

Supporting information

Multiscale Quantum Refinement Approaches for Metalloproteins

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1. Protein structure preparation

In our quantum refinement applications, three protein structures taken from protein data bank (PDB) were used as the initial structures for the quantum refinement calculations. Before the quantum refinement calculations, protonated state of amino acid residues was checked. WHATCHECK^{1,2} was also used to check the quality of protein structures. Moreover, the rotamer of Asn, Gln, His residues and ligands were checked and determined on the basis of their local structures and hydrogen bond network. Furthermore, pKa values of amino acid residues were calculated by PROPKA 3.0 program at the pH of crystallization and hydrogen atoms were added by PDB2PQR 2.0.0 program.^{3,4}

A. Rusticyanin (RC)

Protonation state: HID39, HID57, HIE85, HID128, CYM138, HIE143; the other titratable residues remain the standard protonation state.

The flipped residues: His57, Gln139

B. Histone acetyltransferase

Protonation state: HID513, CYM540, CYM543, HID556, CYM563, HID579, HID586, HIE603, HIP627, HID743, HID755; ASP520 (anionic amide form); the other titratable residues remain the standard protonation state.

The flipped residues: His579, His603, His627, Gln717, Gln731, Asn734

C. Amyloid- β (20-34) with L-isoAsp23

Protonation state: PHE20 (with $-\text{NH}_3^+$ terminus), LEU34 (with $-\text{CO}_2^-$ terminus); the other titratable residues remain the standard protonation state.

2. Crystallography & NMR System (CNS) program preparation

In our quantum refinement calculations, CNS program calculated the crystallographic penalty function and its corresponding derivatives (E_{xray} & ∇E_{xray}) based on the given structure and X-ray structure factors. Therefore, the minimization step is set to zero in the CNS refinement input file. The topology and parameters of the ligands (such as the mutated residue ALY from lysine) for our CNS refinement calculations were downloaded from HIC-UP database⁵. Whereas, AceDRG and the CNS tool (cns_import_cif) were used to generate topology and parameter files for the unknown ligands (such as FCV in histone acetyltransferase).

3. Molecular mechanics force field parameters

Since ONIOM⁶ method implemented in Gaussian 16 package was used,⁷ amber force field parameters implemented were used for our MM calculations except for metal ions and unknown ligands.

For the metal ions, the published Lennard-Jones non-bonded model parameters for copper⁸, zinc⁹ and magnesium¹⁰ ions were used.

RESP (Restrained Electrostatic Potential)¹¹ charges calculated at HF/6-31G(d) level¹² and the similar AMBER atom types were applied for the mutated residue ALY and FCV ligand in the case of the histone acetyltransferase system.

For the magnesium binding site in the histone acetyltransferase, its amide should become deprotonated, due to a short distance between N_{ASP520} and magnesium ion (3.2 Å, Figure S1). The revised force field parameter (RESP atomic charges) for this binding site are given in Table S1, based on standard RESP re-fitting calculations (at HF/6-31(d) level) on a dipeptide model of ILE519 and ASP520.

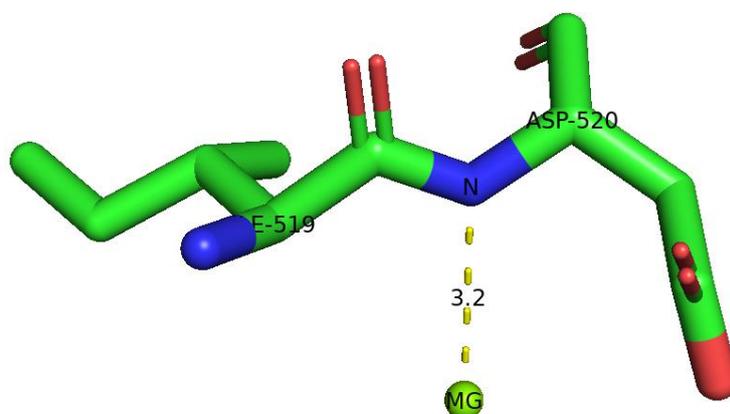


Figure S1. Local structure for the Mg binding site in the histone acetyltransferase

Table S1. RESP charges calculated at HF/6-31G(d) level and atom type in the histone acetyltransferase

ALY604:										
Atom type	N	H	CT	CT	CT	CT	CT	N	C	O
charge	-0.6081	0.3518	-0.0206	-0.5133	-0.0226	-0.1307	-0.3000	-0.5793	0.8771	-0.6258
Atom type	CT	HC	HC	HC	H	H1	H1	HC	HC	HC
charge	-0.5526	0.1531	0.1531	0.1531	0.3012	0.1854	0.1854	0.1013	0.1013	0.0858
Atom type	HC	HC	HC	H1	C	O				
charge	0.0858	0.1942	0.1942	0.1364	0.6616	-0.5675				
FCV801:										
Atom type	CA	HA	CA	HA	CA	HA	CA	H4	NC	CA
charge	-0.5492	0.1812	0.1657	0.1179	-0.4574	0.1792	0.3857	0.0690	-0.6868	0.7469
Atom type	CA	CA	CA	CA	HA	F	HA	CA	HA	CA
charge	-0.0215	-0.2847	0.3872	-0.2887	0.1919	-0.2275	0.1708	-0.2444	0.1746	-0.0696
Atom type	C	O	N	H	NT	H	SO	O	O	CA
charge	0.7728	-0.5062	-0.5160	0.3593	-0.5628	0.4651	0.9182	-0.5210	-0.5210	-0.0973
Atom type	CA	HA	CA	HA	CA	HA	CA	HA	CA	F
charge	-0.0200	0.1535	-0.2395	0.1789	-0.0465	0.1653	-0.3351	0.2012	0.4473	-0.2365
ILE519:										
Atom type	N	CT	C	O	CT	CT	CT	CT	H1	HC
charge	-0.5562	-0.4434	1.1689	-0.9351	0.3264	0.0677	-0.1574	-0.2506	0.2117	0.0255
Atom type	HC	HC	HC	HC	HC	H	HC	HC	HC	
charge	0.0255	-0.0476	-0.0201	-0.0201	0.0323	0.3057	0.0323	0.0255	0.0323	
ASP520:										
Atom type	N	CT	C	O	CT	C	O2	O2	H1	HC
charge	-1.0512	0.4485	0.5530	-0.6284	-0.3790	0.9318	-0.8712	-0.8712	-0.0426	0.0434
Atom type	HC									
charge	0.0434									

4. Definition of ONIOM layers and optimized regions

A. Rusticyanin (RC)

ONIOM layers were defined with the copper ion as the center atom:

High layer: all residues within a radius ~ 4.0 Å to the Cu center (117 atoms, including 17 link atoms):

PRO52, HIE85, SER86, CYM138, ILE140, HIE143, MET148, CU156

Medium layer for the ONIOM3 cases: all residues within a radius ~ 8.0 Å to the Cu center, (449 atoms, including 15 link atoms and the high-layer atoms):

ALA43, ALA44, VAL45, LEU46, PRO50, PHE51, SER53, PHE54, GLU55, THR75, PHE76, ILE77, ASN78, THR79, ASN80, LYS81, GLY82, PHE83, GLY84, PHE87, ASP88, GLY110, PHE111, SER112, TYR136, VAL137, GLN139, ILE140, PRO141, GLY142, HIE143, ALA144, ALA145, THR146, GLY147, MET148, PHE149,

HOH212, HOH221, HOH238, PHE51, PRO52, SER53, GLY84, HIE85, SER86, PHE87, VAL137, CYM138, GLN139, ILE140, HIE143, MET148, CU156

Optimized regions:

R1a: all atoms in the high layer (117 atoms):

PHE51, PRO52, SER53, GLY84, HIE85, SER86, PHE87, VAL137, CYM138, GLN139, ILE140, HIE143, MET148 and CU156

R2a: all residues within a radius of ~ 8.0 Å to the Cu center (396 atoms):

ALA44, VAL45, PHE51, PRO52, SER53, PHE54, PHE76, ASN78, ASN80, PHE83, GLY84, HIE85, SER86, PHE87, PHE111, SER112, VAL137, CYM138, GLN139, ILE140, PRO141, GLY142, HIE143, ALA144, THR146, MET148, CU156, HOH212, HOH221, HOH238

R3a: all atoms in the medium layer for the ONIOM3 cases (449 atoms):

ALA43, ALA44, VAL45, LEU46, PRO50, PHE51, PRO52, SER53, PHE54, GLU55, THR75, PHE76, ILE77, ASN78, THR79, ASN80, LYS81, GLY82, PHE83, GLY84, HIE85, SER86, PHE87, ASP88, GLY110, PHE111, SER112, TYR136, VAL137, CYM138, GLN139, ILE140, PRO141, GLY142, HIE143, ALA144, ALA145, THR146, GLY147, MET148, PHE149, CU156, HOH212, HOH221, HOH238

B. Histone acetyltransferase

ONIOM layers were defined with the zinc ion and FCV ligand as the center atoms:

High layer: FCV ligand and all residues within a ~ 4.0 Å to the Zn center (112 atoms, including 8 link atoms):

CYM540, CYM543, HID556 and CYM560, FCV801, ZN802

Medium layer: all residues within a radius ~ 3.0 Å to the FCV center and all residues within a radius ~ 5.0 Å to the Zn center (592 atoms, including 24 link atoms and the high-layer atoms):

GLU541, TYR542, LEU544, LYS545, TYR546, GLN561, TRP562, ARG563, LEU599, PHE600, LEU601, ASP602, CYS646, ILE647, MET648, ILE649, LEU650, TYR653, GLN654, ARG655, ARG656, GLY657, TYR658, GLY659, ARG660, PHE661, LEU662, ILE663, ALA664, LEU683, SER684, ASP685, LEU686, GLY687, LYS688, LEU689, SER690, TYR691, ARG692, SER693, TYR694, TRP695, HOH904, HOH938, HOH950, HOH951, HOH981, HOH983, HOH1008, HOH1022, LEU539, CYM540, GLU541, TYR542, CYM543, LEU544, PHE555, HID556, LEU557, GLN559, CYM560, GLN561, FCV801, ZN802

Optimized regions:

R1b: all atoms in the high layer (112 atoms):

LEU539, CYM540, GLU541, TYR542, CYM543, LEU544, PHE555, HID556, LEU557, GLN559, CYM560, GLN561, FCV801, ZN802

R2b: all residues within a radius of ~ 3.0 Å to the FCV center and all residues within a radius to ~ 5.0 Å around the Zn center (528 atoms):

LEU539, CYM540, GLU541, TYR542, CYM543, LEU544, LYS545, PHE555, HID556, LEU557, GLN559, CYM560, GLN561, TRP562, PHE600, LEU601, ILE647, MET648, ILE649, GLN654, ARG655, ARG656, GLY657, TYR658, GLY659, ARG660, ILE663, SER684, LEU686, GLY687, SER690, SER693, TYR694, FCV801, ZN802, HOH904, HOH938, HOH950, HOH951, HOH981, HOH983, HOH1008, HOH1022

R3b: all atoms in the medium layer for ONIOM3 cases (592 atoms).

LEU539, CYM540, GLU541, TYR542, CYM543, LEU544, LYS545, TYR546, PHE555, HID556, LEU557, GLN559, CYM560, GLN561, TRP562, ARG563, LEU599, PHE600, LEU601, ASP602, CYS646, ILE647, MET648, ILE649, LEU650, TYR653, GLN654, ARG655, ARG656, GLY657, TYR658, GLY659, ARG660, PHE661, LEU662, ILE663, ALA664, LEU683, SER684, ASP685, LEU686, GLY687, LYS688, LEU689, SER690, TYR691, ARG692, SER693, TYR694, TRP695, FCV801, ZN802, HOH904, HOH938, HOH950, HOH951, HOH981, HOH983, HOH1008, HOH1022

5. Energy expression for multicentered (MC) ONIOM schemes

ONIOM2:

$$E(\mathbf{1C-ONIOM2}) = E_{\text{Low}}(\text{Real}) + E_{\text{High}}(\text{Model}_1 + \text{Model}_2) - E_{\text{Low}}(\text{Model}_1 + \text{Model}_2)$$

$$E(\mathbf{2C-ONIOM2}) = E_{\text{Low}}(\text{Real}) + E_{\text{High}}(\text{Model}_1) - E_{\text{Low}}(\text{Model}_1) \\ + E_{\text{High}}(\text{Model}_2) - E_{\text{Low}}(\text{Model}_2)$$

ONIOM3:

$$E(\mathbf{1C-ONIOM3}) = E_{\text{Low}}(\text{Real}) + E_{\text{Medium}}(\text{intermediate}) - E_{\text{Low}}(\text{intermediate}) \\ + E_{\text{High}}(\text{Model}_1 + \text{Model}_2) - E_{\text{Medium}}(\text{Model}_1 + \text{Model}_2)$$

$$E(\mathbf{2C-ONIOM3}) = E_{\text{Low}}(\text{Real}) + E_{\text{Medium}}(\text{intermediate}) - E_{\text{Low}}(\text{intermediate}) \\ + E_{\text{High}}(\text{Model}_1) - E_{\text{Medium}}(\text{Model}_1) \\ + E_{\text{High}}(\text{Model}_2) - E_{\text{Medium}}(\text{Model}_2)$$

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7. Quantum refined results of Rusticyanin (RC)

Table S2. Our quantum refined key structural results for the copper binding site using different DFT functionals (B3LYP, B3LYP-D3, or M06L) and basis set (6-31G(d) or SDD for copper) in the ONIOM(QM/MM) scheme with the R1a-optimized region and ω_α value of 1.0. **M6** R2a results are used as reference for RMSD and MAD computations.

	M1	M2	M3	M4
Cu-N _{H85}	2.14	2.14	2.14	2.16
Cu-N _{H143}	1.96	1.96	1.96	1.99
Cu-S _{C138}	2.26	2.26	2.26	2.27
Cu-S _{M148}	2.87	2.88	2.86	2.88
RMSD (bonds)	0.02	0.02	0.02	0.00
MAD (bonds)	0.02	0.02	0.02	0.00
N _{H85} -Cu-N _{H143}	102.1	102.5	101.8	102.4
N _{H85} -Cu-S _{C138}	127.5	127.1	127.4	127.0
N _{H85} -Cu-S _{M148}	88.0	88.0	88.2	88.0
S _{M148} -Cu-S _{C138}	105.8	105.8	105.8	105.7
N _{H143} -Cu-S _{C138}	120.9	121.0	121.1	121.3
RMSD (angles)	0.5	0.4	0.5	0.3
MAD (angles)	0.5	0.3	0.5	0.2
R/R _{free}	0.162/0.221	0.162/0.22	0.163/0.221	0.162/0.221

Table S3. Our key structural results for the copper binding site from quantum refinement (ω_α value of 1.0) in the ONIOM(QM/MM) scheme with the R1a-optimized region in protein and optimization of R1a-optimized region in gas phase using B3LYP/6-31G(d) and B3LYP-D3/6-31G(d) (in parenthesis).

	Protein	Gas
Cu-N _{H85}	2.14(2.14)	1.99(2.00)
Cu-N _{H143}	1.96(1.96)	1.98(1.95)
Cu-S _{C138}	2.26(2.26)	2.23(2.22)
Cu-S _{M148}	2.87(2.88)	2.46(2.41)
N _{H85} -Cu-N _{H143}	102.1(102.5)	96.3(98.0)
N _{H85} -Cu-S _{C138}	127.5(127.1)	139.8(135.0)
N _{H85} -Cu-S _{M148}	88.0(88.0)	88.6(88.9)
S _{M148} -Cu-S _{C138}	105.8(105.8)	109.2(106.6)
N _{H143} -Cu-S _{C138}	120.9(121.0)	94.5(93.4)

Table S4. RSZD scores of residues around the Cu(II) binding site in the rusticyanin protein from quantum refinement approaches using B3LYP/6-31G(d) (**M1**) and B3LYP-D3/6-31G(d) (**M2**) with ω_α value of 1.0. RSZD scores of the FCV binding site were also given.

	X-ray	M1	M2
PRO52	1.3	1.3	1.4
HIE85	1.4	0.2	0.3
SER86	2.3	0.5	0.6
CYM138	1.0	0.8	0.8
ILE140	0.3	0.3	0.3
HIE143	1.5	0.4	0.4
MET148	0.8	0.9	0.8
Cu(II)	2.7	3.1	3.0
Sum	11.3	7.5	7.6

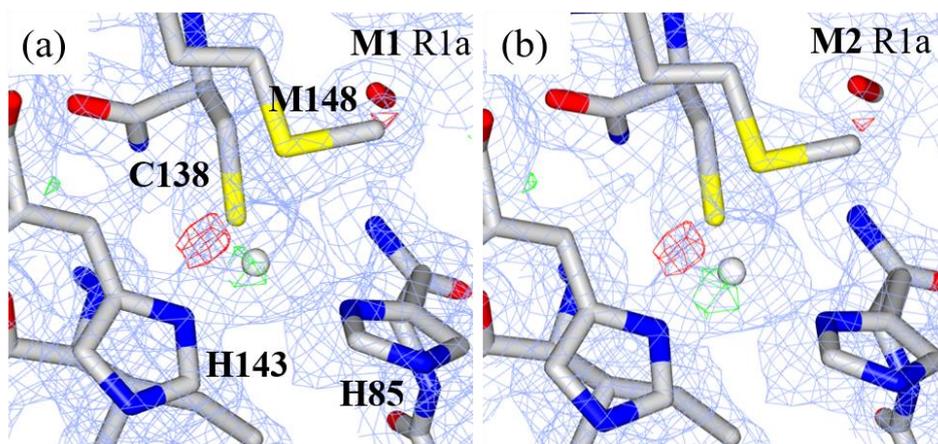


Figure S2. Structures for the Cu(II) binding site in the rusticyanin protein from various quantum refinement schemes with ω_α value of 1.0 using (a) **M1** (with the R1a-optimized region), (b) **M2** (with the R1a-optimized region), including the electron density map (2mFo-DFc maps, contoured at 1.0 σ (blue), mFo-DFc maps, contoured at +3.0 σ (green), and mFo-DFc maps, contoured at -3.0 σ (red)).

Table S5. Our quantum refined key structural results for the copper binding site using mechanical embedding (ONIOM-ME) and electrostatic embedding (ONIOM-EE; in parenthesis) ONIOM (**M1**) schemes with the R1a- and R2a-optimized regions and ω_α value of 1.0. **M6** R2a results are used as reference for RMSD and MAD computaions.

	M1 R1a	M1 R2a
Cu-N _{H85}	2.14(2.14)	2.14(2.14)
Cu-N _{H143}	1.96(1.98)	1.96(1.98)
Cu-S _{C138}	2.26(2.26)	2.26(2.25)
Cu-S _{M148}	2.87(2.88)	2.87(2.88)
RMSD (bonds)	0.02(0.02)	0.01(0.01)
MAD (bonds)	0.02(0.02)	0.01(0.01)
N _{H85} -Cu-N _{H143}	102.1(102.0)	102.6(102.4)
N _{H85} -Cu-S _{C138}	127.5(127.4)	126.8(126.9)
N _{H85} -Cu-S _{M148}	88.0(88.0)	88.2(88.2)
S _{M148} -Cu-S _{C138}	105.8(105.9)	105.6(105.7)
N _{H143} -Cu-S _{C138}	120.9(121.0)	121.4(121.4)
RMSD (angles)	0.5(0.5)	0.2(0.2)
MAD (angles)	0.5(0.5)	0.1(0.1)
R/R _{free}	0.162/0.221 (0.162/0.221)	0.162/0.216 (0.162/0.216)

Table S6. Our quantum refined key structural results for the copper binding site using different multiscale schemes with different optimized regions (R1a, R2a or R3a). Different values of the weighting factor (1.0 and 0.606 (in parenthesis)) are used. The key structural results from the X-ray crystal structure were also given. **M6** R2a results are used as reference for RMSD and MAD computaions.

	M1 R1a	M1 R2a	M5 R1a	M5 R3a	M6 R1a	M6 R2a	X-ray
Cu-N _{H85}	2.14(2.11)	2.14(2.11)	2.17(2.14)	2.16(2.14)	2.17(2.14)	2.16(2.14)	2.04
Cu-N _{H143}	1.96(1.97)	1.98(1.98)	1.98(1.99)	2.00(1.99)	2.00(1.98)	1.99(1.98)	1.89
Cu-S _{C138}	2.26(2.25)	2.26(2.25)	2.26(2.25)	2.25(2.25)	2.26(2.25)	2.26(2.25)	2.26
Cu-S _{M148}	2.87(2.87)	2.88(2.88)	2.87(2.88)	2.88(2.88)	2.87(2.87)	2.88(2.88)	2.88
RMSD (bonds)	0.02(0.02)	0.01(0.01)	0.01(0.00)	0.00(0.00)	0.01(0.00)	0.00(0.00)	0.08(0.07)
MAD (bonds)	0.02(0.01)	0.01(0.01)	0.01(0.00)	0.00(0.00)	0.01(0.00)	0.00(0.00)	0.06(0.05)
N _{H85} -Cu-N _{H143}	102.1(102.1)	102.6(102.8)	101.8(102.1)	102.0(102.3)	102.1(102.1)	102.5(102.3)	105.4
N _{H85} -Cu-S _{C138}	127.5(127.5)	126.8(126.6)	127.4(127.1)	127.2(126.9)	127.2(127.0)	126.7(126.9)	127.9
N _{H85} -Cu-S _{M148}	88.0(87.6)	88.2(88.2)	88.0(87.8)	88.2(88.0)	87.9(87.9)	88.5(88.2)	85.3
S _{M148} -Cu-S _{C138}	105.8(105.7)	105.6(105.5)	105.8(105.7)	105.4(105.5)	105.7(105.8)	105.6(105.6)	105.5
N _{H143} -Cu-S _{C138}	120.9(121.2)	121.4(121.5)	121.3(121.6)	121.8(121.9)	121.3(121.5)	121.5(121.6)	119.1
RMSD (angles)	0.5(0.4)	0.2(0.3)	0.5(0.2)	0.3(0.2)	0.4(0.2)	0.0(0.0)	2.3(2.3)
MAD (angles)	0.5(0.4)	0.1(0.2)	0.4(0.2)	0.3(0.1)	0.4(0.2)	0.0(0.0)	2.0(1.9)
R	0.162(0.163)	0.162(0.162)	0.163(0.163)	0.162(0.162)	0.162(0.163)	0.161(0.162)	0.163
R _{free}	0.221(0.221)	0.216(0.216)	0.221(0.221)	0.215(0.215)	0.220(0.221)	0.216(0.217)	0.223

Table S7. Strain energy (ΔE , kcal/mol) at B3LYP/6-31G(d) level for the R1a-optimized active-site region in the copper protein determined by various quantum refinement schemes. Different values of the weighting factor (1.0 and 0.606 (values given in parenthesis)) are used

	ΔE
X-ray	258.0
M1 R1a	88.74(82.05)
M1 R2a	89.85(80.44)
M5 R1a	93.15(82.88)
M5 R3a	91.57(82.31)
M6 R1a	92.85(82.64)
M6 R2a	89.92(82.53)

Table S8. Atomic displacements of copper binding site using different multiscale schemes with different optimized regions (R1a, R2a or R3a). Different values of the weighting factor 1.0 and 0.606 (values given in parenthesis) are used

	M1 R1a	M1 R2a	M5 R1a	M5 R3a	M6 R1a	M6 R2a
HIE85						
N	0.07(0.05)	0.10(0.09)	0.07(0.03)	0.11(0.09)	0.06(0.03)	0.09(0.08)
CA	0.05(0.04)	0.07(0.08)	0.04(0.02)	0.07(0.06)	0.03(0.03)	0.06(0.06)
C	0.05(0.07)	0.09(0.11)	0.05(0.07)	0.07(0.09)	0.05(0.08)	0.09(0.10)
O	0.07(0.06)	0.09(0.09)	0.08(0.08)	0.09(0.09)	0.08(0.09)	0.10(0.10)
CB	0.10(0.09)	0.11(0.09)	0.13(0.11)	0.12(0.11)	0.13(0.12)	0.12(0.11)
CG	0.11(0.08)	0.12(0.10)	0.13(0.11)	0.13(0.11)	0.13(0.11)	0.14(0.11)
ND1	0.08(0.07)	0.08(0.07)	0.11(0.09)	0.10(0.08)	0.11(0.10)	0.10(0.09)
CD2	0.09(0.09)	0.09(0.07)	0.12(0.10)	0.11(0.09)	0.12(0.11)	0.10(0.10)
CE1	0.06(0.06)	0.09(0.09)	0.05(0.05)	0.08(0.08)	0.05(0.05)	0.07(0.06)
NE2	0.05(0.06)	0.07(0.08)	0.05(0.06)	0.07(0.08)	0.05(0.05)	0.07(0.06)
CYM138						
N	0.13(0.15)	0.15(0.14)	0.13(0.13)	0.13(0.13)	0.13(0.14)	0.14(0.14)
CA	0.04(0.04)	0.03(0.04)	0.04(0.03)	0.05(0.03)	0.04(0.03)	0.03(0.03)
C	0.07(0.06)	0.09(0.08)	0.09(0.07)	0.10(0.07)	0.10(0.06)	0.09(0.06)
O	0.02(0.02)	0.02(0.02)	0.02(0.01)	0.01(0.01)	0.02(0.01)	0.01(0.01)
CB	0.06(0.07)	0.05(0.06)	0.05(0.05)	0.04(0.04)	0.04(0.05)	0.03(0.04)
SG	0.08(0.08)	0.08(0.07)	0.09(0.10)	0.08(0.09)	0.09(0.10)	0.08(0.08)
HIE143						
N	0.00(0.00)	0.02(0.02)	0.00(0.00)	0.03(0.04)	0.00(0.00)	0.04(0.04)
CA	0.04(0.05)	0.06(0.05)	0.06(0.06)	0.07(0.08)	0.06(0.06)	0.08(0.07)
C	0.04(0.05)	0.07(0.08)	0.04(0.05)	0.06(0.06)	0.05(0.05)	0.06(0.05)
O	0.05(0.06)	0.10(0.10)	0.06(0.06)	0.10(0.10)	0.06(0.06)	0.10(0.09)
CB	0.08(0.08)	0.11(0.11)	0.11(0.11)	0.13(0.11)	0.13(0.10)	0.12(0.10)
CG	0.09(0.11)	0.12(0.12)	0.12(0.13)	0.13(0.13)	0.13(0.12)	0.12(0.12)
ND1	0.14(0.15)	0.15(0.13)	0.17(0.17)	0.17(0.15)	0.19(0.16)	0.16(0.14)
CD2	0.11(0.12)	0.13(0.11)	0.15(0.15)	0.15(0.13)	0.17(0.14)	0.14(0.12)
CE1	0.00(0.00)	0.03(0.03)	0.00(0.00)	0.05(0.04)	0.00(0.00)	0.04(0.04)
NE2	0.00(0.00)	0.06(0.05)	0.00(0.00)	0.05(0.04)	0.00(0.00)	0.05(0.04)
MET148						
N	0.00(0.00)	0.03(0.03)	0.00(0.00)	0.03(0.04)	0.00(0.00)	0.03(0.04)
CA	0.04(0.05)	0.04(0.04)	0.04(0.05)	0.03(0.02)	0.04(0.05)	0.03(0.02)
C	0.08(0.09)	0.07(0.07)	0.11(0.13)	0.06(0.06)	0.12(0.12)	0.09(0.06)
O	0.06(0.08)	0.09(0.09)	0.07(0.07)	0.09(0.09)	0.08(0.07)	0.09(0.09)
CB	0.03(0.03)	0.04(0.03)	0.04(0.03)	0.04(0.04)	0.04(0.03)	0.04(0.04)
CG	0.06(0.08)	0.08(0.08)	0.07(0.07)	0.08(0.07)	0.08(0.07)	0.07(0.07)
SD	0.00(0.00)	0.03(0.03)	0.00(0.00)	0.05(0.04)	0.00(0.00)	0.05(0.05)
CE	0.00(0.00)	0.05(0.04)	0.00(0.00)	0.04(0.04)	0.00(0.00)	0.06(0.06)
Cu	0.02(0.01)	0.02(0.01)	0.02(0.02)	0.02(0.02)	0.02(0.02)	0.02(0.02)

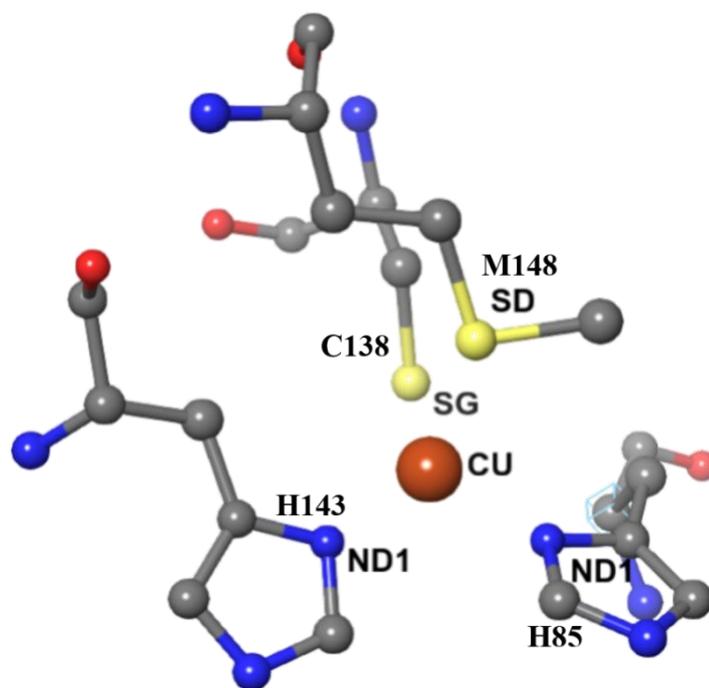


Figure S3. Local structure for the Cu binding site in X-ray crystal structure of the rusticyanin (RC).

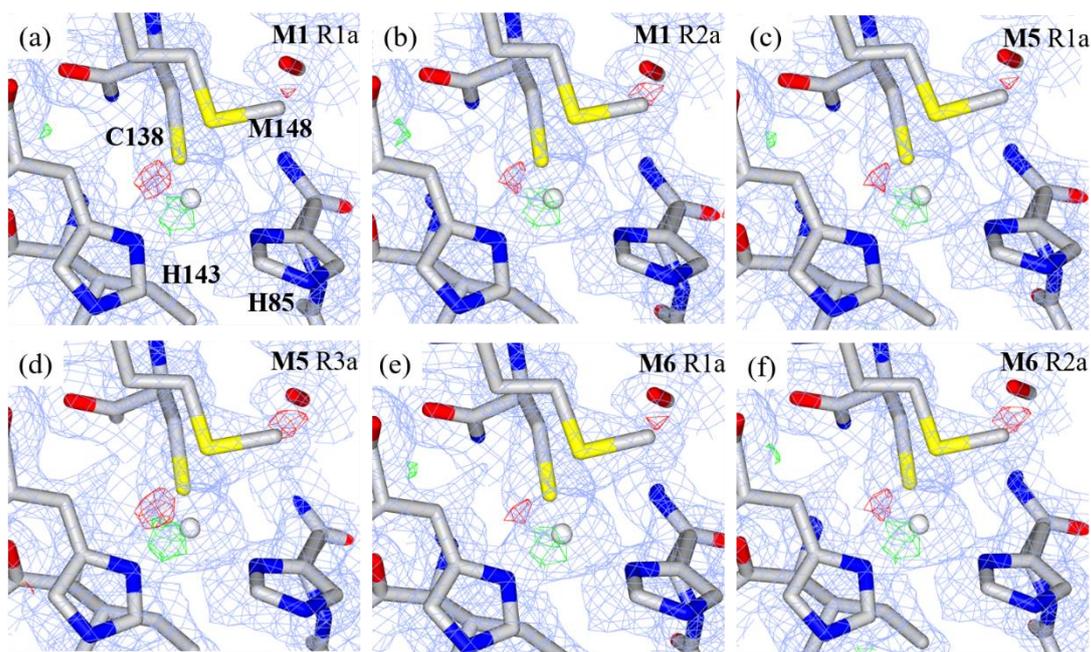


Figure S4. Structures for the Cu binding site in the rusticyanin (RC) protein from various quantum refinement schemes with ω_α value of 0.606 using (a) **M1** (with the R1a-optimized region), (b) **M1** (with the R2a-optimized region), (c) **M5** (with the R1a-optimized region), (d) **M5** (with the R3a-optimized region), (e) **M6** (with the R1a-optimized region) and (f) **M6** (with the R2a-optimized region), including the electron density map (2mFo-DFc maps, contoured at 1.0 σ (blue), mFo-DFc maps, contoured at +3.0 σ (green), and mFo-DFc maps, contoured at -3.0 σ (red)).

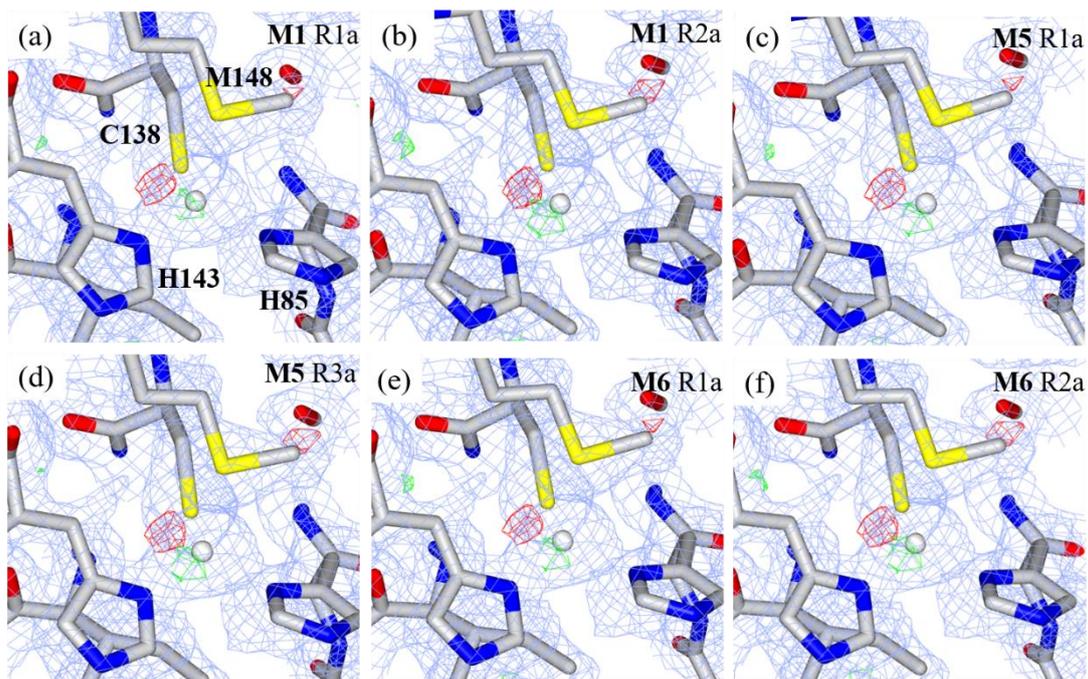


Figure S5. Structures for the Cu binding site in the rusticyanin (RC) protein from various quantum refinement schemes with ω_α value of 1.0 using (a) **M1** (with the R1a-optimized region), (b) **M1** (with the R2a-optimized region), (c) **M5** (with the R1a-optimized region), (d) **M5** (with the R3a-optimized region), (e) **M6** (with the R1a-optimized region) and (f) **M6** (with the R2a-optimized region), including the electron density map (2mFo-DFc maps, contoured at 1.0 σ (blue), mFo-DFc maps, contoured at +3.0 σ (green), and mFo-DFc maps, contoured at -3.0 σ (red)).

8. Quantum refined results of histone acetyltransferase

Table S9. Our key structural results for the zinc binding site from quantum refinement (ω_α value of 1.0) in the ONIOM(QM/MM) scheme with the R1b-optimized region in protein and optimization of R1b-optimized region in gas phase using B3LYP/6-31G(d) and B3LYP-D3/6-31G(d) (in parenthesis).

	Protein	Gas
Zn-S _{C540}	2.39(2.41)	2.33(2.33)
Zn-S _{C543}	2.34(2.34)	2.17(2.16)
Zn-N _{H556}	2.09(2.07)	2.07(2.05)
Zn-S _{C560}	2.35(2.32)	2.19(2.19)
N _{H556} -Zn-S _{C540}	103.3(97.7)	100.8(100.1)
N _{H556} -Zn-S _{C543}	98.2(97.6)	97.2(97.7)
N _{H556} -Zn-S _{C560}	109.3(108.6)	104.7(104.6)
S _{C540} -Zn-S _{C543}	113.7(108.7)	110.9(111.1)
S _{C540} -Zn-S _{C560}	111.0(117.7)	110.7(110.6)
S _{C543} -Zn-S _{C560}	119.3(121.6)	127.6(127.7)

Table S10. RSZD scores of residues around the Zn(II) binding site in the histone acetyltransferase from quantum refinement approaches using B3LYP/6-31G(d) (**M1**) and B3LYP-D3/6-31G(d) (**M2**) with ω_α value of 1.0. RSZD scores of the FCV binding site were also given.

	X-ray	M1	M2
CYM540	0.6	2.1	2.1
CYM543	1.5	1.7	1.8
HID556	3.0	0.6	0.5
CYM560	1.7	1.6	1.6
Zn	2.7	3.6	3.6
Sum ^a (Zn(II) center)	9.5	9.6	9.6
FCV	1.7	1.2	1.3

a: The sum for Zn(II) center is the sum of CYM540, CYM543, HID556, CYM560 and Zn(II).

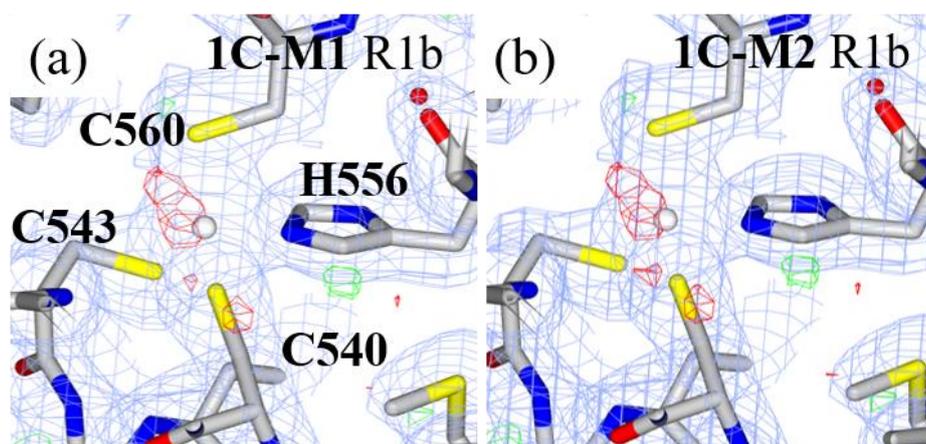


Figure S6. Structures for the Zinc active-site in the MYST histone acetyltransferase KAT6A/B protein from various quantum refinement schemes with ω_α value of 1.0 using (a) 1C-M1 (with the R1b-optimized region), (b) 1C-M2 (with the R1b-optimized region), including the electron density map (2mFo-DFc maps, contoured at 1.0 σ (blue), mFo-DFc maps, contoured at +3.0 σ (green), and mFo-DFc maps, contoured at -3.0 σ (red)).

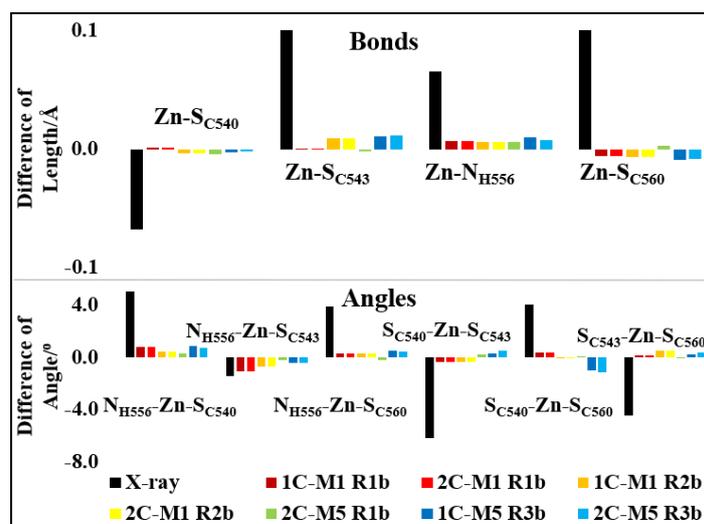


Figure S7. Difference in the key bond lengths and bond angles involving the zinc metal-ligand in our quantum refinement with ω_α value of 1.667 of the histone acetyltransferase using different methods compared to that obtained from the most reliable 1C-M5 scheme with R1b-optimized region (detailed data are given in Tables S12 and S14).

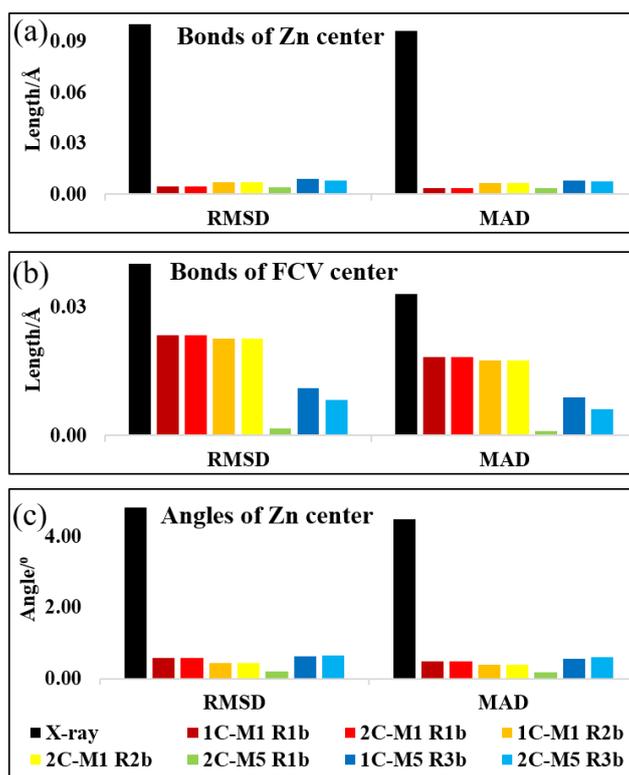


Figure S8. RMSD and MAD analysis of the refined (a) bond lengths for the Zn(II) center; (b) bond lengths for the FCV center; (c) bond angles around the Zn(II) center of the histone acetyltransferase obtained using different methods with ω_α value of 1.667, which are compared to that obtained from the most reliable **1C-M5** scheme with R1b-optimized region (detailed data are given in Tables S12 and S14).

The key results for the conventional two- and three-layer ONIOM-based quantum refinements (**M1** and **M5**) are compared and summarized in Figures S7-S8 and Tables S12-S17. In comparison with our quantum refinement calculations with ω_α value of 1.667 (suggested by CNS) and 1.0 (Tables S16-S17), their maximum difference of the metal-ligand bond lengths on the Zn(II) site between various quantum refinement schemes is less than 0.03 Å and that of the related angle is less than 0.7°. The computed RSZD scores for these ω_α values are also similar with a deviation of less than 0.2 (Table S11). In addition, the R and R_{free} factors for these ω_α values are computed to be identical. These results reveal that our quantum refinement

calculations give similar local geometries for the two different ω_α cases. Hereafter, the refined results for ω_α value of 1.667 are mainly discussed.

Table S11. RSZD scores of residues around the Zn(II) binding site in the histone acetyltransferase from various quantum refinement approaches with ω_α value of 1.667 and 1.0 (in parenthesis). RSZD scores of the FCV binding site were also given.

		M1 R1b	M1 R2b	M5 R1b	M5 R3b	M7 R1b ^a	M8 R1b ^a	X-ray
CYM540	1C	2.0(2.1)	2.0(2.1)	1.9(2.1)	2.0(2.1)	-	-	
	2C	2.0(2.1)	2.2(2.2)	1.9(2.1)	1.9(2.1)	(2.3)	(2.3)	0.6
CYM543	1C	1.4(1.7)	1.3(1.6)	1.3(1.6)	1.3(1.5)	-	-	
	2C	1.4(1.7)	1.3(1.6)	1.3(1.6)	1.2(1.6)	(2.0)	(1.9)	1.5
HID556	1C	0.8(0.6)	0.8(0.8)	0.5(0.8)	0.9(1.1)	-	-	
	2C	0.8(0.5)	2.0(1.2)	0.5(0.6)	0.8(0.8)	(0.6)	(0.7)	3.0
CYM560	1C	1.9(1.6)	1.9(1.7)	1.7(1.6)	1.8(1.7)	-	-	
	2C	1.9(1.6)	1.7(1.7)	1.6(1.5)	1.8(1.7)	(1.4)	(1.5)	1.7
Zn	1C	3.7(3.6)	3.9(3.8)	3.7(3.4)	3.7(3.4)	-	-	
	2C	3.8(3.5)	3.9(3.7)	3.7(3.5)	3.8(3.3)	(3.5)	(3.3)	2.7
Sum ^b (Zn(II) center)	1C	9.8(9.6)	9.9(10.0)	9.1(9.5)	9.7(9.8)	-	-	
	2C	9.9(9.4)	11.1(10.4)	9.0(9.3)	9.5(9.5)	(9.8)	(9.7)	9.5
FCV	1C	1.1(1.2)	1.0(1.0)	0.9(1.0)	0.8(1.0)	-	-	
	2C	1.1(1.2)	1.0(1.0)	0.9(1.1)	0.7(1.1)	(1.2)	(1.1)	1.7

a: values computed by the **2C-M7** and **2C-M8** schemes with the CCSD-in-DFT method as the QM method. b: The sum for Zn(II) center is the sum of CYM540, CYM543, HID556, CYM560 and Zn(II).

Compared to the X-ray crystal structure, the refined Zn-S_{C540} bond obtained by different multiscale schemes (**M1** and **M5**) becomes longer by 0.07 Å, while the Zn-S_{C543}, Zn-N_{H556} and Zn-S_{C560} bonds become shorter by 0.11-0.12, 0.05-0.06 and 0.08-0.09 Å, respectively (Figure S7). In addition, our different quantum refinement calculations generally provide similar active-site bonding based on their RMSD, MAD and RSZD scores. Compared to the best computational combination (**1C-M5** R1b), the RMSD and MAD values for the bonds involving the zinc ion refined by different approaches deviate by 0.01 and 0.01 Å only (Figure S8), respectively. Similarly, the RMSD and MAD values for the bond angles refined by different

approaches deviate by approximately 0.1-0.7 ° and 0.1-0.6 °, respectively. Likewise, the RSZD scores of the zinc and FCV centers refined by different approaches deviate by less than 1.3 and 0.2, respectively (Table S11). The electron density maps are almost identical relative to those by **1C-M5** R1b (Figures S10 and S14). These computational results show again that different quantum refinement schemes generally lead to the similar active-site geometry.

Furthermore, compared to the X-ray crystal structure, the strain energy of the R1b-optimized region (which was calculated as the QM energy difference between the fully-optimized R1b-optimized geometry in vacuum and the quantum refined R1b-optimized geometry extracted from the protein at B3LYP/6-31G(d) level) is considerably decreased by more than 17.0-24.2 kcal/mol and 61.9-66.3 kcal/mol for the FCV and zinc centers, respectively, after these quantum refinement calculations (**M1** and **M5**; Figure S9 and Table S23).

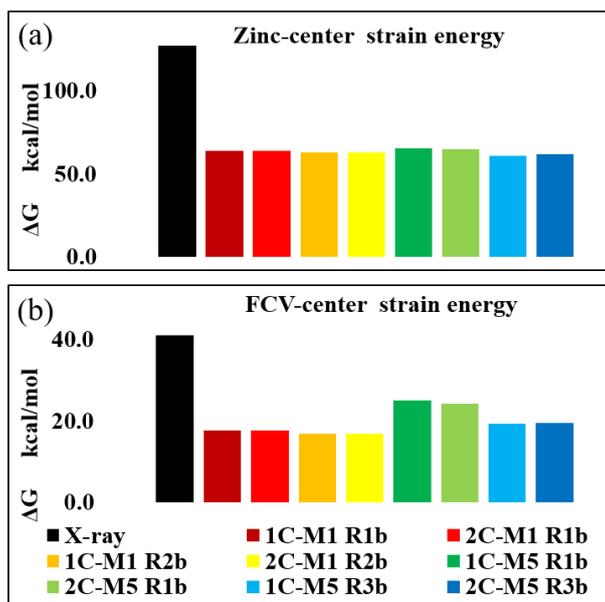


Figure S9. Strain energy (ΔE , kcal/mol) at B3LYP/6-31G(d) level for the R1b-optimized region for (a) the Zn(II) center and (b) the FCV center in the histone acetyltransferase determined by various quantum refinement schemes.

However, the computed RZSD scores of Zn(II) center for the different quantum refined calculations (**M1** and **M5**) become higher than that obtained from the X-ray crystal structure by 0.4-1.7 . As shown in Figures S10 and S14, a less positive (green contours) difference density around the zinc ion was observed after these quantum refinement calculations. Moreover, the key atomic displacement for these refined results (Figure S12a and Tables S21-S22) with respect to the X-ray crystal structure show that the zinc metal moves only 0.07-0.08 Å, whereas the Zn-ligated N_εHID556 atom was found to have the largest displacement (0.18-0.22 Å) than the other Zn-ligated S_{CYM540}, S_{CYM543} and S_{CYM560} atoms (0.12-0.17 Å) and the Zn(II) metal (0.07-0.08 Å). On the basis of the RSZD scores results (Table S11), that for the sum of the zinc center modestly raises from 9.5 (crystal structure) to 9.1-9.8 (for the small R1b-optimized region with **M1** and **M5** approaches) and 9.7-9.9 (for the larger R2b- and R3b-optimized regions with **M1** and **M5** approaches). These **M1**- and **M5**-refined results reveal that the RSZD score for the Zn(II) binding site which is positioned on the surface of the protein obviously becomes larger with the larger optimization region. Therefore, the flexible Zn(II) binding on this protein surface (Figure S12b) should be attributed to the more negative (red contours) difference density around the zinc center, and the flexible optimization region on the protein surface should be carefully selected in quantum refinement calculations.

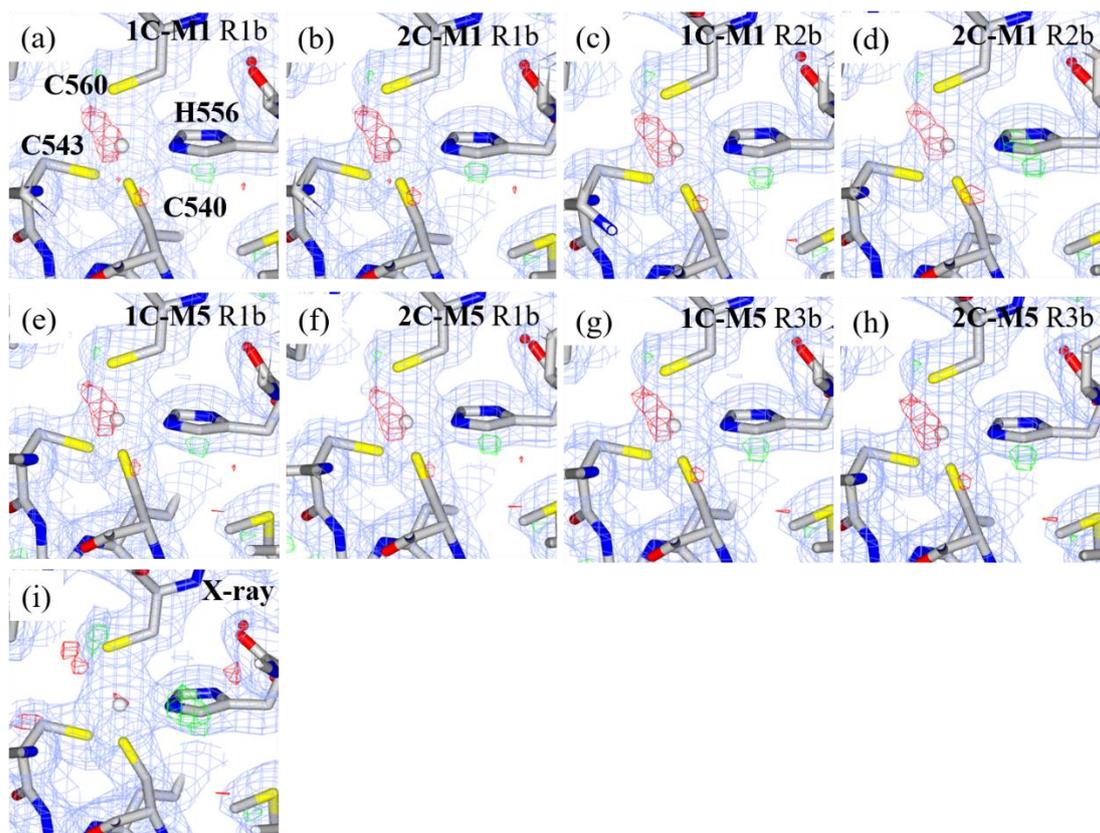


Figure S10. Structures for the Zinc active-site in the MYST histone acetyltransferase KAT6A/B protein from various quantum refinement schemes with ω_α value of 1.667 using (a) **1C-M1** (with the R1b-optimized region), (b) **2C-M1** (with the R1b-optimized region), (c) **1C-M1** (with the R2b-optimized region), (d) **2C-M1** (with the R2b-optimized region), (e) **1C-M5** (with the R1b-optimized region), (f) **2C-M5** (with the R1b-optimized region), (g) **1C-M5** (with the R3b-optimized region), (h) **2C-M5** (with the R3b-optimized region) and (i) the X-ray crystal structure, including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)).

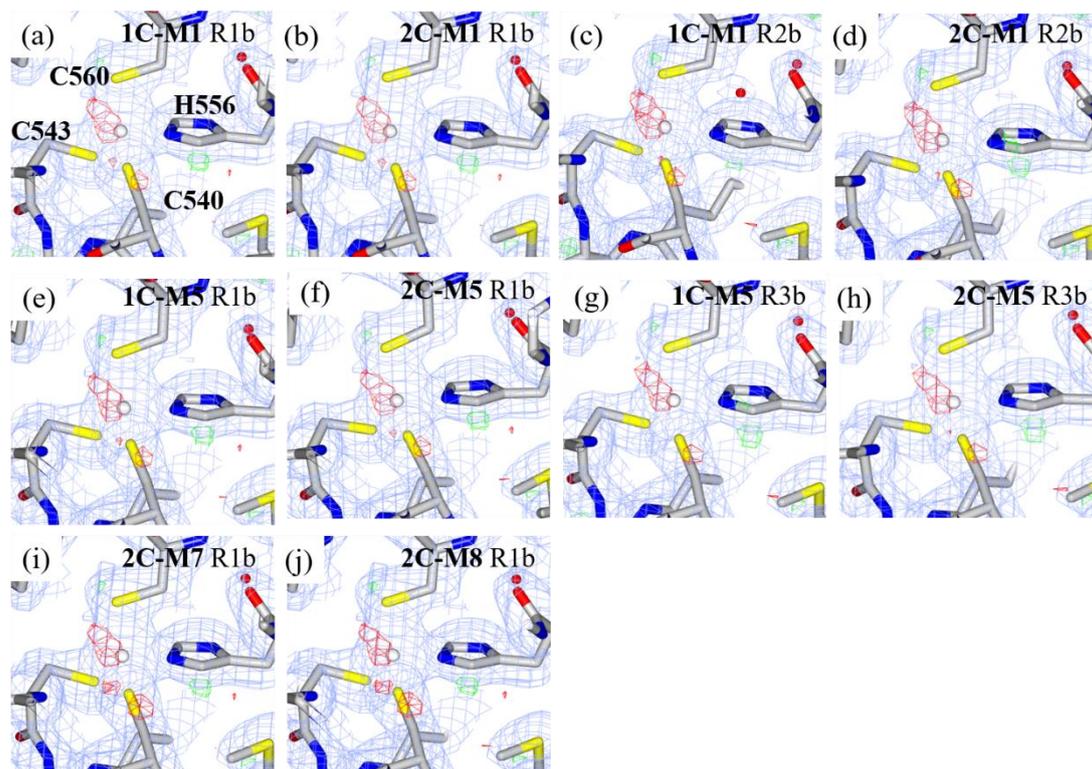


Figure S11. Structures for the Zn binding site in the histone acetyltransferase protein from various quantum refinement schemes with ω_α value of 1.0 using (a) **1C-M1** (with the R1b-optimized region), (b) **2C-M1** (with the R1b-optimized region), (c) **1C-M1** (with the R2b-optimized region), (d) **2C-M1** (with the R2b-optimized region), (e) **1C-M5** (with the R1b-optimized region), (f) **2C-M5** (with the R1b-optimized region), (g) **1C-M5** (with the R3b-optimized region), (h) **2C-M5** (with the R3b-optimized region), (i) **2C-M7** (with the R1b-optimized region) and (j) **2C-M8** (with the R1b-optimized region), including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)).

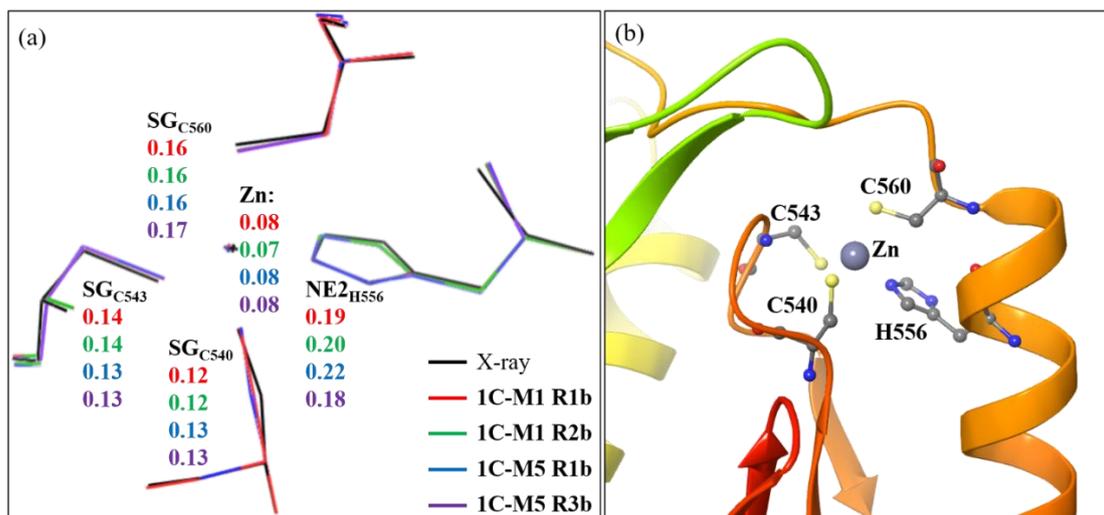


Figure S12. (a) Superposition of the Zinc binding site in the histone acetyltransferase protein from X-ray structure (black) and quantum refinements with ω_α value of 1.667 using **1C-M1** (with the R1b-optimized region, red), **1C-M1** (with the R2b-optimized region, green), **1C-M5** (with the R1b-optimized region, blue), **1C-M5** (with the R3b-optimized region, purple). The atomic displacements (Å) of the key atoms in our quantum refinement calculations relative to the X-ray crystal structure are given. (b) The flexible Zinc binding site in X-ray structure of the histone acetyltransferase protein.

