The Elusive 5'-Deoxyadenosyl Radical in Coenzyme-B_{12}-Mediated Reactions

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SUPPORTING INFORMATION

(66 pages)

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Full Citation for Reference 54

D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, R. Luo, K.M. Merz, B. Wang, D.A. Pearlman, M. Crowley, S. Brozell, V. Tsui, H. Gohlke, J. Mongan, V. Hornak, G. Cui, P. Beroza, C. Schafmeister, J.W. Caldwell, W.S. Ross, and P.A. Kollman (2004), AMBER 8, University of California, San Francisco.

Text S1 Metadynamics (MTD)

To choose the parameters for the MTD simulations, we first determined a low-resolution free energy surface (FES) from constrained MD simulations in 2D. The simulation time required to fill this surface with potential hills, t_{tot}, was estimated[1] as:

$$t_{tot} = \frac{\overline{F}}{w}\tau_G\left(\frac{\overline{S}}{\delta s}\right)^d \qquad (1)$$

where F is an estimate of the depth of the FES in the region of interest (~ 80 kJ mol^{-1}), w is the depth of the hills (typically chosen so that $F/w > 20$, hence we used 3.7 kJ mol^{-1}), τ_G is the time between the addition of a new potential hill (~ 0.005 ps), S is the dimension of the system (~ 4 Å), δs the half-width of the potential hills (typically chosen so that $S/\delta s > 10$; here we used 0.3 Å), and d the dimensionality (i.e., 2). With these parameters, the FES can be explored in ~ 20 ps. The accuracy of the FES reconstruction can be estimated, using a formula given in reference 1, by:

$$\varepsilon = C(d)\sqrt{\frac{\overline{S}\delta s w}{D\tau_G\beta}}, \qquad (2)$$

where ε is the error, $C(d)$ is a constant equal to ~ 0.3 in the two-dimensional case, β is $1/kT$, and D is the average diffusion coefficient of the CVs that we measured to be ~ 4 Å^2/ps. For the chosen parameters the error was found to be ~ 2.8 kJ mol^{-1}.

Figures

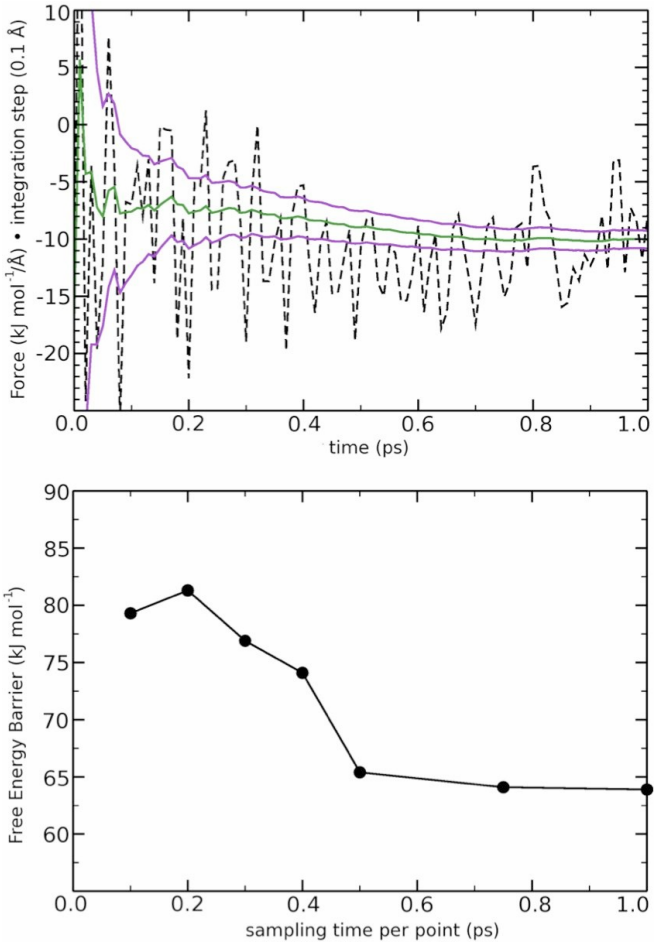

Figure S1 The top panel depicts the convergence of the mean constraint force for a chosen point in the PMF calculations for the Co–C homolysis step (Co–C5' = 2.54 Å). The green line is the running average, and the purple lines show the limits of a 97.5% confidence interval. After 1 ps (~10,000 MD steps) of sampling time, the work performed by the force can be calculated with a statistical precision of ~2 kJ mol^{-1}.

The bottom panel displays the free energy barrier computed for the Co–C5' cleavage as a function of the sampling time per point. It shows that a sampling time of 0.5 ps (or ~ 5,000 MD steps) per point is sufficient to converge the PMF to a precision of < 3 kJ mol^{-1}.

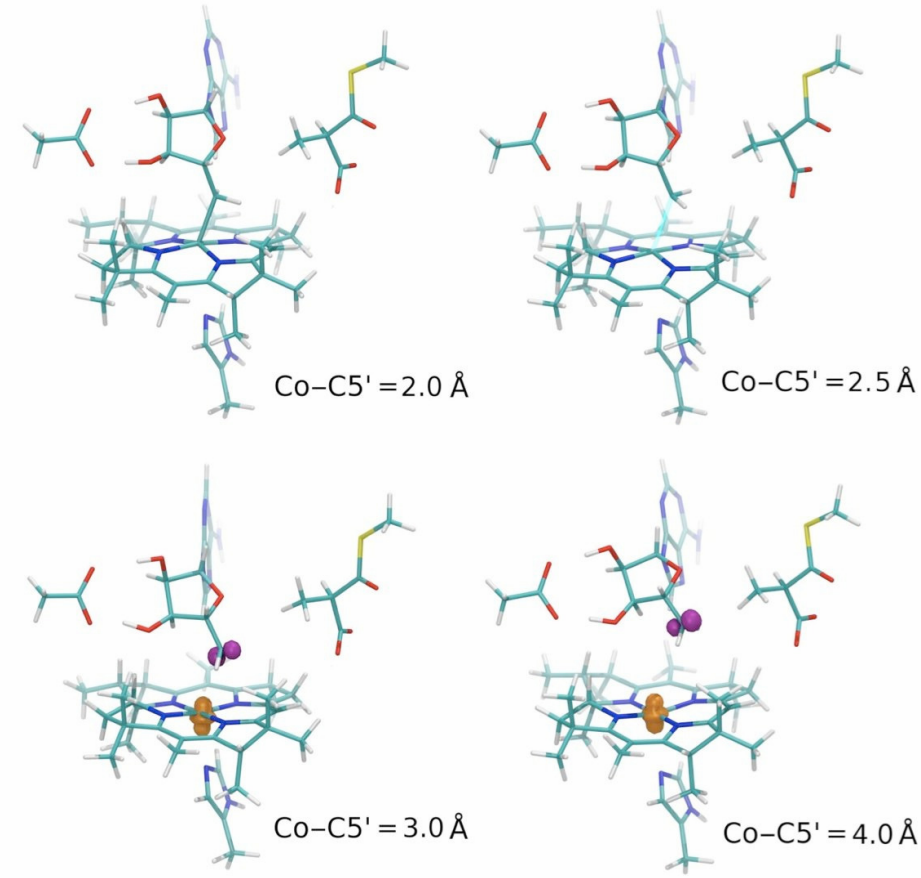

Figure S2 Spin density, computed as the difference between the α-electron and β-electron densities, as a function of the Co–C5' distance. The spin density is already visible at a Co–C5' distance of ~3 Å, and the radical center is fully formed at ~3.9 Å.

