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IMPLEMENTATION AND APPLICATION OF THE MMFF94 FORCE FIELD

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IMPLEMENTATION AND APPLICATION OF THE MMFF94 FORCE FIELD

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MMFF94 is implemented for molecular mechanics calculation in the quantum chemistry polarizable force field program (QuanPol). As a general force field for organic molecules, the availability of MMFF94 expends the capability of the QuanPol program. The MMFF94 force field atom type determination and parameter matching methods are established and corresponding program routines are written in the FORTRAN language. In this implementation, the MMFF94 atom types can be determined automatically from the connectivity of the input atoms with no or minimum information of formal charges. This implementation of MMFF94 is validated using the 761 standard tests, thus is a complete implementation. MMFF94 molecular dynamics (MD) simulation is used to study the stability of a 21-residue antimicrobial peptide named MSI-78, which is an amphipathic alpha-helical peptide designed as a synthetic analog to the Magainin family peptides. The MD simulation shows that the MSI-78 peptide exhibits random coil structure in aqueous solvent, but alpha-helical structure in the 2,2,2-trifluoroethanol/water (50:50 V/V) solvent. These results are in good agreement with experiments. The MD simulation also suggests that the preferential stabilization of the folded alpha-helical structure of MSI-78 in the 2,2,2-trifluoroethanol/water solvent is due to its lower dielectric constant as compared to aqueous solvent.

Table of Contents

List of Abbreviations

QM	Quantum Mechanics
MM	Molecular Mechanics
QuanPol	Quantum Chemistry Polarizable Force Field program
MMFF94	Merck Molecular Force Field 94
DFT	Density Function Theory
HF	Hartree-Fock
CHARMM	Chemistry at Harvard Molecular Mechanics
AMBER	Assisted Model Building with Energy Refinement
OPLS-AA	Optimized Potentials for Liquid Simulations-All Atom
MD	Molecular Dynamics
PBC	Periodic Boundary Condition
TZP	Core double zeta, valence triple zeta, polarized basis set
6-31G*	A valence double-zeta polarized basis set defined for the atoms H-Zn
MP2	Second order Møller-Plesset perturbation theory method
MP4SDQ	Fourth-order Moller-Plesset perturbation theory and omits the contribution of triple excitations
GAMESS	General Atomic and Molecular Electronic Structure System
AMP	Antimicrobial peptides
TFE	2,2,2-Trifluoroethanol

CHAPTER 1 Introduction

1.1 Overview

Quantum mechanics (QM) methods were established in the 1920s. The milestone of QM theory is the proposition of the time-dependent Schrödinger equation, which states that a wavefunction can fully specify the state of a system.[1] As a very accurate method but limited by its computational cost, QM methods can be hardly used for large size system. Molecular mechanics (MM) methods have been wieldy applied in condensed phases and bio-molecular simulations.[2] Comparing to QM methods, MM methods show their advantage in computational efficiency but disadvantage in accuracy. Due to the lack of description of electronic structure, MM methods cannot be used to simulate chemical reactions. Combined QM/MM method was proposed by Warshel and Levitt in 1976,[3] which could combine the advantages of QM and MM methods. Recently we developed QuanPol as a full spectrum and seamless QM/MM program.[4] In QuanPol, MM force fields include Chemistry at Harvard Molecular Mechanics (CHARMM), Assisted Model Building with Energy Refinement (AMBER), Optimized Potentials for Liquid Simulations-All Atom (OPLS-AA), and MMFF94.

In QuanPol, the implementation of MMFF94 includes three parts: automatic atom-type determination, parameter searching, and the interface with the QuanPol program. As a general force field, the implementation of MMFF94 improves MM calculation capability of QuanPol, and provides a basis for the development of a more general force field.

1.2 Theoretical background

1.2.1 Molecular mechanics force field

Molecular mechanics (MM) methods model molecular system in classical mechanics, and can be generally used in molecular geometry optimization and molecular dynamics simulation. The atoms are treated as classical mass points linked by interatomic interactions, which include bonded terms relating to atoms that are linked by covalent bonds, and nonbonded terms describing the long-range electrostatic and van der Waals interactions. The total potential energy of the system in molecular mechanics is calculated as the sum of individual energy terms defined for a force field. The parameters in the force fields are optimized according to experimental or high-level QM calculated results.

In some popular force fields (e.g. AMBER,[5] CHARMM,[6] GROMOS,[7] CFF,[8] MMFF,[9] MM3,[10] MM4,[11] UFF,[12]) the potential energy is given in analytical formula.

The potential energy in MM force field can be written:

$$E_{MM} = E_{bond} + E_{ang} + E_{tors} + E_{vdw} + E_{ele} + E_{cross} \quad (1.1)$$

where E_{bond} is the bonding energy between atoms. E_{ang} is the angle bending energy between two atoms bonded to a third atom. E_{tors} is the energy associated with the rotational motion of bonds. E_{vdw} describes the energy combined repulsion and dispersion Van der Waals interactions between two atoms. E_{ele} represents the energy in the system due to electrostatic interactions. E_{cross} stands for a hybrid effect of coupling energy terms.

1.2.2 Molecular dynamics simulation

Molecular dynamics simulation method can sample the system successfully by integrating Newton's law of motions. It is generally used in chemical physics, material science and biological science. The limitation of MD simulation is the weakness in description of quantum effect.[13] The direct result of MD simulation is a time-correlated trajectory that specifies the positions and velocities of all the particles. The macroscopic observables such as pressure, heat capacities, etc., can be generated via statistical mechanics. This computational method calculates the time-dependent behavior of a N-body system. The system will reach dynamic equilibrium when all thermodynamic properties of the system no longer change with time. In MD simulation, the simulation size (number of particles), time-step and total time duration must be carefully designed to guarantee the job can be finished within a reasonable time period. To match with laboratory conditions, NPT (constant particle number, pressure and temperature) ensemble is usually used in the biological system simulations.

In MD simulation, cumulative errors in numerical integration can be minimized with proper selection of algorithms, but not eliminated completely. The *Verlet*[14] integration algorithm and a modified Beeman[15] integration algorithm are implemented in QuanPol for MD simulation. The content below is a brief description of integration algorithm in MD simulation.

As the centers that divide most mass of an atom, nuclei are good model points to carry out the dynamic simulation in classical mechanics. The expression of Newton's second law can be written as:

$$-\frac{dV}{d\boldsymbol{r}} = m\frac{d^2\boldsymbol{r}}{dt^2} \tag{1.2}$$

where V is the potential energy at position $\boldsymbol{r}$. As a vector, $\boldsymbol{r}$ can give lengths and directions for all the particles.

A set of position $\boldsymbol{r}_i$, that interval Δt (time step) can be presented as Taylor expansion:

$$\begin{aligned}\boldsymbol{r}_{i+1} &= \boldsymbol{r}_i + \frac{\partial \boldsymbol{r}}{\partial t}(\Delta t) + \frac{1}{2}\frac{\partial^2 \boldsymbol{r}}{\partial^2 t}(\Delta t)^2 + \frac{1}{6}\frac{\partial^3 \boldsymbol{r}}{\partial^3 t}(\Delta t)^3 + \ldots \\ \boldsymbol{r}_{i+1} &= \boldsymbol{r}_i + \boldsymbol{v}_i(\Delta t) + \frac{1}{2}\boldsymbol{a}_i(\Delta t)^2 + \frac{1}{6}\boldsymbol{b}_i(\Delta t)^3 + \ldots\end{aligned} \tag{1.3}$$

where $\boldsymbol{v}_i$ are the velocities of all particles. $\boldsymbol{a}_i$ are the acceleration; $\boldsymbol{b}_i$ are the hyper accelerations of all particles. Substitute Δt with $-\Delta t$, we can get:

$$\boldsymbol{r}_{i+1} = \boldsymbol{r}_i - \boldsymbol{v}_i(\Delta t) + \frac{1}{2}\boldsymbol{a}_i(\Delta t)^2 - \frac{1}{6}\boldsymbol{b}_i(\Delta t)^3 + \ldots \tag{1.4}$$

sum Eq. (1.3) and Eq. (1.4), we get:

$$\begin{aligned}\boldsymbol{r}_{i+1} &= (2\boldsymbol{r}_i - \boldsymbol{r}_{i-1}) + \boldsymbol{a}_i(\Delta t)^2 + \ldots \\ \boldsymbol{a}_i &= \frac{F_i}{m_i} = -\frac{1}{m_i}\frac{dV}{d\boldsymbol{r}_i}\end{aligned} \tag{1.5}$$

Verlet[14] integration algorithm solves Newton's equation numerically. The accurate description of motions requires short step-time, but calls for more compute cost.

A modified Beeman[15] integration algorithm computes the positions $\boldsymbol{r}_{i+1}$ using full predictor-corrector scheme.

$$\boldsymbol{r}_{i+1} = \boldsymbol{r}_i - \boldsymbol{v}_i(\Delta t) + \frac{2}{3}\boldsymbol{a}_i(\Delta t)^2 - \frac{1}{6}\boldsymbol{a}_{i-1}(\Delta t)^2 + \ldots \tag{1.6}$$

Predicted velocities $\boldsymbol{v}_{i+1}$ will be derived as

$$\boldsymbol{v}_{i+1} = \boldsymbol{v}_i + \frac{3}{2}\boldsymbol{a}_i\Delta t - \frac{1}{2}\boldsymbol{a}_{i-1}\Delta t + ... \tag{1.7}$$

Velocities can be corrected by applying the $\boldsymbol{a}_{i+1}$ at position $\boldsymbol{r}_i$ and predicted $\boldsymbol{v}_i$

$$\boldsymbol{v}_{i+1} = \boldsymbol{v}_i + \frac{5}{12}\boldsymbol{a}_{i+1}\Delta t + \frac{2}{3}\boldsymbol{a}_i\Delta t - \frac{1}{12}\boldsymbol{a}_{i-1}\Delta t + ... \tag{1.8}$$

In QuanPol, the initial velocities to all mass points was assigned by applying the method developed by Zhou et al.[16]

1.2.3 Physical properties in MD simulation

In MD simulations, temperature can be calculated from the velocities:

$$T = \sum_{i=1}^{N} \frac{m_i v_i^2}{N_{df} k_b} \tag{1.9}$$

Here, v_i is velocity of particle i. m_i is mass of particle i, N is the total number of particle, N_{df} is the number of degrees of freedom in the system, k_b is the Boltzmann constant.

The Berendsen thermostat[17] algorithm and Andersen thermostat[18] algorithm are used to re-scale velocities of particles in molecular dynamics simulation to control the simulation temperature. The Berendsen thermostat algorithm is very efficient for relaxing a system to the target temperature. In Berendsen thermostat algorithm, the temperature of a system is coupled to an external heat bath with fixed temperature of T_0. The velocities are scaled at each step, such that the rate of change of temperature is proportional to the difference in temperature:

$$\frac{dT(t)}{dt} = \frac{T_0 - T(t)}{\tau} \tag{1.10}$$

Herein, t is time. $T(t)$ is the temperature of system at time t. τ is the coupling parameter, which determines how tightly the bath and the system are coupled together (commonly default as 200 fs). This method gives an exponential decay of the system towards the desired temperature. The scaling factor for the velocities is:

$$\lambda = \left\{ 1 + \frac{\Delta t}{\tau} \left[\frac{T_0}{T(t - \frac{\Delta t}{2})} - 1 \right] \right\}^{1/2} \tag{1.11}$$

Many methods can be used to determine pressure. In QuanPol, Pressure P is computed with the virial equation:

$$P = \frac{1}{3V} \left[\sum_i^N m_i v_i^2 - \sum_i^N \sum_{j>i}^N (r_{ij} \cdot f_{ij}) + U_{Ewald}^{reci} \right] \tag{1.12}$$

In this equation, v_i is velocity of particle i, m_i is mass of particle i. N is the total number of particle, V is the volume of the master periodic boundary condition (PBC) box, r_{ij} is the vector from mass point i to point j, f_{ij} is the pair-wise force from mass point i to point j. U_{Ewald}^{reci} is the reciprocal term in Ewald summation[19].

The Berendsen barostat algorithm[17] is implemented to control the pressure. In Berendsen barostat, the pressure is set toward a desired value by changing the dimensions of the simulation cell size by scaling factor (for each dimension) in each MD step. Equations of motion are modified with a first order relaxation of P towards a reference P_0

$$\left(\frac{dP}{dt} \right)_{bath} = \frac{P_0 - P}{\tau_P} \tag{1.13}$$

The scaling factor is

$$\mu = \left[1 - \frac{\beta \Delta t}{\tau_P} (P_0 - P(t) \right]^{1/3} \tag{1.14}$$

Where P_0 is the desired value of pressure, τ_p (commonly default as 200 fs) the coupling time constant for the pressure scaling and β (typically set as $4.9 \times 10^{-5}\ bar^{-1}$) the isothermal compressibility of the system. The scaling is done for all components of the atom positions as well as the simulation cell dimensions. Particle coordinates $\boldsymbol{r}_i$ are scaled as

$$r_i^{'} = \mu r_i \tag{1.15}$$

1.2.4 Peptide folding simulation

The methodology we applied in this project is long time molecular dynamics simulation, which strictly distinct from experimental studies. *ab initio* MD folding simulations are low efficient due to random pathway, and high opportunity cost. Implicit solvent model and umbrella sampling are commonly used to get energy minimum point on energy landscapes. In order to get reasonable results, long-time (more than 1 microsecond) simulation processes is required. Thus, this work is unaffordable for an ordinary compute cluster. Since MIS-78 (name of an antimicrobial peptide) is known to have an alpha-helix structure, the strategy of this study is starting MD simulation from an alpha-helix structure to test the stabilization mechanism, which has significant advantage in time saving. To track the folding level, hydrogen bond distances between oxygen in C=O on *i* residue and N on *i+4* residue will be monitored during MD simulation. The distance within 3.5 Å is acceptable.