Table S12. Our quantum refined key structural results with ω_α value of 1.667 for the zinc binding site using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase. The two-center (2C) ONIOM approximation was also used (values given in parenthesis). The key structural results from the X-ray crystal structure were also given. **1C-M5** R1b results are used as reference for RMSD and MAD computations.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
Zn-S _{C540}	2.33(2.33)	2.33(2.33)	2.33(2.33)	2.33(2.33)	2.26
Zn-S _{C543}	2.17(2.17)	2.17(2.17)	2.16(2.16)	2.17(2.17)	2.28
Zn-N _{H556}	2.07(2.07)	2.08(2.09)	2.08(2.08)	2.08(2.07)	2.13
Zn-S _{C560}	2.19(2.19)	2.19(2.19)	2.20(2.20)	2.19(2.19)	2.28
RMSD (bonds)	0.00(0.00)	0.01(0.01)	0.00(0.00)	0.01(0.01)	0.10
MAD (bonds)	0.00(0.00)	0.01(0.01)	0.00(0.00)	0.01(0.01)	0.10
N _{H556} -Zn-S _{C540}	100.8(100.5)	100.8(101.9)	101.2(100.8)	101.8(101.1)	107.8
N _{H556} -Zn-S _{C543}	97.2(97.5)	97.3(96.8)	97.6(97.9)	97.6(98.0)	96.7
N _{H556} -Zn-S _{C560}	104.7(104.7)	104.7(104.7)	104.7(104.5)	105.1(105.1)	108.1
S _{C540} -Zn-S _{C543}	110.9(110.9)	111.0(110.8)	111.2(111.3)	111.5(111.8)	105.2
S _{C540} -Zn-S _{C560}	110.7(110.7)	110.1(110.3)	110.1(110.1)	109.2(108.9)	114.0
S _{C543} -Zn-S _{C560}	127.6(127.7)	128.1(127.8)	127.4(127.5)	127.5(127.6)	123.0
RMSD (angles)	0.6(0.6)	0.4(0.4)	0.0(0.2)	0.6(0.7)	4.8
MAD (angles)	0.5(0.5)	0.4(0.4)	0.0(0.2)	0.5(0.6)	4.5
R/	0.218(0.218/	0.218(0.217/	0.218(0.218/	0.217(0.217/	0.210/
R _{free}	0.244(0.244)	0.244(0.243)	0.244(0.244)	0.243(0.243)	0.241

Table S13. Our quantum refined key structural results with ω_α value of 1.0 for the zinc binding site using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase. The two-center (2C) ONIOM approximation was also used (values given in parenthesis). The key structural results from the X-ray crystal structure were also given. **1C-M5** R1b results are used as reference for RMSD and MAD computaions.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
Zn-S _{C540}	2.33(2.33,2.35 ^a)	2.33(2.33)	2.33(2.33,2.35 ^a)	2.33(2.33)	2.26
Zn-S _{C543}	2.17(2.17,2.19)	2.17(2.17)	2.16(2.16,2.19)	2.17(2.17)	2.28
Zn-N _{H556}	2.07(2.07,2.08)	2.08(2.09)	2.08(2.08,2.09)	2.08(2.07)	2.13
Zn-S _{C560}	2.19(2.19,2.22)	2.19(2.19)	2.20(2.20,2.22)	2.19(2.19)	2.28
RMSD (bonds)	0.01(0.01,0.02)	0.01(0.00)	0.00(0.00,0.02)	0.01(0.01)	0.09
MAD (bonds)	0.00(0.01,0.01)	0.00(0.00)	0.00(0.00,0.02)	0.00(0.01)	0.08
N _{H556} -Zn-S _{C540}	100.8(100.5,100.7)	100.8(101.9)	101.2(100.8,101.1)	101.8(101.1)	107.8
N _{H556} -Zn-S _{C543}	97.2(97.5,97.0)	97.3(96.8)	97.6(97.9,97.5)	97.6(98.0)	96.7
N _{H556} -Zn-S _{C560}	104.7(104.7,104.9)	104.7(104.7)	104.7(104.5,104.8)	105.1(105.1)	108.1
S _{C540} -Zn-S _{C543}	110.9(110.9,110.9)	111.0(110.8)	111.2(111.3,111.3)	111.5(111.8)	105.2
S _{C540} -Zn-S _{C560}	110.7(110.7,110.7)	110.1(110.3)	110.1(110.1,110.2)	109.2(108.9)	114.0
S _{C543} -Zn-S _{C560}	127.6(127.7,127.7)	128.1(127.8)	127.4(127.5,127.4)	127.5(127.6)	123.0
RMSD (angles)	0.4(0.4,0.5)	0.4(0.5)	0.0(0.3,0.1)	0.5(0.6)	4.6
MAD (angles)	0.3(0.3,0.4)	0.3(0.4)	0.0(0.2,0.1)	0.4(0.5)	4.2
R/	0.218(0.218,0.218)/	0.218(0.217)/	0.218(0.218,0.218)/	0.217(0.217)/	0.214/
R _{free}	0.244(0.244,0.244)	0.244(0.243)	0.244(0.244,0.244)	0.243(0.243)	0.241

a: values computed by the **2C-M7** and **2C-M8** method with the CCSD-in-DFT method as the QM method.

Table S14. Our quantum refined key structural results with ω_α value of 1.667 for the FCV ligand using different multiscale schemes with different optimized regions (R1b, R2b or R3b). The two-center (2C) ONIOM approximation (values given in parenthesis) was also used. **1C-M5** R1b results are used as reference for RMSD and MAD computaions.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
C2-C7	1.40(1.40)	1.40(1.40)	1.42(1.42)	1.41(1.41)	1.39
C2-C3	1.41(1.42)	1.41(1.40)	1.43(1.44)	1.42(1.43)	1.39
C6-C7	1.40(1.40)	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.39
C7-F1	1.37(1.37)	1.37(1.37)	1.38(1.38)	1.38(1.38)	1.36
C6-C5	1.39(1.39)	1.39(1.39)	1.41(1.41)	1.40(1.40)	1.38
C5-C4	1.40(1.40)	1.40(1.39)	1.41(1.41)	1.40(1.40)	1.39
C4-C3	1.41(1.41)	1.40(1.40)	1.39(1.40)	1.40(1.40)	1.39
C2-S1	1.86(1.86)	1.85(1.87)	1.81(1.81)	1.83(1.82)	1.82
S1-O3	1.46(1.46)	1.47(1.47)	1.48(1.48)	1.48(1.48)	1.47
S1-O2	1.46(1.47)	1.47(1.47)	1.49(1.49)	1.48(1.48)	1.46
S1-N1	1.66(1.66)	1.66(1.67)	1.67(1.66)	1.67(1.66)	1.70
N1-N2	1.37(1.37)	1.38(1.40)	1.38(1.38)	1.39(1.38)	1.40
N2-C1	1.39(1.39)	1.39(1.39)	1.40(1.40)	1.40(1.40)	1.45
C1-O1	1.23(1.23)	1.23(1.23)	1.27(1.27)	1.26(1.27)	1.19
C1-C8	1.48(1.48)	1.48(1.49)	1.44(1.44)	1.46(1.45)	1.52
C8-C9	1.41(1.41)	1.41(1.41)	1.44(1.44)	1.43(1.43)	1.38
C9-C10	1.39(1.39)	1.39(1.39)	1.38(1.38)	1.38(1.38)	1.38
C10-F2	1.36(1.36)	1.35(1.35)	1.37(1.37)	1.36(1.36)	1.36
C10-C11	1.40(1.40)	1.40(1.39)	1.40(1.40)	1.40(1.40)	1.39
C11-C12	1.41(1.41)	1.41(1.40)	1.43(1.43)	1.42(1.42)	1.39
C12-C18	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.38
C18-C8	1.39(1.39)	1.39(1.38)	1.40(1.40)	1.39(1.40)	1.38
C12-C13	1.48(1.48)	1.47(1.46)	1.47(1.47)	1.46(1.47)	1.38
C13-C14	1.38(1.38)	1.38(1.38)	1.39(1.39)	1.39(1.39)	1.38
C14-C15	1.39(1.39)	1.39(1.38)	1.39(1.38)	1.38(1.39)	1.38
C15-C16	1.39(1.40)	1.39(1.39)	1.40(1.40)	1.40(1.40)	1.39
C16-C17	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.39
C17-N3	1.35(1.35)	1.35(1.35)	1.36(1.36)	1.35(1.36)	1.32
C13-N3	1.34(1.34)	1.34(1.34)	1.36(1.35)	1.35(1.35)	1.32
RMSD	0.02(0.02)	0.02(0.02)	0.00(0.00)	0.01(0.01)	0.04
MAD	0.02(0.02)	0.02(0.02)	0.00(0.00)	0.01(0.01)	0.03

Table S15. Our quantum refined key structural results with ω_α value of 1.0 for the FCV ligand using different multiscale schemes with different optimized regions (R1b, R2b or R3b). The two-center (2C) ONIOM approximation (values given in parenthesis) was also used. **1C-M5** R1b results are used as reference for RMSD and MAD computaions.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
C2-C7	1.40(1.40,1.40 ^a)	1.40(1.40)	1.42(1.42,1.42 ^a)	1.41(1.41)	1.39
C2-C3	1.41(1.42,1.41)	1.41(1.40)	1.43(1.44,1.44)	1.42(1.43)	1.39
C6-C7	1.40(1.40,1.40)	1.39(1.39)	1.39(1.39,1.39)	1.39(1.39)	1.39
C7-F1	1.37(1.37,1.37)	1.37(1.37)	1.38(1.38,1.38)	1.38(1.38)	1.36
C6-C5	1.39(1.39,1.39)	1.39(1.39)	1.41(1.41,1.41)	1.40(1.40)	1.38
C5-C4	1.40(1.40,1.40)	1.40(1.39)	1.41(1.41,1.41)	1.40(1.40)	1.39
C4-C3	1.41(1.41,1.41)	1.40(1.40)	1.39(1.40,1.40)	1.40(1.40)	1.39
C2-S1	1.86(1.86,1.86)	1.85(1.87)	1.81(1.81,1.81)	1.83(1.82)	1.82
S1-O3	1.46(1.46,1.46)	1.47(1.47)	1.48(1.48,1.48)	1.48(1.48)	1.47
S1-O2	1.46(1.47,1.47)	1.47(1.47)	1.49(1.49,1.49)	1.48(1.48)	1.46
S1-N1	1.66(1.66,1.66)	1.66(1.67)	1.67(1.66,1.66)	1.67(1.66)	1.70
N1-N2	1.37(1.37,1.37)	1.38(1.40)	1.38(1.38,1.38)	1.39(1.38)	1.40
N2-C1	1.39(1.39,1.39)	1.39(1.39)	1.40(1.40,1.40)	1.40(1.40)	1.45
C1-O1	1.23(1.23,1.23)	1.23(1.23)	1.27(1.27,1.27)	1.26(1.27)	1.19
C1-C8	1.48(1.48,1.48)	1.48(1.49)	1.44(1.44,1.44)	1.46(1.45)	1.52
C8-C9	1.41(1.41,1.41)	1.41(1.41)	1.44(1.44,1.44)	1.43(1.43)	1.38
C9-C10	1.39(1.39,1.39)	1.39(1.39)	1.38(1.38,1.38)	1.38(1.38)	1.38
C10-F2	1.36(1.36,1.36)	1.35(1.35)	1.37(1.37,1.37)	1.36(1.36)	1.36
C10-C11	1.40(1.40,1.40)	1.40(1.39)	1.40(1.40,1.40)	1.40(1.40)	1.39
C11-C12	1.41(1.41,1.41)	1.41(1.40)	1.43(1.43,1.43)	1.42(1.42)	1.39
C12-C18	1.39(1.39,1.39)	1.39(1.39)	1.39(1.39,1.39)	1.39(1.39)	1.38
C18-C8	1.39(1.39,1.39)	1.39(1.38)	1.40(1.40,1.40)	1.39(1.40)	1.38
C12-C13	1.48(1.48,1.48)	1.47(1.46)	1.47(1.47,1.47)	1.46(1.47)	1.38
C13-C14	1.38(1.38,1.38)	1.38(1.38)	1.39(1.39,1.39)	1.39(1.39)	1.38
C14-C15	1.39(1.39,1.39)	1.39(1.38)	1.39(1.38,1.38)	1.38(1.39)	1.38
C15-C16	1.39(1.40,1.40)	1.39(1.39)	1.40(1.40,1.40)	1.40(1.40)	1.39
C16-C17	1.39(1.39,1.39)	1.39(1.39)	1.39(1.39,1.39)	1.39(1.39)	1.39
C17-N3	1.35(1.35,1.35)	1.35(1.35)	1.36(1.36,1.36)	1.35(1.36)	1.32
C13-N3	1.34(1.34,1.34)	1.34(1.34)	1.36(1.35,1.35)	1.35(1.35)	1.32
RMSD	0.02(0.02,0.02)	0.02(0.02)	0.00(0.00,0.00)	0.01(0.00)	0.04
MAD	0.01(0.01,0.01)	0.01(0.02)	0.00(0.00,0.00)	0.01(0.00)	0.03

a: values computed by the **2C-M7** and **2C-M8** method with the CCSD-in-DFT method as the QM method.

Table S16. Our quantum refined key structural results for the zinc binding site using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase. Different values of the weighting factor (1.0 and 1.667 (in parenthesis)) are used. The key structural results from the X-ray crystal structure were also given. **1C-M5** R1b results are used as reference for RMSD and MAD computations.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
Zn-S _{C540}	2.33(2.33)	2.33(2.32)	2.33(2.33)	2.33(2.32)	2.26
Zn-S _{C543}	2.17(2.14)	2.17(2.15)	2.16(2.14)	2.17(2.15)	2.28
Zn-N _{H556}	2.07(2.07)	2.08(2.07)	2.08(2.06)	2.08(2.07)	2.13
Zn-S _{C560}	2.19(2.17)	2.19(2.17)	2.20(2.17)	2.19(2.16)	2.28
RMSD (bonds)	0.01(0.00)	0.01(0.01)	0.00(0.00)	0.01(0.01)	0.09(0.10)
MAD (bonds)	0.00(0.00)	0.00(0.01)	0.00(0.00)	0.00(0.01)	0.08(0.10)
N _{H556} -Zn-S _{C540}	100.8(101.8)	100.8(101.5)	101.2(101.0)	101.8(101.9)	107.8
N _{H556} -Zn-S _{C543}	97.2(97.1)	97.3(97.4)	97.6(98.1)	97.6(97.7)	96.7
N _{H556} -Zn-S _{C560}	104.7(104.5)	104.7(104.5)	104.7(104.2)	105.1(104.7)	108.1
S _{C540} -Zn-S _{C543}	110.9(111.1)	111.0(111.0)	111.2(111.4)	111.5(111.7)	105.2
S _{C540} -Zn-S _{C560}	110.7(110.3)	110.1(109.9)	110.1(109.9)	109.2(109.0)	114.0
S _{C543} -Zn-S _{C560}	127.6(127.6)	128.1(128.0)	127.4(127.5)	127.5(127.7)	123.0
RMSD (angles)	0.4(0.6)	0.4(0.4)	0.0(0.0)	0.5(0.6)	4.6(4.8)
MAD (angles)	0.3(0.5)	0.3(0.4)	0.0(0.0)	0.4(0.5)	4.2(4.5)
R/	0.218(0.218/	0.218(0.217/	0.218(0.218/	0.217(0.217/	0.214/
R _{free}	0.244(0.244)	0.244(0.243)	0.244(0.244)	0.243(0.243)	0.241

Table S17. Our quantum refined key structural results for the FCV ligand using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase. Different values of the weighting factor (1.0 and 1.667 (in parenthesis)) are used. The key structural results from the X-ray crystal structure were also given. **1C-M5** R1b results are used as reference for RMSD and MAD computaions.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
C2-C7	1.40(1.40)	1.40(1.40)	1.42(1.42)	1.41(1.41)	1.39
C2-C3	1.41(1.41)	1.41(1.41)	1.43(1.45)	1.42(1.42)	1.39
C6-C7	1.40(1.40)	1.39(1.40)	1.39(1.40)	1.39(1.40)	1.39
C7-F1	1.37(1.38)	1.37(1.38)	1.38(1.39)	1.38(1.39)	1.36
C6-C5	1.39(1.38)	1.39(1.39)	1.41(1.41)	1.40(1.40)	1.38
C5-C4	1.40(1.39)	1.40(1.39)	1.41(1.41)	1.40(1.40)	1.39
C4-C3	1.41(1.40)	1.40(1.40)	1.39(1.40)	1.40(1.40)	1.39
C2-S1	1.86(1.88)	1.85(1.88)	1.81(1.82)	1.83(1.85)	1.82
S1-O3	1.46(1.47)	1.47(1.48)	1.48(1.48)	1.48(1.48)	1.47
S1-O2	1.46(1.47)	1.47(1.47)	1.49(1.50)	1.48(1.49)	1.46
S1-N1	1.66(1.64)	1.66(1.64)	1.67(1.64)	1.67(1.64)	1.70
N1-N2	1.37(1.40)	1.38(1.40)	1.38(1.37)	1.39(1.39)	1.40
N2-C1	1.39(1.39)	1.39(1.40)	1.40(1.40)	1.40(1.40)	1.45
C1-O1	1.23(1.23)	1.23(1.23)	1.27(1.27)	1.26(1.26)	1.19
C1-C8	1.48(1.48)	1.48(1.48)	1.44(1.43)	1.46(1.45)	1.52
C8-C9	1.41(1.41)	1.41(1.42)	1.44(1.45)	1.43(1.44)	1.38
C9-C10	1.39(1.39)	1.39(1.39)	1.38(1.38)	1.38(1.38)	1.38
C10-F2	1.36(1.36)	1.35(1.36)	1.37(1.37)	1.36(1.37)	1.36
C10-C11	1.40(1.39)	1.40(1.40)	1.40(1.41)	1.40(1.40)	1.39
C11-C12	1.41(1.41)	1.41(1.41)	1.43(1.44)	1.42(1.42)	1.39
C12-C18	1.39(1.38)	1.39(1.39)	1.39(1.39)	1.39(1.38)	1.38
C18-C8	1.39(1.39)	1.39(1.38)	1.40(1.40)	1.39(1.39)	1.38
C12-C13	1.48(1.46)	1.47(1.46)	1.47(1.48)	1.46(1.46)	1.38
C13-C14	1.38(1.37)	1.38(1.38)	1.39(1.39)	1.39(1.38)	1.38
C14-C15	1.39(1.38)	1.39(1.38)	1.39(1.39)	1.38(1.38)	1.38
C15-C16	1.39(1.39)	1.39(1.39)	1.40(1.40)	1.40(1.40)	1.39
C16-C17	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.39(1.39)	1.39
C17-N3	1.35(1.35)	1.35(1.35)	1.36(1.37)	1.35(1.36)	1.32
C13-N3	1.34(1.34)	1.34(1.34)	1.36(1.35)	1.35(1.35)	1.32
RMSD	0.02(0.02)	0.02(0.02)	0.00(0.00)	0.01(0.01)	0.04(0.04)
MAD	0.01(0.02)	0.01(0.02)	0.00(0.00)	0.01(0.01)	0.03(0.03)

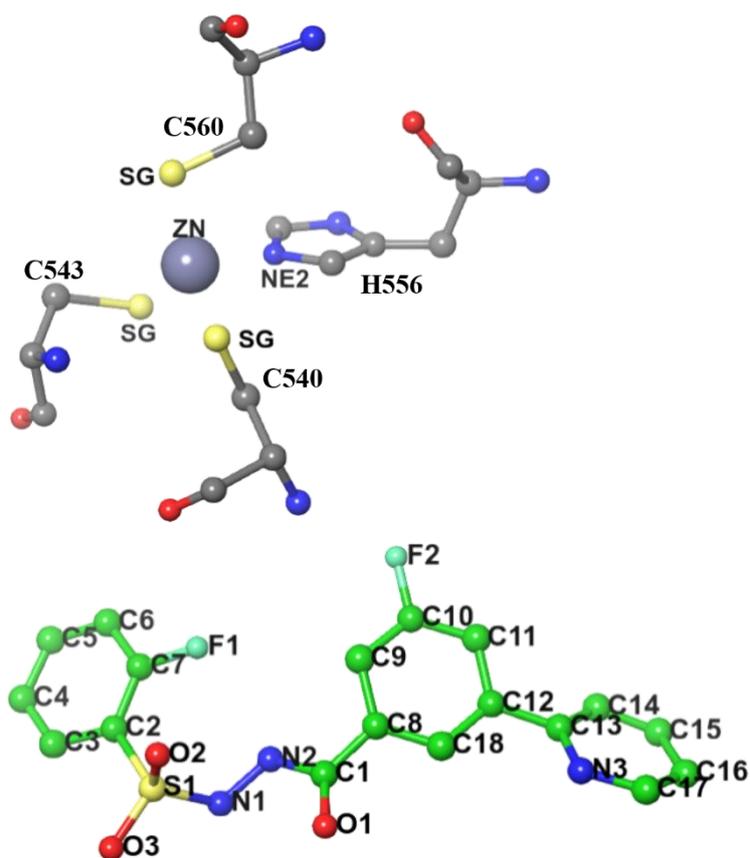


Figure S13. Local structure for the Zn and FCV binding site in X-ray crystal structure of the histone acetyltransferase.

Table S18. RSZD scores of residues around the Zn binding site in the histone acetyltransferase from various quantum refinement calculations with ω_α value of 1.667. The two-center (2C) ONIOM approximation was also used (values given in parenthesis).

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
CYM540	2.0(2.0)	2.0(2.2)	1.9(1.9)	2.0(1.9)	0.6
CYM543	1.4(1.4)	1.3(1.3)	1.3(1.3)	1.3(1.2)	1.5
HID556	0.8(0.8)	0.8(2.0)	0.5(0.5)	0.9(0.8)	3.0
CYM560	1.9(1.9)	1.9(1.7)	1.7(1.6)	1.8(1.8)	1.7
Zn	3.7(3.8)	3.9(3.9)	3.7(3.7)	3.7(3.8)	2.7
Sum (Zn center)	9.8(9.9)	9.9(11.1)	9.1(9.0)	9.7(9.5)	9.5
FCV	1.1(1.1)	1.0(1.0)	0.9(0.9)	0.8(0.7)	1.7

Table S19. RSZD scores of residues around the Zn binding site in the histone acetyltransferase from various quantum refinement calculations with ω_α value of 1.0. The two-center (2C) ONIOM approximation was also used (values given in parenthesis).

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
CYM540	2.1(2.1, 2.3 ^a)	2.1(2.2)	2.1(2.1, 2.3 ^a)	2.1(2.1)	0.6
CYM543	1.7(1.7, 2.0)	1.6(1.6)	1.6(1.6, 1.9)	1.5(1.6)	1.5
HID556	0.6(0.5, 0.6)	0.8(1.2)	0.8(0.6, 0.7)	1.1(0.8)	3.0
CYM560	1.6(1.6, 1.4)	1.7(1.7)	1.6(1.5, 1.5)	1.7(1.7)	1.7
Zn	3.6(3.5, 3.5)	3.8(3.7)	3.4(3.5, 3.3)	3.4(3.3)	2.7
Sum (Zn center)	9.6(9.4, 9.8)	10.0(10.4)	9.5(9.3, 9.7)	9.8(9.5)	9.5
FCV	1.2(1.2, 1.2)	1.0(1.0)	1.0(1.1, 1.1)	1.0(1.1)	1.7

a: values computed by the **2C-M7** and **2C-M8** method with the CCSD-in-DFT method as the QM method.

Table S20. RSZD scores of residues around the Zn binding site in the histone acetyltransferase from various quantum refinement calculations using 1C-ONIOM methods with ω_α value of 1.0 and 1.667 (values given in parenthesis).

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	X-ray
CYM540	2.0(2.1)	2.0(2.1)	1.9(2.1)	2.0(2.1)	0.6
CYM543	1.4(1.7)	1.3(1.6)	1.3(1.6)	1.3(1.5)	1.5
HID556	0.8(0.6)	0.8(0.8)	0.5(0.8)	0.9(1.1)	3.0
CYM560	1.9(1.6)	1.9(1.7)	1.7(1.6)	1.8(1.7)	1.7
Zn	3.7(3.6)	3.9(3.8)	3.7(3.4)	3.7(3.4)	2.7
Sum (Zn center)	9.8(9.6)	9.9(10.0)	9.1(9.5)	9.7(9.8)	9.5
FCV	1.1(1.2)	1.0(1.0)	0.9(1.0)	0.8(1.0)	1.7

Table S21. Atomic displacements of zinc center through our quantum refinements using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase with ω_α value of 1.667. The two-center (2C) ONIOM approximation was also used (values given in parenthesis).

	M1 R1b	M1 R2b	M5 R1b	M5 R3b
CYM540				
N	0.08(0.08)	0.07(0.04)	0.05(0.05)	0.06(0.06)
CA	0.05(0.05)	0.04(0.01)	0.04(0.04)	0.03(0.03)
CB	0.13(0.13)	0.13(0.06)	0.21(0.21)	0.15(0.19)
SG	0.12(0.12)	0.12(0.11)	0.13(0.13)	0.13(0.13)
C	0.05(0.05)	0.04(0.01)	0.04(0.04)	0.03(0.03)
O	0.07(0.07)	0.06(0.04)	0.07(0.07)	0.07(0.08)
CYM543				
N	0.18(0.18)	0.17(0.10)	0.16(0.16)	0.17(0.18)
CA	0.14(0.14)	0.14(0.11)	0.12(0.12)	0.14(0.14)
CB	0.06(0.06)	0.07(0.04)	0.07(0.06)	0.06(0.07)
SG	0.14(0.14)	0.14(0.12)	0.13(0.13)	0.13(0.13)
C	0.07(0.07)	0.08(0.04)	0.08(0.08)	0.09(0.09)
O	0.08(0.08)	0.09(0.04)	0.12(0.11)	0.11(0.11)
HID556				
N	0.11(0.11)	0.10(0.06)	0.10(0.10)	0.11(0.12)
CA	0.12(0.12)	0.11(0.05)	0.13(0.13)	0.12(0.13)
CB	0.12(0.12)	0.12(0.03)	0.16(0.15)	0.13(0.15)
CG	0.10(0.10)	0.11(0.03)	0.14(0.14)	0.11(0.13)
CD2	0.13(0.13)	0.14(0.05)	0.17(0.16)	0.14(0.14)
ND1	0.16(0.16)	0.16(0.07)	0.18(0.18)	0.17(0.17)
CE1	0.20(0.20)	0.21(0.09)	0.23(0.22)	0.20(0.20)
NE2	0.19(0.19)	0.20(0.08)	0.22(0.21)	0.18(0.18)
C	0.08(0.08)	0.08(0.05)	0.06(0.06)	0.07(0.07)
O	0.26(0.26)	0.25(0.14)	0.29(0.29)	0.26(0.27)
CYM560				
N	0.05(0.05)	0.04(0.03)	0.05(0.05)	0.06(0.09)
CA	0.05(0.05)	0.06(0.03)	0.06(0.05)	0.08(0.10)
CB	0.12(0.12)	0.12(0.04)	0.13(0.13)	0.10(0.12)
SG	0.16(0.16)	0.16(0.14)	0.16(0.16)	0.17(0.17)
C	0.02(0.02)	0.03(0.03)	0.04(0.03)	0.03(0.05)
O	0.07(0.07)	0.08(0.03)	0.15(0.14)	0.12(0.14)
ZN802				
ZN	0.08(0.08)	0.07(0.07)	0.08(0.08)	0.08(0.08)

Table S22. Atomic displacements of zinc center through our quantum refinements using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase with ω_α value of 1.0. The two-center (2C) ONIOM approximation was also used (values given in parenthesis).

	M1 R1b	M1 R2b	M5 R1b	M5 R3b
CYM540				
N	0.06(0.06)	0.06(0.07)	0.04(0.04)	0.05(0.05)
CA	0.03(0.03)	0.03(0.04)	0.02(0.02)	0.02(0.02)
CB	0.18(0.18)	0.17(0.09)	0.18(0.17)	0.13(0.17)
SG	0.13(0.13)	0.13(0.12)	0.13(0.13)	0.13(0.14)
C	0.04(0.04)	0.03(0.03)	0.03(0.03)	0.02(0.02)
O	0.07(0.07)	0.07(0.06)	0.07(0.07)	0.07(0.08)
CYM543				
N	0.15(0.15)	0.15(0.14)	0.13(0.13)	0.14(0.16)
CA	0.12(0.13)	0.14(0.12)	0.11(0.12)	0.12(0.13)
CB	0.08(0.08)	0.06(0.06)	0.05(0.06)	0.04(0.05)
SG	0.13(0.13)	0.13(0.13)	0.12(0.13)	0.12(0.12)
C	0.05(0.05)	0.07(0.06)	0.06(0.06)	0.07(0.08)
O	0.05(0.05)	0.08(0.07)	0.09(0.09)	0.09(0.10)
HID556				
N	0.12(0.12)	0.12(0.11)	0.10(0.10)	0.11(0.12)
CA	0.14(0.14)	0.13(0.10)	0.11(0.12)	0.11(0.13)
CB	0.15(0.16)	0.14(0.09)	0.14(0.14)	0.12(0.15)
CG	0.13(0.13)	0.12(0.08)	0.13(0.13)	0.11(0.13)
CD2	0.14(0.15)	0.14(0.10)	0.13(0.15)	0.11(0.14)
ND1	0.15(0.16)	0.14(0.13)	0.16(0.18)	0.16(0.17)
CE1	0.22(0.24)	0.22(0.18)	0.20(0.22)	0.18(0.21)
NE2	0.21(0.22)	0.21(0.17)	0.20(0.22)	0.17(0.20)
C	0.08(0.09)	0.08(0.08)	0.06(0.07)	0.07(0.08)
O	0.25(0.26)	0.24(0.21)	0.25(0.26)	0.23(0.25)
CYM560				
N	0.06(0.06)	0.08(0.04)	0.06(0.06)	0.08(0.12)
CA	0.06(0.06)	0.07(0.04)	0.05(0.04)	0.07(0.09)
CB	0.11(0.12)	0.12(0.10)	0.11(0.12)	0.09(0.10)
SG	0.13(0.13)	0.14(0.13)	0.13(0.13)	0.14(0.14)
C	0.03(0.03)	0.04(0.04)	0.02(0.02)	0.02(0.02)
O	0.07(0.07)	0.09(0.06)	0.06(0.05)	0.06(0.08)
ZN802				
ZN	0.07(0.07)	0.07(0.07)	0.07(0.08)	0.07(0.07)

Table S23. Strain energy (ΔE , kcal/mol) at B3LYP/6-31G(d) level for the R1b-optimized region of the FCV and Zn centers in the histone acetyltransferase determined by various quantum refinement schemes with ω_α value of 1.667. The two-center (2C) ONIOM approximation (values given in parenthesis) was also used.

	ΔE	
	FCV	Zn
X-ray	41.1	127.2
M1 R1b	17.6(17.6)	64.1(64.1)
M1 R2b	16.9(16.9)	63.1(63.1)
M5 R1b	25.0(24.1)	65.3(64.8)
M5 R3b	19.3(19.5)	60.9(62.0)

Table S24. Strain energy (ΔE , kcal/mol) at B3LYP/6-31G(d) level for the R1b-optimized region of the FCV and Zn centers in the histone acetyltransferase determined by various quantum refinement schemes with ω_α value of 1.0. The two-center (2C) ONIOM approximation (values given in parenthesis) was also used.

	ΔE	
	FCV	Zn
X-ray	41.1	127.2
M1 R1b	13.9(14.1)	55.9(56.6)
M1 R2b	12.5(13.1)	55.8(56.2)
M5 R1b	16.3(17.4)	55.4 (56.1)
M5 R3b	14.3(15.0)	53.7(54.9)

Table S25. Strain energy (ΔE , kcal/mol) at B3LYP/6-31G(d) level for the R1b-optimized region of the FCV and Zn centers in the histone acetyltransferase determined by various quantum refinement schemes. Different values of the weighting factor (1.0 and 1.667 (values given in parenthesis)) are used.

	ΔE	
	FCV	Zn
X-ray	41.1	127.2
M1 R1b	13.9(17.6)	55.9(64.1)
M1 R2b	12.5(16.9)	55.8(63.1)
M5 R1b	16.3(25.0)	55.4(65.3)
M5 R3b	14.3(19.3)	53.7(60.9)

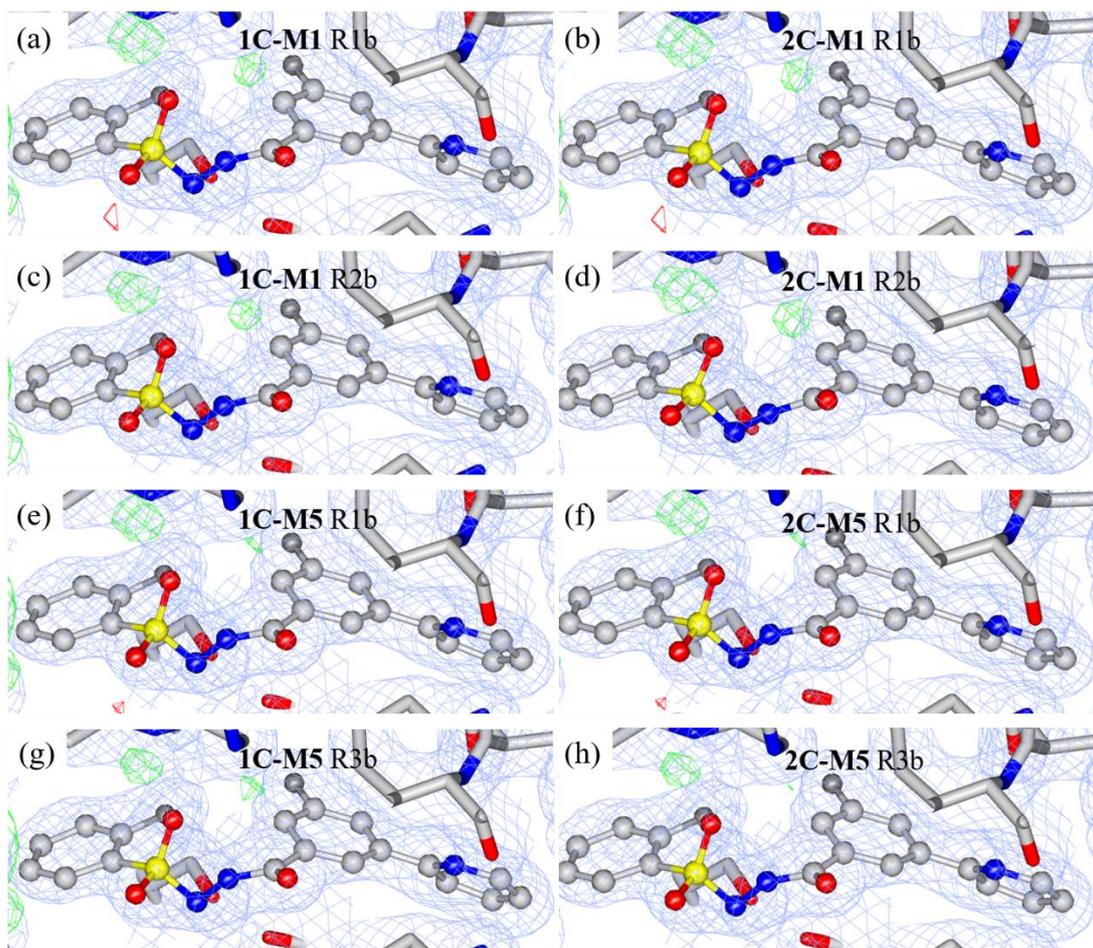


Figure S14. Structures for the FCV binding site in the histone acetyltransferase protein from various quantum refinement schemes with ω_α value of 1.667 using (a) **1C-M1** (with the R1b-optimized region), (b) **2C-M1** (with the R1b-optimized region), (c) **1C-M1** (with the R2b-optimized region), (d) **2C-M1** (with the R2b-optimized region), (e) **1C-M5** (with the R1b-optimized region), (f) **2C-M5** (with the R1b-optimized region), (g) **1C-M5** (with the R3b-optimized region), (h) **2C-M5** (with the R3b-optimized region), including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)).

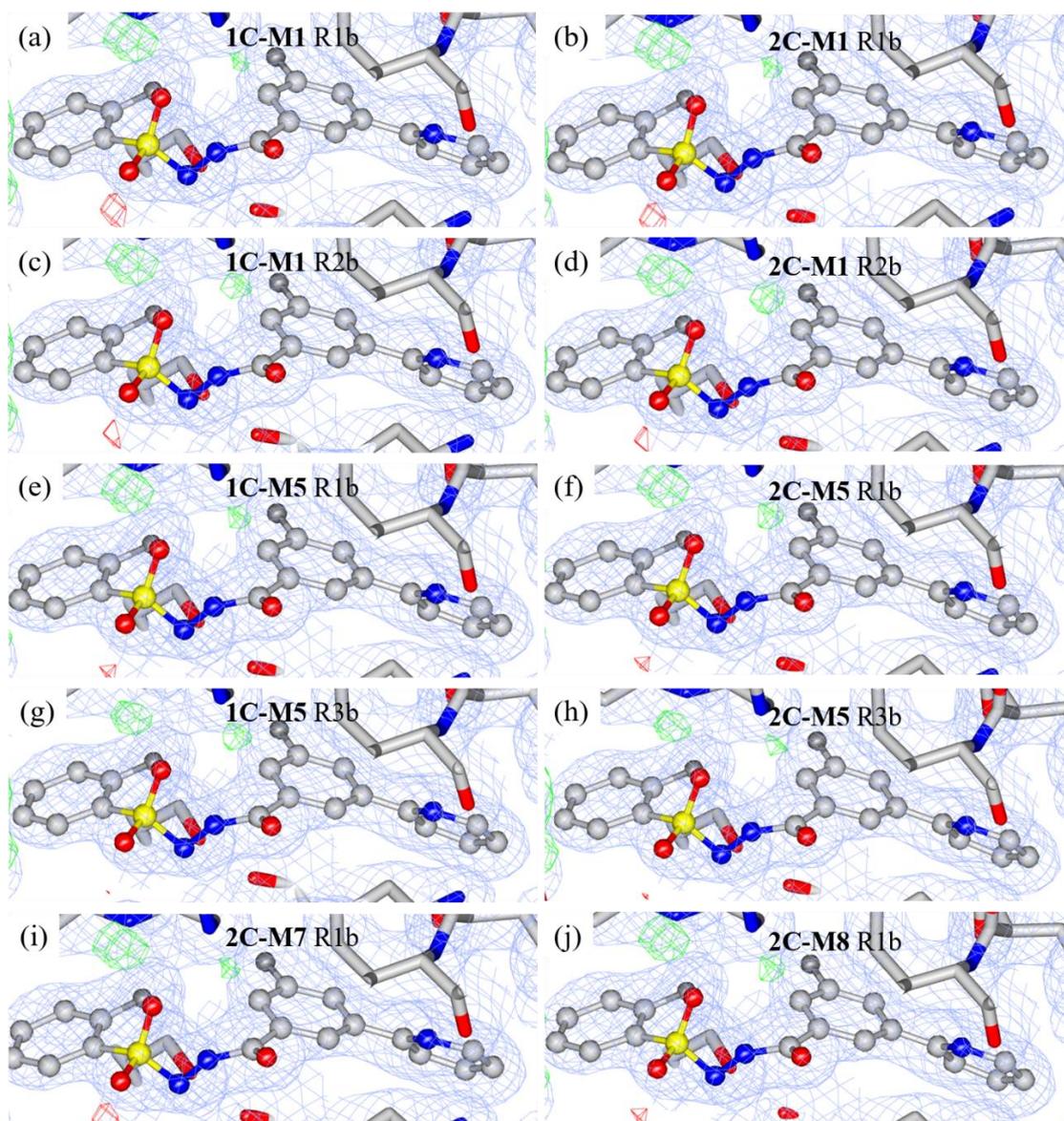


Figure S15. Structures for the FCV binding site in the histone acetyltransferase protein from various quantum refinement schemes with ω_α value of 1.0 using (a) **1C-M1** (with the R1b-optimized region), (b) **2C-M1** (with the R1b-optimized region), (c) **1C-M1** (with the R2b-optimized region), (d) **2C-M1** (with the R2b-optimized region), (e) **1C-M5** (with the R1b-optimized region), (f) **2C-M5** (with the R1b-optimized region), (g) **1C-M5** (with the R3b-optimized region), (h) **2C-M5** (with the R3b-optimized region), (i) **2C-M7** (with the R1b-optimized region) and (j) **2C-M8** (with the R1b-optimized region), including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)).

Table S26. Our quantum refined key structural results with different ω_α values for the zinc binding site using **1C-M1** R1b. The key structural results from the X-ray crystal structure were also given.

	1.0	1.667	3.0	5.0	10.0	20.0	X-ray
Zn-S _{C540}	2.33	2.33	2.33	2.32	2.31	2.29	2.26
Zn-S _{C543}	2.17	2.14	2.11	2.10	2.07	2.07	2.28
Zn-N _{H556}	2.07	2.07	2.06	2.06	2.10	2.14	2.13
Zn-S _{C560}	2.19	2.17	2.14	2.13	2.12	2.11	2.28
N _{H556} -Zn-S _{C540}	100.8	101.8	101.2	101.8	101.2	100.7	107.8
N _{H556} -Zn-S _{C543}	97.2	97.1	97.3	97.3	96.8	97.9	96.7
N _{H556} -Zn-S _{C560}	104.7	104.5	104.4	104.8	105.0	105.7	108.1
S _{C540} -Zn-S _{C543}	110.9	111.1	111.3	111.4	111.8	111.2	105.2
S _{C540} -Zn-S _{C560}	110.7	110.3	109.7	109.6	109.3	109.3	114.0
S _{C543} -Zn-S _{C560}	127.6	127.6	128.2	127.6	128.1	127.6	123.0

Table S27. RSZD scores of residues around the Zn(II) binding site in the histone acetyltransferase from various quantum refinement approaches using **1C-M1** R1b with different ω_α values. RSZD scores of the FCV binding site were also given. Results for X-ray were taken from the experimental structure without our further refinement.

	1.0	1.667	3.0	5.0	10.0	20.0	X-ray
CYM540	2.1	2.0	1.8	1.7	1.6	1.2	0.6
CYM543	1.7	1.4	1.1	1.2	1.8	2.1	1.5
HID556	0.6	0.8	0.4	0.5	0.7	0.7	3.0
CYM560	1.6	1.9	2.3	2.2	2.4	2.2	1.7
Zn(II)	3.6	3.7	4.3	3.9	4.3	3.8	2.7
Sum ^a (Zn center)	9.6	9.8	9.9	9.5	10.8	10.0	9.5
FCV	1.2	1.1	0.6	0.5	0.1	0.1	1.7

a: The sum for Zn center is the sum of CYM540, CYM543, HID556, CYM560 and Zn.

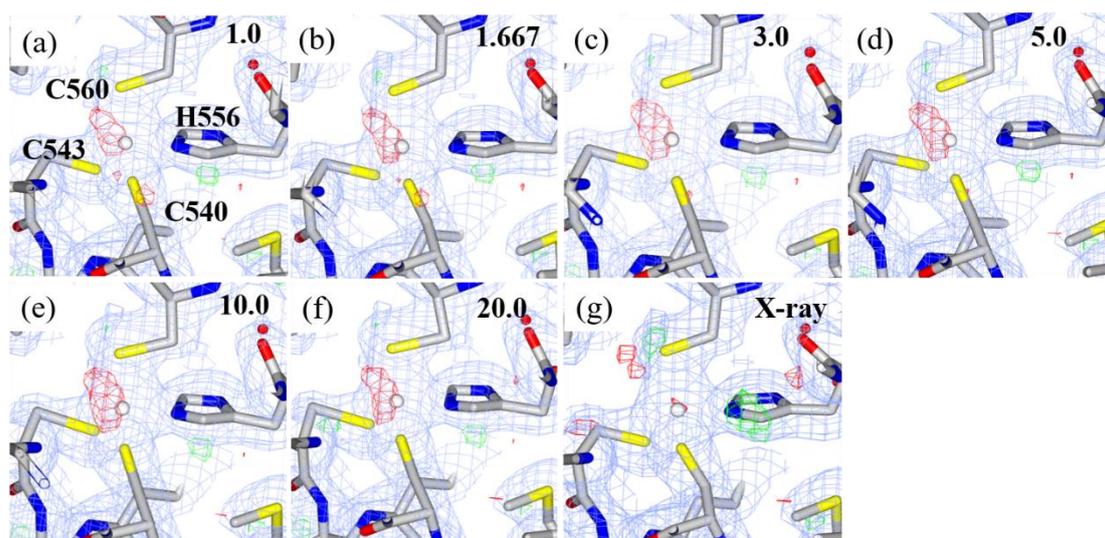


Figure S16. Structures for the Zinc(II) active-site in the MYST histone acetyltransferase KAT6A/B protein from various quantum refinement schemes with different ω_α values using **1C-M1** (with the R1b-optimized region), (a) 1.0, (b) 1.667, (c) 3.0, (d) 5.0, (e) 10.0, (f) 20.0 and (g) the X-ray crystal structure, including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)). Results for X-ray were taken from the experimental structure without our further refinement.

Table S28. Our quantum refined key structural results with ω_α value of 1.667 for the zinc binding site using different multiscale schemes with different optimized regions (R1b, R2b or R3b) for histone acetyltransferase including individual B factors for all atoms. The two-center (2C) ONIOM approximation was also used (values given in parenthesis). The key structural results from the X-ray crystal structure were also given. **1C-M5** R1b results are used as reference for RMSD and MAD computations.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	M7 R1b	M8 R1b	X-ray
Zn-S _{C540}	2.35(2.36)	2.36(2.36)	2.35(2.36)	2.36(2.37)	(2.36)	(2.37)	2.26
Zn-S _{C543}	2.15(2.14)	2.14(2.14)	2.15(2.14)	2.15(2.15)	(2.16)	(2.17)	2.28
Zn-N _{H556}	2.06(2.07)	2.07(2.07)	2.09(2.08)	2.09(2.09)	(2.08)	(2.09)	2.13
Zn-S _{C560}	2.18(2.18)	2.17(2.17)	2.18(2.18)	2.18(2.18)	(2.19)	(2.21)	2.28
RMSD (bonds)	0.01(0.01)	0.01(0.01)	0.00(0.01)	0.01(0.01)	(0.01)	(0.02)	0.10
MAD (bonds)	0.01(0.01)	0.01(0.01)	0.00(0.01)	0.00(0.01)	(0.01)	(0.02)	0.09
N _{H556} -Zn-S _{C540}	100.4(100.6)	100.1(100.1)	101.4(100.5)	100.9(100.9)	(100.7)	(100.7)	107.8
N _{H556} -Zn-S _{C543}	97.6(96.6)	96.5(96.6)	97.2(97.2)	97.0(96.9)	(96.4)	(96.8)	96.7
N _{H556} -Zn-S _{C560}	105.2(106.0)	105.8(105.9)	105.3(105.9)	106.3(106.3)	(106.1)	(106.2)	108.1
S _{C540} -Zn-S _{C543}	110.8(110.0)	110.3(110.3)	110.9(110.4)	110.4(110.4)	(110.0)	(110.3)	105.2
S _{C540} -Zn-S _{C560}	109.9(109.6)	108.7(108.7)	109.5(109.1)	108.4(108.4)	(109.7)	(109.2)	114.0
S _{C543} -Zn-S _{C560}	128.1(129.2)	130.1(130.1)	128.1(129.1)	129.4(129.3)	(129.1)	(129.0)	123.0
RMSD (angles)	0.5(0.8)	1.1(1.1)	0.0(0.6)	0.8(0.8)	(0.8)	(0.7)	4.6
MAD (angles)	0.3(0.7)	1.0(1.0)	0.0(0.6)	0.8(0.7)	(0.7)	(0.6)	4.2
R/ R _{free}	0.221(0.221)/ 0.235(0.235)	0.220(0.220)/ 0.236(0.236)	0.221(0.221)/ 0.235(0.235)	0.220(0.220)/ 0.235(0.235)	(0.221)/ (0.235)	(0.221)/ (0.235)	0.214/ 0.241

Table S29. Our quantum refined key structural results with ω_α value of 1.667 for the FCV ligand using different multiscale schemes with different optimized regions (R1b, R2b or R3b) including individual B factors for all atoms. The two-center (2C) ONIOM approximation (values given in parenthesis) was also used. **1C-M5** R1b results are used as reference for RMSD and MAD computaions.

	M1 R1b	M1 R2b	M5 R1b	M5 R3b	M7 R1b	M8 R1b	X-ray
C2-C7	1.40(1.40)	1.40(1.40)	1.42(1.42)	1.41(1.41)	(1.40)	(1.42)	1.39
C2-C3	1.42(1.41)	1.41(1.41)	1.43(1.43)	1.42(1.42)	(1.41)	(1.43)	1.39
C6-C7	1.41(1.40)	1.40(1.40)	1.39(1.39)	1.39(1.39)	(1.40)	(1.39)	1.39
C7-F1	1.39(1.39)	1.38(1.38)	1.39(1.39)	1.39(1.39)	(1.39)	(1.40)	1.36
C6-C5	1.39(1.38)	1.39(1.39)	1.40(1.40)	1.39(1.39)	(1.38)	(1.40)	1.38
C5-C4	1.40(1.39)	1.40(1.40)	1.40(1.40)	1.40(1.40)	(1.39)	(1.40)	1.39
C4-C3	1.41(1.41)	1.41(1.41)	1.40(1.40)	1.40(1.41)	(1.41)	(1.40)	1.39
C2-S1	1.88(1.88)	1.86(1.87)	1.85(1.83)	1.84(1.84)	(1.88)	(1.83)	1.82
S1-O3	1.47(1.47)	1.47(1.47)	1.49(1.49)	1.48(1.48)	(1.47)	(1.49)	1.47
S1-O2	1.48(1.48)	1.48(1.48)	1.50(1.50)	1.50(1.50)	(1.48)	(1.50)	1.46
S1-N1	1.64(1.65)	1.65(1.65)	1.65(1.65)	1.65(1.65)	(1.65)	(1.65)	1.70
N1-N2	1.38(1.40)	1.38(1.38)	1.41(1.40)	1.40(1.40)	(1.40)	(1.40)	1.40
N2-C1	1.40(1.40)	1.40(1.40)	1.40(1.41)	1.41(1.41)	(1.40)	(1.41)	1.45
C1-O1	1.23(1.23)	1.23(1.23)	1.27(1.27)	1.27(1.26)	(1.23)	(1.27)	1.19
C1-C8	1.47(1.47)	1.47(1.47)	1.44(1.44)	1.45(1.45)	(1.47)	(1.44)	1.52
C8-C9	1.42(1.42)	1.43(1.43)	1.44(1.45)	1.44(1.44)	(1.42)	(1.45)	1.38
C9-C10	1.39(1.39)	1.39(1.39)	1.38(1.38)	1.38(1.38)	(1.39)	(1.38)	1.38
C10-F2	1.36(1.36)	1.36(1.36)	1.37(1.38)	1.37(1.37)	(1.36)	(1.38)	1.36
C10-C11	1.40(1.39)	1.40(1.40)	1.39(1.40)	1.40(1.40)	(1.40)	(1.40)	1.39
C11-C12	1.42(1.41)	1.41(1.41)	1.42(1.43)	1.42(1.42)	(1.41)	(1.43)	1.39
C12-C18	1.39(1.39)	1.39(1.39)	1.38(1.38)	1.38(1.38)	(1.39)	(1.38)	1.38
C18-C8	1.39(1.39)	1.39(1.39)	1.40(1.40)	1.39(1.39)	(1.39)	(1.40)	1.38
C12-C13	1.48(1.46)	1.48(1.48)	1.45(1.46)	1.45(1.45)	(1.46)	(1.46)	1.38
C13-C14	1.38(1.37)	1.38(1.38)	1.38(1.38)	1.38(1.38)	(1.37)	(1.38)	1.38
C14-C15	1.39(1.38)	1.39(1.39)	1.38(1.38)	1.38(1.38)	(1.39)	(1.38)	1.38
C15-C16	1.40(1.39)	1.39(1.39)	1.40(1.40)	1.40(1.40)	(1.39)	(1.40)	1.39
C16-C17	1.39(1.38)	1.39(1.39)	1.38(1.38)	1.39(1.39)	(1.38)	(1.38)	1.39
C17-N3	1.36(1.35)	1.36(1.36)	1.36(1.36)	1.36(1.36)	(1.35)	(1.36)	1.32
C13-N3	1.34(1.34)	1.34(1.34)	1.35(1.35)	1.35(1.35)	(1.34)	(1.35)	1.32
RMSD	0.02(0.02)	0.02(0.02)	0.00(0.00)	0.00(0.00)	(0.02)	(0.01)	0.04
MAD	0.01(0.01)	0.01(0.01)	0.00(0.00)	0.00(0.00)	(0.01)	(0.00)	0.03

Table S30. Strain energy (ΔE , kcal/mol) at B3LYP/6-31G(d) level for the R1b-optimized region of the FCV and Zn centers in the histone acetyltransferase

determined by various quantum refinement schemes with ω_α value of 1.667 including individual B factors for all atoms. The two-center (2C) ONIOM approximation (values given in parenthesis) was also used.

	ΔE	
	FCV	Zn
X-ray	41.1	127.2
M1 R1b	18.1(18.1)	63.1(63.1)
M1 R2b	18.1(18.1)	63.1(63.1)
M5 R1b	23.7(23.5)	63.2(62.9)
M5 R3b	20.8(20.8)	60.6(60.3)

9. Quantum refined results of Amyloid- β

In addition to the main ONIOM-type QM/MM- or QM/SE/MM-based quantum refinement calculations for the two metalloproteins, a small amyloid- β (20-34) protein with L-isoAsp23 (Figure S17a), which contains 223 atoms, was refined by a complete DFT, fragmentation DFT or GFN2-xTB method (**M9-M11**) briefly. B3LYP-D3/def2-SVP¹³⁻¹⁴ with an efficient RIJCOSX algorithm¹⁵ implemented in ORCA 4.2.1 program¹⁶ (**M9**) were also used. Moreover, a generalized energy-based fragmentation (GEBF)¹⁷⁻²⁰ method at the B3LYP-D3/6-31G(d) level implemented in LSQC 2.3 code²¹ (**M10**) was also used. Finally, full SE quantum refinement calculation with an efficient GFN2-xTB implemented in xTB 6.1 code was examined (**M11**). All atoms were fully relaxed in this monomer cluster model. Moreover, a full geometry optimization for this monomer protein using the GFN2-xTB method in the gas phase without experimental data was performed and the results obtained compared with our quantum refinement results.

Quantum refinement calculations with ω_α value of 0.269 or 1.0 were conducted. Different from our previous two applications, the choice of ω_α values show some influence on R and R_{free} factors (Table S31). When ω_α was set to 1.0, the R factors are slightly improved. However, R factors increase by ~ 0.02 , when CNS-suggested value of 0.269 was used. Pleasingly, as shown in Figure S18b, our quantum refinement calculations using the monomer structure and different computational methods (**M9-M11**) were found to give a very similar overall protein structure compared to the X-ray crystal structure with a very small RMSD value (0.08-0.09 with ω_α value of 1.0; 0.12-0.14 with ω_α value of 0.269). Moreover, slightly reduced R/R_{free} factors by these three methods with ω_α value of 1.0 were also observed (0.245/0.256-0.257 vs. X-ray: 0.246/0.263; see Table S31). While, significantly increased R/R_{free} factors by the GFN2-xTB method without experimental data was found (0.560/0.569)^a. From the electron density maps (Figures S19-S20), the reduction of the negative (red contours) difference density closed to the O atom of IAS23 in the resultant electron density maps indicates that the discrepancy with experimental observations was minimized.

^a The R/R_{free} factors are different with the PDB database values, because we use CCP4i2 Remac5 for all R/R_{free} factors computations, which is different from the original program.

The RSZD scores (Table S32) are decreased by 0.4-3.2, compared to the X-ray structure. These results suggest that the non-natural amino acid residue L-isoAsp23 can be well described by the experimental refinement approach or quantum refinement approach. In contrast, normal geometry optimization for the monomer protein structure using the GFN2-xTB method in the absence of the experimental data leads to a substantial structural change with a RMSD value of 2.92 (Figure S18a). A few intramolecular H-bonds were also found to be formed without the experimental data (Figure S17b). Alternatively, in the absence of experimental constrains, one may use periodic boundary conditions (PBC) and full optimization of biomolecules to obtain the protein structures. Overall, our quantum refinement calculations are shown to provide an excellent protein structure using the monomer structure (as a cluster model) and afford a flexible combination with different computational methods (such as fragmentation DFT methods).

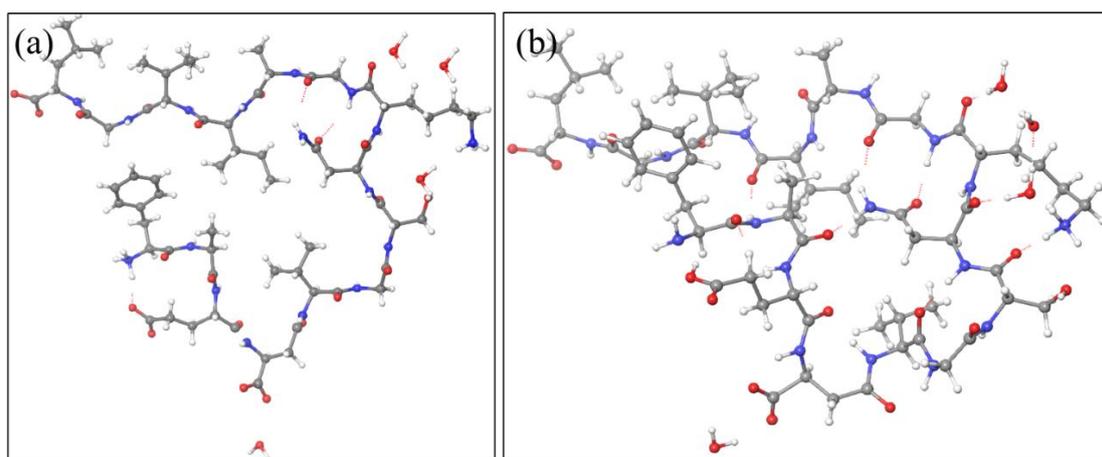


Figure S17. Structures for the amyloid- β (20–34) protein from: (a) the X-ray crystal structure and (b) the full geometry optimization by the GFN2-xTB method in gas phase.

