

## **Supporting Information**

**for**

# **Computational evidence for intramolecular hydrogen bonding and nonbonding X...O interactions in 2'-haloflavonols**

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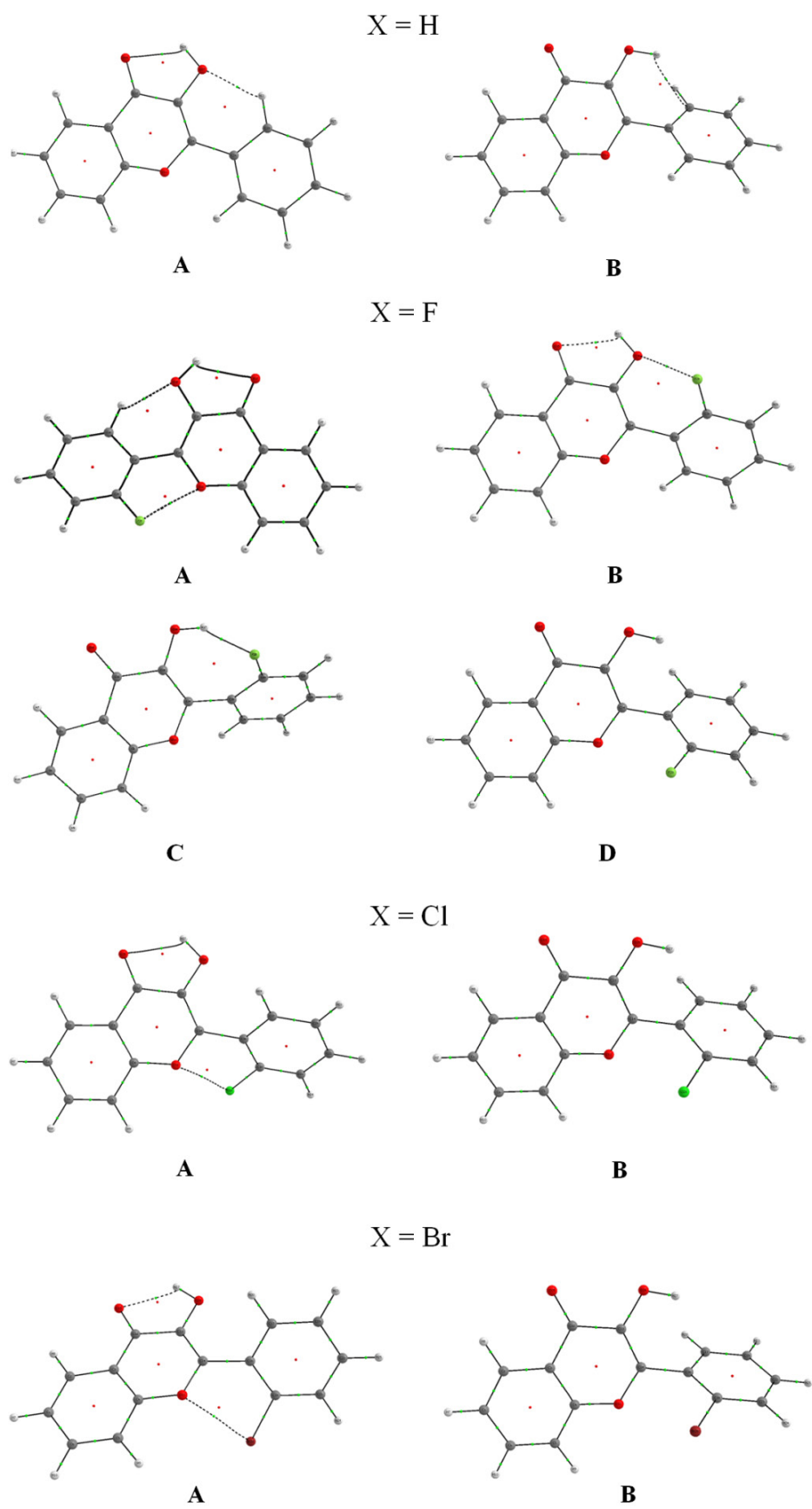
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**Optimized structures for all minima of 2'-haloflavonols and the corresponding Cartesian coordinates**

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S1. Stable conformers for the 2'-X-flavonols (X = H, F, Cl and Br).