1.2.5 Dielectric constant calculation

As an important indicator for the thermodynamic polarization of a system, dielectric constant (relative static permittivity) will be calculated during the MD simulation by applying the equation:

$$\varepsilon = 1 + \frac{4\pi(\langle M^2 \rangle - \langle M \rangle^2)}{3\varepsilon_0 \langle T \rangle \langle V \rangle k_B} \tag{1.16}$$

Where, M is the total dipole moment. ε_0 is the vacuum permittivity, usually taken as 1. k_B is the Boltzmann-constant. T is tempter. V is volume. ⟨ ⟩ means take an average.

CHAPTER 2 Implementation of MMFF94

2.1 Introduction

MMFF94 is a molecular modeling force field developed in 1994 and reported in 1996.[9, 20, 21] MMFF94 is designed to deal with condensed-phase processes in molecular dynamics simulation and molecular geometry optimization in proteins and other biological systems. MMFF94s, a variant of MMFF94, provides a better match to the time-averaged static molecular geometry. The parameters in MMFF94s have a slight difference in the energy term of out-of-plane bending and torsion interactions on planarize certain types of delocalized trigonal nitrogen atoms.

The core part of MMFF94 is derived from QM computational data (e.g. HF[22]/6-31G*[23], MP2[24]/6-31G[23]*) and evaluated at a defined approximation to high-level QM computational data (e.g. MP4SDQ[24]/TZP[25], MP2[24]/TZP[25]). The parameters are assigned according to the experimental results or high-level QM computation data, and can be classified into seven energy terms. For each energy term, the parameters will be addressed by matching atom-types and energy-term-types. Operating mechanisms and policies of this system are described in great details in the literature[9, 20, 21]. The descriptions of potential energy functions and implementation strategy are presented below.

2.2 Potential energy functions

Aiming to achieve high accuracy for calculation, well-characterized equations are applied in each energy division. The following is a complete description of the force field presented in articles of MMFF94.[9, 20, 21]

The total potential energy is expressed as the summary of:

$$E_{MMFF} = \sum EB_{ij} + \sum EA_{ijk} + \sum EBA_{ijk} + \sum EOOP_{ijk;l} + \sum ET_{ijkl} + \sum EvdW_{ij} + \sum EQ_{ij} \qquad (2.1)$$

$\sum EB_{ij}$: for the sum of Bond stretching energy

$\sum EA_{ijk}$: for the sum of Angle bending energy

$\sum EBA_{ijk}$: for the sum of Stretch-bend interaction energy

$\sum EOOP_{ijk;l}$: the sum of Out-of-plane bending at tricoordinate centers energy

$\sum ET_{ijkl}$: for the sum of Torsion interactions energy

$\sum EvdW_{ij}$: for the sum of Van der Waals interactions energy

$\sum EQ_{ij}$: for the sum of Electrostatic interactions energy

Bond stretching interactions was represented via equation:

$$EB_{ij} = 143.9325 \frac{kb_{ij}}{2} \Delta r_{ij}^2 \left(1 + cs\Delta r_{ij} + \frac{7}{12} cs^2 \Delta r_{ij}^2\right) \qquad (2.2)$$

Here, $\Delta r_{ij} = r_{ij} - r_{ij}^0$, the difference of distance between atom i and atom j to the reference bond length. kb_{ij} is the force constant between the atoms. $cs = -2\text{Å}^{-1}$ is the "cubic-stretch" constant, aiming to fit the fourth order expansion of a Morse function.[26, 27]

MMFF94 represents angle bending interaction via equation:

$$EA_{ij} = 0.043844 \frac{ka_{ijk}}{2} \Delta v_{ijk}^2 \left(1 + cb\Delta v_{ijk}\right) \tag{2.3}$$

where $\Delta v_{ijk} = v_{ijk} + v_{ijk}^0$, difference between angle of atom *i, j, k* to the reference angle. ka_{ijk} is the force constant this angle. $cb = -0.4\ rad^{-1}$ is the "cubic-bend" constant. For the angle between delocalized single bonds or small rings, MMFF94 will present the energy by equation:

$$EA_{ij} = 143.9325 ka_{ijk} \left(1 + \cos \Delta v_{ijk}\right) \tag{2.4}$$

As a cross term, related to bending interactions and stretching interactions, stretch-bending interactions is presented as:

$$EBA_{ijk} = 2.51210(kba_{IJK} \Delta r_{ij} + kba_{KJI} \Delta r_{kj}) \Delta v_{ijk} \tag{2.5}$$

Δr and Δv have the same definition in stretching and bending. kba_{IJK} and kba_{KJI} are force constants, which the $i - j$ and $k - j$ stretches to the $i - j - k$ bend.

The out-of-plane bending interactions are normally represented by MMFF94 as:

$$EOOP_{ijkl} = 0.043844 \frac{koop_{ijkl}}{2} \chi_{ijkl}^2 \tag{2.6}$$

In this equation, χ_{ijkl} is the Wilson angle (**Figure 1**) between the $j - l$ bond and the $i - j - k$ plane and $koop_{ijkl}$ is the angle force constant. l atom can be rotated with $i.k.j$ will always be the center of this Wilson angle.

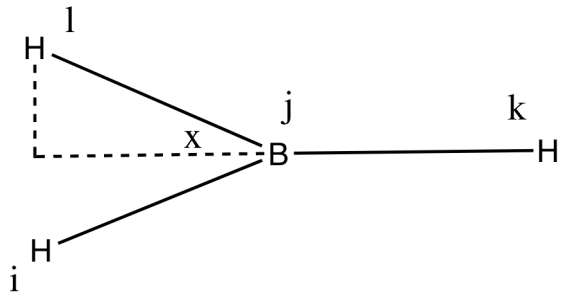

Figure 1. Out-of-plane angle in MMFF94

For torsional bending interactions, MMFF94 uses the potential energy representation:

$$ET_{ijkl} = \frac{1}{2}\left[V_1(1+\cos\phi) + V_2(1+\cos 2\phi) + V_3(1+\cos 3\phi)\right] \tag{2.7}$$

Herein, V_1, V_2, and V_3 are constants, which depend on orbital hybridization condition of the atoms (atom types). ϕ is the $i-j-k-l$ torsion angle (**Figure 2**).

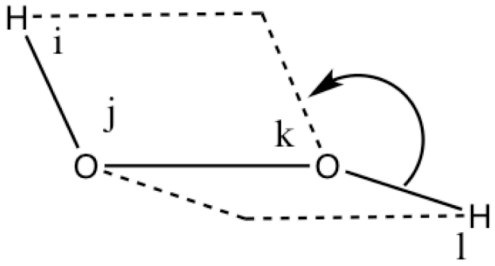

Figure 2. Torsion angle in MMFF94

MMFF94 utilizes the following representation (buffered-14-7) for Van der Waals

interactions:

$$EvdW_{ij} = \varepsilon_{IJ}\left[\left(\frac{1.07R_{IJ}^{*}}{R_{ij}+0.07R_{IJ}^{*}}\right)^{7}\left(\frac{1.12R_{IJ}^{*7}}{R_{ij}^{7}+0.12R_{IJ}^{*7}}-2\right)\right] \tag{2.8}$$

Here, the minimum-energy separations between i, j, R_{ij}^{*} expressed as:

$$R_{ij}^{*} = \frac{1}{2}\left(R_{II}^{*}+R_{JJ}^{*}\right)\left[1+0.2\left(1-e^{-12r_{ij}^{2}}\right)\right] \tag{2.9}$$

and

$$R_{II}^{*} = A_I a_I^{0.25} \tag{2.10}$$

$$r_{IJ} = \frac{R_{II}^{*}-R_{JJ}^{*}}{R_{II}^{*}+R_{JJ}^{*}} \tag{2.11}$$

a_I in Eq. (2.10) is the atomic polarizability of atom type I. A_i and G_i is scale factors

The well-depth is presented in the Slater-Kirkwood expression:

$$\varepsilon_{IJ} = \frac{181.16G_I G_J a_I a_J}{R_{IJ}^{*6}\left[\left(\frac{a_I}{N_I}\right)^{\frac{1}{2}}+\left(\frac{a_J}{N_J}\right)^{\frac{1}{2}}\right]} \tag{2.12}$$

Herein, when any of i, j is hydrogen bond acceptor or donor, the formation of Eq. (2.9) and Eq. (2.12) will be different. For details, please refer to the literatures.[9, 20, 21] Owing to choose of the buffered-14-7 style potential, MMFF94 bypass the interactions of 1–2, 1–3, or 1–4 pairs. Thus, 1–2, 1–3, and 1–4 exclusion lists must be generated in the neighbor list.

Electrostatic interactions are represented in the buffered columbic form.

$$EQ_{ij} = 332.07\frac{Q_i Q_j}{D(R_{ij}+\delta)^{n}} \tag{2.13}$$

D is the dielectric constant. D and n are usually taken as 1. Q_i and Q_j are the poplar on atom *i, j*. 1–4 electrostatic interactions are scaled by 0.75.

In these energy terms, MMFF94 force field also sets the rules for types in bond, angle, torsion, streach-bend energy terms.

The bond-type is taken as '0' for all ordinary bond, but taken as '1' when a formally single bond between sp- or sp2-hybridized atoms of types that can participate in multiple (double or triple) bonding.

Table 2.1. Angle-type matching mechanism

Type	Structural significance
0	The angle i-j-k is a "normal" bond angle
1	Either bond i-j or bond j-k has a bond type of 1
2	Bonds i-j and j-k each have bond types of 1; the sum is 2
3	The angle occurs in a three-membered ring
4	The angle occurs in a four-membered ring
5	In a three-membered ring and the sum of the bond types is 1
6	In a three-membered ring and the sum of the bond types is 2
7	In a four-membered ring and the sum of the bond types is 1
8	In a four-membered ring and the sum of the bond types is 2

Table 2.2. Stretch-bend-type matching mechanism

Stretch-bend-type	Angle-type	Bond-type (ij)	Bond-type (jk)
0	0	0	0
1	1	1	0
2	2	0	1
3	2	1	1
4	4	0	0
5	3	0	0
6	5	1	0
7	5	0	1
8	6	1	1
9	7	1	0
10	7	0	1
11	8	1	1

Table 2.3. Torsion-type matching mechanism

Torsion-type (IJKL)	Structural significance
0	Normal torsion angle
1	Bond-type (JK) is 1
2	Bond-type (JK) is 0, Bond-type (IJ) or Bond-type (KL) is 1
4	IJKL In a four-membered ring
5	IJKL In a five-membered ring

2.3 Implementation and computational methods

The implementation work is presented in three parts. The first part is a global analysis of molecular information, which can determine bond-orders and type of functional groups. Based on the molecular information, the atom-types will be assigned. In the other part, the parameters of all the energy terms will be assigned by matching the atom-types and energy-term-types in force field parameter file. The last part is the interface with the QuanPol program.

In QuanPol, MMFF94 is started from reading the input of GAMESS[28, 29] input file format (.inp). In this kind of input file, only atoms and coordinates are given. QuanPol assigns the MMFF94 types of atoms according to their chemical environments (e.g. neighbored atoms, hybridization).

The first task in the project is to set up a determining system, which can do molecular information analysis.

Determining whether a covalent bond formed between two atoms can be a complicated problem. As the preparation work, it seams to be infeasible to run a QM calculation to get the bond list information for a system with thousands of atoms.

Therefore, we simplified the bond list preparation work by comparing the distances between atoms to the covalent radii by John Emsley[30] (For most elements). The accepted radii for two atoms can be presented as:

$$D_{radii} = \alpha_i R_i + \alpha_j R_j \tag{2.14}$$

where R_i, R_j is the covalent radii of atom i and j. α is the scan factor and normally taken as 1.2. When atom i is hydrogen α will be equal to 1.0.

Based on the information of bond list, the connection relation of each atom will be obtained. And some bond-order can be uniquely determined. For example, the bond connected to H must be single bond, and C atom forming four bonds should form four single bonds. With the known bond order information, applying the logical inference, some more bond order can be determined step by step. For those that cannot be assigned bond order after logical inference, some reasonable speculation will be carried out. In this program, self-inspection work will be followed after the bond order determination work is finished. If some mistake is found, the program will return to the speculate section to continue though other reasonable pathways. The warning or error message will be printed out, when the mistake is unsolvable.