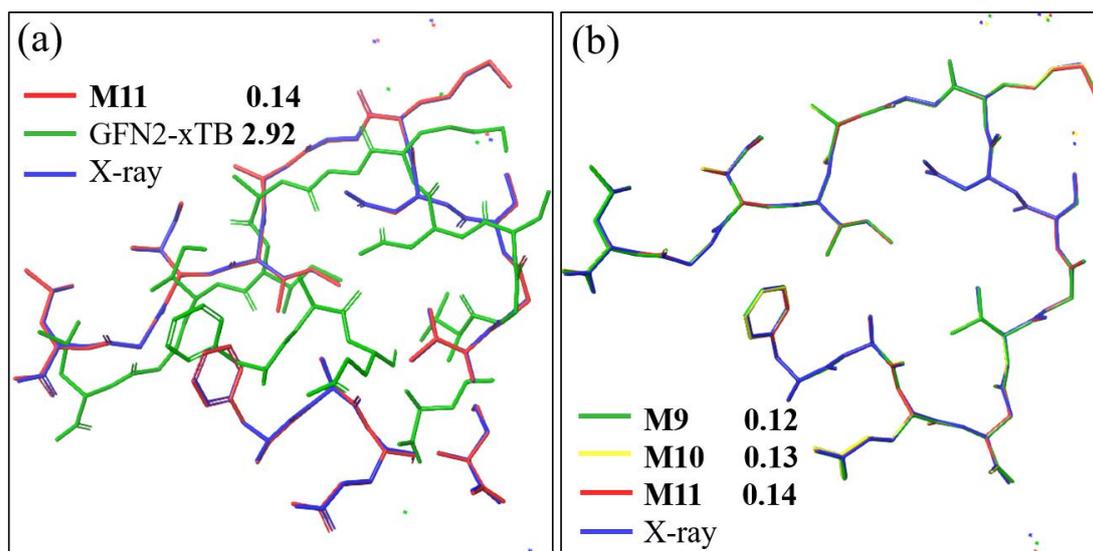


Figure S18. Superposition of the amyloid- β structure: (a) X-ray crystal structure (blue line), our quantum refined results obtained by the GFN2-xTB method (M11, red line; normal optimization without experimental data, green line) and (b) X-ray crystal structure (blue line), our quantum refined results with ω_α value of 0.269 obtained by different computational methods (M9, green line; M10, yellow line; M11, red line). RMSD values were determined based on the positions of the heavy atoms (non-hydrogen).

Table S31. Our quantum refined R and R_{free} factors and RMSD values based on positions of the heavy atoms (non-hydrogen) of the Amyloid- β protein using different computational methods with ω_α value of 0.269 and 1.0 (in parenthesis).

	M9	M10	M11	GFN2-xTB	X-ray
R	0.266(0.245)	0.267(0.245)	0.268(0.245)	0.560	0.246
R_{free}	0.280(0.257)	0.279(0.256)	0.282(0.257)	0.569	0.263
RMSD	0.12(0.09)	0.13(0.09)	0.14(0.08)	2.92	0.00

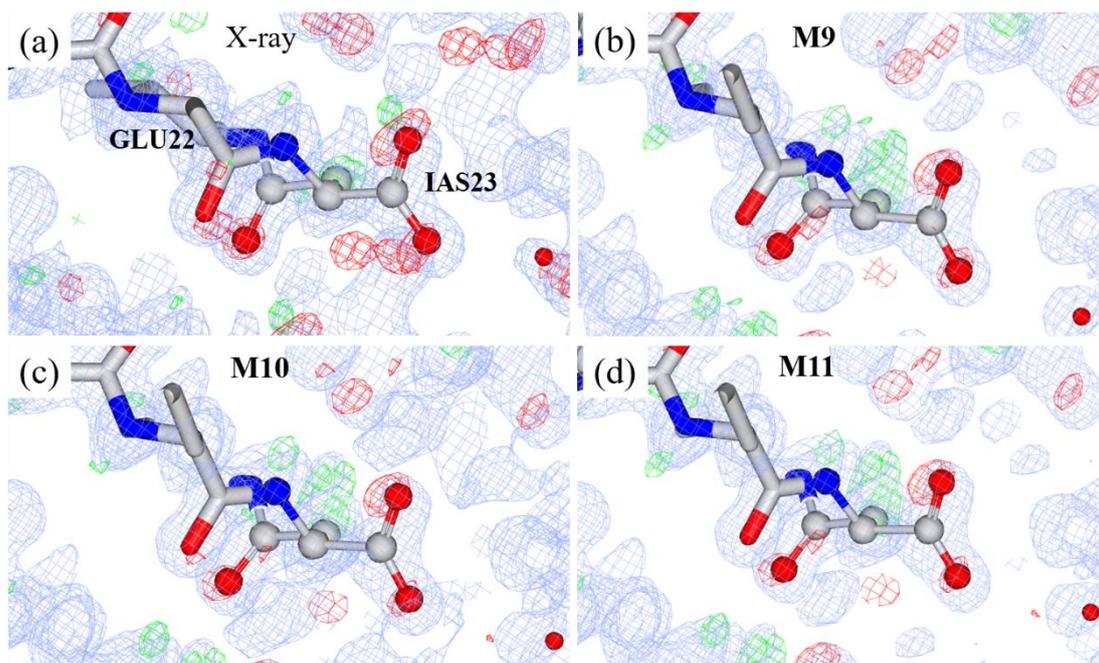


Figure S19. Structures for the L-isoaspartic acid (IAS) in the amyloid- β protein from (a) the X-ray crystal structure and various quantum refinement schemes with ω_α value of 0.269 using (b) **M9**, (c) **M10**, (d) **M11**, including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)).

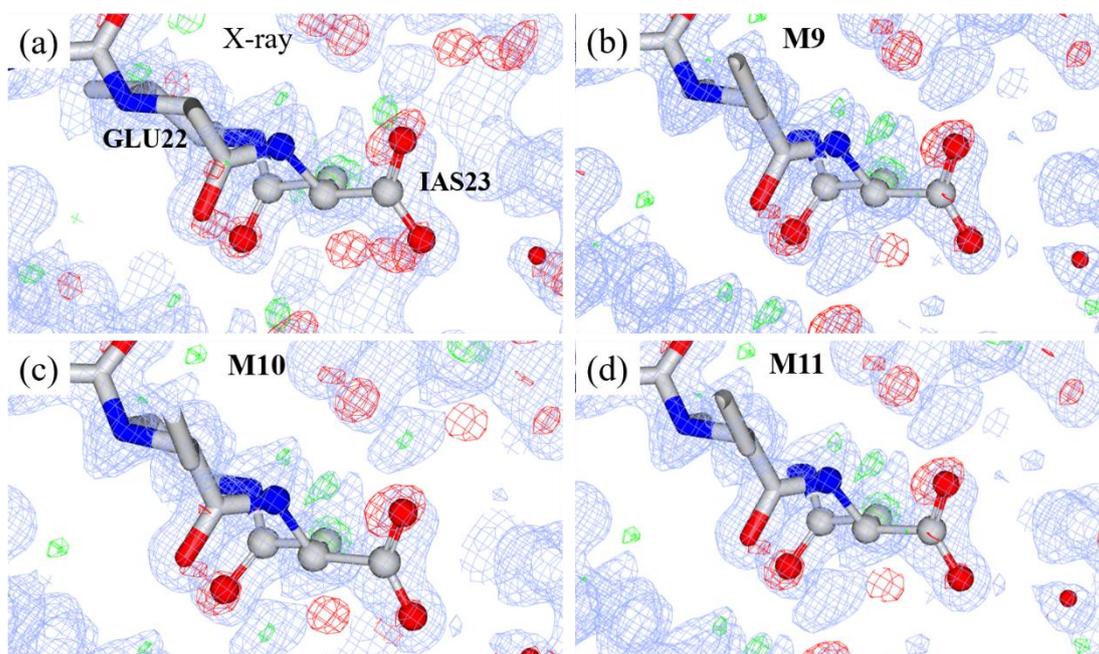


Figure S20. Structures for the L-isoaspartic acid (IAS) in the amyloid- β protein from (a) the X-ray crystal structure and various quantum refinement schemes with ω_α value of 1.0 using (b) **M9**, (c) **M10**, (d) **M11**, including the electron density map ($2mF_o-DF_c$ maps, contoured at 1.0σ (blue), mF_o-DF_c maps, contoured at $+3.0 \sigma$ (green), and mF_o-DF_c maps, contoured at -3.0σ (red)).

Table S32. RSZD scores of residues of the Amyloid- β protein using different computational methods with ω_α value of 0.269 and 1.0 (in parenthesis).

	X-ray	M9	M10	M11
PHE20	1.0	0.2(0.8)	0.1(0.9)	0.1(0.8)
ALA21	0.6	0.8(0.6)	1.1(0.7)	1.0(0.6)
GLU22	1.3	0.8(1.2)	1.6(1.1)	0.8(1.2)
IAS23	4.2	0.2(3.7)	0.1(3.9)	0.2(3.7)
VAL24	0.7	4.0(0.2)	4.0(0.2)	3.9(0.2)
GLY25	3.3	0.5(3.4)	0.5(3.6)	0.6(3.4)
SER26	4.8	2.8(3.8)	2.9(3.6)	2.7(3.8)
ASN27	2.4	2.3(2.4)	2.4(2.4)	2.2(2.4)
LYS28	0.7	3.1(0.8)	3.8(0.8)	3.0(0.8)
GLY29	2.9	0.7(3.1)	0.5(3.1)	0.8(3.1)
ALA30	3.5	3.0(4.3)	2.9(4.4)	2.5(4.3)
ILE31	0.7	4.3(1.0)	4.5(1.1)	4.1(1.0)
ILE32	0.7	1.3(1.0)	1.0(0.9)	1.3(1.0)
GLY33	0.3	0.3(0.1)	0.4(0.1)	0.4(0.1)
LEU34	0.1	0.3(0.0)	0.4(0.0)	0.4(0.0)
Sum	27.2	24.6(26.4)	26.2(26.8)	24.0(26.4)

10. Cartesian coordinates of the quantum refinement results

A. Cartesian coordinates of all optimized regions for Rusticyanin (RC)

QM/MM R1a (B3LYP/6-31G(d):Amber) mechanical embedding $\omega_c=0.606$

C	7.55004347	3.24440157	12.93181343	O	-6.56560798	3.89054607	12.70208114
C	7.13291798	4.14961944	11.77800995	N	-4.51159013	4.61501248	12.02207668
O	7.98132382	4.55973181	11.00097198	C	-4.28069155	5.40052268	13.22602998
N	5.80659312	4.48548801	11.73814437	C	-4.58497854	6.88690580	12.94850859
C	4.68223021	3.94816357	12.53373920	O	-4.18865823	7.44875845	11.91925291
C	3.99186529	2.82505812	11.72627279	C	-2.79102258	5.23039419	13.63894729
O	3.86429536	2.87956139	10.50742461	S	-2.46231683	6.22510006	15.12751620
C	3.77601788	5.19424589	12.68696323	H	-3.88909591	4.74106994	11.22954230
C	3.92094409	5.86614225	11.30927501	H	-4.92185432	4.99649947	14.00967774
C	5.41253863	5.66574651	10.94664964	H	-2.59581110	4.18185708	13.87293100
H	4.98127523	3.58231314	13.52060326	H	-2.13734830	5.55277201	12.82373723
H	2.74982916	4.91658060	12.92657965	N	-5.27914818	7.51853149	13.92674936
H	4.16801163	5.83155882	13.49020505	C	-5.68850308	8.92314693	13.78214548
H	3.28844021	5.36669808	10.57276982	C	-4.66815673	9.91965784	14.36584187
H	3.65086803	6.92382581	11.34348062	O	-4.84837163	11.12323042	14.25064085
H	5.56950360	5.50266327	9.87812818	H	-5.65951047	7.03265132	14.73862163
H	6.02541094	6.52337136	11.25146755	H	-5.79606369	9.17452414	12.72606091
N	3.52838974	1.75377178	12.42984722	N	-3.55395013	9.45448935	14.95059122
C	2.87955976	0.62382556	11.74867027	C	-2.55779500	10.44163269	15.42081372
H	3.72000217	1.59606073	13.41365416	C	-2.06039873	11.18610427	14.19245641
C	-1.19768600	6.69016405	21.93730110	O	-1.63988817	10.51878398	13.23494371
C	-1.98299267	6.38325708	20.69201893	C	-1.39590706	9.80758834	16.17265622
O	-3.06648589	6.88568683	20.45764332	C	-1.95905915	9.17251210	17.44883449
N	-1.38674237	5.45537496	19.90950321	C	-0.29051226	10.86475787	16.47514154
C	-1.99542130	5.12439943	18.61600903	C	-0.85777857	8.59590734	18.35098932
C	-3.47919305	4.68544272	18.79685831	H	-3.42479018	8.45022170	14.99971654
O	-3.88006122	4.20824117	19.84934933	H	-3.07395174	11.11976894	16.09552435
C	-1.20363313	3.97837273	17.97948478	H	-0.97036979	9.02487854	15.53417160
C	0.26400634	4.26474878	17.90434888	H	-2.51844104	9.92133085	18.02517686
C	1.29155912	3.80244328	18.71340888	H	-2.65931622	8.36843873	17.19280288
N	0.81029796	4.99568870	16.89152703	H	0.12831858	11.33340079	15.57622361
C	2.11849031	4.97707303	17.03099152	H	0.55955767	10.41067430	16.99895180
N	2.44955620	4.26650579	18.13488971	H	-0.66789532	11.66640531	17.12156600
H	-0.54220887	4.99563468	20.22547484	H	-0.28630408	7.81229767	17.83231431
H	-1.97409005	6.01007570	17.97475918	H	-1.29471626	8.16401295	19.24819875
H	-1.37330767	3.05227740	18.54294320	H	-0.14580685	9.36576615	18.66456359
H	-1.59695081	3.81172339	16.97203672	C	0.73408869	8.44698170	11.22696621
H	1.30194254	3.20722863	19.60506979	C	0.24440880	7.79117239	12.51408324
H	2.84772340	5.44985218	16.39076764	C	1.10535184	8.14410745	13.69278346
H	3.40205051	4.11584428	18.46241710	C	2.08361514	9.10666461	13.79704767
N	-4.27146429	4.83288181	17.67794654	N	0.99875995	7.46295193	14.90272450
C	-5.64622812	4.33245222	17.67242751	C	1.89827233	8.03579255	15.72794610
C	-5.73753407	3.23903336	16.59034541	N	2.56569994	9.01794033	15.09651729
O	-4.87029079	3.14161330	15.73060064	H	-0.80185130	8.07417738	12.67285930
C	-6.70115085	5.42936769	17.38354870	H	0.26703883	6.70876279	12.35804855
O	-6.48291670	5.97422245	16.07575826	H	2.47964632	9.83752059	13.10929464
H	-3.88425750	5.11221220	16.78488151	H	2.07959399	7.76130445	16.75492803
H	-5.82230763	3.91375004	18.66736941	H	3.29295689	9.59501134	15.50045615
H	-7.70068786	4.98151518	17.43316583	C	0.15298353	3.49823199	9.52582605
H	-6.62776137	6.21817766	18.13830975	C	0.27749759	4.19982587	10.89855162
H	-7.37603010	5.92706952	15.64557175	C	-0.02916590	3.17241275	11.97266968
N	-6.81299220	2.41284882	16.67379389	S	0.49673266	3.81401569	13.61938975
C	-7.15276786	1.44305430	15.62573488	C	0.03850144	2.38317186	14.62968456
H	-7.48080538	2.45274419	17.44211500	H	1.30522301	4.56082355	10.98736972
C	-5.92917906	3.50961634	10.40358452	H	-0.39450457	5.06138577	10.93838624
C	-5.71788340	4.00576895	11.83909879	H	-1.09964302	2.95322620	12.01099094
				H	0.49602956	2.23016709	11.80908674
				H	-1.00525978	2.10978168	14.46703063
				H	0.67430602	1.53103879	14.40110106
				H	0.17407186	2.64861243	15.67762650
				Cu	-0.23133990	5.99199098	15.34708459

**QM/MM R2a (B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_a=0.606$**

N 0.23726650 -1.96655459 17.88130322
C 0.89034138 -0.80871317 17.28884248
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H	-3.79225722	14.78888735	14.16094039	H	-1.03004423	2.18629029	14.57647166
H	-1.95032964	13.42382232	16.12796972	H	0.58497112	1.49351331	14.29622583
H	-3.64150071	13.02407689	15.69701193	H	0.31920216	2.60146868	15.65685364

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O -1.97209892 11.14837698 8.89915797
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H -2.61591939 10.13871276 11.93029723
H -3.51956550 9.04002318 11.37459735
O 2.39152318 11.81916700 18.51223457
H 2.12757267 12.57744857 17.98336678
H 2.83940804 12.21634411 19.26462415

QM/SE/MM R1a (B3LYP/6-31G(d):xTB:Amber)
mechanical embedding $\omega_\alpha=0.606$

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C 3.79532675 5.18045019 12.67943036
C 3.92962045 5.84921197 11.29705758
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H 5.01855130 3.57432994 13.51553643
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H 3.29242894 5.35181977 10.56410840
H 3.66875403 6.90995165 11.30374440
H 5.55465963 5.47574753 9.85173219
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H -2.59287356 4.17589980 13.83506878
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O -1.63439100 10.54969851 13.23221675
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C -1.97146979 9.17889839 17.42726385
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C -0.86396808 8.60819387 18.32578247
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H -0.29055718 7.83533426 17.80069941
H -1.30168869 8.16050644 19.21542280
H -0.15991832 9.38368508 18.64622177
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C 1.09503017 8.15478613 13.67595219
C 2.07431900 9.11620734 13.75658200
N 1.01041195 7.47489596 14.88954179
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H 2.45486695 9.84240040 13.05677911
H 2.10756306 7.77961206 16.72259031
H 3.30612457 9.61570351 15.44130704
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C 0.22126249 4.20521573 10.89363715
C 0.00322141 3.15166993 11.96510703
S 0.49575444 3.81371813 13.61479810
C 0.07910528 2.36104326 14.61530170
H 1.20938479 4.67353880 10.97545557
H -0.55191703 4.98186770 10.94363641
H -1.04562799 2.84051675 12.00467232
H 0.61800620 2.26488520 11.79506708
H -0.95466710 2.04920858 14.43747218
H 0.76034900 1.53455092 14.39449747
H 0.19340600 2.64181530 15.66252977

Cu -0.23750203 5.99320940 15.34635263

**QM/SE/MM R3a (B3LYP/6-31G(d):xTB:Amber)
mechanical embedding $\omega_c=0.606$**

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N 0.25960607 -2.00381811 17.87172446
C 0.88790980 -0.84653080 17.27797933
C 2.43451036 -0.88843100 17.63427370
O 2.80285372 -0.81404053 18.79626829
C 0.32669429 0.47119012 17.81302300
H -0.03664570 -2.00694881 18.84006625
H 0.75468678 -0.92235860 16.19709184
H -0.41345626 0.27690984 18.58771247
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H 1.10833897 1.08230476 18.25250354
N 3.19774627 -0.96874364 16.55475186
C 4.67096226 -0.93574767 16.53770984
C 5.20583617 -1.89985917 17.62761082
O 5.61072990 -1.51948727 18.70731339
C 5.22926091 0.49898344 16.78631417
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H 7.36993736 0.67529325 17.23491259
H 7.03719967 -0.36665978 15.87233308
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H	-3.34265033	-3.97514434	19.97989607	C	-1.93250451	6.38722140	20.76640403
H	-3.28493871	-3.20277091	22.85230808	O	-3.01870347	6.90083323	20.49926841
N	-1.52025732	-1.46543229	22.36603481	H	0.11242498	8.27323552	21.41385523
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C	0.75781753	-0.73399407	22.81055163	H	-1.79053732	7.39715666	22.65509996
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C	-1.01012153	0.93659126	22.46028719	C	-1.99478100	5.14791855	18.64871034
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N	-0.01001167	3.10993184	22.83398969	O	-3.87033350	4.19952556	19.86750422
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H	-2.00028429	-1.41166005	23.25813271	C	0.26563777	4.26008223	17.93166734
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C	3.00908056	-1.66198424	22.66961513	H	-1.37978812	3.06670290	18.57657617
C	4.12891319	-0.61953806	22.49668091	H	-1.60440903	3.83898704	17.00519097
O	5.27002535	-0.80490910	22.88222569	H	1.28074845	3.16581122	19.62514045
C	3.44205327	-3.00412880	22.07446706	H	2.83991397	5.43314022	16.41097181
H	1.61062415	-1.47635376	21.12325211	H	3.42352059	4.09079194	18.45974459
H	2.87095857	-1.79196425	23.74137503	N	-4.25653116	4.82621691	17.69003764
N	3.74477655	0.53075777	21.90613510	C	-5.63000780	4.30945480	17.66814171
C	4.70325975	1.52276695	21.51048695	C	-5.72483387	3.22528725	16.57588252
C	4.79377464	2.64609371	22.54801269	O	-4.85367528	3.11838754	15.72064567
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C	4.30393074	2.09996048	20.14330130	O	-6.49385850	5.96838620	16.08696031
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H	2.78268479	0.67439381	21.61667645	H	-6.62619206	6.19569582	18.14508642
H	5.68090000	1.03723990	21.45447732	H	-7.38379415	5.94735945	15.64945959
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H	6.93465006	1.74761174	20.00978015	C	-8.56071569	1.71829696	15.19405455
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H	6.68343987	1.97906277	23.02753304	C	-8.32956936	-1.62299463	14.74668386
C	5.40290403	7.37737485	24.14635102	C	-5.94931406	-1.61153758	14.49007216
C	4.33673452	7.84775315	23.17163582	C	-8.39443186	-2.65068644	13.81403271
O	4.21125141	9.03529871	22.99772054	C	-6.02620485	-2.63083501	13.56407256
N	3.63059504	6.91770979	22.52500315	C	-7.25770784	-3.14973092	13.22861105
C	2.56802241	7.36565956	21.63583179	H	-7.48936176	2.48069006	17.40056888
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C	2.84616475	6.95939739	20.17216973	H	-7.79088866	-0.15548095	16.85987594
C	4.12625566	7.59947860	19.76715644	H	-9.22473008	-1.23006420	15.20202476
C	5.33945760	7.00050208	20.09927346	H	-4.98863842	-1.19679108	14.75590146
C	4.09974211	8.83518009	19.13857129	H	-9.35619940	-3.06617540	13.54775601
C	6.51348796	7.65389761	19.80446596	H	-5.13225074	-3.01169125	13.09475737
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C	6.48924732	8.88475574	19.18167391	N	-8.69848684	2.46901788	14.09811335
H	3.65231326	5.92757309	22.71648325	C	-10.03264247	2.88332358	13.64387092
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C	-6.41513611	6.18155563	22.44386309	H	-11.11389081	8.83314781	15.21266141
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C	-7.52937196	5.44197576	10.20870156	H	-1.85549567	15.48280943	12.88442535
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QM/SE R1a (B3LYP/6-31G(d):xTB) mechanical embedding $\omega_c=0.606$

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H	0.74586525	1.53086383	14.39695088	H	5.60964494	5.40978919	9.86479864
H	0.19360177	2.64403993	15.66565427	H	6.08876236	6.43635177	11.22597712
Cu	-0.23633214	5.99164018	15.34522613	N	3.50282320	1.72283330	12.43179276
				C	2.91651637	0.61450162	11.70261744
				C	2.09064582	-0.21872133	12.68396990
				O	2.32777191	-0.17876123	13.88993953
				C	3.97204419	-0.32574272	11.03436061
				O	4.77675566	-1.04191195	11.95192741
N	0.25508524	-1.98030858	17.90194649	H	3.55369496	1.60780347	13.43945252
C	0.88897420	-0.84148797	17.28292243	H	2.29849358	1.02610302	10.89754716
C	2.43638341	-0.87995255	17.62659659	H	3.41483677	-1.07749571	10.46979980
O	2.79821312	-0.82061819	18.79877570				

QM/SE R2a (B3LYP/6-31G(d):xTB) mechanical embedding $\omega_c=0.606$

H	4.58990357	0.27367114	10.35644405	H	5.70375313	1.06116915	21.47621532
H	5.49672224	-0.47086706	12.29464832	H	4.11495977	1.26348013	19.48710696
N	1.17493655	-0.98870593	12.10639778	H	3.39032862	2.65963938	20.28173302
C	0.45205479	-2.02235142	12.82227124	H	6.94211655	1.75946163	20.02209059
C	1.00093854	-3.42876871	12.50637966	H	7.32973515	3.22730494	19.17827880
O	1.42121646	-3.70651480	11.37915724	N	3.60639130	6.92609826	22.54742336
C	-1.01001353	-2.01338323	12.34445515	C	2.55384646	7.37906179	21.64269068
C	-1.82915106	-0.79106530	12.70040495	C	1.24073395	6.67333887	21.98969242
C	-2.25784557	-0.58218323	14.01190002	O	1.27113748	5.51328051	22.37090840
C	-2.22168069	0.10640730	11.70565879	C	2.84137935	6.96916945	20.18652204
C	-3.08068516	0.48671223	14.31533259	C	4.13653052	7.57858050	19.78701831
C	-3.02141834	1.18652651	12.03283602	C	5.33395400	6.96110382	20.13970901
C	-3.46048695	1.37864952	13.33477707	C	4.13611981	8.80229395	19.13818860
H	1.05874177	-1.00488130	11.09220311	C	6.52425894	7.58782329	19.84784218
H	0.53133089	-1.82874559	13.89361360	C	5.33710225	9.42040495	18.84704777
H	-0.95240415	-2.09344586	11.25710770	C	6.52718900	8.81027926	19.20641262
H	-1.51067206	-2.90421811	12.73274566	H	3.64025988	5.93401525	22.74468069
H	-1.96423094	-1.28071670	14.78254162	H	2.48431325	8.46441511	21.74034570
H	-1.87808469	-0.03562093	10.69194867	H	2.87873363	5.87900608	20.14527718
H	-3.41173943	0.65497470	15.32990365	H	2.02549585	7.32315958	19.54787960
H	-3.32640766	1.87734336	11.26109114	H	5.32546383	6.00571685	20.63768128
H	-4.09489236	2.21400600	13.58346105	H	3.20360848	9.27597904	18.86536570
N	-6.91960972	-4.87913521	20.30953492	H	7.45840398	7.13101374	20.12414521
C	-5.91465570	-3.93879540	19.91638881	H	5.34932073	10.36979370	18.33539565
C	-5.01273219	-3.60173401	21.12463150	H	7.46436832	9.29511637	18.97631323
O	-5.52909878	-3.23642935	22.16671293	N	0.09787537	7.34383230	21.80080272
C	-6.57972553	-2.62305796	19.47281500	C	-1.17631206	6.70122984	22.06286513
C	-5.54991234	-1.58140151	19.14887514	C	-1.94150276	6.38692384	20.75771277
C	-4.57216099	-1.82526675	18.20623258	O	-3.02474385	6.90358337	20.49299217
C	-5.56739256	-0.36370684	19.79742830	H	0.10367868	8.28519264	21.44249468
C	-3.65034169	-0.83980047	17.90219123	H	-1.00128729	5.76471426	22.59310909
C	-4.64287189	0.62184962	19.52078529	H	-1.81355392	7.34431865	22.67059881
C	-3.67706367	0.37214698	18.55186901	N	-1.38149464	5.46229011	19.94900006
H	-7.56480711	-4.63149380	21.05788795	C	-1.99336975	5.14130822	18.64109356
H	-5.32738375	-4.39460191	19.11769483	C	-3.47596331	4.69410690	18.79040118
H	-7.18856780	-2.82982648	18.58740377	O	-3.88387158	4.19817541	19.85283269
H	-7.23641135	-2.27283132	20.26702675	C	-1.20005095	3.98224997	18.01409624
H	-4.53925953	-2.76515663	17.67903060	C	0.27420465	4.25745898	17.93310912
H	-6.32854562	-0.18571886	20.54091500	C	1.30169851	3.77596009	18.73139733
H	-2.88515199	-1.03730034	17.16537153	N	0.80904127	4.99798522	16.92106629
H	-4.66361352	1.56905628	20.03542267	C	2.11431935	4.97087374	17.05558480
H	-2.95057540	1.13496534	18.31172784	N	2.46187938	4.25015962	18.15283070
N	-1.51373841	-1.48951797	22.35391917	H	-0.52378376	5.00538673	20.22620470
C	-0.54874186	-0.46197373	22.00442246	H	-1.94933333	6.00834972	17.97855852
C	0.76737578	-0.73932997	22.77185164	H	-1.36646590	3.06008176	18.58028241
O	0.81964135	-0.48866058	23.96375629	H	-1.59049871	3.82709996	17.00467045
C	-1.00194364	0.92515657	22.47046704	H	1.29350795	3.16271901	19.62175095
C	0.05593269	1.95612344	22.14573234	H	2.84010584	5.44846589	16.41584954
N	-0.00885939	3.10357554	22.82337037	H	3.43422064	4.10475108	18.46159451
O	0.95176660	1.70676389	21.34928720	N	-4.26088287	4.82588827	17.68217861
H	-1.98571028	-1.44101593	23.25260743	C	-5.64158786	4.30832957	17.66180142
H	-0.38599219	-0.49191952	20.92817982	C	-5.73654876	3.21318109	16.57872881
H	-1.90280755	1.21508349	21.91924823	O	-4.87232559	3.11969221	15.71217109
H	-1.25257309	0.92632198	23.52744403	C	-6.67926437	5.42498076	17.36027338
H	-0.75444583	3.27618198	23.48070568	O	-6.47571675	5.97525686	16.07050112
H	0.68330842	3.82551445	22.65840135	H	-3.84507602	5.12679249	16.79962099
N	3.75941321	0.53541329	21.88648810	H	-5.84877893	3.89833893	18.65348061
C	4.72443695	1.54456281	21.51891666	H	-7.67960597	4.98344508	17.40872446
C	4.78661591	2.67099807	22.56503694	H	-6.60967232	6.21225197	18.12054367
O	3.90367820	3.45907352	22.80342324	H	-7.33923588	5.93444483	15.60236340
C	4.32034730	2.11162517	20.14983161	N	-6.81758746	2.38752133	16.66288207
C	5.35706345	2.99910308	19.53007211	C	-7.13300814	1.42495577	15.60262450
N	6.64303831	2.64064794	19.63624072	C	-8.58975372	1.72301800	15.18908984
O	5.02575532	4.01442872	18.93839238	O	-9.51306928	1.34477486	15.88927072
H	2.79847597	0.69321801	21.59277509	C	-6.99889451	-0.01950306	16.13097772

C	-7.09781931	-1.08926735	15.08549881	O	-4.21068375	7.44922736	11.92810090
C	-8.33245903	-1.62490348	14.74415196	C	-2.79528264	5.23467206	13.63226955
C	-5.95039883	-1.59894111	14.49201452	S	-2.46369160	6.21874687	15.13249845
C	-8.39188234	-2.65275603	13.81238357	H	-3.89883040	4.78883045	11.22099850
C	-6.02345346	-2.61998209	13.56624754	H	-4.90343958	4.96806207	14.01838500
C	-7.25096845	-3.14604151	13.22754017	H	-2.58843403	4.17807190	13.81538877
H	-7.47725370	2.46543901	17.43522963	H	-2.16409258	5.59025011	12.81183479
H	-6.45491778	1.61068284	14.76683379	N	-5.26424928	7.53399732	13.95160193
H	-6.03996296	-0.08623481	16.64704659	C	-5.66552829	8.92146834	13.79274947
H	-7.79583044	-0.15600852	16.86360779	C	-4.64206589	9.93035062	14.36702756
H	-9.23116607	-1.23815784	15.19625910	O	-4.82390535	11.12616556	14.26662922
H	-4.99143572	-1.18063761	14.75709627	C	-7.02092013	9.16924393	14.47241848
H	-9.35021212	-3.07322552	13.54366069	C	-8.15317492	8.48327197	13.69938869
H	-5.12535878	-2.99190759	13.09865253	C	-9.48535276	9.16079137	14.05672861
H	-7.31640328	-3.94875122	12.50744335	N	-10.24991622	8.49858817	14.93900037
N	-8.04753501	6.97852665	20.76581600	O	-9.80351873	10.22468558	13.57213325
C	-6.63254815	7.01114720	21.16437074	H	-5.55661684	7.03618773	14.79246819
C	-6.41230165	6.15807610	22.44437227	H	-5.74869962	9.12782058	12.71797682
O	-7.14999595	6.22163039	23.41993551	H	-6.99080506	8.78807747	15.49351974
C	-6.18920856	8.45334169	21.44373198	H	-7.19574091	10.24553016	14.49909998
C	-6.18836829	9.29724215	20.19882826	H	-8.00686136	8.62432869	12.62659387
C	-5.43562040	8.92941601	19.09490400	H	-8.20106813	7.41876215	13.92787731
C	-6.96946921	10.45167303	20.11139905	H	-11.13517389	8.89444671	15.21138245
C	-5.45382105	9.70507494	17.93848778	H	-9.95541205	7.60326042	15.30356072
C	-6.99809285	11.21566148	18.95077396	N	-3.52506441	9.43499851	14.93505169
C	-6.23674525	10.84664942	17.85114811	C	-2.58204754	10.44108728	15.43709389
H	-8.54532599	7.85875394	20.73756211	C	-2.07965606	11.19479580	14.22816011
H	-6.03621523	6.57111326	20.36143510	O	-1.65815940	10.56719933	13.24274584
H	-6.83695107	8.89513961	22.20053809	C	-1.41143897	9.81219848	16.17164586
H	-5.16985198	8.39651492	21.83459305	C	-1.96931565	9.16580654	17.44715698
H	-4.80685211	8.05280710	19.13060027	C	-0.32164358	10.89145839	16.45627158
H	-7.56908289	10.75387267	20.95794411	C	-0.86094370	8.60432510	18.35448464
H	-4.85752193	9.39814143	17.09430806	H	-3.30004280	8.44422787	14.97827683
H	-7.60645698	12.10595508	18.91670726	H	-3.12476767	11.10001068	16.11719099
H	-6.25120039	11.43504096	16.94799904	H	-0.97391364	9.04403364	15.52319222
N	-5.35010128	5.35648320	22.39415215	H	-2.54804089	9.90222656	18.01995909
C	-4.99924840	4.44618623	23.48230007	H	-2.65349798	8.35364569	17.18014760
C	-4.10622463	5.15279276	24.50214278	H	0.05058362	11.35491625	15.53655464
O	-3.48380435	6.15695047	24.23290384	H	0.53982298	10.46329902	16.97393384
C	-4.20400166	3.27691832	22.89780092	H	-0.71469134	11.67942876	17.11036860
O	-2.98848407	3.66843389	22.32127227	H	-0.27595470	7.83504202	17.83665147
H	-4.72459871	5.38675551	21.59931718	H	-1.29313006	8.15362936	19.24344002
H	-5.92124036	4.10445408	23.95730229	H	-0.16226948	9.38338329	18.67791176
H	-3.97027032	2.56463988	23.69227482	N	-2.14925851	12.51235950	14.25394916
H	-4.83462547	2.77295872	22.15588880	C	-1.73541801	13.31962349	13.08026309
H	-3.17120324	3.97295755	21.40850197	C	-0.35918811	12.87738412	12.55800294
N	-6.83081578	2.39635781	10.37219604	O	0.61777011	12.74520433	13.28126158
C	-5.92342593	3.51963256	10.34109429	C	-1.69480157	14.73140081	13.66366631
C	-5.70551241	4.01833044	11.79174814	C	-2.83431130	14.70870136	14.67256211
O	-6.56348115	3.89717045	12.66407611	C	-2.67152756	13.33358286	15.31840352
C	-6.46025560	4.68289510	9.47861871	H	-2.48771872	13.23702179	12.29214007
C	-7.02328635	4.20046502	8.11941568	H	-0.73859007	14.89269860	14.16635595
C	-7.53622125	5.43335640	10.24901756	H	-1.82276968	15.48819328	12.89365594
H	-7.67281863	2.50359514	10.93844464	H	-2.78193209	15.51752951	15.39596523
H	-4.97287801	3.15400862	9.94055544	H	-3.78761945	14.77080668	14.14929670
H	-5.61264531	5.34544526	9.28774201	H	-1.93342128	13.38772206	16.12721660
H	-8.01693929	4.59270715	7.93887444	H	-3.61647398	12.95493533	15.70378562
H	-6.38115018	4.53575616	7.30912260	N	-0.35880829	12.63894263	11.23409579
H	-7.08718915	3.12148454	8.05896366	C	0.79620306	12.22028349	10.48068004
H	-8.15938878	4.75206813	10.81922047	C	1.02693918	10.73419339	10.32146255
H	-8.17533803	5.95991753	9.55004652	O	1.70286544	10.34159578	9.37904398
H	-7.10047906	6.15861542	10.93286508	H	-1.23019164	12.76469617	10.72723479
N	-4.51111479	4.62129303	12.01192863	H	0.76027445	12.65721770	9.48181997
C	-4.28995084	5.40230376	13.23109630	H	1.68679240	12.59590937	11.00428185
C	-4.58933534	6.88602882	12.97623497	N	0.51393532	9.91225598	11.24800352

C	0.81738205	8.49468211	11.21216322	H	1.99594638	12.45835976	18.16213291
C	0.24571817	7.77663244	9.95357142	H	2.94929567	11.92777011	19.26495647
O	0.96183231	7.02946772	9.30326584				
C	0.29536451	7.80045042	12.47246279				
C	1.13461996	8.15453179	13.67457457				
C	2.10282748	9.12056880	13.79809511				
N	1.01009005	7.46592624	14.87989601				
C	1.88362311	8.03685290	15.72105967				
N	2.56152448	9.02777605	15.10887000				
H	-0.08494187	10.27162413	11.98506418				
H	1.90527597	8.36924169	11.13350870				
H	-0.75189861	8.09643211	12.64067158				
H	0.32535884	6.71701651	12.31034063				
H	2.49713502	9.85179866	13.11163184				
H	2.05031669	7.76268559	16.74997200				
H	3.27586904	9.60902547	15.52514900				
N	-1.04122106	7.97273037	9.66740674				
C	-1.61845806	7.35549089	8.48132456				
C	-0.90102315	7.82992197	7.20730758				
O	-0.69220114	7.05798653	6.27123690				
C	-3.12294024	7.68888267	8.40172978				
H	-1.63619167	8.58555378	10.23224682				
H	-1.47311781	6.27046258	8.54826850				
H	-3.38373275	8.07318788	7.42489036				
H	-3.37698420	8.43548892	9.14482836				
H	-3.72020923	6.80320019	8.58838315				
N	2.11615797	8.52295329	6.94162234				
C	3.42272898	7.93118165	6.77026501				
C	3.36051477	6.39941885	6.78993748				
O	4.36340436	5.74072830	7.01059669				
C	4.42552544	8.45359624	7.81906770				
C	4.95609175	9.83894435	7.42910313				
O	3.84000659	8.47707559	9.08182318				
H	1.73522783	8.57037814	7.87672412				
H	3.78036367	8.24125784	5.77931423				
H	5.23087690	7.71543907	7.88595987				
H	3.17060470	9.18436261	9.10896587				
H	5.20973163	10.40292121	8.32202318				
H	4.21973010	10.39724434	6.85784583				
H	5.85945688	9.74340372	6.83267963				
N	0.76991223	4.24189729	8.46339101				
C	0.16267570	3.43829467	9.50550275				
C	-1.34016392	3.18081007	9.19261660				
O	-2.23666075	3.84239318	9.69513805				
C	0.26003365	4.14549152	10.87955740				
C	-0.02376425	3.13483605	11.97174940				
S	0.49052282	3.81208461	13.61115310				
C	0.06388245	2.37328907	14.62158292				
H	0.83196336	5.25135993	8.57737201				
H	0.68920619	2.47874952	9.52928589				
H	1.27652509	4.54919087	10.96096766				
H	-0.46264653	4.96920266	10.90207942				
H	-1.08777944	2.88860709	12.02742186				
H	0.55100267	2.21554325	11.82918512				
H	-0.97671609	2.07482201	14.46137368				
H	0.72631691	1.53228138	14.39828805				
H	0.19490154	2.66085278	15.66536418				
Cu	-0.23588210	5.99109864	15.34514680				
O	-1.92187596	11.14694972	8.88046181				
H	-2.51312666	11.64886773	8.30493389				
H	-2.45117379	10.78151840	9.60296523				
O	-2.94765578	9.74976826	11.06503445				
H	-2.52479049	10.12096859	11.85888433				
H	-3.48399815	8.99640035	11.37557203				
O	2.31928952	11.66357925	18.59119580				
H	7.55601702	3.23895574	12.94002613				
C	7.13494017	4.13054551	11.77506278				
O	7.98809307	4.52634918	10.99688364				
N	5.80657527	4.46394215	11.74325369				
C	4.68034982	3.91880267	12.55002308				
C	3.99030083	2.81179824	11.73549315				
O	3.85996121	2.87444892	10.51749580				
C	3.77477103	5.15514052	12.74270427				
C	3.89114187	5.83476968	11.35804739				
C	5.39168601	5.65895447	10.97808254				
H	5.00245261	3.54371541	13.51690726				
H	2.75664565	4.86413595	12.97659720				
H	4.16362052	5.78947532	13.54197790				
H	3.25807697	5.33572855	10.62940061				
H	3.61753572	6.88598166	11.41034267				
H	5.52571989	5.50735282	9.91102810				
H	5.98343101	6.52338118	11.28502751				
N	3.50532439	1.75549479	12.44070406				
C	2.87663564	0.62364963	11.75034028				
H	3.73093566	1.59656576	13.41744426				
C	-1.18901663	6.69532811	21.94931742				
C	-1.96103542	6.38751942	20.69764450				
O	-3.05154266	6.87410910	20.46130613				
N	-1.36745266	5.44996268	19.92875319				
C	-1.99126909	5.13327175	18.62856549				
C	-3.47066137	4.68152809	18.79314701				
O	-3.88720413	4.21636853	19.84729369				
C	-1.20590805	4.00102319	17.97009421				
C	0.26756415	4.27380973	17.90636234				
C	1.28281951	3.78546620	18.72448272				
N	0.82359339	4.99675157	16.91233120				
C	2.12362086	4.96326611	17.05204009				
N	2.44756660	4.23627102	18.15468220				
H	-0.52374350	4.98944833	20.24240488				
H	-1.97691011	6.03003043	18.00884677				
H	-1.38228811	3.07346011	18.51634711				
H	-1.59478268	3.85336057	16.96579912				
H	1.23448100	3.18440297	19.60713590				
H	2.85772958	5.43130394	16.41806289				
H	3.39458939	4.06624113	18.48617141				
N	-4.25900205	4.82236358	17.65489897				
C	-5.64065481	4.32273901	17.66753860				
C	-5.74278057	3.23954416	16.58281759				
O	-4.87060640	3.13608062	15.72976678				
C	-6.69705110	5.42455093	17.37574112				
O	-6.46214010	5.98650414	16.08279337				
H	-3.86226087	5.13314489	16.77784189				
H	-5.80191052	3.87990292	18.64981439				
H	-7.69246186	4.98111889	17.40759316				
H	-6.62602390	6.19853467	18.14222503				
H	-7.33294131	5.93891785	15.61675508				
N	-6.81884468	2.41272344	16.67698476				
C	-7.15034427	1.44404043	15.62362158				
H	-7.49396765	2.46741263	17.43882529				
C	-5.93290811	3.51036513	10.39740230				
C	-5.72284702	4.02111045	11.83238248				
O	-6.56034236	3.89370300	12.69814786				
N	-4.51522845	4.62696103	12.01226661				

N	-5.27425028	7.50996963	13.93705114	H	2.75196008	4.91401033	12.95996031
C	-5.68708587	8.91558969	13.78089354	H	4.17517916	5.82648776	13.50963549
C	-4.67322579	9.92736733	14.36594789	H	3.27447425	5.34224626	10.59744901
O	-4.84085808	11.12810183	14.24877977	H	3.64908144	6.90414466	11.35416004
H	-5.64083063	7.00400147	14.74494910	H	5.55653246	5.47169350	9.87770567
H	-5.79589504	9.14603818	12.72054130	H	6.02910952	6.49719373	11.23824567
N	-3.55697179	9.45919844	14.94191960	N	3.49782309	1.76037832	12.44442379
C	-2.56342833	10.44986677	15.41977093	C	2.87473218	0.62545062	11.75107674
C	-2.06083944	11.18866828	14.19877021	H	3.65398524	1.61601870	13.43706581
O	-1.64805030	10.52278646	13.23682410	C	-1.19178252	6.69213461	21.94833465
C	-1.41548826	9.80327935	16.16213724	C	-1.96217000	6.39034448	20.69083201
C	-1.97041441	9.16730683	17.44234878	O	-3.05556362	6.87651456	20.46086158
C	-0.29714915	10.86187267	16.47693211	N	-1.37305992	5.45352296	19.91779094
C	-0.86544995	8.58238893	18.33812144	C	-1.98658046	5.14280507	18.60297884
H	-3.43978954	8.45575766	15.00500556	C	-3.47320024	4.70268190	18.79214837
H	-3.09341166	11.14514050	16.04628512	O	-3.87611245	4.21080583	19.83998685
H	-1.00067545	9.01836715	15.52758210	C	-1.21462005	3.99209732	17.97545491
H	-2.52061184	9.91844650	18.01398058	C	0.25471887	4.26867178	17.90980211
H	-2.67008215	8.37024789	17.18277231	C	1.28483594	3.79409408	18.73011562
H	0.09973671	11.32037249	15.56777894	N	0.81351800	4.99255348	16.91771652
H	0.53518034	10.39019437	16.99661536	C	2.11581592	4.96709719	17.04590201
H	-0.69284564	11.65235920	17.11977166	N	2.44488708	4.25143996	18.15047245
H	-0.30995785	7.80133880	17.80559385	H	-0.53062529	4.98778026	20.22669886
H	-1.30460198	8.15227318	19.23253650	H	-1.95846261	6.03638118	17.97030362
H	-0.15620528	9.35572839	18.63901032	H	-1.39312579	3.06485571	18.53294390
C	0.74253284	8.45137062	11.22707123	H	-1.60114969	3.83577794	16.96644954
C	0.25403180	7.79010578	12.50361252	H	1.30064566	3.19839702	19.61943640
C	1.10570980	8.14015934	13.69170674	H	2.84282402	5.43734568	16.40378328
C	2.08451089	9.10156232	13.79288522	H	3.39626353	4.09347561	18.47588323
N	0.98190898	7.45724040	14.89899966	N	-4.26684356	4.82449041	17.65790955
C	1.88958126	8.03270025	15.72508743	C	-5.65600926	4.33875396	17.66661565
N	2.56581493	9.01364920	15.09949250	C	-5.74059494	3.24640121	16.58319625
H	-0.78720143	8.08191708	12.66034586	O	-4.86884742	3.14260192	15.73176397
H	0.26028675	6.71238190	12.34078417	C	-6.70912276	5.44586353	17.37267654
H	2.45652062	9.81216584	13.07460117	O	-6.45972176	5.98033828	16.06954845
H	2.05869615	7.75030149	16.75058116	H	-3.89457351	5.09989201	16.75712993
H	3.29446226	9.58325529	15.51093060	H	-5.83822438	3.91988753	18.66093007
C	0.15586423	3.49104819	9.51756131	H	-7.71139773	5.00369330	17.41971594
C	0.26526084	4.17947444	10.90037558	H	-6.63559783	6.23639645	18.13120051
C	-0.01489369	3.16125444	11.98099320	H	-7.34700315	5.92250534	15.63036415
S	0.49485476	3.81878559	13.61824151	N	-6.81472755	2.41645153	16.67507633
C	0.06452331	2.38207940	14.62046369	C	-7.14842404	1.44216018	15.62595273
H	1.27788540	4.57276408	11.00154969	H	-7.49133350	2.47732525	17.43410858
H	-0.42520066	5.02336126	10.94945358	C	-5.92913419	3.51225335	10.39717928
H	-1.07860442	2.90611190	11.98583774	C	-5.71053371	4.01586378	11.83490325
H	0.51234371	2.22543852	11.79040568	O	-6.55988944	3.90278012	12.69473379
H	-0.95854261	2.05966486	14.42404578	N	-4.49793730	4.61075798	12.02925355
H	0.74343527	1.55742908	14.41549093	C	-4.28262462	5.40060227	13.23719720
H	0.15237589	2.64732496	15.67395085	C	-4.58254683	6.88487339	12.96015289
Cu	-0.23422335	5.98942165	15.34483501	O	-4.20243835	7.45098107	11.91986146
QM/MM R1a (B3LYP-D3/6-31G(d):Amber)				C	-2.77303902	5.23508123	13.63856422
mechanical embedding $\omega_c=1.0$				S	-2.47134308	6.22319053	15.13029820
C	7.55365985	3.23551505	12.94007050	H	-3.85613602	4.73749431	11.25212671
C	7.13287175	4.12773271	11.77610426	H	-4.91503361	4.99247064	14.03116500
O	7.98461388	4.51998544	10.99253475	H	-2.56775725	4.18507665	13.86394033
N	5.80442154	4.45766343	11.73678593	H	-2.11991149	5.56678135	12.82354903
C	4.68205222	3.92512783	12.55739271	N	-5.27509334	7.52110241	13.93726680
C	3.98117799	2.82149643	11.74668720	C	-5.68595507	8.92386199	13.78269362
O	3.87579942	2.86837662	10.52465805	C	-4.67154455	9.93181794	14.37112509
C	3.77638913	5.18633507	12.71288011	O	-4.83807364	11.13263571	14.24926986
C	3.91508458	5.84600062	11.23364188	H	-5.65768071	7.04957613	14.75574384
C	5.41398238	5.63929676	10.94466806	H	-5.79208037	9.17603957	12.72728633
H	4.98303717	3.56570344	13.54117223	N	-3.55149614	9.46243317	14.94227415
				C	-2.56215947	10.45708837	15.42255733
				C	-2.05487073	11.19072822	14.20223661

O	-1.65309813	10.52149592	13.23794376	C	-1.19038137	6.69317506	21.95066779
C	-1.39828892	9.80210060	16.14452678	C	-1.95632383	6.38664707	20.69128057
C	-1.97265483	9.15216913	17.40672488	O	-3.04365923	6.87616908	20.45149832
C	-0.27937549	10.85843604	16.45567511	N	-1.35928561	5.45045261	19.92307974
C	-0.86434148	8.55417154	18.29177649	C	-1.98649062	5.13954473	18.63195603
H	-3.42150427	8.45865787	14.98186561	C	-3.46260824	4.68706852	18.78582477
H	-3.07146420	11.12363948	16.10786607	O	-3.88275977	4.22538888	19.84079793
H	-0.97707214	9.02847169	15.49431510	C	-1.20037350	4.02175329	17.96131175
H	-2.52391842	9.89091854	17.99699584	C	0.26994853	4.28784930	17.90508077
H	-2.67400642	8.35484970	17.14318687	C	1.27249029	3.78955000	18.73212881
H	0.14482864	11.34010801	15.56507976	N	0.82417652	5.00407507	16.92080175
H	0.57121739	10.39350046	16.96533315	C	2.12316360	4.96654211	17.06055592
H	-0.65122583	11.65043140	17.11674798	N	2.44104212	4.23343636	18.16768182
H	-0.29753627	7.77503428	17.75106753	H	-0.51427309	4.98249112	20.23442718
H	-1.30058884	8.10568520	19.18667025	H	-1.97358319	6.05708456	18.01128459
H	-0.14444908	9.31320164	18.61686739	H	-1.38642167	3.07935111	18.50680900
C	0.73982601	8.44795362	11.22936163	H	-1.59668390	3.87599836	16.93940855
C	0.24181444	7.78067039	12.50489436	H	1.19070843	3.18933065	19.61032942
C	1.10338005	8.14006962	13.68314584	H	2.86528803	5.43175956	16.42884171
C	2.08480503	9.10141623	13.77798590	H	3.38550374	4.05422551	18.50637784
N	0.98179233	7.45613681	14.89420072	N	-4.25911480	4.84287866	17.66069346
C	1.88794322	8.03773112	15.72262821	C	-5.63250843	4.33048367	17.66878267
N	2.56126588	9.01373674	15.08919187	C	-5.73757647	3.24842412	16.58399707
H	-0.80405246	8.06436085	12.66471455	O	-4.87562884	3.13909021	15.72448888
H	0.26612622	6.69561211	12.35401380	C	-6.69439330	5.41562844	17.37040715
H	2.49728841	9.83255318	13.10041160	O	-6.45797511	5.97716215	16.08770476
H	2.05842619	7.76242953	16.74988151	H	-3.86358511	5.16791397	16.78408570
H	3.28901349	9.58888399	15.49353226	H	-5.78751752	3.87333781	18.65653082
C	0.15641736	3.49401168	9.52531575	H	-7.70141807	4.96415268	17.39331364
C	0.25177293	4.21207507	10.90830345	H	-6.63170442	6.19146046	18.15023762
C	-0.01062586	3.15381223	11.95672520	H	-7.32062524	5.92126506	15.60245571
S	0.49871641	3.81639418	13.61212150	N	-6.81515197	2.42235503	16.67652895
C	0.04330494	2.39884255	14.63493044	N	-7.14862325	1.44719126	15.62421839
H	1.27015038	4.60935025	10.99784363	H	-7.49408549	2.47430046	17.43464279
H	-0.45351587	5.05081890	10.95905463	C	-5.93180923	3.51064241	10.39903762
H	-1.07449258	2.90045963	12.00083946	C	-5.72102349	4.01535119	11.84076911
H	0.54861468	2.23173131	11.79118856	O	-6.56452588	3.89949453	12.69819803
H	-0.99694718	2.11826334	14.45436638	N	-4.51482767	4.62445164	12.02075794
H	0.69394511	1.55050802	14.43004240	C	-4.25909000	5.37266129	13.24106697
H	0.15305892	2.68323671	15.68288529	C	-4.57511022	6.86577392	12.95497555
Cu	-0.23376323	5.99105727	15.34617122	O	-4.18781458	7.44836150	11.92922532
				C	-2.76078469	5.21803580	13.66634531
				S	-2.47400347	6.22544484	15.12989855
				H	-3.86782321	4.67489928	11.23978715
				H	-4.93698609	5.00921793	14.01950437
				H	-2.55787444	4.17658635	13.92444708
				N	-2.12259608	5.53944364	12.84002177
				N	-5.26648415	7.50207961	13.93922188
				C	-5.68995302	8.90805320	13.77538567
				C	-4.67426846	9.92081680	14.36094070
				O	-4.84212544	11.12200666	14.24356202
				H	-5.62543745	6.98903876	14.74345898
				H	-5.80367484	9.12808367	12.71156264
				N	-3.56398412	9.45227247	14.94511395
				C	-2.56001145	10.43766040	15.42392073
				C	-2.06221753	11.18791439	14.20349502
				O	-1.65002597	10.52583531	13.23869330
				C	-1.42005435	9.78465226	16.16649742
				C	-1.95626817	9.14873742	17.44666329
				C	-0.30625042	10.83606176	16.48419891
				C	-0.85329459	8.55968299	18.32561642
				H	-3.45273673	8.44690512	15.01263900
				H	-3.09992673	11.15217998	16.03263581
				H	-1.00651800	8.98290233	15.52057050
				H	-2.50725079	9.91206395	18.02729142

**QM/MM R1a (M06L/6-31G(d):Amber)
mechanical embedding $\omega_c=1.0$**

C	7.54970230	3.23426425	12.93993185
C	7.12535496	4.13536935	11.77967202
O	7.97334233	4.52349666	10.99318629
N	5.79832910	4.47200409	11.75676159
C	4.66871739	3.92621778	12.55341964
C	3.99563677	2.81749500	11.73473929
O	3.86388308	2.87950629	10.51766116
C	3.76587465	5.14255199	12.75815278
C	3.87352165	5.81872798	11.37363274
C	5.37028328	5.65779034	11.00320562
H	5.00225293	3.54426989	13.52991839
H	2.73397488	4.83640913	12.99328233
H	4.15198909	5.78590691	13.56999189
H	3.23601979	5.30787273	10.63697467
H	3.58782820	6.87913470	11.42775853
H	5.50994117	5.50642800	9.92221559
H	5.95858965	6.53983296	11.31533465
N	3.51096645	1.76146297	12.43632424
C	2.87722399	0.62781814	11.74960002
H	3.71908979	1.59993927	13.41661297

H -2.67233426 8.34510091 17.18542474
H 0.08508080 11.29991821 15.56139833
H 0.53250993 10.35242187 17.00821488
H -0.70907385 11.63373681 17.13384172
H -0.30203903 7.76760843 17.77519993
H -1.28721879 8.12485743 19.23109494
H -0.13115872 9.33972466 18.62224040
C 0.74032223 8.44853361 11.22917432
C 0.26669982 7.78761836 12.51954721
C 1.10806034 8.13482223 13.70479703
C 2.08463615 9.10367291 13.80283599
N 0.98691166 7.45649495 14.90173373
C 1.89460949 8.03277355 15.72955210
N 2.56785300 9.01651875 15.10742807
H -0.78794593 8.07701819 12.67262517
H 0.26068177 6.69990017 12.34778260
H 2.43763679 9.80518389 13.07075902
H 2.06162887 7.74417025 16.75736886
H 3.29544130 9.58674656 15.52047367
C 0.15713026 3.48990151 9.52021201
C 0.27363268 4.16165347 10.91367343
C -0.01837272 3.16706345 11.99975588
S 0.49439576 3.82086813 13.62051061
C 0.06508090 2.38792399 14.61210749
H 1.29582324 4.55528012 11.02159043
H -0.40730595 5.02300611 10.95949182
H -1.08554497 2.91252744 11.98433318
H 0.48480097 2.21931852 11.80230755
H -0.95337050 2.05827120 14.41699583
H 0.74200856 1.56454585 14.41523853
H 0.14730938 2.65176081 15.66399273
Cu -0.23396043 5.98908589 15.34491291

