2
assign (resid 2 and name HG* ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HD1 ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HD2 ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 3 and name HA ) (resid 4 and name HN ) 1.8 0.0 1.0
assign (resid 4 and name HA ) (resid 5 and name HN ) 1.8 0.0 1.0
assign (resid 4 and name HD* ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HG1*) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HG2*) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HG2*) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HA ) (resid 6 and name HN ) 1.8 0.0 1.0
assign (resid 5 and name HB ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG11) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG12) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG2*) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HA ) (resid 7 and name HN ) 1.8 0.0 1.0
assign (resid 6 and name HB1 ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HB2 ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HD1*) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HD2*) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HN ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 7 and name HA ) (resid 8 and name HN ) 1.8 0.0 1.0
assign (resid 7 and name HN ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 7 and name HB1 ) (resid 8 and name HN ) 1.8 0.0 2.2
assign (resid 7 and name HB2 ) (resid 8 and name HN ) 1.8 0.0 2.2
assign (resid 8 and name HA ) (resid 9 and name HN ) 1.8 0.0 2.2
assign (resid 8 and name HN ) (resid 9 and name HN ) 1.8 0.0 2.2
assign (resid 8 and name HB* ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HA ) (resid 10 and name HN ) 1.8 0.0 1.0
assign (resid 9 and name HN ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HD2*) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HD2*) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HB1 ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HB2 ) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 9 and name HD1*) (resid 10 and name HN ) 1.8 0.0 3.2
assign (resid 10 and name HA ) (resid 11 and name HN ) 1.8 0.0 1.0

```

[illegible]

```

assign (resid 24 and name HD2*) (resid 23 and name HN ) 1.8 0.0 3.2
assign (resid 25 and name HG* ) (resid 24 and name HN ) 1.8 0.0 3.2
assign (resid 25 and name HA ) (resid 24 and name HN ) 1.8 0.0 3.2
assign (resid 25 and name HA ) (resid 26 and name HN ) 1.8 0.0 1.0
assign (resid 25 and name HG* ) (resid 26 and name HN ) 1.8 0.0 3.2
assign (resid 26 and name HN ) (resid 27 and name HN ) 1.8 0.0 3.2
assign (resid 26 and name HA ) (resid 27 and name HN ) 1.8 0.0 1.0
assign (resid 26 and name HB ) (resid 27 and name HN ) 1.8 0.0 2.2
assign (resid 26 and name HG* ) (resid 27 and name HN ) 1.8 0.0 3.2
assign (resid 27 and name HA ) (resid 28 and name HN ) 1.8 0.0 1.0
assign (resid 27 and name HB1 ) (resid 28 and name HN ) 1.8 0.0 3.2
assign (resid 27 and name HB2 ) (resid 28 and name HN ) 1.8 0.0 3.2
assign (resid 28 and name HA ) (resid 29 and name HN ) 1.8 0.0 2.2
assign (resid 28 and name HN ) (resid 29 and name HN ) 1.8 0.0 3.2
assign (resid 28 and name HB ) (resid 29 and name HN ) 1.8 0.0 1.0
assign (resid 28 and name HG* ) (resid 29 and name HN ) 1.8 0.0 3.2
assign (resid 29 and name HN ) (resid 30 and name HN ) 1.8 0.0 1.0