After the types of all the atoms are assigned, the parameters will be addressed by matching atom-types and energy-term-types. The type of torsion parameters could have type conflict but not denote in the original MMFF94 papers. The rank of priority is found to be 1, 4, 2, 5, 0.

Actually, not all the parameters can be matched exactly. Some universal matching rules might be needed in some specific conditions. Furthermore, the parameter file does not cover all the required data that may be needed. Thus, the empirical method will be

used to determine or estimate the missing parameters. Applying the rules presented in the original MMFF94 paper,[20] most of the missing parameters can be computed correctly. However, empirical parameter calculation preformed in our program has some bifurcations to what is presented in Halgren's article.[20]

$$r_{IJ}^0 = r_I^0 + r_J^0 - c\left|\chi_I - \chi_J\right|^n - \delta \tag{2.15}$$

where r_I^0 and r_J^0 stand for covalent radii for type *I, J. c* is the proportionality constant, which is taken to be 0.05 and to be 0.085 when atom *i* or *j* is hydrogen. χ_I and χ_J are Pauling-scale electronegativities defined by Allred and Rochow[31]. The shrinkage factor δ was given as 0.008 Å, which conflicts with test molecule results, and was tested to be 0.0. The flow charts of this program are displayed in **Figure 3** and **Figure 4**.

2.4 Result and discussion

Along with the force field, developers of MMFF94 published a test package with 761 test molecules for MMFF94 and 261 test molecules for MMFF94s, which are computed by OPTIMOL and BatchMin.[32] The following comparison is made between OPTIMOL and QuanPol. The computed results of MMFF94 (**APPEDIX A**) and results of MMFF94s (**APPEDIX B**) matched well with the results of OPTIMOL.

The statistics results are shown in **Table 2.4**. The differences are found to be numeric errors caused by precision arithmetic differences rather than systematic errors. The conclusion is that our implementation in QuanPol is a complete implementation of MMFF94

Table 2.4. The maximum energy (kcal/mol) difference that computed by QuanPol and OPTIMOL in 761 MMFF94 and 264 MMF94s test molecules for each energy term and total potential energy

Energy term	$\Delta \boldsymbol{E}$ in MMFF94	$\Delta \boldsymbol{E}$ in MMFF94s
Maximum Bond stretching	0.00551458	0.00000497
Maximum Angle Bending	-0.00565146	0.00039698
Maximum Stretch-bending	0.00421940	0.00001730
Maximum Torsional bending	0.00616807	-0.00144961
Maximum Out-of-plane bending	-0.00167208	0.00006910
Maximum Van der Waals	-0.00591332	-0.00014757
Maximum Electrostatic interactions	-0.01615691	-0.00981167
Maximum Total energy	0.01141437	-0.00970263

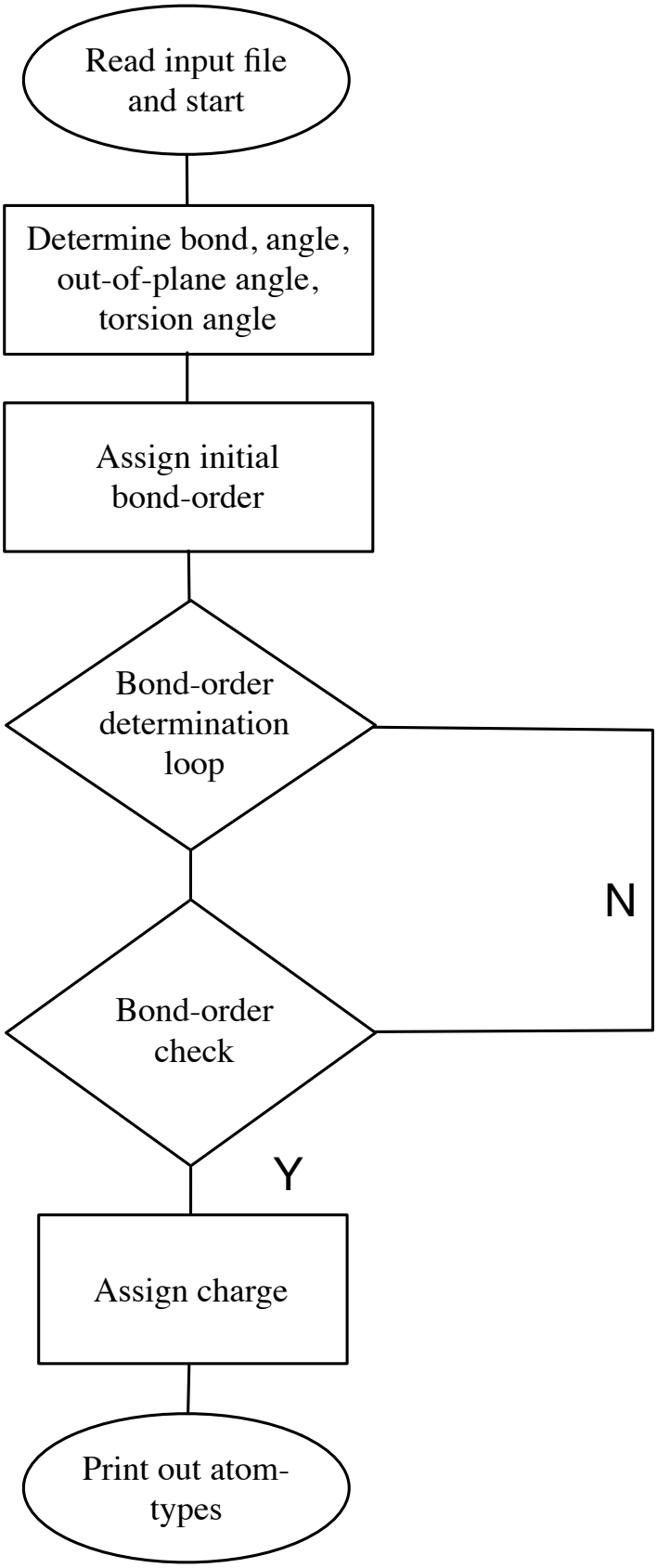

Figure 3. Flow chart of atom-type assigning

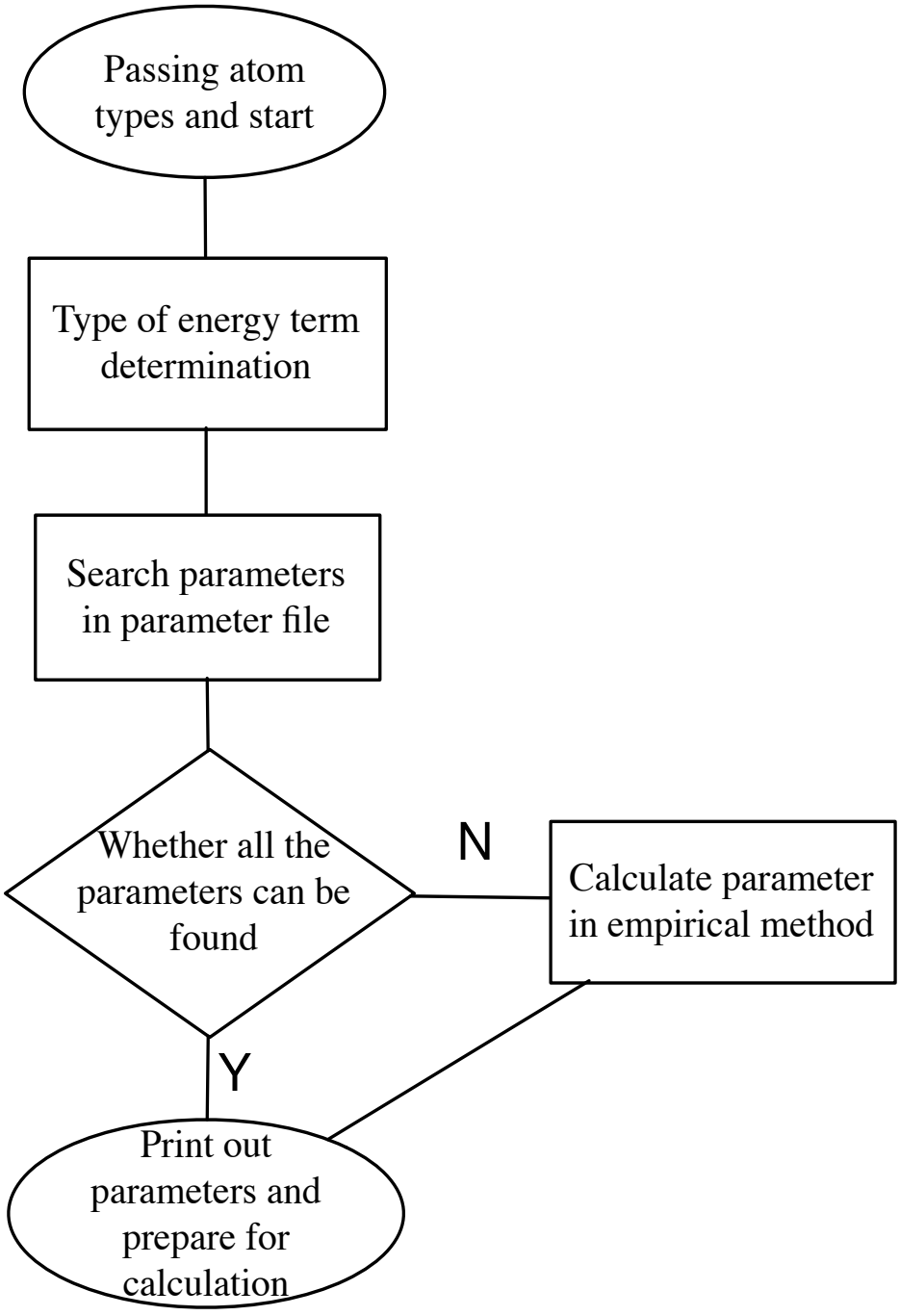

Figure 4. Flow chart of parameter matching

CHAPTER 3 Peptide folding in different solvents

3.1 introductions

Since antibiotics were abused during the last 30 years, antibiotic resistance has become a major clinical and growing public health problem. Besides these conventional antibiotics, large amount of other antibacterial agents were introduced and studied, including polymers, quaternary ammonium and Titanium compounds[33]. However, they all suffer from some side effects, like high cytotoxicity, short-term bacterial protection, or hypersensibility.[34] Antimicrobial peptides (AMPs) are an attractive and new choice for antibiofilm coatings. AMPs are naturally occurring or synthetic substances that can destroy bacteria, fungi, and human cancer cells through permeation of cell membrane without harming mammalian cells.[35] AMPs have attracted more and more attention due to their properties that can overcome the limitations of other antibacterial materials. In this chapter, we chose magainin peptide (MSI-78) as the research subject. MSI-78 was firstly isolated from the frog Xenopus laevis skin, which has a high antimicrobial activity.[36]

MSI-78 is a 22-residue synthetic peptide with the amino acid sequence:

Gly Ile Gly Lys Phe Leu Lys Lys Ala Lys Lys Phe Gly Lys Ala Phe Val Lys Ile Leu Lys Lys -NH_2

Its C-terminus amidation was reported to increase antimicrobial activities of peptides.[37] Previous studies have shown that MSI-78 adopts random coils in aqueous solutions and forms alpha-helix in the presence of lipids or detergents.[38] This project is a MD simulation for MSI-78 in water and 2,2,2-Tribromoethanol (TFE) 50% (V/V)

solution, trying to figure out the structure difference, and to study the mechanism of stabilization.

3.3 Computational methods

MSI-78 structure preparation

The experimental geometry information of MSI-78 was unknown. The MSI-78 geometry used in this project was artificially made by applying the backbone geometry of MSI-594[39], which has a similar protein sequence to MSI-78. The residues that can be protonated in MSI-78 are Lysine. The pK_a of Lysine is roughly equal to 11, so all the Lysine residues were set to be protonated. The Protein Data Bank[40] format file (.pdb) of MSI-78 is shown in **APPENDIX C**.

MD simulation in water:

PBC box was set to be $45\times45\times45$ Å^3, filled with 2705 water molecules, 3 Na^+, 13 Cl^- ions (corresponding to 150 mmol/L ionic strength). The MD simulation was preformed in two steps. The first step is carried out in NPT (constant particle number, pressure and temperature) ensemble for 1 ns, with T = 298.15K, P = 1 bar and with time step size 1 fs. N and O atoms on backbone of MSI-78 fixed. In the second step, the equilibrium trajectory was be used to start new MD simulation for 5 ns at same condition, with distances between 13 and 78, 61 and 141, 122 and 195, 176 and 244, 277 and 350 (atom numbers in PDB file) tracked. The computing time cost is about 75 hours on an

eight-node Linux cluster with a gigabit network. Each node has two Dual Core AMD Opteron 275 Processors (four cores per node and total 32 cores) running at 2.2 GHz.