**QM/MM R1a (B3LYP/6-31G(d) SDD:Amber)
mechanical embedding $\omega_c=1.0$**

C 7.55470972 3.23647839 12.94046195
C 7.13965265 4.12847615 11.77455820
O 7.99266044 4.52121147 10.99216164
N 5.81246450 4.46151340 11.73390316
C 4.68723492 3.92868136 12.54926356
C 3.98819576 2.82099320 11.73753435
O 3.87303600 2.86768790 10.51635038
C 3.78703053 5.18309428 12.70759401
C 3.92697114 5.84974890 11.32231000
C 5.42625188 5.64373123 10.94585428
H 4.98822302 3.56351570 13.53389555
H 2.76091178 4.91018859 12.95424651
H 4.18725595 5.82049204 13.50731451
H 3.28638264 5.35036985 10.59150676
H 3.66281998 6.90923812 11.35515740
H 5.57088405 5.48090367 9.87483664
H 6.04273822 6.50108795 11.24366286
N 3.50508124 1.76179386 12.44049939
C 2.87595092 0.62626713 11.75097617
H 3.68155717 1.61719983 13.42931483
C -1.19084896 6.69289199 21.94919570
C -1.96101158 6.39108431 20.69308685
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C	-4.58431803	6.88416362	12.96853572	N	0.53858828	9.91438557	11.24644233
O	-4.21007172	7.45440241	11.93258698	C	0.81559101	8.47297231	11.20704822
C	-2.77018384	5.23882861	13.63120810	C	0.24969873	7.75215508	9.95174822
S	-2.46822065	6.22095076	15.12837102	O	0.98842765	7.02922701	9.30203221
H	-3.86137993	4.78507942	11.23242612	C	0.30867242	7.79895175	12.48268565
H	-4.90808959	4.96867308	14.01923023	C	1.14111297	8.15809140	13.67969863
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C	-7.03840315	9.15656802	14.49434244	H	-0.74015246	8.08807415	12.63448629
C	-8.15175004	8.49638185	13.67658930	H	0.33478774	6.71607950	12.32009913
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H	-5.64277641	7.04503846	14.76952851	N	-1.04437610	7.88903841	9.65638568
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C	-2.56556743	10.43485125	15.44990061	H	-3.74073326	6.74974628	8.56973652
C	-2.06598652	11.19366696	14.24962147	N	2.14581993	8.56066555	6.93167091
O	-1.67100399	10.55008723	13.25950138	C	3.46812454	7.93891372	6.78583449
C	-1.39933858	9.80080172	16.17576959	C	3.35515422	6.41897193	6.78285330
C	-1.97829299	9.15799605	17.43358860	O	4.36753117	5.74192812	7.00368663
C	-0.29475076	10.87529676	16.48531748	C	4.45314863	8.43625596	7.84085327
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H	-3.40748737	8.44099708	14.97997261	O	3.82058936	8.53858780	9.06306236

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H 3.90945715 8.22915461 5.83144122
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H 3.15997819 9.24443300 8.98654597
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H 4.27956218 10.38157536 6.85262201
H 5.92082117 9.68455350 6.92021655
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C -0.02997844 3.13535283 11.97030016
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**QM/MM R2a (B3LYP/6-31G(d):Amber)
electrostatic embedding $\omega_{\alpha}=1.0$**

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C	-6.59881548	-2.62506815	19.46589887	C	-1.20598717	6.69689462	22.08057455
C	-5.56170719	-1.57901830	19.13713007	C	-1.94125675	6.39449643	20.75995586
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H	-7.19327374	-2.82147026	18.57066820	O	-3.88234899	4.19623287	19.85542558
H	-7.26868174	-2.26959669	20.25165944	C	-1.21527954	4.00187561	18.00713799
H	-4.56252654	-2.77489580	17.66090818	C	0.25613863	4.26869573	17.92787008
H	-6.34894763	-0.20618987	20.54298882	C	1.28301248	3.78844614	18.73899499
H	-2.87886916	-1.04129211	17.15267004	N	0.80954920	4.98818573	16.92533664
H	-4.66745645	1.57629969	20.06947455	C	2.11199197	4.96503616	17.04834443
H	-2.92842844	1.13405846	18.32491977	N	2.43933042	4.24523277	18.15239575
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C	-0.53758405	-0.46137772	22.00068334	H	-1.95494936	6.05595800	18.02063165
C	0.76455762	-0.76172778	22.76020065	H	-1.39663914	3.07410733	18.56848858
O	0.81972839	-0.48461315	23.95478797	H	-1.61244451	3.84459348	16.99869909
C	-1.00780218	0.93173268	22.46020463	H	1.29273359	3.18965364	19.63106199
C	0.04254796	1.97159152	22.14993721	H	2.84501721	5.43341255	16.40878181
N	0.00912568	3.10638265	22.82513196	H	3.39254023	4.08566308	18.47420968
O	0.93489758	1.73452000	21.35819485	N	-4.26716056	4.82126403	17.68213790
H	-2.04379224	-1.44642904	23.20419663	C	-5.65595378	4.32416324	17.67592489
H	-0.33263907	-0.45022601	20.93102001	C	-5.73992189	3.23566717	16.58513001
H	-1.89272447	1.19105342	21.87902016	O	-4.86178599	3.14208005	15.73257361
H	-1.28200247	0.94424904	23.51536978	C	-6.71041894	5.43895748	17.37256131
H	-0.73408310	3.25710276	23.49541276	O	-6.47538389	5.96883449	16.06677724
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N	3.77458467	0.54064790	21.87776334	H	-5.83822756	3.90763013	18.67050068
C	4.71171501	1.57172512	21.49529435	H	-7.71290721	4.99463841	17.41881577
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C	5.35296493	3.00198309	19.52947403	C	-7.13702813	1.42244725	15.60855024
N	6.62623682	2.64879832	19.62849046	C	-8.57188539	1.72287598	15.17555274
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H	4.08705645	1.29810124	19.45683130	C	-8.34883292	-1.62017376	14.75158739
H	3.36936335	2.67140661	20.24045918	C	-5.93593296	-1.61673658	14.48227940
H	6.88450795	1.77178854	20.04598727	C	-8.40857679	-2.66262918	13.80719988
H	7.32159265	3.23027638	19.17865635	C	-6.01803478	-2.65099445	13.54915860
N	3.62210889	6.94353809	22.54061503	C	-7.26129921	-3.16579928	13.21909395
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O	1.25366344	5.50594565	22.32919803	H	-6.01776219	-0.09886910	16.62344612
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C	4.14531355	7.62388834	19.75299666	H	-9.24759499	-1.22904220	15.20946007
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C	4.10181464	8.87609979	19.11979576	H	-9.36847072	-3.08167058	13.53829400
C	6.55382783	7.66079841	19.77877343	H	-5.13334128	-3.04694618	13.07137787
C	5.30426463	9.52832854	18.82221675	H	-7.33507770	-3.96766712	12.49629671
C	6.52204639	8.91005692	19.15812676	N	-8.04046643	6.98237633	20.75117630
H	3.72189964	5.96157841	22.75719852	C	-6.62574289	7.04228855	21.18979826
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H	-4.81301336	8.04092815	19.14738854	C	-0.29454176	10.87502695	16.48495255
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H	-4.86753138	9.37440181	17.08537800	H	-3.40774909	8.44108007	14.98019052
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C	-4.19538554	3.24291417	22.90816667	H	-0.67688021	11.66791417	17.14070130
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H	-4.76615346	5.38509775	21.55359537	H	-1.30477296	8.13680563	19.23083856
H	-5.87413548	4.05856535	23.96001656	H	-0.16373907	9.35231060	18.66018654
H	-3.96698960	2.53606707	23.70724886	N	-2.15493090	12.52169194	14.27469898
H	-4.80072706	2.73748147	22.15486452	C	-1.74103358	13.35002467	13.11641815
H	-3.24362190	3.95209607	21.40140692	C	-0.36619740	12.94098908	12.54038510
N	-6.79329777	2.39860783	10.37659313	O	0.61715558	12.74290913	13.27689621
C	-5.91627435	3.56850291	10.34597715	C	-1.70908457	14.76585001	13.69698754
C	-5.69925023	4.03773334	11.80196427	C	-2.85387882	14.73146161	14.70551049
O	-6.54067732	3.90437202	12.67553575	C	-2.67153419	13.35375639	15.33837393
C	-6.45561296	4.69851318	9.45533722	H	-2.50877485	13.31075492	12.35072280
C	-7.00174111	4.24706062	8.06596725	H	-0.76158133	14.94912582	14.21054964
C	-7.57376807	5.42406126	10.18264796	H	-1.86341367	15.52175552	12.92644990
H	-7.62788533	2.47704131	10.95674453	H	-2.77592272	15.53851576	15.43598642
H	-4.95154188	3.24011615	9.96205042	H	-3.81405458	14.77573252	14.18613404
H	-5.61985457	5.37966665	9.28163097	H	-1.92551967	13.42557562	16.13279412
H	-7.99780713	4.62696950	7.84845447	H	-3.62653091	13.00684478	15.73296476
H	-6.32295350	4.61267789	7.29877565	N	-0.34414003	12.65571063	11.23755708
H	-7.05896873	3.17189250	7.95054322	C	0.81063236	12.23726129	10.43312421
H	-8.20589208	4.72532884	10.73394532	C	1.03854079	10.75089171	10.31741931
H	-8.19699308	5.93565664	9.45730698	O	1.70674755	10.34084094	9.37758295
H	-7.15425738	6.15240366	10.87923836	H	-1.22411723	12.77136008	10.74204406
N	-4.49201516	4.62316437	12.01716416	H	0.71763221	12.64929711	9.42671212
C	-4.28299161	5.39759074	13.23851475	H	1.70946573	12.65382462	10.88664819
C	-4.58585955	6.88458664	12.97454020	N	0.53887826	9.91466929	11.24681189
O	-4.20924988	7.45625008	11.93075919	C	0.81597177	8.47338817	11.20723245
C	-2.77017561	5.23923555	13.63330951	C	0.25004847	7.75261675	9.95173550
S	-2.46697853	6.22172690	15.13111789	O	0.98851286	7.02951090	9.30165142
H	-3.86595428	4.78702228	11.23306950	C	0.30881035	7.79881603	12.48273145
H	-4.90759720	4.96944782	14.02322176	C	1.14111799	8.15777911	13.68006056
H	-2.56201919	4.18840428	13.84852298	C	2.11206406	9.12523662	13.80032860
H	-2.12863701	5.58578003	12.81555331	N	1.00381698	7.46498368	14.88676604
N	-5.26476498	7.52042834	13.95000089	C	1.88970570	8.05018183	15.73427687
C	-5.68576145	8.92457112	13.79859086	N	2.56223789	9.03325395	15.11726472
C	-4.66444612	9.92246395	14.37887247	H	-0.02231976	10.32397880	11.98862441
O	-4.83397295	11.12210640	14.25161330	H	1.90093349	8.35028644	11.15908684
C	-7.03843542	9.15602987	14.49438083	H	-0.74033790	8.08751995	12.63481466
C	-8.15233010	8.49652034	13.67659418	H	0.33519015	6.71580075	12.32007489
C	-9.50167059	9.12884173	14.06669451	H	2.52611324	9.86215508	13.12935919
N	-10.26075785	8.49169014	14.92152590	H	2.05262109	7.77842080	16.76574162
O	-9.83161447	10.20330220	13.60702611	H	3.27788189	9.61296622	15.54036804
H	-5.64222188	7.04049254	14.77004315	N	-1.04441927	7.88883620	9.65677574
H	-5.80438066	9.15911098	12.73970867	C	-1.64295368	7.32108203	8.44521462
H	-7.02479622	8.74831219	15.50747175	C	-0.92566021	7.83328930	7.19502839
H	-7.24515315	10.22643181	14.56335498	O	-0.68085096	7.06138872	6.25938992
H	-7.98872239	8.64750734	12.61105098	C	-3.15421017	7.65806654	8.41309004
H	-8.16350494	7.42503005	13.86094150	H	-1.63384919	8.47001314	10.24528332
H	-11.11470981	8.95778659	15.15622832	H	-1.52560083	6.23592861	8.47637731

H	-3.42356633	8.08535295	7.45664995	N	3.47688893	1.74436052	12.45393845
H	-3.42726065	8.37772917	9.17444220	C	2.86911386	0.62868675	11.75770340
H	-3.74022087	6.75064356	8.56958350	H	3.73126539	1.56027502	13.41706829
N	2.14575461	8.56062719	6.93164012	C	-1.17528952	6.70477974	21.94341706
C	3.46795396	7.93874835	6.78598038	C	-1.94612093	6.38400813	20.68522621
C	3.35511475	6.41884401	6.78295390	O	-3.05712050	6.86407452	20.46821866
O	4.36745498	5.74142535	7.00450615	N	-1.36770281	5.45064650	19.92033764
C	4.45290689	8.43597666	7.84124068	C	-1.99453532	5.13283041	18.62050971
C	4.98581176	9.82652701	7.47279440	C	-3.47080223	4.68516333	18.78140182
O	3.81956880	8.53756408	9.06362900	O	-3.88556017	4.21821867	19.84817093
H	1.72681079	8.63375231	7.84934940	C	-1.20337565	4.00139291	17.96645195
H	3.90965153	8.22881557	5.83196428	C	0.27258798	4.26892660	17.91898388
H	5.27582781	7.72898705	7.94639919	C	1.27936064	3.76492456	18.75343767
H	3.15912637	9.24372161	8.98684110	N	0.83795746	4.98481915	16.93379591
H	5.22394154	10.40347602	8.36612599	C	2.13340276	4.95646456	17.08662182
H	4.27853980	10.38156814	6.85442602	N	2.45300180	4.22217500	18.19220816
H	5.91950274	9.68579912	6.92134774	H	-0.52092085	4.98855452	20.22013056
N	0.78714576	4.22949747	8.48400168	H	-1.98236045	6.03776300	18.00043693
C	0.15265010	3.43166552	9.53133346	H	-1.38856595	3.06396980	18.51683844
C	-1.32651766	3.16165157	9.19970656	H	-1.60096765	3.86256049	16.95181934
O	-2.23425846	3.83567512	9.69652274	H	1.20554627	3.15058511	19.64571759
C	0.26407031	4.16335767	10.90573025	H	2.87536857	5.43087495	16.45844617
C	-0.02971377	3.13532951	11.97071265	H	3.40892587	4.05251373	18.52957158
S	0.49376843	3.81302276	13.60892952	N	-4.25609677	4.83008328	17.65275495
C	0.05275734	2.38445882	14.61052677	C	-5.64195509	4.32893814	17.66450242
H	0.84155631	5.24075735	8.55902244	C	-5.74900866	3.23882794	16.57449266
H	0.66482013	2.47193406	9.61948301	O	-4.87592957	3.12790282	15.72454529
H	1.29010758	4.53415602	10.99182507	C	-6.70607522	5.42147892	17.37134265
H	-0.41528878	5.02106045	10.93612109	O	-6.47204940	5.98207596	16.08111454
H	-1.09883450	2.90841803	12.01792975	H	-3.83992533	5.14994142	16.77672348
H	0.50640923	2.19484851	11.82420217	H	-5.79503579	3.88209827	18.65690118
H	-0.99151049	2.10159597	14.45597215	H	-7.70210608	4.95429443	17.40716709
H	0.69349964	1.52888339	14.38588180	H	-6.64740878	6.21019266	18.13602351
H	0.18825678	2.65758516	15.65785981	H	-7.33736162	5.92979290	15.60223165
Cu	-0.23459750	5.99060642	15.34509304	N	-6.82689503	2.40488998	16.66199827
O	-1.97817736	11.16518039	8.89811960	C	-7.14660629	1.42918506	15.61638150
H	-2.59697851	11.66498332	8.33708729	H	-7.44776353	2.39938039	17.46403059
H	-2.52080485	10.88297201	9.65425555	C	-5.94668982	3.49721890	10.38282336
O	-2.95170670	9.78455998	11.08793453	C	-5.73418557	4.01602464	11.82422440
H	-2.62617463	10.15382385	11.92928544	O	-6.58454466	3.90246371	12.70029799
H	-3.54716412	9.06995908	11.37615184	N	-4.53827848	4.61936603	12.01150442
O	2.34673329	11.73572787	18.59522708	C	-4.26749145	5.37893144	13.23743662
H	1.95798267	12.56174472	18.29812378	C	-4.57931566	6.86903182	12.96994793
H	2.93622114	12.00542681	19.30465071	O	-4.20936159	7.44658677	11.91996302
QM/SE/MM R1a (B3LYP/6-31G(d):xTB:Amber)				C	-2.75825522	5.20859067	13.64883432
mechanical embedding $\omega_c=1.0$				S	-2.47645762	6.22233828	15.13202456
C	7.56421223	3.23042539	12.94920434	H	-3.89808679	4.68821572	11.23204250
C	7.13926312	4.13373041	11.77934541	H	-4.93093947	5.01028074	14.02454822
O	8.00112752	4.50565859	10.98461371	H	-2.56091679	4.16556558	13.91824598
N	5.81805631	4.46541793	11.73256882	H	-2.12591456	5.53809603	12.81598576
C	4.70057916	3.90412334	12.55028927	N	-5.26277537	7.52392602	13.94576619
C	3.99630822	2.78486032	11.74542070	C	-5.68017311	8.90655940	13.78518091
O	3.86704116	2.85341702	10.52323575	C	-4.66109651	9.94365130	14.36694976
C	3.78806108	5.13629300	12.75132005	O	-4.82139847	11.13703565	14.25417027
C	3.88730037	5.81932022	11.35660714	H	-5.59741724	7.01333750	14.75953576
C	5.38585646	5.65767808	10.97119695	H	-5.76203217	9.10271194	12.70814238
H	5.04611483	3.52481897	13.51838325	N	-3.54499470	9.44403713	14.93104297
H	2.76338323	4.82979192	12.98933784	C	-2.57912460	10.45577409	15.41127462
H	4.17853025	5.78136520	13.55749514	C	-2.07531371	11.19742000	14.19751553
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H	3.60380303	6.87789758	11.40895634	C	-1.43530185	9.81500242	16.15271158
H	5.51967926	5.50506570	9.89440192	C	-1.97330928	9.16683211	17.43337548
H	5.97290640	6.53735350	11.28240210	C	-0.32313853	10.88671199	16.46879602
				C	-0.85696149	8.58806304	18.32499406
				H	-3.38119060	8.44484929	15.02508790

H -3.14993769 11.17382385 16.01023564
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H -2.53567350 9.92096784 18.01391249
H -2.67032380 8.35797636 17.16637043
H 0.04950965 11.34855345 15.54108352
H 0.51580298 10.41496785 16.99088070
H -0.74662420 11.67412760 17.11856880
H -0.29961753 7.81202065 17.77723906
H -1.29664616 8.14838878 19.22278896
H -0.15269690 9.38164240 18.62295026
C 0.73621299 8.46744807 11.23809242
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S 0.49386985 3.81731233 13.61359953
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H 0.81666956 1.55660277 14.39449947
H 0.16085367 2.63250269 15.65691404
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**QM/SE/MM R3a (B3LYP/6-31G(d):xTB:Amber)
mechanical embedding $\omega_c=1.0$**

C -0.54296368 -4.25386591 17.89556527
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O 2.80377714 -0.81003751 18.79324040
C 0.32709282 0.47694841 17.79669388
H -0.05182618 -1.98549789 18.83773517
H 0.73932269 -0.91211230 16.19391625
H -0.41114970 0.28222187 18.57497435
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H 1.10738883 1.09036662 18.23283611
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H 2.77087718 -0.98595617 15.62162083
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H 5.16744268 0.71575995 17.85547052
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H 7.03237906 -0.36795251 15.89676736
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H 3.57184249 1.90440774 16.55517004
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C 6.66764639 4.90226442 15.83862544
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H 9.13281999 4.49262669 13.59829803
H 6.69819376 3.92947986 16.31388607
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H 3.69369853 6.88961781 11.38057951
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O 4.74778254 -1.05421208 11.94109096
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H 3.36290526 -1.10233011 10.45404342
H 4.51991991 0.23467196 10.30733789
H 5.45908874 -0.43965070 12.21124185
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O 1.39195895 -3.68992202 11.36524415
C -0.99831194 -2.00600406 12.33548530
C -1.83271808 -0.78656526 12.68852448
C -2.26361534 -0.59572579 14.00630374
C -2.22286826 0.12460540 11.70255662
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H	-1.47772653	-2.91354381	12.71880732	C	5.33955514	2.98935085	19.53206940
H	-1.95878098	-1.30230864	14.76689230	N	6.62424519	2.59760182	19.65000985
H	-1.88866962	-0.00648648	10.68381436	O	5.03017139	4.00127727	18.93618936
H	-3.41605968	0.62744269	15.33267597	H	2.78455423	0.64486575	21.62886569
H	-3.34020090	1.89098845	11.28307800	H	5.66575250	1.07150697	21.44596927
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C	1.32763042	-5.65372041	13.30972027	H	6.88374465	1.73066320	20.09156502
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C	-3.68383979	0.35564861	18.55164560	C	4.15706853	8.84941262	19.15907307
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O	0.79826429	-0.47023158	23.99121495	N	-1.35614727	5.45824586	19.97095822
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H	-2.06177396	-1.38921713	23.21474319	C	0.26267136	4.27002236	17.92887915
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H	-1.89432501	1.18252765	21.82540527	N	0.83089891	4.98902034	16.93873899
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O	5.28298974	-0.81125057	22.87370256	H	1.21565318	3.15155724	19.64108371
C	3.43993464	-3.00418514	22.07672331	H	2.86897717	5.41598025	16.44501687
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H	2.87671163	-1.79576431	23.75276951	N	-4.25319256	4.81799382	17.67492265
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H	-5.13348132	-3.02759306	13.09247948	C	-8.15061697	8.50878575	13.70035611
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H	-7.60185741	12.10877230	18.87450715	H	0.52041219	10.41553215	17.00834061
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C	-6.55607887	1.33155330	9.57168390	C	-1.74370486	13.30908249	13.11081968
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H	-3.80307772	14.75682746	14.15761132	N	0.78952207	4.25559517	8.47478267
H	-1.91835777	13.41383935	16.14795135	C	0.16177687	3.44627801	9.48878302
H	-3.60665320	12.96722274	15.74278952	C	-1.34276492	3.17684394	9.19770253
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C	0.79799134	12.22295790	10.47939363	C	0.25976681	4.13287073	10.88579572
C	1.03838591	10.74440709	10.32928122	C	-0.03115267	3.12916984	11.97691116
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C	0.81888082	8.49065465	11.19874516	H	-0.44773423	4.97225309	10.93050353
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O	0.98607204	7.01877307	9.29150361	H	0.49769003	2.18661600	11.80414991
C	0.30658264	7.79677084	12.46917109	H	-0.94832459	2.03215151	14.38664993
C	1.14300818	8.15954829	13.67245055	H	0.77234271	1.54797598	14.38667011
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N	1.01907401	7.47658453	14.87781711	N	-1.51567548	2.22319001	8.29413998
C	1.91015252	8.06077580	15.71172997	C	-2.81185177	1.76948045	7.88442790
N	2.57721696	9.05281249	15.08510125	H	-0.73590178	1.77699720	7.82343937
H	-0.03580972	10.27810684	12.01598674	Cu	-0.23663376	5.99543502	15.34599391
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H	-0.74518779	8.08410809	12.63804972	H	-2.60289327	11.68597383	8.35255870
H	0.33206655	6.71053463	12.31141174	H	-2.45896383	10.86370008	9.66255356
H	2.47309059	9.85268856	13.05622033	O	-2.94068595	9.77951772	11.07243368
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H	3.29455341	9.63144418	15.50180859	H	-3.50244952	9.06621779	11.42399118
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O	-0.68427765	7.03985925	6.26931151				
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N	-0.61466073	9.07513806	7.19611884	N	5.80708599	4.46663316	11.73248955
C	0.09547110	9.65405657	6.07181337	C	4.69804174	3.91758790	12.56337979
C	1.48050313	9.06641045	5.84609090	C	3.98482889	2.79362103	11.77711503
O	2.00653138	9.06385447	4.75088101	O	3.86324185	2.85859787	10.54879737
C	0.26983908	11.14965839	6.27269242	C	3.79504072	5.16244215	12.74815156
H	-0.88841971	9.68437892	7.96345412	C	3.89494606	5.82792761	11.35169587
H	-0.49545125	9.48380752	5.16611673	C	5.38344853	5.65038737	10.96083385
N	2.09577182	8.57442413	6.93089271	H	5.04240636	3.54981669	13.53207479
C	3.38708101	7.95928605	6.78233904	H	2.77650960	4.87061702	12.99918257
C	3.33708560	6.43198171	6.78484830	H	4.19654165	5.80700275	13.53899239
O	4.35460527	5.77607629	6.95472981	H	3.25214777	5.32195804	10.63277715
C	4.39651773	8.39948292	7.86082573	H	3.62289205	6.88368641	11.39017506
C	4.99523559	9.76672269	7.50085086	H	5.50722392	5.48918693	9.88687980
O	3.79214533	8.45353764	9.10053066	H	5.97723447	6.52202873	11.25517922
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H	3.78362461	8.31057868	5.81786420	C	2.87207025	0.63121356	11.75613957
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H	3.13886814	9.17630928	9.10216128	C	-1.17596205	6.70384423	21.94368457
H	5.22726480	10.31207603	8.41501107	C	-1.94522974	6.38454934	20.68512363
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N	2.11885970	5.88269187	6.56175374	C	-1.99768273	5.13474586	18.60925437
C	2.01644841	4.47887756	6.34650553	C	-3.47546778	4.69101890	18.77405985
C	1.36728023	3.62851183	7.43466375	O	-3.89316741	4.20993854	19.84114307
O	1.31968740	2.40800500	7.32159751	C	-1.20662654	3.99262785	17.96459796

QM/SE R1a (B3LYP/6-31G(d):xTB) mechanical embedding $\omega_c=1.0$

C 0.26321066 4.25997135 17.91866218
C 1.26958855 3.76444403 18.75673144
N 0.83691866 4.97618972 16.93448990
C 2.13435040 4.94626219 17.08208272
N 2.44294219 4.21989438 18.19116306
H -0.52559876 4.98411604 20.20852738
H -1.98055920 6.02816055 17.98981335
H -1.39327657 3.05956502 18.51749162
H -1.59780832 3.84293907 16.95056453
H 1.20970053 3.15747514 19.64985551
H 2.87640661 5.41469511 16.45317216
H 3.39753616 4.05387308 18.52748572
N -4.26037113 4.81855034 17.65720493
C -5.65347583 4.33281954 17.65633535
C -5.74926039 3.24259967 16.57007957
O -4.87159735 3.12355000 15.72384273
C -6.70590275 5.44209995 17.34460168
O -6.45079976 5.98495579 16.06457822
H -3.85444570 5.12131930 16.77186905
H -5.83264838 3.89866156 18.63898882
H -7.70629159 4.99906583 17.36637039
H -6.64489778 6.21805444 18.11000184
H -7.30050506 5.93196228 15.57695812
N -6.82897237 2.41276316 16.66710453
C -7.14627514 1.43459571 15.62191988
H -7.44976051 2.44142183 17.47583692
C -5.94395104 3.49579446 10.38241350
C -5.72887367 4.01694592 11.82517733
O -6.57925819 3.90290093 12.69601672
N -4.53174255 4.62153516 12.02204627
C -4.26820244 5.39293022 13.24197354
C -4.57394742 6.87738861 12.97526043
O -4.21634184 7.44955022 11.91656475
C -2.75073914 5.21276533 13.63860399
S -2.47519335 6.21938937 15.13214989
H -3.88225063 4.69703991 11.24852795
H -4.91481118 5.02632476 14.03024458
H -2.55394460 4.17158766 13.88387679
H -2.12309597 5.53376799 12.80705691
N -5.25633248 7.52752802 13.94737197
C -5.68232594 8.90869976 13.78482253
C -4.66014948 9.93848285 14.36944955
O -4.82298705 11.13162835 14.25182474
H -5.59526512 7.02966475 14.76988595
H -5.77403755 9.11007569 12.71397329
N -3.54182892 9.44579234 14.93958453
C -2.57829062 10.46185836 15.41848342
C -2.07107994 11.20079393 14.20042301
O -1.64420306 10.54644317 13.23486780
C -1.43013886 9.81634470 16.15393292
C -1.97006806 9.17513856 17.42034546
C -0.31846884 10.88437007 16.46597428
C -0.85683907 8.59516120 18.30877440
H -3.36771970 8.45178273 15.03423918
H -3.13936521 11.17025246 16.02498831
H -1.00843059 9.03002466 15.51087226
H -2.52983102 9.92509701 18.00089570
H -2.66667605 8.37165060 17.15472804
H 0.05864000 11.34590311 15.55082280
H 0.52102848 10.41594548 16.98516344
H -0.72728891 11.66907413 17.11361063
H -0.30048724 7.82400113 17.77045951
H -1.28986266 8.15504426 19.19941385
H -0.15329099 9.37496425 18.61171610
C 0.73585070 8.46804645 11.24130028

C 0.22217701 7.78646065 12.50978761
C 1.10372352 8.15715987 13.67969728
C 2.07972191 9.12365971 13.74224402
N 1.00813805 7.48723334 14.89376349
C 1.92728131 8.06834107 15.69782249
N 2.58704045 9.04852057 15.04229911
H -0.81853102 8.09364790 12.69516030
H 0.22428688 6.70655742 12.34488730
H 2.43581573 9.82916727 13.01073671
H 2.11411317 7.79084985 16.72357946
H 3.32051930 9.62029736 15.43694204
C 0.16597347 3.49973827 9.51098301
C 0.22211787 4.19428309 10.90450743
C -0.01640809 3.14365301 11.96971516
S 0.49664240 3.81675833 13.61226143
C 0.08428639 2.35948880 14.59577268
H 1.21003544 4.64994739 11.01507642
H -0.52182040 4.99107627 10.96075295
H -1.06520161 2.83468658 11.95300492
H 0.55467282 2.23370007 11.77731550
H -0.93468171 2.02553002 14.39170361
H 0.78118445 1.54497340 14.39250190
H 0.16741649 2.63365615 15.64468314
Cu -0.23369446 5.99147929 15.34497135

QM/SE R2a (B3LYP/6-31G(d):xTB) mechanical embedding $\omega_{\alpha}=1.0$

N 0.25272291 -1.97479171 17.89218912
C 0.88263274 -0.84451925 17.26432926
C 2.44563664 -0.88968410 17.61429639
O 2.79881372 -0.81102375 18.78962803
C 0.34251253 0.49194270 17.77626552
H -0.03864366 -1.92499593 18.86045077
H 0.73487323 -0.92651566 16.18332675
H -0.39131360 0.31725424 18.56543497
H -0.14901069 1.03714922 16.97357306
H 1.12961781 1.11234999 18.20030626
N 3.19773581 -0.96209663 16.54659388
C 4.67889690 -0.94394290 16.55551058
C 5.24443196 -1.91566407 17.64099257
O 5.60163521 -1.52858274 18.74319590
C 5.22656323 0.51001153 16.79729344
C 6.73746237 0.57682038 16.39212615
C 4.43877839 1.56916485 16.02497158
H 2.79763253 -0.99426953 15.61750531
H 5.00077327 -1.27063488 15.56324338
H 5.16091794 0.70781890 17.87185384
H 7.36600126 0.71330193 17.27252508
H 7.05056567 -0.35101858 15.90762732
H 6.92198583 1.39553846 15.70153667
H 3.55684565 1.90413407 16.57560109
H 4.11015800 1.13195634 15.08240861
H 5.06447626 2.43586697 15.80902813
N 8.45916027 2.17218271 12.55423073
C 7.57014283 3.17990531 13.05332520
C 7.12897492 4.06624650 11.85068144
O 7.98296039 4.45782341 11.04721671
C 8.25533382 4.07775800 14.10036166
C 7.40618834 5.17360924 14.70383055
C 6.65840311 4.94002849 15.84646956
C 7.32069687 6.44007007 14.11249285
C 5.85706131 5.93817473 16.38889134
C 6.53369608 7.42818995 14.64932348
C 5.79744503 7.18923852 15.79250748

H	9.34242982	2.46278754	12.17858436	H	-7.55287806	-4.61750522	21.05729791
H	6.71158271	2.65150085	13.46976801	H	-5.31869012	-4.39079543	19.11130904
H	8.60974498	3.41201426	14.90108450	H	-7.19522986	-2.82658858	18.58106545
H	9.11238094	4.54658389	13.59945457	H	-7.24525266	-2.27077399	20.27168822
H	6.69636337	3.96970888	16.32877094	H	-4.58086105	-2.77257370	17.66948578
H	7.90124448	6.64509086	13.22286347	H	-6.32050826	-0.20053440	20.55304716
H	5.28850320	5.72976475	17.28577629	H	-2.90667605	-1.05300969	17.15145263
H	6.49733486	8.39593393	14.16667299	H	-4.63948293	1.56167581	20.04313841
H	5.16599742	7.95348862	16.22637205	H	-2.94212285	1.11270292	18.31128818
N	5.81955506	4.41904582	11.76790013	N	-1.51243172	-1.49607480	22.35279525
C	4.68295960	3.90883305	12.57783043	C	-0.54509511	-0.47007199	21.99577481
C	3.98217780	2.80089673	11.77055728	C	0.77422291	-0.73914285	22.77217334
O	3.86419145	2.86946961	10.54377665	O	0.81035902	-0.48586825	23.96088330
C	3.79395818	5.17433412	12.72139127	C	-0.99859885	0.92389299	22.45942201
C	3.95190534	5.83435718	11.33376917	C	0.05916618	1.94986699	22.13110451
C	5.44911658	5.60714320	10.96597700	N	0.01595584	3.08974679	22.83335605
H	4.99925344	3.53736172	13.55353763	O	0.94456085	1.70416771	21.33022803
H	2.76476528	4.91435258	12.96528907	H	-2.01814659	-1.40382556	23.22865659
H	4.19957970	5.80571369	13.52084526	H	-0.35401294	-0.53360971	20.92519468
H	3.31179283	5.34570130	10.59818950	H	-1.90175494	1.19696160	21.89305560
H	3.70906196	6.89787718	11.34435023	H	-1.25711849	0.92934094	23.51754657
H	5.59164169	5.43619792	9.89844354	H	-0.70440615	3.23757060	23.52353015
H	6.07039666	6.45601242	11.26728211	H	0.71128952	3.81101340	22.68880535
N	3.49231282	1.73649597	12.44290055	N	3.75598055	0.53565543	21.89115960
C	2.93396460	0.62576361	11.71093462	C	4.70075383	1.55429437	21.52397103
C	2.10894241	-0.22412579	12.67922209	C	4.78539239	2.67975700	22.56101161
O	2.32815407	-0.17359971	13.89131540	O	3.90926672	3.46545326	22.80959318
C	3.96219037	-0.36452472	11.03286834	C	4.30264431	2.12798897	20.14524536
O	4.76914892	-1.05310976	11.97716762	C	5.34987707	2.99764185	19.53366695
H	3.61361966	1.60673268	13.44243505	N	6.63443696	2.62228048	19.64467946
H	2.30359778	1.04409942	10.91768739	O	5.02696078	4.00682605	18.93285300
H	3.38848068	-1.11911596	10.48222980	H	2.79842394	0.69706018	21.59250552
H	4.56948820	0.21278092	10.32266558	H	5.68972128	1.08468610	21.46964785
H	5.49653897	-0.46851803	12.27947421	H	4.08963797	1.27639135	19.48318167
N	1.18421019	-0.98134722	12.10504766	H	3.37748511	2.68830583	20.27664176
C	0.46692466	-2.01465314	12.83398980	H	6.90251758	1.75585216	20.08049520
C	1.01337829	-3.42630001	12.51000439	H	7.36729675	3.17229505	19.21842191
O	1.41016847	-3.71572924	11.37401156	N	3.65101922	6.92287551	22.51436930
C	-0.98752383	-2.01707808	12.34632138	C	2.57468037	7.37542067	21.63147451
C	-1.82197506	-0.79575232	12.69213277	C	1.25105696	6.68114281	21.97519755
C	-2.25924831	-0.59272744	14.00752987	O	1.26324781	5.51963045	22.34686387
C	-2.21812159	0.11106582	11.70211557	C	2.84902230	6.97528091	20.16633850
C	-3.07779677	0.47627930	14.31330757	C	4.14471477	7.58471870	19.77679977
C	-3.02421925	1.18146045	12.04085110	C	5.33638560	6.94411780	20.12644425
C	-3.46394209	1.37208221	13.34434473	C	4.15407804	8.81764749	19.14706195
H	1.03204722	-1.00767740	11.09694961	C	6.53021719	7.55923643	19.84481044
H	0.59660443	-1.82960125	13.90639683	C	5.36340192	9.42579490	18.86700444
H	-0.92551806	-2.08377518	11.25258938	C	6.54077195	8.78807359	19.22013658
H	-1.47550386	-2.92177585	12.73003949	H	3.68322789	5.92966310	22.70295065
H	-1.95509309	-1.30071747	14.77021435	H	2.49993657	8.45971915	21.76935728
H	-1.88077031	-0.02029124	10.68214080	H	2.87096372	5.88071393	20.11561864
H	-3.41304711	0.64354773	15.32935453	H	2.04405941	7.34507533	19.51824965
H	-3.33824671	1.87914701	11.27559300	H	5.31582134	5.98016982	20.61163056
H	-4.10038067	2.20400275	13.60918027	H	3.22462465	9.30481345	18.87767909
N	-6.90789783	-4.88303012	20.31493078	H	7.46919110	7.09748442	20.10646055
C	-5.91840854	-3.94240895	19.91034719	H	5.40544485	10.38709783	18.37377877
C	-5.00897164	-3.58890410	21.12277862	H	7.48729120	9.26840876	19.00080083
O	-5.53577257	-3.24516876	22.16250143	N	0.11607418	7.36530653	21.79244900
C	-6.58621597	-2.62283562	19.47311046	C	-1.15745242	6.72873019	22.07450356
C	-5.55565214	-1.58476326	19.14748539	C	-1.91741586	6.39534159	20.75952256
C	-4.59614276	-1.82807611	18.19676823	O	-3.01384295	6.88688442	20.49384423
C	-5.56051778	-0.37261819	19.80179881	H	0.10541210	8.29946015	21.41763207
C	-3.66599919	-0.84975189	17.89709138	H	-0.98888804	5.80442961	22.62904410
C	-4.63719918	0.61268065	19.52929453	H	-1.79986910	7.38685696	22.66530962
C	-3.67525437	0.35235576	18.55141205	N	-1.36433515	5.46218994	19.96039205

C	-1.98959726	5.15464137	18.64062685	H	-7.59506627	12.11410130	18.89573195
C	-3.47269359	4.70027435	18.79113351	H	-6.25277151	11.42788820	16.92207228
O	-3.88301788	4.19538083	19.84923533	N	-5.35079829	5.36052489	22.39181200
C	-1.20922409	3.99689612	18.00764497	C	-4.98984695	4.43740143	23.47416529
C	0.26626007	4.25915890	17.93824351	C	-4.09681017	5.13961218	24.49873822
C	1.29055733	3.75985669	18.74660322	O	-3.49684413	6.15552347	24.24081747
N	0.81713753	4.98973286	16.94434009	C	-4.20147279	3.27051093	22.89870311
C	2.11688672	4.95357510	17.07131764	O	-2.98541875	3.67175471	22.32368665
N	2.45558907	4.22326993	18.16732045	H	-4.73417959	5.39422582	21.59216963
H	-0.50409789	5.00175451	20.22238854	H	-5.91519764	4.11503598	23.96437982
H	-1.95629007	6.04102347	18.00579354	H	-3.97223195	2.55187171	23.69586633
H	-1.38915714	3.07024525	18.56635109	H	-4.82926407	2.76985695	22.14561794
H	-1.59954787	3.84878144	16.99807448	H	-3.17280793	3.97804503	21.41482829
H	1.27335745	3.14458921	19.63493465	N	-6.81905873	2.39523977	10.38355235
H	2.84581166	5.42668387	16.43323598	C	-5.92998702	3.52482148	10.32961312
H	3.42377543	4.06359921	18.47691667	C	-5.70363068	4.03629788	11.78466546
N	-4.25958999	4.81883721	17.67158605	O	-6.54725378	3.89519957	12.66750959
C	-5.65214634	4.31823279	17.66576135	C	-6.44013427	4.67517270	9.44819112
C	-5.74516039	3.22554590	16.57797740	C	-7.03016284	4.18006543	8.09906596
O	-4.87285321	3.12785748	15.72026770	C	-7.49774235	5.44642071	10.20710824
C	-6.69930280	5.43456008	17.35130419	H	-7.65595019	2.50050876	10.95810595
O	-6.46213425	5.97576744	16.06568527	H	-4.97357817	3.13720618	9.95294703
H	-3.85636637	5.11618392	16.78255203	H	-5.57965843	5.32159816	9.21936090
H	-5.84397929	3.89814959	18.65581170	H	-8.02558139	4.58036881	7.93312488
H	-7.69996033	4.99201251	17.38209399	H	-6.39401836	4.49771010	7.27010101
H	-6.63723594	6.22225983	18.11160739	H	-7.09986733	3.09489824	8.06560933
H	-7.31603006	5.92435381	15.58202847	H	-8.11344089	4.77658024	10.80636807
N	-6.82105283	2.39011780	16.65913368	H	-8.15335665	5.96332735	9.50730527
C	-7.12524111	1.42144163	15.60139461	H	-7.04774891	6.18946377	10.86991841
C	-8.58706664	1.71501366	15.17832967	N	-4.50264797	4.62104265	12.01013503
O	-9.50537425	1.35362702	15.88885668	C	-4.27920924	5.39248447	13.23578609
C	-7.00471324	-0.02604992	16.12100959	C	-4.58063021	6.87704312	12.98414719
C	-7.09715539	-1.10213736	15.08413017	O	-4.21852732	7.45577094	11.93372929
C	-8.33926602	-1.62153032	14.74272754	C	-2.76811066	5.22995943	13.62990010
C	-5.95618578	-1.62250229	14.49278726	S	-2.46940305	6.21764525	15.13223415
C	-8.39141285	-2.64924730	13.80693847	H	-3.86685705	4.76246797	11.23306461
C	-6.02867125	-2.64044521	13.56672478	H	-4.90247898	4.97519996	14.02411431
C	-7.25863045	-3.14930790	13.22858745	H	-2.55856850	4.17804277	13.83201389
H	-7.48016376	2.43058258	17.43525815	H	-2.14276797	5.58485809	12.80534161
H	-6.46942959	1.59973451	14.74411092	N	-5.25372376	7.52188348	13.96140758
H	-6.03291817	-0.10024462	16.62165007	C	-5.66290472	8.90491184	13.80208060
H	-7.80950591	-0.15514245	16.85359644	C	-4.64803709	9.93518060	14.37307808
H	-9.23551695	-1.22411622	15.19635139	O	-4.81857950	11.12736373	14.25932030
H	-4.99109727	-1.21335617	14.76225048	C	-7.01334938	9.15901873	14.48897553
H	-9.35444389	-3.06295203	13.53181294	C	-8.15101122	8.48707802	13.71439617
H	-5.13680581	-3.03224436	13.09960857	C	-9.49287124	9.17313803	14.05377469
H	-7.32857406	-3.95219279	12.50394023	N	-10.26251057	8.52614387	14.94224999
N	-8.05199835	6.97938284	20.77412352	O	-9.80179647	10.22733833	13.54924531
C	-6.62980319	7.02816717	21.17617187	H	-5.56196798	7.02619002	14.79733666
C	-6.41186887	6.16127328	22.45378698	H	-5.75317844	9.10895050	12.72938390
O	-7.14062250	6.22476166	23.43279288	H	-6.99107405	8.77402774	15.51384154
C	-6.16943763	8.46764260	21.45066633	H	-7.17830591	10.23966874	14.53025391
C	-6.18078565	9.29999829	20.20406454	H	-8.00220245	8.60942994	12.63668344
C	-5.43614089	8.92858086	19.09973990	H	-8.19579628	7.42044556	13.95220466
C	-6.95979047	10.46247412	20.10731608	H	-11.13656948	8.96369113	15.18076286
C	-5.46226515	9.70042489	17.93406713	H	-9.98347440	7.63973295	15.34020729
C	-6.99157915	11.21842806	18.93900377	N	-3.52591285	9.43319544	14.93226693
C	-6.23789527	10.84593315	17.83254181	C	-2.58225852	10.44550785	15.44207353
H	-8.54857389	7.85956533	20.77298455	C	-2.08229140	11.19092238	14.24001214
H	-6.04450787	6.59380284	20.35842263	O	-1.66396926	10.56885198	13.24859439
H	-6.81308219	8.91535598	22.21621496	C	-1.41901648	9.80898392	16.16667299
H	-5.13899752	8.41092868	21.82663966	C	-1.98152918	9.15680327	17.42911152
H	-4.81086072	8.04572436	19.13749462	C	-0.31765217	10.88622524	16.47543186
H	-7.55842864	10.77182657	20.95534932	C	-0.86996547	8.58453153	18.32870878
H	-4.87082904	9.38466309	17.08683972	H	-3.32709759	8.43968815	15.01140278

H	-3.13689708	11.11774863	16.09394388	H	1.73422746	8.57697646	7.88137778
H	-0.98242118	9.04163489	15.51685631	H	3.77308203	8.27992588	5.78620465
H	-2.55584058	9.89205143	18.00720654	H	5.22142087	7.67301783	7.88466525
H	-2.66400406	8.34790354	17.15278826	H	3.17689819	9.17555229	9.08166226
H	0.06207292	11.35706976	15.56317600	H	5.22896875	10.36120518	8.34104095
H	0.53404493	10.44018974	16.99455992	H	4.26084615	10.37974425	6.85382210
H	-0.72124487	11.66740404	17.13217492	H	5.89622759	9.69719861	6.85470127
H	-0.29072073	7.81857597	17.79742974	N	0.77753060	4.24160458	8.47210867
H	-1.30558246	8.12954492	19.21578364	C	0.16048270	3.43621140	9.50164163
H	-0.17107473	9.36321390	18.65186221	C	-1.34894804	3.17536267	9.19421104
N	-2.17092556	12.50609808	14.27197073	O	-2.23868381	3.84691972	9.69170440
C	-1.74175804	13.31766132	13.09107492	C	0.22791545	4.14088170	10.89699194
C	-0.35888860	12.89244255	12.56552969	C	-0.00340099	3.10803583	11.97488777
O	0.62219820	12.75129973	13.28648145	S	0.49266330	3.81544411	13.60503925
C	-1.69256576	14.72907280	13.69371675	C	0.07023271	2.37675686	14.60545517
C	-2.84055557	14.70280289	14.69234133	H	0.82774881	5.25155127	8.58237376
C	-2.67030704	13.32960303	15.33692896	H	0.67292704	2.46986839	9.54732468
H	-2.49707868	13.27574871	12.30303401	H	1.22362039	4.59317104	10.98688114
H	-0.73565031	14.89017406	14.20271139	H	-0.53070321	4.93133249	10.93983194
H	-1.81770959	15.48828273	12.92003221	H	-1.05615315	2.80954619	12.00977651
H	-2.77191510	15.51046954	15.42307196	H	0.58781832	2.20303568	11.80987615
H	-3.79756168	14.77032454	14.16760652	H	-0.95987530	2.05795418	14.41921635
H	-1.92372880	13.38597876	16.14538457	H	0.75423193	1.54816273	14.40046316
H	-3.61697746	12.95118677	15.73106495	H	0.17143454	2.66246476	15.65300330
N	-0.35969676	12.64750210	11.24475569	Cu	-0.23430662	5.99110400	15.34520580
C	0.78432755	12.21730704	10.47610462	O	-1.94633151	11.16473561	8.88883144
C	1.02931265	10.74027212	10.33094945	H	-2.57439913	11.64474831	8.33693443
O	1.69565476	10.35186616	9.38299517	H	-2.43530257	10.82298554	9.64968891
H	-1.22085083	12.76346126	10.71786862	O	-2.94829932	9.76924170	11.07179424
H	0.74488021	12.64259761	9.47003001	H	-2.52949226	10.16905510	11.85364689
H	1.67506803	12.61916470	10.98767615	H	-3.48888525	9.04337160	11.43137516
N	0.52209131	9.91164247	11.26170675	O	2.31848147	11.73965347	18.63290822
C	0.82446449	8.49871686	11.20253223	H	1.95295392	12.58524644	18.36720239
C	0.25305346	7.76002451	9.94305481	H	2.95308565	11.93317372	19.32618000
O	0.98051401	7.02771191	9.29639579				
C	0.30402508	7.79555763	12.46208624				
C	1.14294981	8.15935609	13.66440874				
C	2.10948119	9.12980359	13.77555616				
N	1.01167101	7.47252127	14.87383605				
C	1.89448898	8.05807424	15.71343326				
N	2.56761451	9.04544547	15.09284181				
H	-0.05581546	10.26478288	12.01803688				
H	1.91436346	8.36627171	11.13395983				
H	-0.74478589	8.08162782	12.63399123				
H	0.33810815	6.71201093	12.29757660				
H	2.50194229	9.85582127	13.08294231				
H	2.05687735	7.78497151	16.74338389				
H	3.28153289	9.62707211	15.50966259				
N	-1.03796503	7.94047040	9.66540343				
C	-1.61839839	7.33943284	8.47099210				
C	-0.90266356	7.83130686	7.20323877				
O	-0.68957161	7.05804029	6.26580474				
C	-3.12619537	7.69355528	8.39886095				
H	-1.62931741	8.53309981	10.25099488				
H	-1.49143040	6.24756620	8.52667029				
H	-3.37477165	8.10921876	7.42790902				
H	-3.36625755	8.43340552	9.15791257				
H	-3.74031404	6.81207165	8.56907518				
N	2.10939306	8.53004598	6.94474006				
C	3.40872201	7.94011649	6.76830535				
C	3.36010883	6.40832610	6.78728560				
O	4.37696602	5.76199058	6.98279099				
C	4.42416829	8.42313113	7.81893754				
C	4.98025299	9.80662538	7.43699219				
O	3.84542643	8.46798000	9.07249044				

B. Cartesian coordinates of all optimized regions for MYST histone acetyltransferase KAT6A/B in complex with WM-1119

1C QM/MM R1b (B3LYP/6-31G(d):Amber) mechanical embedding $\omega_{\alpha}=1.667$ including B factors

C	21.94073594	-10.35563768	-4.21855206
C	22.25680035	-8.89111460	-4.42034794
O	21.41952270	-8.01360077	-4.34741474
N	23.52996977	-8.66526497	-4.77018317
C	23.90058430	-7.38390579	-5.36880287
C	23.06594641	-7.23776731	-6.66608127
O	23.13422709	-8.10399219	-7.53808421
C	25.39047247	-7.37436441	-5.83033538
S	25.81305002	-5.71741486	-6.50323110
H	24.14347636	-9.46732353	-4.90655694
H	23.71433881	-6.57919738	-4.65694980
H	25.58275533	-8.18348918	-6.53751208
H	25.98596062	-7.56832590	-4.92767633
N	22.36986906	-6.08586207	-6.79301186
C	21.45646356	-5.93158302	-7.92156576
H	22.15885922	-5.52481623	-5.97314360
C	24.31464426	-4.85997693	-10.21425324
C	25.25336528	-5.90171697	-10.73698499
O	25.25373829	-6.08482209	-11.95030613
N	26.00908195	-6.59718043	-9.82452832
C	26.84244165	-7.67002402	-10.30689395
C	26.23521058	-9.07205678	-10.12487182
O	26.77423595	-10.09028589	-10.57260122
C	28.24684731	-7.59498332	-9.72360581
S	28.23655950	-8.13574302	-7.88059322
H	25.99026924	-6.32500688	-8.83902927
H	26.90939709	-7.53808048	-11.39042380
H	28.63143703	-6.57859683	-9.82395200
H	28.89435646	-8.28298561	-10.27102847
N	25.07706370	-9.11595236	-9.41687339
C	24.41120315	-10.40462451	-9.18060668
H	24.60144550	-8.30389824	-9.04658929
C	29.87618767	-4.49139904	2.80734460
C	30.08809079	-4.51304251	1.25997262
O	30.68177758	-3.65189688	0.65538702
N	29.50878361	-5.57056662	0.64034629
C	29.56468735	-5.63294728	-0.82963224
C	29.06034466	-4.33597995	-1.43967688
O	29.79331547	-3.73646848	-2.21400992
C	28.84073746	-6.85845777	-1.37065211
C	28.94490551	-6.94732431	-2.85614620
H	29.27409099	-7.75211230	-0.91376376
H	28.96143463	-6.24735463	1.16406704
H	30.62154031	-5.65715345	-1.11010517
H	27.78226465	-6.81356902	-1.10188711
C	28.13636501	-6.45547340	-3.86218308
H	30.87958019	-7.83143239	-3.02821072
H	27.22424926	-5.88777328	-3.77790857
C	29.81360910	-7.47099245	-4.82354680
N	30.00621728	-7.59005678	-3.49266547
N	28.65468046	-6.87895189	-5.03036549
H	30.47767511	-7.84755967	-5.58167924
N	27.83963988	-3.88198010	-1.05152279
C	27.28004636	-2.64030923	-1.54927257
H	27.30420088	-4.36721450	-0.33308501
C	32.66577007	-1.85125542	-2.42098860
C	32.41206854	-1.96660021	-3.93852705

O	33.16291283	-1.50130576	-4.79179252
N	31.30915677	-2.66681769	-4.23063886
C	30.98417770	-3.03901006	-5.61684253
C	30.87574310	-1.72773794	-6.40635342
O	30.13257839	-0.83792937	-6.06463419
C	29.67282759	-3.82665333	-5.59210692
S	29.19530776	-4.40310987	-7.28267219
H	30.76041128	-3.03843701	-3.47109740
H	31.78348960	-3.67165832	-6.01940026
H	28.89035625	-3.17958298	-5.18586834
H	29.81214063	-4.67407763	-4.91775721
N	31.60211060	-1.61416253	-7.51677801
C	31.62350322	-0.46811741	-8.37660949
H	32.39354180	-2.18616113	-7.66946925
C	7.68880347	-15.97673983	-16.35325433
H	7.13257647	-16.36225543	-17.19389092
C	8.07429751	-16.79164897	-15.30030228
H	7.86120392	-17.85116936	-15.32508937
C	8.75144409	-16.18649120	-14.24483267
H	9.12710908	-16.74867484	-13.41609152
C	8.97153808	-14.81993887	-14.27158004
H	9.54166155	-14.35231068	-13.47793470
N	8.49562773	-13.99473752	-15.23625285
C	7.91284040	-14.62527482	-16.26793244
C	7.39481130	-13.77933435	-17.35077773
C	7.52223061	-14.20235981	-18.69358602
C	7.00241290	-13.37208453	-19.69119257
C	6.41159701	-12.14712662	-19.40456826
H	6.01918558	-11.54881197	-20.19725982
F	7.07150359	-13.77176911	-20.99464842
H	8.05665654	-15.12083328	-18.92672037
C	6.80395267	-12.56484880	-17.02726152
H	6.71249257	-12.31380973	-15.98116706
C	6.26512854	-11.77640741	-18.04021655
C	5.46015755	-10.60241534	-17.66963750
O	5.69970977	-9.85429347	-16.72119726
N	4.37078163	-10.33592303	-18.51532000
H	3.97189627	-11.04969422	-19.13329522
N	3.43949500	-9.35347169	-18.20192869
H	3.37743513	-9.17809524	-17.19840049
S	3.59506388	-7.95862163	-19.05943988
O	4.97173062	-7.56611062	-19.42231035
O	2.81214898	-6.88746735	-18.42152319
C	2.76969810	-8.39279158	-20.68427117
C	1.62025016	-7.67156497	-21.07773761
H	1.13308883	-6.98731600	-20.39278126
C	1.05119937	-7.92944969	-22.34462582
H	0.10994536	-7.47349478	-22.61951817
C	1.61488253	-8.88265105	-23.19477280
H	1.16039281	-9.12052380	-24.15482562
C	2.78757877	-9.53083345	-22.84397326
H	3.27404571	-10.22876551	-23.52268338
C	3.35393759	-9.28994509	-21.58860604
F	4.52475627	-9.96797300	-21.28809894
Zn	28.08282134	-6.23748601	-6.90668687

2C QM/MM R1b (B3LYP/6-31G(d): Amber) mechanical embedding $\omega_{\alpha}=1.667$ including B factors

C	21.94065383	-10.35660226	-4.21796255
C	22.25676507	-8.89284205	-4.41784677
O	21.41823759	-8.01610196	-4.34941772
N	23.52907014	-8.66573171	-4.76820555

C 23.89428628 -7.38413281 -5.36705444
 C 23.06616102 -7.23908515 -6.66790198
 O 23.13233313 -8.10403293 -7.54099225
 C 25.38776150 -7.36245005 -5.80512050
 S 25.81298731 -5.71851560 -6.50550616
 H 24.15995629 -9.46132829 -4.86008770
 H 23.69496636 -6.58157053 -4.65824777
 H 25.60936820 -8.19462591 -6.47494296
 H 25.95842157 -7.51415464 -4.87846596
 N 22.37169965 -6.08620884 -6.79433588
 C 21.45674831 -5.93146554 -7.92169412
 H 22.17726240 -5.51288425 -5.97904153
 C 24.31461549 -4.86000499 -10.21462396
 C 25.25233279 -5.90181226 -10.73965827
 O 25.25256455 -6.08443937 -11.95299700
 N 26.00829874 -6.59638467 -9.82762056
 C 26.83988764 -7.67180148 -10.30537404
 C 26.23418744 -9.07134604 -10.12438768
 O 26.77600259 -10.08702595 -10.57387776
 C 28.24000842 -7.59508404 -9.71940008
 S 28.23633803 -8.13575648 -7.87888816
 H 25.98296595 -6.32806300 -8.84143109
 H 26.91980225 -7.54587826 -11.38763681
 H 28.60924794 -6.57463224 -9.81913536
 H 28.88859847 -8.27629639 -10.27267762
 N 25.07696397 -9.11669047 -9.41625384
 C 24.41111603 -10.40499349 -9.18039961
 H 24.60474750 -8.30546403 -9.04015425
 C 29.87623099 -4.49086641 2.80923437
 C 30.08817135 -4.51108980 1.26356670
 O 30.68328274 -3.65183601 0.65747339
 N 29.50595536 -5.56786367 0.64611109
 C 29.56958081 -5.62417131 -0.82107572
 C 29.06277246 -4.33272222 -1.43439918
 O 29.79018989 -3.74824887 -2.22417912
 C 28.85040508 -6.84606310 -1.37064259
 C 28.95538229 -6.94510910 -2.85108420
 H 29.28936164 -7.73464256 -0.91556327
 H 28.94803511 -6.23536671 1.17141215
 H 30.62784502 -5.64873920 -1.09294465
 H 27.79363324 -6.79460689 -1.10706485
 C 28.14856222 -6.45812300 -3.85861791
 H 30.87733549 -7.86139421 -3.01969768
 H 27.24131889 -5.88991929 -3.75976508
 C 29.82037751 -7.47877812 -4.81256436
 N 30.01058324 -7.59668037 -3.48329915
 N 28.66430906 -6.88299721 -5.02778369
 H 30.49612830 -7.85988106 -5.55402845
 N 27.84172445 -3.87858118 -1.04748173
 C 27.28029118 -2.63972220 -1.54913806
 H 27.32750434 -4.34015400 -0.29870801
 C 32.66602620 -1.85116211 -2.42104443
 C 32.41388506 -1.96602268 -3.93938426
 O 33.16747564 -1.50594137 -4.79209824
 N 31.30767404 -2.66250475 -4.22895362
 C 30.97900904 -3.03703490 -5.61508636
 C 30.86816274 -1.72804221 -6.40511183
 O 30.12900710 -0.83634312 -6.06029987
 C 29.66991845 -3.82452316 -5.59602032
 S 29.19577273 -4.40336761 -7.28480868
 H 30.75713690 -3.01767822 -3.46237852
 H 31.77836421 -3.66837424 -6.01669841
 H 28.88565061 -3.17622672 -5.19703894
 H 29.80922385 -4.67370988 -4.92636085
 N 31.59932925 -1.60650108 -7.50826083