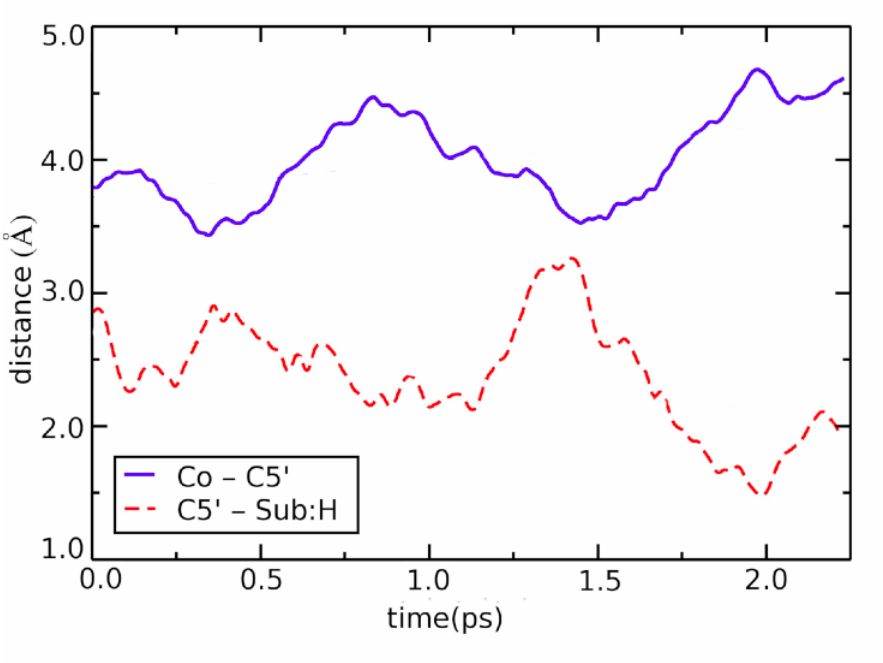

Figure S3 Unconstrained QM/MM trajectories of the dAdo• radical as it advances toward the substrate in the active site of MCM, showing the Co–C5' and C5'–Sub:H distances as a function of simulation time.

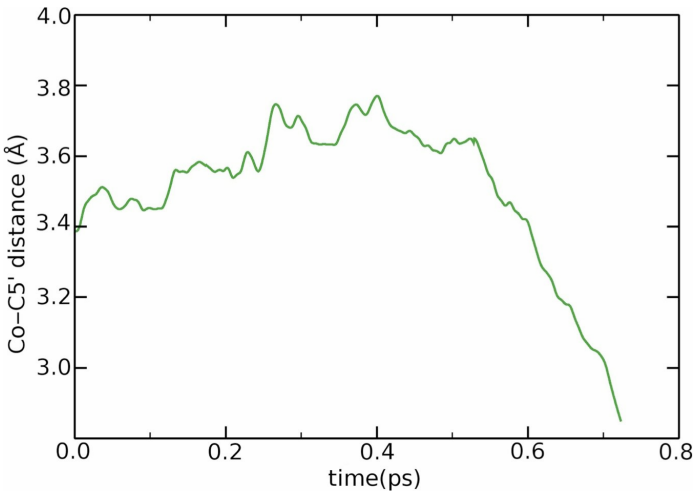

Figure S4 Unconstrained QM/MM trajectories of the dAdo• radical with an initial Co–C5' separation of 3.4 Å. In these simulations, the broken Co–C5' bond is re-formed in less than 1 ps.

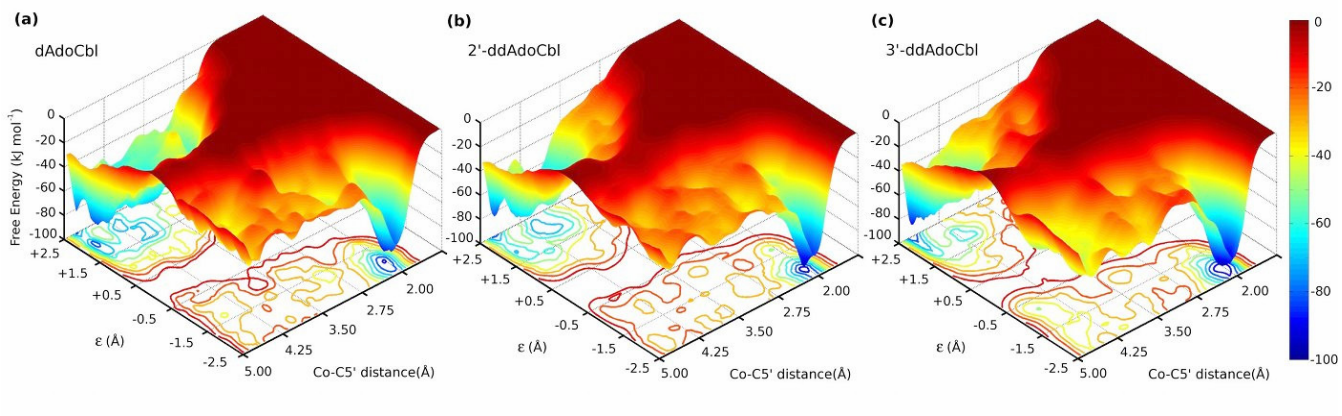

Figure S5 Free energy surfaces (kJ mol^{-1}) for the homolytic cleavage of the Co–C5' bond of dAdoCbl and H-atom abstraction by $dAdo^{\bullet}$ from substrate computed with metadynamics (MTD) for (a) dAdoCbl, (b) 2'-ddAdoCbl, and (c) 3'-ddAdoCbl. The results are consistent with the constrained MD calculations (Fig. 4b). Trajectories were run for only ~5 ps, as we were only interested in the location of the saddle points on these free energy surfaces.

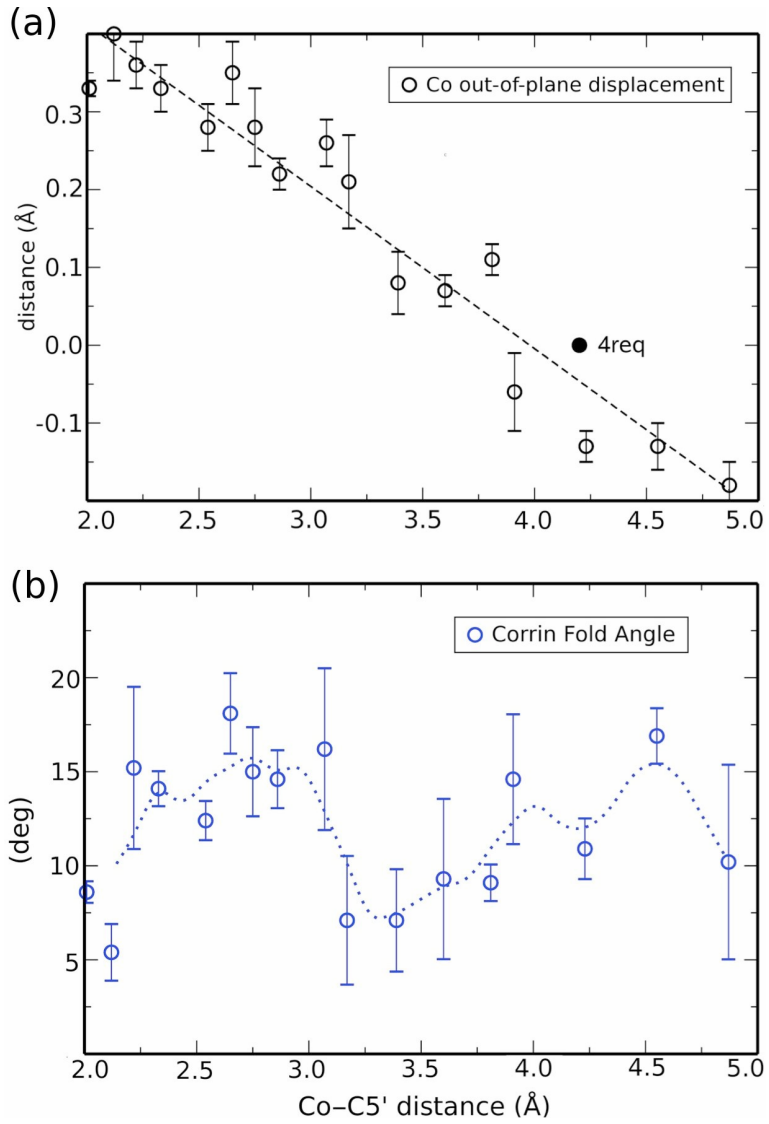

Figure S6 **(a)** Cobalt out-of-plane displacement. The position of the cobalt is measured with respect to a horizontal plane that minimizes all the distances to the corrin 23 heavy atoms in the mean-square sense. The atoms belonging to the corrin ring side chains were not included to determine the position of the plane. The position of the crystal structure (pdb code: 4REQ) is indicated on the figure. On the basis of the metal-to-ligand charge-transfer transitions in this system,[2] it was suggested that the Co 3d orbitals are stabilized by the enzyme through a reduction in charge donation from one or several of the cobalt ligands. The observation that the position of the Co ion relative to the corrin plane is correlated with the Co–C5' distance in the simulation is certainly consistent with this interpretation. (**b**) Average amplitude of vibrations, and average value of the fold angle in the simulations, as a function of the Co–C5' distance.