MD simulation in 50% (V/V) TFE

Initial PBC box was set to be $45 \times 45 \times 45$ $Å^3$, and prepared by filled with 349 TFE and 1428 water molecules (roughly 50% volume ratio). 3 Na^+, 13 Cl^- ions (corresponding to 150 mmol/L ionic strength) were added. The MD simulation was also preformed in two steps. The first step is carried out in NPT (constant particle number, pressure and temperature) ensemble for 1 ns, with T = 298.15K, P = 1 bar and with time step size 1 fs. N and O atoms on backbone of MSI-78 fixed. After reliminary equilibrium, the average temperature of system is 298.0151281789 K, and the average pressure of system is 1.0326227614 bar. In the second step, the equilibrium trajectory was be used to start new MD simulation for 5 ns at same condition, with distances between 13 and 78, 61 and 141, 122 and 195, 176 and 244, 277 and 350 (atom numbers in PDB file) tracked.

Dielectric constant of water

PBC box was set to be $30 \times 30 \times 30$ $Å^3$ filled with 855 water molecules. The preliminary equilibrium was taken for 1 ns in NPT ensemble, with T = 298.15K, P= 1 bar and time step size 1 fs. The dielectric constant was investigated another MD simulation at the same conditions for 5 ns, which start with equilibrium trajectory.

Dielectric constant of 50% (V/V) TFE/water mixture

PBC box was set to be $40 \times 40 \times 40$ $Å^3$ filled with 128 TFE molecules and 512 water molecules. The preliminary equilibrium was taken for 1 ns in NPT ensemble, with T = 298.15K, P= 1 bar and time step size 1 fs. The dielectric constant was investigated another MD simulation at the same conditions for 5 ns, which start with equilibrium trajectory.

3.4 Result and Discussion

Circular Dichroism (CD) spectroscopy results (**Figure 4**) show that MSI-78 shows a random coil structure in aqueous solution, but alpha-helix structure in 50% TFE (V/V) solutions.

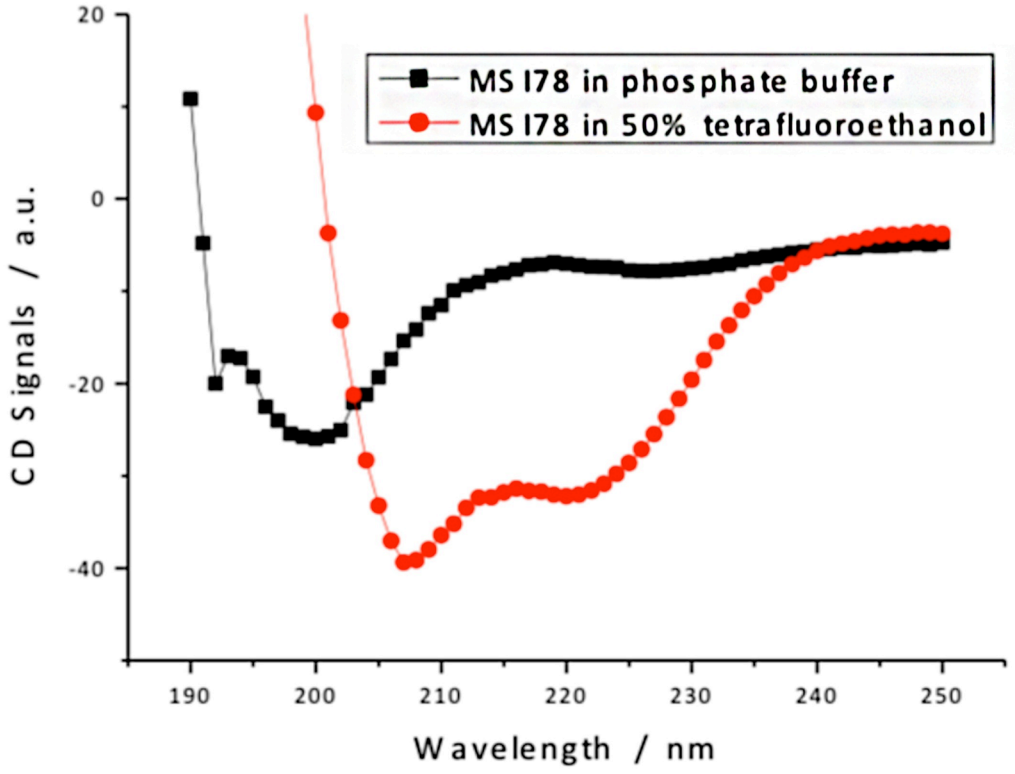

Figure 4. Circular Dichroism spectroscopy of MSI-78 sample is preparing in 10 $\mu mol/L$ Experimental result of CD, and tested on Aviv CD spectrometer, in 50mmol/L ionic strength solution, provided by Dr.

The theoretical result can fully explain experimental result. The MD simulation result is shown in **Figure 5**. In 50% (V/V) TFE water mixture solvent, the average distances between oxygen in C=O on *i* residue and N on *i+4* residue fluctuations in a small range to that of initial geometry (i.e. typical alpha-helix structure). On the other hand, MSI-78 starts to unfold and keeps random coil structure in aqueous solution.

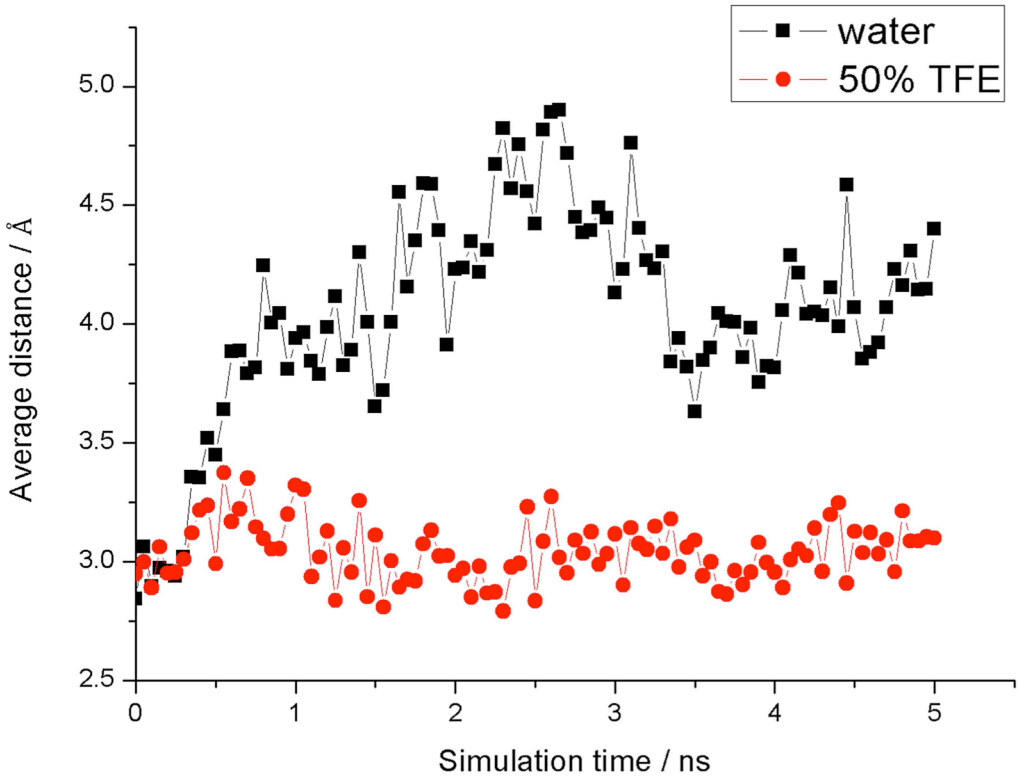

Figure 5. Trend of average distances between oxygen in C=O on *i* residue and N on *i+4* residue over simulation time in 5 ns.

The MD simulation results of dielectric constant are shown in **Figure 6**. Even though the difference between experimental and computational value is obviously, the

relative tendency of dielectric constant property can be used to explain the different solvation effect. In Bron's theory,[41] the solvation free energy correspond to the dielectric constant, distances and strength of opposite partial charge. Bron proposed the favorable change in free energy for transferring the ions from vacuum to water as:

$$-\Delta G = (q^2 / 2r)[1-(1/D)] \quad (3.1)$$

In which D is dielectric constant, r is partial charged atom distance, q is partial charge of atom.

A propertied dielectric constant solvation environment could induce the peptide to the alpha-helix structure.

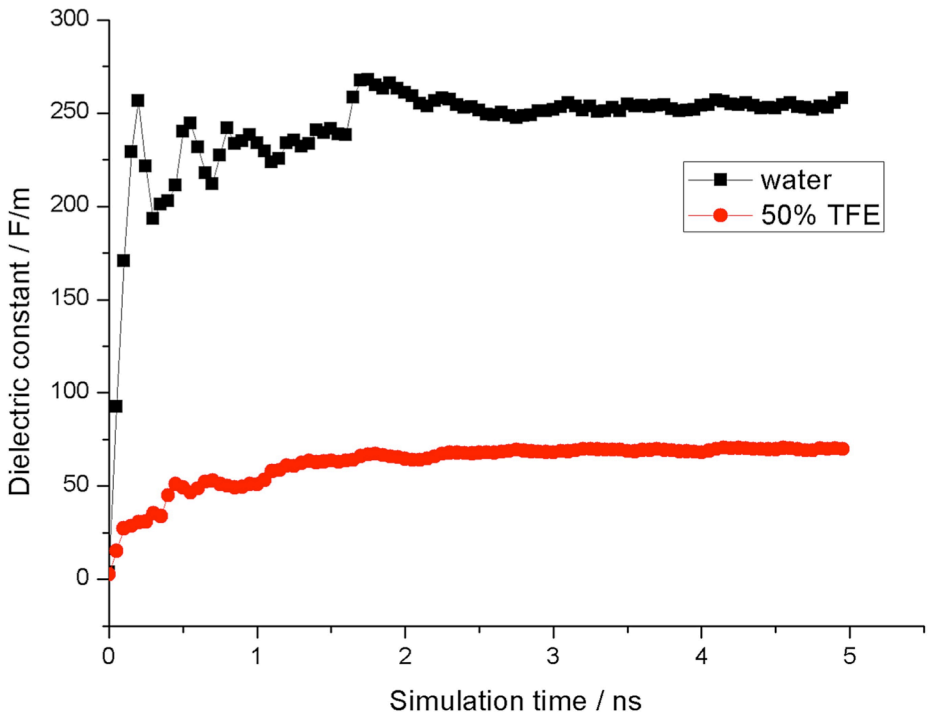

Figure 6. Dielectric constants of water (250) and 50% (V/V) TFE/water solution (70).

TFE is known as a cosolvent on the stability of peptides. To a get better comprehensive understanding of secondary structure-inducing capabilities of TFE, we used MD simulations to study the mechanism. Based on the simulation results, the dielectric constant in TFE/water mixture solution is lower than water. As we know, a lower dielectric constant solution could increase electrostatic interactions. The conception of dielectric constant effect is commonly used in the study of protein and DNA folding.[42] The same conception is also utilized in the study of crystallization.[43] In this specific project, TFE/water cosolvent increases the interactions between opposite polarized atoms in an appropriate level, which means the backbone hydrogen bond strength is enhanced, and side chain interactions are not overemphasized

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APPENDIX A

Comparison between MMFF94 force field energy (kcal/mol) of 761 test molecules computed in QuanPol program and OPTIMOL program is shown in following table. The maximum energy difference is 0.01141437 kcal/mol accrued on FETRUR molecule.