C 31.62300226 -0.46750000 -8.37629476
 H 32.31158620 -2.24903296 -7.72863222
 C 7.67526289 -15.97232178 -16.35287639
 H 7.10350078 -16.36263605 -17.17946250
 C 8.06677831 -16.78719023 -15.30384379
 H 7.85356707 -17.84615069 -15.32383328
 C 8.75148577 -16.18776450 -14.25176533
 H 9.13343324 -16.75602588 -13.43244480
 C 8.97672251 -14.82370532 -14.27762952
 H 9.55629664 -14.35521333 -13.49353330
 N 8.50269673 -13.99852091 -15.23996862
 C 7.91118093 -14.62435505 -16.26859371
 C 7.39862577 -13.77943728 -17.34587210
 C 7.53174736 -14.19790213 -18.68650360
 C 7.00644394 -13.37443576 -19.68215963
 C 6.41180628 -12.15525702 -19.38797941
 H 6.00739141 -11.55457971 -20.16827843
 F 7.07340221 -13.77373711 -20.98518007
 H 8.07503660 -15.10568702 -18.92220733
 C 6.79894065 -12.57420264 -17.01698223
 H 6.68000429 -12.33459191 -15.97385243
 C 6.26125406 -11.78502183 -18.02695749
 C 5.45540065 -10.60537130 -17.66499850
 O 5.70499292 -9.85428072 -16.72104638
 N 4.36140917 -10.33301319 -18.49931058
 H 3.96013710 -11.03335892 -19.13044198
 N 3.43218147 -9.33318938 -18.19105720
 H 3.44319646 -9.11224421 -17.19402449
 S 3.59184975 -7.94893492 -19.06656689
 O 4.97622498 -7.57219112 -19.41651792
 O 2.80945312 -6.87054454 -18.43578956
 C 2.76424923 -8.38377803 -20.69464331
 C 1.61229815 -7.67344220 -21.08687147
 H 1.12110719 -6.99617528 -20.40242164
 C 1.04370381 -7.93997574 -22.34978018
 H 0.09654219 -7.49677972 -22.61980748
 C 1.60863587 -8.89277528 -23.19608508
 H 1.14799064 -9.13746602 -24.15024171
 C 2.78322836 -9.53444350 -22.84544575
 H 3.26757874 -10.23574609 -23.51968610
 C 3.34877393 -9.28422144 -21.59426917
 F 4.51959999 -9.96019119 -21.29063924
 Zn 28.08268870 -6.23738754 -6.90737083

**1C QM/MM R2b (B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_c=1.667$ including B
factors**

C 21.94167691 -10.35519930 -4.21859036
 C 22.25983100 -8.89540303 -4.43123794
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H	0.16492210	-9.77227537	-12.62529715	C	5.95473878	-7.33020417	-23.17227775
H	-2.10888036	-12.79695359	-15.47788808	C	7.07450779	-6.70960647	-23.99515282
H	-1.59887969	-11.15456410	-15.14039125	O	7.18533774	-6.98362151	-25.19329156
H	0.35979108	-7.92536346	-14.87850951	C	4.74941206	-6.38990055	-23.10126553
H	1.46075166	-7.91308876	-13.49619273	C	4.14710030	-6.04849233	-24.48970117
N	3.59004280	-5.59935357	-15.80953250	C	2.94402527	-5.14570545	-24.21853022
C	3.71062688	-4.12343854	-15.85732493	N	2.22718116	-4.75101895	-25.42905695
C	4.28080393	-3.61720468	-17.18969082	C	1.13198790	-3.97963354	-25.46477999
O	4.54489276	-2.43337492	-17.35667678	N	0.59437089	-3.53423375	-24.33640005
C	4.51464908	-3.60905765	-14.66379653	N	0.61007354	-3.59636058	-26.60360234
C	3.67927760	-3.51822867	-13.39642468	H	3.81055949	-6.95163761	-24.99865792
C	4.55951054	-3.71918081	-12.17215475	H	5.67302723	-8.25317076	-23.68491078
N	3.86582963	-3.26283886	-10.94742561	H	2.60461121	-5.05668195	-26.32713141
C	3.43051409	-4.04924817	-9.96385979	H	4.86540987	-5.51453712	-25.10739880
N	3.44078899	-5.35280477	-10.08584867	H	-0.23082661	-3.05433528	-26.66564412
N	2.98521155	-3.54807213	-8.83984963	H	0.96180726	-3.99962225	-27.46417785
H	2.88411634	-4.26044086	-13.38423179	H	6.05841298	-7.20806559	-21.01946190
H	2.72336224	-3.66721116	-15.77194146	H	3.28676332	-4.25093507	-23.70134838
H	3.82458754	-2.26879832	-10.79524293	H	2.24546206	-5.68679656	-23.58007065
H	3.22737284	-2.52331154	-13.35331491	H	-0.21446180	-2.93629702	-24.38744903
H	2.73301996	-4.18055797	-8.10566790	H	0.82571363	-4.08021292	-23.53995961
H	2.94213112	-2.55548316	-8.71775128	H	5.02219643	-5.46356270	-22.60874642
H	4.40510561	-6.17668584	-15.98391100	H	3.97982967	-6.86451729	-22.50593274
H	5.48109202	-3.14418947	-12.27989520	N	9.61930907	-9.43391052	-24.94600453
H	4.83564340	-4.77246989	-12.11784624	C	9.06730048	-10.21469515	-26.06961163
H	3.22759596	-6.00988698	-9.35798819	C	9.19588883	-9.39457679	-27.37060193
H	3.85221974	-5.71151277	-10.92724023	O	9.79528165	-9.85451920	-28.31723117
H	4.90883656	-2.61306679	-14.87908089	C	7.61294367	-10.69826543	-25.80389854
H	5.36147916	-4.26638254	-14.49458053	C	7.58437527	-11.69399394	-24.63716609
N	4.30075950	-4.47855201	-18.21179204	C	7.09907439	-11.41797837	-27.05795194
C	4.75900332	-4.10891130	-19.55827588	C	6.17805508	-11.89230143	-24.08038461
C	6.23998996	-4.46303082	-19.87440209	H	9.68783571	-11.10407632	-26.20030879
O	6.59945991	-4.44179145	-21.06438243	H	6.08247051	-11.76593096	-26.89662006
H	4.05604444	-5.43934978	-18.00111488	H	7.07868116	-10.73701204	-27.90482636
H	4.14850128	-4.64163084	-20.28390454	H	6.98655143	-9.83344827	-25.58329962
H	4.64416554	-3.03531993	-19.71608867	H	8.01095900	-12.64393128	-24.94960370
N	7.04827179	-4.82472444	-18.86348892	H	8.20358376	-11.32477641	-23.82535714
C	8.46002208	-5.18542155	-19.00901524	H	5.56174474	-12.35394636	-24.84978206
C	8.61184467	-6.50301033	-19.75109010	H	9.04824798	-9.21506303	-24.14240686
O	9.39819246	-6.55769845	-20.69231932	H	6.23228386	-12.56020251	-23.22760353
C	9.16741143	-5.24705518	-17.62111213	H	7.73994068	-12.26389121	-27.28982476
C	9.11557897	-3.93368361	-16.87070018	H	5.74787593	-10.93532743	-23.79409717
C	9.98835247	-2.87140881	-17.14693757	N	6.59450517	-20.99399810	-19.57814771
C	8.16452347	-3.79497052	-15.85165357	C	6.07987226	-20.91097797	-18.20205194
C	9.90961903	-1.67336510	-16.40702186	C	4.58281412	-20.56968892	-18.30855374
C	8.06339652	-2.60405022	-15.10263788	O	4.08718745	-20.17253374	-19.39297612

C	6.81290042	-19.87036195	-17.36902842	H	1.08847455	-11.70984707	-25.88610671
O	6.65452106	-18.58717064	-17.94219228	H	4.06263353	-11.74804345	-29.28173479
H	7.17126506	-20.27322915	-19.99392350	H	3.90161137	-7.90248204	-27.33784843
H	6.18655086	-21.88276585	-17.71627438	H	3.23076246	-11.57055335	-27.03817414
H	7.87311298	-20.12392825	-17.32321711	H	3.32831543	-10.06572430	-26.11667465
H	6.41080517	-19.86665805	-16.35660932	H	6.34315923	-7.40823927	-31.21503281
H	7.53709099	-18.35446804	-18.30143237	C	7.70843886	-15.97509670	-16.35732213
N	3.14382709	-17.89151541	-16.99721397	H	7.18297045	-16.35710459	-17.22131005
C	3.07660392	-16.45518114	-17.25547308	C	8.08994520	-16.79554545	-15.30579727
C	3.61599907	-16.03991949	-18.63506246	H	7.87716759	-17.85620933	-15.33985909
O	3.11344021	-15.09542106	-19.27366576	C	8.75499658	-16.19172034	-14.24120173
C	3.79652848	-15.71799285	-16.14355908	H	9.10596682	-16.76106229	-13.40015445
C	3.77689980	-14.18648434	-16.26490668	C	8.96571195	-14.81802121	-14.27099437
C	2.34963924	-13.64984828	-16.44617269	H	9.51887603	-14.34904410	-13.46440155
C	4.35662048	-13.60970593	-14.95072217	N	8.49305590	-13.98899110	-15.23843801
H	5.37026919	-13.98011918	-14.79915266	C	7.90795703	-14.61606575	-16.27141143
H	4.36087553	-12.52448601	-14.98732782	C	7.38541760	-13.76706991	-17.36012338
H	3.74750736	-13.93909271	-14.10785750	C	7.49736467	-14.19346226	-18.70239944
H	3.82627116	-18.25541776	-16.33193413	C	6.99734349	-13.34713120	-19.70531189
H	1.72891110	-14.00932706	-15.62752340	C	6.40368075	-12.12196859	-19.43318485
H	2.37295399	-12.56231224	-16.43252252	H	6.02530008	-11.52967468	-20.24326563
H	1.92981500	-13.97539245	-17.39177788	F	7.07755072	-13.75417788	-21.00260079
H	2.02557921	-16.17042495	-17.22731882	H	8.00276903	-15.13117759	-18.94076543
H	4.39255719	-13.85229727	-17.09712970	C	6.80399425	-12.54005590	-17.04577244
H	4.83805938	-16.03631020	-16.12799610	H	6.74251856	-12.27659394	-15.99830329
H	3.34640066	-16.00080595	-15.19157750	C	6.25697771	-11.75982097	-18.05807012
N	4.67659225	-16.67359499	-19.07315384	C	5.45147351	-10.59672681	-17.67078108
C	5.15102067	-16.56427740	-20.44462921	O	5.67652423	-9.86168743	-16.71240015
C	4.04589609	-16.96500139	-21.44601065	N	4.38146984	-10.33272342	-18.53897362
O	3.83199139	-16.20164989	-22.35445547	H	4.00570133	-11.07225282	-19.14050780
H	5.08259719	-17.40446691	-18.49096439	N	3.42712604	-9.38323484	-18.22493344
H	5.45611632	-15.54195767	-20.65095803	H	3.25223102	-9.28582572	-17.22419667
H	6.00591795	-17.22539100	-20.59007687	S	3.59320842	-7.96692403	-19.04576016
N	1.57121543	-14.23929555	-21.63483890	O	4.96950286	-7.56269044	-19.40692671
C	2.20385140	-13.04215909	-22.16201855	O	2.80959309	-6.89733379	-18.41067294
C	2.47230844	-13.19451922	-23.69120903	C	2.78554652	-8.38296249	-20.67449869
O	2.28904236	-12.23104583	-24.40183305	C	1.64482594	-7.64696539	-21.06486693
C	3.55285529	-12.80739442	-21.41111992	H	1.16905685	-6.95421383	-20.37872013
O	3.32860194	-12.57049730	-19.97254224	C	1.07331188	-7.88523925	-22.33448252
H	2.08694866	-14.82843553	-20.98985044	H	0.15831025	-7.38516024	-22.63556717
H	1.55931446	-12.17757296	-22.00782686	C	1.63464418	-8.83474948	-23.19223338
H	4.07800648	-11.99968204	-21.89565145	H	1.19021596	-9.04450648	-24.16349882
H	4.18247217	-13.69048975	-21.52824835	C	2.79367842	-9.50795909	-22.83626664
H	3.22131926	-13.46809986	-19.58929393	H	3.27945183	-10.19794971	-23.52281776
N	-0.99883750	-13.04004213	-25.47347320	C	3.36373997	-9.27976969	-21.58022235
C	-1.45653366	-11.65281278	-25.47030359	F	4.53375268	-9.95655528	-21.29022520
C	-0.66362526	-10.83090403	-26.48354622	Zn	28.08310060	-6.23441893	-6.91254238
O	-1.22483587	-9.98396742	-27.18873217	O	-2.10866911	-6.04256302	-23.95331848
H	-0.53228664	-13.43689858	-24.67127450	H	-2.82318363	-5.47642944	-23.60749244
H	-2.50410694	-11.62695972	-25.77878544	H	-2.40863869	-6.92076016	-23.69985219
N	0.67171976	-11.00497996	-26.48387746	O	7.34923536	-19.80969014	-13.53894323
C	1.54953190	-10.22820919	-27.35080014	H	8.21335279	-19.44180396	-13.27932953
C	1.19398743	-10.53481715	-28.82444176	H	7.37769770	-20.69639980	-13.16246258
O	0.99670514	-9.59211710	-29.57115729	O	9.24761494	-17.93744864	-18.98035543
C	3.05284262	-10.49714501	-27.07707917	H	9.88002556	-17.25031981	-18.68045914
C	3.96209270	-9.90944935	-28.14926714	H	9.82421427	-18.65692144	-19.25857282
C	4.24641463	-8.53730260	-28.13563460	O	5.98280948	-7.01653550	-16.77148116
C	4.35371555	-10.70957192	-29.23851011	H	6.45367046	-6.72544003	-15.96780510
C	5.07797717	-7.99940447	-29.13299739	H	6.21328141	-7.95313267	-16.83508129
C	5.18882584	-10.19025308	-30.24466932	O	26.49407347	-0.90809781	-4.84887327
C	5.57533737	-8.84254521	-30.15167148	H	27.11630126	-0.82001480	-4.11396664
O	6.50627272	-8.33288739	-30.97361666	H	26.76582713	-1.71735874	-5.29123432
H	1.36322101	-9.16562933	-27.20062766	O	0.73163336	-10.02469854	-18.02520022
H	5.38984116	-6.97171014	-29.10147345	H	-0.04357004	-10.48686893	-18.41286294
H	5.55535257	-10.79684564	-31.05977438	H	1.46921835	-10.39186484	-18.52008374

O 4.78284773 -18.68717480 -14.47386265
H 5.70325743 -18.92087106 -14.25649973
H 4.28543008 -19.33738352 -13.96613729
O -0.45920945 -6.70337312 -25.86136120
H -0.90434201 -7.26849694 -26.50326302
H -1.17567613 -6.40192276 -25.27242006

1C QM/SE/MM R1b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.667$ including B factors

C 22.27282083 -8.92436286 -4.42227427
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N 23.53837507 -8.67713073 -4.77428101
C 23.88304980 -7.39000885 -5.37305674
C 23.06228446 -7.24443947 -6.68301598
O 23.12358015 -8.11387364 -7.55527362
C 25.38118965 -7.35371153 -5.80320518
S 25.81328984 -5.71118521 -6.50623255
H 24.17088853 -9.46491764 -4.89901889
H 23.67499577 -6.58504626 -4.66699980
H 25.61219351 -8.18796499 -6.47116225
H 25.94870544 -7.50149457 -4.87250544
N 22.37015149 -6.08667505 -6.82285062
H 22.18530785 -5.53217017 -5.99245907
C 25.24718822 -5.90687421 -10.75098074
O 25.31336158 -6.06205639 -11.97150991
N 26.00186049 -6.60828800 -9.83420844
C 26.81625749 -7.70200019 -10.30136128
C 26.19822323 -9.10300030 -10.09931884
O 26.73394933 -10.11837609 -10.56596256
C 28.22155186 -7.61440034 -9.73143668
S 28.24190562 -8.13569583 -7.88272360
H 25.94545417 -6.37904354 -8.83797259
H 26.90496134 -7.58879721 -11.38476573
H 28.58639509 -6.59407556 -9.83674701
H 28.86962921 -8.30351285 -10.27529691
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O 30.68396685 -3.64159089 0.66424795
N 29.50389409 -5.54982158 0.66329845
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C 28.84631869 -6.83038305 -1.35760628
C 28.95200900 -6.93540881 -2.83369861
H 29.28815715 -7.71803202 -0.89805243
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H 30.87747561 -7.86993980 -2.99690440
H 27.24715365 -5.88434272 -3.75490344
C 29.81876104 -7.49090502 -4.79874186
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H 30.49980038 -7.87662278 -5.53189687
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H 27.30385568 -4.30862731 -0.32511636
C 32.42369638 -1.94868818 -3.92966428
O 33.17702618 -1.49391053 -4.78339235
N 31.31296847 -2.64457324 -4.22686395
C 30.98152882 -3.02620492 -5.61507439

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O 30.15586434 -0.81196375 -6.06692522
C 29.67030981 -3.81184381 -5.59589917
S 29.19049258 -4.40115858 -7.28619986
H 30.76020083 -3.00346363 -3.46461345
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C 7.67288075 -15.97897930 -16.35347904
H 7.10274574 -16.37015453 -17.18292180
C 8.06107037 -16.79202514 -15.30657368
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C 8.74715162 -16.20117339 -14.24361682
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C 8.98835576 -14.83965900 -14.27236954
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C 6.99847225 -13.37705990 -19.67255946
C 6.40902276 -12.16377845 -19.38906030
H 6.01638929 -11.54942029 -20.15907412
F 7.06879065 -13.78185518 -20.98555304
H 8.09168246 -15.10117388 -18.91949460
C 6.81970936 -12.57387807 -17.00903535
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N 4.37640109 -10.33595694 -18.50871951
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H 3.55270960 -9.04716104 -17.19979058
S 3.60440355 -7.95152205 -19.08189228
O 5.01545224 -7.56410083 -19.41430173
O 2.84216728 -6.84951033 -18.42777548
C 2.78782262 -8.36381023 -20.67449526
C 1.61505893 -7.65250859 -21.07210734
H 1.13174418 -6.98355929 -20.37798311
C 1.04862584 -7.92583885 -22.32286981
H 0.09715891 -7.47927580 -22.58582536
C 1.60016400 -8.88732757 -23.18173506
H 1.12033448 -9.13950154 -24.11935631
C 2.78181361 -9.54109609 -22.83009421
H 3.22430617 -10.26824557 -23.49767169
C 3.35866355 -9.27951807 -21.59634826
F 4.52580587 -9.97865558 -21.29498351
Zn 28.08199226 -6.24092961 -6.90505020

2C QM/SE/MM R1b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.667$ including B factors

C 22.27376086 -8.92401909 -4.42405813
O 21.42461151 -8.05582481 -4.33631712
N 23.54034655 -8.67759477 -4.77800900
C 23.88937278 -7.39052448 -5.37514304
C 23.06297665 -7.24353414 -6.68179139
O 23.12546412 -8.11355236 -7.55362070
C 25.38497484 -7.36376479 -5.82153118
S 25.81703024 -5.71280535 -6.50591722

H	24.15900389	-9.46928969	-4.93862774	C	7.39887418	-13.77971386	-17.33920017
H	23.68918464	-6.58519808	-4.66677282	C	7.52061587	-14.21296579	-18.69289436
H	25.59496241	-8.18059185	-6.51648312	C	6.99625299	-13.37294943	-19.67956574
H	25.97125889	-7.54265887	-4.90966546	C	6.40888684	-12.15533434	-19.39974519
N	22.36938213	-6.08815422	-6.82047407	H	6.02487910	-11.54312886	-20.17955044
H	22.17566048	-5.54100761	-5.98682763	F	7.06937273	-13.77711203	-20.99268897
C	25.24773667	-5.90755002	-10.75006497	H	8.07779925	-15.11323972	-18.92378817
O	25.31471763	-6.06130246	-11.97071284	C	6.82388890	-12.56693472	-17.01562358
N	26.00079286	-6.61150979	-9.83386652	H	6.71750344	-12.31814478	-15.97030979
C	26.81881899	-7.70219860	-10.30415291	C	6.26877395	-11.76096129	-18.01660346
C	26.20097959	-9.10504290	-10.10073757	C	5.46708418	-10.61835485	-17.66049753
O	26.73449642	-10.12178899	-10.56613248	O	5.69652227	-9.83850761	-16.67972258
C	28.22711433	-7.61391126	-9.73513758	N	4.38507064	-10.33602372	-18.52299379
S	28.24193601	-8.13476475	-7.88507891	H	3.96115907	-11.04581327	-19.11582277
H	25.94532653	-6.38213969	-8.83736586	N	3.45702203	-9.34164259	-18.19323517
H	26.89699205	-7.58463266	-11.38807391	H	3.52504456	-9.08373163	-17.20086298
H	28.60284417	-6.59754011	-9.84252653	S	3.60679041	-7.95764818	-19.07873042
H	28.87504188	-8.30687187	-10.27352100	O	5.01318583	-7.55701701	-19.41727381
N	25.05664557	-9.15201435	-9.36423206	O	2.84628534	-6.86135057	-18.41667979
H	24.59372175	-8.32858386	-9.00524261	C	2.78993308	-8.37320243	-20.66486725
C	30.09147482	-4.49105299	1.28289158	C	1.62050896	-7.64709063	-21.06303678
O	30.68571979	-3.64151630	0.66505304	H	1.14030847	-6.97371530	-20.36684392
N	29.50535786	-5.54961127	0.65952982	C	1.05357347	-7.91454334	-22.31653842
C	29.55728365	-5.60836494	-0.81203715	H	0.10640380	-7.45834281	-22.58078472
C	29.05045499	-4.31949962	-1.44055792	C	1.60104830	-8.87866394	-23.17815093
O	29.79488422	-3.73545363	-2.21558149	H	1.12179875	-9.12820622	-24.11755439
C	28.83867103	-6.83884381	-1.35669089	C	2.78146988	-9.53951153	-22.82776844
C	28.94380793	-6.93701111	-2.83721442	H	3.22237221	-10.26796712	-23.49727054
H	29.27505698	-7.72962412	-0.89566706	C	3.36109572	-9.28411777	-21.59186344
H	28.94480430	-6.22219812	1.17469172	F	4.52822008	-9.98732933	-21.29327171
H	30.61340130	-5.63355602	-1.09575597	Zn	28.08231401	-6.24165852	-6.90615848
H	27.78021213	-6.79654024	-1.09335674				
C	28.14475046	-6.45016877	-3.85410615				
H	30.87888328	-7.84787925	-3.00357367				
H	27.23631331	-5.87952836	-3.76907133				
C	29.81357413	-7.48535989	-4.80721906				
N	29.99994395	-7.61247032	-3.46626923				
N	28.66263664	-6.87729364	-5.01748947	C	21.94235593	-10.35441323	-4.21923405
H	30.48339685	-7.87048296	-5.55298867	C	22.26213096	-8.89486943	-4.42683948
N	27.82703598	-3.85418433	-1.07090545	O	21.42258707	-8.01927272	-4.34633861
H	27.28543437	-4.33191098	-0.35234398	N	23.53417164	-8.67665758	-4.78455333
C	32.42067854	-1.95009883	-3.92931273	C	23.89355583	-7.39534152	-5.38780835
O	33.17274397	-1.49090806	-4.78085563	C	23.07461744	-7.24669929	-6.69724290
N	31.31251101	-2.64901593	-4.22817084	O	23.12874591	-8.13033821	-7.55514783
C	30.98196696	-3.02927033	-5.61608048	C	25.38353526	-7.36442034	-5.81668671
C	30.87469587	-1.72220190	-6.41715338	S	25.81678803	-5.71693765	-6.50245878
O	30.16564873	-0.80814908	-6.06769466	H	24.14804832	-9.47563419	-4.92435699
C	29.67005631	-3.81466158	-5.59213057	H	23.68607490	-6.59087292	-4.68517898
S	29.19030220	-4.40133969	-7.28474687	H	25.59703691	-8.17908706	-6.50867519
H	30.76059826	-3.01877855	-3.47086145	H	25.96653131	-7.54172180	-4.90466163
H	31.78302433	-3.66621409	-6.01264769	N	22.39336607	-6.08868686	-6.84980670
H	28.88946380	-3.16295139	-5.19076003	C	21.47687488	-5.96277464	-7.96253623
H	29.80628489	-4.66214112	-4.91612583	C	22.17619051	-5.64169626	-9.30394485
N	31.60841649	-1.59977940	-7.52279749	O	21.56568092	-5.75563631	-10.34942644
H	32.12995217	-2.37270204	-7.85802255	C	20.49320556	-4.87081719	-7.64678233
C	7.68135978	-15.98286114	-16.35596184	H	20.93182619	-6.90049926	-8.10598104
H	7.12312775	-16.37117369	-17.19605006	H	22.23909599	-5.51084407	-6.02737978
C	8.06534423	-16.79711722	-15.30741963	N	23.43905266	-5.18534741	-9.15261499
H	7.84775264	-17.85456029	-15.32258423	C	24.28962152	-4.79077336	-10.23530244
C	8.74624951	-16.20553379	-14.23976785	C	25.23403167	-5.87009104	-10.73709497
H	9.11492094	-16.80790262	-13.43236881	O	25.27754317	-6.06812498	-11.95352447
C	8.98376836	-14.84181903	-14.26688271	C	25.10063870	-3.57070430	-9.88367227
H	9.56474477	-14.35982168	-13.48979655	C	24.25439009	-2.42767539	-9.42218032
N	8.51872528	-14.00438168	-15.23324954	C	23.30333541	-1.84842535	-10.24981436
C	7.91107569	-14.62515009	-16.26862814	C	24.39152719	-1.92964815	-8.10914418

1C QM/SE/MM R3b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.667$ including B factors

C	21.94235593	-10.35441323	-4.21923405
C	22.26213096	-8.89486943	-4.42683948
O	21.42258707	-8.01927272	-4.34633861
N	23.53417164	-8.67665758	-4.78455333
C	23.89355583	-7.39534152	-5.38780835
C	23.07461744	-7.24669929	-6.69724290
O	23.12874591	-8.13033821	-7.55514783
C	25.38353526	-7.36442034	-5.81668671
S	25.81678803	-5.71693765	-6.50245878
H	24.14804832	-9.47563419	-4.92435699
H	23.68607490	-6.59087292	-4.68517898
H	25.59703691	-8.17908706	-6.50867519
H	25.96653131	-7.54172180	-4.90466163
N	22.39336607	-6.08868686	-6.84980670
C	21.47687488	-5.96277464	-7.96253623
C	22.17619051	-5.64169626	-9.30394485
O	21.56568092	-5.75563631	-10.34942644
C	20.49320556	-4.87081719	-7.64678233
H	20.93182619	-6.90049926	-8.10598104
H	22.23909599	-5.51084407	-6.02737978
N	23.43905266	-5.18534741	-9.15261499
C	24.28962152	-4.79077336	-10.23530244
C	25.23403167	-5.87009104	-10.73709497
O	25.27754317	-6.06812498	-11.95352447
C	25.10063870	-3.57070430	-9.88367227
C	24.25439009	-2.42767539	-9.42218032
C	23.30333541	-1.84842535	-10.24981436
C	24.39152719	-1.92964815	-8.10914418

C	22.54571781 -0.76760877 -9.82373915	C	24.89854097 -13.85121236 -4.12911153
C	23.59571914 -0.89565580 -7.66599640	H	26.23738580 -14.13969646 -5.72856318
C	22.68918678 -0.28530974 -8.52488490	C	29.87642389 -4.48901804 2.80743862
O	22.01553736 0.82823964 -8.08591688	C	30.09409099 -4.50203636 1.26424678
H	23.62110377 -4.54393001 -11.06794936	O	30.68533311 -3.64203265 0.65773434
H	21.80974392 -0.34932532 -10.48360898	N	29.51313746 -5.56088847 0.64599284
H	23.71528381 -0.49617211 -6.67883629	C	29.56560303 -5.61738194 -0.81829936
H	23.85985379 -5.31075796 -8.23472763	C	29.05575303 -4.32482432 -1.43543876
H	25.12891274 -2.34577367 -7.45216067	O	29.77753803 -3.72980162 -2.22384976
H	23.14307259 -2.23820172 -11.24111396	C	28.84329301 -6.84365062 -1.35804838
H	25.66612554 -3.24890181 -10.75368006	C	28.95276614 -6.94895573 -2.83491434
H	25.80319654 -3.81326609 -9.08848733	H	29.27349521 -7.73259600 -0.89300725
H	22.41391754 1.64011932 -8.42211592	H	28.95436180 -6.22700389 1.17253586
N	25.99980655 -6.57885988 -9.83119578	H	30.62079218 -5.64665631 -1.10080977
C	26.81844227 -7.66946635 -10.30669761	H	27.78828711 -6.79527640 -1.09509363
C	26.20499796 -9.07435742 -10.11123866	C	28.15785125 -6.46365474 -3.85191454
O	26.74547109 -10.08896384 -10.57327581	H	30.88046317 -7.86906768 -2.99363656
C	28.22376711 -7.59786973 -9.73369999	H	27.24861073 -5.89797997 -3.77312821
S	28.24759529 -8.14465534 -7.89314345	C	29.82598062 -7.50169774 -4.79758267
H	25.96449716 -6.34161462 -8.83564058	N	30.00659313 -7.62439621 -3.45936394
H	26.90492166 -7.54721246 -11.38814836	N	28.67999219 -6.89115311 -5.01440459
H	28.60851247 -6.58596268 -9.82725078	H	30.49663694 -7.88792675 -5.54064594
H	28.86748826 -8.28396935 -10.28158623	N	27.83683733 -3.87712793 -1.04286821
N	25.05632100 -9.11633456 -9.38481654	C	27.27826719 -2.63905941 -1.54909625
C	24.39732265 -10.38661446 -9.15559211	H	27.30871224 -4.36214470 -0.31965026
C	25.18428382 -11.36502399 -8.28346346	C	32.66455425 -1.85341088 -2.42329706
O	24.84009635 -12.52961171 -8.12688660	C	32.41679646 -1.97471158 -3.94347622
C	23.92580466 -11.10371503 -10.43675880	O	33.16520052 -1.50026733 -4.78981450
C	22.97237977 -10.22905341 -11.25192134	N	31.32156575 -2.68955511 -4.24301479
C	22.49533756 -11.00644688 -12.48540354	C	30.98415104 -3.04274693 -5.63310056
C	21.75352536 -9.82085912 -10.43940657	C	30.87159399 -1.72697755 -6.42265572
H	22.06837466 -9.22660439 -9.59517857	O	30.15712492 -0.82216724 -6.05682126
H	21.08546501 -9.24195809 -11.05021257	C	29.67107760 -3.82331547 -5.60688110
H	21.25319758 -10.71157782 -10.07255730	S	29.16662296 -4.39060570 -7.28692503
H	24.64750506 -8.28895410 -8.97166334	H	30.76898837 -3.05395481 -3.48251648
H	21.98362212 -11.90895387 -12.17020860	H	31.77633577 -3.67652076 -6.04249569
H	21.82401711 -10.38995122 -13.05992450	H	28.89905608 -3.17682503 -5.18697322
H	23.34665138 -11.28635387 -13.09243888	H	29.81178133 -4.67680390 -4.94300042
H	23.48367072 -10.16280082 -8.60063764	N	31.56870806 -1.58802679 -7.55078818
H	23.49222762 -9.33262758 -11.57431126	C	31.55431489 -0.40545664 -8.34621571
H	23.41644117 -12.01216762 -10.14011760	C	30.64913733 -0.54442507 -9.57634755
H	24.78732609 -11.33576117 -11.04569073	O	30.28904759 0.42106668 -10.22164774
N	26.23770176 -10.83354612 -7.61982491	C	33.00361561 -0.10007440 -8.72663592
C	26.89269920 -11.70471940 -6.64566762	H	31.16203452 0.42053820 -7.75231988
C	25.84832203 -12.11249461 -5.53708911	H	32.16725484 -2.32082790 -7.85615908
O	25.17601038 -11.27260407 -4.98858998	N	30.22845600 -1.79093586 -9.83296395
C	28.05752931 -10.98560209 -5.99160496	C	29.18139741 -2.01141876 -10.83623999
C	28.65402881 -11.78306628 -4.84535538	C	27.94090666 -1.18720416 -10.49688796
C	29.95511488 -11.13058317 -4.32770069	O	27.41032801 -1.15225293 -9.41278282
C	30.34666479 -11.81941986 -3.00944205	C	28.78207754 -3.48486865 -10.96224891
N	31.78578462 -11.67581158 -2.76435007	C	29.83575661 -4.33427168 -11.57927163
H	27.23390753 -12.61900819 -7.14120176	C	31.18566806 -4.22444691 -11.42443492
H	29.79848408 -11.36276882 -2.19310207	C	29.62522732 -5.45223757 -12.44911435
H	30.11111115 -12.87615203 -3.06861848	N	31.83711878 -5.20005082 -12.13436608
H	27.93641472 -11.80611113 -4.02939534	C	30.91144133 -5.98340572 -12.75479850
H	28.86379805 -12.80265172 -5.14798771	C	28.49876700 -6.11696686 -12.92615107
H	32.11652695 -12.30345294 -2.02589243	C	31.06755656 -7.17469178 -13.45571152
H	32.33638001 -11.90737640 -3.61534257	C	28.66698844 -7.31552349 -13.58145682
H	32.01923455 -10.71084046 -2.47942248	C	29.92517245 -7.83859087 -13.85773023
H	29.80190863 -10.07168827 -4.18512045	H	30.01469478 -8.73470657 -14.43453295
H	30.72077304 -11.29695906 -5.07714037	H	29.58543529 -1.64454741 -11.78700329
H	26.60170129 -9.91336193 -7.83945613	H	32.83300722 -5.31150070 -12.22183890
H	27.75193047 -10.00834835 -5.64288740	H	27.51761956 -5.71942452 -12.75718426
H	28.83041075 -10.84408404 -6.74399592	H	27.80097042 -7.85475960 -13.89000732
N	25.77481122 -13.41567811 -5.19610601	H	32.05255088 -7.52829820 -13.70055019

H	31.72733562 -3.49021255 -10.87319211	H	10.50509788 -16.58567105 -21.68084298
H	30.36933090 -2.51708812 -9.14032557	H	12.06861525 -14.80253562 -22.27307493
H	27.89901016 -3.55753914 -11.59018200	H	10.59429288 -13.21631549 -20.17305783
H	28.54876757 -3.88166221 -9.97686129	H	12.17112845 -12.78010042 -20.81236459
N	27.43419175 -0.49464490 -11.53579607	H	9.61327151 -13.01663972 -22.41227078
C	26.12731097 0.15140242 -11.47717085	H	12.11621601 -17.42993727 -20.18966812
H	27.94595285 -0.38065280 -12.40983798	H	10.40484159 -11.53551682 -21.91262214
C	14.00742517 -19.32486299 -8.43976762	H	9.68291781 -15.48482234 -20.55030515
C	12.58256894 -19.02992183 -8.88598750	H	11.19672370 -12.60367297 -23.06898900
O	11.66498721 -19.12743371 -8.10885034	N	12.19423490 -14.21944363 -18.07171520
N	12.46556699 -18.62168110 -10.17117789	C	11.97177877 -14.17529900 -16.59864227
C	11.18009709 -18.24156650 -10.70873880	C	11.95024653 -12.72332505 -16.24657886
C	10.79943164 -19.00365582 -11.95432770	O	12.89227871 -12.00820951 -16.53219591
O	9.74657124 -18.76806506 -12.53107111	C	13.02951965 -14.91022050 -15.81251601
C	11.04914652 -16.73553234 -10.93086434	C	12.65419862 -15.13111956 -14.25927938
C	11.55465377 -15.97157996 -9.74015679	S	12.77736683 -13.58098547 -13.37542930
C	10.78578981 -15.89929601 -8.57201897	C	14.55316298 -13.26157453 -13.56946083
C	12.77819158 -15.31079826 -9.80101241	H	11.61261483 -15.42854832 -14.22762074
C	11.26999082 -15.19375936 -7.47446240	H	14.89084601 -12.68282178 -12.72333910
C	13.25165167 -14.61960751 -8.70220601	H	15.08236967 -14.20910462 -13.58695876
C	12.49358593 -14.55482496 -7.53366051	H	14.73144031 -12.72292158 -14.49019235
H	12.88681677 -14.03684034 -6.68319419	H	13.21171056 -15.88849931 -16.23407205
H	10.45246175 -18.55162824 -9.94919988	H	13.30067555 -15.90417149 -13.87060492
H	10.67951444 -15.15532406 -6.59098841	H	12.91894526 -13.61704196 -18.46725826
H	14.21362246 -14.14719022 -8.76190784	H	11.00145665 -14.65198741 -16.44540765
H	13.28125153 -18.50054266 -10.76317160	H	13.95141056 -14.33853804 -15.83764195
H	13.37024081 -15.38170908 -10.69622091	N	10.79188799 -12.27637061 -15.72637028
H	9.83810003 -16.39839549 -8.52301050	C	10.67213557 -10.91582242 -15.21766043
H	10.00727588 -16.48615490 -11.08128586	C	10.55507679 -11.05241025 -13.66286864
H	11.63143927 -16.44131847 -11.79634541	O	9.89466765 -11.93276815 -13.13398094
N	11.60708901 -19.99221460 -12.32201911	C	9.41848979 -10.22391496 -15.72801847
C	11.31282624 -20.75750784 -13.49626782	C	9.40970277 -10.11986293 -17.27296998
C	11.32401728 -22.22060932 -13.13491779	C	9.24442583 -8.84794583 -15.11003662
O	12.21712147 -22.72153854 -12.48898374	C	10.50271888 -9.19318712 -17.74919598
C	12.30779731 -20.45759605 -14.63698049	H	11.56649298 -10.36050733 -15.47363862
C	12.27014534 -18.99636567 -15.04859582	H	8.32955580 -8.39701415 -15.46431387
C	13.37958147 -18.76325298 -16.05997016	H	9.17806102 -8.94805425 -14.03272342
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O 4.77648370 -18.69792216 -14.48880416
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H -0.81737428 -7.44210354 -26.30379010
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2C QM/SE/MM R3b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_{\alpha}=1.667$ including B factors

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S 25.81188667 -5.71585913 -6.50274049
H 24.14957123 -9.47583484 -4.92118669
H 23.68390764 -6.59224778 -4.68519771
H 25.59802074 -8.17849443 -6.50489386
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H	27.93640018	-11.80438478	-4.02946962	C	30.91203949	-5.98358546	-12.75462424
H	28.86256170	-12.80276377	-5.14610646	C	28.49947808	-6.11763274	-12.92563779
H	32.11605264	-12.30267259	-2.02568762	C	31.06836250	-7.17414249	-13.45665168
H	32.33611935	-11.90781494	-3.61533947	C	28.66780367	-7.31514049	-13.58277632
H	32.01973190	-10.71056997	-2.48042195	C	29.92622982	-7.83749914	-13.85962508
H	29.80256739	-10.07286882	-4.18632085	H	30.01586073	-8.73234065	-14.43730103
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C	29.87660853	-4.48869047	2.80772447	H	27.90024722	-3.55766295	-11.59037656
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N	29.51269963	-5.56015475	0.64627548	C	26.12699723	0.15112271	-11.47693681
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C	28.84441723	-6.84302288	-1.35779430	O	11.66470664	-19.12905292	-8.10898536
C	28.95386418	-6.94908509	-2.83466322	N	12.46517480	-18.62210093	-10.17099121
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H	30.62088782	-5.64581595	-1.09957988	O	9.74619043	-18.76747798	-12.53130693
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O	33.16605999	-1.50179735	-4.78959806	H	9.83882052	-16.39787844	-8.52227046
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C	10.24551794 -15.55875026 -21.47041222	H	6.67372655 -8.26313125 -11.71972708
C	10.57016863 -12.56496954 -22.18689195	H	4.57987539 -10.61603315 -13.50336040
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O	12.89210176 -12.00721014 -16.53196373	N	-1.63778899 -12.08809801 -14.94461946
C	13.02924942 -14.90956194 -15.81270409	N	-0.41494117 -13.90357328 -13.94760871
C	12.65303829 -15.13030187 -14.26021003	H	2.16652857 -10.24380650 -14.01798992
S	12.77774808 -13.58167080 -13.37480452	H	2.22424914 -8.14607078 -16.39616732
C	14.55376556 -13.26295213 -13.56936440	H	0.72886263 -12.03555454 -12.69863623
H	11.61152714 -15.42677168 -14.22931812	H	1.15114812 -10.19122483 -15.46990185
H	14.89198531 -12.68499455 -12.72375004	H	-1.18057124 -14.50993035 -14.20075503
H	15.08216293 -14.21026789 -13.58741830	H	-0.01535394 -14.15520016 -13.05046511
H	14.73192970 -12.72453723 -14.48957597	H	4.31269959 -8.89873315 -15.53797460
H	13.21098289 -15.88749974 -16.23374420	H	-0.84290560 -9.96073917 -14.10771919
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H	12.91965246 -13.61669902 -18.46875606	H	-2.02295310 -12.79594117 -15.54954201
H	11.00201276 -14.65069250 -16.44700432	H	-1.46482856 -11.19200825 -15.36642956
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C	9.41812205 -10.22352281 -15.72738382	O	4.54953835 -2.48185956 -17.32311921
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H	8.44655321 -9.72465525 -17.55648753	H	2.67794918 -3.81728841 -15.76222470
H	11.46775121 -9.59244085 -17.44911308	H	3.79473541 -2.34050354 -10.81015195
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H	10.08552053 -8.21258453 -15.33344958	H	2.69553800 -2.68398907 -8.79050789
H	10.39959498 -8.19710226 -17.34854629	H	4.42262171 -6.20995730 -16.02389028
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H	11.91087415 -9.52108904 -13.31157700	H	3.31676372 -6.11142199 -9.40163622
C	7.89735789 -6.08073966 -12.13764772	H	3.91837596 -5.84971067 -10.91220975
C	6.87468438 -6.76378875 -13.06430268	H	4.88586939 -2.68701392 -14.92978840
O	6.61540862 -6.34073088 -14.16635006	H	5.31962378 -4.33765465 -14.47832101
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H	4.14264761	-4.59443769	-20.26500750	C	7.61604574	-11.64910026	-24.61517875
H	4.68790009	-3.03897766	-19.55088622	C	7.11067332	-11.36615139	-27.03392773
N	7.02453343	-4.84709384	-18.83136849	C	6.21314958	-11.91123547	-24.11010172
C	8.42301083	-5.18349333	-19.00446347	H	9.73619478	-11.06956101	-26.15866254
C	8.58724952	-6.49871921	-19.77029055	H	6.08738376	-11.66648950	-26.86136700
O	9.39615002	-6.56371214	-20.67856015	H	7.13463010	-10.68322649	-27.86768550
C	9.17326408	-5.24896352	-17.63134878	H	7.03544288	-9.80516634	-25.56081237
C	9.10444573	-3.95046505	-16.88755183	H	8.09053835	-12.57528342	-24.91757033
C	9.95684320	-2.89311688	-17.13799208	H	8.19185951	-11.22062480	-23.80374577
C	8.17431172	-3.80198299	-15.87535482	H	5.62880647	-12.36002118	-24.90602943
C	9.88904090	-1.72636969	-16.40605764	H	9.00293916	-9.11998278	-24.17601952
C	8.06875701	-2.63151395	-15.14072106	H	6.26696264	-12.59581202	-23.28242142
C	8.95614720	-1.58539787	-15.37264553	H	7.71173515	-12.23118984	-27.26155986
O	8.78789555	-0.44472888	-14.66708915	H	5.74768197	-10.98461377	-23.81384121
H	8.89563330	-4.40136724	-19.60272265	N	8.75190519	-8.16432274	-27.37131658
H	10.58420562	-0.92708182	-16.58594386	C	8.84974772	-7.32505707	-28.54791177
H	7.33578473	-2.54814691	-14.36836212	H	8.25521650	-7.76544748	-26.58692100
H	6.63520330	-4.90100336	-17.89680150	C	6.58969445	-21.92076189	-21.79764284
H	7.51443923	-4.61698125	-15.64517568	C	6.21540378	-22.03059166	-20.30638962
H	10.71095811	-2.97102570	-17.89400551	O	5.51742192	-22.93016760	-19.88486193
H	10.20390030	-5.45464698	-17.87200283	N	6.58455511	-20.95531600	-19.60359106
H	8.75861916	-6.04766214	-17.03507856	C	6.10546422	-20.90583963	-18.22475257
H	9.63412172	0.11395237	-14.78284091	C	4.59899375	-20.55885810	-18.34683873
N	7.79253653	-7.52348532	-19.37929116	O	4.09718101	-20.19880454	-19.40726471
C	7.78709069	-8.77917971	-20.07603082	C	6.80683719	-19.84459839	-17.39066246
C	7.39496442	-8.59555302	-21.61603831	O	6.64642324	-18.56324279	-17.96410978
O	7.96878417	-9.24161004	-22.46851835	H	7.28456015	-20.30668918	-19.93919926
H	7.07732840	-7.34813508	-18.68373192	H	6.22296583	-21.88909740	-17.76546483
H	8.78276706	-9.21835834	-20.10012598	H	7.86187899	-20.10257741	-17.30425637
H	7.08139209	-9.46628877	-19.62533366	H	6.36236690	-19.82931587	-16.39573779
N	6.50761377	-7.58610034	-21.82844437	H	7.52886386	-18.29538766	-18.30043730
C	5.96204095	-7.33209767	-23.13782544	N	3.93277000	-20.54849896	-17.16592309
C	7.07410616	-6.70047117	-24.00209075	C	2.51749596	-20.23127823	-17.17061910
O	7.19170238	-6.98127264	-25.18564706	C	2.35146447	-18.74427647	-17.58203836
C	4.74979917	-6.41087627	-23.07817218	O	1.52121486	-18.35294357	-18.38421386
C	4.14651973	-6.05115254	-24.45610624	C	1.92455245	-20.50876666	-15.78876816
C	2.93693989	-5.16107754	-24.20191452	H	4.31552931	-21.06287699	-16.38161653
N	2.27400786	-4.74323272	-25.40823891	H	1.98253687	-20.83347106	-17.90702865
C	1.14791509	-4.00364758	-25.43365755	N	3.21194487	-17.89294014	-17.00509015
N	0.66067367	-3.50291327	-24.23894312	C	3.09744250	-16.46653607	-17.24614572
N	0.68988240	-3.51756329	-26.60520359	C	3.61774115	-16.06345665	-18.63318006
H	3.81409579	-6.93997422	-24.97928909	O	3.11006578	-15.15228759	-19.30116711
H	5.67486801	-8.26885834	-23.63463219	C	3.82244759	-15.70126208	-16.16717955
H	2.64741798	-5.05570777	-26.30446958	C	3.77594916	-14.17528542	-16.25195858
H	4.86884036	-5.51887482	-25.05380301	C	2.35309390	-13.68084238	-16.46413389
H	-0.25275814	-3.16955624	-26.66943542	C	4.33086928	-13.62784346	-14.92217811
H	1.00436686	-3.96579190	-27.45952942	H	5.34002205	-13.97129668	-14.76522594
H	5.97677942	-7.31387588	-21.00575452	H	4.30006934	-12.54960326	-14.93594230
H	3.26402234	-4.28074552	-23.65385332	H	3.71311171	-13.97592199	-14.10100476
H	2.22779881	-5.72698883	-23.59135602	H	3.88274111	-18.24922958	-16.32296063
H	-0.24787746	-3.05879359	-24.33279741	H	1.72545124	-14.03069152	-15.64937551
H	0.78311510	-4.15962171	-23.48924551	H	2.35136313	-12.59791856	-16.44315168
H	5.01295693	-5.49100410	-22.57226961	H	1.97124360	-14.02482153	-17.40619831
H	3.98084769	-6.92670337	-22.51045774	H	2.03811002	-16.20017759	-17.22398523
N	7.75366634	-5.75397196	-23.33606150	H	4.41303909	-13.80845219	-17.05089122
C	8.91851202	-5.13407263	-23.92996000	H	4.87018449	-15.98564025	-16.17582305
H	7.60877129	-5.58253842	-22.34922060	H	3.40260526	-15.99044614	-15.20735662
C	11.29384618	-8.06821768	-23.87305515	N	4.66504390	-16.72690771	-19.06830569
C	10.87738344	-8.98568545	-25.03405831	C	5.13651209	-16.53095228	-20.42165363
O	11.70382290	-9.33556849	-25.85993609	C	4.04893395	-16.92969396	-21.45447692
N	9.58709193	-9.38611921	-24.95100128	O	3.82217986	-16.18345211	-22.37794833

O	21.42063857	-8.01790473	-4.34986592	H	29.80984801	-4.67253907	-4.92630369
N	23.52792260	-8.66482181	-4.76907916	N	31.59783875	-1.60620356	-7.50550317
C	23.89464868	-7.38700718	-5.36713765	C	31.62322509	-0.46738690	-8.37684343
C	23.06546307	-7.23964510	-6.66944239	H	32.31487521	-2.24660412	-7.72732145
O	23.13089562	-8.10209151	-7.53968613	C	7.67619198	-15.97266621	-16.35304340
C	25.38728585	-7.35691680	-5.80949028	H	7.10526556	-16.36263485	-17.18046685
S	25.80835503	-5.71665459	-6.50477240	C	8.06731548	-16.78754457	-15.30378601
H	24.15961566	-9.46176574	-4.86297495	H	7.85391872	-17.84653647	-15.32404306
H	23.69485059	-6.58058026	-4.65760738	C	8.75144245	-16.18777121	-14.25140810
H	25.60709337	-8.19504793	-6.47872976	H	9.13298667	-16.75572854	-13.43152528
H	25.95931350	-7.51781168	-4.88051707	C	8.97630035	-14.82356635	-14.27721491
N	22.37200360	-6.08981625	-6.79345017	H	9.55533975	-14.35515025	-13.49255791
C	21.45687274	-5.93119478	-7.92202629	N	8.50225172	-13.99826135	-15.23970186
H	22.17694716	-5.51297751	-5.97838188	C	7.91137399	-14.62447960	-16.26856921
C	24.31358558	-4.85876801	-10.21384602	C	7.39831418	-13.77953614	-17.34618528
C	25.25416471	-5.90418948	-10.74149895	C	7.53124109	-14.19826321	-18.68698826
O	25.25342018	-6.08404794	-11.94889138	C	7.00632224	-13.37431105	-19.68278373
N	26.00892366	-6.59737626	-9.82808700	C	6.41197946	-12.15473448	-19.38901899
C	26.83990208	-7.67152183	-10.30490730	H	6.00814585	-11.55428302	-20.17006057
C	26.23427013	-9.07339612	-10.12878016	F	7.07357741	-13.77345765	-18.58580234
O	26.77205430	-10.08672623	-10.57681326	H	8.07403550	-15.10672591	-18.92253443
C	28.23894960	-7.59886081	-9.71256138	C	6.79924090	-12.57368881	-17.01762132
S	28.23838425	-8.15068800	-7.88539896	H	6.68201540	-12.33338809	-15.97425771
H	25.98439894	-6.33120828	-8.83851371	C	6.26164428	-11.78445712	-18.02781126
H	26.91923773	-7.54489791	-11.38920545	C	5.45569233	-10.60524001	-17.66527197
H	28.61075072	-6.57576419	-9.82134117	O	5.70456368	-9.85440229	-16.72092926
H	28.88901548	-8.27706703	-10.27818352	N	4.36201270	-10.33320608	-18.50057629
N	25.08019504	-9.11687977	-9.41712108	H	3.96074663	-11.03439266	-19.13067887
C	24.41083148	-10.40521118	-9.18036592	N	3.43274272	-9.33456730	-18.19185065
H	24.60384509	-8.30516936	-9.04000924	H	3.43920989	-9.11626004	-17.19420350
C	29.87597387	-4.49083214	2.81070020	S	3.59207829	-7.94958049	-19.06621681
C	30.09002231	-4.51001911	1.26044428	O	4.97596990	-7.57192890	-19.41696461
O	30.68173359	-3.65439951	0.65890257	O	2.80962003	-6.87165081	-18.43476784
N	29.50663000	-5.56634861	0.64586121	C	2.76466956	-8.38431891	-20.69399149
C	29.56754018	-5.62491396	-0.82000874	C	1.61276225	-7.67328634	-21.08631276
C	29.06408619	-4.33207150	-1.43544634	H	1.12171617	-6.99567731	-20.40174915
O	29.78910189	-3.74765535	-2.22284014	C	1.04415999	-7.93932627	-22.34950428
C	28.85029517	-6.84559719	-1.37008616	H	0.09729161	-7.49551505	-22.61980249
C	28.95396443	-6.94583529	-2.84964089	C	1.60894577	-8.89226475	-23.19603283
H	29.28937817	-7.73608798	-0.91404919	H	1.14873348	-9.13656939	-24.15056512
H	28.94887046	-6.23608821	1.17188168	C	2.78343449	-9.53429576	-22.84540977
H	30.62842998	-5.64867156	-1.09391679	H	3.26806935	-10.23535590	-23.51995370
H	27.79219433	-6.79546190	-1.10562895	C	3.34916899	-9.28453171	-21.59400757
C	28.14917649	-6.46027068	-3.85853782	F	4.52000965	-9.96072343	-21.29062810
H	30.87816429	-7.85969650	-3.01925125	Zn	28.08092433	-6.23401021	-6.90730545
H	27.23946599	-5.88896973	-3.75944666				
C	29.81084277	-7.47678653	-4.81330066				
N	30.01258289	-7.59612577	-3.48257776				
N	28.66842539	-6.88753734	-5.02553612				
H	30.49677466	-7.85966970	-5.55473717				
N	27.84491702	-3.87907740	-1.04813792				
C	27.28002262	-2.63940483	-1.54939069	C	22.27401658	-8.92022241	-4.42330374
H	27.32568509	-4.34231316	-0.30086210	O	21.42733192	-8.05536294	-4.33582911
C	32.66620370	-1.85100711	-2.41941337	N	23.54044048	-8.67556138	-4.78315713
C	32.41393324	-1.96564375	-3.94238416	C	23.89241636	-7.39442869	-5.37702940
O	33.16443939	-1.50658488	-4.79020278	C	23.06361428	-7.24364703	-6.68469664
N	31.30906487	-2.66271416	-4.22921402	O	23.12674562	-8.11162044	-7.55190567
C	30.97885828	-3.03444167	-5.61169838	C	25.38772754	-7.35257865	-5.83505796
C	30.86941394	-1.72413939	-6.40332914	S	25.80846324	-5.70999815	-6.50521253
O	30.13311942	-0.83496361	-6.05927666	H	24.15589591	-9.47059527	-4.95025578
C	29.67130921	-3.82536030	-5.60463377	H	23.69067369	-6.58186507	-4.66724850
S	29.20147092	-4.39242911	-7.29064155	H	25.58574938	-8.18187292	-6.53099025
H	30.75543372	-3.02022576	-3.46213470	H	25.97656715	-7.55818967	-4.91991863
H	31.78053971	-3.66749618	-6.01687860	N	22.36684002	-6.09183529	-6.81790638
H	28.88643207	-3.17462405	-5.19544363	H	22.18174874	-5.54150746	-5.98171035

2C WF-in-DFT/SE/MM R1b (2C-CCSD-in-B3LYP/6-31G(d):xTB:Amber) mechanical embedding $\omega_c=1.667$ including B factors

