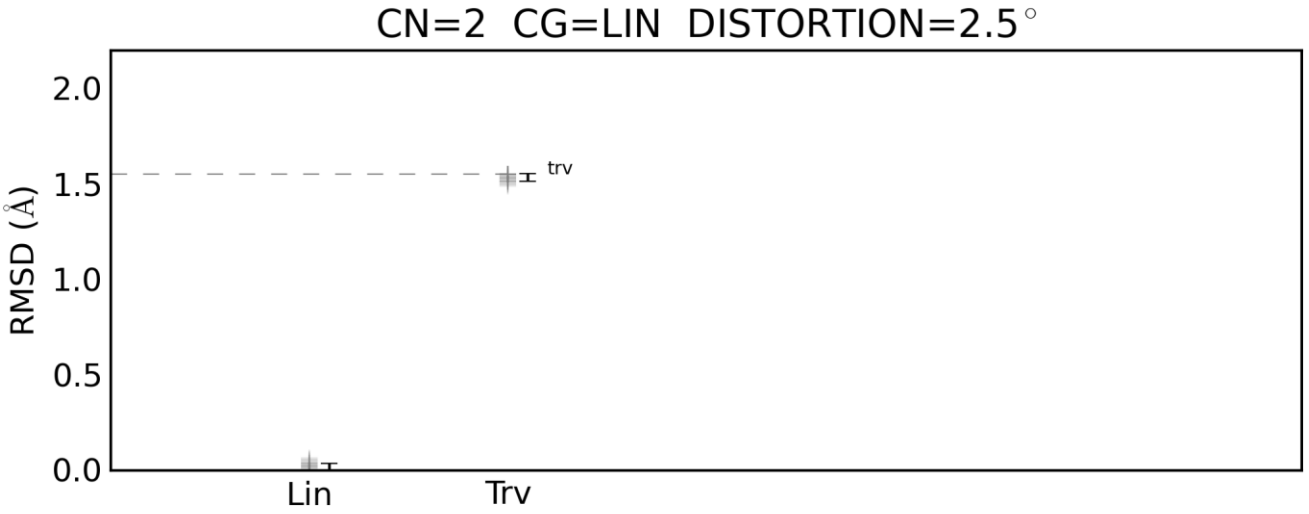
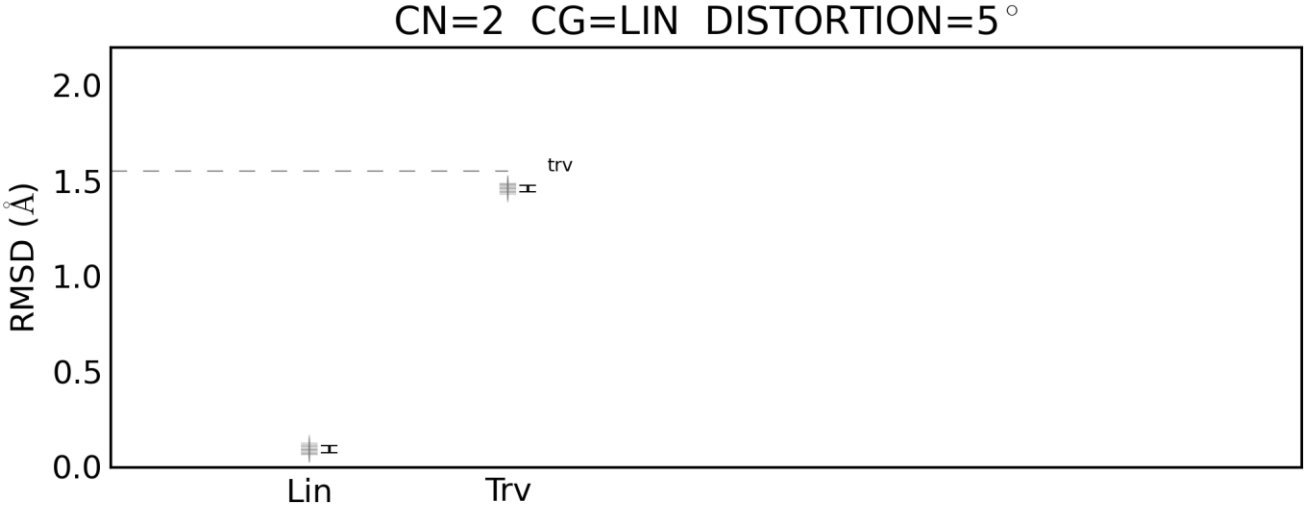
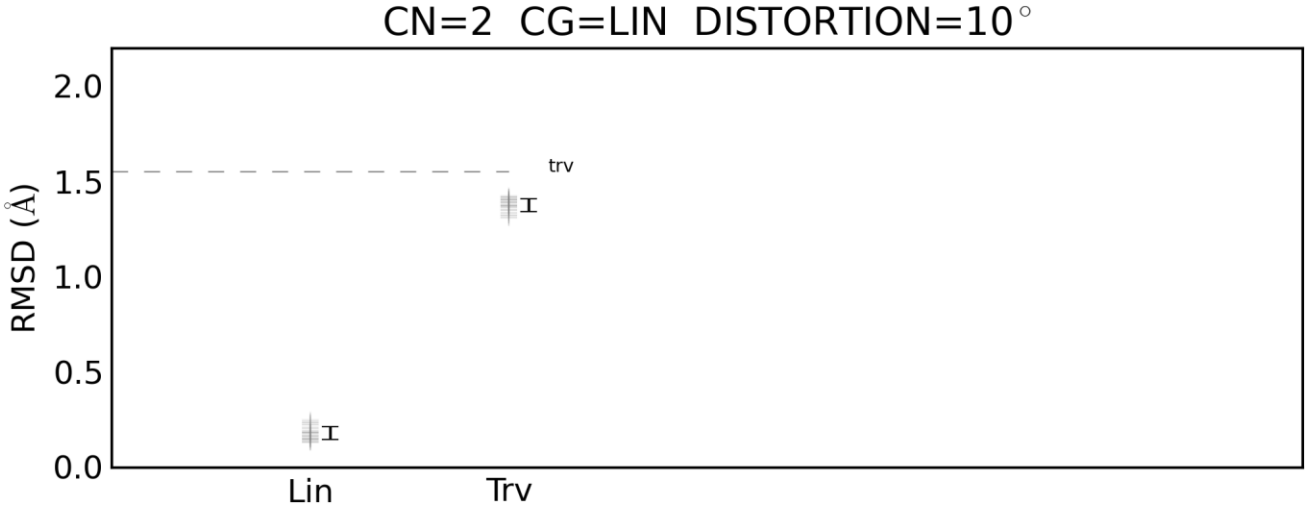
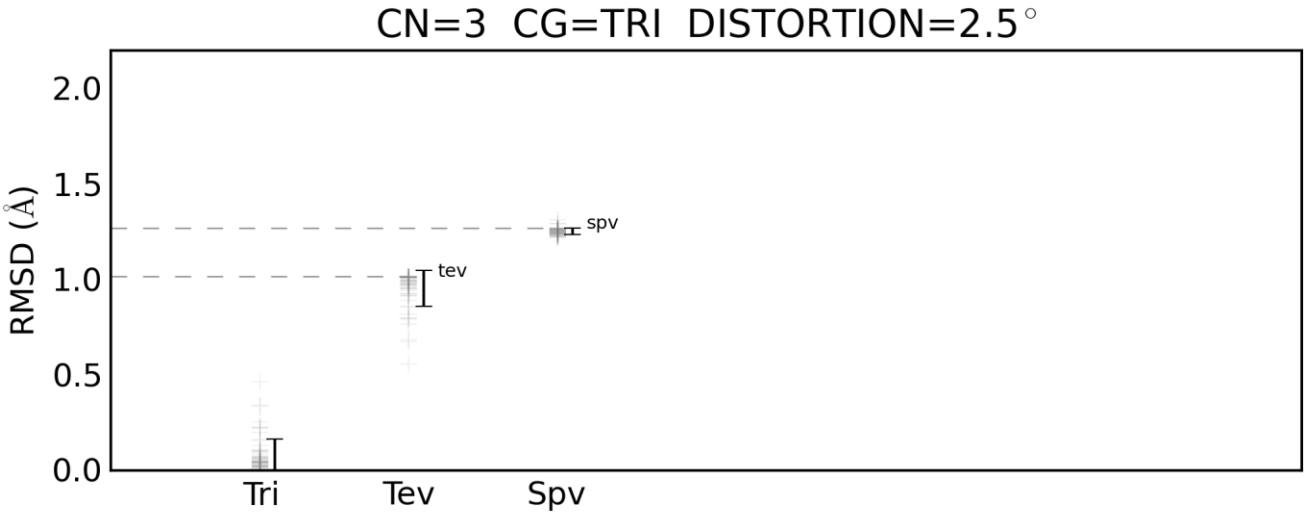
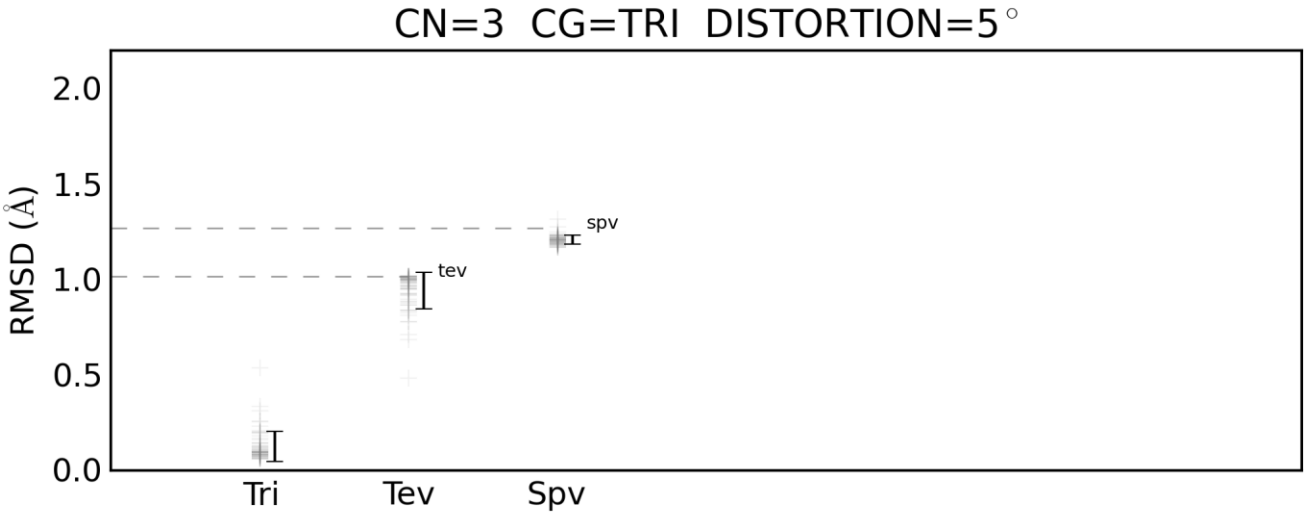
Figure S3. Plots showing the distribution of the RMSD values calculated for every geometry tested on the structures of the CSD-derived data set (CN = coordination number, CG = coordination geometry, DISTORTION = tolerated distortion of ligand-metal-ligand angles)