Structure name/Conformational Index	OPTIMOL	QuanPol
AGLYSL01	26.87431	26.87367
AMHTAR01	66.18011	66.17897
AMPTRB10	-18.73262	-18.73109
ARGIND11	-207.43598	-207.43029
BAOXLM01	278.92570	278.91954
BBSPRT10	-13.55387	-13.55318
BEVJER10	18.75343	18.75389
BEWCUB	52.60970	52.61068
BEWKUJ04	-4.78796	-4.78660
BIHKEI01	-42.47323	-42.47138
BIPDEJ02	-70.08179	-70.07948
BIPJUF10	33.27498	33.27538
BIPYCL01	148.41423	148.41156
BITNAT10	65.11954	65.11859
BIYBIU10	51.30021	51.30008
BODKOU	23.36915	23.36926
BSALAP01	6.84068	6.84154
BUPSLB10	56.93022	56.92987
BUPSLD10	-16.46525	-16.46406
BUYTIY10	122.43528	122.43360
BUYTOE10	144.89777	144.89567
BUYXEY10	-2.24767	-2.24682
BYITOT02	27.10908	27.10946
CABWEH10	64.52122	64.52031
CAFORM07	0.01281	0.01281
CAGREH10	-259.51340	-259.50641
CALXES20	-35.97705	-35.97498
CAMALD03	36.83909	36.83840
CEFMEN	33.08425	33.08515
CETROI01	126.08934	126.08730
CEWCUC10	113.91582	113.91419
CEWVIJ10	-123.17150	-123.16803
CEWYIM30	66.77530	66.76901
CIHWUL10	15.14485	15.14474

CIJXOI10	27.48125	27.48142
CIKSEU10	-38.93481	-38.93300
CILBII	-46.87953	-46.87653
CILDOQ	-33.26989	-33.26849
CILWUP11	0.68501	0.68531
CIMRUL10	39.87555	39.87557
CINVIE	38.90984	38.91051
CIPVOM	-2.84100	-2.84040
CIPYAB10	34.87235	34.87261
CISMOG	32.82537	32.82511
CISPOJ	69.57227	69.57169
CITDIS	32.12371	32.12369
CITNOI10	32.01892	32.01887
CITPEA10	34.82777	34.82778
CITSED10	28.49078	28.49014
CIVCEP02	-182.12144	-182.11613
CIVLAU02	16.12615	16.12707
CIXWAH	-15.95417	-15.95321
CIYNUT	68.95129	68.94994
CIZFIA	-18.99671	-18.99542
CIZJAW	7.48409	7.48412
CIZWUD	30.42557	30.42550
CIZYEP	47.66782	47.66795
CIZZUG	-49.57596	-49.57415
COBKIN01	9.80521	9.80549
COCXUN	24.42247	24.42294
COGDEH	106.99152	106.98995
COGYAY	39.56560	39.56521
COHKOZ	58.62058	58.61945
COJFIQ	74.97484	74.97388
COKDEL	11.80918	11.80945
COKROJ	46.31871	46.31848
COLZUY	43.67995	43.67991
COMDIR	46.29230	46.29235
COMKAQ	-7.61770	-7.61711
COMWOQ	31.05100	31.05064
COMWUW	23.74581	23.74591
CONBAI	-127.16493	-127.16094
CONFAM	-44.68386	-44.68253
CONLIA	40.26758	40.26766
CORDOC	57.69573	57.69517
CORWUB10	-84.01803	-84.01568
COSFAR	0.08159	0.08210
COSSEI	-73.95317	-73.95087
COSWIQ	27.25872	27.25912
COTMON	23.49300	23.49333

COTPEG	43.95150	43.95071
COTRIM	46.34354	46.34354
COVHUQ	-34.84357	-34.84302
COVMAB	54.88679	54.88626
COVXIU	-136.04527	-136.04087
COWTIR	-71.22739	-71.22496
COXBAS	-5.38669	-5.38614
COXZEU	-142.02636	-142.02246
COYMOS	2.84235	2.84340
COYNAF	78.55952	78.55833
COYVIV	-76.17420	-76.17176
CUBTUO	62.99488	62.99408
CUCDAF	62.58536	62.58500
CUCHOX	12.51668	12.51720
CUCHUD	107.86578	107.86400
CUDJAM	64.03198	64.03130
CUDNEU	46.57412	46.57350
CUDPAS	122.63660	122.63480
CUDPOG	39.36271	39.36300
CUDREY	-26.29199	-26.29131
CUFFAK	48.34575	48.34629
CUGBEL	-6.31517	-6.31443
CUGGOA	90.33658	90.33540
CUGLOF	25.29487	25.29590
CUJYUB10	77.34274	77.34190
CULGEV10	6.39875	6.39916
CULHIA10	22.96006	22.95994
CULVEK	-28.97125	-28.96973
CUNVAI	124.07957	124.07815
CUNVEM	34.52853	34.52853
CURZIY	39.43648	39.43624
CUVFOO	-43.92628	-43.92485
CUVGAB	78.85250	78.85110
CUVJOS	97.11218	97.10999
CUYRAP	43.42514	43.42506
CYANAM01	-36.48459	-36.48372
CYGUAN01	-254.74397	-254.73620
DABHAP	-61.26979	-61.26702
DABLIB	-0.78636	-0.78576
DACSAB	-81.87365	-81.87113
DACYIP	7.01608	7.01680
DADDAN	-14.11976	-14.11868
DADLAV	31.84138	31.84118
DADLEZ	39.20451	39.20403
DAFKIE	18.68792	18.68810
DAFPUV	31.94967	31.94915

DAGTUA	65.93412	65.93308
DAHBAP	41.42849	41.42842
DAHNAB	1.89669	1.89659
DAJXER	-80.97047	-80.96760
DAKBAS	20.14939	20.15047
DAKCEX	6.83065	6.83134
DAKDOI	52.07023	52.07067
DANCUQ	-32.45004	-32.44908
DAPSUO03	65.72509	65.72466
DARDEF	-16.98389	-16.98289
DARPOB10	-56.15408	-56.15166
DARXID	66.08694	66.08667
DARZEB	-2.51092	-2.51001
DAVWEC	-44.65652	-44.65360
DAVXED	-64.35191	-64.34823
DAWXII	42.33212	42.33151
DAWYUV	20.92222	20.92256
DAYWEF	-244.65194	-244.64591
DAZVEF	69.37451	69.37377
DEBMOM01	-62.78120	-62.77921
DECJAW	5.45573	5.45618
DECKUR	-59.58237	-59.58013
DECRIM	-36.93866	-36.93709
DEDCIY	42.76261	42.76237
DEDSIO	1.32068	1.32127
DEFGIE	30.40441	30.40467
DEFLEF	-296.27657	-296.26761
DEFPUZ	-103.20611	-103.20336
DEFTUD	-19.28221	-19.28040
DEFVAL	13.92912	13.93008
DEFYUI	17.23114	17.23110
DEGLUW	-57.99964	-57.99801
DEGRIQ	-13.92177	-13.91941
DEKRUG	-50.14814	-50.14646
DEMBIG	23.79651	23.79655
DEPKEO	96.11090	96.10956
DERZUV	72.73796	72.73760
DESWUT	41.10067	41.09991
DESYOP	26.36673	26.36622
DEWHOC	87.84014	87.83934
DEWJEU	45.49318	45.49263
DEXCIS	-6.20874	-6.20791
DEXGIW	-60.11998	-60.11805
DEZDUH	50.63786	50.63746
DEZNIF	85.50222	85.50097
DEZXEL	15.13713	15.13764

DHOADS01	37.43734	37.43716
DICKIJ	69.01570	69.01508
DICPUA	39.00857	39.00818
DICRAI	22.87059	22.87055
DICYIX	-1.45480	-1.45464
DICYOD	14.86818	14.86860
DIDYOE	60.09139	60.09061
DIFSIU	83.35147	83.35105
DIGCOL	34.17032	34.16992
DIGCUR	-17.62974	-17.62890
DIGLEK	87.73651	87.73596
DIHTET	9.87683	9.87703
DIKGAF	-14.94346	-14.94220
DIKGEJ	-4.20762	-4.20678
DIKWID	145.34404	145.34121
DIKYUR	37.45468	37.45415
DILCOQ	-52.82481	-52.82304
DIMYIH10	61.29056	61.28986
DIPDAH10	7.20477	7.20574
DIPDIP10	-35.68081	-35.67984
DIRMIA	2.70519	2.70520
DISHES	13.80187	13.80232
DISJOE	76.64152	76.64044
DITRAZ	25.28388	25.28368
DITYAG10	46.54242	46.54219
DIVJUN	86.58284	86.58189
DIVTUX	23.87164	23.87202
DIVVEJ	-315.34316	-315.33542
DIVWEK	47.22938	47.22971
DIWCOB	179.17218	179.16881
DIXJEZ	25.43315	25.43328
DIYDIY	42.18619	42.18594
DIYPOQ	-48.43392	-48.43163
DIYPUW	22.27500	22.27498
DIZPUX	9.74056	9.74097
DMEOXA01	53.54773	53.54674
DOCCIH	99.11440	99.11291
DOCFIK	132.94633	132.94375
DOCWUN	83.14102	83.14019
DODNOZ	-309.76326	-309.75549
DODNUF	-196.30290	-196.29823
DOJPAT	23.11220	23.11229
DONFOB	-154.02320	-154.01851
DOSNOO	-156.15561	-156.15145
DOTNIJ	40.54214	40.54234
DOTVEN	-218.60040	-218.59465

DOTWOY	-2.76358	-2.76258
DOWDEY	-104.77712	-104.77397
DOXXAP	-15.64479	-15.64386
DOXZOF	65.56067	65.55990
DOZFON	167.54961	167.54630
DOZNIP	-239.04493	-239.03825
DUBNET	-20.67230	-20.67082
DUDMUK	52.64434	52.64368
DUGMUN	83.65885	83.65755
DUGWIL01	-157.51276	-157.50855
DUJHEV	4.35715	4.35765
DUJMEA	143.61644	143.61400
DUKVAG	-37.53122	-37.53022
DUKWUB	-0.47215	-0.47152
DULTIN	79.77418	79.77309
DUMHIC	42.98219	42.98213
DUMPAC	-47.19370	-47.19099
DUPHEB	31.37985	31.38031
DUPTAJ	113.43678	113.43460
DURDID	71.65295	71.65164
DUTHIJ	136.91955	136.91757
DUVHUX10	64.08285	64.08210
DUVXIB	-72.46526	-72.46309
DUWGAD	-12.37378	-12.37279
DUWKUB	56.68430	56.68388
DUWRIW	81.67334	81.67223
DUXTIZ	97.25524	97.25321
DUXWUO	54.56841	54.56790
DUXXAV	76.64426	76.64324
DUYNOA	66.17564	66.17531
DUYPES	30.51992	30.52126
DUYRAQ	65.03902	65.03848
FACMIF	76.52254	76.52159
FACREG	113.76824	113.76627
FACYAJ	41.11543	41.11510
FADMIG	58.93381	58.93318
FADVEL	-106.77293	-106.77000
FADVUB	-32.54552	-32.54416
FAGBUK	187.30066	187.29832
FAGCOF	-87.57240	-87.56969
FAGLII	21.99812	21.99807
FAGVEO	90.19710	90.19551
FAGZOC	214.30851	214.30435
FAHPUZ	-47.69082	-47.68848
FAHSUC	-58.35213	-58.34967
FAHYUI	65.43368	65.43318

FAHZET	-142.34477	-142.34046
FAJWIW	-217.77066	-217.76493
FAMHAC	-20.44858	-20.44743
FAMYUN	-21.88548	-21.88483
FAPLUD	-389.23990	-389.23024
FARMAM	15.32885	15.32924
FARSOG	-39.74204	-39.74008
FARWEA	-61.01925	-61.01721
FASGUB	81.36854	81.36728
FASJIS	41.65550	41.65572
FATLIV	-56.35494	-56.35246
FAXFUF10	-104.90436	-104.90161
FAXVAB	-172.35653	-172.35137
FAXVEF	42.51885	42.51827
FAXVIJ	67.72316	67.72261
FAZBAJ	13.14753	13.14771
FAZKUM	35.83595	35.83553
FBATNB	112.60951	112.60893
FECXEQ	89.73554	89.73440
FEGSEP	-82.52081	-82.51914
FEHDAX	-17.65295	-17.65217
FEJJEJ	3.65242	3.65295
FEJKIO	198.60780	198.60393
FELYIE	17.32218	17.32202
FELYUQ	68.22311	68.22252
FEMGEJ	19.89068	19.89059
FENCOQ	41.71703	41.71642
FENHAH	35.23240	35.23168
FENJIR	-21.19718	-21.19533
FENJOX	2.49167	2.49274
FENJUD	-13.90365	-13.90273
FENNUH	-44.53683	-44.53494
FENYIG	12.36498	12.36565
FEPWAY	-136.46417	-136.46054
FEPWOM	-15.19947	-15.19892
FESCAH	-66.59850	-66.59667
FESMIZ	70.03626	70.03548
FETRUR	-433.93729	-433.92588
FETWOQ	-16.43906	-16.43788
FEVNUP	-29.92782	-29.92637
FEYLUQ	-73.24187	-73.23903
FEZPOP	1.20616	1.20648
FEZRUX	39.90989	39.91028
FIBLIL	86.78845	86.78748
FICDOK	87.69205	87.69042
FIFGUW	41.81489	41.81493