C	25.25096854	-5.91047805	-10.75127341	H	8.07207037	-15.11722032	-18.92519171
O	25.31840868	-6.06224332	-11.96725416	C	6.82580787	-12.56399122	-17.01815806
N	26.00198104	-6.61621594	-9.83459703	H	6.72709407	-12.31192216	-15.97198963
C	26.82149949	-7.70297790	-10.30260957	C	6.26958496	-11.75813311	-18.01944748
C	26.20227646	-9.10908824	-10.10612773	C	5.46771162	-10.61725083	-17.66111899
O	26.73110230	-10.12270230	-10.56834487	O	5.69467564	-9.83746351	-16.67936049
C	28.22846060	-7.62201394	-9.71649631	N	4.38755872	-10.33680712	-18.52707656
S	28.24443861	-8.16262148	-7.89800247	H	3.96398325	-11.05063454	-19.11518942
H	25.94441315	-6.38946290	-8.83424360	N	3.45870117	-9.34680318	-18.19616704
H	26.89782582	-7.58478883	-11.39213759	H	3.51533038	-9.09722107	-17.20141739
H	28.60790014	-6.59958662	-9.85007660	S	3.60790504	-7.95990892	-19.07742365
H	28.87762798	-8.30616065	-10.28539637	O	5.01245898	-7.55395440	-19.41859862
N	25.05988406	-9.15251783	-9.36542652	O	2.84691037	-6.86630593	-18.41266477
H	24.59609337	-8.32620532	-9.00622246	C	2.79103689	-8.37642175	-20.66150838
C	30.09490135	-4.48874988	1.27999165	C	1.62310837	-7.64527344	-21.05991338
O	30.68508105	-3.64107295	0.66440396	H	1.14471625	-6.96960246	-20.36345822
N	29.50541141	-5.54657372	0.65843343	C	1.05576188	-7.91010247	-22.31410065
C	29.55446074	-5.61025308	-0.80941921	H	0.11051064	-7.44957712	-22.57905127
C	29.05412728	-4.31824181	-1.44211508	C	1.60122000	-8.87552024	-23.17644187
O	29.79565467	-3.73331304	-2.21278393	H	1.12252912	-9.12333676	-24.11681634
C	28.83821823	-6.83862599	-1.35411792	C	2.78106093	-9.53919454	-22.82648558
C	28.94246427	-6.94057146	-2.83277260	H	3.22140998	-10.26772493	-23.49686466
H	29.27511552	-7.73444595	-0.88917386	C	3.36183826	-9.28637375	-21.59005159
H	28.94959221	-6.22399267	1.17663915	F	4.52942354	-9.99018740	-21.29258692
H	30.61565358	-5.63412665	-1.09938744	Zn	28.08229227	-6.23943430	-6.90760889
H	27.77611815	-6.79979924	-1.08792538				
C	28.14643133	-6.45826869	-3.85223103				
H	30.88489769	-7.84125393	-3.00079998				
H	27.23282742	-5.87859369	-3.77011509				
C	29.80014173	-7.48459562	-4.80430773				
N	30.00484660	-7.61318323	-3.46296810				
N	28.67164716	-6.88846234	-5.01116411	C	21.93944613	-10.35331763	-4.22240600
H	30.48076568	-7.87142480	-5.55694993	C	22.24711678	-8.89009438	-4.43052047
N	27.82942410	-3.85491270	-1.07210843	O	21.40507677	-8.01104709	-4.35332935
H	27.28168546	-4.34365411	-0.36174909	N	23.51659206	-8.66762391	-4.80148808
C	32.41914184	-1.95042669	-3.93183107	C	23.89512661	-7.38418327	-5.38185053
O	33.16672750	-1.49092330	-4.78081610	C	23.07111559	-7.22670851	-6.68330161
N	31.31131119	-2.65242182	-4.22934957	O	23.13859188	-8.07986952	-7.57063711
C	30.98000832	-3.02598536	-5.61127276	C	25.39655539	-7.36389985	-5.80518457
C	30.87825210	-1.71778939	-6.41655249	S	25.83226407	-5.73231388	-6.52612871
O	30.17665092	-0.80434488	-6.06524190	H	24.15640266	-9.45877900	-4.86323560
C	29.66889114	-3.81869669	-5.61331106	H	23.69715714	-6.58462769	-4.66647169
S	29.20429000	-4.37799384	-7.29667101	H	25.61906533	-8.20853974	-6.46303163
H	30.75757213	-3.02762882	-3.47089103	H	25.95387648	-7.50611250	-4.86711745
H	31.78689967	-3.66441485	-6.01448904	N	22.36560731	-6.08516244	-6.79319254
H	28.89167735	-3.16140425	-5.18566862	C	21.45927119	-5.92812617	-7.91957611
H	29.80842443	-4.66005060	-4.91539096	H	22.17853706	-5.50864658	-5.97892831
N	31.60765078	-1.60307658	-7.52526058	C	24.31486653	-4.85811935	-10.21474579
H	32.10302936	-2.39139668	-7.87494003	C	25.24487132	-5.91039522	-10.73133102
C	7.68460720	-15.98404754	-16.35653576	O	25.23447530	-6.11408071	-11.94258079
H	7.13081347	-16.37159102	-17.20030424	N	26.00545653	-6.59576077	-9.80983388
C	8.06703263	-16.79860430	-15.30709063	C	26.82900289	-7.67672881	-10.28695168
H	7.84931414	-17.85623247	-15.32361054	C	26.22641367	-9.06824193	-10.09786026
C	8.74618073	-16.20680597	-14.23796221	O	26.74788981	-10.09032721	-10.56097945
H	9.11321109	-16.80961028	-13.42916944	C	28.23959229	-7.58526367	-9.73395265
C	8.98224033	-14.84245938	-14.26480068	S	28.26866263	-8.13034854	-7.89379493
H	9.56034223	-14.35978146	-13.48526342	H	25.98388834	-6.32308543	-8.82540577
N	8.51714565	-14.00442748	-15.23168467	H	26.89595249	-7.55724581	-11.37274839
C	7.91127307	-14.62536177	-16.26871556	H	28.59855887	-6.56162439	-9.84548621
C	7.39807665	-13.77922213	-17.34040785	H	28.87880172	-8.27007088	-10.29680699
C	7.51798033	-14.21351622	-18.69493393	N	25.07419824	-9.10777799	-9.38506322
C	6.99501959	-13.37122908	-19.68185653	C	24.40941007	-10.40627415	-9.17346176
C	6.40856619	-12.15203676	-19.40391364	H	24.59659740	-8.29911484	-9.01208674
H	6.02806015	-11.54044248	-20.18722898	C	29.87806132	-4.48938831	2.81336424
F	7.06900551	-13.77563570	-20.99507306	C	30.09617890	-4.49756591	1.26552990
				O	30.70774033	-3.64774975	0.66713150

**1C QM/MM R1b (B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_c=1.667$**

C 29.81902853 -7.49664207 -4.80786695
 N 30.00825497 -7.61858845 -3.48026315
 N 28.69096002 -6.86503760 -5.03619436
 H 30.50402263 -7.87620633 -5.54319101
 N 27.85637192 -3.88136069 -1.06099211
 C 27.28387922 -2.64301718 -1.55367409
 H 27.35770026 -4.33168861 -0.29529576
 C 32.66420188 -1.85217980 -2.42419056
 C 32.40871777 -1.95394187 -3.94353821
 O 33.14157200 -1.46687712 -4.79935685
 N 31.31010926 -2.66008055 -4.23300159
 C 30.97290830 -3.04544144 -5.62207325
 C 30.85228002 -1.73641041 -6.40541404
 O 30.11795301 -0.84834532 -6.04921432
 C 29.67050361 -3.84550204 -5.59063133
 S 29.20124914 -4.43223459 -7.28315264
 H 30.76722999 -3.02038537 -3.46383014
 H 31.77564142 -3.67388641 -6.02451255
 H 28.88354501 -3.19468465 -5.19672190
 H 29.82234090 -4.68965110 -4.91716009
 N 31.59436960 -1.60679279 -7.50426318
 C 31.62338604 -0.46992919 -8.37291724
 H 32.28578413 -2.26665338 -7.73542324
 C 7.66110544 -15.95918612 -16.33719272
 H 7.09241853 -16.35285774 -17.16507728
 C 8.05894735 -16.77378231 -15.29270215
 H 7.84886502 -17.83302646 -15.31297229
 C 8.75846140 -16.17339312 -14.24790709
 H 9.14650876 -16.74365204 -13.43505021
 C 8.98671883 -14.80776520 -14.27595491
 H 9.56942834 -14.33658507 -13.49745903
 N 8.48999357 -13.98241365 -15.22685751
 C 7.90089015 -14.60937149 -16.25662288
 C 7.40080713 -13.76541088 -17.33926226
 C 7.53583783 -14.18371532 -18.67822447
 C 7.00446657 -13.36555224 -19.67495162
 C 6.39767782 -12.15530050 -19.37478358
 H 5.99718318 -11.55254492 -20.15521717
 F 7.06991621 -13.75276216 -20.97780989
 H 8.08192686 -15.08882850 -18.91352648
 C 6.79004419 -12.56689538 -17.01204173
 H 6.66314443 -12.33164691 -15.96926354
 C 6.24736103 -11.78577171 -18.01941370
 C 5.43915867 -10.60120416 -17.66011842
 O 5.68052764 -9.85717058 -16.70934093
 N 4.35073094 -10.33189822 -18.48605329
 H 3.95292062 -11.02285240 -19.12969271
 N 3.43855050 -9.31173115 -18.19925405
 H 3.45227777 -9.08587246 -17.20118728
 S 3.59560356 -7.93555360 -19.07494153
 O 4.97777293 -7.56026268 -19.42263930
 O 2.80765830 -6.86715280 -18.43389273
 C 2.75434125 -8.38327682 -20.70054572
 C 1.60599423 -7.67285010 -21.10091413
 H 1.11555503 -6.99606387 -20.41534507
 C 1.03591969 -7.94116941 -22.35660243
 H 0.08603516 -7.50385204 -22.62394105
 C 1.60975165 -8.88606399 -23.20173095
 H 1.14952032 -9.13532214 -24.15481030
 C 2.78553822 -9.52954722 -22.85320168
 H 3.27151337 -10.23202206 -23.52340383
 C 3.34167691 -9.28399659 -21.59484121
 F 4.51753761 -9.94335655 -21.28784901
 Zn 28.06978765 -6.24300435 -6.91161499

1C QM/MM R2b (B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_c=1.667$

C 21.93966067 -10.35383512 -4.22263429
 C 22.25008786 -8.89404235 -4.43464929
 O 21.40679393 -8.01662041 -4.35798531
 N 23.51810333 -8.67352726 -4.81053851
 C 23.89957060 -7.38713607 -5.38603167
 C 23.07839871 -7.22991711 -6.68764304
 O 23.15003720 -8.08555410 -7.57272592
 C 25.40062597 -7.36565891 -5.80445120
 S 25.83733548 -5.73704570 -6.52277826
 H 24.15429720 -9.46589494 -4.88255968
 H 23.69507764 -6.59085372 -4.66991110
 H 25.62180275 -8.20093341 -6.47175194
 H 25.96333201 -7.52030786 -4.87409099
 N 22.36630037 -6.09352000 -6.79580487
 C 21.46142823 -5.93202511 -7.92004894
 H 22.17298557 -5.52317886 -5.97789701
 N 23.47776561 -5.21751011 -9.14223368
 C 24.31571012 -4.81272101 -10.25452396
 C 25.23696899 -5.89817082 -10.75600185
 O 25.22565418 -6.13742887 -11.96174898
 C 25.10431644 -3.59641681 -9.91020746
 C 24.27231485 -2.43752392 -9.45177934
 C 23.30035041 -1.87294645 -10.29602249
 C 24.43499124 -1.93904078 -8.12566421
 C 22.52409144 -0.78693738 -9.83881938
 C 23.62010985 -0.89973806 -7.66315274
 C 22.67637978 -0.30578452 -8.51732371
 O 22.05015284 0.81586013 -8.11233242
 H 23.66431372 -4.53090953 -11.08261658
 H 21.79274299 -0.37006896 -10.49237550
 H 23.77513565 -0.49492710 -6.68629207
 H 23.88612445 -5.31254764 -8.21737336
 H 25.19996359 -2.33736039 -7.48454039
 H 23.15086733 -2.27014388 -11.28235876
 H 25.66421636 -3.26140161 -10.77790476
 H 25.80799246 -3.84014467 -9.11831721
 H 22.47990837 1.61978618 -8.42298224
 N 25.99689458 -6.57387441 -9.82716176
 C 26.81708954 -7.66552675 -10.29049041
 C 26.20732371 -9.05532332 -10.09680378
 O 26.73573690 -10.07337858 -10.56006327
 C 28.23161189 -7.57566694 -9.73507159
 S 28.27247037 -8.13414031 -7.90041096
 H 25.98043914 -6.29039438 -8.84561461
 H 26.88550699 -7.55174240 -11.37617823
 H 28.59798034 -6.55482353 -9.84201145
 H 28.87245357 -8.25486079 -10.30010733
 N 25.04277381 -9.09194785 -9.39702376
 C 24.37958892 -10.39358003 -9.16000734
 C 25.17764597 -11.36482586 -8.29634104
 O 24.79990365 -12.54554007 -8.16495142
 C 23.88425097 -11.09192153 -10.45114109
 C 22.95075832 -10.19346939 -11.26933093
 C 22.45248170 -10.96243486 -12.50470454
 C 21.71526816 -9.81017953 -10.46598859
 H 22.04085697 -9.19877906 -9.63507706
 H 21.06423393 -9.21586464 -11.08159298
 H 21.22944879 -10.70634748 -10.08643036
 H 24.61852375 -8.28061785 -8.96741362
 H 21.94430426 -11.87325627 -12.19179077
 H 21.79025032 -10.32325544 -13.07128872

H	23.31861051	-11.22927544	-13.10665296	H	32.29816886	-2.25483907	-7.74036585
H	23.46906376	-10.21102380	-8.60186155	N	30.18797031	-1.81784940	-9.82127554
H	23.46885488	-9.29980676	-11.58401012	C	29.15952385	-2.01467326	-10.86015879
H	23.34771124	-11.99832373	-10.18551255	C	27.91529759	-1.20367518	-10.54020050
H	24.72696401	-11.34394040	-11.07454647	O	27.41915245	-1.15064906	-9.41742645
N	26.23568758	-10.87029760	-7.62318217	C	28.79628701	-3.48969292	-10.98457459
C	26.87042941	-11.71864300	-6.60110422	C	29.85210627	-4.34134957	-11.57330772
C	25.83731789	-12.12049593	-5.51263440	C	31.19122831	-4.23248093	-11.41895524
O	25.15935370	-11.25864781	-4.97697308	C	29.65794237	-5.46412839	-12.45558266
C	28.05346077	-10.98903084	-5.98286788	N	31.83958390	-5.18564120	-12.15919214
C	28.65998982	-11.80110160	-4.84510073	C	30.93995537	-6.01885154	-12.75035594
C	29.96340657	-11.14569069	-4.34246289	C	28.52761748	-6.13234261	-12.95253561
C	30.36439144	-11.82357364	-3.01387880	C	31.09221427	-7.20863080	-13.45059806
N	31.79356245	-11.68638184	-2.77711721	C	28.67501479	-7.35935746	-13.60191472
H	27.21068565	-12.62642028	-7.10026736	C	29.93968179	-7.88462105	-13.87321022
H	29.80109409	-11.34992623	-2.20694144	H	30.03140153	-8.77189923	-14.44625063
H	30.10592668	-12.88148685	-3.06911505	H	29.55610901	-1.66346911	-11.81320067
H	27.94845323	-11.79448094	-4.02250613	H	32.83809818	-5.30581422	-12.22693613
H	28.86128300	-12.82272394	-5.15203157	H	27.54639699	-5.74255070	-12.76379351
H	32.10241061	-12.30183626	-2.03879612	H	27.79715229	-7.87793940	-13.89947584
H	32.33315829	-11.93166816	-3.60884250	H	32.07705413	-7.55931048	-13.67392761
H	32.02442162	-10.73803303	-2.49203674	H	31.69211826	-3.48773954	-10.83709910
H	29.80305873	-10.09079212	-4.17485183	H	30.33132633	-2.54311597	-9.12775757
H	30.72221433	-11.31367340	-5.10179414	H	27.92832673	-3.57152190	-11.63503855
H	26.54536193	-9.92474305	-7.82967810	H	28.53877882	-3.90369026	-10.01630937
H	27.75269943	-10.00926802	-5.62237497	N	12.44898487	-18.60440877	-10.13055902
H	28.82175477	-10.88860051	-6.74710089	C	11.16164132	-18.22621457	-10.70006264
C	29.87757315	-4.48860296	2.81212480	C	10.80430302	-18.99870972	-11.94185656
C	30.09718423	-4.49382370	1.26665390	O	9.73997619	-18.77422741	-12.49889184
O	30.70655520	-3.64036569	0.67003933	C	11.06801296	-16.72939676	-10.91898024
N	29.50446268	-5.53667055	0.64275641	C	11.56338972	-15.94141481	-9.74060649
C	29.57852237	-5.61173130	-0.82734585	C	10.78333009	-15.87877734	-8.55914307
C	29.07538681	-4.32576772	-1.44281398	C	12.81209028	-15.30027193	-9.81430527
O	29.79714274	-3.74895345	-2.23717528	C	11.28258391	-15.17380068	-7.45514184
C	28.84726441	-6.83531260	-1.37542552	C	13.29974740	-14.61637980	-8.69628152
C	28.95494026	-6.94528219	-2.84979578	C	12.53253727	-14.55109170	-7.51282099
H	29.27934084	-7.72428389	-0.91084999	H	12.92592017	-14.03992241	-6.66012848
H	28.96211822	-6.21648003	1.16880529	H	10.38162636	-18.48613260	-9.98832035
H	30.63730507	-5.64718778	-1.09652776	H	10.70439206	-15.14105764	-6.56781428
H	27.79104983	-6.77899578	-1.10788783	H	14.26770129	-14.16127302	-8.75366156
C	28.15671255	-6.46081091	-3.85534651	H	13.27791460	-18.51855711	-10.71071567
H	30.87242938	-7.86911872	-3.01609697	H	13.40670579	-15.38420426	-10.70450804
H	27.25109830	-5.88598978	-3.76582757	H	9.83788857	-16.38145037	-8.50366338
C	29.81608892	-7.48483494	-4.80946233	H	10.03346554	-16.44358891	-11.07196565
N	30.00675864	-7.60402334	-3.48158946	H	11.66313383	-16.45306022	-11.77991997
N	28.68606539	-6.85560356	-5.03158187	N	11.59873241	-19.98139503	-12.32854723
H	30.49150027	-7.86553614	-5.55349806	C	11.29344809	-20.77178613	-13.50367545
N	27.85073961	-3.88121109	-1.05767139	C	11.28198595	-22.22846420	-13.15176451
C	27.28251122	-2.64183660	-1.55368053	O	12.20973120	-22.71567724	-12.50944642
H	27.34070886	-4.34452988	-0.30728697	C	12.28891215	-20.45570818	-14.63944161
C	32.66329690	-1.85241594	-2.42387228	C	12.25661504	-19.00178468	-15.06918141
C	32.40524152	-1.95648180	-3.94128071	C	13.35521850	-18.80415538	-16.10397458
O	33.12070622	-1.44133847	-4.79491727	C	10.90869357	-18.65917845	-15.68317476
N	31.32599480	-2.68954537	-4.23512615	H	10.14421402	-18.78414417	-14.93655265
C	30.98113492	-3.05533260	-5.62544812	H	10.94724390	-17.63021578	-16.00672483
C	30.86064314	-1.73893004	-6.40308369	H	10.71933059	-19.32710669	-16.52118667
O	30.12300950	-0.85356089	-6.04455227	H	12.43932585	-20.18067303	-11.80591847
C	29.67358513	-3.84919878	-5.58708565	H	13.21411434	-19.45224307	-16.96817861
S	29.18342601	-4.41970199	-7.27787047	H	13.33620115	-17.79569096	-16.46008660
H	30.78330097	-3.05691076	-3.46944825	H	14.32519362	-18.99011397	-15.65084139
H	31.77860100	-3.68259265	-6.03667525	H	10.30339103	-20.54629544	-13.88878319
H	28.89340772	-3.20296481	-5.17710837	H	12.42948826	-18.34126627	-14.23257385
H	29.82294888	-4.69768903	-4.91973100	H	12.04677072	-21.08289380	-15.49205477
N	31.59204726	-1.60840153	-7.50933168	H	13.28912014	-20.68846833	-14.29177297
C	31.62021256	-0.47004896	-8.37149217	N	12.73602677	-16.67261300	-20.53240655

C	12.42014525 -15.29071504 -20.26103610	H	4.58505097 -10.60871260 -13.47175879
C	11.79139629 -15.20353639 -18.84816349	H	5.02644014 -10.00439777 -11.85808545
O	10.93973795 -16.02980626 -18.47058184	H	8.32577340 -12.82861950 -12.48940541
C	11.51306274 -14.70909810 -21.35304175	O	5.28227159 -12.61337922 -11.87924144
C	11.23376125 -13.25368327 -21.07460540	N	7.42970289 -13.13123287 -12.10998335
C	10.22333669 -15.52361806 -21.48241422	H	7.28865919 -14.04291329 -11.69915346
C	10.56900929 -12.52192333 -22.21407323	N	3.73055358 -8.28477750 -14.96226455
H	13.34373065 -14.71855993 -20.24854116	C	2.43429650 -7.77600699 -15.41529834
H	9.64904015 -15.13212200 -22.31079146	C	2.45150159 -6.25282015 -15.45207887
H	10.47646868 -16.55245348 -21.69207319	O	1.43903168 -5.63317424 -15.15674646
H	12.03910131 -14.77054192 -22.29807828	C	1.32184050 -8.29901687 -14.47051301
H	10.57267964 -13.17621020 -20.21292043	C	1.24365469 -9.82854878 -14.44241365
H	12.16276354 -12.74815495 -20.84626029	C	0.05021459 -10.25800206 -13.61171887
H	9.60499980 -12.97373838 -22.42951909	N	0.03689671 -11.70119669 -13.39524373
H	12.10524382 -17.40716536 -20.24972046	C	-0.68484305 -12.57114615 -14.08244643
H	10.41452411 -11.49206263 -21.91276849	N	-1.51091496 -12.16316249 -15.01018992
H	9.65060144 -15.43267541 -20.56700438	N	-0.56771898 -13.85983102 -13.85708105
H	11.21116597 -12.57332180 -23.09037829	H	2.13863618 -10.24261560 -13.99355875
N	12.20367552 -14.21053712 -18.07567159	H	2.16633405 -8.13844288 -16.40387651
C	11.97792923 -14.14780962 -16.60576158	H	0.67154938 -12.06231781 -12.68515533
C	11.95434465 -12.71409541 -16.25084497	H	1.11740295 -10.19573162 -15.45682131
O	12.90718638 -12.00084638 -16.52891829	H	-1.13220263 -14.54236605 -14.33476551
C	13.02817181 -14.88640001 -15.80516367	H	0.01414003 -14.18116206 -13.09708547
C	12.65624236 -15.11475404 -14.27838871	H	4.29298358 -8.90964191 -15.52866537
S	12.78726272 -13.58755586 -13.36049197	H	-0.86525111 -9.94865170 -14.11229731
C	14.55608004 -13.25366093 -13.56412973	H	0.08806224 -9.76477657 -12.64454532
H	11.62617824 -15.44690037 -14.25134658	H	-2.06299286 -12.82803194 -15.514445806
H	14.92561172 -12.66613205 -12.73030778	H	-1.55673235 -11.18302942 -15.21027167
H	15.10114904 -14.19825442 -13.59440908	H	0.36660937 -7.90828440 -14.81761303
H	14.73849482 -12.72517490 -14.49612357	H	1.49214344 -7.94527901 -13.45585963
H	13.18812121 -15.84099262 -16.24825899	N	3.57152535 -5.60973652 -15.81015630
H	13.29930431 -15.88914410 -13.87563226	C	3.68893369 -4.13131734 -15.85247500
H	12.90839051 -13.60067382 -18.49456617	C	4.27787288 -3.62543251 -17.16470812
H	11.00517041 -14.59448152 -16.39999934	O	4.56370306 -2.44444775 -17.31067602
H	13.96722753 -14.34863464 -15.85874670	C	4.48241488 -3.62529534 -14.65945628
N	10.80836658 -12.24631333 -15.75149834	C	3.64789257 -3.52016571 -13.39528253
C	10.67240660 -10.88974215 -15.19118860	C	4.50830216 -3.75952744 -12.17138383
C	10.53682481 -11.05903418 -13.65154684	N	3.81092377 -3.32110125 -10.94217144
O	9.80327408 -11.92152342 -13.16182518	C	3.38976120 -4.13766762 -9.98438729
C	9.42709059 -10.20498496 -15.72709053	N	3.46664836 -5.42491112 -10.12370598
C	9.40609694 -10.09738852 -17.26587684	N	2.88333144 -3.69888864 -8.86815943
C	9.21330853 -8.82409033 -15.10373336	H	2.83641008 -4.23938624 -13.40010870
C	10.51507416 -9.17585528 -17.73831503	H	2.70385240 -3.67427647 -15.76867006
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H	8.29840692 -8.38446681 -15.48219242	H	3.23625911 -2.51324812 -13.33048379
H	9.11581384 -8.94461508 -14.03294220	H	2.60706613 -4.35434695 -8.16106037
H	8.56302935 -10.80402236 -15.46596490	H	2.77658412 -2.71354054 -8.74303063
H	9.54905475 -11.07913222 -17.69081440	H	4.37455475 -6.19243177 -16.01992987
H	8.45600586 -9.67666262 -17.55921511	H	5.44365663 -3.21209738 -12.25656699
H	11.47690576 -9.57479889 -17.42674158	H	4.74911542 -4.82013108 -12.14039477
H	10.04372524 -12.89883953 -15.64990096	H	3.25850450 -6.09999562 -9.41112219
H	10.50384399 -9.15280930 -18.81520579	H	3.96701211 -5.77577494 -10.91742702
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C	5.36097573 -10.11998871 -12.88579239	H	4.03275966 -5.43556234 -17.99224046
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H	7.44301697 -10.48492481 -12.41259463	C	8.59330179 -6.48784013 -19.72000028
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C	9.97550161 -2.87172907 -17.12785780	N	6.60489128 -20.99262056 -19.57946497
C	8.15713602 -3.79609037 -15.85255240	C	6.08698552 -20.90021387 -18.19635702
C	9.87788609 -1.67305963 -16.40427912	C	4.59230711 -20.56673105 -18.29994476
C	8.06288562 -2.62655744 -15.08515857	O	4.09754145 -20.18360238 -19.39319820
C	8.94607590 -1.56387099 -15.32973192	C	6.81882549 -19.84989659 -17.38644973
O	8.77991572 -0.42415730 -14.63356375	O	6.67836860 -18.56824025 -17.98085131
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H	6.63659275 -4.83497370 -17.90125256	H	6.39614872 -19.82403952 -16.38519970
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H	10.73017158 -2.95990729 -17.88133754	N	3.13703895 -17.88591693 -16.99640177
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H	8.77049978 -6.02958074 -16.99965191	C	3.60880981 -16.05448658 -18.64900008
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N	7.81544889 -7.52777948 -19.35613414	C	3.80487875 -15.70366989 -16.16980255
C	7.79893247 -8.79841846 -20.06748993	C	3.77319901 -14.18006247 -16.23850620
C	7.39169835 -8.56783141 -21.57629533	C	2.35353512 -13.65655163 -16.42536321
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H	7.15006685 -7.35569777 -18.61500004	H	5.32794461 -13.99340869 -14.75960415
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H	7.09692574 -9.49229721 -19.61623948	H	3.69723409 -13.99738234 -14.08475208
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O	7.18832245 -6.96900686 -25.19195812	H	1.96839950 -13.99103540 -17.37677587
C	4.73758970 -6.41178747 -23.10944516	H	2.02130699 -16.15797657 -17.22591823
C	4.13840379 -6.05982846 -24.49425728	H	4.39950124 -13.81041915 -17.03866973
C	2.93543517 -5.16034719 -24.23281458	H	4.84849635 -15.99024232 -16.19317725
N	2.23886572 -4.76529214 -25.44949669	H	3.38112588 -16.00325158 -15.21461257
C	1.14175213 -4.00218984 -25.48679022	N	4.66750163 -16.69636180 -19.07807133
N	0.60510712 -3.54965380 -24.36115002	C	5.15872491 -16.55743987 -20.44933457
N	0.62615551 -3.61997808 -26.62564957	C	4.05749748 -16.96495263 -21.45608743
H	3.79218635 -6.95272662 -25.00526301	O	3.86015243 -16.19700264 -22.36796251
H	5.67678239 -8.25479334 -23.68241144	H	5.07523478 -17.42316192 -18.48993190
H	2.63205481 -5.05994588 -26.34363661	H	5.44539759 -15.52551181 -20.63448057
H	4.85780691 -5.51042727 -25.08716707	H	6.02496269 -17.20148994 -20.60284065
H	-0.21741880 -3.08394059 -26.68450212	N	1.58537750 -14.26601807 -21.66196010
H	1.00172201 -3.98447487 -27.49346940	C	2.20634884 -13.05059872 -22.16694176
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H	3.28170527 -4.27048317 -23.71346067	O	2.32485871 -12.22368171 -24.40200686
H	2.22649572 -5.70485923 -23.61208083	C	3.55133406 -12.79919400 -21.41598328
H	-0.22369764 -2.98570599 -24.41631593	O	3.32370698 -12.58737820 -19.97855649
H	0.92333947 -3.96383353 -23.51980622	H	2.09737008 -14.87469689 -21.03080597
H	4.98657179 -5.48910555 -22.60209643	H	1.55984463 -12.19293838 -21.99812684
H	3.97105472 -6.92269820 -22.54904504	H	4.05332763 -11.97180858 -21.88851833
N	9.61278947 -9.42238143 -24.96073307	H	4.19359841 -13.66966602 -21.54947066
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C	7.62812380 -10.67942458 -25.82200088	C	-0.64096804 -10.85219831 -26.48941993
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F 4.52794363 -9.92891654 -21.28698139
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H 6.21200440 -7.98542221 -16.86207741

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H 5.69040634 -18.93410874 -14.28751665
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**2C QM/MM R2b (B3LYP/6-31G(d): Amber)
mechanical embedding $\omega_{\alpha}=1.667$**

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C	21.71526816	-9.81017953	-10.46598859	S	29.18342601	-4.41970199	-7.27787047
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H	21.22944879	-10.70634748	-10.08643036	H	28.89340772	-3.20296481	-5.17710837
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H	21.94430426	-11.87325627	-12.19179077	N	31.59204726	-1.60840153	-7.50933168
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C	26.87042941	-11.71864300	-6.60110422	C	29.85210627	-4.34134957	-11.57330772
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C	9.19621842	-9.39523911	-27.37744508	N	-1.01159788	-13.04812973	-25.46768621
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 H 0.10580568 -7.48092797 -22.64216969
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 H 6.21200440 -7.98542221 -16.86207741
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 H -0.07133587 -10.50402632 -18.46274884
 H 1.42693052 -10.31182645 -18.65238519
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1C QM/SE/MM R1b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
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 H 8.02310545 -15.13359226 -18.92727988
 C 6.82996132 -12.51953004 -17.03851550
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 H 0.13784142 -7.36919148 -22.57253590
 C 1.60572617 -8.83580848 -23.17258606
 H 1.13874933 -9.06816616 -24.12428519

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 C 3.36139607 -9.30916806 -21.57062590
 F 4.54019973 -9.99533921 -21.28170774
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2C QM/SE/MM R1b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
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 S 25.83579805 -5.72714899 -6.52249581
 H 24.09635486 -9.48032030 -5.09952940
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C	29.68648101	-3.85831103	-5.57782549	H	23.69347277	-6.58960090	-4.68959628
S	29.19833737	-4.42621914	-7.28077307	H	25.58844563	-8.17777121	-6.53555508
H	30.80990728	-3.12220077	-3.50243068	H	25.98198499	-7.56262610	-4.92257637
H	31.79217936	-3.67388955	-6.03772730	N	22.38653397	-6.08325395	-6.84704626
H	28.90443641	-3.22675648	-5.14674518	C	21.47882281	-5.95725563	-7.96224494
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N	31.60997185	-1.62040818	-7.54497831	O	21.56126554	-5.81377111	-10.35561503
H	31.99970269	-2.44138867	-7.97352894	C	20.48982790	-4.86935086	-7.64942759
C	7.70084550	-15.97490091	-16.33175113	H	20.93080333	-6.89639795	-8.10223553
H	7.18906768	-16.36084449	-17.20597125	H	22.22012269	-5.51427624	-6.02087443
C	8.08001002	-16.78953443	-15.27691093	N	23.42373924	-5.18636493	-9.17084674
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C	8.76790038	-16.19264612	-14.20863745	C	25.22231151	-5.89207672	-10.73766789
H	9.13671887	-16.79460812	-13.39142392	O	25.25803221	-6.09736350	-11.95407903
C	8.99275348	-14.81940626	-14.24444788	C	25.10230282	-3.59804592	-9.91359396
H	9.55181789	-14.32523426	-13.45231670	C	24.26595193	-2.44638123	-9.45869581
N	8.49557490	-13.98284883	-15.20600495	C	23.30438460	-1.87274038	-10.28009723
C	7.90198550	-14.60284262	-16.25426977	C	24.40519987	-1.95613698	-8.13461128
C	7.38723076	-13.75191496	-17.34486221	C	22.54107504	-0.79234848	-9.83903639
C	7.49095605	-14.19505302	-18.70596409	C	23.60900065	-0.92908604	-7.68326603
C	6.97209371	-13.33725170	-19.69683790	C	22.69427924	-0.31664053	-8.53958796
C	6.37751735	-12.11576164	-19.43137430	O	22.03209863	0.79423664	-8.09026480
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F	7.05594905	-13.72348045	-21.01123832	H	21.80241366	-0.36357596	-10.49322118
H	8.01584528	-15.13090363	-18.92750868	H	23.71584750	-0.53350671	-6.69028143
C	6.82837311	-12.51951365	-17.03935673	H	23.84810458	-5.31143851	-8.25431642
H	6.80200656	-12.23835815	-15.98832193	H	25.13855899	-2.38350073	-7.47700542
C	6.25716731	-11.72508040	-18.04234532	H	23.13998544	-2.25506677	-11.27478322
C	5.45958278	-10.59393298	-17.66465200	H	25.66670316	-3.28524578	-10.79145620
O	5.65932570	-9.82363130	-16.67174654	H	25.81173316	-3.83630150	-9.11906283
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H	3.40994618	-9.21529824	-17.22858219	C	26.19299035	-9.07539503	-10.08436967
S	3.62126604	-7.97052766	-19.07255935	O	26.71533445	-10.09522104	-10.55757856
O	4.99851277	-7.49855613	-19.43655806	C	28.22494173	-7.58273837	-9.74519135
O	2.85622697	-6.92406045	-18.36019659	S	28.28080452	-8.13998382	-7.90917320
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C	1.64115623	-7.63571813	-21.04784754	H	26.87527753	-7.56427475	-11.37582724
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C	1.06497616	-7.87428119	-22.30270218	H	28.86692407	-8.26709928	-10.30239926
H	0.14376993	-7.36277945	-22.57513972	N	25.04233598	-9.11412382	-9.36278008
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H	1.14009626	-9.06338949	-24.12472231	C	25.17375424	-11.37620893	-8.30029251
C	2.78337053	-9.52734142	-22.82437159	O	24.82191060	-12.53928822	-8.13572670
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				H	21.81955803	-10.32521608	-13.09306548
				H	23.33618394	-11.24089878	-13.12254017
				H	23.46863037	-10.17928144	-8.59872245
				H	23.49312112	-9.30119966	-11.56663305
				H	23.38784394	-12.00912763	-10.16348708
				H	24.77100430	-11.33826497	-11.06196604
				N	26.21479056	-10.83606763	-7.61515320
				C	26.87196561	-11.71087502	-6.65449577
				C	25.83123016	-12.12185126	-5.54080263
				O	25.17137709	-11.27703134	-4.98105559

1C QM/SE/MM R3b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_{\alpha}=1.667$

C	21.94126857	-10.35051432	-4.22419597
C	22.25418007	-8.89143491	-4.44250367
O	21.41128062	-8.01405868	-4.34952080
N	23.52430939	-8.67546724	-4.81768198
C	23.89728852	-7.39005715	-5.40131637
C	23.07798669	-7.23041366	-6.70796290
O	23.13850600	-8.10371004	-7.58059725
C	25.39582866	-7.36565773	-5.83015769
S	25.84285697	-5.72614468	-6.52176980

C	28.02659892	-10.97923928	-5.98621901	C	29.18716940	-1.99505020	-10.87355588
C	28.65049542	-11.80912961	-4.87825927	C	27.95109674	-1.17026211	-10.51960763
C	29.93814849	-11.13000786	-4.34349044	O	27.42023676	-1.12544384	-9.43351178
C	30.33720351	-11.83279277	-3.03024472	C	28.78349923	-3.46932969	-10.97470645
N	31.77163792	-11.69641969	-2.78424944	C	29.83638022	-4.32947094	-11.57993536
H	27.22060315	-12.62234003	-7.15472242	C	31.18532665	-4.22640485	-11.41993813
H	29.78763748	-11.39105147	-2.20427438	C	29.62507583	-5.44674441	-12.45258056
H	30.10457756	-12.89232236	-3.10337608	N	31.83324713	-5.20332465	-12.12375233
H	27.93822558	-11.87730583	-4.05677436	C	30.91079895	-5.98951982	-12.74349523
H	28.88865128	-12.81081532	-5.21791553	C	28.49577955	-6.11079522	-12.93885392
H	32.10883772	-12.32839401	-2.04954672	C	31.06352977	-7.19555959	-13.42149721
H	32.32668149	-11.91923216	-3.63569952	C	28.66243285	-7.32240391	-13.57594967
H	32.00772426	-10.73322031	-2.49127957	C	29.92049576	-7.85955261	-11.83241598
H	29.76619246	-10.07458263	-4.18170788	H	30.00851764	-8.77276551	-14.38549095
H	30.71199964	-11.26914845	-5.09283931	H	29.58402720	-1.64257885	-11.83302267
H	26.59874773	-9.92823171	-7.85009723	H	32.82998318	-5.31609808	-12.20997788
H	27.69572469	-10.02046049	-5.60374961	H	27.51347124	-5.70333820	-12.78304828
H	28.78991570	-10.79103916	-6.74152331	H	27.79327882	-7.85911451	-13.88609705
N	25.76353801	-13.42704580	-5.19586379	H	32.04945124	-7.56464997	-13.65078892
C	24.89697945	-13.85116827	-4.13083612	H	31.73659234	-3.49360479	-10.86982821
H	26.19958655	-14.15312837	-5.74710110	H	30.36501340	-2.48952169	-9.17086298
C	29.87738705	-4.48726081	2.81045623	H	27.89600967	-3.54899445	-11.60135897
C	30.09721461	-4.49108311	1.26276390	H	28.54567672	-3.85133723	-9.98129678
O	30.70300399	-3.63809201	0.66485736	N	27.43870512	-0.47357451	-11.55082024
N	29.50808323	-5.54016383	0.63874008	C	26.13040339	0.15449985	-11.47770303
C	29.57335687	-5.61539075	-0.83129121	H	27.93938186	-0.35846061	-12.43089118
C	29.07166490	-4.32333917	-1.44876909	C	14.00414517	-19.32631751	-8.43486537
O	29.79780904	-3.72859220	-2.22663739	C	12.58045847	-19.03032025	-8.87981331
C	28.83612195	-6.83938290	-1.37074588	O	11.65566567	-19.11972444	-8.10230809
C	28.95235999	-6.94916480	-2.84375844	N	12.47688478	-18.59478114	-10.15752490
H	29.25637154	-7.73136126	-0.89383927	C	11.19537141	-18.22692070	-10.69905820
H	28.97011033	-6.22446614	1.16317149	C	10.81545245	-18.99708218	-11.93611428
H	30.62964891	-5.65986555	-1.11339056	O	9.76643452	-18.75949310	-12.51582975
H	27.77939349	-6.78242369	-1.10554757	C	11.05541139	-16.72390793	-10.93307647
C	28.16685666	-6.46398289	-3.85958416	C	11.57063706	-15.96115257	-9.73972147
H	30.87713081	-7.87236939	-2.99936919	C	10.80301316	-15.89118335	-8.56472998
H	27.25849011	-5.89121425	-3.79276168	C	12.80130452	-15.30586365	-9.80038187
C	29.81951672	-7.50651354	-4.80641633	C	11.28916734	-15.18066294	-7.47466709
N	30.00201557	-7.63348774	-3.46720399	C	13.28379683	-14.62511446	-8.69694785
N	28.70021232	-6.86306231	-5.02989642	C	12.52171409	-14.55818957	-7.52597738
H	30.48990381	-7.89529246	-5.55302184	H	12.91419049	-14.03848211	-6.67334785
N	27.84715013	-3.88409634	-1.06035184	H	10.46527188	-18.53190411	-9.93637499
C	27.28148377	-2.64221502	-1.55395437	H	10.69850692	-15.13791266	-6.58835516
H	27.31862204	-4.37524016	-0.34172896	H	14.24953370	-14.15610812	-8.75195836
C	32.66140136	-1.85458605	-2.42719094	H	13.29144140	-18.49140570	-10.75317264
C	32.40766150	-1.95967538	-3.94895724	H	13.39053338	-15.37428632	-10.69970150
O	33.11897403	-1.42609269	-4.79128125	H	9.85102764	-16.38663493	-8.51837270
N	31.33818599	-2.70695064	-4.25979159	H	10.01007583	-16.47785500	-11.08503355
C	30.99027370	-3.05794725	-5.65523822	H	11.63563722	-16.43077348	-11.80422450
C	30.86810618	-1.73812419	-6.43581989	N	11.61766351	-19.99395965	-12.30000587
O	30.17056615	-0.83136567	-6.04635806	C	11.29861419	-20.75060583	-13.47619499
C	29.68155796	-3.85083468	-5.60397254	C	11.31825989	-22.21139649	-13.11715337
S	29.16818726	-4.42420672	-7.28683546	O	12.23375423	-22.71795511	-12.50834127
H	30.80580566	-3.11172852	-3.50594726	C	12.28201411	-20.45189335	-14.63520386
H	31.78242087	-3.68885889	-6.07330063	C	12.23577006	-18.99645646	-15.05671778
H	28.91101300	-3.20548284	-5.17580783	C	13.33878261	-18.76788286	-16.07845755
H	29.84250547	-4.70139989	-4.93946357	C	10.87410606	-18.65127439	-15.64995359
N	31.56531652	-1.59529583	-7.57232578	H	10.11417083	-18.76781193	-14.89439471
C	31.55426755	-0.40753148	-8.35957459	H	10.88461472	-17.63210452	-16.00259407
C	30.67042173	-0.52796828	-9.61470639	H	10.67164865	-19.32115939	-16.48209529
O	30.32793812	0.43905355	-10.27072995	H	12.47507588	-20.19990562	-11.81150385
C	33.00663004	-0.10090071	-8.72718175	H	13.19392586	-19.40473428	-16.94771310
H	31.15655911	0.41463990	-7.76306921	H	13.31980696	-17.73873009	-16.41459492
H	32.08301154	-2.36443439	-7.94570272	H	14.31382416	-18.97622007	-15.65508975
N	30.24789027	-1.77275307	-9.87735420	H	10.29880151	-20.45698985	-13.79867076

H	12.39919473 -18.34459853 -14.20179275	C	11.29029442 -10.40657471 -11.44556413
H	12.01954097 -21.07973475 -15.48078457	H	11.90658477 -9.53007626 -13.31270721
H	13.28511143 -20.71043926 -14.30591245	C	7.89832056 -6.08053557 -12.13455221
N	10.24494756 -22.87619158 -13.56381045	C	6.86560589 -6.75262238 -13.05176581
C	10.13342367 -24.32164228 -13.36917201	O	6.61048240 -6.32322761 -14.14931732
H	9.59930757 -22.47925367 -14.23359036	N	6.44559762 -7.96150420 -12.65396183
C	14.09735237 -18.54641718 -21.17681653	C	5.62004516 -8.76975256 -13.48890197
C	13.89434970 -17.05586811 -21.07073759	C	4.30252775 -7.98011041 -13.74786687
O	14.71224501 -16.27339792 -21.45967844	O	3.92559800 -7.15152188 -12.93321317
N	12.72264838 -16.68782138 -20.52828465	C	5.34924969 -10.13028313 -12.89761416
C	12.42615044 -15.30977775 -20.26711283	C	6.62232452 -10.97838325 -12.89003772
C	11.79957693 -15.21999829 -18.83911403	C	6.37486070 -12.30378927 -12.28276060
O	10.95257558 -16.03804871 -18.45983280	H	6.92758679 -11.15191603 -13.92842122
C	11.50595452 -14.71415596 -21.34670791	H	6.12667189 -8.87992795 -14.45724140
C	11.23739965 -13.26361425 -21.06440315	H	7.44155146 -10.47787958 -12.40007509
C	10.22764551 -15.54378919 -21.47304254	H	6.65838130 -8.26016017 -11.71041638
C	10.56527049 -12.54428763 -22.20496689	H	4.58760008 -10.62628512 -13.49475557
H	13.37629119 -14.77409635 -20.27842997	H	4.97786593 -10.03828867 -11.87905452
H	9.62997888 -15.14584557 -22.27948318	H	8.29994198 -12.86960801 -12.58981216
H	10.48509161 -16.57166182 -21.69181685	O	5.25367307 -12.59156594 -11.86632569
H	12.05120727 -14.78731300 -22.28716887	N	7.43303523 -13.11777087 -12.12981168
H	10.59336620 -13.18998677 -20.18256528	H	7.30300810 -14.07067556 -11.81982412
H	12.17182029 -12.75999225 -20.83124739	N	3.76075619 -8.24843857 -14.97710985
H	9.60349670 -12.99434624 -22.42424922	C	2.46577627 -7.76232743 -15.40685893
H	12.09435256 -17.40117846 -20.19020274	C	2.45955070 -6.23686887 -15.44537879
H	10.40179079 -11.50947120 -21.93554277	O	1.45383013 -5.61792660 -15.15874832
H	9.66777290 -15.47278169 -20.54895501	C	1.35161478 -8.28179708 -14.46727440
H	11.18827569 -12.58924955 -23.09234220	C	1.27623319 -9.81053798 -14.45625899
N	12.17193331 -14.18316253 -18.08229979	C	0.09082473 -10.24225624 -13.60795157
C	11.97728689 -14.17591262 -16.59670958	N	0.01804383 -11.64632988 -13.31720343
C	11.95897988 -12.72772786 -16.23948468	C	-0.66998434 -12.53283202 -14.08515142
O	12.90607953 -12.01997145 -16.52588712	N	-1.62975169 -12.08083031 -14.95696278
C	13.03562273 -14.91284573 -15.81829599	N	-0.41144386 -13.89200117 -13.96433793
C	12.66134559 -15.13140249 -14.26684312	H	2.17926252 -10.23617388 -14.062515783
S	12.77568913 -13.57684125 -13.37367587	H	2.22124832 -8.12570604 -16.40296383
C	14.54486711 -13.23281308 -13.56949898	H	0.75264416 -12.03123448 -12.72540845
H	11.62382028 -15.44454270 -14.22085670	H	1.15533716 -10.17741623 -15.47436500
H	14.87160917 -12.64792942 -12.72027876	H	-1.19013313 -14.49479635 -14.19054476
H	15.08615151 -14.17661346 -13.58577310	H	-0.00354967 -14.14810181 -13.07118747
H	14.71803417 -12.68981708 -14.49136368	H	4.31335790 -8.88842967 -15.55025634
H	13.22159730 -15.89091125 -16.24418284	H	-0.83909056 -9.94477100 -14.09040891
H	13.32443036 -15.88878757 -13.86602835	H	0.13014230 -9.73027313 -12.64609168
H	12.90963717 -13.58432492 -18.45639996	H	-1.99656556 -12.79243807 -15.56705089
H	11.00550208 -14.65432149 -16.44070373	H	-1.42561619 -11.20285425 -15.40481141
H	13.95680317 -14.33675325 -15.84412761	H	0.40926173 -7.86735161 -14.81275067
N	10.79217278 -12.27563194 -15.74117997	H	1.54072346 -7.92237159 -13.45864564
C	10.67774556 -10.91353427 -15.23015858	N	3.59632534 -5.63766339 -15.83105067
C	10.54248616 -11.05188782 -13.67116604	C	3.68689600 -4.18784202 -15.86311357
O	9.85893873 -11.92207497 -13.15699586	C	4.28282460 -3.65115153 -17.17031498
C	9.42506025 -10.22289655 -15.73345080	O	4.57100497 -2.47689406 -17.31505230
C	9.39228469 -10.12525151 -17.27810303	C	4.47077576 -3.65149825 -14.67535123
C	9.25068479 -8.84063693 -15.11213458	C	3.63836254 -3.54547895 -13.41157015
C	10.48796243 -9.19222596 -17.74895688	C	4.50706689 -3.77302395 -12.18863765
H	11.57716149 -10.36110550 -15.48037490	N	3.84104380 -3.32816571 -10.97701358
H	8.33781617 -8.38426392 -15.47445471	C	3.44504713 -4.14993742 -9.97995162
H	9.17463630 -8.93841516 -14.03271966	N	3.25904681 -5.47465764 -10.21395789
H	8.56835903 -10.83424701 -15.44463373	N	3.08007386 -3.63692518 -8.76264341
H	9.53369754 -11.11555262 -17.69077746	H	2.83292365 -4.27269326 -13.41497026
H	8.42315356 -9.73512718 -17.56045230	H	2.66377504 -3.80821081 -15.77731497
H	11.45769676 -9.58606168 -17.45597361	H	3.81924719 -2.34090372 -10.80188443
H	9.98941215 -12.89409209 -15.59578989	H	3.19958145 -2.54914978 -13.34254589
H	10.48528530 -9.13325747 -18.82820178	H	2.57110646 -4.28261263 -8.18110413
H	10.09730008 -8.20482724 -15.33220556	H	2.72575682 -2.69715625 -8.77831408
H	10.37630155 -8.19221770 -17.35521550	H	4.42245519 -6.19343775 -16.03265901
N	11.34353764 -10.28296028 -12.92883591	H	5.44769263 -3.22785584 -12.27823856

H	4.73868644	-4.83428495	-12.12546687	C	8.92289118	-5.13448542	-23.92742657
H	3.29670391	-6.11346437	-9.42048622	H	7.63390371	-5.59811314	-22.34063117
H	3.83157305	-5.85797162	-10.95060566	C	11.29232766	-8.07323074	-23.87669680
H	4.87129224	-2.67393152	-14.93397242	C	10.87106095	-8.98204082	-25.04540229
H	5.30515463	-4.32880567	-14.48617729	O	11.69831828	-9.32138987	-25.87437940
N	4.27750185	-4.52556229	-18.20130919	N	9.57893484	-9.39763848	-24.96655606
C	4.76556935	-4.11607990	-19.49464841	C	9.07304659	-10.21584321	-26.06274925
C	6.24240496	-4.47763568	-19.85798845	C	9.21621777	-9.41695842	-27.38471017
O	6.59494802	-4.42275328	-21.04221378	O	9.80573429	-9.86693761	-28.32662855
H	4.01770531	-5.49460783	-18.05045529	C	7.62723062	-10.69454377	-25.83041284
H	4.14960461	-4.57418867	-20.26897577	C	7.57868896	-11.65146398	-24.64732936
H	4.70568920	-3.02407968	-19.53979965	C	7.12477116	-11.38542811	-27.08138028
N	7.01483766	-4.84180992	-18.82451290	C	6.17613618	-11.89074327	-24.13992644
C	8.42272940	-5.17731971	-18.97813713	H	9.73005907	-11.08801627	-26.17421695
C	8.58096059	-6.48567374	-19.74019750	H	6.09972987	-11.70167210	-26.92092930
O	9.38776986	-6.54200766	-20.65493153	H	7.14735899	-10.70567900	-27.92102035
C	9.16341097	-5.24567296	-17.59052400	H	7.02000829	-9.81441529	-25.61622611
C	9.09697137	-3.92852880	-16.86886483	H	8.04717722	-12.58784270	-24.93832097
C	9.95321321	-2.87550387	-17.12173409	H	8.16056331	-11.22498003	-23.83288431
C	8.17050305	-3.77585969	-15.85253583	H	5.58169274	-12.33400948	-24.93581296
C	9.86574071	-1.69247108	-16.41411483	H	8.99182558	-9.14501367	-24.18962776
C	8.07546830	-2.61678259	-15.09928289	H	6.21577620	-12.57534865	-23.30537390
C	8.95166984	-1.56465504	-15.34652368	H	7.74019414	-12.24778405	-27.29535574
O	8.78583811	-0.43369619	-14.62862441	H	5.72395353	-10.95299354	-23.84597674
H	8.90537445	-4.39512328	-19.57221892	N	8.74037513	-8.17543930	-27.38530276
H	10.55502423	-0.88570126	-16.59834836	C	8.84823536	-7.32536146	-28.54605145
H	7.35190802	-2.53547380	-14.31491262	H	8.24007907	-7.78120829	-26.60100054
H	6.62672746	-4.86459311	-17.88905209	C	6.59359662	-21.92030832	-21.79991568
H	7.51059209	-4.59419622	-15.61809572	C	6.23320887	-22.03540259	-20.30803359
H	10.70877667	-2.95535847	-17.87961130	O	5.53516755	-22.93761182	-19.89153921
H	10.19375395	-5.46858554	-17.82950007	N	6.59122873	-20.95112292	-19.60925902
H	8.73067938	-6.03692052	-16.99243140	C	6.12493903	-20.90759504	-18.21528849
H	9.62793174	0.13254065	-14.74926466	C	4.62235295	-20.55895977	-18.32237909
N	7.78518391	-7.50863844	-19.35412496	O	4.11880132	-20.20885651	-19.39091833
C	7.80179964	-8.76290418	-20.04539229	C	6.83905527	-19.84828129	-17.39445127
C	7.39932665	-8.57387689	-21.59482046	O	6.65131777	-18.55912319	-17.96047430
O	7.95929554	-9.22994988	-22.44842874	H	7.27639844	-20.29179200	-19.95379103
H	7.06676172	-7.33959089	-18.66129762	H	6.24900271	-21.89770812	-17.76606828
H	8.80369234	-9.19158485	-20.07423003	H	7.90211005	-20.09437895	-17.32999349
H	7.09721731	-9.45956586	-19.60121786	H	6.41565554	-19.83794359	-16.38615124
N	6.51988010	-7.56335565	-21.81345889	H	7.52360523	-18.28077032	-19.31171475
C	5.97192391	-7.33841234	-23.12821086	N	3.96169984	-20.53940105	-17.13706003
C	7.08274887	-6.70744636	-23.99363085	C	2.53983278	-20.23847232	-17.16141710
O	7.18978190	-6.96338994	-25.18270725	C	2.34899152	-18.74772659	-17.57470089
C	4.76344179	-6.41494954	-23.07590328	O	1.51078111	-18.38207085	-18.37786804
C	4.15983211	-6.07476763	-24.46620052	C	1.92425287	-20.51093143	-15.79033630
C	2.93813073	-5.18934003	-24.22158707	H	4.33088520	-21.06968234	-16.35712783
N	2.26103228	-4.80057494	-25.43011320	H	2.01884017	-20.84725768	-17.90556727
C	1.14294583	-4.04865778	-25.45796288	N	3.20108104	-17.88281396	-17.00488573
N	0.65219044	-3.56522475	-24.25579770	C	3.08540505	-16.45950995	-17.25091122
N	0.68315102	-3.56645255	-26.63009739	C	3.61137118	-16.06472689	-18.64094409
H	3.83406000	-6.97551175	-24.97915549	O	3.11583308	-15.15828965	-19.32268324
H	5.68751492	-8.28487225	-23.61205609	C	3.82088225	-15.69521227	-16.17645980
H	2.64893688	-5.09877280	-26.32455664	C	3.76832007	-14.17079334	-16.26313885
H	4.88082447	-5.54201423	-25.07041324	C	2.34236205	-13.67436963	-16.47995485
H	-0.26089422	-3.22046384	-26.70250416	C	4.31718240	-13.61366886	-14.93993431
H	1.00462553	-4.01026887	-27.48412828	H	5.33014578	-13.95703864	-14.77544754
H	5.98143651	-7.29075529	-20.99647316	H	4.29710353	-12.53135338	-14.95995726
H	3.25345642	-4.29541640	-23.68195168	H	3.69829719	-13.95453558	-14.11320862
H	2.23540921	-5.75530607	-23.59822530	H	3.87548069	-18.22784950	-16.32092166
H	-0.23948739	-3.08572187	-24.35910675	H	1.70862993	-14.02495872	-15.66715167
H	0.69472296	-4.28826219	-23.55589528	H	2.34037680	-12.58812575	-16.46485407
H	5.03085781	-5.48317235	-22.58823595	H	1.95909907	-14.01527176	-17.42733108
H	3.98968609	-6.91556078	-22.49570252	H	2.02419769	-16.19280958	-17.23122868
N	7.76259243	-5.76164997	-23.33109627	H	4.40319933	-13.80888855	-17.07009158

H	4.86979422	-15.98585191	-16.18455652	C	8.06755817	-16.78455571	-15.29825222
H	3.40146147	-15.98455720	-15.21248516	H	7.84966255	-17.84211670	-15.31831820
N	4.65537708	-16.73486120	-19.07261934	C	8.76599736	-16.19219847	-14.24044088
C	5.14180426	-16.51624933	-20.42608227	H	9.14418350	-16.78848605	-13.43256603
C	4.05841420	-16.91476328	-21.46661347	C	9.00020640	-14.82277410	-14.27569025
O	3.84923570	-16.16581413	-22.39107965	H	9.58498305	-14.33698303	-13.50240840
H	5.12009519	-17.43964078	-18.50214508	N	8.51109295	-13.98725245	-15.23213099
H	5.38142388	-15.46508449	-20.58733370	C	7.89942045	-14.60389735	-16.26580291
H	6.03141112	-17.12463583	-20.58579793	C	7.39748140	-13.76224704	-17.34596174
N	3.38352890	-18.06172085	-21.29160805	C	7.51363701	-14.19641292	-18.69673633
C	2.28384429	-18.49266053	-22.16789878	C	6.99412680	-13.35303448	-19.68685056
H	3.64212271	-18.70772617	-20.54795757	C	6.38223008	-12.14750740	-19.40103933
C	-0.21892821	-15.82577368	-21.26966975	H	6.01271373	-11.53626433	-20.19313025
C	0.32352223	-14.61223263	-21.99414654	F	7.07584112	-13.73271730	-20.99624863
O	-0.42818053	-14.00176774	-22.73305432	H	8.05426253	-15.10792165	-18.92685732
N	1.57848723	-14.27836127	-21.69164625	C	6.81209566	-12.54986303	-17.02831594
C	2.16698122	-13.05286187	-22.16646747	H	6.72331246	-12.29253420	-15.98182758
C	2.47927115	-13.16859561	-23.70473794	C	6.24600728	-11.76075818	-18.02563239
O	2.34407780	-12.19790700	-24.40952622	C	5.44533866	-10.60764399	-17.66541763
C	3.51813944	-12.76564563	-21.40897811	O	5.65846180	-9.84718628	-16.67821024
O	3.30811911	-12.56384110	-19.98032550	N	4.37769129	-10.33958100	-18.53064185
H	2.08517851	-14.79723489	-20.98257054	H	3.96612984	-11.06111230	-19.12164729
H	1.49279036	-12.20519798	-22.02601642	N	3.44970861	-9.34558582	-18.22418524
H	3.97236235	-11.87854133	-21.82109402	H	3.45685674	-9.12794346	-17.21864019
H	4.17823184	-13.62040156	-21.56420353	S	3.60348575	-7.95621867	-19.08511453
H	3.24432025	-13.44122414	-19.57416509	O	4.99603390	-7.54729729	-19.42635593
N	2.80538747	-14.36202041	-24.17406703	O	2.83098030	-6.88325246	-18.41284485
C	3.07333290	-14.52082505	-25.60718477	C	2.78028160	-8.38113782	-20.68181547
H	3.15801941	-15.09928222	-23.57483640	C	1.62794516	-7.64834650	-21.08531796
C	-0.57268130	-15.19133509	-26.42371091	H	1.16076751	-6.95751495	-20.39559699
C	-1.14229331	-13.78420788	-26.53940716	C	1.05243540	-7.90760889	-22.33613394
O	-1.61404594	-13.34839781	-27.56210842	H	0.12666018	-7.42364401	-22.61524279
N	-1.00278424	-13.05119161	-25.44466150	C	1.60879500	-8.86311649	-23.19395916
C	-1.45430259	-11.68250874	-25.51800713	H	1.14056643	-9.09812634	-24.14213033
C	-0.65105844	-10.86041809	-26.53044330	C	2.78475454	-9.53097554	-22.84570051
O	-1.17487589	-10.02253965	-27.24143092	H	3.22863705	-10.25974922	-23.51235102
C	-1.40822698	-11.10856079	-24.10459023	C	3.35219815	-9.28770928	-21.59195620
H	-0.63863818	-13.40097615	-24.57259342	F	4.52778694	-9.95964346	-21.28182431
H	-2.49543641	-11.65311713	-25.86433910	Zn	28.07132634	-6.25160132	-6.90925493
N	0.69581293	-11.06858221	-26.51346532	O	-2.06705675	-5.89948902	-23.83673221
C	1.55393702	-10.22149829	-27.33010115	H	-2.87323080	-5.44535044	-23.50842197
C	1.18147721	-10.47189713	-28.84088390	H	-2.11288899	-6.75734414	-23.40726437
O	1.00332452	-9.55725145	-29.59585264	O	7.33725916	-19.80118092	-13.52143235
C	3.06850914	-10.48497198	-27.09111505	H	8.19331807	-19.41810423	-13.27051545
C	3.95296129	-9.89826561	-28.17763912	H	7.29701616	-20.65473130	-13.07814108
C	4.27708175	-8.55427890	-28.15042788	O	9.18410687	-17.88858389	-19.01570740
C	4.33917250	-10.66565064	-29.26187939	H	9.86622799	-17.26128921	-18.71380237
C	5.08525006	-8.01993835	-29.13207423	H	9.64402678	-18.54676417	-19.54668865
C	5.16004665	-10.16184108	-30.25309224	O	5.96598586	-7.06764494	-16.81658114
C	5.56250049	-8.83603996	-30.16360389	H	6.35861116	-6.81000850	-15.96283348
O	6.50708365	-8.34298420	-30.99129206	H	5.97115905	-8.04329963	-16.81488540
H	1.34638790	-9.16152818	-27.16275448	O	26.48523063	-0.93217449	-4.86024112
H	5.39103022	-6.98926547	-29.09682171	H	27.12928731	-0.80483508	-4.14697169
H	5.49584365	-10.76486146	-31.07415027	H	26.62183567	-1.81691568	-5.21244991
H	1.12382680	-11.64789092	-25.80225462	O	0.68555472	-10.03041521	-18.09130439
H	4.04077745	-11.69892219	-29.30718017	H	-0.10246744	-10.50957000	-18.45411549
H	3.97487573	-7.93058855	-27.32619618	H	1.41583820	-10.32735908	-18.63521269
H	3.22678993	-11.55836963	-27.06189257	O	4.76710353	-18.66100665	-14.47075280
H	3.34266643	-10.05177819	-26.13543624	H	5.69118099	-18.88976355	-14.27119402
H	6.36331517	-7.39102257	-31.16943210	H	4.26345726	-19.22098287	-13.86874755
N	1.14872638	-11.75736678	-29.18264821	O	-0.47226573	-6.69947401	-25.81498839
C	0.80767637	-12.22207600	-30.51402524	H	-0.80849900	-7.43194339	-26.33754685
H	1.36762523	-12.50474155	-28.53441989	H	-1.21107482	-6.36800178	-25.29499693
C	7.67541671	-15.96790468	-16.34402422				
H	7.12990383	-16.36009959	-17.19034476				