assign (resid 29 and name HA ) (resid 30 and name HN ) 1.8 0.0 1.0
assign (resid 29 and name HB1 ) (resid 30 and name HN ) 1.8 0.0 3.2
assign (resid 29 and name HB2 ) (resid 30 and name HN ) 1.8 0.0 3.2
assign (resid 30 and name HN ) (resid 31 and name HN ) 1.8 0.0 3.2
assign (resid 30 and name HA ) (resid 31 and name HN ) 1.8 0.0 1.0
assign (resid 30 and name HA ) (resid 29 and name HN ) 1.8 0.0 3.2
assign (resid 30 and name HB ) (resid 29 and name HN ) 1.8 0.0 3.2
assign (resid 30 and name HB ) (resid 31 and name HN ) 1.8 0.0 1.0
assign (resid 30 and name HG1*) (resid 31 and name HN ) 1.8 0.0 3.2
assign (resid 30 and name HG1*) (resid 29 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HN ) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HA ) (resid 32 and name HN ) 1.8 0.0 1.0
assign (resid 31 and name HB ) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HG1*) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HG2*) (resid 32 and name HN ) 1.8 0.0 3.2
assign (resid 32 and name HN ) (resid 33 and name HN ) 1.8 0.0 3.2
assign (resid 32 and name HB* ) (resid 33 and name HN ) 1.8 0.0 3.2
assign (resid 34 and name HN ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 34 and name HA ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 34 and name HB* ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB1 ) (resid 36 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB2 ) (resid 36 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HN ) (resid 36 and name HN ) 1.8 0.0 1.0
assign (resid 35 and name HA ) (resid 36 and name HN ) 1.8 0.0 2.2
assign (resid 36 and name HN ) (resid 37 and name HN ) 1.8 0.0 2.2
assign (resid 36 and name HA ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 36 and name HA ) (resid 37 and name HN ) 1.8 0.0 1.0
assign (resid 36 and name HB* ) (resid 37 and name HN ) 1.8 0.0 3.2
assign (resid 36 and name HB* ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 37 and name HN ) (resid 38 and name HN ) 1.8 0.0 3.2
assign (resid 37 and name HA ) (resid 38 and name HN ) 1.8 0.0 1.0
assign (resid 37 and name HB* ) (resid 38 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HN ) (resid 39 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HA ) (resid 39 and name HN ) 1.8 0.0 1.0
assign (resid 38 and name HB1 ) (resid 39 and name HN ) 1.8 0.0 2.2
assign (resid 38 and name HB2 ) (resid 39 and name HN ) 1.8 0.0 3.2
assign (resid 39 and name HN ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 39 and name HB* ) (resid 40 and name HN ) 1.8 0.0 2.2
assign (resid 40 and name HN ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HD* ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HG2*) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 41 and name HD2*) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 42 and name HB1 ) (resid 43 and name HN ) 1.8 0.0 3.2

```

```

assign (resid 42 and name HG2 ) (resid 43 and name HN ) 1.8 0.0 2.2
assign (resid 42 and name HA ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 42 and name HA ) (resid 43 and name HN ) 1.8 0.0 1.0
assign (resid 42 and name HD1 ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 42 and name HD1 ) (resid 43 and name HN ) 1.8 0.0 3.2
assign (resid 43 and name HN ) (resid 44 and name HN ) 1.8 0.0 1.0
assign (resid 43 and name HA1 ) (resid 44 and name HN ) 1.8 0.0 3.2