FIGYID	-4.04373	-4.04347
FIHXID	-36.90498	-36.90297
FIKJAK	42.79221	42.79194
FIKZOO10	11.54801	11.54836
FILGEM	17.37940	17.38000
FILNOD	57.68163	57.68097
FINBIN	74.95031	74.94973
FINPEX	1.60801	1.60860
FITGIY	3.76800	3.76918
FITSEG	-18.54718	-18.54649
FITTIL	-72.20689	-72.20464
FIVNUT	10.99905	10.99973
FIVRAD	-71.32750	-71.32518
FIXPIL	19.19788	19.19858
FIYBIY	-78.13514	-78.13251
FIZGEA	63.61449	63.61383
FIZGOK	-86.77461	-86.77208
FIZJED	57.67889	57.67821
FOBJUB01	-5.71683	-5.71622
FODTUN	7.86517	7.86597
FOGBIM	24.03593	24.03580
FOGVIG01	-287.57893	-287.57103
FOHXEF	-155.90357	-155.89919
FOHYAC	49.52196	49.52116
FOJBEL	12.83602	12.83598
FOJPAV	10.54302	10.54365
FONCOA	47.11940	47.11909
FORGOI	30.14956	30.14951
FORHEZ	19.85843	19.85853
FORJIF	35.83388	35.83409
FORJUR	44.65007	44.65023
FORTAH	87.87463	87.87376
FOSDIA	44.94385	44.94400
FOVHUT	-294.74544	-294.73783
FOVJIJ	22.56614	22.56612
FOVRAJ	104.46793	104.46639
FOVRUD	96.48010	96.47904
FOWBEY	27.87889	27.87883
FOWPOW	60.55950	60.55936
FOWVES	-7.43616	-7.43559
FOWZAS	41.93185	41.93200
FOYMAH	-4.87726	-4.87993
FOYNUC	53.98090	53.98024
FUCMIZ	-25.93021	-25.92947
FUCMUL	18.31930	18.31890
FUCTIG01	6.41462	6.41458

FUCWIJ	71.19690	71.19636
FUCWOP	-33.35464	-33.35271
FUDPOJ	99.29055	99.28949
FUDXUX	14.66699	14.66675
FUFDIT	-61.71479	-61.71268
FUGWIN	-8.81522	-8.81401
FUHFAP	15.71718	15.71685
FUHSEG	22.72121	22.72154
FULRAF	98.97744	98.97547
FUNSIQ	-67.11554	-67.11350
FUNXOB	54.89022	54.88982
FUPJUV	81.27769	81.27676
FUPKIK	-38.02337	-38.02199
FUPKOQ	67.68032	67.67971
FUPTOZ	111.63852	111.63674
FUPZEV	24.61971	24.61977
FUSPEO	1.30439	1.30446
FUTCEC	63.33738	63.33675
FUTZEZ	-8.61144	-8.61119
FUVDOP	28.54770	28.54802
FUVMUE	55.78149	55.78086
FUVNEP	72.90969	72.91002
FUVXOJ	75.49849	75.49757
FUWMOZ	-206.64659	-206.64058
FUWTUM	32.55406	32.55382
FUXXAX	-360.41364	-360.40373
FUXZED	-11.21303	-11.21209
GADHEY	43.51385	43.51449
GAFNUW	48.79520	48.79552
GAHPIO	26.65978	26.65952
GAJTEQ	-56.77015	-56.76827
GAKGOO	2.67700	2.67762
GAKNEL	42.83176	42.83154
GAKNIP	12.55811	12.55812
GAKPEN	37.10128	37.10074
GAKTAN	75.15214	75.15146
GANHUY	60.73197	60.73075
GAPMEP	58.68366	58.68265
GAVKOD	89.18747	89.18552
GAVMEV	4.85701	4.85749
GAWWOQ	-109.87689	-109.87366
GEHBOK	-51.42718	-51.42472
GEHPUE	12.98179	12.98155
GEHXEW	-19.02522	-19.02375
GEJYOJ	-54.17030	-54.16874
GEKXEZ	47.02326	47.02235

GEMCEG	19.14746	19.14743
GEMCOQ	37.25987	37.25938
GEMDAD	67.23109	67.23018
GERCUB	108.97947	108.97743
GESCIQ	-29.47462	-29.47297
GESNIB	67.12883	67.12843
GESSUS	-18.73026	-18.72930
GETFIU	26.71721	26.71758
GETFOA	35.62475	35.62519
GETJOE	-70.29989	-70.29729
GEWTAD	51.09590	51.09549
GEXGIZ	68.34325	68.34206
GEYWOW	11.93576	11.93680
GICTIV01	115.40014	115.39806
GIDJUY	3.48286	3.48362
GIDMEL	-81.78540	-81.78233
GIDTIW	-196.65519	-196.64900
GIFRAO	14.02576	14.02661
GIGCEE	42.32187	42.32219
GIGMUE	44.82306	44.82261
GIHZEC	18.85082	18.85163
GIJMOB01	24.15189	24.15195
GIKJIT	37.86562	37.86507
GIKNOD	-25.31661	-25.31493
GIKTUP	-36.16502	-36.16363
GIMJIV	85.50402	85.50355
GINMUL	-6.11131	-6.11043
GIPHES	-25.55737	-25.55596
GIRDOA01	-12.93127	-12.92999
GOHVUU	-157.88177	-157.87732
GOJCIR	130.47050	130.46841
GOJKIZ	19.84592	19.84620
GUANCH01	-102.11644	-102.11357
HYTPRD01	41.66664	41.66666
ISTZCN10	-33.40207	-33.40189
JABGAU	58.72261	58.72261
JADLIJ	24.70380	24.70370
JADXER	60.29233	60.29207
JAHKOS	38.38559	38.38534
JAHTOB	61.73877	61.73853
JAHYEW	36.60584	36.60567
JAKGUX	50.86397	50.86374
JAKJOU	53.34609	53.34571
JALSOE	36.00393	36.00399
JAMREU	-90.81299	-90.80879
JANDOR	68.91078	68.91153

JANMAM	97.69500	97.69352
JAPFAH	30.49033	30.49074
JATBIP	-4.42045	-4.41969
JATCOW	-65.81452	-65.81254
JATLOF	-377.45704	-377.44726
JATMEW	-130.46676	-130.46271
JAVGAO	52.27513	52.27476
JAWJIA	-79.23239	-79.22895
JAWMAV	33.08004	33.07949
JAWVEI	26.97104	26.97099
JAWZEM	99.41011	99.40788
JAZGOG	28.41242	28.41303
JAZVIP10	-26.12245	-26.12084
JAZZOZ10	-32.67302	-32.67121
JEBFEB01	-30.89478	-30.89292
JECVES	99.89048	99.88874
JECVUI	-82.36050	-82.35804
JECYIZ	-10.09203	-10.09132
JEFRAN	-210.24982	-210.24338
JEHCUU01	-57.90105	-57.89897
JEHXOJ	88.72617	88.72445
JELKUG	73.20361	73.20215
JELREX	-14.54886	-14.54731
JELRIB	-26.11275	-26.11127
JEMHIS	-8.33007	-8.32993
JEMWUT	27.84541	27.84533
JESFES	-342.47108	-342.46289
JETJUN	-122.48312	-122.48053
JEVXIR	42.45553	42.45531
JEWFAS	-165.02652	-165.02196
JEWPIK	59.51936	59.51889
JEXREJ	-92.70123	-92.69741
JEYBUK	2.50214	2.50255
JIDHIN	47.98424	47.98382
JIFYUS	-80.05364	-80.05120
JIGCIL	52.17531	52.17466
JIGRAS	46.95941	46.95889
JIHVEB	83.07172	83.07017
JIKHUG	-40.26738	-40.26542
JILWUW	116.51674	116.51486
JINDAL	48.34693	48.34667
JINDOZ	3.59888	3.60036
JIRJID	-13.19969	-13.19924
JISZAM	-32.18179	-32.17964
JITMII	36.88547	36.88520
JIWKOP	13.05414	13.05504

JIXBAT	58.99277	58.99237
JIYJAC	32.58200	32.58203
JIYREO	64.27237	64.27113
JIYTOA	-14.13829	-14.13755
JIZWUK	-4.13028	-4.12927
JOFDUD	-11.44908	-11.44884
KAFXIY	100.47867	100.47702
KAGBOJ	78.37129	78.37126
KAKGOS	27.94946	27.95003
KAMCUW	-45.49517	-45.49292
KAMJAJ	28.53248	28.53287
KANWEB	1.60201	1.60290
KANZOO	15.28037	15.28183
KAPCUZ	68.97469	68.97353
KARYAD	31.61636	31.61675
KASBAH	-77.62909	-77.62648
KASBOV	7.17020	7.17100
KATNAU	157.86556	157.86312
KAVFUI	93.83083	93.82901
KAVTEG	-0.39200	-0.39148
KECSIU	141.51878	141.51631
KECSUG	146.47715	146.47424
KEDYAT	14.65953	14.65983
KEFJEK	7.25573	7.25633
KEJFOU	-99.02540	-99.02252
KEMFAJ	45.98424	45.98411
KENHOA	-29.17778	-29.17632
KEPKIZ	61.81628	61.81526
KESNEB	85.44380	85.44344
KEWJIF	-24.71146	-24.71068
KHDFRM11	-20.67992	-20.67946
KIBDII	-145.90465	-145.90021
KIBFAC	-21.88719	-21.88584
KICCUU	-8.77274	-8.77245
KICGAE	52.12669	52.12670
KICLAJ	3.16372	3.16447
KIGKIU	8.18255	8.18286
KIKVUV	45.65486	45.65517
KIMLEX01	0.26622	0.26622
KINKUN	85.26987	85.26864
KINTUW	-11.88791	-11.88741
KINWEJ	78.78392	78.78378
KINWIN	-50.54032	-50.53847
KIRCAP	255.83493	255.83125
KIRCOD	-4.49523	-4.49459
KITREK	-81.64657	-81.64310

KIYGAA	26.60510	26.60491
KOBXOO	33.68958	33.68953
KOBYOP	23.88117	23.88075
KOBZEG	95.02469	95.02401
KOCWUU	30.67330	30.67319
KODFUE	18.59940	18.59960
KOFKIZ	-99.88830	-99.88451
KOFMEX	-65.48715	-65.48498
KOFNIC	-60.92107	-60.91873
KOHVEI	47.44503	47.44433
KOHVIM	40.77334	40.77297
KOJGOF	90.29853	90.29743
KOJKID	2.90851	2.90926
KOJZOY	-31.79265	-31.79103
KOKMIG	-92.24143	-92.23864
KOLCUJ	117.98880	117.98723
MAPMIP03	34.02492	34.02466
MENBZS01	44.15542	44.15504
METBZC10	29.12095	29.12112
NAESCB01	-36.35711	-36.35555
NHOXAL06	118.48950	118.48699
PHOSLA10	112.07078	112.06860
PHOSLB10	-92.64081	-92.63762
PIMTAZ01	22.57669	22.57704
QUICNA01	-8.50687	-8.50576
SABNOY	-164.85434	-164.84948
SACXAV	15.28467	15.28472
SADXAW	-177.99006	-177.98507
SAFFOU	16.71277	16.71249
SAFFUA	39.61979	39.61898
SAFKAL	-73.74664	-73.74457
SAHSOJ	29.28905	29.28954
SAHSUP	-49.72910	-49.72685
SAKGUG	26.03383	26.03519
SALVEG	-65.30963	-65.30754
SAMFUH	76.00269	76.00165
SAMXUZ	-64.19365	-64.19154
SANKEX10	98.14771	98.14636
SAVDOI	22.57240	22.57343
SAWKEG10	-41.22035	-41.21882
SEBPEU01	60.07828	60.07754
SECDAF	-6.53837	-6.53622
SEFRAW	-45.24984	-45.24829
SEFYIL	-131.25092	-131.24749
SEGFIT	80.75242	80.75154
SEGJAP	35.61354	35.61408

SEGLAR	85.70341	85.70174
SEGNEX	29.82309	29.82319
SEGWEG	37.46823	37.46804
SEHBEM	28.74491	28.74536
SEJDAM	61.79333	61.79256
SEKKIC	38.05399	38.05360
SEKPED	-67.45408	-67.45196
SEKPIH	9.55143	9.55157
SELFIY	77.47071	77.46997
SEMDIX	-30.86340	-30.86190
SEMXOX	30.67184	30.67268
SETHAA	-4.49051	-4.48957
SETLIM	74.07649	74.07595
SEYVUN	43.93074	43.93006
SEYWUO	-39.99911	-39.99677
SEZMEP	66.22117	66.22054
SICNUN	55.76478	55.76535
SICPEZ	38.87320	38.87316
SICSEC	73.44743	73.44660
SIDFIU	33.96223	33.96281
SIDRUS	17.24568	17.24629
SINMIL	-32.59558	-32.59400
SIYLOB	35.54398	35.54387
SIZJIU	132.88205	132.88030
SIZWUT	57.15654	57.15558
SLFNMB04	-75.26360	-75.26120
SOGVOZ	107.39049	107.38866
SOHXOC	-153.83106	-153.82653
SOJNEK	-2.22516	-2.22452
SOMKIO	25.04375	25.04384
SONZIE	-18.83751	-18.83650
SOPZEC	-13.45857	-13.45795
SORBIK	77.59603	77.59519
SURDOX02	93.02783	93.02593
TACGIN	79.70690	79.70546
TACLEO	21.61532	21.61591
TAFKIU	12.68068	12.68091
TAFXIH	80.02713	80.02697
TAFZIJ	44.29657	44.29623
TAGVIG	-103.49420	-103.49121
TAHMOE	-11.22592	-11.22529
TAJPUP	80.83233	80.83196
TAJSUS	91.68004	91.67913
TAJVUV	14.55410	14.55380
TAJWAC	28.09963	28.09967
TAKHES	31.54540	31.54504