References

(1) Laio A.; Laio, Rodriguez-Fortea, A.; Gervasio, F. L.; Ceccarelli, M.; Parrinello, M. *J. Phys. Chem. B.* **2005**, *109*, 6714–6721.

(2) Brooks A. J.; Vlasie M.; Banerjee R.; Brunold T. C. *J. Am. Chem. Soc.* **2005**, *127*, 16522–16528.

Table S1. Parameters Used in the Classical MD Simulations

The classical parameters were derived for a state in which the Co-C bond of AdoCbl was broken. This required the derivation of additional parameters for cob(II)alamin (B12), 5'-deoxyadenosine (5AD), and methylmalonyl-CoA (MCA).

The valence and relevant van der Waals parameters for B12 were adapted from Marques and Brown,[3] whereas standard AMBER valence and van der Waals parameters were used in conjunction with the *parmchk* utility of the AMBER for 5AD and MCA. RESP charges for selected conformers of all three units were derived from the electrostatic potentials obtained at the IEFPCM-B3LYP/cc-pVTZ level of theory, using a value of 4.335 for the dielectric constant (consistent with ff03). For the Co atom of B12, the Douglas-Kroll correlation consistent polarized valence triple-ζ basis set (cc-pVTZ-DK) of Peterson and co-workers was used[4] in conjunction with a Merz-Kollman radius of 1.8 Å.

The actual RESP charges for B12 were derived from a two-conformer fit using base-on and base-off structures. The final unit used in the classical simulations was actually a juxtaposition of His610 and B12 (named H12 below) with an additional bond between the Co atom and N_{ax}. The parameters for the atoms later treated by DFT in the CPMD QM/MM calculations do not play a role in these latter calculations as the relevant interactions are treated quantum mechanically. Both the classical and the QM/MM descriptions provide good agreement with the relevant crystal structures.

(3) Marques, H. M.; Brown, K. L. *Inorg. Chem.* **1995**, *34*, 3733-3740.
(4) (a) Balabanov N. B.; Peterson K. A. *J. Chem. Phys.* **2005**, *123*, 064107-1–064107-15. (b) Balabanov N. B.; Peterson K. A. *J. Chem. Phys.* **2006**, *125*, 074110.

Cob(II)alamin – frcmod

```
# Parameter file for cob(II)alamin
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U2   12.01      0.616
U3   12.01      0.616
U4   12.01      0.616
UA   12.01      0.616
M1   12.01      0.616
DP   14.01      0.53
DQ   14.01      0.53
DR   14.01      0.53
DS   14.01      0.53
D1   14.01      0.53
D2   14.01      0.53
D3   14.01      0.53
DA   14.01      0.53
K1   16.00      0.434
```

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K3	16.00	0.465
K4	16.00	0.465
FO	30.97	1.538
KO	58.93	

BOND

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DQ	KO	158	1.860
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DA	KO	120	1.967
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U4	KO	150	1.965
CL	KO	121	2.300
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K3	FO	432	1.585
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K3	V	331	0.942
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U4	U4	DP	U3	1	10.0	130.0	3.
U4	U4	DP	KO	1	0.5	280.0	3.
U4	U4	U4	DP	1	0.5	275.0	3.
U4	U4	U4	DQ	1	2.0	250.0	3.
DP	U4	U4	DQ	1	10.0	265.0	2.
U4	U4	U4	U3	1	0.2	0.0	3.
U4	U4	U4	U4	1	0.2	0.0	3.
U1	KO	DS	U3	1	0.0	0.0	2.
U1	KO	DR	U3	1	0.0	0.0	2.
U1	KO	DQ	U3	1	0.0	0.0	2.
U1	KO	DP	U3	1	0.0	0.0	2.
U1	KO	DP	U4	1	0.0	0.0	2.
U1	KO	DQ	U4	1	0.0	0.0	2.
DP	KO	U1	N1	1	0.0	0.0	2.
DR	KO	U1	N1	1	0.0	0.0	2.
DS	KO	U1	N1	1	0.0	0.0	2.
DQ	KO	U1	N1	1	0.0	0.0	2.
DA	KO	U1	N1	1	0.0	0.0	2.
U1	KO	DA	UA	1	0.0	0.0	2.
U3	U3	M1	V	1	-0.2	0.0	3.
U3	U4	U4	U3	1	-2.5	0.0	3.
U3	DR	KO	DQ	1	0.0	0.0	3.
U3	DR	KO	U1	1	0.0	0.0	3.
U3	DR	U3	U3	1	6.0	170.0	2.
U3	DR	U3	U4	1	-0.3	0.0	1.
U3	DP	KO	U1	1	0.0	0.0	3.
U3	DP	KO	DA	1	0.0	0.0	3.
U4	U3	DP	U4	1	3.0	180.0	3.
U4	U3	U3	V	1	1.3	180.0	2.
V	U4	U3	DR	1	-0.2	0.0	1.
U3	U3	U3	DS	1	5.0	190.0	2.
DR	U3	U3	V	1	15.0	180.0	2.
V	U3	U3	DS	1	15.0	180.0	2.
U4	U4	U3	D2	1	-0.2	360.0	1.
U4	U4	U3	K1	1	-0.3	360.0	1.
V	U4	U4	U4	1	0.2	360.0	3.
U4	U3	U3	U3	1	5.0	350.0	1.
U4	U3	U3	M1	1	11.0	180.0	2.
V	U4	U4	V	1	0.2	360.0	3.
U3	U3	U4	U4	1	-0.3	360.0	1.
U3	U3	U4	V	1	-0.3	360.0	1.
DP	U3	U4	V	1	-0.2	360.0	1.
DP	U4	U4	V	1	0.3	360.0	3.
U4	DP	KO	DR	1	0.2	360.0	1.
U4	DP	KO	DS	1	0.0	0.0	3.
U4	DP	KO	U1	1	0.0	0.0	3.
U4	DP	KO	DA	1	0.0	0.0	3.