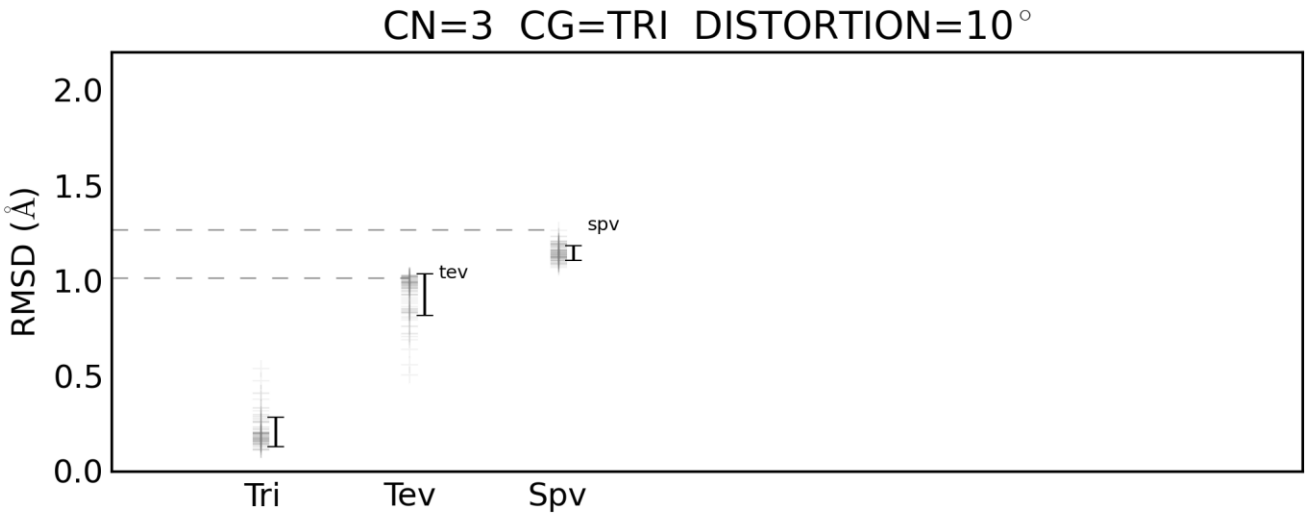

CN=2 CG=LIN DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
trv
Lin
Trv

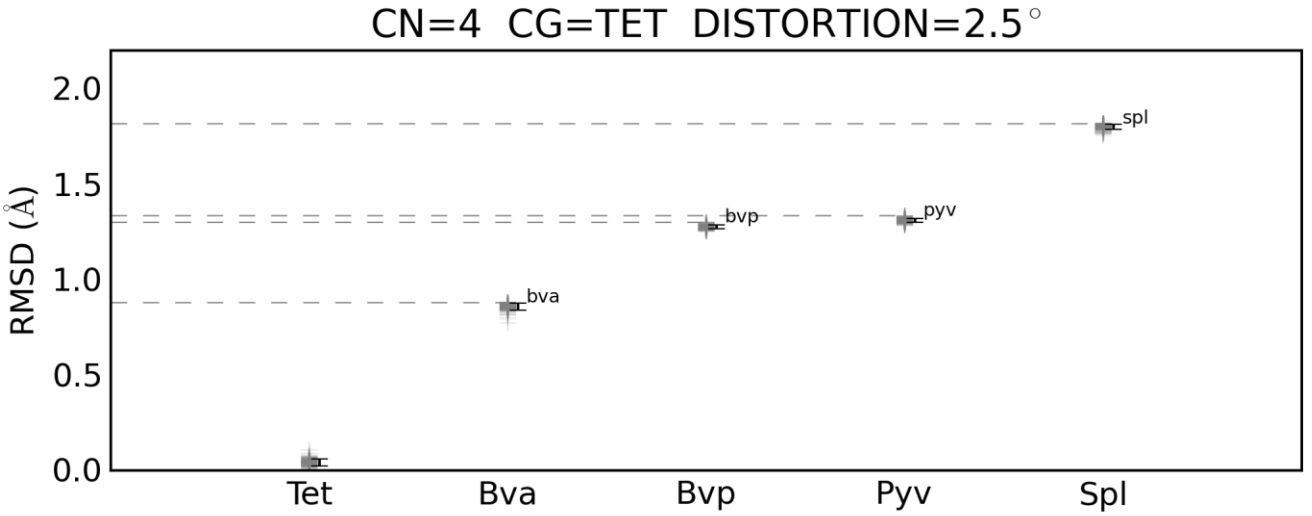

CN=2 CG=LIN DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
trv
Lin
Trv

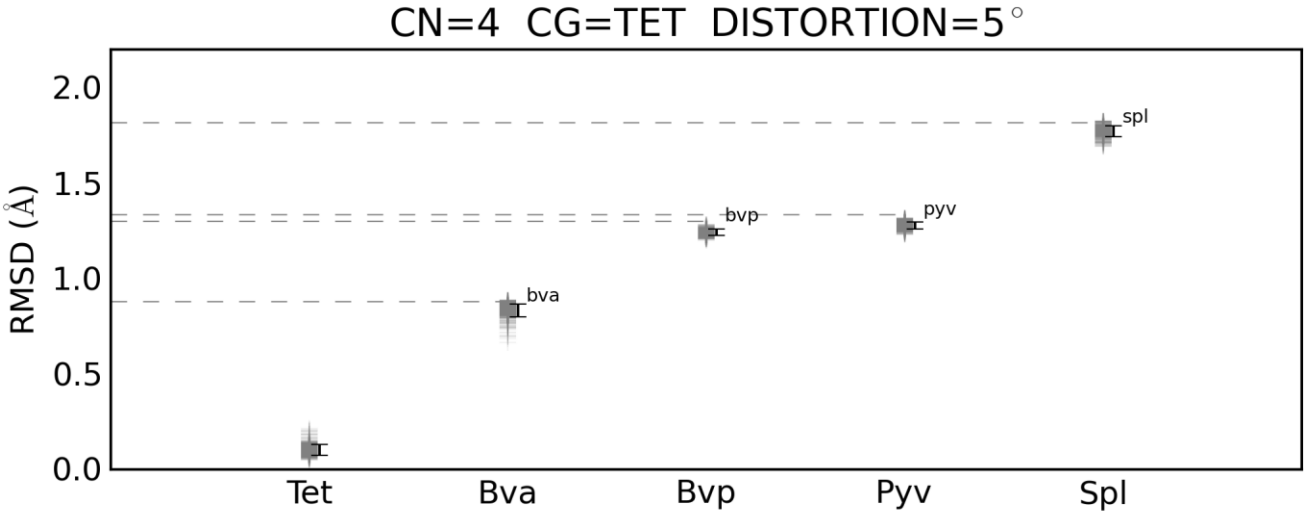

CN=2 CG=LIN DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
trv
Lin
Trv

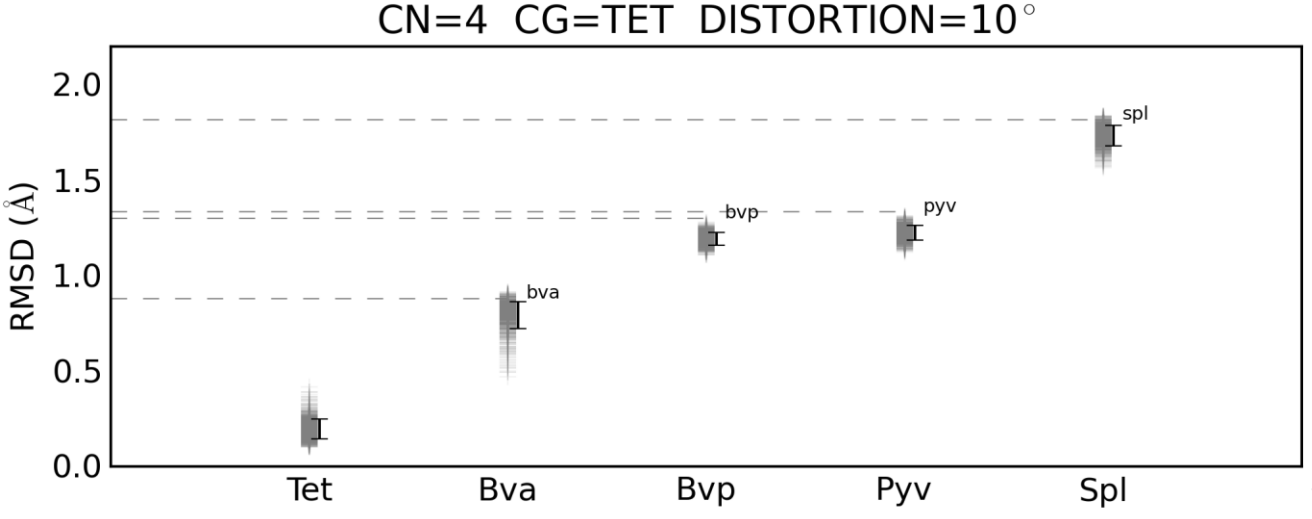

CN=3 CG=TRI DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
spv
tev
Tri
Tev
Spv