assign (resid 43 and name HA2 ) (resid 44 and name HN ) 1.8 0.0 3.2
assign (resid 44 and name HN ) (resid 45 and name HN ) 1.8 0.0 1.0
assign (resid 44 and name HA ) (resid 45 and name HN ) 1.8 0.0 2.2
assign (resid 44 and name HB1 ) (resid 45 and name HN ) 1.8 0.0 3.2
assign (resid 44 and name HB2 ) (resid 45 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HN ) (resid 46 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HA ) (resid 46 and name HN ) 1.8 0.0 1.0
assign (resid 45 and name HB ) (resid 46 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HB ) (resid 44 and name HN ) 1.8 0.0 2.2
assign (resid 45 and name HG11) (resid 46 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HD* ) (resid 46 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HG2*) (resid 44 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HG2*) (resid 46 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HG11) (resid 46 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HG12) (resid 46 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HD* ) (resid 44 and name HN ) 1.8 0.0 3.2
assign (resid 46 and name HA ) (resid 47 and name HN ) 1.8 0.0 1.0
assign (resid 46 and name HB* ) (resid 47 and name HN ) 1.8 0.0 2.2
assign (resid 47 and name HN ) (resid 48 and name HN ) 1.8 0.0 2.2
assign (resid 47 and name HA ) (resid 48 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HB1 ) (resid 48 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HG1 ) (resid 48 and name HN ) 1.8 0.0 3.2
assign (resid 47 and name HG2 ) (resid 48 and name HN ) 1.8 0.0 3.2
assign (resid 48 and name HN ) (resid 49 and name HN ) 1.8 0.0 1.0
assign (resid 48 and name HB1 ) (resid 49 and name HN ) 1.8 0.0 2.2
assign (resid 48 and name HB2 ) (resid 48 and name HN ) 1.8 0.0 3.2
assign (resid 49 and name HN ) (resid 50 and name HN ) 1.8 0.0 1.0
assign (resid 49 and name HA ) (resid 50 and name HN ) 1.8 0.0 3.2
assign (resid 49 and name HB1 ) (resid 50 and name HN ) 1.8 0.0 3.2
assign (resid 49 and name HB2 ) (resid 50 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HN ) (resid 51 and name HN ) 1.8 0.0 1.0
assign (resid 50 and name HA ) (resid 49 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HA ) (resid 51 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HB ) (resid 51 and name HN ) 1.8 0.0 2.2
assign (resid 50 and name HB ) (resid 49 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HD* ) (resid 49 and name HN ) 1.8 0.0 3.2
assign (resid 50 and name HG2*) (resid 51 and name HN ) 1.8 0.0 3.2
assign (resid 51 and name HN ) (resid 52 and name HN ) 1.8 0.0 1.0
assign (resid 51 and name HA ) (resid 52 and name HN ) 1.8 0.0 2.2
assign (resid 51 and name HB ) (resid 52 and name HN ) 1.8 0.0 2.2
assign (resid 51 and name HG* ) (resid 52 and name HN ) 1.8 0.0 3.2
assign (resid 52 and name HN ) (resid 53 and name HN ) 1.8 0.0 1.0
assign (resid 52 and name HA ) (resid 53 and name HN ) 1.8 0.0 3.2
assign (resid 52 and name HB* ) (resid 51 and name HN ) 1.8 0.0 3.2
assign (resid 52 and name HB* ) (resid 53 and name HN ) 1.8 0.0 2.2
assign (resid 53 and name HN ) (resid 54 and name HN ) 1.8 0.0 1.0
assign (resid 53 and name HA ) (resid 54 and name HN ) 1.8 0.0 3.2
assign (resid 53 and name HG1*) (resid 54 and name HN ) 1.8 0.0 3.2
assign (resid 53 and name HG2*) (resid 54 and name HN ) 1.8 0.0 3.2