DS	U3	U4	U4	1	6.4	230.0	3.
KO	DA	UA	UA	1	10.0	180.0	2.
KO	DA	UA	V	1	10.0	180.0	2.
KO	DA	UA	DA	1	10.0	180.0	2.
U3	U4	U4	V	1	0.2	0.0	3.
V	U4	U3	DS	1	-0.2	0.0	1.
V	U4	U4	DQ	1	-0.1	180.0	2.
V	U4	DQ	U3	1	-0.4	180.0	2.
U4	U3	D2	V	1	1.3	180.0	2.
V	U4	U3	K1	1	-0.3	360.0	1.
D2	U3	U4	V	1	-0.3	360.0	1.
V	D2	U3	K1	1	1.3	180.0	2.
U4	U3	D2	U4	1	1.3	180.0	2.
K1	U3	D2	U4	1	1.3	180.0	2.
U3	D2	U4	U4	1	-0.3	360.0	1.
U3	D2	U4	V	1	-0.3	360.0	1.
V	D2	U4	U4	1	0.9	360.0	3.
D2	U4	U4	U4	1	0.2	0.0	3.
D2	U4	U4	K3	1	0.5	0.0	3.
D2	U4	U4	V	1	0.5	0.0	3.
U4	DA	UA	UA	1	10.0	180.0	2.
UA	DA	UA	UA	1	10.0	180.0	2.
DA	UA	UA	DA	1	10.0	180.0	2.
DA	UA	UA	UA	1	10.0	180.0	2.
DA	UA	UA	V	1	15.0	180.0	2.
UA	DA	U4	U4	1	6.0	-30.0	4.
DA	U4	U4	U4	1	0.1	180.0	2.
DA	U4	U4	K3	1	0.1	180.0	2.
DA	U4	U4	V	1	0.1	180.0	2.
UA	DA	U4	K3	1	0.0	0.0	3.
DA	U4	K3	U4	1	0.1	180.0	2.
U4	DA	U4	V	1	0.0	0.0	3.
UA	DA	UA	DA	1	10.0	180.0	2.
U4	DA	UA	DA	1	10.0	180.0	2.
UA	DA	UA	V	1	10.0	180.0	2.
U4	DA	UA	V	1	12.5	180.0	2.
V	D2	U4	V	1	0.2	0.0	3.
UA	DA	U4	V	1	0.0	0.0	3.
UA	UA	UA	UA	1	10.0	180.0	2.
V	UA	UA	UA	1	8.5	180.0	2.
UA	UA	UA	U4	1	9.9	180.0	2.
V	UA	UA	U4	1	12.5	180.0	2.
UA	UA	U4	V	1	-0.2	0.0	3.
U4	UA	UA	U4	1	1O.O	180.0	2.
K3	U4	U4	U4	1	0.2	0.0	3.
K3	U4	U4	K3	1	0.2	0.0	3.
V	U4	U4	K3	1	0.2	0.0	3.

U4	U4	K3	V	1	0.9	360.0	1.
U4	U4	K3	U4	1	0.7	360.0	3.
V	U4	K3	U4	1	0.7	360.0	3.
U4	U4	K3	FO	1	0.7	360.0	3.
V	U4	K3	V	1	0.2	360.0	3.
V	U4	K3	FO	1	0.7	360.0	3.
U4	K3	FO	K3	1	0.7	360.0	3.
U4	K3	FO	K1	1	0.4	360.0	3.
U2	KO	DP	U3	1	0.0	0.0	2.
U4	KO	DA	UA	1	0.0	0.0	2.
U4	DP	KO	U4	1	0.0	0.0	2.
U3	DR	KO	U4	1	0.0	0.0	2.
U3	DS	KO	U4	1	0.0	0.0	2.
U3	DQ	KO	U4	1	0.0	0.0	2.
U4	DQ	KO	U4	1	0.0	0.0	2.
U3	DP	KO	U4	1	0.0	0.0	2.
F	U4	KO	DP	1	0.0	0.0	2.
F	U4	KO	DQ	1	0.0	0.0	2.
F	U4	KO	DR	1	0.0	0.0	2.
F	U4	KO	DS	1	0.0	0.0	2.
F	U4	KO	DA	1	0.0	0.0	2.
U4	U4	KO	DP	1	0.0	0.0	2.
U4	U4	KO	DQ	1	0.0	0.0	2.
U4	U4	KO	DR	1	0.0	0.0	2.
U4	U4	KO	DS	1	0.0	0.0	2.
U4	U4	KO	DA	1	0.0	0.0	2.
U4	U4	U4	KO	1	0.5	230.0	2.
K3	U4	U4	KO	1	5.0	230.0	2.
KO	U4	U4	V	1	0.0	0.0	2.
U4	DA	UA	DP	1	10.0	180.0	2.
UA	DA	UA	DP	1	10.0	180.0	2.
DA	UA	DP	UA	1	10.0	180.0	2.
DA	UA	UA	D3	1	10.0	180.0	2.
DA	UA	UA	DP	1	10.0	180.0	2.
UA	UA	UA	D3	1	10.0	180.0	2.
V	UA	UA	D3	1	10.0	180.0	2.
UA	UA	D3	V	1	-0.2	0.0	3.
UA	UA	D3	LP	1	-0.2	0.0	3.
UA	UA	UA	DP	1	10.0	180.0	2.
V	UA	UA	DP	1	10.0	180.0	2.
UA	UA	DP	UA	1	10.0	180.0	2.
V	UA	UA	V	1	10.0	180.0	2.
DP	UA	D3	V	1	-0.2	0.0	3.
DP	UA	D3	LP	1	-0.2	0.0	3.
D3	UA	DP	UA	1	10.0	180.0	2.
UA	DP	UA	DP	1	10.0	180.0	2.
UA	DP	UA	V	1	10.0	180.0	2.

DA	UA	K3	V	1	-0.2	0.0	3.
DA	UA	D3	LP	1	-0.2	0.0	3.
D3	UA	DA	UA	1	10.0	180.0	2.
DP	U4	K3	U4	1	0.1	180.0	2.
DP	U4	U4	U4	1	0.1	180.0	2.
DP	U4	U4	K3	1	0.1	180.0	2.
DP	U4	U4	V	1	0.1	180.0	2.
UA	DP	U4	U4	1	6.0	-30.0	4.
UA	DP	U4	K3	1	0.0	0.0	3.
UA	DP	U4	V	1	0.0	0.0	3.
U4	DP	UA	DP	1	10.0	180.0	2.
U4	DP	UA	V	1	12.5	180.0	2.
U4	DP	UA	DA	1	10.0	180.0	2.
U4	DP	UA	UA	1	10.0	180.0	2.
V	DA	UA	DA	1	1.0	180.0	2.
V	DA	UA	V	1	1.0	180.0	2.
V	DA	UA	UA	1	1.0	180.0	2.
V	DA	UA	DP	1	1.0	180.0	2.
U1	KO	DP	U3	1	0.0	0.0	2.
U1	KO	DR	U3	1	0.0	0.0	2.
U1	KO	DS	U3	1	0.0	0.0	2.
U1	KO	DQ	U3	1	0.0	0.0	2.
U1	KO	DQ	U4	1	0.0	0.0	2.
U1	KO	DA	UA	1	0.0	0.0	2.
U1	KO	DP	U4	1	0.0	0.0	2.
DP	KO	DA	UW	1	1.0	180.0	2.
DQ	KO	DA	UW	1	1.0	180.0	2.
DR	KO	DA	UW	1	1.0	180.0	2.
DS	KO	DA	UW	1	1.0	180.0	2.
DP	KO	DA	UR	1	1.0	180.0	2.
DQ	KO	DA	UR	1	1.0	180.0	2.
DR	KO	DA	UR	1	1.0	180.0	2.
DS	KO	DA	UR	1	1.0	180.0	2.
U4	KO	DA	UW	1	0.0	0.0	2.
U4	KO	DA	UR	1	0.0	0.0	2.

IMPROPER

U3-U4-DP-KO	0.25	180.0	2.
U3-U4-DQ-KO	0.25	180.0	2.
U3-U3-DR-KO	0.25	180.0	2.
U3-U3-DS-KO	0.25	180.0	2.
U3-U4-U3-DP	0.25	180.0	2.
U3-U4-U3-DQ	0.25	180.0	2.
U3-U4-U3-DR	0.25	180.0	2.
U3-U3-U3-M1	0.25	180.0	2.
U3-U4-U3-DS	0.25	180.0	2.
UA-UA-DA-KO	0.25	180.0	2.

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UA-UA-DA-U4     1.25        180.0   2.
UA-UA-UA-DA     1.25        180.0   2.
UA-UA-UA-U4     1.25        180.0   2.
UA-UA-UA-V      1.25        180.0   2.
V-V-D2-U3       0.50  180.0   2.
U4-D2-U3-K1     0.50        180.0   2.
U4-V-D2-U3      0.25 180.0   2.
V-U3-U3-U3      0.25 180.0   2.