TAMMAV	46.27017	46.26968
TANHAR	51.35225	51.35200
TAPJUP	19.89126	19.89183
TAPSAE	34.83021	34.83013
TCYMPH02	26.38037	26.37987
TMTCHD01	89.46568	89.46443
VABLIT	13.61554	13.61622
VABROF	53.81788	53.81749
VACRUM	107.76910	107.76722
VAJFAN	50.90003	50.89946
VALTEH	-16.71883	-16.71810
VALWOU	-156.37291	-156.36807
VAPZOB10	105.60153	105.60008
VASDOI	13.85039	13.85052
VATKAC	88.96469	88.96346
VAWDUS	-19.81119	-19.81012
VAWMOV	159.94275	159.93984
VAWWAR	108.23634	108.23549
VAYKUB	-45.36228	-45.36041
VAZHUZ	53.65497	53.65464
VECSAX	-44.65044	-44.64883
VEDTED	-201.69887	-201.69336
VEHCOA	26.73428	26.73388
VEHZOX	-34.32136	-34.31976
VEJWOW	53.96769	53.96719
VEKMON	28.23453	28.23504
VENYUI	29.55129	29.55142
VETWAS	30.41711	30.41718
VEVDIJ	60.52869	60.52816
VEWZOM	-9.37968	-9.37781
VEXKOY	67.06387	67.06298
VEXMOA	101.95271	101.95152
VEYBIK	-63.59484	-63.59328
VEYWAX	73.03787	73.03635
VEZBUX	62.20201	62.20116
VICGAP	5.33694	5.33804
VICGET	-12.61650	-12.61498
VICKIB	40.26154	40.26172
VICPOM	-66.75993	-66.75777
VIDKUO	51.29373	51.29300
VIFFEV	34.35377	34.35367
VIGPEG	-35.74854	-35.74656
VIGTUA	124.75411	124.75260
VIHHID	55.16481	55.16430
VIKVIU	2.63326	2.63368
VIKYAP	87.86543	87.86488

VIMHII	0.00000	0.00000
VIPXAT	-162.40026	-162.39571
VIRBON	-9.52358	-9.52285
VIWCOT	16.54360	16.54377
VIXRID	37.57932	37.57882
VIXXOP	52.43194	52.43090
VIYPAU	81.46682	81.46576
VOBLAZ	11.51405	11.51474
VOBWOY	-25.40316	-25.40196
VOFBOH	7.85016	7.85078
VOFCAU	22.37171	22.37188
VOJGEG	-18.40802	-18.40750
VOJJIN	-8.99563	-8.99468
VUWXUG	201.69806	201.69367
VUXGOK	40.70548	40.70500
VUXPUZ	-50.22075	-50.21911
VUXREL	-4.36876	-4.36843
ZZZIZA01	35.42935	35.42893
ZZZMVU10	66.05382	66.05269
ZZZVCQ01	-24.07079	-24.07009
AR14A	5.70457	5.70446
CA04A	21.28839	21.28799
CE05A	15.67142	15.67129
CO01A	0.05416	0.05417
CO08A	22.31754	22.31702
HL08A	9.72664	9.72665
IM02A	7.42929	7.42922
NC10A	9.82297	9.82277
NC13A	9.89880	9.89858
NH10A	0.00000	0.00000
NH20A	3.64241	3.64242
NH22A	-1.24400	-1.24401
NH23A	17.23512	17.23458
OH10A	1.51461	1.51461
SR01A	0.00000	0.00000
SR05A	-3.28926	-3.28933
SR07A	12.91164	12.91170
AN05A	5.28439	5.28435
AN06A	0.68272	0.68272
AN08A	-14.52414	-14.52374
AN11A	-5.70233	-5.70218
AN12A	-15.08050	-15.08014
HL11A	4.68132	4.68134
HL13A	0.88660	0.88659
NO03A	-0.17493	-0.17491
NX02A	1.89613	1.89624

OC02A	14.28224	14.28211
PO02A	0.00211	0.00211
PO05A	-109.74485	-109.74217
PR01A	0.00000	0.00000
PR02A	0.18897	0.18897
PR03A	0.37672	0.37672
PR04A	6.98708	6.98703
SI02A	-0.02915	-0.02915
SI03A	-15.26744	-15.26707
SO07A	-80.21965	-80.21717
SO12A	-142.92206	-142.91853
SO15A	14.98726	14.98710
SO16A	0.62880	0.62891
SO18A	2.10304	2.10306
BRMW1	-13.13210	-13.13170
CA2PW3	-129.29119	-129.28734
CLMW1	-14.30054	-14.30011
CU1PW1	-23.88920	-23.88849
CU2PW3	-162.18769	-162.18232
FE2PW3	-156.84605	-156.84098
FE3PW3	-262.64650	-262.63811
FMW1	-20.44875	-20.44807
H3OPW1	-28.28397	-28.28306
KPW1	-18.26556	-18.26502
LIPW1	-32.35420	-32.35319
MG2PW3	-177.29756	-177.29210
NAPW	-24.09511	-24.09433
OHMW1	-21.72690	-21.72620
ZN2PW3	-158.88980	-158.88470
ERULE_01	-21.51511	-21.51473
ERULE_02	29.79957	29.79874
ERULE_03	-2.93518	-2.92992
ERULE_04	-2.31007	-2.31019
ERULE_05	4.88443	4.88437
ERULE_06	1.58172	1.58164
ERULE_07	3.16775	3.16779
ERULE_08	34.41382	34.41340

APPENDIX B

Comparison between MMFF94s force field energy (kcal/mol) of 264 test molecules computed in QuanPol program and OPTIMOL program is shown in following table. The maximum energy difference is -0.00970263 kcal/mol accrued on JATLOF molecule.

Structure name/Conformational Index	OPTIMOL	QuanPol
BEWCUB	60.39329	60.39415
BEWKUJ04	-3.72160	-3.72027
BIPDEJ02	-70.71969	-70.71739
BIYBIU10	50.76674	50.76659
BODKOU	24.78704	24.78704
BUYTIY10	124.43150	124.42977
BUYTOE10	145.00516	145.00304
BUYXEY10	-0.27671	-0.27591
BYITOT02	27.91649	27.91685
CALXES20	-32.52189	-32.51994
CEFMEN	34.32892	34.32966
CEWVIJ10	-124.21039	-124.20694
CILDOQ	-33.12081	-33.11944
CIMRUL10	40.60342	40.60339
CIPVOM	-0.72042	-0.71986
CITNOI10	32.14000	32.13992
CITPEA10	34.92805	34.92805
CIVCEP02	-183.69591	-183.69061
CIZFIA	-18.84123	-18.83995
CIZYEP	47.94793	47.94805
CIZZUG	-50.38411	-50.38232
COBKIN01	9.76832	9.76858
COJFIQ	76.37728	76.37622
COKROJ	47.84747	47.84718
CONBAI	-128.38792	-128.38396
CORWUB10	-84.17203	-84.16968
COSFAR	-0.32265	-0.32214
COSSEI	-74.79135	-74.78907
COTMON	23.45601	23.45633
COVXIU	-134.79631	-134.79195
COXZEU	-137.01509	-137.01137
COYMOS	9.71340	9.71435
COYNAF	78.56980	78.56859
COYVIV	-75.19612	-75.19373
CUDJAM	70.95668	70.95592

CUDPOG	39.05770	39.05798
CUGBEL	-6.55666	-6.55594
CUNVAI	124.69107	124.68961
CYGUAN01	-252.74851	-252.74081
DABHAP	-60.56143	-60.55870
DADLAV	34.24441	34.24415
DADLEZ	41.82027	41.81973
DAFKIE	18.30074	18.30089
DAFPUV	32.02843	32.02789
DAHBAP	40.92177	40.92168
DAJXER	-80.40995	-80.40712
DAKBAS	20.34466	20.34573
DAKDOI	53.42879	53.42914
DAPSUO03	67.69552	67.69504
DARDEF	-15.28369	-15.28271
DARPOB10	-56.30806	-56.30572
DARXID	70.44689	70.44655
DARZEB	-2.38238	-2.38149
DAWXII	41.75020	41.74958
DECKUR	-58.89113	-58.88893
DEDCIY	42.33964	42.33939
DEDSIO	1.38380	1.38438
DEFGIE	30.80484	30.80503
DEFLEF	-291.33061	-291.32193
DEFPUZ	-103.57884	-103.57612
DEFTUD	-18.79281	-18.79103
DEFVAL	14.92181	14.92267
DEFYUI	18.15664	18.15657
DEGRIQ	-4.21483	-4.21256
DEKRUG	-50.03897	-50.03733
DEMBIG	23.43951	23.43954
DERZUV	73.03326	73.03286
DESWUT	41.23092	41.23014
DESYOP	27.78867	27.78812
DEWHOC	87.97683	87.97602
DEXCIS	-3.85232	-3.85158
DEXGIW	-59.86089	-59.85897
DHOADS01	38.08002	38.07979
DICYOD	14.87073	14.87114
DIGLEK	87.74065	87.74007
DILCOQ	-50.93866	-50.93698
DIPDAH10	7.20554	7.20649
DIVVEJ	-315.49715	-315.48941
DIXJEZ	26.20209	26.20218
DIYPOQ	-48.18582	-48.18356
DIYPUW	36.04408	36.04395

DOCWUN	83.01077	83.00993
DOSNOO	-155.68967	-155.68556
DOTNIJ	40.68258	40.68277
DOTVEN	-218.72250	-218.71678
DOWDEY	-104.41882	-104.41572
DOZFON	167.98368	167.98032
DOZNIP	-231.48346	-231.47708
DUBNET	-13.26130	-13.26003
DUJHEV	4.80071	4.80120
DUKVAG	-37.43120	-37.43023
DUPHEB	31.38371	31.38413
DUVXIB	-73.17786	-73.17570
DUWKUB	59.93657	59.93604
DUXTIZ	97.86577	97.86372
DUXWUO	54.91869	54.91817
DUXXAV	76.92999	76.92896
FACMIF	76.95781	76.95685
FADMIG	64.51876	64.51802
FAHSUC	-56.31124	-56.30883
FAJWIW	-217.92465	-217.91893
FAMYUN	-20.30626	-20.30562
FAPLUD	-389.04269	-389.03309
FARWEA	-59.26574	-59.26381
FASGUB	84.25905	84.25773
FATLIV	-56.22143	-56.21899
FBATNB	116.44155	116.44090
FECXEQ	90.59095	90.58976
FEGSEP	-81.74333	-81.74170
FEHDAX	-17.74516	-17.74440
FEJJEJ	5.06019	5.06063
FELYIE	16.47982	16.47965
FELYUQ	68.60682	68.60620
FENHAH	34.00068	33.99995
FENJIR	-18.10610	-18.10430
FENJOX	2.19640	2.19744
FENJUD	-15.21762	-15.21671
FENNUH	-43.19268	-43.19083
FENYIG	14.92653	14.92714
FESCAH	-66.56849	-66.56667
FESMIZ	71.48832	71.48745
FETWOQ	-14.88655	-14.88539
FEVNUP	-29.97066	-29.96924
FEYLUQ	-71.67171	-71.66895
FEZPOP	1.21949	1.21980
FEZRUX	39.92355	39.92389
FIBLIL	89.66122	89.66015

FIHXID	-37.48035	-37.47835
FIKJAK	43.12263	43.12233
FIKZOO10	11.55329	11.55363
FILGEM	17.13041	17.13100
FITGIY	6.73276	6.73456
FITTIL	-72.03820	-72.03599
FIVNUT	10.87125	10.87188
FIVRAD	-71.71064	-71.70835
FODTUN	7.79404	7.79481
FOGVIG01	-281.87064	-281.86299
FOHXEF	-155.80331	-155.79895
FOJPAV	11.21920	11.21981
FONCOA	50.43187	50.43147
FORJUR	45.59708	45.59719
FOSDIA	45.65771	45.65783
FOVHUT	-292.26552	-292.25803
FOVRUD	96.90400	96.90290
FOWPOW	60.10552	60.10536
FUCWIJ	71.19746	71.19689
FUCWOP	-32.83328	-32.83141
FUFDIT	-61.57594	-61.57389
FUGWIN	-8.56321	-8.56204
FULRAF	99.46117	99.45949
FUPKOQ	68.20535	68.20467
FUTCEC	63.33868	63.33803
FUVMUE	55.63187	55.63120
FUVNEP	73.82036	73.82065
GADHEY	48.27966	48.28022
GAHPIO	26.96887	26.96859
GAKGOO	2.84878	2.84938
GAVKOD	89.21401	89.21203
GEHPUE	12.86901	12.86872
GEHXEW	-13.14292	-13.14154
GEJYOJ	-53.83818	-53.83664
GESCIQ	-25.13707	-25.13553
GEWTAD	51.11093	51.11051
GEYWOW	11.26051	11.26154
GIDMEL	-78.74552	-78.74258
GIDTIW	-196.64811	-196.64201
GIFRAO	15.62748	15.62828
GINMUL	-6.10962	-6.10876
GOHVUU	-152.39677	-152.39262
GUANCH01	-102.22404	-102.22121
HYTPRD01	40.72762	40.72760
JABGAU	58.73751	58.73749
JAKJOU	54.35681	54.35638