2C QM/SE/MM R3b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.667$

C	21.94130761	-10.34954627	-4.22487254	H	21.18582913	-10.66949809	-10.14458355
C	22.25461464	-8.89027182	-4.44514589	H	24.57523605	-8.30960057	-8.96905505
O	21.41396197	-8.01173075	-4.34532705	H	21.91726059	-11.81107218	-12.26155190
N	23.52570241	-8.67724078	-4.82196312	H	21.83000614	-10.27820394	-13.14935702
C	23.90375455	-7.38918091	-5.40121120	H	23.31545604	-11.23370057	-13.16253884
C	23.07602608	-7.22919465	-6.70303396	H	23.48591524	-10.18809667	-8.57300452
O	23.13708388	-8.10704002	-7.57180597	H	23.50455288	-9.28790791	-11.56815379
C	25.39603153	-7.37961569	-5.86446560	H	23.35659310	-12.01120620	-10.16268845
S	25.84263162	-5.72334884	-6.51833425	H	24.74836357	-11.38232005	-11.07056084
H	24.09847449	-9.48259013	-5.05860835	N	26.22122226	-10.83554533	-7.62021982
H	23.71084711	-6.58904055	-4.68339788	C	26.87627503	-11.71090770	-6.65946367
H	25.53580429	-8.15563246	-6.62225983	C	25.82913924	-12.13054699	-5.54800442
H	26.02011960	-7.64033217	-4.99985265	O	25.18702176	-11.28128184	-4.97606563
N	22.37969204	-6.08519454	-6.84405890	C	27.99104855	-10.93956245	-5.96186725
C	21.47241666	-5.96053282	-7.95950307	C	28.67907738	-11.82167356	-4.92618018
C	22.16479535	-5.65878565	-9.30775236	C	29.92192657	-11.09836600	-4.32866371
O	21.56647754	-5.83072786	-10.35160761	C	30.33083815	-11.86002385	-3.04358707
C	20.48843465	-4.86950567	-7.64841733	N	31.76257672	-11.70785267	-2.78060358
H	20.92391516	-6.89894120	-8.09907486	H	27.24577444	-12.61332858	-7.16449974
H	22.19881847	-5.52272505	-6.01700176	H	29.76609621	-11.48628228	-2.19145018
N	23.40820679	-5.15658465	-9.15867295	H	30.12165294	-12.92132624	-3.17548207
C	24.27022963	-4.80672747	-10.24146340	H	27.97512546	-12.02648181	-4.11751045
C	25.21211050	-5.88210203	-10.71632569	H	28.98700988	-12.76853522	-5.36378311
O	25.25402771	-6.06041394	-11.93636093	H	32.11305548	-12.35231046	-2.05968877
C	25.10799767	-3.59881895	-9.93791527	H	32.33002256	-11.90364120	-3.63122840
C	24.26912648	-2.45029608	-9.47430378	H	31.98236659	-10.74825920	-2.46247404
C	23.30665357	-1.87097972	-10.29648443	H	29.68749756	-10.05970226	-4.11784319
C	24.39192499	-1.99568951	-8.13278856	H	30.71788994	-11.14076660	-5.07012308
C	22.54487928	-0.78965010	-9.84649314	H	26.64561985	-9.94709090	-7.86255504
C	23.59080331	-0.97488502	-7.66997709	H	27.58087489	-10.04360378	-5.50048759
C	22.69815418	-0.33663205	-8.53665672	H	28.71943112	-10.61792788	-6.70853662
O	22.05239582	0.78016332	-8.07890883	N	25.76124203	-13.43537866	-5.20032686
H	23.61377522	-4.60491006	-11.09954372	C	24.89579973	-13.85206304	-4.13102706
H	21.81458488	-0.33296297	-10.49935091	H	26.12148689	-14.16573727	-5.79890149
H	23.65418929	-0.61211349	-6.65795032	C	29.87748201	-4.48803737	2.80690417
H	23.83288752	-5.24826681	-8.24016751	C	30.10035068	-4.49240657	1.25698900
H	25.09807864	-2.46376315	-7.46786614	O	30.70167128	-3.63322401	0.66426089
H	23.14859614	-2.23676040	-11.30331124	N	29.52069447	-5.54391386	0.62600964
H	25.65551222	-3.31366938	-10.83897772	C	29.56978920	-5.62467021	-0.84827892
H	25.83934046	-3.83106307	-9.15935991	C	29.07188569	-4.32232781	-1.45709810
H	22.35047431	1.57737318	-8.53153104	O	29.80200665	-3.70366577	-2.21459754
N	25.98364161	-6.58325313	-9.81128009	C	28.81931822	-6.85235243	-1.37004465
C	26.80137777	-7.67079596	-10.29036229	C	28.93512975	-6.95421769	-2.85034655
C	26.18842592	-9.07176428	-10.08337023	H	29.23341705	-7.74655831	-0.88397137
O	26.71386352	-10.09170482	-10.55411729	H	29.00643210	-6.24756902	1.14777100
C	28.22627642	-7.56961194	-9.75284514	H	30.62064283	-5.67901671	-1.15223663
S	28.28111822	-8.13913324	-7.91551027	H	27.76079551	-6.80115493	-1.09556521
H	25.93844080	-6.35030525	-8.81427755	C	28.15231834	-6.46505748	-3.86972549
H	26.84915046	-7.54598227	-11.37746123	H	30.87341497	-7.84273112	-2.99549090
H	28.60524416	-6.55099957	-9.84689287	H	27.23342378	-5.89889365	-3.83525036
H	28.87534925	-8.24701863	-10.31194204	C	29.81902846	-7.50245892	-4.81566324
N	25.03575394	-9.11860607	-9.36135570	N	29.99738788	-7.62630441	-3.47320523
C	24.38237809	-10.40842361	-9.16339165	N	28.69756624	-6.86343433	-5.03587103
C	25.18314637	-11.38146910	-8.30267743	H	30.47266066	-7.89881288	-5.57901501
O	24.83459065	-12.54477440	-8.12304241	N	27.84738419	-3.88583063	-1.06296289
C	23.88917334	-11.11023621	-10.46035789	C	27.28130414	-2.64276140	-1.55364598
C	22.95500502	-10.18497326	-11.27819926	H	27.29054266	-4.41164540	-0.39175382
C	22.46800790	-10.92130506	-12.55485706	C	32.66055773	-1.85561942	-2.42762130
C	21.70364048	-9.77503946	-10.48414144	C	32.40578989	-1.95891996	-3.94920940
H	21.97808186	-9.17928474	-9.61928794	O	33.09176713	-1.38239246	-4.78329940
H	21.04302645	-9.18533764	-11.10702807	N	31.36229715	-2.74149744	-4.27107845
				C	31.00603417	-3.07270796	-5.66808588
				C	30.87944865	-1.74499729	-6.44448231
				O	30.19634800	-0.82936034	-6.04718919
				C	29.70480619	-3.88011560	-5.59721236

S	29.16411748 -4.42080525 -7.28529071	O	12.23432310 -22.71798360 -12.50209092
H	30.87504248 -3.22477516 -3.53218820	C	12.27031373 -20.46172925 -14.62677420
H	31.79402190 -3.69970212 -6.10334715	C	12.21556822 -19.00124199 -15.05887185
H	28.93809606 -3.26422453 -5.11996573	C	13.32867453 -18.80294796 -16.08475678
H	29.90053475 -4.74270964 -4.95442721	C	10.84607899 -18.64438170 -15.65324657
N	31.56843486 -1.60414226 -7.58908416	H	10.07944673 -18.73023854 -14.89498741
C	31.55132365 -0.41028684 -8.36619369	H	10.85400275 -17.63191749 -16.03672723
C	30.66320080 -0.52992202 -9.61861943	H	10.61882531 -19.32991334 -16.46920013
O	30.31007899 0.43981190 -10.26472901	H	12.48538336 -20.22077173 -11.81755954
C	33.00620198 -0.10092957 -8.72772702	H	13.18135710 -19.46964850 -16.93292156
H	31.15309450 0.40604004 -7.76195913	H	13.33221606 -17.78677395 -16.46226604
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C	3.07949354 -16.45870260 -17.25280813	C	5.55937263 -8.83950217 -30.16486642
C	3.60889137 -16.05805469 -18.64137656	O	6.50951600 -8.34895020 -30.99002851
O	3.11431820 -15.14924939 -19.32140833	H	1.33776277 -9.16443160 -27.13406528

H 5.33660845 -6.97328790 -29.14299669
H 5.53127008 -10.76888470 -31.08165831
H 1.13428996 -11.65571971 -25.81614663
H 4.07128234 -11.72226615 -29.29613950
H 3.90779854 -7.92026952 -27.35900035
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H 3.35806511 -10.07744334 -26.11556709
H 6.38271853 -7.39685221 -31.18683214
N 1.14732009 -11.74878021 -29.18272963
C 0.80768517 -12.22007608 -30.51280578
H 1.37772210 -12.49600308 -28.53810225
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H 7.16896510 -16.37234813 -17.19649597
C 8.08659214 -16.79591906 -15.28902146
H 7.86929680 -17.85573065 -15.31678608
C 8.78277721 -16.20543209 -14.22496916
H 9.16289545 -16.80274019 -13.40995797
C 9.00259182 -14.82951030 -14.26517651
H 9.58115195 -14.34027665 -13.48573685
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C 7.89559297 -14.60288578 -16.26418622
C 7.38216438 -13.75280812 -17.35237650
C 7.48073669 -14.18630335 -18.71072198
C 6.97511328 -13.32834576 -19.70410233
C 6.37255660 -12.11234299 -19.43321191
H 6.02422530 -11.50359230 -20.24607007
F 7.06847373 -13.71226904 -21.00943338
H 7.99123074 -15.11935717 -18.94605665
C 6.81652965 -12.52172016 -17.04845263
H 6.76731661 -12.23875607 -16.00218833
C 6.25230638 -11.73250021 -18.04910799
C 5.45555462 -10.59084822 -17.66908754
O 5.64849543 -9.83262844 -16.67746879
N 4.39995368 -10.35481423 -18.54872748
H 4.01931611 -11.11205807 -19.11670064
N 3.46207165 -9.38701779 -18.24991243
H 3.38067880 -9.22756017 -17.24093052
S 3.61318022 -7.97556519 -19.07749777
O 4.99100977 -7.52755987 -19.43454657
O 2.83783036 -6.92679141 -18.38718435
C 2.79692958 -8.39807291 -20.66739465
C 1.65730689 -7.64017720 -21.06563864
H 1.21328316 -6.93191939 -20.37335975
C 1.07528724 -7.87063283 -22.32387440
H 0.17423341 -7.33944223 -22.61656234
C 1.62345096 -8.83097475 -23.18599011
H 1.16596484 -9.03282535 -24.14881140
C 2.78650961 -9.52735429 -22.83649389
H 3.22422550 -10.25507037 -23.51151438
C 3.36225489 -9.30342178 -21.57827208
F 4.53928573 -9.97650986 -21.27368897
Zn 28.07085179 -6.25181499 -6.91357939
O -2.07869539 -6.03951880 -23.84950698
H -2.82653933 -5.54439648 -23.45652318
H -2.30856994 -6.96220113 -23.70031526
O 7.34988097 -19.80489596 -13.52491210
H 8.18689920 -19.38074016 -13.27577947
H 7.40226492 -20.69455432 -13.16007849
O 9.21595193 -17.91417356 -18.99904977
H 9.83039275 -17.20224345 -18.73991947
H 9.75254016 -18.71552882 -18.99130893
O 5.96475481 -7.06872391 -16.81599269
H 6.37833723 -6.80988980 -15.97273247
H 5.94758839 -8.04424863 -16.79993383
O 26.49620731 -0.90467254 -4.84945503

H 27.12018715 -0.74970922 -4.12281802
H 26.77479647 -1.70778257 -5.29782087
O 0.68848989 -10.04602204 -18.07531948
H -0.10019583 -10.51137560 -18.45355680
H 1.44095584 -10.48759808 -18.47288518
O 4.76692924 -18.65836160 -14.46756212
H 5.69337698 -18.83973455 -14.23619891
H 4.28008616 -19.32292961 -13.96412614
O -0.45900623 -6.68935282 -25.85267914
H -0.75204924 -7.37572644 -26.45861493
H -1.23500701 -6.38377378 -25.37499171

**1C QM/MM R1b (B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_c=1.0$**

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O 21.41108921 -8.00960815 -4.34545664
N 23.53503612 -8.67605689 -4.80411180
C 23.91787549 -7.39753976 -5.40113065
C 23.07991681 -7.24086502 -6.68265989
O 23.14898444 -8.09330856 -7.56888026
C 25.40001678 -7.38945164 -5.85267950
S 25.82711505 -5.73153736 -6.51886608
H 24.09838922 -9.49284652 -5.03161321
H 23.72815056 -6.59755706 -4.68415430
H 25.55967682 -8.16438892 -6.60544609
H 26.02084062 -7.63484327 -4.98353118
N 22.35028720 -6.11441320 -6.78418845
C 21.46135612 -5.93336637 -7.92126503
H 22.13271485 -5.56811383 -5.95676126
C 24.31831765 -4.87394999 -10.22379946
C 25.23593845 -5.94242589 -10.76212339
O 25.21136996 -6.17372885 -11.96656667
N 26.00118413 -6.60734773 -9.83795050
C 26.84889883 -7.68707897 -10.30258804
C 26.24353331 -9.08592472 -10.11518146
O 26.78270146 -10.10228366 -10.56105122
C 28.26139703 -7.61737820 -9.71812790
S 28.26814310 -8.15190141 -7.90587389
H 25.98727394 -6.30701549 -8.86060562
H 26.90747822 -7.56019609 -11.38855418
H 28.67075954 -6.60973129 -9.82890548
H 28.90015293 -8.30962168 -10.27203540
N 25.08432739 -9.12689643 -9.41752925
C 24.40766283 -10.41278491 -9.17844111
H 24.60594096 -8.31043135 -9.06007984
C 29.87817528 -4.49498073 2.80826416
C 30.09495677 -4.49941419 1.27080674
O 30.69198448 -3.62939268 0.67802758
N 29.50992954 -5.54967995 0.63980357
C 29.57580524 -5.63518937 -0.82450341
C 29.07141300 -4.33858643 -1.44720761
O 29.78645085 -3.74086622 -2.23131576
C 28.83772894 -6.87263135 -1.35155167
C 28.93908926 -6.97301092 -2.83647659
H 29.25802528 -7.76569522 -0.87049419
H 29.02141136 -6.26640275 1.16732984
H 30.62882155 -5.67370122 -1.11904521
H 27.78019921 -6.83262440 -1.06738308
C 28.12967692 -6.49791188 -3.83830895
H 30.89581728 -7.78280282 -3.01749562
H 27.20252683 -5.94618956 -3.78164896
C 29.81148913 -7.46633668 -4.81715753

N 30.00920109 -7.59464100 -3.48152903
N 28.66940535 -6.85670018 -5.03035008
H 30.46574610 -7.83157908 -5.59721035
N 27.85256765 -3.88440279 -1.05061726
C 27.28078540 -2.64087560 -1.55470601
H 27.29623966 -4.39952405 -0.37025262
C 32.65987311 -1.85137456 -2.42376192
C 32.40663147 -1.96154267 -3.93672340
O 33.11166590 -1.41052363 -4.77871949
N 31.34477120 -2.71796787 -4.23776177
C 30.99983839 -3.05349699 -5.62158799
C 30.85116691 -1.73901573 -6.39585931
O 30.04745770 -0.89899051 -6.06390044
C 29.69265709 -3.85210770 -5.59576024
S 29.22370031 -4.40819248 -7.29232904
H 30.83215305 -3.15950052 -3.49070593
H 31.79263897 -3.67219546 -6.05570252
H 28.91173772 -3.21808036 -5.16844368
H 29.84460050 -4.70358580 -4.93012070
N 31.61471285 -1.61221805 -7.49283714
C 31.62667725 -0.47282199 -8.36952449
H 32.50774013 -2.07814804 -7.50439093
C 7.68471435 -15.96989805 -16.32764272
H 7.15410770 -16.35667439 -17.18644805
C 8.08536547 -16.77971068 -15.27354528
H 7.87951488 -17.84269107 -15.29525238
C 8.76398032 -16.16023852 -14.22394487
H 9.13719193 -16.70956087 -13.37949096
C 8.96795810 -14.78789153 -14.25756802
H 9.51947526 -14.32007988 -13.44624653
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C 7.90434255 -14.60670895 -16.26092031
C 7.40277191 -13.75597248 -17.36064833
C 7.51273934 -14.18908385 -18.69887828
C 6.99604958 -13.35966213 -19.69944024
C 6.38256285 -12.14413535 -19.41833831
H 5.99881512 -11.56548972 -20.24337581
F 7.06727109 -13.73808013 -21.00009127
H 8.02334834 -15.12779879 -18.92749323
C 6.81114471 -12.53265474 -17.04978993
H 6.76851441 -12.25637067 -16.00218431
C 6.25366979 -11.75970980 -18.06547028
C 5.44751656 -10.58564582 -17.68069822
O 5.66404679 -9.85659889 -16.71829348
N 4.36683542 -10.34635916 -18.52338226
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N 3.45262550 -9.37030267 -18.22558534
H 3.22503624 -9.29878698 -17.23684728
S 3.58947211 -7.95387617 -19.07196456
O 4.94973632 -7.54928880 -19.43317752
O 2.79013509 -6.93641528 -18.38734715
C 2.76480010 -8.40178718 -20.67371982
C 1.61023973 -7.69366092 -21.07283464
H 1.12549317 -7.00306885 -20.38688654
C 1.04346529 -7.92939116 -22.33799107
H 0.11433345 -7.44678299 -22.62354314
C 1.63106192 -8.85382811 -23.20497409
H 1.20464923 -9.06766148 -24.18381427
C 2.80019921 -9.51607479 -22.84510920
H 3.29876691 -10.19849095 -23.53263587
C 3.35202423 -9.29646620 -21.58052432
F 4.52253467 -9.93848673 -21.27580296
Zn 28.07147894 -6.23697008 -6.91430175

**2C-QM/MM R1b (2C-B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_a=1.0$**

C 21.94153684 -10.35320693 -4.21756948
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O 21.40914360 -8.00855989 -4.34590485
N 23.53342678 -8.67456013 -4.80286262
C 23.91777213 -7.39549912 -5.39944653
C 23.07838414 -7.23967113 -6.68185299
O 23.14740770 -8.09274325 -7.56836132
C 25.40288719 -7.39172046 -5.85119977
S 25.82725919 -5.73133967 -6.51897700
H 24.09428878 -9.49078397 -5.03708802
H 23.73028308 -6.59310961 -4.68088592
H 25.57082418 -8.16859346 -6.60377872
H 26.02153264 -7.63518097 -4.97798151
N 22.34896726 -6.11347621 -6.78402544
C 21.46105368 -5.93350598 -7.92167542
H 22.11944617 -5.57439277 -5.95523701
C 24.31761457 -4.87366287 -10.22317811
C 25.23736041 -5.94100951 -10.75872829
O 25.21322500 -6.17194809 -11.96300208
N 26.00206088 -6.60566837 -9.83397913
C 26.84957788 -7.68419968 -10.30219385
C 26.24295675 -9.08429002 -10.11502957
O 26.78125665 -10.10108675 -10.56210454
C 28.26509189 -7.61359530 -9.71993029
S 28.26876748 -8.15131350 -7.90527335
H 25.99378651 -6.30492145 -8.85643304
H 26.90204568 -7.55402063 -11.38859443
H 28.67643906 -6.60451782 -9.82941207
H 28.90484328 -8.30725562 -10.27369497
N 25.08353838 -9.12655179 -9.41709690
C 24.40735329 -10.41278517 -9.17857558
H 24.60230921 -8.31300549 -9.05751317
C 29.87723156 -4.49535641 2.80773540
C 30.09335957 -4.50221628 1.26996096
O 30.68908627 -3.63162195 0.67620185
N 29.50999256 -5.55356290 0.63950184
C 29.57428371 -5.64034596 -0.82487516
C 29.07007086 -4.34245774 -1.44581137
O 29.78978205 -3.74419167 -2.22531331
C 28.83267098 -6.87824669 -1.35197999
C 28.93281576 -6.97145764 -2.83856055
H 29.25179160 -7.77623199 -0.87494573
H 29.02070960 -6.27132070 1.16445235
H 30.62870145 -5.67197208 -1.11985138
H 27.77257179 -6.83854130 -1.06775663
C 28.12227099 -6.48772077 -3.83646170
H 30.88845178 -7.78512169 -3.02718673
H 27.19957211 -5.92453459 -3.77730644
C 29.79927591 -7.46275325 -4.82347147
N 30.00023736 -7.59574331 -3.48813182
N 28.65870257 -6.84759006 -5.03024310
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N 27.85132390 -3.88584304 -1.05100556
C 27.28140227 -2.64110886 -1.55452871
H 27.29099532 -4.40017163 -0.37356287
C 32.65969250 -1.85107410 -2.42408467
C 32.40712144 -1.95862993 -3.93732062
O 33.11350098 -1.40832313 -4.77956887
N 31.34502743 -2.71463971 -4.23852519
C 31.00038888 -3.05577505 -5.62086580
C 30.85377988 -1.74001722 -6.39664761
O 30.05064107 -0.90002179 -6.06352850

C	29.68875355	-3.85246734	-5.58802782	H	25.56710674	-8.17134488	-6.60187659
S	29.22360688	-4.40790256	-7.28946680	H	26.01855220	-7.63576913	-4.97594764
H	30.82404056	-3.14753004	-3.49328999	N	22.34926215	-6.11772076	-6.78325111
H	31.79333421	-3.67868385	-6.05354688	C	21.46107778	-5.93400548	-7.92160564
H	28.90599054	-3.21652519	-5.16174600	H	22.12661595	-5.57106475	-5.95434124
H	29.83660272	-4.70339492	-4.91735052	C	24.31697550	-4.87176880	-10.22349076
N	31.61777182	-1.61215246	-7.49366311	C	25.23891351	-5.94393673	-10.75987268
C	31.62683512	-0.47299928	-8.36903534	O	25.21526296	-6.17191167	-11.96039134
H	32.51991410	-2.06393278	-7.49896153	N	26.00353336	-6.60824076	-9.83591008
C	7.68332993	-15.97174981	-16.33122188	C	26.85061237	-7.68462313	-10.30002319
H	7.14982769	-16.35494452	-17.19101879	C	26.24407831	-9.08807467	-10.12101136
C	8.08064354	-16.78259614	-15.27785984	O	26.77853777	-10.10073378	-10.56549025
H	7.86918838	-17.84489098	-15.30123491	C	28.26205922	-7.62128201	-9.70281209
C	8.76172203	-16.16396061	-14.22800682	S	28.27180418	-8.17554679	-7.91605271
H	9.13650211	-16.71541053	-13.38591399	H	25.99209424	-6.31166646	-8.85359415
C	8.96702678	-14.79155597	-14.25823841	H	26.90487071	-7.55591419	-11.39133778
H	9.51927723	-14.32445097	-13.44713104	H	28.67533945	-6.60606167	-9.83434721
N	8.48486308	-13.97787309	-15.22478193	H	28.90467826	-8.30610450	-10.28426844
C	7.90697816	-14.60895147	-16.26033494	N	25.08690327	-9.12707435	-9.41800245
C	7.40510073	-13.75539083	-17.36061006	C	24.40777631	-10.41315851	-9.17868336
C	7.51726651	-14.19121360	-18.69863513	H	24.60255627	-8.31200184	-9.05747485
C	6.99729990	-13.36220487	-19.69815401	C	29.87705108	-4.49523112	2.80969280
C	6.38442861	-12.14623242	-19.41557371	C	30.09573656	-4.50004105	1.26721912
H	5.99878549	-11.56725043	-20.23926874	O	30.68892693	-3.63186490	0.67694100
F	7.06493418	-13.74088625	-20.99817065	N	29.51096325	-5.55040914	0.64057750
H	8.03122066	-15.13012989	-18.92706716	C	29.57219206	-5.63926260	-0.82056224
C	6.81310529	-12.53210898	-17.04725107	C	29.07345689	-4.34011494	-1.44669622
H	6.77150253	-12.25813190	-15.99812263	O	29.78956844	-3.74506925	-2.22598485
C	6.25456578	-11.75932134	-18.06293531	C	28.83558230	-6.87371900	-1.34980388
C	5.44520963	-10.58732458	-17.67856141	C	28.93529031	-6.97378027	-2.83321706
O	5.65577097	-9.86225190	-16.71080406	H	29.25599307	-7.77478906	-0.86911282
N	4.37097918	-10.33965810	-18.53158030	H	29.02120446	-6.26926270	1.16829047
H	3.98660573	-11.07775991	-19.12895437	H	30.63189261	-5.67162151	-1.11854870
N	3.45543884	-9.36754320	-18.22268146	H	27.77318554	-6.83628673	-1.06419559
H	3.23843607	-9.28920835	-17.23052379	C	28.12832077	-6.49751914	-3.83508693
S	3.58856762	-7.95218915	-19.07068835	H	30.89402783	-7.78546873	-3.02075629
O	4.95011461	-7.55298709	-19.43530274	H	27.19986696	-5.92897142	-3.77422823
O	2.78859080	-6.93435894	-18.38670917	C	29.79003083	-7.46374073	-4.81824750
C	2.76206430	-8.40221895	-20.67186151	N	30.00618407	-7.59829614	-3.48142016
C	1.60555054	-7.69232510	-21.07255243	N	28.66938610	-6.86180680	-5.02281850
H	1.11793504	-7.00278980	-20.38486395	H	30.45536019	-7.83083373	-5.60467344
C	1.03976770	-7.93134877	-22.33892121	N	27.85496631	-3.88571094	-1.05177038
H	0.10599404	-7.45714708	-22.62271565	C	27.28090200	-2.64052465	-1.55529056
C	1.62948984	-8.85573117	-23.20665591	H	27.29304673	-4.40216641	-0.37312482
H	1.20219583	-9.07617849	-24.18419817	C	32.66085911	-1.85121830	-2.42163830
C	2.80094016	-9.51517090	-22.84848521	C	32.40688180	-1.95887349	-3.93921789
H	3.30300783	-10.19877379	-23.53506603	O	33.10972177	-1.41031308	-4.77826264
C	3.35016717	-9.29503611	-21.58164535	N	31.34554339	-2.71637518	-4.23798560
F	4.52148162	-9.93805435	-21.27856923	C	30.99874808	-3.05077710	-5.61423331
Zn	28.07125793	-6.23642753	-6.91435390	C	30.85402125	-1.73522569	-6.39420581
				O	30.05468585	-0.89684033	-6.06054019
				C	29.69000357	-3.85447573	-5.60957038
				S	29.23614043	-4.38821137	-7.30051318
				H	30.82119323	-3.15160925	-3.49047231
				H	31.79666326	-3.67469621	-6.05392230
				H	28.90849768	-3.21442129	-5.16093527
				H	29.84045080	-4.70138039	-4.92051548
				N	31.61655780	-1.61027503	-7.48996139
				C	31.62695260	-0.47130737	-8.37094229
				H	32.51569234	-2.06849007	-7.50289230
				C	7.68376341	-15.97129562	-16.33049861
				H	7.15068171	-16.35532479	-17.18984958
				C	8.08173986	-16.78194089	-15.27686254
				H	7.87139376	-17.84440438	-15.29987505
				C	8.76216096	-16.16320436	-14.22708814

2C-WF-in-DFT/MM R1b (2C-CCSD-in-B3LYP/6-31G(d):Amber) mechanical embedding $\omega_c=1.0$

C	21.94185129	-10.35473871	-4.21709651
C	22.25555358	-8.88196799	-4.43220532
O	21.41091266	-8.01019941	-4.34629469
N	23.53226225	-8.67376975	-4.80590608
C	23.91733414	-7.40137134	-5.40033495
C	23.07775355	-7.24204234	-6.68506926
O	23.14765101	-8.09151013	-7.56757283
C	25.40208560	-7.37640936	-5.85766426
S	25.81557519	-5.72671803	-6.51801373
H	24.09663836	-9.49165726	-5.03460135
H	23.72588269	-6.59221213	-4.68144432

H	9.13603244	-16.71415581	-13.38417633	C	23.61504559	-0.90589461	-7.65656323
C	8.96706886	-14.79096673	-14.25813471	C	22.68293059	-0.30360269	-8.52648393
H	9.51891234	-14.32357359	-13.44669215	O	22.03722728	0.81740117	-8.13444581
N	8.48535396	-13.97782179	-15.22499822	H	23.65860063	-4.53984485	-11.08461328
C	7.90630014	-14.60843707	-16.26054549	H	21.79883969	-0.33076982	-10.50187088
C	7.40468077	-13.75545198	-17.36071873	H	23.73389609	-0.52787759	-6.65594680
C	7.51615589	-14.19079303	-18.69874111	H	23.88872583	-5.26493966	-8.20580832
C	6.99693550	-13.36171449	-19.69850515	H	25.15943199	-2.39786053	-7.45528482
C	6.38401312	-12.14574173	-19.41625649	H	23.17187580	-2.24797479	-11.30803718
H	5.99851919	-11.56700825	-20.24022991	H	25.66635519	-3.26926047	-10.79950016
F	7.06523294	-13.74042531	-20.99858470	H	25.84560186	-3.83784549	-9.14038443
H	8.02914962	-15.12973010	-18.92720127	H	22.55067608	1.60070308	-8.35330727
C	6.81274145	-12.53221530	-17.04794801	N	25.98348437	-6.56970431	-9.84417904
H	6.77048082	-12.25791304	-15.99911553	C	26.81962769	-7.66345588	-10.29663846
C	6.25410448	-11.75956249	-18.06353925	C	26.20984309	-9.05933626	-10.10766651
C	5.44527978	-10.58722388	-17.67922779	O	26.75801753	-10.06859071	-10.55840420
O	5.65779485	-9.86100420	-16.71252316	C	28.23486554	-7.60446985	-9.71669915
N	4.37028002	-10.34098591	-18.52944449	S	28.27225437	-8.15048248	-7.90687533
H	3.98866564	-11.07916257	-19.12945383	H	25.96762231	-6.27305229	-8.86596570
N	3.45474571	-9.36822212	-18.22350654	H	26.88897391	-7.54305731	-11.38267681
H	3.23483793	-9.29160455	-17.23192864	H	28.64325536	-6.59629322	-9.83105108
S	3.58873962	-7.95253985	-19.07111799	H	28.86208532	-8.29707875	-10.28426067
O	4.95014540	-7.55231270	-19.43490435	N	25.04175885	-9.10837517	-9.41736236
O	2.78868469	-6.93510111	-18.38660357	C	24.38128432	-10.40554587	-9.16695514
C	2.76249322	-8.40217109	-20.67233069	C	25.18683591	-11.37176245	-8.29442724
C	1.60662467	-7.69259770	-21.07266538	O	24.80718774	-12.54541311	-8.15497978
H	1.11952479	-7.00292475	-20.38537045	C	23.86808066	-11.08723596	-10.46770206
C	1.04064599	-7.93081244	-22.33873341	C	22.93819424	-10.17336486	-11.29132315
H	0.10780722	-7.45476260	-22.62285431	C	22.44705973	-10.93778457	-12.53410135
C	1.62954188	-8.85542092	-23.20612816	C	21.68893462	-9.77798062	-10.49510874
H	1.20257512	-9.07423843	-24.18405232	H	21.98223438	-9.14621675	-9.66069786
C	2.80059641	-9.51547402	-22.84766239	H	21.01863599	-9.20689064	-11.12825394
H	3.30180755	-10.19877890	-23.53448864	H	21.19600692	-10.67246551	-10.11914525
C	3.35031194	-9.29554201	-21.58137957	H	24.58912316	-8.30150254	-9.00747738
F	4.52175309	-9.93819659	-21.27784714	H	21.91042876	-11.83311104	-12.22585657
Zn	28.07258036	-6.23429361	-6.91766063	H	21.80403793	-10.29720830	-13.13203163

**1C QM/MM R2b (B3LYP/6-31G(d):Amber)
mechanical embedding $\omega_c=1.0$**

C	21.94185370	-10.35375643	-4.21758034	H	23.31276020	-11.98656806	-10.20124091
C	22.25696289	-8.88934834	-4.43527578	H	24.70709066	-11.38812897	-11.09250861
O	21.40814789	-8.01462162	-4.35628552	N	26.24831828	-10.89165072	-7.62177712
N	23.53407859	-8.67720612	-4.80583719	C	26.88622675	-11.71893248	-6.58639583
C	23.91686267	-7.39692789	-5.39949079	C	25.84788684	-12.11724484	-5.51134447
C	23.08386511	-7.24132542	-6.68510190	O	25.16897360	-11.25053858	-4.97586041
O	23.15089081	-8.09656849	-7.56893949	C	28.05644214	-10.95830957	-5.96085620
C	25.39924974	-7.38485628	-5.83625718	C	28.69082389	-11.80326864	-4.85404526
S	25.83105628	-5.73362717	-6.51267081	C	29.96927174	-11.13052878	-4.32209735
H	24.12034945	-9.48956991	-4.98588720	C	30.38085379	-11.86240762	-3.02790092
H	23.72111774	-6.59673785	-4.68245718	N	31.80610665	-11.67057308	-2.74469226
H	25.56752469	-8.17053103	-6.57702437	H	27.24351936	-12.62864755	-7.07389283
H	26.00870941	-7.61944836	-4.95414607	H	29.77393661	-11.48397910	-2.19866754
N	22.35367944	-6.11685816	-6.78747870	H	30.17326171	-12.92856180	-3.15388870
C	21.46377060	-5.93668491	-7.92132242	H	27.98266447	-11.88670290	-4.02951016
H	22.15221446	-5.55452475	-5.96619203	H	28.93002378	-12.80057688	-5.22372107
N	23.48148494	-5.22794029	-9.13438795	H	32.11917786	-12.30273642	-2.02164879
C	24.31277337	-4.81369759	-10.25508263	H	32.37274179	-11.87615391	-3.56978921
C	25.22365277	-5.90330681	-10.77104221	H	31.99120597	-10.72182357	-2.42818052
O	25.20205221	-6.14820013	-11.97321694	H	29.77458512	-10.08456879	-4.10755726
C	25.11800409	-3.59133269	-9.91476130	H	30.74039753	-11.21960372	-5.08889621
C	24.27374958	-2.43586398	-9.44694650	H	26.57113918	-9.95145373	-7.83401370
C	23.30924557	-1.86501877	-10.30510301	H	27.71745696	-10.00358137	-5.55523733
C	24.42356024	-1.95871033	-8.11571697	H	28.81078838	-10.77595666	-6.72817050
C	22.52674618	-0.78103108	-9.84954406	C	29.87489511	-4.49593270	2.80736160
				C	30.09415344	-4.49804838	1.27254654

O	30.68696542	-3.62588968	0.67779277	C	11.07361451	-16.71311541	-10.94584060
N	29.50965901	-5.54749776	0.64277706	C	11.56639914	-15.91713654	-9.75917968
C	29.57843303	-5.62600211	-0.81879431	C	10.78894956	-15.86300028	-8.57596983
C	29.07135609	-4.33202110	-1.44024929	C	12.82727089	-15.28884451	-9.81642372
O	29.77693791	-3.73896354	-2.23788717	C	11.29421039	-15.17631317	-7.45686208
C	28.83931621	-6.85830790	-1.35152019	C	13.32284986	-14.61632935	-8.68702385
C	28.94062805	-6.96321030	-2.83174642	C	12.55681128	-14.56027455	-7.50109437
H	29.26208194	-7.75108993	-0.87361100	H	12.96071523	-14.06999166	-6.62891911
H	29.01240745	-6.25856079	1.17083538	H	10.35764018	-18.45096740	-9.98154764
H	30.63249888	-5.66597103	-1.11131096	H	10.71813206	-15.15712619	-6.55893682
H	27.78176048	-6.81180607	-1.07079808	H	14.30638431	-14.17451728	-8.73229927
C	28.13288527	-6.49345149	-3.83581614	H	13.25836434	-18.48601571	-10.69909219
H	30.89400612	-7.79190591	-3.00585136	H	13.43204069	-15.36853688	-10.70938691
H	27.20648040	-5.94136123	-3.77384354	H	9.83495702	-16.36871203	-8.52512683
C	29.81914137	-7.45661885	-4.80680595	H	10.04201541	-16.42311695	-11.14127641
N	30.01313083	-7.58102643	-3.47202000	H	11.67757429	-16.46239672	-11.81735731
N	28.67612711	-6.85041124	-5.02662322	N	11.58568355	-19.96978811	-12.34907685
H	30.48615239	-7.82032197	-5.57520456	C	11.29505474	-20.76625973	-13.52715536
N	27.85276465	-3.88163713	-1.04379781	C	11.29036576	-22.22512809	-13.16845670
C	27.28106579	-2.64032827	-1.55445441	O	12.20190186	-22.69969467	-12.49485753
H	27.30492799	-4.38274257	-0.34581991	C	12.30752384	-20.45804361	-14.64391354
C	32.66053881	-1.85303693	-2.42403705	C	12.26027669	-19.00472263	-15.11232690
C	32.40925740	-1.96050996	-3.93706992	C	13.35059516	-18.85861541	-16.17223733
O	33.09520487	-1.38501429	-4.77830458	C	10.90213942	-18.65414935	-15.72868935
N	31.36623155	-2.74272114	-4.23979597	H	10.12406428	-18.73932336	-14.98090854
C	31.00878674	-3.06375316	-5.62442637	H	10.93427459	-17.63382157	-16.09904965
C	30.85333419	-1.74351928	-6.39154694	H	10.68948894	-19.34245659	-16.54625032
O	30.03853419	-0.91308812	-6.05909226	H	12.43567919	-20.16986470	-11.84257455
C	29.69905117	-3.85643357	-5.59276770	H	13.19852908	-19.57066379	-16.98434023
S	29.20191732	-4.39360050	-7.28668304	H	13.33880664	-17.86869845	-16.59793625
H	30.87001972	-3.19950236	-3.48935233	H	14.32483566	-19.03765018	-15.71954902
H	31.79468497	-3.68317354	-6.07137698	H	10.29905216	-20.55057395	-13.90896427
H	28.92719723	-3.22507156	-5.14525224	H	12.45962127	-18.31974003	-14.29260754
H	29.85963859	-4.71730957	-4.93970252	H	12.09594111	-21.11086096	-15.48932267
N	31.61272302	-1.61232493	-7.49231817	H	13.31045951	-20.68769685	-14.28256763
C	31.62447834	-0.47262436	-8.36740246	N	12.73499080	-16.67201117	-20.52173198
H	32.50902944	-2.07135369	-7.50536975	C	12.40760054	-15.28580098	-20.25338338
N	30.17010424	-1.81923390	-9.80822218	C	11.78577170	-15.20822118	-18.84309442
C	29.15725419	-2.01665589	-10.85173943	O	10.93985854	-16.03451039	-18.46242709
C	27.91548368	-1.19912669	-10.53119935	C	11.50261339	-14.71445891	-21.35995826
O	27.43083833	-1.14614031	-9.39992206	C	11.22067478	-13.24251125	-21.07790389
C	28.79468333	-3.49105999	-10.97855124	C	10.20703168	-15.53647186	-21.51605747
C	29.86281642	-4.33665491	-11.57226262	C	10.56125552	-12.50909971	-22.23538632
C	31.20444359	-4.21339382	-11.41577397	H	13.32714587	-14.70227996	-20.24401731
C	29.66911260	-5.47526812	-12.44893406	H	9.64004869	-15.15816609	-22.36265343
N	31.84688185	-5.18175898	-12.15429520	H	10.44496466	-16.57776710	-21.72003209
C	30.94863917	-6.04055267	-12.73603856	H	12.05436980	-14.77127891	-22.29704074
C	28.53623564	-6.13937431	-12.95738310	H	10.56268699	-13.16476583	-20.21208106
C	31.09788231	-7.24770374	-13.43016060	H	12.15163116	-12.73141376	-20.84200841
C	28.67705140	-7.37861478	-13.60216570	H	9.59101895	-12.95002947	-22.45497249
C	29.94242996	-7.93389600	-13.85131570	H	12.07715995	-17.38200619	-20.24471693
H	30.02225164	-8.86752385	-14.37952829	H	10.41555082	-11.46913732	-21.95498904
H	29.56068829	-1.68173565	-11.80851328	H	9.60440266	-15.45434412	-20.61671955
H	32.84768569	-5.27679018	-12.23598454	H	11.20054746	-12.56806481	-23.11613971
H	27.55469814	-5.72232396	-12.78971981	N	12.21812264	-14.23116716	-18.05994875
H	27.79076417	-7.89908429	-13.89986369	C	11.97525726	-14.15540794	-16.60468234
H	32.08499029	-7.62868025	-13.62560187	C	11.95407548	-12.70222141	-16.25936692
H	31.71325029	-3.46393538	-10.82763654	O	12.91380959	-11.98986933	-16.52778926
H	30.29476500	-2.54850918	-9.11588390	C	13.04166142	-14.90332240	-15.81592204
H	27.92633106	-3.57633327	-11.63273046	C	12.69370310	-15.12689146	-14.29871607
H	28.51902551	-3.90063673	-10.00939961	S	12.78161151	-13.59809163	-13.35644138
N	12.42974512	-18.59710066	-10.12393062	C	14.53700086	-13.19387336	-13.55666399
C	11.14127630	-18.21542252	-10.69896756	H	11.68625418	-15.53197403	-14.23391276
C	10.77937988	-19.00140916	-11.94208747	H	14.87526996	-12.56913195	-12.73153687
O	9.70889400	-18.78179359	-12.49491685	H	15.11976218	-14.11486581	-13.56806303

H	14.69593844	-12.66675494	-14.49619981	H	1.45578816	-7.91781873	-13.46031193
H	13.19795584	-15.86526200	-16.27378782	N	3.56281979	-5.58472693	-15.80164174
H	13.38746779	-15.85303665	-13.87441620	C	3.69327280	-4.10683217	-15.85992881
H	12.92407719	-13.60981440	-18.45721525	C	4.27399449	-3.60784403	-17.18163877
H	11.00712295	-14.60192812	-16.37911011	O	4.54216552	-2.42514705	-17.34186641
H	13.97581807	-14.35554297	-15.88905457	C	4.49919818	-3.60034676	-14.66481468
N	10.81793951	-12.23356661	-15.74240586	C	3.65341214	-3.49978826	-13.39826272
C	10.67102565	-10.88752187	-15.17679158	C	4.54629569	-3.66330520	-12.17411190
C	10.54232506	-11.07342000	-13.64866289	N	3.84597655	-3.23143455	-10.94590112
O	9.78917672	-11.92449206	-13.16519045	C	3.42031588	-4.02503538	-9.97360917
C	9.41982193	-10.20319059	-15.73009603	N	3.48402304	-5.31828295	-10.08999056
C	9.40214460	-10.10867868	-17.27662732	N	2.92657905	-3.54639375	-8.86679113
C	9.20992347	-8.80744972	-15.11319156	H	2.87668891	-4.26177949	-13.37667249
C	10.51276591	-9.18456742	-17.77812340	H	2.70806635	-3.64478862	-15.78241365
H	11.54490748	-10.27284495	-15.39074562	H	3.76819747	-2.23881110	-10.80033702
H	8.33307525	-8.33175324	-15.54382558	H	3.17958448	-2.51506219	-13.37203706
H	9.05404619	-8.90783115	-14.04306969	H	2.68816838	-4.18303532	-8.13031757
H	8.56289369	-10.81239796	-15.45191908	H	2.84611231	-2.55571808	-8.73719798
H	9.52334691	-11.09738976	-17.71689229	H	4.37499320	-6.16639818	-15.9791519
H	8.43963906	-9.70889761	-17.58233281	H	5.44676612	-3.05793848	-12.29010350
H	11.48288073	-9.55928254	-17.45695206	H	4.86089293	-4.70655269	-12.11674565
H	10.06216877	-12.88613419	-15.58847918	H	3.26128143	-5.97739826	-9.36461462
H	10.50844837	-9.17460105	-18.86217151	H	3.93685428	-5.66746078	-10.91326889
H	10.08947391	-8.18167805	-15.26497053	H	4.90205079	-2.60696475	-14.87536174
H	10.37643886	-8.16619624	-17.42373093	H	5.34172918	-4.26416074	-14.49434780
N	6.48738439	-7.95818863	-12.67390151	N	4.32187670	-4.47063143	-18.19849096
C	5.62339941	-8.75768482	-13.49936091	C	4.77966197	-4.10399109	-19.54682314
C	4.31779590	-8.00023380	-13.75838654	C	6.24960274	-4.45186587	-19.85933055
O	3.89612963	-7.17792983	-12.92793768	O	6.61335852	-4.43814196	-21.04609736
C	5.35447559	-10.11724691	-12.88168198	H	4.08123785	-5.43270161	-17.98791518
C	6.62576895	-10.97924245	-12.89847652	H	4.16985949	-4.63952745	-20.27083977
C	6.39813630	-12.31569482	-12.27685706	H	4.66265759	-3.03097241	-19.70665590
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H	6.12345206	-8.90510844	-14.45576559	C	8.45848626	-5.17372018	-16.398374119
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H	6.76696138	-8.28545968	-11.75772673	O	9.39640569	-6.54682244	-20.67146567
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O	1.41603433	-5.61712309	-15.17150176	H	10.54536220	-0.83868697	-16.60425748
C	1.31455395	-8.29494962	-14.47459150	H	7.32062516	-2.49664489	-14.29584322
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C	-0.65680304	-12.58790588	-14.07780456	H	10.19676324	-5.48339845	-17.78120448
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H	1.14114717	-10.21525621	-15.44393720	O	7.96115281	-9.20254183	-22.45708731
H	-1.06176089	-14.56306216	-14.36742325	H	7.17865741	-7.34537944	-18.61152423
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H	-0.85212487	-9.91917685	-14.03462734	N	6.44207078	-7.63788252	-21.83590338
H	0.15561502	-9.78478203	-12.59574714	C	5.94455227	-7.32897024	-23.17823884
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C	2.90441417 -5.19015094 -24.25040787	H	4.84486871 -16.02499600 -16.13106532
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H	5.67616011 -8.25616425 -23.69105294	H	5.07780954 -17.42833688 -18.48505968
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H	6.02459421 -7.20865428 -21.02079215	C	2.48827486 -13.18498145 -23.68937319
H	3.23543137 -4.28677654 -23.73931968	O	2.29844243 -12.21294026 -24.39529672
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H	-0.25272025 -2.99658037 -24.49782697	O	3.32645072 -12.59537310 -19.99740503
H	0.75442402 -4.15841915 -23.63884437	H	2.09529793 -14.85334851 -21.00819750
H	5.00542959 -5.45691552 -22.64300158	H	1.58731851 -12.19392423 -22.00433875
H	3.96567127 -6.85817162 -22.50785987	H	4.09415301 -12.01156132 -21.88121973
N	9.62219680 -9.43434783 -24.97407583	H	4.19573157 -13.71437807 -21.52508632
C	9.06979610 -10.22008463 -26.09608305	H	3.21959630 -13.49121567 -19.61095198
C	9.19801828 -9.39882958 -27.38974852	N	-1.00993012 -13.04449886 -25.46453089
O	9.78390577 -9.85295166 -28.34603147	C	-1.45158940 -11.65340688 -25.47120248
C	7.61650672 -10.68935178 -25.84160704	C	-0.64176923 -10.82937604 -26.47384719
C	7.56632341 -11.67276476 -24.66054531	O	-1.20155169 -9.99563650 -27.18895200
C	7.08807924 -11.40136237 -27.09286640	H	-0.54513310 -13.44222283 -24.66242186
C	6.15458336 -11.87954217 -24.12406165	H	-2.49639766 -11.61737287 -25.78714574
H	9.68470050 -11.11305661 -26.22553620	N	0.69539976 -10.98479622 -26.47253003
H	6.07055641 -11.74835637 -26.93495470	C	1.56590737 -10.21488499 -27.36273996
H	7.06995652 -10.72194897 -27.94253378	C	1.20583869 -10.53049722 -28.83231993
H	6.99663067 -9.81813721 -25.62485157	O	0.99779932 -9.59955928 -29.59921389
H	7.99848019 -12.62476995 -24.96081468	C	3.06543417 -10.48265270 -27.08732711
H	8.17209485 -11.29542498 -23.84134355	C	3.96133796 -9.89933499 -28.17063110
H	5.54577723 -12.35000580 -24.89395887	C	4.27708215 -8.53098257 -28.14410573
H	9.04764597 -9.21643843 -24.17220098	C	4.35810997 -10.70701501 -29.25314011
H	6.20083366 -12.54047031 -23.26382820	C	5.10635168 -7.99683222 -29.14074395
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H	5.71862771 -10.92247115 -23.84580488	C	5.58832262 -8.83735894 -30.16939389
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C	4.59081648 -20.55526849 -18.29800609	H	5.42763154 -6.97193425 -29.10914430
O	4.09286429 -20.16362222 -19.38020378	H	5.54981726 -10.78874867 -31.08031655
C	6.83389423 -19.84386677 -17.38812770	H	1.12253656 -11.68420057 -25.87569854
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**2C-QM/MM R2b (2C-B3LYP/6-31G(d):Amber)
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H	29.81436390	-10.10511127	-4.19279059	H	30.34252891	-2.54781161	-9.11761592
H	30.71708538	-11.35770294	-5.09174558	H	27.95110848	-3.56904566	-11.63837814
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C	3.06832312	-16.44839458	-17.24979172	C	8.05328423	-16.77143694	-15.29657248
C	3.61329077	-16.06398765	-18.63224475	H	7.84081715	-17.83086140	-15.31300614
O	3.10680290	-15.14115542	-19.28858442	C	8.75835749	-16.17361678	-14.25706736

H	9.13806210 -16.75275487 -13.44135991	C	22.27484563 -8.92226598 -4.43701792
C	8.98540777 -14.80742960 -14.28438494	O	21.41898472 -8.05412142 -4.32981081
H	9.56433152 -14.33783913 -13.50038976	N	23.54490886 -8.68977876 -4.81724373
N	8.51242270 -13.99043779 -15.24272096	C	23.90497039 -7.40225217 -5.40690613
C	7.90240108 -14.60637538 -16.26586258	C	23.07432975 -7.24325915 -6.69717227
C	7.41565807 -13.75770558 -17.34362203	O	23.13578968 -8.10267385 -7.58070980
C	7.54813520 -14.17184235 -18.67550402	C	25.39039227 -7.37905919 -5.84903155
C	7.01666499 -13.36187750 -19.67011070	S	25.83087033 -5.72561906 -6.51896265
C	6.38632232 -12.16670547 -19.36138427	H	24.10611457 -9.49243194 -5.08961625
H	5.97958017 -11.56248490 -20.14319321	H	23.70013683 -6.60603809 -4.69039038
F	7.08852127 -13.74690264 -20.96608018	H	25.54964914 -8.15480546 -6.60033714
H	8.08334488 -15.08238797 -18.91340512	H	26.01258191 -7.62465751 -4.98145484
C	6.78499382 -12.57019578 -17.00900378	N	22.34659427 -6.11679007 -6.81293970
H	6.65170410 -12.33511794 -15.96739313	H	22.16348303 -5.56719052 -5.97725226
C	6.23109319 -11.79494338 -18.01440709	C	25.22419259 -5.94081586 -10.77059107
C	5.42568280 -10.59895420 -17.65483434	O	25.26245552 -6.14288986 -11.98457208
O	5.67610766 -9.85744310 -16.70857147	N	25.98744748 -6.62061454 -9.84687074
N	4.32962863 -10.33202623 -18.46892061	C	26.82314846 -7.71684737 -10.30136369
H	3.94407126 -11.01818728 -19.12399327	C	26.20781588 -9.11701122 -10.09205231
N	3.41268009 -9.30802572 -18.18560305	O	26.73237025 -10.13484507 -10.55818589
H	3.47759669 -9.05389800 -17.19802990	C	28.24087133 -7.63563001 -9.73058277
S	3.58389557 -7.91994044 -19.09890586	S	28.27386602 -8.15001739 -7.91298948
O	4.97428237 -7.57461518 -19.41224764	H	25.92791166 -6.37156873 -8.85560390
O	2.78334698 -6.86285749 -18.45838153	H	26.88983669 -7.60443740 -11.38693262
C	2.75231356 -8.36984986 -20.70842111	H	28.64584047 -6.63005567 -9.85113885
C	1.59005901 -7.68877240 -21.10584664	H	28.87947837 -8.33372439 -10.27496178
H	1.09925330 -7.00923570 -20.42353182	N	25.06542222 -9.15793989 -9.35987174
C	1.02234547 -7.96153775 -22.35648635	H	24.60023019 -8.32974708 -9.01586894
H	0.08074956 -7.51493280 -22.63818210	C	30.09957728 -4.47253265 1.29410590
C	1.61161910 -8.89047005 -23.20946753	O	30.69758479 -3.61022227 0.69277879
H	1.15837920 -9.13437017 -24.16627078	N	29.51142437 -5.52465724 0.65899723
C	2.79233421 -9.52557972 -22.85363897	C	29.56975929 -5.60871973 -0.80797718
H	3.28686398 -10.21845518 -23.52640328	C	29.06326230 -4.31812808 -1.44803172
C	3.34331792 -9.27232915 -21.60084474	O	29.78857327 -3.72665374 -2.22669439
F	4.51493068 -9.90438495 -21.27942875	C	28.83544843 -6.85206758 -1.33207342
Zn	28.07230211 -6.23863472 -6.91176801	C	28.93683844 -6.96747271 -2.81522515
O	-2.02926157 -5.78114103 -23.88547456	H	29.25983452 -7.73813842 -0.83950145
H	-2.87411954 -5.34636510 -23.65829683	H	29.01847050 -6.24257532 1.18112364
H	-2.03688759 -6.53875609 -23.30051002	H	30.61992502 -5.65371920 -1.11078122
O	7.30982453 -19.76597207 -13.49803681	H	27.78021439 -6.81587064 -1.04690303
H	8.19338840 -19.43788431 -13.24998837	C	28.14607735 -6.48913481 -3.83195190
H	7.27623060 -20.62997438 -13.07204287	H	30.89642888 -7.79297044 -2.98684830
O	9.13910144 -17.86134361 -18.99294155	H	27.22490503 -5.92998668 -3.78734207
H	9.88288929 -17.28788272 -18.71466321	C	29.81277837 -7.49604652 -4.79902130
H	9.50008309 -18.34921432 -19.73754749	N	29.99912396 -7.63573302 -3.44956499
O	5.97571714 -7.04440088 -16.78762548	N	28.68462521 -6.85940272 -5.01801270
H	6.41721261 -6.77013845 -15.96143335	H	30.46205236 -7.88567542 -5.56921301
H	6.20839505 -7.98044699 -16.86168025	N	27.83944663 -3.85833922 -1.07199100
O	26.46596446 -0.95621527 -4.84736431	H	27.27116835 -4.37697892 -0.40390902
H	27.13195739 -0.86675617 -4.15259835	C	32.41852766 -1.93865759 -3.92514332
H	26.59955286 -1.84471639 -5.18853373	O	33.11555639 -1.37701699 -4.76125953
O	0.72643947 -9.98511228 -18.10446721	N	31.35495812 -2.70315290 -4.23901115
H	-0.04964111 -10.47356391 -18.45822506	C	30.99693344 -3.04312847 -5.62527266
H	1.44127990 -10.26944985 -18.67871309	C	30.84501959 -1.73116174 -6.40876463
O	4.77996249 -18.65505289 -14.46165944	O	30.09822587 -0.85070778 -6.04908317
H	5.69295239 -18.95023299 -14.29038808	C	29.69412668 -3.84623710 -5.59608986
H	4.27769995 -19.18079025 -13.83123476	S	29.21630693 -4.40597635 -7.29410108
O	-0.39396870 -6.77788977 -25.72226987	H	30.86238817 -3.17166571 -3.49505593
H	-0.85427526 -7.39842631 -26.29750220	H	31.79072673 -3.66225461 -6.05856899
H	-1.09708092 -6.40096866 -25.16396787	H	28.91429454 -3.21893424 -5.16314277
		H	29.85516378 -4.70255034 -4.93678029
		N	31.59025076 -1.59516201 -7.51311181
		H	32.08605064 -2.38990395 -7.85735911
		C	7.68142283 -15.97792447 -16.32942998
		H	7.15826662 -16.37298690 -17.19119503