NONBON
V    1.4590      0.0150
U1   1.9080      0.0860
U2   1.9080      0.0860
U3   1.9080      0.0860
U4   1.9080      0.1094
M1   1.9080      0.1094
UA   1.9080      0.0860
DP   1.8240      0.1700
DQ   1.8240      0.1700
DR   1.8240      0.1700
DS   1.8240      0.1700
D1   1.8240      0.1700
D2   1.8240      0.1700
D3   1.8240      0.1700
DA   1.8240      0.700
K1   1.6612      0.2100
K2   1.6612      0.2100
K3   1.6612      0.2100
K4   1.6612      0.2100
FO   2.100       0.200
KO   1.9080      0.1094
```

Cob(II)alamin frcmod file with bond to lower axial ligand

```
#  Modification
MASS

BOND
NB      KO      120     2.47

ANGLE
CV      NB      KO      16.56   127.00
NB      KO      DP      156.00 92.00
NB      KO      DR      156.00 87.00
NB      KO      DQ      156.00  92.00
NB      KO      DS      156.00  87.00
CR      NB      KO      16.56   127.00
```

DIHE
CV NB KO DP 1 0.0 0.0 3.
CV NB KO DQ 1 0.0 0.0 3.
CV NB KO DR 1 0.0 0.0 3.
CV NB KO DS 1 0.0 0.0 3.
U4 DP KO NB 1 0.0 0.0 2.
U3 DP KO NB 1 0.0 0.0 2.
U3 DR KO NB 1 0.0 0.0 3.
U3 DS KO NB 1 0.0 0.0 2.
U3 DQ KO NB 1 0.0 0.0 3.
U4 DQ KO NB 1 0.0 0.0 2.
CR NB KO DP 1 0.0 0.0 3.
CR NB KO DQ 1 0.0 0.0 3.
CR NB KO DR 1 0.0 0.0 3.
CR NB KO DS 1 0.0 0.0 3.

IMPROPER
CV-CR-NB-KO 0.25 180.0 2.

NONBON

H12.lib file

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"H" "H" 0 1 131072 2 1 0.351000
"CA" "CT" 0 1 131072 3 6 0.119100
"HA" "H1" 0 1 131072 4 1 0.137800
"CB" "CT" 0 1 131072 5 6 -0.122600
"HB2" "HC" 0 1 131072 6 1 0.086300
"HB3" "HC" 0 1 131072 7 1 0.086300
"CG" "CC" 0 1 131072 8 6 -0.001500
"ND1" "NA" 0 1 131072 9 7 -0.205800
"HD1" "H" 0 1 131072 10 1 0.318300
"CE1" "CR" 0 1 131072 11 6 0.147300
"HE1" "H5" 0 1 131072 12 1 0.122200
"NE2" "NB" 0 1 131072 13 7 -0.601500
"CD2" "CV" 0 1 131072 14 6 0.043700
"HD2" "H4" 0 1 131072 15 1 0.110200
"CO" "KO" 0 1 131072 16 27 0.092500
"N21" "DP" 0 1 131072 17 7 0.104200
"C1" "U4" 0 1 131072 18 6 0.036200
"C20" "U4" 0 1 131072 19 6 -0.053400
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"H37" "V" 0 1 131072 21 1 0.044400

"H38" "V" 0 1 131072 22 1 0.044400
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"C25" "U4" 0 1 131072 24 6 -0.053700
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"H40" "V" 0 1 131072 26 1 0.029100
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"C27" "U3" 0 1 131072 29 6 0.474700
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"H42" "V" 0 1 131072 34 1 0.027300
"H43" "V" 0 1 131072 35 1 0.027300
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"C31" "U4" 0 1 131072 38 6 -0.285400
"C32" "U3" 0 1 131072 39 6 0.753400
"O34" "K1" 0 1 131072 40 8 -0.651100
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"C35" "M1" 0 1 131072 50 6 -0.003100
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"C50" "U3" 0 1 131072 99 6 0.395700
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"H71" "V" 0 1 131072 106 1 -0.007600
"H72" "V" 0 1 131072 107 1 -0.007600
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"C2R" "U4" 0 1 131072 140 6 0.106900
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"C1R" "U4" 0 1 131072 143 6 0.098400
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56.900000 48.323000 77.725000
57.126000 47.694000 78.483000
57.010000 48.058000 76.442000
57.372000 47.099000 76.070000
56.602000 49.160000 75.789000
56.242000 50.122000 76.678000
55.888000 51.089000 76.321000
57.048000 49.859000 73.462000
56.149000 48.488000 73.065000
54.645000 48.538000 73.048000
54.029000 48.371000 74.441000
54.285000 49.214000 75.047000
54.408000 47.478000 74.893000
52.965000 48.303000 74.353000
54.223000 47.374000 72.053000
52.762000 46.906000 72.209000
52.438000 47.078000 73.215000
52.696000 45.861000 71.988000
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54.427000 47.862000 70.594000
54.436000 46.720000 69.589000
55.512000 46.198000 69.273000
53.298000 46.274000 69.053000
52.474000 46.201000 69.616000
53.269000 46.012000 68.088000
55.376000 48.354000 70.541000
53.674000 48.559000 70.294000
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54.486000 44.028000 72.688000
53.586000 43.099000 73.454000
53.174000 42.114000 72.853000
53.220000 43.297000 74.711000
53.612000 44.054000 75.233000
52.549000 42.690000 75.138000
55.263000 43.455000 72.225000
53.914000 44.515000 71.926000
54.422000 45.590000 74.142000
55.999000 44.894000 73.922000
56.502000 47.272000 72.786000
57.838000 46.764000 72.867000
58.026000 45.281000 72.494000
57.848000 44.671000 73.354000
59.025000 45.124000 72.146000
57.335000 45.018000 71.720000
58.869000 47.583000 73.256000

58.710000 48.918000 73.608000
59.919000 49.459000 73.716000
61.041000 48.453000 73.716000
60.309000 47.122000 73.383000
60.410000 46.055000 74.465000
60.093000 46.465000 75.401000
61.423000 45.723000 74.546000
59.782000 45.227000 74.209000
60.847000 46.657000 71.990000
62.221000 45.967000 72.106000
63.218000 46.574000 72.546000
62.230000 44.718000 71.707000
61.991000 43.987000 72.347000
62.476000 44.497000 70.763000
60.996000 47.542000 71.408000
60.223000 46.003000 71.417000
61.619000 48.404000 75.187000
60.488000 48.741000 76.214000
60.903000 48.262000 77.579000
60.205000 47.445000 78.208000
62.035000 48.711000 78.156000
62.037000 48.965000 79.123000
62.873000 48.791000 77.617000
59.612000 48.197000 75.928000
60.223000 49.775000 76.297000
62.376000 49.156000 75.270000
62.051000 47.466000 75.468000
61.794000 48.707000 73.000000
60.147000 50.816000 73.834000
59.141000 51.731000 73.854000
57.812000 51.457000 73.774000
57.190000 52.691000 74.025000
58.127000 53.713000 74.584000
59.428000 53.225000 73.970000
59.579000 53.684000 72.480000
59.267000 54.702000 72.388000
58.971000 53.066000 71.853000
60.604000 53.596000 72.183000
60.698000 53.569000 74.777000
60.432000 53.765000 75.795000
61.164000 54.435000 74.357000
61.378000 52.743000 74.740000
58.173000 53.534000 76.182000
58.686000 54.859000 76.832000
58.264000 54.895000 78.314000
57.184000 54.272000 78.587000
58.959000 55.515000 79.207000

58.596000 55.635000 80.130000
59.863000 55.876000 78.975000
58.218000 55.681000 76.332000
59.747000 54.996000 76.783000
58.892000 52.771000 76.400000
57.259000 53.270000 76.671000
57.802000 54.699000 74.325000
55.871000 53.025000 73.818000
55.236000 54.369000 74.100000
55.014000 54.446000 75.144000
54.333000 54.462000 73.534000
55.913000 55.149000 73.821000
55.090000 51.953000 73.318000
55.505000 50.761000 73.032000
54.411000 49.972000 72.480000
53.111000 50.695000 72.754000
53.589000 52.120000 72.982000
53.989000 52.814000 71.616000
53.997000 53.876000 71.745000
53.277000 52.551000 70.862000
54.962000 52.483000 71.320000
52.668000 53.072000 73.699000
52.430000 52.599000 75.183000
51.961000 53.884000 75.868000
52.715000 54.540000 76.549000
50.699000 54.163000 75.634000
50.138000 55.290000 76.354000
49.841000 54.922000 77.810000
49.106000 56.055000 78.549000
49.062000 55.829000 79.594000
48.112000 56.147000 78.161000
49.633000 56.975000 78.405000
48.891000 53.828000 77.699000
49.138000 52.490000 78.544000
50.498000 52.392000 79.053000
48.502000 51.385000 77.761000
48.115000 52.709000 79.827000
46.750000 52.929000 79.606000
45.929000 51.653000 79.537000
46.765000 50.561000 79.241000
47.090000 49.999000 79.949000
45.341000 51.637000 80.970000
44.920000 52.980000 81.135000
46.098000 53.772000 80.751000
45.609000 55.150000 80.294000
44.802000 54.913000 79.076000
43.869000 54.952000 79.298000

46.455000 55.756000 80.041000
45.011000 55.665000 81.017000
46.701000 53.913000 81.623000
46.350000 51.283000 81.977000
46.149000 51.277000 83.361000
47.326000 50.894000 83.959000
48.262000 50.670000 82.939000
47.599000 50.929000 81.815000
48.045000 50.856000 80.845000
47.408000 50.802000 85.364000
46.261000 51.119000 86.090000
46.226000 51.053000 87.597000
45.496000 51.743000 87.967000
47.189000 51.310000 87.988000
45.968000 50.062000 87.905000
45.025000 51.518000 85.454000
43.821000 51.841000 86.243000
44.088000 51.946000 87.275000
43.103000 51.055000 86.138000
43.400000 52.760000 85.889000
44.972000 51.601000 84.038000
44.066000 51.898000 83.552000
48.291000 50.507000 85.892000
44.493000 51.002000 81.116000
45.156000 51.762000 78.804000
46.627000 53.460000 78.685000
50.704000 54.613000 78.362000
49.223000 55.577000 75.881000
50.807000 56.124000 76.343000
50.118000 53.651000 75.000000
53.362000 52.293000 75.609000
51.702000 51.830000 75.339000
51.722000 53.024000 73.201000
52.953000 54.102000 73.742000
52.085000 50.470000 71.615000
50.714000 51.047000 71.967000
50.173000 50.721000 73.015000
50.140000 51.873000 71.113000
49.526000 52.588000 71.446000
50.319000 51.783000 70.133000
51.981000 49.416000 71.454000
52.423000 50.922000 70.706000
52.698000 50.348000 73.678000
54.502000 49.898000 71.416000
61.141000 51.204000 73.915000
55.621000 45.917000 71.418000
56.824000 51.659000 81.112000

56.282000 50.980000 82.006000
!entry.H12.unit.residueconnect table int c1x int c2x int c3x int c4x int c5x int c6x
1 195 0 0 0 0
!entry.H12.unit.residues table str name int seq int childseq int startatomx str restype int imagingx
"H12" 1 197 1 "?" 0
!entry.H12.unit.residuesPdbSequenceNumber array int
0
!entry.H12.unit.solventcap array dbl
-1.000000
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!entry.H12.unit.velocities table dbl x dbl y dbl z
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5AD.lib

!!index array str
"5AD"
!entry.5AD.unit.atoms table str name str type int typex int resx int flags int seq int elmnt dbl chg
"C8" "CK" 0 1 131072 1 6 0.167900
"N7" "NB" 0 1 131072 2 7 -0.648300
"C5" "CB" 0 1 131072 3 6 0.127100
"C4" "CB" 0 1 131072 4 6 0.299800
"N9" "N*" 0 1 131072 5 7 0.003900
"N3" "NC" 0 1 131072 6 7 -0.656300
"C2" "CQ" 0 1 131072 7 6 0.513900
"N1" "NC" 0 1 131072 8 7 -0.727700
"C6" "CA" 0 1 131072 9 6 0.584000
"N6" "N2" 0 1 131072 10 7 -0.743200
"C1'" "CT" 0 1 131072 11 6 0.046900
"C2'" "CT" 0 1 131072 12 6 0.017700
"C3'" "CT" 0 1 131072 13 6 0.067800
"C4'" "CT" 0 1 131072 14 6 0.178700
"C5'" "CT" 0 1 131072 15 6 -0.260600
"O4'" "OS" 0 1 131072 16 8 -0.372700
"O3'" "OH" 0 1 131072 17 8 -0.651200
"O2'" "OH" 0 1 131072 18 8 -0.611700
"H1" "H5" 0 1 131072 19 1 0.152300