## S2. Optimized structures for 2'-X-flavonols:

**X = H**

### Conformer A

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,5,B5,4,A4,3,D3,0  
H,1,B6,2,A5,3,D4,0  
H,2,B7,1,A6,6,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,5,A8,4,D7,0  
O,4,B10,3,A9,2,D8,0  
C,3,B11,2,A10,1,D9,0  
C,12,B12,3,A11,2,D10,0  
C,13,B13,12,A12,3,D11,0  
O,12,B14,3,A13,2,D12,0  
C,14,B15,13,A14,12,D13,0  
C,16,B16,14,A15,13,D14,0  
C,16,B17,14,A16,13,D15,0  
C,17,B18,16,A17,14,D16,0  
H,17,B19,16,A18,14,D17,0  
C,18,B20,16,A19,14,D18,0  
H,18,B21,16,A20,14,D19,0  
C,21,B22,18,A21,16,D20,0  
H,19,B23,17,A22,16,D21,0  
H,21,B24,18,A23,16,D22,0  
H,23,B25,21,A24,18,D23,0  
O,13,B26,12,A25,3,D24,0  
H,27,B27,13,A26,12,D25,0

Variables:

B1=1.38116693  
B2=1.40703418  
B3=1.40025312  
B4=1.39949105  
B5=1.38373876  
B6=1.08336361  
B7=1.08321129  
B8=1.08290359  
B9=1.08398138  
B10=1.35806881  
B11=1.45562765  
B12=1.45961276  
B13=1.36744807  
B14=1.23701555  
B15=1.46810621  
B16=1.40808849  
B17=1.40782297  
B18=1.38935293  
B19=1.08084534  
B20=1.39120169  
B21=1.07885843  
B22=1.39318453  
B23=1.08421473  
B24=1.08412969  
B25=1.08412392  
B26=1.35255706  
B27=0.97927312  
A1=120.25402114  
A2=118.96880778  
A3=121.11615706

A4=118.88121459  
A5=120.25099798  
A6=121.77880056  
A7=119.28715259  
A8=119.35585371  
A9=121.98105292  
A10=122.5647566  
A11=115.89453525  
A12=122.37309043  
A13=125.46150417  
A14=128.60829376  
A15=119.694646  
A16=121.92328323  
A17=120.75499977  
A18=119.58094557  
A19=120.37271665  
A20=119.92075696  
A21=120.71246104  
A22=119.5015909  
A23=119.22531728  
A24=120.32464275  
A25=114.04175915  
A26=104.01454434  
D1=-0.00220703  
D2=0.00294222  
D3=-0.00216584  
D4=-179.99856675  
D5=179.99988276  
D6=179.99757097  
D7=179.9999285  
D8=-179.99929166  
D9=179.99562653  
D10=-179.98803548  
D11=-0.02903441  
D12=0.01213897  
D13=-179.96876076  
D14=179.93217436  
D15=-0.07154779  
D16=-179.99798178  
D17=-0.00373198  
D18=179.99856924  
D19=-0.00375349  
D20=0.00110149  
D21=179.99828314  
D22=-179.99782877  
D23=-179.99958033  
D24=179.98860175  
D25=0.00966111

## Conformer B

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,5,B5,4,A4,3,D3,0  
H,1,B6,2,A5,3,D4,0  
H,2,B7,1,A6,6,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,5,A8,4,D7,0  
O,4,B10,3,A9,2,D8,0  
C,3,B11,2,A10,1,D9,0  
C,12,B12,3,A11,2,D10,0  
C,13,B13,12,A12,3,D11,0  
O,12,B14,3,A13,2,D12,0  
C,14,B15,13,A14,12,D13,0  
C,16,B16,14,A15,13,D14,0  
C,16,B17,14,A16,13,D15,0  
C,17,B18,16,A17,14,D16,0  
H,17,B19,16,A18,14,D17,0  
C,18,B20,16,A19,14,D18,0  
H,18,B21,16,A20,14,D19,0  
C,21,B22,18,A21,16,D20,0  
H,19,B23,17,A22,16,D21,0  
H,21,B24,18,A23,16,D22,0  
H,23,B25,21,A24,18,D23,0  
O,13,B26,12,A25,3,D24,0  
H,27,B27,13,A26,12,D25,0

Variables:

B1=1.38233893  
B2=1.4059077  
B3=1.39802672  
B4=1.39871463  
B5=1.38432111  
B6=1.0834752  
B7=1.08328717  
B8=1.08301566  
B9=1.08401249  
B10=1.36349337  
B11=1.47509212  
B12=1.47226595  
B13=1.36252391  
B14=1.22227611  
B15=1.47570937  
B16=1.40413432  
B17=1.40353536  
B18=1.39323155  
B19=1.08429178  
B20=1.39043015  
B21=1.08295438  
B22=1.39519344  
B23=1.08394182  
B24=1.0840604  
B25=1.08388964  
B26=1.3596579  
B27=0.96513194  
A1=120.54308429  
A2=118.50147701  
A3=121.52669292  
A4=118.8421706  
A5=120.20805404  
A6=121.80577291  
A7=119.25402256  
A8=119.43136061  
A9=121.70951345  
A10=121.10569104  
A11=113.89499172  
A12=121.55634731

A13=123.43936127  
A14=125.76204341  
A15=121.08414055  
A16=120.06956677  
A17=120.45566128  
A18=119.9536916  
A19=120.4358136  
A20=119.36751651  
A21=120.33740169  
A22=119.59396281  
A23=119.63924092  
A24=120.14938572  
A25=114.55831158  
A26=109.94002008  
D1=-0.08800948  
D2=0.09635249  
D3=-0.05922609  
D4=-179.94934329  
D5=-179.84660385  
D6=179.72395581  
D7=179.94233798  
D8=179.66032551  
D9=-179.2145768  
D10=179.27066144  
D11=2.12694214  
D12=-0.15498182  
D13=179.37003567  
D14=-44.57574492  
D15=136.18944471  
D16=179.63745079  
D17=-2.96485214  
D18=-179.64516585  
D19=0.1563781  
D20=-0.26623349  
D21=179.44500549  
D22=179.58666864  
D23=179.96559541  
D24=-177.35644831  
D25=168.61603958

$$\mathbf{X} = \mathbf{F}$$

## Conformer A

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,1,B5,2,A4,3,D3,0  
H,1,B6,6,A5,5,D4,0  
H,4,B7,3,A6,2,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,1,A8,2,D7,0  
O,3,B10,2,A9,1,D8,0  
C,2,B11,1,A10,6,D9,0  
C,12,B12,2,A11,1,D10,0  
C,13,B13,12,A12,2,D11,0  
O,12,B14,2,A13,1,D12,0  
O,13,B15,12,A14,2,D13,0  
H,16,B16,13,A15,12,D14,0  
C,14,B17,13,A16,12,D15,0  
C,18,B18,14,A17,13,D16,0  
C,18,B19,14,A18,13,D17,0  
C,19,B20,18,A19,14,D18,0  
H,19,B21,18,A20,14,D19,0  
C,20,B22,18,A21,14,D20,0  
C,23,B23,20,A22,18,D21,0  
H,21,B24,19,A23,18,D22,0  
H,23,B25,20,A24,18,D23,0  
H,24,B26,23,A25,20,D24,0  
F,20,B27,18,A26,14,D25,0

Variables:

B1=1.40759653  
B2=1.40204224  
B3=1.39951865  
B4=1.38318459  
B5=1.38075606  
B6=1.08319638  
B7=1.08275271  
B8=1.08397494  
B9=1.08338757  
B10=1.3586117  
B11=1.45733994  
B12=1.46000771  
B13=1.36170075  
B14=1.23578592  
B15=1.35241875  
B16=0.97738951  
B17=1.47004062  
B18=1.40476859  
B19=1.40045527  
B20=1.38956148  
B21=1.0815568  
B22=1.3850104  
B23=1.39208637  
B24=1.08324285  
B25=1.08284683  
B26=1.08367301  
B27=1.35207956  
A1=118.83556492  
A2=121.19611459  
A3=118.85026555  
A4=120.29320683  
A5=121.77750712  
A6=119.11524807



A7=119.36582758  
A8=120.22746403  
A9=122.06523099  
A10=122.30462338  
A11=115.42487666  
A12=121.92141341  
A13=125.67591027  
A14=115.26749093  
A15=104.34442218  
A16=125.97406825  
A17=120.8620474  
A18=122.17632986  
A19=121.25263946  
A20=118.6903306  
A21=122.65840356  
A22=119.07083319  
A23=119.67032537  
A24=118.98495142  
A25=119.64038522  
A26=119.6856544  
D1=0.04846074  
D2=0.00819975  
D3=-0.08046305  
D4=-179.91327343  
D5=-179.82725351  
D6=-179.94617704  
D7=-179.980777  
D8=179.75975362  
D9=-179.89263687  
D10=179.7665228  
D11=-0.31870042  
D12=0.45642484  
D13=-179.21397538  
D14=1.0884314  
D15=-179.65050727  
D16=-40.16881133  
D17=139.94517422  
D18=-179.09370519  
D19=0.9209714  
D20=179.07102497  
D21=0.25940026  
D22=179.62445343  
D23=179.65697226  
D24=179.96026948  
D25=-2.6053541