1C QM/SE/MM R1b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.0$

C	8.08071707 -16.79025954 -15.28073365	S	28.27466540 -8.14957189 -7.91097628
H	7.87317228 -17.85203503 -15.29812842	H	25.93313152 -6.37121826 -8.85207215
C	8.76398552 -16.19630507 -14.21112000	H	26.88516531 -7.60047230 -11.38746127
H	9.13112636 -16.79884199 -13.39273539	H	28.64784905 -6.62031570 -9.84589060
C	8.98628502 -14.82443997 -14.24352691	H	28.88864589 -8.32398376 -10.27593806
H	9.54323093 -14.33359934 -13.44925336	N	25.06417517 -9.15659231 -9.35856702
N	8.51825819 -14.00026621 -15.21494348	H	24.59457749 -8.32960501 -9.01713533
C	7.90572311 -14.60649633 -16.26009979	C	30.09921506 -4.47413760 1.29410880
C	7.40856549 -13.75168837 -17.34770666	O	30.69465478 -3.61162237 0.69073819
C	7.49772254 -14.19550789 -18.70017988	N	29.51154596 -5.52697081 0.66026147
C	6.97860420 -13.35107346 -19.68998706	C	29.56710440 -5.61212210 -0.80616548
C	6.37130981 -12.13927307 -19.41831128	C	29.06020590 -4.32215233 -1.44597827
H	6.00833917 -11.54408945 -20.23772479	O	29.78986158 -3.73274886 -2.22259449
F	7.05904083 -13.73564954 -20.99990650	C	28.83152352 -6.85646307 -1.33130659
H	8.01541241 -15.12784299 -18.92717909	C	28.93028074 -6.96264399 -2.81559709
C	6.84243681 -12.52328253 -17.03971404	H	29.25441886 -7.74965919 -0.84583792
H	6.80622865 -12.23929870 -15.99238810	H	29.01589003 -6.24486665 1.17910821
C	6.26117880 -11.73280922 -18.04209496	H	30.61943999 -5.64555556 -1.11006753
C	5.46124603 -10.59075302 -17.66979585	H	27.77264716 -6.82394094 -1.04706935
O	5.65278610 -9.83206485 -16.66988328	C	28.13799251 -6.47412173 -3.82707334
N	4.39420576 -10.34681112 -18.53799961	H	30.88473102 -7.80260904 -2.99757175
H	4.00149754 -11.09781362 -19.09932164	H	27.22217490 -5.90085119 -3.77769048
N	3.46918520 -9.36836875 -18.22665610	C	29.79431103 -7.49216062 -4.80507478
H	3.46756529 -9.17500617 -17.22256724	N	29.98703664 -7.63600748 -3.45631310
S	3.61584822 -7.95335808 -19.09423347	N	28.66996622 -6.84695020 -5.01513673
O	5.00063123 -7.52216306 -19.42904790	H	30.43368768 -7.88643162 -5.58453326
O	2.83529196 -6.92679238 -18.37139492	N	27.83697533 -3.85952123 -1.07140162
C	2.79581191 -8.38546127 -20.64394101	H	27.26639620 -4.37530780 -0.40301778
C	1.63077178 -7.65113350 -21.04193172	C	32.41949790 -1.93727423 -3.92579588
H	1.17172651 -6.95461790 -20.34728747	O	33.12451484 -1.38827063 -4.76423363
C	1.05409854 -7.88832103 -22.28954473	N	31.34822821 -2.69033237 -4.23620559
H	0.13024008 -7.38010742 -22.56028449	C	30.99301093 -3.03884911 -5.61980011
C	1.60624917 -8.83580306 -23.16857177	C	30.84002922 -1.72649399 -6.40459657
H	1.14153477 -9.05665763 -24.12262422	O	30.08533152 -0.85161591 -6.05024783
C	2.78046751 -9.52452238 -22.81507938	C	29.68885829 -3.84537729 -5.58825941
H	3.22261847 -10.24668955 -23.49146426	S	29.21643361 -4.40699311 -7.29024595
C	3.36006454 -9.29732601 -21.57434268	H	30.83881989 -3.13962094 -3.49248959
F	4.52861288 -9.96530307 -21.28016985	H	31.79294271 -3.65935224 -6.04757112
Zn	28.07209169 -6.24260600 -6.91164462	H	28.90367070 -3.21607316 -5.15844518

2C-QM/SE/MM R1b (2C-B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.0$

C	22.27368070 -8.92165207 -4.43761382	C	8.07162905 -16.79161749 -15.28549548
O	21.41696811 -8.05327573 -4.33124994	H	7.85632065 -17.85223449 -15.30219147
N	23.54393240 -8.68959135 -4.81701209	C	8.75850729 -16.19672703 -14.21748425
C	23.90400734 -7.40169816 -5.40623619	H	9.12510546 -16.80253639 -13.40244181
C	23.07301050 -7.24438028 -6.69830865	C	8.98566573 -14.82586293 -14.24652251
O	23.13382398 -8.10272164 -7.58264334	H	9.54641624 -14.33566960 -13.45415776
C	25.39389884 -7.37628187 -5.84057692	N	8.51702700 -13.99830788 -15.21637914
S	25.83082000 -5.72400942 -6.51830370	C	7.90904930 -14.60910133 -16.26044981
H	24.10531162 -9.49063061 -5.09443742	C	7.41317040 -13.75352576 -17.34780672
H	23.69665804 -6.60302907 -4.68847966	C	7.50933005 -14.20161667 -18.69880500
H	25.57355933 -8.16092871 -6.58322181	C	6.98301611 -13.35901220 -19.68643607
H	26.00949983 -7.60905463 -4.96176661	C	6.37411307 -12.14821694 -19.41086110
N	22.34554624 -6.11615779 -6.81128456	H	6.00888142 -11.55193250 -20.22741729
H	22.14539900 -5.58245449 -5.97022543	F	7.05911373 -13.74302388 -20.99650371
C	25.22682718 -5.93874075 -10.76857827	H	8.03794106 -15.13042558 -18.92488290
O	25.26683441 -6.13806164 -11.98331988	C	6.84353462 -12.52807859 -17.03438045
N	25.98810115 -6.61976039 -9.84406238	H	6.80618865 -12.24694388 -15.98540864
C	26.82404637 -7.71505654 -10.29967156	C	6.25990810 -11.73781801 -18.03525816
C	26.20688779 -9.11612376 -10.09144317	C	5.45903360 -10.59690637 -17.66229366
O	26.72907727 -10.13484061 -10.55837716	O	5.64769546 -9.84208290 -16.65631435
C	28.24409949 -7.62953863 -9.73040358	N	4.40014507 -10.33473838 -18.54482226

H 3.98451177 -11.07898311 -19.09937240
 N 3.47438723 -9.36054049 -18.22211886
 H 3.47357044 -9.15702153 -17.21994070
 S 3.61339690 -7.94908075 -19.09359746
 O 5.00356632 -7.53383510 -19.42822362
 O 2.83506433 -6.91516566 -18.37493222
 C 2.78968321 -8.38454020 -20.64311304
 C 1.61918481 -7.65066250 -21.04412188
 H 1.15302239 -6.95940487 -20.34517801
 C 1.04585814 -7.89819566 -22.29265661
 H 0.11217349 -7.40808687 -22.55975726
 C 1.60336023 -8.84388374 -23.17215741
 H 1.13774077 -9.07865392 -24.12318948
 C 2.78252168 -9.52574593 -22.82030818
 H 3.22854572 -10.25037734 -23.49535565
 C 3.35755949 -9.29388560 -21.57714533
 F 4.52742866 -9.96335344 -21.28379828
 Zn 28.07141853 -6.24244516 -6.91290544

2C-WF-in-DFT/SE/MM R1b (2C-CCSD-in-B3LYP/6-31G(d):xTB:Amber) mechanical embedding $\omega_c=1.0$

C 22.27396529 -8.91579513 -4.43615126
 O 21.41993970 -8.05462177 -4.33226126
 N 23.54223392 -8.68827411 -4.81908027
 C 23.90313792 -7.40639765 -5.40643779
 C 23.07119189 -7.24609028 -6.70070267
 O 23.13218084 -8.10093772 -7.58113311
 C 25.39219778 -7.36381633 -5.84596673
 S 25.81817685 -5.71904104 -6.51740637
 H 24.10704260 -9.49106793 -5.09263927
 H 23.69299142 -6.60212614 -4.68796419
 H 25.57060854 -8.16255439 -6.58297151
 H 26.00702729 -7.60973454 -4.96082454
 N 22.34593472 -6.12072428 -6.80941120
 H 22.15103104 -5.57994425 -5.96850357
 C 25.23119697 -5.94355012 -10.77121905
 O 25.26861222 -6.13840508 -11.97900333
 N 25.98963730 -6.62207639 -9.84479619
 C 26.82449292 -7.71506512 -10.29852429
 C 26.20699735 -9.11935080 -10.09808161
 O 26.72402520 -10.13401213 -10.56340576
 C 28.24172191 -7.63693303 -9.71701669
 S 28.27863884 -8.17498789 -7.92208727
 H 25.93431840 -6.37669650 -8.84823436
 H 26.88662068 -7.60052306 -11.38975779
 H 28.64784102 -6.62258589 -9.84994263
 H 28.88824418 -8.32471195 -10.28632865
 N 25.06798478 -9.15681486 -9.36042736
 H 24.59538062 -8.32851024 -9.01606038
 C 30.10168118 -4.47238915 1.28927478
 O 30.69297711 -3.61379272 0.69115380
 N 29.51243366 -5.52468869 0.66046565
 C 29.56517554 -5.61210681 -0.80327339
 C 29.06327553 -4.32061502 -1.44692485
 O 29.78914639 -3.73355295 -2.22226033
 C 28.83340472 -6.85355057 -1.33027916
 C 28.93122854 -6.96442270 -2.81226441
 H 29.25702140 -7.74931446 -0.84223885
 H 29.01588771 -6.24416326 1.18142116
 H 30.62195135 -5.64573947 -1.10935669
 H 27.77249240 -6.82241034 -1.04490592
 C 28.14185655 -6.48050661 -3.82626422
 H 30.88799923 -7.80305556 -2.99400091

H 27.22202176 -5.90256733 -3.77554347
 C 29.78251315 -7.49114526 -4.80318541
 N 29.99159450 -7.63760017 -3.45221268
 N 28.67977642 -6.85822602 -5.01019078
 H 30.43986801 -7.88771738 -5.58084559
 N 27.84070860 -3.86052545 -1.07198706
 H 27.26782623 -4.37775236 -0.40221448
 C 32.41899065 -1.93696776 -3.93114870
 O 33.12068244 -1.38972389 -4.76358393
 N 31.35034014 -2.69210826 -4.23683933
 C 30.99252089 -3.03460162 -5.61460953
 C 30.84254172 -1.72058282 -6.40172699
 O 30.09211990 -0.84869046 -6.04774297
 C 29.69040275 -3.84647670 -5.60586797
 S 29.22745773 -4.38693556 -7.30164601
 H 30.83639091 -3.14286090 -3.49123041
 H 31.79608518 -3.65709915 -6.04854482
 H 28.90564585 -3.21311004 -5.15785655
 H 29.84445907 -4.69813618 -4.92446938
 N 31.58045666 -1.59059679 -7.50701043
 H 32.15701228 -2.35002717 -7.79106107
 C 7.67867217 -15.97919319 -16.33439409
 H 7.15247750 -16.36853476 -17.19828696
 C 8.07217037 -16.79141610 -15.28507132
 H 7.85745591 -17.85211588 -15.30177800
 C 8.75886359 -16.19662585 -14.21701337
 H 9.12547972 -16.80214073 -13.40174406
 C 8.98575494 -14.82579486 -14.24643575
 H 9.54626801 -14.33554536 -13.45393648
 N 8.51733272 -13.99835861 -15.21635069
 C 7.90878761 -14.60885432 -16.26044575
 C 7.41289304 -13.75340574 -17.34773311
 C 7.50850915 -14.20119394 -18.69882192
 C 6.98265702 -13.35857099 -19.68655668
 C 6.37387718 -12.14775832 -19.41126487
 H 6.00860998 -11.55149571 -20.22780616
 F 7.05897898 -13.74274998 -20.99658487
 H 8.03634031 -15.13011134 -18.92494950
 C 6.84335285 -12.52788386 -17.03467159
 H 6.80556807 -12.24674656 -15.98585740
 C 6.25970535 -11.73773554 -18.03557685
 C 5.45898667 -10.59662901 -17.66295030
 O 5.64815838 -9.84137693 -16.65735407
 N 4.39937296 -10.33579212 -18.54400178
 H 3.98560844 -11.08018971 -19.09940531
 N 3.47377556 -9.36091792 -18.22233415
 H 3.47328667 -9.15782983 -17.21993646
 S 3.61337087 -7.94938326 -19.09371472
 O 5.00350456 -7.53316343 -19.42831348
 O 2.83480678 -6.91596679 -18.37479094
 C 2.79004699 -8.38447061 -20.64333362
 C 1.61990285 -7.65085381 -21.04414940
 H 1.15422934 -6.95923247 -20.34562412
 C 1.04632735 -7.89769568 -22.29250265
 H 0.11329384 -7.40639273 -22.55990031
 C 1.60341773 -8.84354453 -23.17187450
 H 1.13782040 -9.07731761 -24.12309250
 C 2.78230056 -9.52573077 -22.81991493
 H 3.22797895 -10.25016925 -23.49502585
 C 3.35760708 -9.29416663 -21.57703060
 F 4.52753550 -9.96330267 -21.28346445
 Zn 28.07196175 -6.23909730 -6.91200497

1C QM/SE/MM R3b (B3LYP/6-31G(d):xTB:Amber) mechanical embedding
 $\omega_c=1.0$

C	21.94416514	-10.35261693	-4.21816128	H	21.23092762	-10.70511417	-10.09319338
C	22.26071489	-8.88920541	-4.43779550	H	24.62470683	-8.30783927	-8.97353446
O	21.41083976	-8.01620802	-4.34259202	H	21.96464523	-11.86837487	-12.20760675
N	23.53584780	-8.67829995	-4.81431451	H	21.82612686	-10.34923802	-13.09639917
C	23.90099292	-7.39893842	-5.41448999	H	23.33588225	-11.25797319	-13.11766990
C	23.08534360	-7.24524264	-6.71445028	H	23.47636152	-10.17483268	-8.59117769
O	23.13658553	-8.11712469	-7.58656283	H	23.48309310	-9.30993737	-11.56952251
C	25.39084292	-7.36225324	-5.81101427	H	23.40051521	-12.01109863	-10.16654832
S	25.83764933	-5.72826370	-6.51510108	H	24.77373427	-11.33934928	-11.05788040
H	24.12571997	-9.48599447	-4.99853877	N	26.21475961	-10.85134807	-7.61446505
H	23.67905432	-6.59897804	-4.70932510	C	26.87063960	-11.71757796	-6.65170885
H	25.59837035	-8.16664108	-6.51797637	C	25.83542793	-12.10959873	-5.55199594
H	25.97470463	-7.55913953	-4.90544281	O	25.17801757	-11.26091414	-4.98936815
N	22.38148138	-6.10770756	-6.85118091	C	28.03714739	-10.98954936	-5.99254861
C	21.48689612	-5.96761924	-7.97307391	C	28.64761825	-11.80193498	-4.86293985
C	22.18167626	-5.66010338	-9.31513788	C	29.93731687	-11.14157101	-4.33810026
O	21.57673340	-5.77860537	-10.36249617	C	30.34082281	-11.82796460	-3.02927889
C	20.50050654	-4.87452871	-7.65170459	N	31.78320760	-11.67005112	-2.76712677
H	20.93229387	-6.90031430	-8.12039820	H	27.21819058	-12.63143948	-7.14585561
H	22.22509151	-5.52813091	-6.03027809	H	29.78571326	-11.40044961	-2.20097550
N	23.44359343	-5.21493372	-9.16998857	H	30.12298168	-12.88870252	-3.09975282
C	24.28829663	-4.81512780	-10.25805120	H	27.93284475	-11.86078959	-4.04662358
C	25.21703868	-5.90678445	-10.76393505	H	28.87421848	-12.80984132	-5.19044305
O	25.24195960	-6.12672118	-11.97577039	H	32.11903095	-12.30198089	-2.03414603
C	25.11123739	-3.59831527	-9.90777648	H	32.33752726	-11.88844179	-3.61852133
C	24.26838608	-2.44907773	-9.44899110	H	32.00006291	-10.70454869	-2.47397740
C	23.31303790	-1.87737387	-10.27872950	H	29.77576922	-10.08266825	-4.19056797
C	24.41028737	-1.95378694	-8.14162399	H	30.70940965	-11.28289519	-5.08685552
C	22.54852042	-0.80191896	-9.84470836	H	26.61210259	-9.94909475	-7.85333318
C	23.62942740	-0.90803791	-7.69910536	H	27.71010797	-10.02488641	-5.62453578
C	22.70993588	-0.30965249	-8.55451527	H	28.79864331	-10.80852302	-6.74710936
O	22.01030834	0.79211650	-8.11842525	N	25.77611996	-13.41325879	-5.19777715
H	23.62055280	-4.57670905	-11.09251544	C	24.90341771	-13.85114353	-4.12701567
H	21.80461271	-0.37675031	-10.49497873	H	26.18725482	-14.13881398	-5.76914757
H	23.73369742	-0.51974835	-6.70462145	C	29.87682768	-4.49376616	2.80922188
H	23.86851326	-5.31187114	-8.25124219	C	30.09523653	-4.49054572	1.27488652
H	25.13093861	-2.39168094	-7.47757187	O	30.69142113	-3.62154507	0.68139302
H	23.14894010	-2.26364128	-11.27147420	N	29.50827727	-5.54109719	0.64497406
H	25.67521234	-3.29165740	-10.78547422	C	29.57945665	-5.61449261	-0.81419357
H	25.82013031	-3.84296215	-9.11953259	C	29.06826642	-4.32476653	-1.44347067
H	22.41904025	1.60825154	-8.42984172	O	29.76991488	-3.73626113	-2.24726420
N	25.98174544	-6.59331801	-9.84701475	C	28.84605339	-6.84563102	-1.34977178
C	26.81302542	-7.69099092	-10.29884087	C	28.95498973	-6.96628674	-2.82325956
C	26.20034712	-9.08913154	-10.09371071	H	29.26386566	-7.73458082	-0.86785594
O	26.73777594	-10.10051391	-10.55859026	H	28.99034152	-6.23848536	1.17189153
C	28.22453503	-7.61498973	-9.72607987	H	30.63255432	-5.65544784	-1.10332827
S	28.28193298	-8.15977070	-7.92063083	H	27.79140927	-6.79428107	-1.08040040
H	25.94347398	-6.33894295	-8.85643805	C	28.16673056	-6.49319003	-3.83786068
H	26.89546295	-7.57739807	-11.38263677	H	30.88962979	-7.85968319	-2.98438729
H	28.61523625	-6.60508596	-9.83395364	H	27.25500561	-5.92571381	-3.77585080
H	28.86096867	-8.29658913	-10.28912722	C	29.82643807	-7.50761447	-4.79266215
N	25.05032114	-9.13254206	-9.37557122	N	30.00933560	-7.63695180	-3.44903277
C	24.37960893	-10.40388945	-9.16040546	N	28.70528023	-6.86797341	-5.02304471
C	25.16883817	-11.37688193	-8.29657269	H	30.49560424	-7.89329980	-5.54129473
O	24.81557501	-12.53644510	-8.12962428	N	27.84999969	-3.87853084	-1.04295391
C	23.90964308	-11.09779220	-10.45255441	C	27.27872556	-2.63885795	-1.55432205
C	22.95770750	-10.21054785	-11.26414640	H	27.31617141	-4.37640973	-0.33264901
C	22.48698184	-10.96782309	-12.51019487	C	32.65840262	-1.85421683	-2.42773560
C	21.73250131	-9.81153663	-10.44768668	C	32.41313859	-1.96264564	-3.94614449
H	22.02885190	-9.21541068	-9.59700765	O	33.11993469	-1.40268568	-4.77490916
H	21.05832958	-9.23117714	-11.05455428	N	31.35666227	-2.72858941	-4.26438189
				C	30.99820427	-3.04963741	-5.65330601
				C	30.84076969	-1.73029035	-6.42525968
				O	30.08569115	-0.86591516	-6.04065106
				C	29.69075505	-3.84482105	-5.62091529

S	29.18837348 -4.40094742 -7.30323411	O	12.23063782 -22.69855162 -12.48927594
H	30.82909485 -3.14911354 -3.51449919	C	12.29473972 -20.45053732 -14.63671527
H	31.78482146 -3.67070589 -6.09183488	C	12.24882566 -18.99792906 -15.08005069
H	28.91938518 -3.21256087 -5.18088205	C	13.35436803 -18.77065872 -16.09986494
H	29.84812387 -4.70170363 -4.96552151	C	10.88882842 -18.65660920 -15.67688519
N	31.53702755 -1.57061511 -7.56011587	H	10.12238166 -18.76104387 -14.92750958
C	31.54567556 -0.38677655 -8.35728411	H	10.89266962 -17.64348814 -16.04263703
C	30.66169023 -0.52230526 -9.60864128	H	10.68180230 -19.33194184 -16.50039053
O	30.32523624 0.43557695 -10.27922829	H	12.45890548 -20.18516861 -11.82619282
C	33.00291971 -0.09742282 -8.72657759	H	13.21250273 -19.41553882 -16.95961214
H	31.15435101 0.44698665 -7.77449429	H	13.33915376 -17.74753041 -16.44327882
H	32.15906389 -2.29331801 -7.86056679	H	14.32517494 -18.97918524 -15.67315904
N	30.23931661 -1.77112926 -9.86257942	H	10.30278740 -20.46181153 -13.82484951
C	29.20032572 -1.98953948 -10.86734508	H	12.40684506 -18.34139989 -14.22818994
C	27.95857758 -1.16915794 -10.51378969	H	12.04955182 -21.08616340 -15.47977310
O	27.43874760 -1.13333211 -9.42227445	H	13.29404857 -20.70463583 -14.29928188
C	28.80055258 -3.46253081 -10.97790258	N	10.26624290 -22.88598107 -13.58605268
C	29.85894909 -4.32026251 -11.58201637	C	10.13968128 -24.32346701 -13.37334067
C	31.20827381 -4.20697601 -11.43143809	H	9.61879838 -22.48794845 -14.25478569
C	29.64449301 -5.45591389 -12.42927709	C	14.10025550 -18.55351859 -21.17853964
N	31.85288029 -5.19909515 -12.12055526	C	13.89447449 -17.05801493 -21.07059621
C	30.92618172 -5.99383859 -12.72587102	O	14.72290199 -16.27891518 -21.45045060
C	28.51277479 -6.11611276 -12.91255330	N	12.72473014 -16.69524626 -20.51798590
C	31.08254425 -7.18212301 -13.43166139	C	12.42222716 -15.31191571 -20.25816412
C	28.68049008 -7.31426402 -13.57223295	C	11.80289965 -15.22117058 -18.84563994
C	29.94113912 -7.84184038 -13.84343055	O	10.95775601 -16.03266697 -18.45813238
H	30.02584914 -8.75014996 -14.40581640	C	11.50559347 -14.71696732 -21.34436692
H	29.60073253 -1.63663645 -11.82332954	C	11.22824522 -13.25933340 -21.05656051
H	32.84911080 -5.30182327 -12.21984769	C	10.22704904 -15.53949556 -21.47558278
H	27.53031901 -5.70966222 -12.76126951	C	10.56308765 -12.54306346 -22.20811262
H	27.81484902 -7.85189151 -13.89010921	H	13.37138300 -14.77840603 -20.27242445
H	32.06682884 -7.54653699 -13.67005643	H	9.62726080 -15.14545851 -22.27923311
H	31.76355554 -3.47229288 -10.89039388	H	10.47397941 -16.56832744 -21.69477303
H	30.37073642 -2.49125713 -9.16238162	H	12.05641226 -14.78463249 -22.27979971
H	27.91283526 -3.54274064 -11.60051340	H	10.58315443 -13.19120669 -20.17924602
H	28.55882894 -3.84208685 -9.98605058	H	12.15847591 -12.75457441 -20.81756525
N	27.43456223 -0.49428917 -11.55505081	H	9.60545626 -12.99229191 -22.43238648
C	26.12776350 0.14944088 -11.47965451	H	12.08700653 -17.40445357 -20.19020067
H	27.94636062 -0.36596350 -12.42666464	H	10.39813192 -11.50893475 -21.94846986
C	14.00102427 -19.32361722 -8.43946266	H	9.66512732 -15.47707697 -20.55499638
C	12.57086379 -19.03375222 -8.87936662	H	11.18952340 -12.58996971 -23.08944370
O	11.65373970 -19.13543199 -8.09851162	N	12.20753003 -14.20386366 -18.08084530
N	12.45480875 -18.59606202 -10.15418916	C	11.97046486 -14.16725727 -16.62140094
C	11.17467821 -18.22307915 -10.69388591	C	11.95311630 -12.70717134 -16.25449733
C	10.79306062 -18.99211344 -11.93768886	O	12.90942296 -12.00044721 -16.51840231
O	9.74284395 -18.74667457 -12.51488348	C	13.03439532 -14.89910365 -15.82181370
C	11.05592577 -16.71419381 -10.93228129	C	12.65746085 -15.11913182 -14.31220636
C	11.56903994 -15.94886478 -9.74201507	S	12.77826829 -13.58182024 -13.36664149
C	10.80967507 -15.87225506 -8.57067215	C	14.54789284 -13.23895672 -13.56730824
C	12.80459675 -15.31073281 -9.79774297	H	11.62258510 -15.43831941 -14.24861036
C	11.29908396 -15.17110473 -7.47959382	H	14.87445985 -12.65788914 -12.71946407
C	13.28895524 -14.62198143 -8.70049391	H	15.08675155 -14.17939200 -13.58962132
C	12.53428418 -14.55155806 -7.53315228	H	14.71622803 -12.68923116 -14.48342315
H	12.92814809 -14.03566532 -6.67935758	H	13.22961999 -15.87042702 -16.26208988
H	10.44404019 -18.51601011 -9.93163483	H	13.31091633 -15.87527203 -13.88854719
H	10.71339238 -15.13191210 -6.58939359	H	12.93245773 -13.59022811 -18.45637654
H	14.25837994 -14.16091135 -8.75867322	H	11.00080133 -14.64101211 -16.46340943
H	13.26897179 -18.49187870 -10.75178404	H	13.95026089 -14.31744579 -15.85553717
H	13.39629713 -15.38529421 -10.69489700	N	10.79417509 -12.26217867 -15.74093722
H	9.85484069 -16.36268944 -8.52225683	C	10.67215653 -10.91291731 -15.21304592
H	10.01471836 -16.46525042 -11.09732117	C	10.55151459 -11.06625152 -13.67389432
H	11.63548217 -16.43357130 -11.80569243	O	9.84760820 -11.92291135 -13.16562585
N	11.60270781 -19.97717547 -12.31846233	C	9.41818042 -10.21891501 -15.73149322
C	11.30209310 -20.74346825 -13.49728747	C	9.40896015 -10.11250635 -17.26858735
C	11.33014847 -22.20918932 -13.13169615	C	9.24661033 -8.84143211 -15.10187453

C	10.51231608 -9.19348373 -17.75149109	C	4.52462052 -3.78858140 -12.17999240
H	11.56928748 -10.35833646 -15.46671801	N	3.87927590 -3.34987194 -10.95967432
H	8.34703136 -8.37297942 -15.47337533	C	3.43017021 -4.16301325 -9.98298895
H	9.16130587 -8.93641955 -14.02704591	N	3.19460005 -5.47696437 -10.22966524
H	8.56512717 -10.83464268 -15.44944298	N	3.07530246 -3.63970973 -8.77065203
H	9.53529253 -11.10184298 -17.68938017	H	2.83931092 -4.25282564 -13.40872789
H	8.44384118 -9.72281084 -17.56455398	H	2.66920219 -3.80422628 -15.77049665
H	11.47686808 -9.59040706 -17.45863871	H	3.86226935 -2.36016203 -10.79070962
H	9.99506813 -12.88599545 -15.59122266	H	3.22967839 -2.54029153 -13.33540808
H	10.50343942 -9.12919525 -18.82735567	H	2.55920910 -4.26312135 -8.17308578
H	10.09575132 -8.20836034 -15.31495008	H	2.77608885 -2.68091308 -8.76198997
H	10.40836939 -8.19451050 -17.35643999	H	4.40698347 -6.19902933 -16.02409964
N	11.34530817 -10.29017166 -12.92588479	H	5.46732161 -3.25203834 -12.27371256
C	11.28671741 -10.39946683 -11.45181386	H	4.74853084 -4.84973498 -12.12232577
H	11.90852496 -9.54030044 -13.31542609	H	3.22016468 -6.11742506 -9.43732642
C	7.90878795 -6.08280570 -12.13535706	H	3.75192491 -5.87349756 -10.97072753
C	6.89151246 -6.76307365 -13.06318957	H	4.89951796 -2.69627220 -14.93415659
O	6.61539858 -6.31823093 -14.15473594	H	5.30789184 -4.35067762 -14.48199465
N	6.45743708 -7.95794318 -12.65074849	N	4.29077109 -4.53507782 -18.19071981
C	5.62180309 -8.75758284 -13.49641934	C	4.77293413 -4.13031152 -19.48399559
C	4.31258448 -7.97185515 -13.75015328	C	6.23716861 -4.48862468 -19.84153826
O	3.90904653 -7.16769478 -12.92524255	O	6.58685641 -4.42510662 -21.02170064
C	5.35017308 -10.12130312 -12.90139135	H	4.02519932 -5.50247891 -18.03677376
C	6.60729018 -10.98680821 -12.91568633	H	4.15123582 -4.58160195 -20.25582490
C	6.35180130 -12.31149331 -12.27744241	H	4.70906843 -3.03955448 -19.53097147
H	6.89721869 -11.17048070 -13.95164132	N	7.01570205 -4.85002164 -18.81723020
H	6.13153227 -8.87655318 -14.45840138	C	8.42221803 -5.17549305 -18.98092442
H	7.43979701 -10.49723044 -12.43756095	C	8.58933845 -6.48392155 -19.75105229
H	6.67593681 -8.26817686 -11.71306440	O	9.38814798 -6.55310072 -20.66852388
H	4.57640785 -10.61281761 -13.48372425	C	9.15790014 -5.24983330 -17.61250583
H	4.98735546 -10.02896983 -11.88171025	C	9.09209091 -3.94525145 -16.86800083
H	8.28306124 -12.86960350 -12.60753080	C	9.94701820 -2.88851005 -17.12354422
O	5.23868642 -12.59320428 -11.84955049	C	8.15968745 -3.79810362 -15.85417950
N	7.42240066 -13.10962108 -12.13109829	C	9.86389979 -1.71214168 -16.40398768
H	7.30069057 -14.06488681 -11.82137888	C	8.06793722 -2.63906023 -15.10723280
N	3.76616996 -8.24866261 -14.96271131	C	8.93935303 -1.58414241 -15.35890918
C	2.46542115 -7.76257954 -15.38551005	O	8.78189030 -0.45830886 -14.62611000
C	2.44430105 -6.23286998 -15.43312940	H	8.89430477 -4.39269582 -19.57980544
O	1.43317258 -5.61529671 -15.16701179	H	10.55265362 -0.90352800 -16.58327229
C	1.35415505 -8.28526295 -14.45607318	H	7.35099988 -2.54677191 -14.31764170
C	1.27222629 -9.81107126 -14.44579298	H	6.62911053 -4.88862855 -16.88219023
C	0.09063728 -10.24546326 -13.58624824	H	7.50783622 -4.61827644 -15.61420555
N	0.02545683 -11.65451385 -13.30018962	H	10.70547764 -2.96377315 -17.87825308
C	-0.65019318 -12.54473032 -14.07298937	H	10.18714711 -5.48038831 -17.84341914
N	-1.61600154 -12.10112267 -14.94458937	H	8.73084860 -6.04614512 -17.01641854
N	-0.38793908 -13.89831427 -13.94852557	H	9.61808204 0.11578504 -14.74186616
H	2.17999248 -10.23632357 -14.02744533	N	7.79426493 -7.50171014 -19.35857608
H	2.23061714 -8.12144691 -16.38470276	C	7.78876280 -8.74901484 -20.07337577
H	0.77681987 -12.03140069 -12.72420779	C	7.40133679 -8.55784617 -21.58939319
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H	-1.40599629 -11.22927429 -15.40335557	O	7.18484231 -6.95507756 -25.17722096
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O	4.56122384 -2.48465105 -17.31414803	N	0.62240544 -3.61319615 -24.28665453
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C	3.65502060 -3.53933414 -13.40178678	H	3.83051208 -6.98520044 -24.97634379

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H	5.01878591	-5.48868565	-22.59396576	H	1.95732074	-14.01087050	-17.41558015
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C	11.29239241	-8.07692388	-23.87629508	N	4.65331397	-16.75811746	-19.07529664
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C	7.63331483	-10.68242033	-25.82600578	N	3.37894375	-18.06689106	-21.27562164
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N	6.60153190	-20.97524547	-19.59695577	C	-1.14641716	-13.78620054	-26.55929904
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C	6.83878827	-19.83509552	-17.40631160	C	-0.65376577	-10.84050726	-26.52148449
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2C-QM/SE/MM R3b (2C-B3LYP/6-31G(d):xTB:Amber) mechanical embedding
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**C. Cartesian coordinates for Amyloid-Beta (20-34)
with L-isoaspartate 23**

Full optimization with xTB

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 H 0.677664 2.568737 2.796887
 H -0.273794 2.615453 1.315550
 H -2.663089 3.539195 1.470442
 H -3.562068 3.132586 2.927250
 H -2.608395 4.612381 2.864185
 H 1.191084 4.636807 1.669151
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 H 0.222927 5.056902 3.079873
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 H -4.603214 1.716418 6.551799
 H -4.668121 3.209268 7.526680
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 C -7.898961 2.842710 4.542612
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 O -9.000791 1.446217 6.169972
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 C -6.836551 2.617329 2.165167
 C -5.751274 1.538191 2.177399
 C -7.413167 2.774642 0.757123
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 H -7.914430 3.932480 4.481365
 H -7.979095 1.142481 3.243312
 H -8.927199 2.534589 2.732319
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 H -5.414410 1.344891 3.193257
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 H -6.621628 2.942843 0.027752
 H -7.952931 1.873850 0.470581
 H -8.102766 3.614367 0.722555
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 C 5.391315 5.039210 20.387956
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 C 6.957840 4.822807 18.361845
 C 7.349556 4.155784 17.055878
 O 7.423816 2.944289 16.918174
 O 6.012605 4.505117 21.301819
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 H 5.590722 3.267311 18.965070
 H 7.703844 4.539761 19.108968
 H 6.964619 5.910903 18.257536
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 H 14.021971 7.778947 7.278887
 H 13.068209 6.869100 6.485644
 O 5.698447 5.191570 24.712998
 H 6.308321 5.760883 24.238737
 H 5.235696 4.723524 24.011536
 O 12.397734 6.563063 0.105674
 H 12.247639 6.697135 1.044501
 H 11.611278 6.110681 -0.210294
 O 15.050291 6.600110 1.137817
 H 14.923088 7.551260 1.116297

H 14.555045 6.278834 0.374568

Quantum refinement with ORCA $\omega_c=0.269$

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 O -0.446760 5.219275 13.323098
 C -2.171071 2.626571 11.986666
 C -2.302563 3.656981 10.868536
 C -3.505450 4.350947 10.645402
 C -1.220286 3.918569 10.006803
 C -3.619392 5.289020 9.607346
 C -1.319818 4.880583 8.988336
 C -2.527011 5.553070 8.780440
 H -1.518873 2.311750 14.038229
 H -1.469484 1.867832 11.622431
 H -3.145239 2.130622 12.130689
 H -4.367158 4.149152 11.289387
 H -0.290026 3.357168 10.125800
 H -4.561316 5.820051 9.449777
 H -0.459745 5.099207 8.349438
 H -2.615825 6.285367 7.972809
 H -3.589652 3.520613 14.146012
 H -2.305417 4.538409 15.694376
 H -2.891840 4.845853 13.404107
 N 0.730614 3.293093 13.012783
 C 2.041989 3.953014 12.892281
 C 2.339381 4.799102 14.174039
 O 2.445509 6.014541 14.144923
 C 2.118871 4.816206 11.630296
 H 0.684095 2.283453 12.956819
 H 2.790382 3.144564 12.850104
 H 3.098349 5.311423 11.567502
 H 1.971265 4.194771 10.735673
 H 1.349824 5.596483 11.673774
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 C 3.667774 3.950555 17.427441
 O 3.704567 2.720448 17.479670
 C 1.224472 4.269257 17.479308
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 C -1.309589 4.115438 17.389013
 O -1.335149 3.452840 18.401206
 O -2.412325 4.254889 16.646501
 H 2.466390 3.047062 15.258990
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 H 1.130395 3.174029 17.527225
 H 1.388331 4.606990 18.513693
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 H -0.045554 4.918240 15.825294
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 C 8.121888 4.554112 14.725685
 C 9.523712 5.149085 14.500824
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H	5.113389	4.731801	12.914583	C	4.507943	2.829065	2.598968
H	5.756852	3.329845	13.806473	C	3.832577	2.195695	3.847328
H	5.309507	4.799969	14.687308	O	3.857230	0.976698	3.993560
N	10.564876	4.286861	14.328818	C	3.731356	2.461688	1.326135
C	11.910759	4.801015	14.168971	H	5.981449	1.343365	2.494871
C	12.164580	5.422150	12.772245	H	4.545326	3.923159	2.697766
O	12.378154	6.620238	12.640447	H	2.690434	2.810076	1.395106
H	10.406982	3.288682	14.395864	H	4.201088	2.934935	0.451391
H	12.100880	5.615550	14.880567	H	3.716024	1.368873	1.195107
H	12.620080	3.978029	14.347660	N	3.185569	3.035379	4.688099
N	12.154684	4.547190	11.696256	C	2.340401	2.597554	5.789894
C	12.487705	4.919947	10.341451	C	0.985319	3.293595	5.545927
C	11.533617	4.260886	9.327597	O	0.933516	4.530224	5.631631
O	11.364219	3.047799	9.299586	C	2.890604	2.920620	7.200298
C	13.936615	4.479572	9.995855	C	4.356979	2.460990	7.390011
O	14.265983	4.696706	8.634698	C	1.956111	2.343319	8.264598
H	11.897629	3.575965	11.843953	C	4.993999	2.845134	8.740056
H	12.413997	6.017648	10.272399	H	3.216561	4.038872	4.534275
H	14.625103	5.002690	10.685221	H	2.250308	1.504830	5.698317
H	14.027000	3.396278	10.170522	H	2.874602	4.022087	7.300533
H	14.271892	5.646214	8.442241	H	4.403901	1.362521	7.277906
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C	10.039080	4.672597	7.383320	H	2.286950	2.626389	9.273657
C	10.578074	5.168714	6.032929	H	0.923136	2.704049	8.148790
O	10.637197	6.373685	5.766672	H	1.944388	1.240292	8.214988
C	8.575191	5.149789	7.560160	H	6.066915	2.593224	8.736630
C	7.709535	4.591461	6.404013	H	4.889917	3.926078	8.940446
O	7.714468	3.387715	6.123844	H	4.526801	2.316021	9.585010
N	7.017803	5.489290	5.675063	N	-0.053874	2.523919	5.163522
H	11.051232	6.115218	8.558768	C	-1.295437	3.088754	4.620788
H	10.041110	3.574713	7.410217	C	-2.488582	2.436849	5.340697
H	8.194976	4.779219	8.523246	O	-2.572028	1.201631	5.367473
H	8.544811	6.250307	7.559200	C	-1.435149	2.809991	3.096180
H	6.510251	5.170445	4.851272	C	-0.148850	3.095679	2.290637
H	7.075989	6.482669	5.858805	C	-2.655110	3.550346	2.530535
N	10.960104	4.217012	5.143949	C	0.215725	4.566401	2.100648
C	11.297310	4.484724	3.758235	H	-0.012692	1.511338	5.231940
C	10.268814	3.928493	2.753519	H	-1.253136	4.166861	4.828840
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C	12.698237	3.946093	3.421898	H	0.693108	2.587701	2.789162
C	13.821094	4.740346	4.079047	H	-0.266355	2.615314	1.303263
C	15.196160	4.321315	3.533065	H	-2.678917	3.503481	1.431172
C	16.267862	5.336022	3.880253	H	-3.592281	3.114275	2.900808
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H	11.021445	3.258881	5.475277	H	1.213671	4.668186	1.640592
H	11.295969	5.578429	3.633550	H	-0.503534	5.080932	1.444616
H	12.755800	2.892230	3.753774	H	0.238513	5.100855	3.063487
H	12.821589	3.952790	2.327295	N	-3.388089	3.271343	5.906247
H	13.666858	5.817664	3.894547	C	-4.627038	2.814222	6.517526
H	13.788925	4.572386	5.170767	C	-5.828176	3.381378	5.727359
H	15.475637	3.332438	3.938623	O	-5.897303	4.603711	5.565031
H	15.153241	4.242070	2.436844	H	-3.269898	4.276298	5.837666
H	17.256690	5.046059	3.494665	H	-4.594892	1.718977	6.577133
H	15.999485	6.324591	3.486831	H	-4.692151	3.227877	7.538009
H	15.548963	5.926303	5.817673	N	-6.724252	2.490023	5.271955
H	16.479972	4.546773	5.842301	C	-7.952803	2.848598	4.572134
H	17.208954	6.032851	5.663991	C	-9.245703	2.321567	5.322401
N	9.313527	3.117628	3.268822	O	-9.042116	1.443091	6.188240
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C	6.953818	3.168015	2.562464	C	-6.861392	2.667392	2.166445
O	6.886894	4.391394	2.672764	C	-5.769493	1.585444	2.157811
H	9.165037	3.092068	4.276025	C	-7.429066	2.865879	0.750705
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H	8.209336	1.412561	2.817129	H	-6.579529	1.499179	5.430485
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H 14.633895 6.208909 0.451689

Quantum refinement with LSQC $\omega_{\bar{a}}=0.269$

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C -3.496101 4.349361 10.661546
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C -1.317385 4.892168 9.010694
C -2.524828 5.559050 8.805144
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H -0.297154 3.341212 10.109228
H -4.552946 5.816883 9.483224
H -0.460766 5.125679 8.383997
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H -2.887707 4.831420 13.389113
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H 1.347999 5.580945 11.659118
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C 3.662072 3.941098 17.422560
O 3.703854 2.704985 17.479756
C 1.201639 4.261390 17.452837
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C -1.339794 4.141308 17.266980
O -1.386823 3.440600 18.262534
O -2.421533 4.314666 16.499001
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H 2.627229 5.662953 16.551132
H 1.084665 3.174191 17.483756
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H -0.174611 5.933005 17.221608
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C 9.521946 5.138721 14.501855
O 9.702849 6.362547 14.505838
C 7.183419 4.947098 13.545030
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C 5.755749 4.414480 13.744351
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H 8.160394 3.458697 14.780851
H 7.155391 6.044998 13.530563
H 7.038465 4.545525 11.396959
H 8.676304 4.982216 11.920958
H 8.013166 3.376682 12.274740
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H 12.143053 5.549106 14.899981
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C 11.534344 4.256810 9.326553
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C 13.934074 4.467037 9.989821
O 14.269240 4.695861 8.619579
H 11.919092 3.560717 11.840371
H 12.405591 6.002315 10.270588
H 14.629535 4.988582 10.662159
H 14.020226 3.388930 10.149193
H 14.313142 5.654853 8.470352
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O 10.635314 6.373476 5.760052
C 8.577259 5.144017 7.562134
C 7.710996 4.580923 6.404942
O 7.713856 3.375162 6.124338
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H 10.058425 3.580852 7.407374
H 8.203875 4.780297 8.522178
H 8.549741 6.238749 7.555830

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H	7.093766	6.479656	5.887021	C	-2.651602	3.590568	2.536036
N	10.963215	4.212974	5.142528	C	0.232587	4.541023	2.102098
C	11.297384	4.476628	3.748252	H	-0.014695	1.508086	5.255335
C	10.273763	3.904952	2.748061	H	-1.248716	4.138076	4.800631
O	10.401142	4.133590	1.554740	H	-1.642454	1.722481	2.966058
C	12.698532	3.933473	3.416379	H	0.677185	2.542388	2.753987
C	13.824584	4.735436	4.069601	H	-0.276636	2.620026	1.270559
C	15.191249	4.311148	3.487643	H	-2.680623	3.627611	1.444740
C	16.264689	5.334894	3.826177	H	-3.593992	3.163109	2.885991
N	16.410375	5.438593	5.345472	H	-2.610490	4.634196	2.872743
H	11.018721	3.256640	5.472419	H	1.227897	4.626641	1.648161
H	11.311484	5.561562	3.618385	H	-0.485685	5.063158	1.460152
H	12.762397	2.890054	3.760067	H	0.257113	5.052999	3.070681
H	12.825275	3.942397	2.328992	N	-3.388981	3.264489	5.895441
H	13.668873	5.806449	3.885271	C	-4.627287	2.808550	6.521130
H	13.812416	4.562054	5.154623	C	-5.829319	3.373423	5.728718
H	15.484185	3.330891	3.887717	O	-5.911481	4.606095	5.595320
H	15.119256	4.235131	2.399600	H	-3.265816	4.266061	5.837678
H	17.242197	5.057734	3.423294	H	-4.594616	1.720754	6.592112
H	15.984396	6.321339	3.457136	H	-4.678255	3.219055	7.535691
H	15.575715	5.877690	5.786309	N	-6.714106	2.481456	5.257628
H	16.507116	4.502173	5.758285	C	-7.950169	2.824051	4.553467
H	17.229036	5.992317	5.617056	C	-9.248761	2.285514	5.298959
N	9.312828	3.100770	3.283487	O	-9.036181	1.432927	6.193748
C	8.311090	2.439040	2.479364	C	-7.967482	2.239480	3.133313
C	6.957838	3.160084	2.558728	C	-6.827829	2.630129	2.154267
O	6.881591	4.387722	2.665821	C	-5.726068	1.554334	2.178453
H	9.159449	3.080757	4.285562	C	-7.396212	2.791856	0.734485
H	8.665264	2.399925	1.444757	O	-10.315892	2.745405	4.833628
H	8.201160	1.408765	2.839995	H	-6.535307	1.494094	5.377937
N	5.873863	2.339509	2.525562	H	-7.965406	3.913138	4.490973
C	4.513707	2.813610	2.602572	H	-7.971362	1.140076	3.222608
C	3.832717	2.185791	3.847394	H	-8.936637	2.525163	2.713514
O	3.850384	0.961381	3.997924	H	-6.385597	3.591025	2.455776
C	3.721720	2.457213	1.334444	H	-4.844413	1.845038	1.594109
H	5.990716	1.336022	2.468634	H	-5.393988	1.356976	3.203767
H	4.543423	3.900826	2.705253	H	-6.106132	0.612541	1.759541
H	2.688687	2.809494	1.417013	H	-6.601237	2.965838	-0.004463
H	4.182500	2.938093	0.466313	H	-7.935487	1.882730	0.435365
H	3.703235	1.372111	1.192056	H	-8.100958	3.630736	0.688475
N	3.183533	3.025723	4.688107	N	4.524648	4.778396	18.025261
C	2.336178	2.593787	5.790063	C	5.600563	4.356826	18.939368
C	0.984834	3.285084	5.541081	C	5.404750	5.027577	20.386478
O	0.932735	4.525662	5.631635	O	4.701635	6.065027	20.373026
C	2.886716	2.913184	7.202083	C	6.962379	4.815107	18.387648
C	4.354491	2.456639	7.391565	C	7.345816	4.154738	17.070452
C	1.953997	2.323432	8.264928	O	7.418686	2.932467	16.933422
C	4.992465	2.841271	8.740232	O	6.020786	4.470917	21.326011
H	3.225870	4.025611	4.538549	H	4.371392	5.778446	18.000319
H	2.237475	1.507459	5.710332	H	5.600697	3.267973	18.975375
H	2.880505	4.008896	7.304939	H	7.717133	4.537769	19.132320
H	4.397796	1.363305	7.291374	H	6.976738	5.910335	18.295159
H	4.966321	2.886999	6.590842	O	14.053661	6.994575	6.866131
H	2.277607	2.585390	9.275291	H	14.106700	7.860069	7.303703
H	0.925271	2.681375	8.150472	H	13.128335	6.910730	6.570712
H	1.948351	1.226027	8.193285	O	5.629306	5.279693	24.881060
H	6.059064	2.588738	8.731214	H	6.359696	5.744101	24.445030
H	4.886155	3.917984	8.930999	H	5.265452	4.767405	24.138963
H	4.519788	2.315192	9.576874	O	11.856927	6.631094	0.565458
N	-0.052935	2.513212	5.157954	H	12.747355	6.952791	0.766665
C	-1.296538	3.065895	4.602756	H	11.957882	6.139600	-0.263804
C	-2.490578	2.428365	5.333222	O	14.820374	6.555387	1.206294
O	-2.577648	1.187411	5.373460	H	15.201618	7.446486	1.231386
C	-1.444106	2.797045	3.071511	H	14.930686	6.279938	0.281490

Quantum refinement with xTB $\omega_c=1.0$

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 C -1.222431 3.922077 10.012362
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 H -0.498302 5.150367 8.367848
 H -2.605059 6.287564 8.007108
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 H -2.458810 4.436591 15.003684
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 C 2.096041 4.825069 11.618670
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 C 7.188494 4.952660 13.540390
 C 7.755793 4.466233 12.198387
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 H -0.241625 2.621568 1.291250
 H -2.644003 3.497523 1.406136
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 H -2.621355 4.592418 2.778298
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 H -0.489153 4.998585 1.390652
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 C -5.817763 3.375887 5.739857
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 H -4.662289 3.178307 7.554091
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 C -6.817731 2.655694 2.158808
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 H 6.441141 5.819695 24.353439
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 H 11.287542 5.590808 0.743253
 H 11.920050 6.142964 -0.565979
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Quantum refinement with ORCA $\omega_c=1.0$

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 C -2.303943 3.667333 10.875036
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 C -3.619014 5.305707 9.605663
 C -1.318245 4.918067 8.993402
 C -2.530458 5.580082 8.791105
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 H -1.456813 1.880007 11.681444
 H -3.163754 2.147870 12.147797
 H -4.380802 4.166086 11.286098
 H -0.281388 3.358941 10.112971
 H -4.568825 5.827986 9.446307
 H -0.466637 5.178097 8.357941
 H -2.619076 6.316951 7.982890
 H -3.628047 3.511727 14.183866
 H -2.439970 4.453378 15.126626
 H -2.946441 4.853066 13.426145
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 C 2.044670 3.946734 12.878634
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 C 2.099360 4.819890 11.602483
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 H 2.805819 3.149208 12.834429

H	3.072823	5.329442	11.529482	H	7.095609	6.487305	5.919811
H	1.952475	4.189056	10.711588	N	10.978601	4.212626	5.135255
H	1.313113	5.583530	11.655082	C	11.313187	4.483844	3.751760
N	2.454440	4.080319	15.281143	C	10.292312	3.928879	2.759159
C	2.488976	4.572804	16.673195	O	10.371842	4.214638	1.565858
C	3.658786	3.961140	17.435663	C	12.729133	3.937639	3.416582
O	3.699646	2.719906	17.499083	C	13.845989	4.754539	4.045545
C	1.206925	4.238452	17.485932	C	15.212014	4.318314	3.426087
C	-0.085945	4.839213	16.950264	C	16.273179	5.361535	3.730735
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O	-2.363342	4.233712	16.514365	H	11.337858	5.577510	3.619475
H	2.496617	3.062160	15.220972	H	12.788683	2.888393	3.774412
H	2.620088	5.662306	16.570203	H	12.865522	3.937699	2.325239
H	1.093443	3.141380	17.505725	H	13.687502	5.829691	3.846757
H	1.347886	4.585551	18.524532	H	13.856044	4.594365	5.141085
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H	-0.034496	4.874190	15.847664	H	15.104232	4.226459	2.332467
N	7.633456	5.005320	16.018736	H	17.248358	5.087245	3.299486
C	8.125575	4.555715	14.707828	H	15.963781	6.341461	3.333052
C	9.536390	5.128082	14.485554	H	15.594394	5.903790	5.670472
O	9.702157	6.377767	14.500570	H	16.559798	4.527477	5.661332
C	7.185507	4.956286	13.533795	H	17.263599	6.045227	5.497099
C	7.763184	4.460234	12.195995	N	9.336714	3.107791	3.263953
C	5.743780	4.439277	13.713442	C	8.318201	2.441144	2.468820
H	7.613300	6.012723	16.158688	C	6.966375	3.161871	2.544334
H	8.160997	3.454020	14.749607	O	6.882000	4.401056	2.666983
H	7.167803	6.063226	13.536551	H	9.168699	3.046899	4.269411
H	7.038524	4.567659	11.366704	H	8.658577	2.388242	1.422538
H	8.688296	4.984976	11.898354	H	8.199907	1.409626	2.848907
H	8.003176	3.379399	12.242480	N	5.870516	2.351442	2.515139
H	5.123295	4.747800	12.854566	C	4.526418	2.820303	2.582650
H	5.740117	3.334465	13.761401	C	3.843195	2.210289	3.860198
H	5.275918	4.809447	14.636276	O	3.849228	0.979549	4.014744
N	10.574902	4.292182	14.335970	C	3.741102	2.472480	1.303992
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C	12.173446	5.407588	12.785886	H	4.548675	3.913806	2.703755
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H	10.457331	3.282502	14.336484	H	4.216354	2.962430	0.438050
H	12.142070	5.580286	14.939556	H	3.733446	1.379830	1.161760
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N	12.169957	4.547495	11.689315	C	2.344292	2.614352	5.784499
C	12.497524	4.917693	10.345112	C	0.991756	3.279301	5.534501
C	11.559775	4.271924	9.320746	O	0.922270	4.540841	5.641338
O	11.355687	3.050199	9.285794	C	2.887849	2.921276	7.200654
C	13.950519	4.468067	10.018909	C	4.361939	2.464775	7.403519
O	14.289077	4.681644	8.666969	C	1.960479	2.348870	8.267906
H	11.942425	3.564406	11.838302	C	5.001424	2.858271	8.761804
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H	14.642200	5.007094	10.697423	H	2.236202	1.520398	5.715869
H	14.035938	3.382618	10.198795	H	2.892106	4.027794	7.290221
H	14.334452	5.640199	8.521380	H	4.401749	1.360772	7.322961
N	10.894465	5.119738	8.476646	H	4.983857	2.890802	6.598045
C	10.052623	4.687193	7.386597	H	2.279600	2.616625	9.287158
C	10.571164	5.146729	6.021633	H	0.923125	2.701567	8.146185
O	10.608692	6.358068	5.709926	H	1.957066	1.241464	8.202653
C	8.583821	5.162299	7.592956	H	6.074900	2.602427	8.759838
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N	7.008858	5.503010	5.689552	N	-0.040349	2.518262	5.163190
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H	10.093284	3.590752	7.407120	C	-2.494275	2.459395	5.323117
H	8.215205	4.801016	8.564057	O	-2.583300	1.196564	5.369236
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Quantum refinement with LSQC $\omega_c=1.0$

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O	12.369296	6.637669	12.659714	H	2.701944	2.819263	1.392221
H	10.432618	3.290035	14.354821	H	4.198645	2.940897	0.442971
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C	11.560774	4.273667	9.320255	O	0.922098	4.542011	5.644195
O	11.352271	3.048783	9.286105	C	2.884202	2.919800	7.201238
C	13.951335	4.471937	10.011277	C	4.362758	2.468300	7.400781
O	14.286994	4.691446	8.651153	C	1.959176	2.348195	8.274583
H	11.923620	3.574656	11.825962	C	5.005391	2.848395	8.762170
H	12.418660	6.013613	10.257285	H	3.224226	4.033904	4.548757
H	14.642869	4.998240	10.683297	H	2.245152	1.520440	5.708369
H	14.037219	3.393811	10.176150	H	2.878183	4.016978	7.293534
H	14.327006	5.652225	8.500851	H	4.405423	1.374117	7.311007
N	10.896356	5.121489	8.474856	H	4.973931	2.895213	6.598649
C	10.052456	4.681360	7.385746	H	2.287600	2.627444	9.278555
C	10.571738	5.146742	6.021751	H	0.927103	2.693266	8.154473
O	10.610753	6.362044	5.712336	H	1.959032	1.248787	8.217824
C	8.586137	5.160761	7.599098	H	6.071726	2.596476	8.750087
C	7.697410	4.609618	6.420469	H	4.898489	3.925796	8.948858
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H	6.453538	5.213319	4.892534	C	-0.130230	3.082431	2.271532
H	7.073797	6.490724	5.888693	C	-2.640427	3.546754	2.475072
N	10.976288	4.211324	5.134861	C	0.239777	4.544378	2.058120
C	11.314414	4.485870	3.750620	H	-0.030194	1.506951	5.248964
C	10.289846	3.924269	2.761153	H	-1.251324	4.164750	4.806983
O	10.368726	4.205958	1.562432	H	-1.609577	1.731292	3.003427
C	12.730036	3.945424	3.399914	H	0.710501	2.599306	2.789236
C	13.842433	4.771923	4.029803	H	-0.237804	2.607581	1.287754
C	15.207015	4.341481	3.412006	H	-2.652870	3.498990	1.384927
C	16.267960	5.380568	3.715185	H	-3.576472	3.105915	2.831495
N	16.430890	5.485971	5.237906	H	-2.632889	4.606023	2.760108
H	11.057971	3.251866	5.453719	H	1.239414	4.609920	1.610954
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H	13.675885	5.838846	3.838801	C	-4.616568	2.808404	6.530799
H	13.851470	4.609091	5.116761	C	-5.834109	3.370497	5.731490
H	15.511574	3.368950	3.824834	O	-5.938792	4.610883	5.596889
H	15.106286	4.253830	2.326542	H	-3.274159	4.291817	5.877646
H	17.237984	5.109404	3.293956	H	-4.583481	1.719484	6.584180
H	15.964942	6.356483	3.329089	H	-4.681543	3.203531	7.551695
H	15.592141	5.917255	5.666444	N	-6.731419	2.484010	5.265255
H	16.544347	4.553600	5.654899	C	-7.959807	2.852863	4.556617
H	17.246990	6.051717	5.491151	C	-9.286170	2.297449	5.252243
N	9.336149	3.105449	3.269453	O	-9.093718	1.403516	6.113920
C	8.318380	2.440376	2.469585	C	-7.965831	2.278997	3.125244
C	6.967923	3.160928	2.551000	C	-6.822212	2.657085	2.142747
O	6.884859	4.404777	2.673814	C	-5.734580	1.559323	2.171521
H	9.188876	3.060179	4.272254	C	-7.396535	2.826603	0.722335
H	8.662236	2.400143	1.431413	O	-10.361011	2.784174	4.821961
H	8.213368	1.411749	2.833942	H	-6.537806	1.493737	5.338297
N	5.871597	2.352202	2.520611	H	-7.967200	3.943114	4.533471
C	4.525701	2.826847	2.583705	H	-7.973001	1.179494	3.212426
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C	7.351819	4.179387	17.066116	O	14.530438	6.451259	1.125312
O	7.409656	2.940198	16.939514	H	13.559181	6.457050	0.938050
O	6.024302	4.483132	21.370648	H	14.929763	6.423892	0.242888
H	4.376639	5.800166	17.957981				