assign (resid 53 and name HB ) (resid 54 and name HN ) 1.8 0.0 2.2
assign (resid 54 and name HN ) (resid 55 and name HN ) 1.8 0.0 1.0
assign (resid 54 and name HB1 ) (resid 55 and name HN ) 1.8 0.0 2.2
assign (resid 54 and name HB2 ) (resid 55 and name HN ) 1.8 0.0 2.2

```

```

assign (resid 54 and name HG ) (resid 53 and name HN ) 1.8 0.0 3.2
assign (resid 55 and name HN ) (resid 56 and name HN ) 1.8 0.0 1.0
assign (resid 55 and name HA ) (resid 56 and name HN ) 1.8 0.0 2.2
assign (resid 55 and name HB1 ) (resid 56 and name HN ) 1.8 0.0 3.2
assign (resid 55 and name HB2 ) (resid 56 and name HN ) 1.8 0.0 3.2
assign (resid 56 and name HN ) (resid 57 and name HN ) 1.8 0.0 1.0
assign (resid 56 and name HA ) (resid 57 and name HN ) 1.8 0.0 3.2
assign (resid 56 and name HB1 ) (resid 57 and name HN ) 1.8 0.0 3.2
assign (resid 56 and name HB2 ) (resid 57 and name HN ) 1.8 0.0 3.2
assign (resid 57 and name HN ) (resid 58 and name HN ) 1.8 0.0 1.0
assign (resid 57 and name HA ) (resid 58 and name HN ) 1.8 0.0 2.2
assign (resid 57 and name HA ) (resid 56 and name HN ) 1.8 0.0 3.2
assign (resid 57 and name HB ) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 57 and name HG2*) (resid 58 and name HN ) 1.8 0.0 3.2
assign (resid 57 and name HG2*) (resid 56 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HN ) (resid 59 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HA ) (resid 59 and name HN ) 1.8 0.0 1.0
assign (resid 58 and name HB ) (resid 59 and name HN ) 1.8 0.0 2.2
assign (resid 58 and name HG2*) (resid 59 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HD* ) (resid 59 and name HN ) 1.8 0.0 3.2
assign (resid 58 and name HD* ) (resid 57 and name HN ) 1.8 0.0 3.2
assign (resid 59 and name HN ) (resid 60 and name HN ) 1.8 0.0 2.2
assign (resid 59 and name HA ) (resid 60 and name HN ) 1.8 0.0 1.0
assign (resid 59 and name HB1 ) (resid 60 and name HN ) 1.8 0.0 3.2
assign (resid 59 and name HB2 ) (resid 60 and name HN ) 1.8 0.0 3.2
assign (resid 59 and name HG1 ) (resid 60 and name HN ) 1.8 0.0 3.2
assign (resid 59 and name HG2 ) (resid 60 and name HN ) 1.8 0.0 3.2
assign (resid 60 and name HN ) (resid 61 and name HN ) 1.8 0.0 1.0
assign (resid 60 and name HA ) (resid 61 and name HN ) 1.8 0.0 3.2
assign (resid 60 and name HB* ) (resid 61 and name HN ) 1.8 0.0 2.2
assign (resid 61 and name HN ) (resid 62 and name HN ) 1.8 0.0 1.0
assign (resid 61 and name HA ) (resid 62 and name HN ) 1.8 0.0 2.2
assign (resid 61 and name HA ) (resid 60 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HN ) (resid 63 and name HN ) 1.8 0.0 1.0
assign (resid 62 and name HA ) (resid 61 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HA ) (resid 63 and name HN ) 1.8 0.0 2.2
assign (resid 62 and name HB2 ) (resid 63 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HG* ) (resid 61 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HN ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HA ) (resid 64 and name HN ) 1.8 0.0 1.0
assign (resid 63 and name HB ) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HB ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HG2*) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HG2*) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HD* ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HD* ) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 63 and name HG1*) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 64 and name HA ) (resid 65 and name HN ) 1.8 0.0 2.2