## Conformer B

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,1,B5,2,A4,3,D3,0  
H,1,B6,6,A5,5,D4,0  
H,4,B7,3,A6,2,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,1,A8,2,D7,0  
O,3,B10,2,A9,1,D8,0  
C,2,B11,1,A10,6,D9,0  
C,12,B12,2,A11,1,D10,0  
C,13,B13,12,A12,2,D11,0  
O,12,B14,2,A13,1,D12,0  
O,13,B15,12,A14,2,D13,0  
H,16,B16,13,A15,12,D14,0  
C,14,B17,13,A16,12,D15,0  
C,18,B18,14,A17,13,D16,0  
C,18,B19,14,A18,13,D17,0  
C,19,B20,18,A19,14,D18,0  
H,19,B21,18,A20,14,D19,0  
C,20,B22,18,A21,14,D20,0  
C,23,B23,20,A22,18,D21,0  
H,21,B24,19,A23,18,D22,0  
H,23,B25,20,A24,18,D23,0  
H,24,B26,23,A25,20,D24,0  
F,20,B27,18,A26,14,D25,0

Variables:

B1=1.40739781  
B2=1.4017715  
B3=1.3994726  
B4=1.38351657  
B5=1.38096023  
B6=1.08323939  
B7=1.08291619  
B8=1.08396978  
B9=1.0833759  
B10=1.36067555  
B11=1.45901531  
B12=1.46135244  
B13=1.35975468  
B14=1.23439964  
B15=1.34756467  
B16=0.9759152  
B17=1.46991948  
B18=1.40461583  
B19=1.39757137  
B20=1.38897271  
B21=1.08309821  
B22=1.38655852  
B23=1.39129381  
B24=1.08333406  
B25=1.0827999  
B26=1.08368873  
B27=1.3475099  
A1=118.7950312  
A2=121.18876971  
A3=118.89419507  
A4=120.35605395  
A5=121.75560066  
A6=119.19376974  
A7=119.37332633  
A8=120.23437875  
A9=122.00691458  
A10=122.13474909  
A11=115.38325745  
A12=121.74520301

A13=125.49023034  
A14=115.76104829  
A15=104.85437273  
A16=126.5831262  
A17=120.38190791  
A18=122.39867746  
A19=121.22603955  
A20=118.56939764  
A21=122.45854212  
A22=119.08244699  
A23=119.8502374  
A24=118.99330316  
A25=119.62146948  
A26=119.52139073  
D1=-0.06719913  
D2=-0.01698537  
D3=0.12026119  
D4=179.87713023  
D5=-179.77034661  
D6=-179.89126212  
D7=179.90569094  
D8=-179.71781144  
D9=179.42657835  
D10=-179.85645328  
D11=-0.9537714  
D12=-0.77726088  
D13=177.43168802  
D14=1.99547077  
D15=178.58098308  
D16=-131.43490456  
D17=49.27195578  
D18=179.07788463  
D19=-0.17401814  
D20=-178.91275759  
D21=-0.74394264  
D22=-179.27625199  
D23=-179.93805005  
D24=179.9400511  
D25=3.34286074

## Conformer C

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,1,B5,2,A4,3,D3,0  
H,1,B6,6,A5,5,D4,0  
H,4,B7,3,A6,2,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,1,A8,2,D7,0  
O,3,B10,2,A9,1,D8,0  
C,2,B11,1,A10,6,D9,0  
C,12,B12,2,A11,1,D10,0  
C,13,B13,12,A12,2,D11,0  
O,12,B14,2,A13,1,D12,0  
O,13,B15,12,A14,2,D13,0  
H,16,B16,13,A15,12,D14,0  
C,14,B17,13,A16,12,D15,0  
C,18,B18,14,A17,13,D16,0  
C,18,B19,14,A18,13,D17,0  
C,19,B20,18,A19,14,D18,0  
H,19,B21,18,A20,14,D19,0  
C,20,B22,18,A21,14,D20,0  
C,23,B23,20,A22,18,D21,0  
H,21,B24,19,A23,18,D22,0  
H,23,B25,20,A24,18,D23,0  
H,24,B26,23,A25,20,D24,0  
F,20,B27,18,A26,14,D25,0

Variables:

B1=1.40582275  
B2=1.39638714  
B3=1.39892738  
B4=1.38435064  
B5=1.38232244  
B6=1.08327779  
B7=1.08303791  
B8=1.08403368  
B9=1.08345851  
B10=1.36242321  
B11=1.4736745  
B12=1.47941495  
B13=1.36469316  
B14=1.22108792  
B15=1.35363756  
B16=0.96443127  
B17=1.47687415  
B18=1.40819401  
B19=1.39474433  
B20=1.38811478  
B21=1.08202786  
B22=1.38373169  
B23=1.39080332  
B24=1.0833126  
B25=1.08264618  
B26=1.08333336  
B27=1.36906118  
A1=118.58131133  
A2=121.544946  
A3=118.78183862  
A4=120.48413552  
A5=121.83486457  
A6=119.32467641  
A7=119.41629691  
A8=120.22605069  
A9=121.64696755  
A10=121.27256663  
A11=114.49585674  
A12=121.05788991

A13=123.24926833  
A14=113.97084283  
A15=110.98374094  
A16=128.13208962  
A17=119.36899268  
A18=124.69357208  
A19=121.58884621  
A20=118.31795366  
A21=123.8484643  
A22=118.67081158  
A23=119.63086313  
A24=119.19354762  
A25=119.75376114  
A26=119.04793851  
D1=-0.15521833  
D2=0.18021096  
D3=0.02953301  
D4=-179.91331818  
D5=-179.70141681  
D6=179.96719726  
D7=-179.9844185  
D8=-179.9000714  
D9=-179.53460628  
D10=179.47691093  
D11=1.13009992  
D12=-0.99631224  
D13=177.31520506  
D14=150.71390648  
D15=173.93092615  
D16=-138.19482591  
D17=42.99059959  
D18=179.90774802  
D19=0.26280105  
D20=-179.95570922  
D21=-0.48811914  
D22=-179.35196235  
D23=-179.76928344  
D24=-179.99728603  
D25=1.12251138

## Conformer D

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,1,B5,2,A4,3,D3,0  
H,1,B6,6,A5,5,D4,0  
H,4,B7,3,A6,2,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,1,A8,2,D7,0  
O,3,B10,2,A9,1,D8,0  
C,2,B11,1,A10,6,D9,0  
C,12,B12,2,A11,1,D10,0  
C,13,B13,12,A12,2,D11,0  
O,12,B14,2,A13,1,D12,0  
O,13,B15,12,A14,2,D13,0  
H,16,B16,13,A15,12,D14,0  
C,14,B17,13,A16,12,D15,0  
C,18,B18,14,A17,13,D16,0  
C,18,B19,14,A18,13,D17,0  
C,19,B20,18,A19,14,D18,0  
H,19,B21,18,A20,14,D19,0  
C,20,B22,18,A21,14,D20,0  
C,23,B23,20,A22,18,D21,0  
H,21,B24,19,A23,18,D22,0  
H,23,B25,20,A24,18,D23,0  
H,24,B26,23,A25,20,D24,0  
F,20,B27,18,A26,14,D25,0

Variables:

B1=1.40625542  
B2=1.3989923  
B3=1.39864302  
B4=1.38397661  
B5=1.38202789  
B6=1.08325348  
B7=1.08289624  
B8=1.08400998  
B9=1.08347239  
B10=1.36326112  
B11=1.47503025  
B12=1.47357497  
B13=1.35903727  
B14=1.22173023  
B15=1.35896271  
B16=0.96519678  
B17=1.47851068  
B18=1.40397347  
B19=1.39797712  
B20=1.3920452  
B21=1.08419874  
B22=1.38524152  
B23=1.39313326  
B24=1.08315381  
B25=1.08285355  
B26=1.08359516  
B27=1.34930512  
A1=118.47278805  
A2=121.53381261  
A3=118.8293332  
A4=120.5433153  
A5=121.8093591  
A6=119.19248913  
A7=119.42298833  
A8=120.20435048  
A9=121.74874044  
A10=120.9838934  
A11=113.71026995  
A12=121.28456302