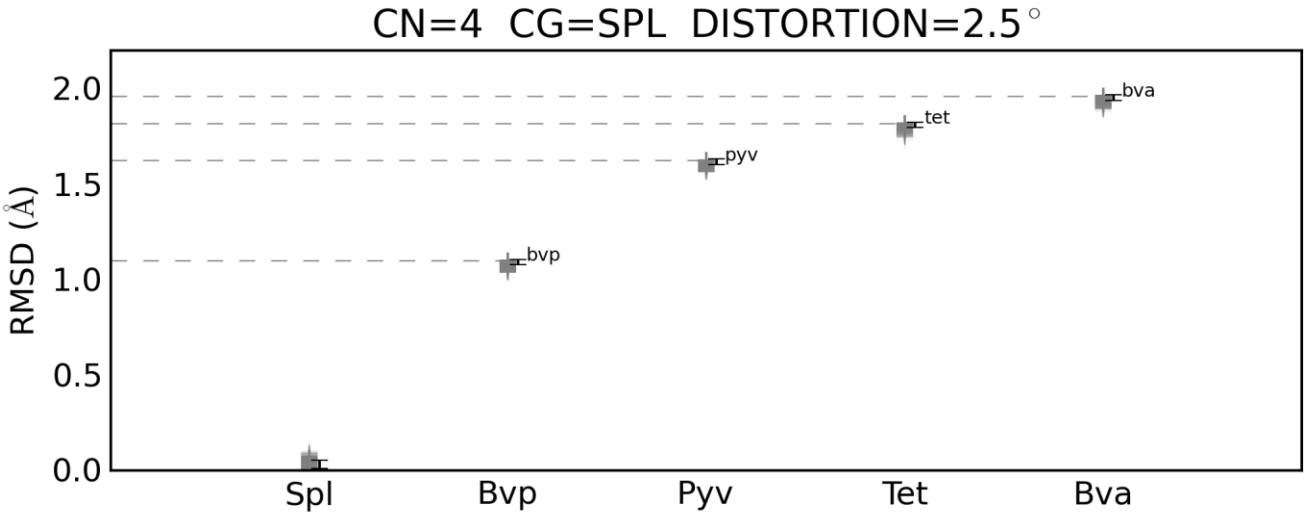

CN=3 CG=TRI DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
spv
tev
Tri
Tev
Spv

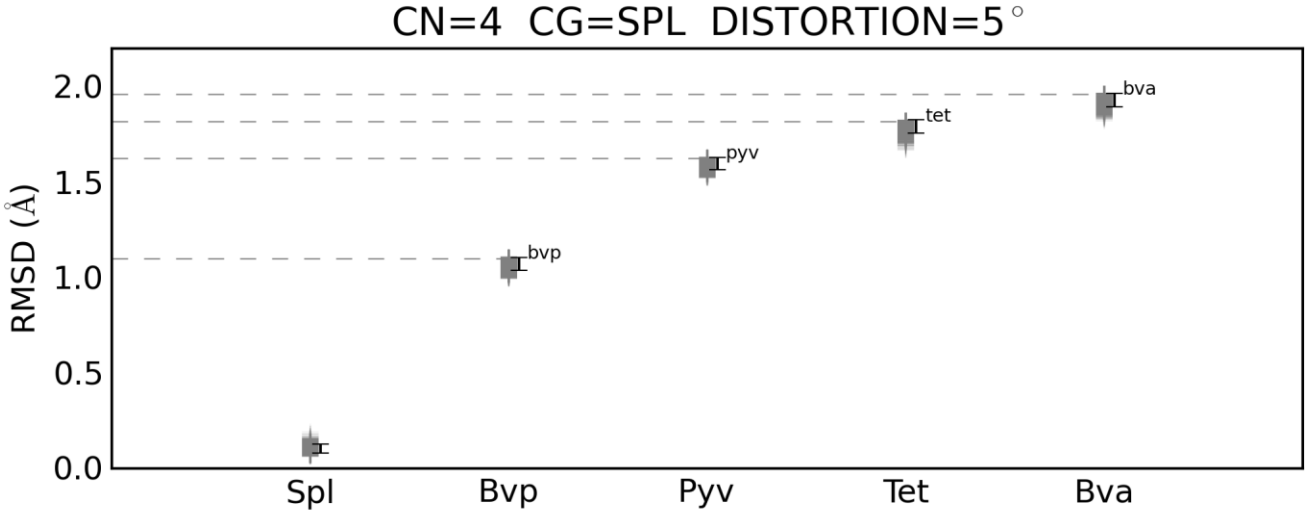

CN=3 CG=TRI DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
spv
tev
Tri
Tev
Spv

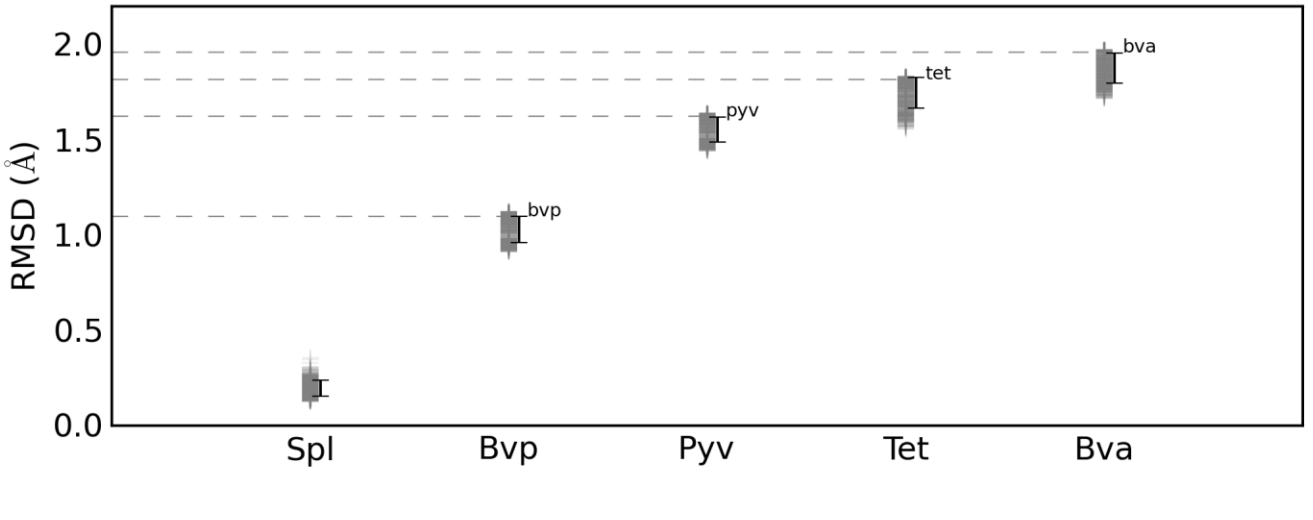

CN=4 CG=TET DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
spl
bvp
pyv
bva
Tet
Bva
Bvp
Pyv
Spl