assign (resid 64 and name HB ) (resid 65 and name HN ) 1.8 0.0 2.2
assign (resid 64 and name HG* ) (resid 65 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HN ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HA ) (resid 66 and name HN ) 1.8 0.0 1.0
assign (resid 65 and name HB* ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HD* ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 66 and name HA ) (resid 67 and name HN ) 1.8 0.0 1.0
assign (resid 66 and name HB1 ) (resid 67 and name HN ) 1.8 0.0 3.2
assign (resid 66 and name HB2 ) (resid 67 and name HN ) 1.8 0.0 3.2
assign (resid 67 and name HN ) (resid 68 and name HN ) 1.8 0.0 3.2
assign (resid 67 and name HA ) (resid 68 and name HN ) 1.8 0.0 1.0
assign (resid 67 and name HB ) (resid 68 and name HN ) 1.8 0.0 2.2

```

[illegible]


```

assign (resid 3 and name HA ) (resid 41 and name HN ) 1.8 0.0 3.2
assign (resid 3 and name HA ) (resid 39 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HA ) (resid 65 and name HA ) 1.8 0.0 2.2
assign (resid 4 and name HD* ) (resid 39 and name HN ) 1.8 0.0 3.2
assign (resid 4 and name HN ) (resid 39 and name HN ) 1.8 0.0 2.2
assign (resid 5 and name HN ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HN ) (resid 64 and name HN ) 1.8 0.0 2.2
assign (resid 5 and name HA ) (resid 39 and name HN ) 1.8 0.0 1.0
assign (resid 5 and name HA ) (resid 38 and name HA ) 1.8 0.0 2.2
assign (resid 5 and name HB ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HD* ) (resid 66 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HG2* ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 5 and name HD* ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HN ) (resid 37 and name HN ) 1.8 0.0 2.2
assign (resid 6 and name HA ) (resid 64 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HA ) (resid 63 and name HA ) 1.8 0.0 3.2
assign (resid 6 and name HB1 ) (resid 37 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HB2 ) (resid 37 and name HN ) 1.8 0.0 3.2
assign (resid 6 and name HD2* ) (resid 63 and name HN ) 1.8 0.0 3.2
assign (resid 7 and name HA ) (resid 36 and name HA ) 1.8 0.0 3.2
assign (resid 7 and name HN ) (resid 62 and name HN ) 1.8 0.0 3.2
assign (resid 14 and name KG1* ) (resid 36 and name HN ) 1.8 0.0 3.2
assign (resid 14 and name HG1* ) (resid 35 and name HN ) 1.8 0.0 3.2
assign (resid 14 and name HG1* ) (resid 36 and name HN ) 1.8 0.0 3.2
assign (resid 14 and name HG2* ) (resid 33 and name HN ) 1.8 0.0 3.2
assign (resid 28 and name HN ) (resid 40 and name HN ) 1.8 0.0 2.2
assign (resid 28 and name HB ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 29 and name HB1 ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 29 and name HB2 ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 30 and name HA ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HN ) (resid 38 and name HN ) 1.8 0.0 2.2
assign (resid 31 and name HN ) (resid 40 and name HN ) 1.8 0.0 3.2
assign (resid 31 and name HB ) (resid 38 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB1 ) (resid 9 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB2 ) (resid 9 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB1 ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HB2 ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 35 and name HA ) (resid 9 and name HN ) 1.8 0.0 3.2