A13=123.62618399  
A14=114.95947278  
A15=109.92061989  
A16=124.34339987  
A17=121.13484813  
A18=121.63007711  
A19=121.13541183  
A20=118.75902205  
A21=122.63079  
A22=118.89749443  
A23=119.83171557  
A24=119.22683828  
A25=119.53433694  
A26=118.98903373  
D1=0.02415587  
D2=0.01265412  
D3=-0.06326635  
D4=-179.87199536  
D5=-179.91718346  
D6=-179.95174006  
D7=-179.97538046  
D8=179.53806559  
D9=-179.53204595  
D10=179.02817132  
D11=1.68393923  
D12=-0.54581177  
D13=-177.92591481  
D14=172.89348469  
D15=178.43200968  
D16=-58.91422552  
D17=121.35242583  
D18=-179.94362541  
D19=-1.29162725  
D20=179.63480712  
D21=0.25498868  
D22=179.61321699  
D23=179.83230408  
D24=179.96091123  
D25=-1.31171269

$$\mathbf{X} = \mathbf{C}\mathbf{I}$$

## Conformer A

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,5,B5,4,A4,3,D3,0  
H,1,B6,2,A5,3,D4,0  
H,2,B7,1,A6,6,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,5,A8,4,D7,0  
O,4,B10,3,A9,2,D8,0  
C,3,B11,2,A10,1,D9,0  
C,12,B12,3,A11,2,D10,0  
C,13,B13,12,A12,3,D11,0  
O,12,B14,3,A13,2,D12,0  
C,14,B15,13,A14,12,D13,0  
C,16,B16,14,A15,13,D14,0  
C,16,B17,14,A16,13,D15,0  
C,17,B18,16,A17,14,D16,0  
H,17,B19,16,A18,14,D17,0  
C,18,B20,16,A19,14,D18,0  
C,21,B21,18,A20,16,D19,0  
H,19,B22,17,A21,16,D20,0  
H,21,B23,18,A22,16,D21,0  
H,22,B24,21,A23,18,D22,0  
O,13,B25,12,A24,3,D23,0  
H,26,B26,13,A25,12,D24,0  
Cl,18,B27,16,A26,14,D25,0

Variables:

B1=1.38079133  
B2=1.40759267  
B3=1.40237188  
B4=1.39951608  
B5=1.38319425  
B6=1.08339862  
B7=1.08322095  
B8=1.08277354  
B9=1.08398444  
B10=1.35912282  
B11=1.45825945  
B12=1.4610936  
B13=1.35894919  
B14=1.23500785  
B15=1.47486578  
B16=1.40290058  
B17=1.40389352  
B18=1.38918345  
B19=1.08257678  
B20=1.39166236  
B21=1.39159984  
B22=1.08338427  
B23=1.08240066  
B24=1.08386869  
B25=1.3520425  
B26=0.97664201  
B27=1.75745825  
A1=120.31912071  
A2=118.79610726  
A3=121.21033421  
A4=118.85808964  
A5=120.22461107  
A6=121.7646442



A7=119.11575433  
A8=119.3721979  
A9=122.03665474  
A10=122.22161424  
A11=115.29471916  
A12=121.80916981  
A13=125.68333127  
A14=125.42598071  
A15=119.05429826  
A16=123.13339575  
A17=121.33434279  
A18=118.5135709  
A19=121.21429431  
A20=119.78331943  
A21=119.84568155  
A22=119.37936091  
A23=119.48708287  
A24=115.60257698  
A25=104.5141405  
A26=121.09559036  
D1=0.07929495  
D2=-0.08364174  
D3=0.03433602  
D4=179.98186594  
D5=179.94269452  
D6=179.90967668  
D7=179.93733442  
D8=-179.68211023  
D9=179.99620295  
D10=-179.72528645  
D11=0.39767902  
D12=-0.27283264  
D13=-179.72305995  
D14=52.05102501  
D15=-128.02723694  
D16=178.77777817  
D17=-1.05365212  
D18=-178.63008765  
D19=-0.48111325  
D20=-179.66376608  
D21=-179.73725307  
D22=-179.96700627  
D23=179.35000261  
D24=-0.88458511  
D25=3.97176791

## Conformer D

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,5,B5,4,A4,3,D3,0  
H,1,B6,2,A5,3,D4,0  
H,2,B7,1,A6,6,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,5,A8,4,D7,0  
O,4,B10,3,A9,2,D8,0  
C,3,B11,2,A10,1,D9,0  
C,12,B12,3,A11,2,D10,0  
C,13,B13,12,A12,3,D11,0  
O,12,B14,3,A13,2,D12,0  
C,14,B15,13,A14,12,D13,0  
C,16,B16,14,A15,13,D14,0  
C,16,B17,14,A16,13,D15,0  
C,17,B18,16,A17,14,D16,0  
H,17,B19,16,A18,14,D17,0  
C,18,B20,16,A19,14,D18,0  
C,21,B21,18,A20,16,D19,0  
H,19,B22,17,A21,16,D20,0  
H,21,B23,18,A22,16,D21,0  
H,22,B24,21,A23,18,D22,0  
O,13,B25,12,A24,3,D23,0  
H,26,B26,13,A25,12,D24,0  
Cl,18,B27,16,A26,14,D25,0