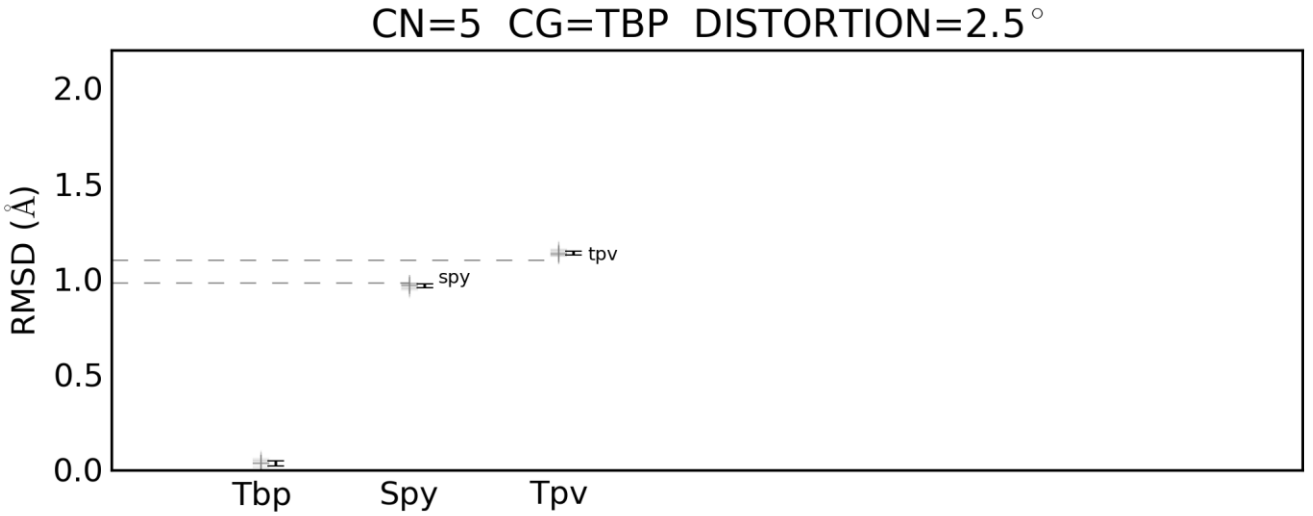

CN=4 CG=TET DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
spl
bvp
pyv
bva
Tet
Bva
Bvp
Pyv
Spl

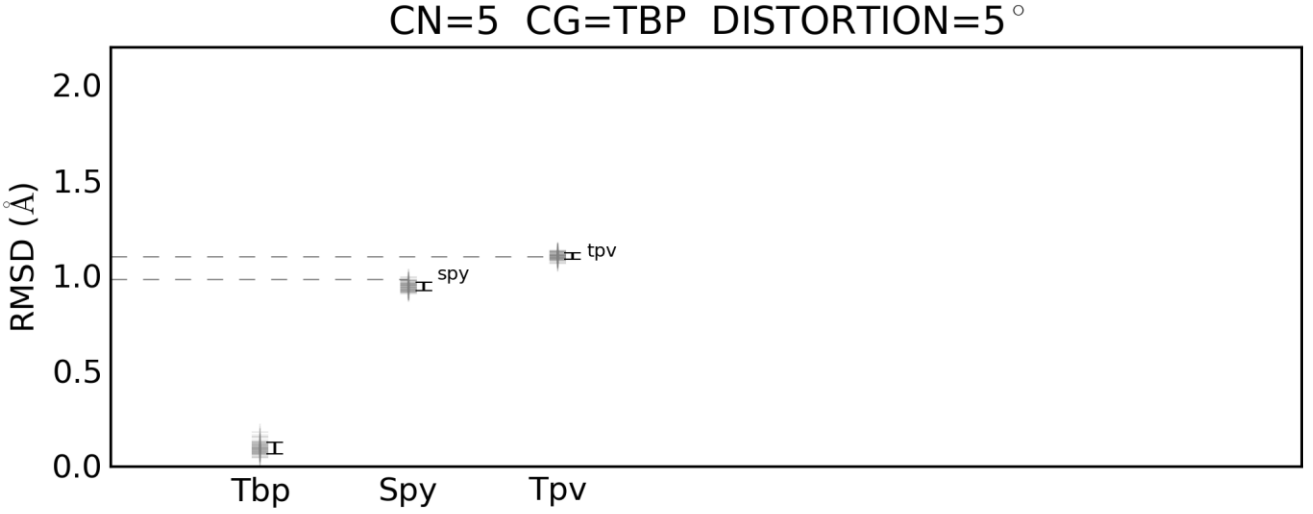

CN=4 CG=TET DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
spl
bvp
pyv
bva
Tet
Bva
Bvp
Pyv
Spl

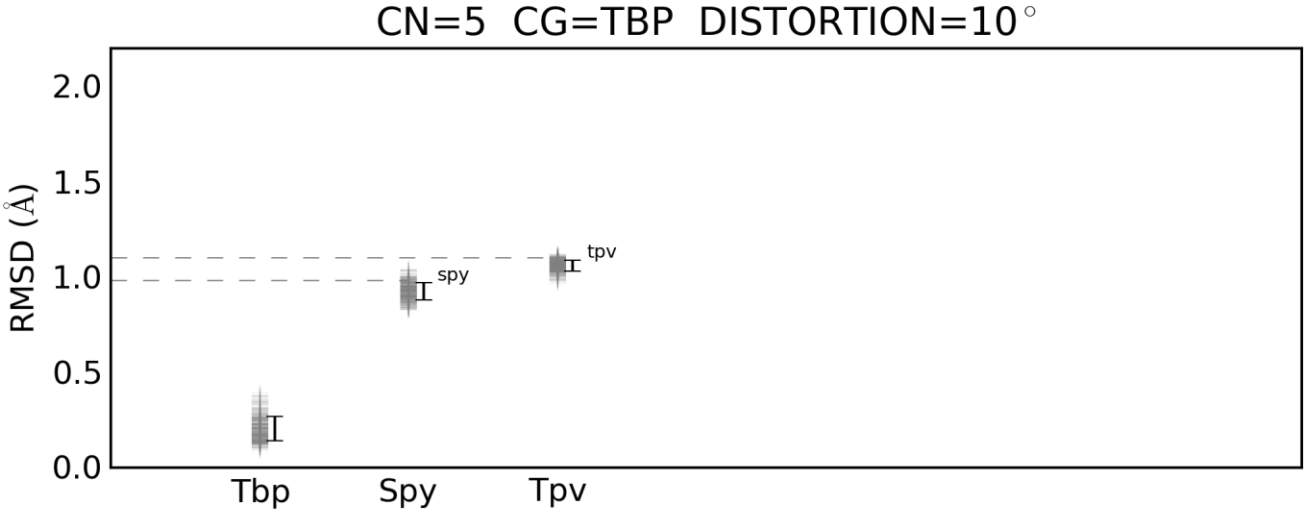

CN=4 CG=SPL DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
bva
tet
pyv
bvp
Spl
Bvp
Pyv
Tet
Bva