```
 "H2" "H5" 0 1 131072 20 1 0.028600
 "H3" "H" 0 1 131072 21 1 0.384300
 "H4" "H" 0 1 131072 22 1 0.384300
 "H5" "H1" 0 1 131072 23 1 0.109600
 "H6" "H2" 0 1 131072 24 1 0.196600
 "H7" "HC" 0 1 131072 25 1 0.079800
 "H8" "HC" 0 1 131072 26 1 0.079800
 "H9" "HC" 0 1 131072 27 1 0.079800
 "H10" "H1" 0 1 131072 28 1 0.142400
 "H11" "H1" 0 1 131072 29 1 0.092500
 "H12" "HO" 0 1 131072 30 1 0.468200
 "H13" "HO" 0 1 131072 31 1 0.465800
!entry.5AD.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl pchg
 "C8" "CK" 0 -1 0.0
 "N7" "NB" 0 -1 0.0
 "C5" "CB" 0 -1 0.0
 "C4" "CB" 0 -1 0.0
 "N9" "N*" 0 -1 0.0
 "N3" "NC" 0 -1 0.0
 "C2" "CQ" 0 -1 0.0
 "N1" "NC" 0 -1 0.0
 "C6" "CA" 0 -1 0.0
 "N6" "N2" 0 -1 0.0
 "C1'" "CT" 0 -1 0.0
 "C2'" "CT" 0 -1 0.0
 "C3'" "CT" 0 -1 0.0
 "C4'" "CT" 0 -1 0.0
 "C5'" "CT" 0 -1 0.0
 "O4'" "OS" 0 -1 0.0
 "O3'" "OH" 0 -1 0.0
 "O2'" "OH" 0 -1 0.0
 "H1" "H5" 0 -1 0.0
 "H2" "H5" 0 -1 0.0
 "H3" "H" 0 -1 0.0
 "H4" "H" 0 -1 0.0
 "H5" "H1" 0 -1 0.0
 "H6" "H2" 0 -1 0.0
 "H7" "HC" 0 -1 0.0
 "H8" "HC" 0 -1 0.0
 "H9" "HC" 0 -1 0.0
 "H10" "H1" 0 -1 0.0
 "H11" "H1" 0 -1 0.0
 "H12" "HO" 0 -1 0.0
 "H13" "HO" 0 -1 0.0
!entry.5AD.unit.boundbox array dbl
 -1.000000
 0.0
```

