Electronic Supplementary Material for PCCP

Modeling the Zn^{+2} binding in the 1-16 region of the amyloid β peptide involved in Alzheimer's disease

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March 27, 2009

Supplementary material

Trajectories:
The CP-MD trajectories of representative model ASP1 is provided in AMBER CRD format (x, y, z for each atom in Å) and compressed using the program BZIP2. The PDB file ASP1_first.pdb contains the t =0 structure and the necessary information for graphical representation. A script file for VMD is also provided.

Parameters used for semiempirical models of Zn-Aβ(1-16) complexes. No torsional parameters have been used (all parameters are set to zero). Atoms not indicated are those in the PARM94 Amber force-field. Atom type X indicates any possible atom involved.

Lennard-Jones parameters for Zn.
ϵ (ZN-ZN) = 0.25104 kJ/mol
σ (ZN-ZN) = 3.296 Å

All the other atoms have the same Lennard-Jones parameters of the corresponding atoms in PARM94 force-field.

Table 1: Summary of atom types

PDB atom name	Atom type
Zn	ZN
Nδ1 (His 6, 14)	NB
Nϵ2 (His 13)	NA
Oδ (Asp)	OA
Oϵ (Glu)	OA
Oη (Tyr)	OB

Table 2: Stretching parameters, energy contribution per pair is given by $U_{str} = k_{str}/2 \ \ (r - r_{eq})^2$, with r the distance between atoms in the pair.

Pair	k_{str} (kJ mol^{-1} Å^{-2})	r_{eq} $\mathring{A}$
ZN-NA	3464.352	2.1
ZN-NB	3464.352	2.1
ZN-OA	3464.352	2.1
ZN-OB	3464.352	2.1

Table 3: Bending parameters, energy contribution per three atoms is given by $U_{ben} = k_{ben}/2 \ (\theta - \theta_{eq})^2$, with θ the bending angle for the two bonds.

Atoms	k_{ben} (kJ mol^{-1} rad^{-2})	θ_{eq} $^\circ$
X-Zn-X	0	-
X-NB-ZN	585.76	121.5
X-NA-ZN	585.76	121.5
X-OA-ZN	0	-
X-OB-ZN	0	-

Table 4: Point charges of Zn binding residues. All atoms not indicated have the standard PARM94 charges.

Atom	q (e)
Zn	0.5
His bonded to Zn via Nϵ2 (His 13)	
Cβ	-0.0191
Hβ	0.0673
Cγ	0.2
Nδ1	-0.3
Hδ1	0.3
Cϵ1	0.32
Hϵ1	0.036
Nϵ2	-0.3
Cδ2	0.1
Hδ2	0.036
His bonded to Zn via Nδ1 (His 6, 14)	
Cβ	0.01877
Hβ	0.06287
Cγ	0.1
Nδ1	-0.3
Cϵ1	0.32
Hϵ1	0.036
Nϵ2	-0.3
Hϵ2	0.3
Cδ2	0.2
Hδ2	0.036