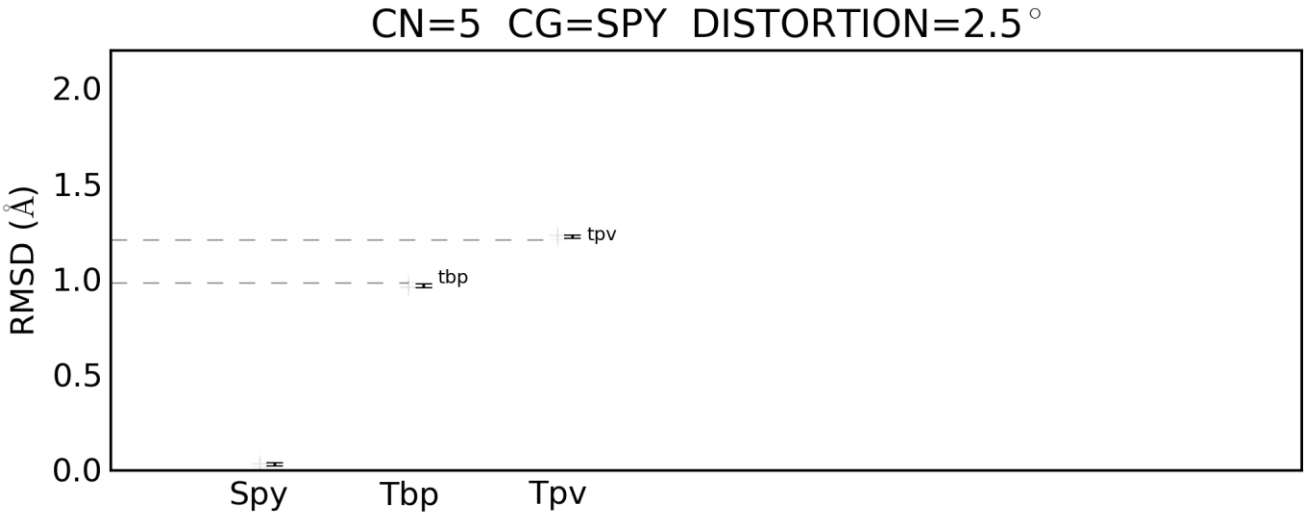

CN=4 CG=SPL DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
bva
tet
pyv
bvp
Spl
Bvp
Pyv
Tet
Bva

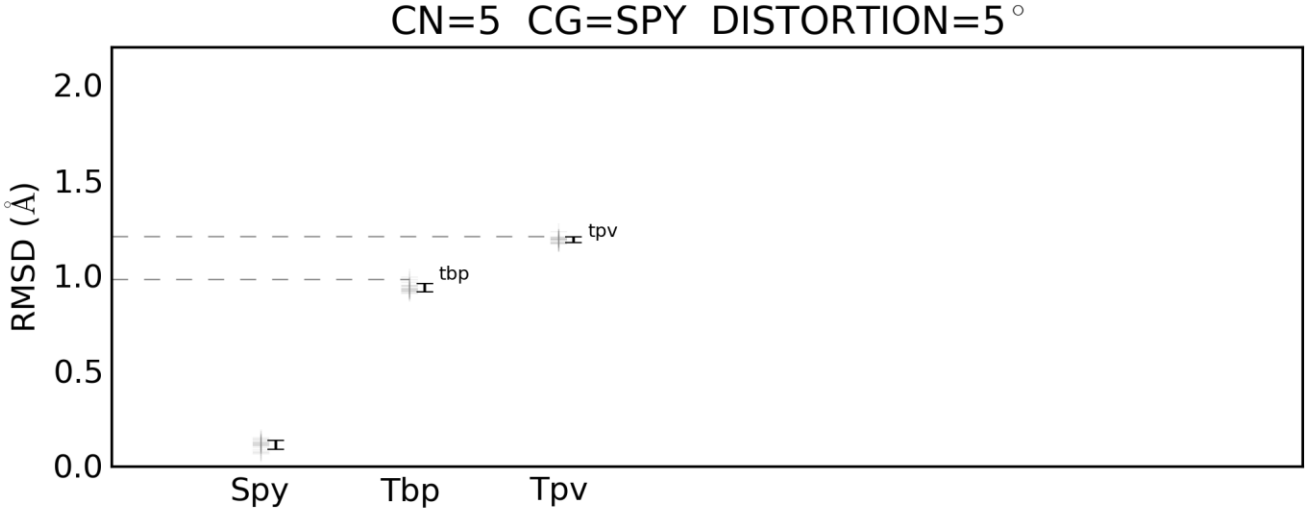

CN=4 CG=SPL DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
bva
tet
pyv
bvp
Spl
Bvp
Pyv
Tet
Bva

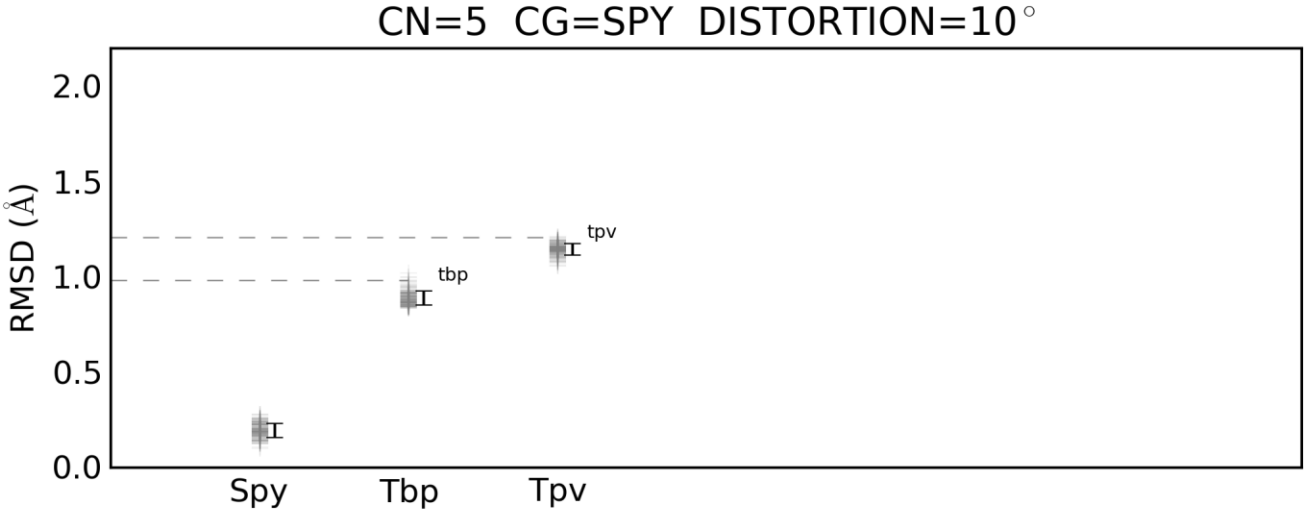

CN=5 CG=TBP DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
tpv
spy
Tbp
Spy
Tpv