assign (resid 36 and name HA ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 36 and name HA ) (resid 8 and name HN ) 1.8 0.0 3.2
assign (resid 37 and name HA ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HA ) (resid 6 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HB1 ) (resid 31 and name HN ) 1.8 0.0 3.2
assign (resid 38 and name HB2 ) (resid 31 and name HN ) 1.8 0.0 3.2
assign (resid 39 and name HB* ) (resid 4 and name HN ) 1.8 0.0 3.2
assign (resid 39 and name HB* ) (resid 28 and name HN ) 1.8 0.0 3.2
assign (resid 39 and name HB* ) (resid 30 and name HN ) 1.8 0.0 3.2
assign (resid 40 and name HG2* ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 42 and name HB1 ) (resid 2 and name HN ) 1.8 0.0 3.2
assign (resid 45 and name HD* ) (resid 65 and name HE* ) 1.8 0.0 3.2
assign (resid 47 and name HB1 ) (resid 65 and name HD* ) 1.8 0.0 3.2
assign (resid 47 and name HB2 ) (resid 65 and name HD* ) 1.8 0.0 3.2
assign (resid 47 and name HB2 ) (resid 65 and name HE* ) 1.8 0.0 3.2
assign (resid 50 and name HG2* ) (resid 65 and name HE* ) 1.8 0.0 3.2
assign (resid 50 and name HG2* ) (resid 65 and name HD* ) 1.8 0.0 3.2
assign (resid 51 and name HG* ) (resid 65 and name HD* ) 1.8 0.0 3.2
assign (resid 55 and name HA ) (resid 63 and name HD* ) 1.8 0.0 3.2
assign (resid 62 and name HA ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HB1 ) (resid 7 and name HN ) 1.8 0.0 3.2
assign (resid 62 and name HB2 ) (resid 7 and name HN ) 1.8 0.0 3.2

```

```

assign (resid 63 and name HG2*) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 64 and name HB ) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HB* ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HA ) (resid 5 and name HN ) 1.8 0.0 3.2
assign (resid 65 and name HE* ) (resid 50 and name HB ) 1.8 0.0 3.2
assign (resid 65 and name HD* ) (resid 4 and name HG2* ) 1.8 0.0 3.2
assign (resid 67 and name HA ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 68 and name HA ) (resid 3 and name HN ) 1.8 0.0 3.2
assign (resid 2 and name HN) (resid 41 and name O) 1.5 0.0 1.0
assign (resid 2 and name N) (resid 41 and name O) 2.4 0.0 1.0
assign (resid 2 and name O) (resid 41 and name HN) 1.5 0.0 1.0
assign (resid 2 and name O) (resid 41 and name N) 2.4 0.0 1.0
assign (resid 3 and name HN) (resid 66 and name O) 1.5 0.0 1.0
assign (resid 3 and name N) (resid 66 and name O) 2.4 0.0 1.0
assign (resid 3 and name O) (resid 66 and name HN) 1.5 0.0 1.0
assign (resid 3 and name O) (resid 66 and name N) 2.4 0.0 1.0
assign (resid 4 and name HN) (resid 39 and name O) 1.5 0.0 1.0
assign (resid 4 and name N) (resid 39 and name O) 2.4 0.0 1.0
assign (resid 4 and name O) (resid 39 and name HN) 1.5 0.0 1.0
assign (resid 4 and name O) (resid 39 and name N) 2.4 0.0 1.0
assign (resid 5 and name HN) (resid 64 and name O) 1.5 0.0 1.0
assign (resid 5 and name N) (resid 64 and name O) 2.4 0.0 1.0
assign (resid 5 and name O) (resid 64 and name HN) 1.5 0.0 1.0
assign (resid 5 and name O) (resid 64 and name N) 2.4 0.0 1.0
assign (resid 6 and name HN) (resid 37 and name O) 1.5 0.0 1.0
assign (resid 6 and name N) (resid 37 and name O) 2.4 0.0 1.0
assign (resid 6 and name O) (resid 37 and name HN) 1.5 0.0 1.0