```
 0.0
 0.0
 0.0
!entry.5AD.unit.childsequence single int
 2
!entry.5AD.unit.connect array int
 0
 0
!entry.5AD.unit.connectivity table  int atom1x  int atom2x  int flags
 1 2 2
 1 5 1
 1 19 1
 2 3 1
 3 4 4
 3 9 4
 4 5 1
 4 6 4
 5 11 1
 6 7 4
 7 8 4
 7 20 1
 8 9 4
 9 10 1
 10 21 1
 10 22 1
 11 12 1
 11 16 1
 11 24 1
 12 13 1
 12 18 1
 12 28 1
 13 14 1
 13 17 1
 13 29 1
 14 15 1
 14 16 1
 14 23 1
 15 25 1
 15 26 1
 15 27 1
 17 30 1
 18 31 1
!entry.5AD.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
```

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 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
!entry.5AD.unit.name single str
 "5AD"
!entry.5AD.unit.positions table  dbl x  dbl y  dbl z
 -0.460000 -1.702000 -0.176000
 -1.711000 -1.936000 0.140000
 -2.333000 -0.701000 0.079000
 -1.423000 0.277000 -0.278000
 -0.239000 -0.379000 -0.435000
 -1.580000 1.597000 -0.451000
 -2.850000 1.830000 -0.207000
 -3.877000 1.057000 0.147000
 -3.646000 -0.263000 0.298000
 -4.664000 -1.028000 0.648000
 1.010000 0.244000 -0.866000
 1.635000 1.142000 0.208000
 2.642000 0.197000 0.855000
 3.112000 -0.622000 -0.346000
 3.692000 -1.987000 -0.041000
 1.929000 -0.774000 -1.117000
```

```
 3.652000 0.934000 1.485000
 2.291000 2.180000 -0.456000
 0.312000 -2.472000 -0.225000
 -3.122000 2.881000 -0.317000
 -4.522000 -2.080000 0.778000
 -5.630000 -0.595000 0.802000
 3.826000 -0.031000 -0.908000
 0.813000 0.814000 -1.761000
 3.917000 -2.518000 -0.959000
 4.618000 -1.885000 0.519000
 3.001000 -2.589000 0.540000
 0.899000 1.528000 0.900000
 2.132000 -0.444000 1.570000
 4.100000 0.418000 2.140000
 2.910000 2.591000 0.136000
!entry.5AD.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int c6x
 0 0 0 0 0 0
!entry.5AD.unit.residues table  str name  int seq  int childseq  int startatomx  str restype  int imagingx
 "5AD" 1 32 1 "?" 0
!entry.5AD.unit.residuesPdbSequenceNumber array int
 0
!entry.5AD.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.5AD.unit.velocities table  dbl x  dbl y  dbl z
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MCA frcmod file

```
#  Modifications to the AMBER95 force field for polyphosphates
MASS
CT 12.01
OS 16.00
P  30.97
H1 1.008
O2 16.00
O3 16.00
MG 24.31

BOND
CT-H1   340.000   1.090        from amber98
CT-OS   320.000   1.410
OS-P    230.000   1.61000
O2-P    525.000   1.480
O3-P    525.000   1.480        by analogy to O2
CT - c3 303.1    1.535        same as c3-c3 SOURCE1 14664    0.0043    0.0048

ANGLE
C -CT-OH   50.000     109.500    analogy with CT-CT-OH
H1-CT-OS   50.000     109.500    from amber
H1-CT-H1   35.000     109.500    from amber
CT-OS-P   100.000     120.500      "
O2-P -O2  140.000     119.900      "
O3-P -O3  140.000     119.90     by analogy to O2
OS-P -O2  100.000     108.230    from amber
OS-P -O3  100.000     108.23     by analogy to O2
OS-P -OS   45.000     102.600    from amber
P -OS-P    12.685     150.000    from amber
H1 - CT - c3 46.4      110.07    same as c3-c3-h1 SOURCE3  457   0.9255   1.1542
CT - c3 - h1 46.4      110.07    same as c3-c3-h1 SOURCE3  457   0.9255   1.1542
CT - c3 - ss 61.1      112.69    same as c3-c3-ss SOURCE3   24   2.0616   2.1842
N - CT - c3  65.9      112.13    same as c3-c3-n SOURCE3   31   1.0775   2.0700
```

```
DIHE
H1-CT-OS-P    3      0.105     000.000      3.000
O2-P -OS-CT   2      1.179     000.000     -3.000
O2-P -OS-CT   2     -0.812     000.000      2.000
CT-OS-P -OS   1     -1.560       0.0        1.0
O2-P -OS-P    2     -0.709       0.0        2.0
O3-P -OS-P    3     -0.255       0.0        3.0
P -OS-P -OS   1      0.897       0.00       1.0
X -CT-c3-X    9      1.400       0.000      3.000   same as X-c3-c3-X  JCC,7,(1986),230

NONBON
  H1         1.3870  0.0157          Veenstra et al JCC,8,(1992),963
  O2         1.6612  0.2100          OPLS
  O3         1.6612  0.2100          OPLS - by analogy to O2
  CT         1.9080  0.1094          Spellmeyer
  P         2.1000  0.2000          JCC,7,(1986),230;
  OS         1.6837  0.1700          OPLS ether
  MG         0.7870  0.8750          (adjusted from Aqvist)
```

MCA.lib file