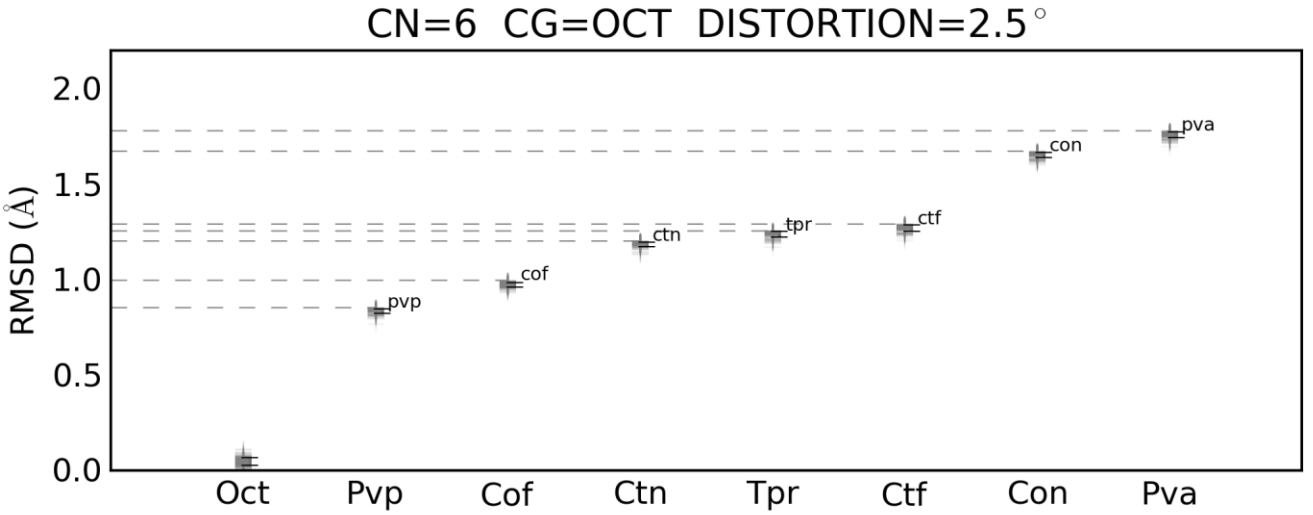

CN=5 CG=TBP DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
tpv
spy
Tbp
Spy
Tpv

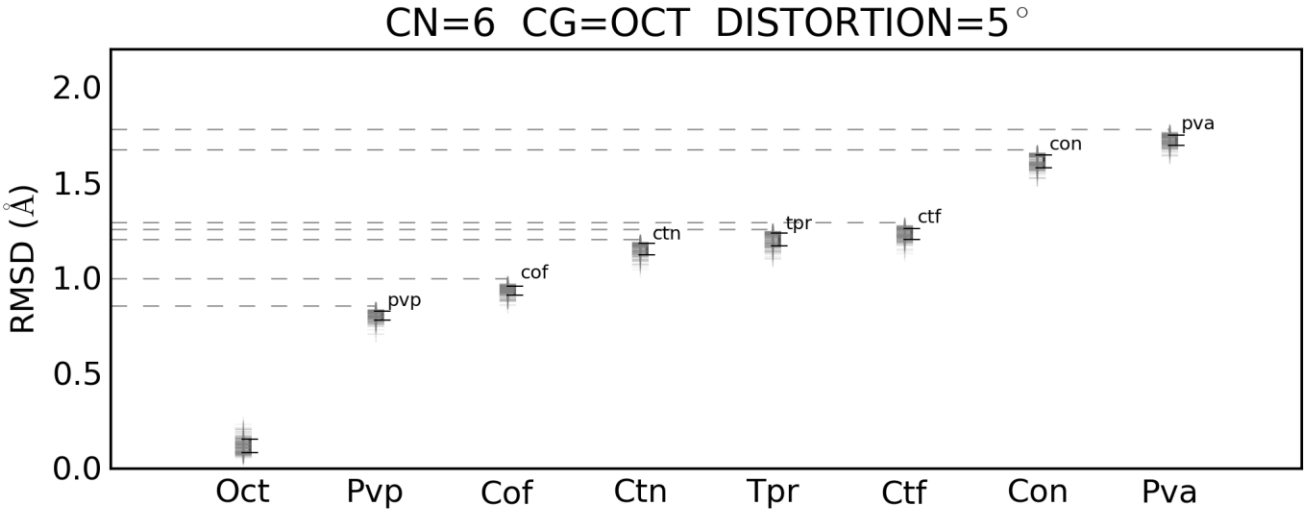

CN=5 CG=TBP DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
tpv
spy
Tbp
Spy
Tpv

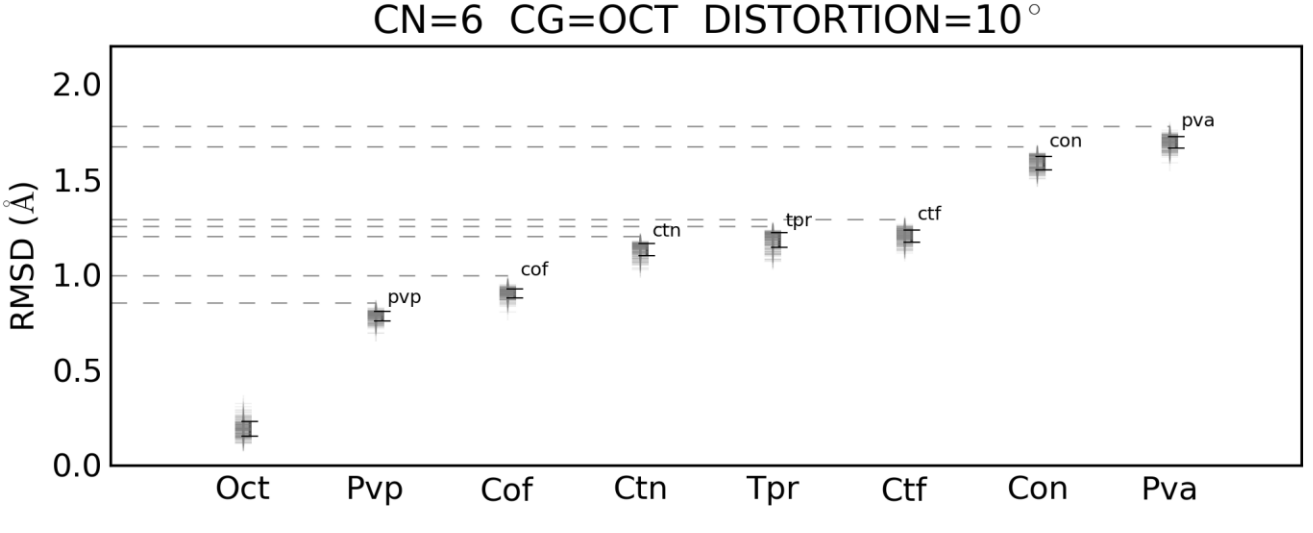

CN=5 CG=SPY DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
tpv
tbp
Spy
Tbp
Tpv