assign (resid 6 and name O) (resid 37 and name N) 2.4 0.0 1.0
assign (resid 7 and name HN) (resid 62 and name O) 1.5 0.0 1.0
assign (resid 7 and name N) (resid 62 and name O) 2.4 0.0 1.0
assign (resid 7 and name O) (resid 62 and name HN) 1.5 0.0 1.0
assign (resid 7 and name O) (resid 62 and name N) 2.4 0.0 1.0
assign (resid 31 and name HN) (resid 38 and name O) 1.5 0.0 1.0
assign (resid 31 and name N) (resid 38 and name O) 2.4 0.0 1.0
assign (resid 31 and name O) (resid 38 and name HN) 1.5 0.0 1.0
assign (resid 31 and name O) (resid 38 and name N) 2.4 0.0 1.0
assign (resid 33 and name HN) (resid 36 and name O) 1.5 0.0 1.0
assign (resid 33 and name N) (resid 36 and name O) 2.4 0.0 1.0
assign (resid 33 and name O) (resid 36 and name HN) 1.5 0.0 1.0
assign (resid 33 and name O) (resid 36 and name N) 2.4 0.0 1.0
assign (resid 17 and name HN) (resid 13 and name O) 1.5 0.0 1.0
assign (resid 17 and name N ) (resid 13 and name O) 2.4 0.0 1.0
assign (resid 18 and name HN) (resid 14 and name O) 1.5 0.0 1.0
assign (resid 18 and name N ) (resid 14 and name O) 2.4 0.0 1.0
assign (resid 19 and name HN) (resid 15 and name O) 1.5 0.0 1.0
assign (resid 19 and name N ) (resid 15 and name O) 2.4 0.0 1.0
assign (resid 20 and name HN) (resid 16 and name O) 1.5 0.0 1.0
assign (resid 20 and name N ) (resid 16 and name O) 2.4 0.0 1.0
assign (resid 21 and name HN) (resid 17 and name O) 1.5 0.0 1.0
assign (resid 21 and name N ) (resid 17 and name O) 2.4 0.0 1.0
assign (resid 22 and name HN) (resid 18 and name O) 1.5 0.0 1.0
assign (resid 22 and name N ) (resid 18 and name O) 2.4 0.0 1.0
assign (resid 50 and name HN) (resid 46 and name O) 1.5 0.0 1.0
assign (resid 50 and name N ) (resid 46 and name O) 2.4 0.0 1.0
assign (resid 51 and name HN) (resid 47 and name O) 1.5 0.0 1.0
assign (resid 51 and name N ) (resid 47 and name O) 2.4 0.0 1.0
assign (resid 52 and name HN) (resid 48 and name O) 1.5 0.0 1.0
assign (resid 52 and name N ) (resid 48 and name O) 2.4 0.0 1.0
assign (resid 53 and name HN) (resid 49 and name O) 1.5 0.0 1.0
assign (resid 53 and name N ) (resid 49 and name O) 2.4 0.0 1.0

```

```
assign (resid 54 and name HN) (resid 50 and name O) 1.5 0.0 1.0
assign (resid 54 and name N ) (resid 50 and name O) 2.4 0.0 1.0
assign (resid 2 and name c) (resid 3 and name n)
(resid 3 and name ca) (resid 3 and name c) 1.0 -139.0 30.0 2
assign (resid 3 and name c) (resid 4 and name n)
(resid 4 and name ca) (resid 4 and name c) 1.0 -139.0 30.0 2
assign (resid 4 and name c) (resid 5 and name n)
(resid 5 and name ca) (resid 5 and name c) 1.0 -139.0 30.0 2
assign (resid 5 and name c) (resid 6 and name n)
(resid 6 and name ca) (resid 6 and name c) 1.0 -139.0 30.0 2
assign (resid 6 and name c) (resid 7 and name n)
(resid 7 and name ca) (resid 7 and name c) 1.0 -139.0 30.0 2
assign (resid 7 and name c) (resid 8 and name n)
(resid 8 and name ca) (resid 8 and name c) 1.0 -139.0 30.0 2
assign (resid 8 and name c) (resid 9 and name n)
(resid 9 and name ca) (resid 9 and name c) 1.0 -57.0 30.0 2
assign (resid 12 and name c) (resid 13 and name n)
(resid 13 and name ca) (resid 13 and name c) 1.0 -57.0 30.0 2
assign (resid 13 and name c) (resid 14 and name n)
(resid 14 and name ca) (resid 14 and name c) 1.0 -57.0 30.0 2
assign (resid 14 and name c) (resid 15 and name n)