```
!!index array str
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!entry.MCA.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq  int elmnt  dbl chg
 "C8" "CK" 0 1 131072 1 6 0.240400
 "H1" "H5" 0 1 131072 2 1 0.105100
 "N9" "N*" 0 1 131072 3 7 -0.040300
 "C4" "CB" 0 1 131072 4 6 0.455900
 "C5" "CB" 0 1 131072 5 6 0.067000
 "N7" "NB" 0 1 131072 6 7 -0.668900
 "N3" "NC" 0 1 131072 7 7 -0.711500
 "C2" "CQ" 0 1 131072 8 6 0.480000
 "H2" "H5" 0 1 131072 9 1 0.047500
 "N1" "NC" 0 1 131072 10 7 -0.773200
 "C6" "CA" 0 1 131072 11 6 0.616400
 "N6" "N2" 0 1 131072 12 7 -0.809000
 "H3" "H" 0 1 131072 13 1 0.373400
 "H4" "H" 0 1 131072 14 1 0.373400
 "C1'" "CT" 0 1 131072 15 6 0.094700
 "H5" "H2" 0 1 131072 16 1 0.141400
 "C2'" "CT" 0 1 131072 17 6 0.143600
 "H6" "H1" 0 1 131072 18 1 0.131300
 "O2'" "OH" 0 1 131072 19 8 -0.699300
 "H7" "HO" 0 1 131072 20 1 0.444100
 "C3'" "CT" 0 1 131072 21 6 0.086200
```

"H8" "H1" 0 1 131072 22 1 0.239000
"O3'" "OS" 0 1 131072 23 8 -0.491500
"C4'" "CT" 0 1 131072 24 6 0.069000
"H9" "H1" 0 1 131072 25 1 0.095000
"O4'" "OS" 0 1 131072 26 8 -0.448000
"C5'" "CT" 0 1 131072 27 6 0.002300
"H10" "H1" 0 1 131072 28 1 0.089000
"H11" "H1" 0 1 131072 29 1 0.089000
"O5'" "OS" 0 1 131072 30 8 -0.286600
"P1" "P" 0 1 131072 31 15 0.810300
"O11" "O2" 0 1 131072 32 8 -0.740700
"O12" "O2" 0 1 131072 33 8 -0.740700
"O6" "OS" 0 1 131072 34 8 -0.393000
"P2" "P" 0 1 131072 35 15 0.789000
"O21" "O2" 0 1 131072 36 8 -0.743800
"O22" "O2" 0 1 131072 37 8 -0.743800
"O7" "OS" 0 1 131072 38 8 -0.175000
"CPB" "CT" 0 1 131072 39 6 0.266700
"H12" "H1" 0 1 131072 40 1 -0.032000
"H13" "H1" 0 1 131072 41 1 -0.032000
"CPA" "CT" 0 1 131072 42 6 0.273900
"CP8" "CT" 0 1 131072 43 6 -0.397300
"H14" "HC" 0 1 131072 44 1 0.095500
"H15" "HC" 0 1 131072 45 1 0.095500
"H16" "HC" 0 1 131072 46 1 0.095500
"CP9" "CT" 0 1 131072 47 6 -0.397300
"H17" "HC" 0 1 131072 48 1 0.095500
"H18" "HC" 0 1 131072 49 1 0.095500
"H19" "HC" 0 1 131072 50 1 0.095500
"CP7" "CT" 0 1 131072 51 6 0.001800
"H20" "H1" 0 1 131072 52 1 0.084600
"OP3" "OH" 0 1 131072 53 8 -0.704100
"H21" "HO" 0 1 131072 54 1 0.459500
"CP6" "C" 0 1 131072 55 6 0.459400
"OP2" "O" 0 1 131072 56 8 -0.555800
"NP2" "N" 0 1 131072 57 7 -0.209400
"H22" "H" 0 1 131072 58 1 0.239300
"CP5" "CT" 0 1 131072 59 6 -0.169900
"H23" "H1" 0 1 131072 60 1 0.096200
"H24" "H1" 0 1 131072 61 1 0.096200
"CP4" "CT" 0 1 131072 62 6 0.054500
"H25" "HC" 0 1 131072 63 1 0.025100
"H26" "HC" 0 1 131072 64 1 0.025100
"CP3" "C" 0 1 131072 65 6 0.494800
"OP1" "O" 0 1 131072 66 8 -0.614600
"NP1" "N" 0 1 131072 67 7 -0.371000
"H27" "H" 0 1 131072 68 1 0.263900

"CP2" "CT" 0 1 131072 69 6 -0.063600
"H28" "H1" 0 1 131072 70 1 0.120700
"H29" "H1" 0 1 131072 71 1 0.120700
"P3" "P" 0 1 131072 72 15 1.159400
"O31" "O3" 0 1 131072 73 8 -0.928500
"O32" "O3" 0 1 131072 74 8 -0.928500
"O33" "O3" 0 1 131072 75 8 -0.928500
"CP1" "c3" 0 1 131072 76 6 0.077000
"H30" "h1" 0 1 131072 77 1 0.063100
"H31" "h1" 0 1 131072 78 1 0.063100
"S" "ss" 0 1 131072 79 16 -0.296000
"CS1" "c" 0 1 131072 80 6 0.392000
"OS1" "o" 0 1 131072 81 8 -0.442700
"CS2" "c3" 0 1 131072 82 6 0.150100
"H32" "hc" 0 1 131072 83 1 -0.020100
"CS4" "c" 0 1 131072 84 6 0.717900
"OS4" "o" 0 1 131072 85 8 -0.787800
"OS5" "o" 0 1 131072 86 8 -0.787800
"CS3" "c2" 0 1 131072 87 6 -0.357400
"H33" "ha" 0 1 131072 88 1 0.114300
"H34" "ha" 0 1 131072 89 1 0.114300
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"N9" "N*" 0 -1 0.0
"C4" "CB" 0 -1 0.0
"C5" "CB" 0 -1 0.0
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"N3" "NC" 0 -1 0.0
"C2" "CQ" 0 -1 0.0
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"N1" "NC" 0 -1 0.0
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"N6" "N2" 0 -1 0.0
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"H4" "H" 0 -1 0.0
"C1'" "CT" 0 -1 0.0
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"H9" "H1" 0 -1 0.0

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"C5'" "CT" 0 -1 0.0
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"O5'" "OS" 0 -1 0.0
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"O12" "O2" 0 -1 0.0
"O6" "OS" 0 -1 0.0
"P2" "P" 0 -1 0.0
"O21" "O2" 0 -1 0.0
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"O7" "OS" 0 -1 0.0
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"H13" "H1" 0 -1 0.0
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"H28" "H1" 0 -1 0.0
"H29" "H1" 0 -1 0.0
"P3" "P" 0 -1 0.0

"O31" "O3" 0 -1 0.0
"O32" "O3" 0 -1 0.0
"O33" "O3" 0 -1 0.0
"CP1" "c3" 0 -1 0.0
"H30" "h1" 0 -1 0.0
"H31" "h1" 0 -1 0.0
"S" "ss" 0 -1 0.0
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"CS3" "c2" 0 -1 0.0
"H33" "ha" 0 -1 0.0
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!entry.MCA.unit.childsequence single int
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!entry.MCA.unit.connect array int
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0
!entry.MCA.unit.connectivity table int atom1x int atom2x int flags
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1 6 2
3 4 1
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4 7 1
5 6 1
5 11 1
7 8 1
8 9 1
8 10 1
10 11 1
11 12 1
12 13 1
12 14 1
15 16 1
15 17 1

15 26 1
17 18 1
17 19 1
17 21 1
19 20 1
21 22 1
21 23 1
21 24 1
23 72 1
24 25 1
24 26 1
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31 32 2
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59 62 1

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65 66 2
65 67 4
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67 69 1
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72 74 2
72 75 2
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80 82 1
82 83 1
82 84 1
82 87 1
84 85 1
84 86 1
87 88 1
87 89 1
!entry.MCA.unit.hierarchy table str abovetype int abovex str belowtype int belowx
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"R" 1 "A" 8
"R" 1 "A" 9
"R" 1 "A" 10
"R" 1 "A" 11
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"R" 1 "A" 14
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!entry.MCA.unit.name single str
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7.322000 2.609000 -0.747000
6.378000 2.337000 -1.170000
8.245000 1.631000 -0.446000
9.295000 2.294000 0.130000
8.945000 3.633000 0.135000
7.688000 3.819000 -0.420000
10.436000 1.762000 0.591000
11.233000 2.720000 1.080000
12.175000 2.387000 1.479000
11.018000 4.039000 1.150000
9.863000 4.550000 0.677000
9.674000 5.876000 0.757000
10.185000 6.311000 1.494000
8.718000 6.158000 0.699000
8.092000 0.194000 -0.695000
9.080000 -0.236000 -0.715000
7.194000 -0.493000 0.339000
6.404000 0.175000 0.630000
7.943000 -0.847000 1.475000
7.932000 -1.814000 1.613000
6.632000 -1.659000 -0.459000

5.708000 -2.029000 -0.045000
7.598000 -2.711000 -0.547000
6.410000 -1.002000 -1.818000
6.601000 -1.713000 -2.611000
7.417000 0.054000 -1.929000
5.058000 -0.346000 -2.027000
5.027000 0.128000 -3.003000
4.260000 -1.065000 -1.942000
4.906000 0.731000 -1.044000
3.686000 0.555000 -0.025000
3.641000 1.705000 0.894000
3.761000 -0.819000 0.516000
2.444000 0.630000 -1.046000
1.386000 -0.510000 -1.518000
2.143000 -1.696000 -1.941000
0.406000 0.167000 -2.382000
0.736000 -0.860000 -0.108000
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0.244000 0.918000 0.773000
-0.967000 0.294000 -0.327000
-0.976000 -0.593000 1.672000
-1.427000 0.521000 2.595000
-0.557000 1.054000 2.962000
-2.062000 1.248000 2.088000
-1.981000 0.145000 3.450000
-0.028000 -1.471000 2.497000
-0.486000 -1.779000 3.441000
0.874000 -0.918000 2.729000
0.299000 -2.347000 1.950000
-2.142000 -1.439000 1.142000
-1.713000 -2.320000 0.678000
-3.003000 -1.845000 2.222000
-2.467000 -2.254000 2.886000
-3.112000 -0.907000 0.113000
-2.814000 -0.610000 -1.056000
-4.358000 -0.784000 0.524000
-4.556000 -1.011000 1.469000
-5.430000 -0.306000 -0.331000
-5.361000 0.768000 -0.462000
-5.310000 -0.737000 -1.313000
-6.782000 -0.672000 0.243000
-6.930000 -0.221000 1.222000
-6.845000 -1.750000 0.388000
-7.918000 -0.263000 -0.651000
-7.758000 0.166000 -1.826000
-9.144000 -0.349000 -0.188000
-9.369000 -0.732000 0.702000

```
 -10.200000 0.077000 -1.150000
 -9.852000 0.964000 -1.649000
 -10.380000 -0.693000 -1.888000
 7.552000 -4.071000 0.345000
 8.652000 -4.941000 -0.213000
 7.815000 -3.675000 1.764000
 6.168000 -4.638000 0.187000
 -11.385000 0.334000 -0.254000
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 -11.731000 -0.594000 0.182000
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 -15.347000 1.168000 -0.067000
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 -16.662000 0.294000 1.631000
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 -15.548000 2.591000 0.367000
 -15.101000 3.393000 -0.195000
 -15.918000 2.783000 1.356000
!entry.MCA.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int c6x
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!entry.MCA.unit.residues table  str name  int seq  int childseq  int startatomx  str restype  int imagingx
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!entry.MCA.unit.solventcap array dbl
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!entry.MCA.unit.velocities table  dbl x  dbl y  dbl z
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 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
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 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
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0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0