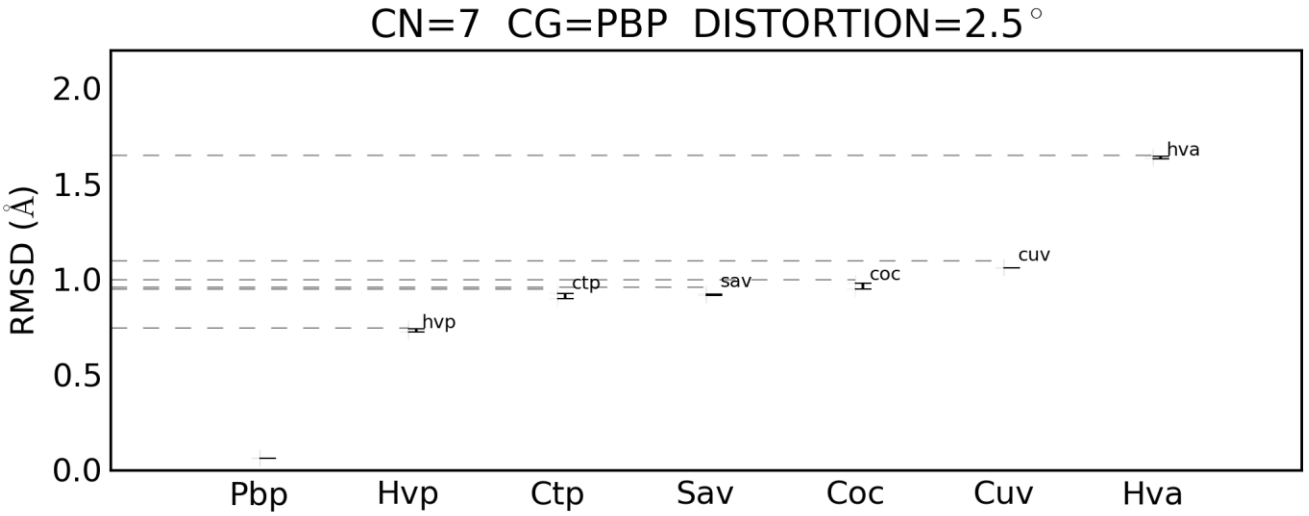

CN=5 CG=SPY DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
tpv
tbp
Spy
Tbp
Tpv

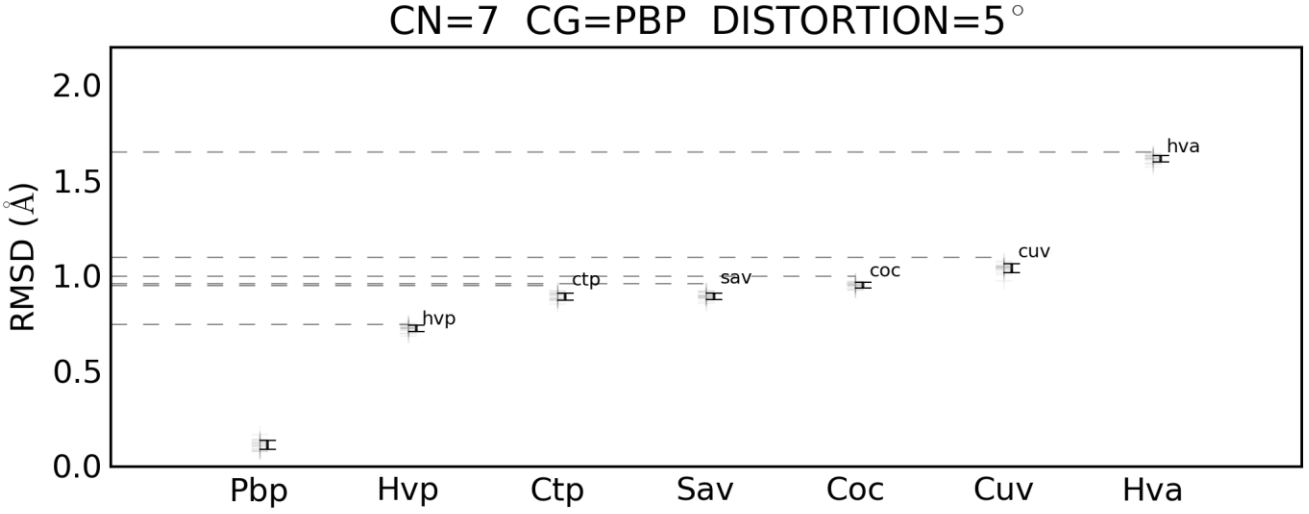

CN=5 CG=SPY DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
tpv
tbp
Spy
Tbp
Tpv

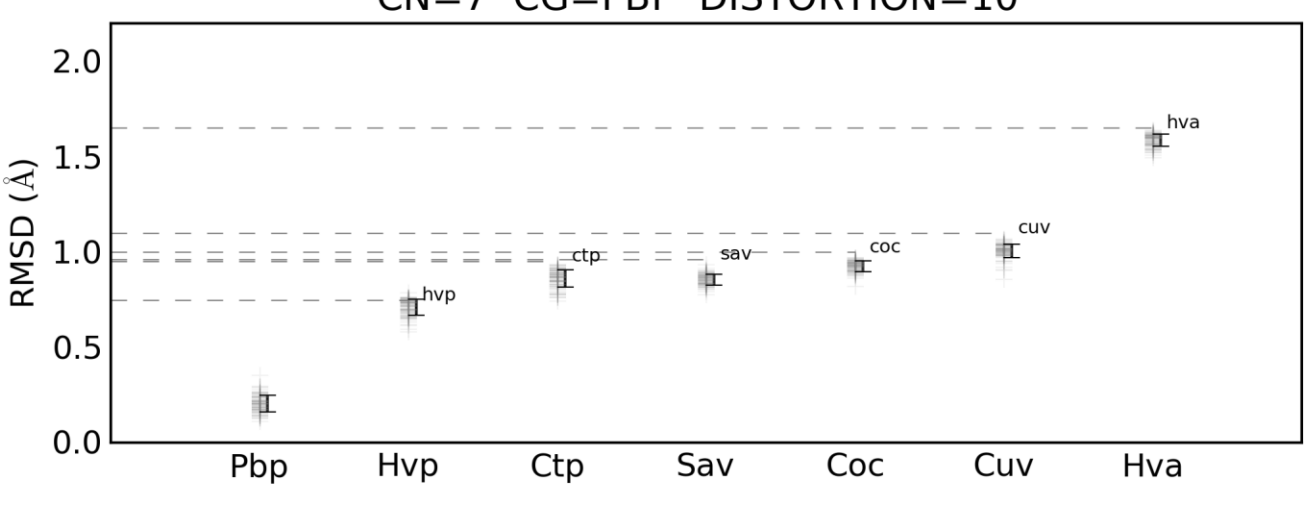

CN=6 CG=OCT DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
pva
con
tpr
ctf
ctn
cof
pvp
Oct
Pvp
Cof
Ctn
Tpr
Ctf
Con
Pva


CN=6 CG=OCT DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
pva
con
tpr
ctf
ctn
cof
pvp
Oct
Pvp
Cof
Ctn
Tpr
Ctf
Con
Pva


CN=6 CG=OCT DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
pva
con
tpr
ctf
ctn
cof
pvp
Oct
Pvp
Cof
Ctn
Tpr
Ctf
Con
Pva


CN=7 CG=PBP DISTORTION=2.5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
hva
cuv
ctp
sav
coc
hvp
Pbp
Hvp
Ctp
Sav
Coc
Cuv
Hva


CN=7 CG=PBP DISTORTION=5°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
hva
cuv
ctp
sav
coc
hvp
Pbp
Hvp
Ctp
Sav
Coc
Cuv
Hva


CN=7 CG=PBP DISTORTION=10°
RMSD (Å)
2.0
1.5
1.0
0.5
0.0
hva
cuv
ctp
sav
coc
hvp
Pbp
Hvp
Ctp
Sav
Coc
Cuv
Hva