(resid 15 and name ca) (resid 15 and name c) 1.0 -57.0 30.0 2
assign (resid 15 and name c) (resid 16 and name n)
(resid 16 and name ca) (resid 16 and name c) 1.0 -57.0 30.0 2
assign (resid 16 and name c) (resid 17 and name n)
(resid 17 and name ca) (resid 17 and name c) 1.0 -57.0 30.0 2
assign (resid 17 and name c) (resid 18 and name n)
(resid 18 and name ca) (resid 18 and name c) 1.0 -57.0 30.0 2
assign (resid 18 and name c) (resid 19 and name n)
(resid 19 and name ca) (resid 19 and name c) 1.0 -57.0 30.0 2
assign (resid 19 and name c) (resid 20 and name n)
(resid 20 and name ca) (resid 20 and name c) 1.0 -57.0 30.0 2
assign (resid 20 and name c) (resid 21 and name n)
(resid 21 and name ca) (resid 21 and name c) 1.0 -57.0 30.0 2
assign (resid 21 and name c) (resid 22 and name n)
(resid 22 and name ca) (resid 22 and name c) 1.0 -57.0 30.0 2
assign (resid 25 and name c) (resid 26 and name n)
(resid 26 and name ca) (resid 26 and name c) 1.0 -139.0 30.0 2
assign (resid 27 and name c) (resid 28 and name n)
(resid 28 and name ca) (resid 28 and name c) 1.0 -139.0 30.0 2
assign (resid 29 and name c) (resid 30 and name n)
(resid 30 and name ca) (resid 30 and name c) 1.0 -57.0 30.0 2
assign (resid 30 and name c) (resid 31 and name n)
(resid 31 and name ca) (resid 31 and name c) 1.0 -139.0 30.0 2
assign (resid 31 and name c) (resid 32 and name n)
(resid 32 and name ca) (resid 32 and name c) 1.0 -139.0 30.0 2
assign (resid 32 and name c) (resid 33 and name n)
(resid 33 and name ca) (resid 33 and name c) 1.0 -139.0 30.0 2
assign (resid 34 and name c) (resid 35 and name n)
(resid 35 and name ca) (resid 35 and name c) 1.0 -139.0 30.0 2
assign (resid 37 and name c) (resid 38 and name n)
(resid 38 and name ca) (resid 38 and name c) 1.0 -139.0 30.0 2
assign (resid 39 and name c) (resid 40 and name n)
(resid 40 and name ca) (resid 40 and name c) 1.0 -139.0 30.0 2
assign (resid 40 and name c) (resid 41 and name n)
(resid 41 and name ca) (resid 41 and name c) 1.0 -139.0 30.0 2
assign (resid 46 and name c) (resid 47 and name n)
(resid 47 and name ca) (resid 47 and name c) 1.0 -57.0 30.0 2
assign (resid 47 and name c) (resid 48 and name n)
(resid 48 and name ca) (resid 48 and name c) 1.0 -57.0 30.0 2
```

assign (resid 49 and name c) (resid 50 and name n)
(resid 50 and name ca) (resid 50 and name c) 1.0 -57.0 30.0 2
assign (resid 50 and name c) (resid 51 and name n)
(resid 51 and name ca) (resid 51 and name c) 1.0 -57.0 30.0 2
assign (resid 51 and name c) (resid 52 and name n)
(resid 52 and name ca) (resid 52 and name c) 1.0 -57.0 30.0 2
assign (resid 54 and name c) (resid 55 and name n)
(resid 55 and name ca) (resid 55 and name c) 1.0 -57.0 30.0 2
assign (resid 57 and name c) (resid 58 and name n)
(resid 58 and name ca) (resid 58 and name c) 1.0 -139.0 30.0 2
assign (resid 61 and name c) (resid 62 and name n)
(resid 62 and name ca) (resid 62 and name c) 1.0 -139.0 30.0 2
assign (resid 62 and name c) (resid 63 and name n)
(resid 63 and name ca) (resid 63 and name c) 1.0 -139.0 30.0 2
assign (resid 63 and name c) (resid 64 and name n)
(resid 64 and name ca) (resid 64 and name c) 1.0 -139.0 30.0 2
assign (resid 64 and name c) (resid 65 and name n)
(resid 65 and name ca) (resid 65 and name c) 1.0 -139.0 30.0 2
assign (resid 65 and name c) (resid 66 and name n)
(resid 66 and name ca) (resid 66 and name c) 1.0 -139.0 30.0 2