Variables:

B1=1.38208611  
B2=1.40623627  
B3=1.39918288  
B4=1.39868978  
B5=1.38397658  
B6=1.08349538  
B7=1.08327918  
B8=1.08292727  
B9=1.08403473  
B10=1.36327939  
B11=1.47541158  
B12=1.47380734  
B13=1.35761748  
B14=1.2215817  
B15=1.48182656  
B16=1.40334785  
B17=1.40360603  
B18=1.39150105  
B19=1.08428954  
B20=1.3917138  
B21=1.39235722  
B22=1.08333784  
B23=1.08245653  
B24=1.08378549  
B25=1.35887291  
B26=0.96526891  
B27=1.75332134  
A1=120.55271704  
A2=118.45441587  
A3=121.5422623  
A4=118.83203397  
A5=120.20248473  
A6=121.79721097  
A7=119.18511923  
A8=119.42795234  
A9=121.73782298  
A10=120.97830265  
A11=113.66463144  
A12=121.26712743

A13=123.63034177  
A14=124.11396412  
A15=119.56465139  
A16=122.52908564  
A17=121.26989442  
A18=118.57664488  
A19=121.22848482  
A20=119.70958789  
A21=119.91083724  
A22=119.46928428  
A23=119.44430407  
A24=115.06378607  
A25=109.86807712  
A26=120.38887613  
D1=-0.03390275  
D2=0.03929922  
D3=-0.0330486  
D4=179.99439752  
D5=-179.92495427  
D6=-179.95562135  
D7=-179.93123515  
D8=179.59568513  
D9=-179.73557368  
D10=179.08481868  
D11=1.187138  
D12=-0.55343503  
D13=178.78170643  
D14=-66.12580276  
D15=114.03769341  
D16=-179.71095246  
D17=-0.76452602  
D18=179.37507628  
D19=0.38629443  
D20=179.68744154  
D21=179.93981235  
D22=179.93548529  
D23=-178.26527403  
D24=174.85766219  
D25=-1.84305651

$$\mathbf{X} = \mathbf{B}\mathbf{r}$$

## Conformer A

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,5,B5,4,A4,3,D3,0  
H,1,B6,2,A5,3,D4,0  
H,2,B7,1,A6,6,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,5,A8,4,D7,0  
O,4,B10,3,A9,2,D8,0  
C,3,B11,2,A10,1,D9,0  
C,12,B12,3,A11,2,D10,0  
C,13,B13,12,A12,3,D11,0  
O,12,B14,3,A13,2,D12,0  
C,14,B15,13,A14,12,D13,0  
C,16,B16,14,A15,13,D14,0  
C,16,B17,14,A16,13,D15,0  
C,17,B18,16,A17,14,D16,0  
H,17,B19,16,A18,14,D17,0  
C,18,B20,16,A19,14,D18,0  
C,21,B21,18,A20,16,D19,0  
H,19,B22,17,A21,16,D20,0  
H,21,B23,18,A22,16,D21,0  
H,22,B24,21,A23,18,D22,0  
O,13,B25,12,A24,3,D23,0  
H,26,B26,13,A25,12,D24,0  
Br,18,B27,16,A26,14,D25,0

Variables:

B1=1.38078019  
B2=1.40761292  
B3=1.40239019  
B4=1.39952115  
B5=1.38320869  
B6=1.08340178  
B7=1.08322564  
B8=1.08276065  
B9=1.08399388  
B10=1.35920645  
B11=1.4582386  
B12=1.46132364  
B13=1.35854855  
B14=1.23490846  
B15=1.47574935  
B16=1.40314077  
B17=1.4036523  
B18=1.38923249  
B19=1.08276889  
B20=1.39198601  
B21=1.39219257  
B22=1.08343868  
B23=1.0821718  
B24=1.0839299  
B25=1.35193923  
B26=0.97656061  
B27=1.91847712  
A1=120.32279302  
A2=118.7969  
A3=121.20508547  
A4=118.86085872  
A5=120.2271412  
A6=121.75866938

A7=119.11908544  
A8=119.37224915  
A9=122.03269431  
A10=122.19933637  
A11=115.28640191  
A12=121.77416046  
A13=125.67431264  
A14=125.35351731  
A15=118.68592228  
A16=123.50116533  
A17=121.36287021  
A18=118.49817619  
A19=121.19522684  
A20=119.78803677  
A21=119.84750938  
A22=119.67705676  
A23=119.45285889  
A24=115.64745164  
A25=104.5436264  
A26=121.44905368  
D1=0.09891844  
D2=-0.12640166  
D3=0.08692578  
D4=179.98504785  
D5=179.96684422  
D6=179.91637897  
D7=179.90146475  
D8=-179.72248863  
D9=179.97691737  
D10=-179.64289539  
D11=0.44795663  
D12=-0.19311474  
D13=-179.69896313  
D14=54.14264789  
D15=-125.96086423  
D16=178.77172098  
D17=-1.07448401  
D18=-178.58629468  
D19=-0.50389343  
D20=-179.67717363  
D21=-179.73490239  
D22=-179.96105352  
D23=179.28727505  
D24=-0.92495036  
D25=4.28608737

## Conformer D

Final structure in terms of initial Z-matrix:

C  
C,1,B1  
C,2,B2,1,A1  
C,3,B3,2,A2,1,D1,0  
C,4,B4,3,A3,2,D2,0  
C,5,B5,4,A4,3,D3,0  
H,1,B6,2,A5,3,D4,0  
H,2,B7,1,A6,6,D5,0  
H,5,B8,4,A7,3,D6,0  
H,6,B9,5,A8,4,D7,0  
O,4,B10,3,A9,2,D8,0  
C,3,B11,2,A10,1,D9,0  
C,12,B12,3,A11,2,D10,0  
C,13,B13,12,A12,3,D11,0  
O,12,B14,3,A13,2,D12,0  
C,14,B15,13,A14,12,D13,0  
C,16,B16,14,A15,13,D14,0  
C,16,B17,14,A16,13,D15,0  
C,17,B18,16,A17,14,D16,0  
H,17,B19,16,A18,14,D17,0  
C,18,B20,16,A19,14,D18,0  
C,21,B21,18,A20,16,D19,0  
H,19,B22,17,A21,16,D20,0  
H,21,B23,18,A22,16,D21,0  
H,22,B24,21,A23,18,D22,0  
O,13,B25,12,A24,3,D23,0  
H,26,B26,13,A25,12,D24,0  
Br,18,B27,16,A26,14,D25,0

Variables:

B1=1.38208547  
B2=1.40628781  
B3=1.3991519  
B4=1.3987034  
B5=1.38401242  
B6=1.08350566  
B7=1.08328061  
B8=1.08293125  
B9=1.08403925  
B10=1.36352327  
B11=1.47556283  
B12=1.47366195  
B13=1.35711961  
B14=1.22155871  
B15=1.48303806  
B16=1.40363734  
B17=1.40349612  
B18=1.39146253  
B19=1.08431723  
B20=1.39209621  
B21=1.39297225  
B22=1.08338566  
B23=1.08222119  
B24=1.08388336  
B25=1.35876866  
B26=0.96526763  
B27=1.9140023  
A1=120.55814204  
A2=118.44684188  
A3=121.54536764  
A4=118.83442715  
A5=120.20207636  
A6=121.79608501  
A7=119.18770203  
A8=119.43020465  
A9=121.73640581  
A10=120.95432854  
A11=113.6373026  
A12=121.25548923

A13=123.62772934  
A14=124.01531991  
A15=119.19519337  
A16=122.87213989  
A17=121.2705297  
A18=118.55353406  
A19=121.20548757  
A20=119.69088568  
A21=119.92129007  
A22=119.77153209  
A23=119.40716908  
A24=115.13134166  
A25=109.84534788  
A26=120.59939184  
D1=0.06188735  
D2=-0.10116758  
D3=0.08733706  
D4=-179.99106646  
D5=179.97802135  
D6=179.97246089  
D7=179.9165649  
D8=-179.68186782  
D9=179.83819806  
D10=-179.17405379  
D11=-0.89600954  
D12=0.53445797  
D13=-178.74442775  
D14=69.54431027  
D15=-110.61157644  
D16=179.66384089  
D17=0.53353587  
D18=-179.40609357  
D19=-0.30993223  
D20=-179.70562736  
D21=-179.92376054  
D22=-179.94956661  
D23=178.50909856  
D24=-175.52311342  
D25=1.78061165