JAMREU	-90.81322	-90.80905
JANDOR	75.84730	75.84793
JAPFAH	30.34289	30.34328
JATCOW	-65.35380	-65.35185
JATLOF	-376.94247	-376.93277
JATMEW	-128.79466	-128.79070
JAWJIA	-79.61377	-79.61044
JAZVIP10	-26.12148	-26.11990
JAZZOZ10	-31.84603	-31.84429
JEBFEB01	-27.51940	-27.51768
JECVUI	-83.81228	-83.80986
JEFRAN	-210.52127	-210.51486
JEHCUU01	-56.55205	-56.55005
JEVXIR	43.85001	43.84974
JEWPIK	65.05058	65.04992
JEXREJ	-92.22862	-92.22485
JIGCIL	52.31659	52.31592
JIKHUG	-40.98226	-40.98031
JITMII	37.34236	37.34206
JIXBAT	62.88898	62.88848
KAKGOS	33.71930	33.71978
KAMCUW	-46.09287	-46.09065
KANZOO	19.09453	19.09586
KATNAU	162.38775	162.38522
KEFJEK	6.95575	6.95632
KEJFOU	-98.71263	-98.70977
KEMFAJ	47.23904	47.23886
KEWJIF	-24.42043	-24.41968
KIBDII	-143.38113	-143.37679
KIGKIU	8.58696	8.58724
KINKUN	85.99501	85.99375
KINWEJ	78.82949	78.82931
KIRCOD	-5.57593	-5.57531
KITREK	-79.69857	-79.69522
KIYGAA	26.81746	26.81724
KOBXOO	40.70583	40.70559
KOBZEG	96.53600	96.53522
KODFUE	17.82845	17.82863
KOFNIC	-55.88915	-55.88692
KOJZOY	-29.91219	-29.91067
KOKMIG	-92.16057	-92.15781
KOLCUJ	118.04535	118.04376
MAPMIP03	34.22587	34.22559
NAESCB01	-36.56278	-36.56122
PHOSLB10	-90.81634	-90.81318
PIMTAZ01	25.49386	25.49416

SABNOY	-165.73632	-165.73148
SADXAW	-179.10884	-179.10387
SAHSOJ	36.66529	36.66565
SALVEG	-65.39838	-65.39632
SAMXUZ	-64.67358	-64.67150
SANKEX10	98.10512	98.10375
SECDAF	-6.17031	-6.16819
SEFRAW	-45.38066	-45.37913
SEFYIL	-130.76279	-130.75938
SEGFIT	80.88802	80.88710
SEGNEX	29.80441	29.80450
SEMXOX	31.88561	31.88640
SETLIM	74.08708	74.08646
SEYWUO	-39.99533	-39.99302
SICNUN	55.28155	55.28209
SIZWUT	57.00842	57.00744
SLFNMB04	-74.24532	-74.24297
SOGVOZ	107.32320	107.32133
SOJNEK	-2.08718	-2.08657
SOMKIO	29.57623	29.57622
SONZIE	-18.20069	-18.19975
SURDOX02	93.88484	93.88289
TAFKIU	13.17824	13.17845
TAGVIG	-103.96695	-103.96397
TAHMOE	-11.29964	-11.29903
TAJPUP	81.51175	81.51136
TAPSAE	35.95843	35.95833
VABLIT	16.84681	16.84742
VACRUM	115.51294	115.51099
VAPZOB10	107.07310	107.07160
VATKAC	89.87814	89.87687
VAWWAR	108.48549	108.48461
VAYKUB	-42.65608	-42.65427
VEDTED	-199.55750	-199.55211
VEHZOX	-33.27933	-33.27781
VEKMON	28.39552	28.39601
VICGAP	14.39407	14.39493
VICGET	-11.20085	-11.19942
VICPOM	-64.16975	-64.16770
VIGPEG	-35.87937	-35.87742
VOBLAZ	12.52118	12.52182
VOJJIN	-7.35152	-7.35060
VUWXUG	201.98216	201.97773
VUXGOK	40.74167	40.74117
ZZZVCQ01	-22.49910	-22.49841

APPENDIX C

The Protein Data Bank format file (.pdb) of MSI-78 is obtained by applying the backbone geometry of MSI-594.

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ATOM      1  N   GLY A   1     -18.453  -7.969  -1.752  1.00  0.00           N
ATOM      2  CA  GLY A   1     -19.515  -7.348  -0.988  1.00  0.00           C
ATOM      3  C   GLY A   1     -19.124  -6.067  -0.279  1.00  0.00           C
ATOM      4  O   GLY A   1     -19.608  -5.815   0.809  1.00  0.00           O
ATOM      5  HA2 GLY A   1     -20.346  -7.214  -1.714  1.00  0.00           H
ATOM      6  HA3 GLY A   1     -19.836  -8.040  -0.248  1.00  0.00           H
ATOM      7  H1  GLY A   1     -18.127  -7.358  -2.519  1.00  0.00           H
ATOM      8  H2  GLY A   1     -17.643  -8.206  -1.137  1.00  0.00           H
ATOM      9  H3  GLY A   1     -18.719  -8.879  -2.177  1.00  0.00           H
ATOM     10  N   ILE A   2     -18.135  -5.277  -0.888  1.00  0.00           N
ATOM     11  CA  ILE A   2     -17.475  -4.217  -0.029  1.00  0.00           C
ATOM     12  C   ILE A   2     -16.969  -3.097  -0.972  1.00  0.00           C
ATOM     13  O   ILE A   2     -15.987  -2.423  -0.678  1.00  0.00           O
ATOM     14  CB  ILE A   2     -16.532  -4.881   0.894  1.00  0.00           C
ATOM     15  CG1 ILE A   2     -16.144  -3.924   2.093  1.00  0.00           C
ATOM     16  CG2 ILE A   2     -15.274  -5.368   0.143  1.00  0.00           C
ATOM     17  CD1 ILE A   2     -15.451  -4.697   3.201  1.00  0.00           C
ATOM     18  H   ILE A   2     -17.737  -5.496  -1.817  1.00  0.00           H
ATOM     19  HA  ILE A   2     -18.322  -3.702   0.551  1.00  0.00           H
ATOM     20  HB  ILE A   2     -17.061  -5.708   1.330  1.00  0.00           H
ATOM     21 HG12 ILE A   2     -15.376  -3.235   1.778  1.00  0.00           H
ATOM     22 HG13 ILE A   2     -16.997  -3.368   2.463  1.00  0.00           H
ATOM     23 HG21 ILE A   2     -15.636  -5.975  -0.726  1.00  0.00           H
ATOM     24 HG22 ILE A   2     -14.649  -4.553  -0.216  1.00  0.00           H
ATOM     25 HG23 ILE A   2     -14.754  -6.005   0.854  1.00  0.00           H
ATOM     26 HD11 ILE A   2     -15.458  -4.042   4.176  1.00  0.00           H
ATOM     27 HD12 ILE A   2     -15.990  -5.602   3.400  1.00  0.00           H
ATOM     28 HD13 ILE A   2     -14.428  -4.930   2.840  1.00  0.00           H
ATOM     29  N   GLY A   3     -17.768  -2.807  -2.050  1.00  0.00           N
ATOM     30  CA  GLY A   3     -17.302  -2.233  -3.300  1.00  0.00           C
ATOM     31  C   GLY A   3     -16.607  -0.847  -3.203  1.00  0.00           C
ATOM     32  O   GLY A   3     -15.565  -0.707  -3.831  1.00  0.00           O
ATOM     33  H   GLY A   3     -18.597  -3.439  -2.113  1.00  0.00           H
ATOM     34  HA2 GLY A   3     -16.688  -3.020  -3.774  1.00  0.00           H
ATOM     35  HA3 GLY A   3     -18.199  -2.009  -3.987  1.00  0.00           H
ATOM     36  N   LYS A   4     -17.177   0.126  -2.383  1.00  0.00           N
ATOM     37  CA  LYS A   4     -16.477   1.415  -2.093  1.00  0.00           C
ATOM     38  C   LYS A   4     -15.135   1.317  -1.411  1.00  0.00           C
ATOM     39  O   LYS A   4     -14.241   2.160  -1.568  1.00  0.00           O
ATOM     40  CB  LYS A   4     -17.376   2.560  -1.407  1.00  0.00           C
ATOM     41  CG  LYS A   4     -17.815   2.199  -0.029  1.00  0.00           C
ATOM     42  CD  LYS A   4     -18.622   3.388   0.619  1.00  0.00           C
ATOM     43  CE  LYS A   4     -19.617   2.931   1.641  1.00  0.00           C
ATOM     44  NZ  LYS A   4     -20.242   4.055   2.197  1.00  0.00           N1+
ATOM     45  H   LYS A   4     -18.156   0.057  -2.154  1.00  0.00           H
ATOM     46  HA  LYS A   4     -16.145   1.835  -3.013  1.00  0.00           H
ATOM     47  HB2 LYS A   4     -16.847   3.547  -1.295  1.00  0.00           H
ATOM     48  HB3 LYS A   4     -18.233   2.784  -2.080  1.00  0.00           H
ATOM     49  HG2 LYS A   4     -18.489   1.379  -0.193  1.00  0.00           H
ATOM     50  HG3 LYS A   4     -17.038   1.913   0.669  1.00  0.00           H
ATOM     51  HD2 LYS A   4     -17.885   4.026   1.114  1.00  0.00           H
ATOM     52  HD3 LYS A   4     -19.203   3.973  -0.150  1.00  0.00           H
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ATOM     53  HE2 LYS A   4     -20.363   2.346   1.124  1.00  0.00           H
ATOM     54  HE3 LYS A   4     -19.108   2.465   2.454  1.00  0.00           H
ATOM     55  HZ1 LYS A   4     -21.043   3.893   2.784  1.00  0.00           H
ATOM     56  HZ2 LYS A   4     -19.640   4.781   2.761  1.00  0.00           H
ATOM     57  HZ3 LYS A   4     -20.649   4.702   1.427  1.00  0.00           H
ATOM     58  N   PHE A   5     -15.044   0.306  -0.479  1.00  0.00           N
ATOM     59  CA  PHE A   5     -13.814   0.262   0.344  1.00  0.00           C
ATOM     60  C   PHE A   5     -12.730  -0.739  -0.331  1.00  0.00           C
ATOM     61  O   PHE A   5     -11.592  -0.672   0.033  1.00  0.00           O
ATOM     62  CB  PHE A   5     -14.095  -0.158   1.835  1.00  0.00           C
ATOM     63  CG  PHE A   5     -15.163   0.689   2.690  1.00  0.00           C
ATOM     64  CD1 PHE A   5     -14.921   2.018   2.776  1.00  0.00           C
ATOM     65  CD2 PHE A   5     -16.178   0.079   3.415  1.00  0.00           C
ATOM     66  CE1 PHE A   5     -15.687   2.730   3.691  1.00  0.00           C
ATOM     67  CE2 PHE A   5     -17.022   0.848   4.268  1.00  0.00           C
ATOM     68  CZ  PHE A   5     -16.772   2.187   4.411  1.00  0.00           C
ATOM     69  H   PHE A   5     -15.815  -0.403  -0.405  1.00  0.00           H
ATOM     70  HA  PHE A   5     -13.372   1.324   0.345  1.00  0.00           H
ATOM     71  HB2 PHE A   5     -14.596  -1.132   1.741  1.00  0.00           H
ATOM     72  HB3 PHE A   5     -13.179  -0.307   2.511  1.00  0.00           H
ATOM     73  HD1 PHE A   5     -14.208   2.494   2.136  1.00  0.00           H
ATOM     74  HD2 PHE A   5     -16.317  -0.991   3.290  1.00  0.00           H
ATOM     75  HE1 PHE A   5     -15.544   3.730   3.821  1.00  0.00           H
ATOM     76  HE2 PHE A   5     -17.661   0.364   4.979  1.00  0.00           H
ATOM     77  HZ  PHE A   5     -17.375   2.853   5.117  1.00  0.00           H
ATOM     78  N   LEU A   6     -13.259  -1.597  -1.270  1.00  0.00           N
ATOM     79  CA  LEU A   6     -12.344  -2.516  -1.826  1.00  0.00           C
ATOM     80  C   LEU A   6     -11.088  -1.841  -2.476  1.00  0.00           C
ATOM     81  O   LEU A   6      -9.962  -2.362  -2.588  1.00  0.00           O
ATOM     82  CB  LEU A   6     -12.969  -3.395  -2.922  1.00  0.00           C
ATOM     83  CG  LEU A   6     -12.137  -4.650  -3.223  1.00  0.00           C
ATOM     84  CD1 LEU A   6     -11.730  -5.533  -2.012  1.00  0.00           C
ATOM     85  CD2 LEU A   6     -12.981  -5.593  -4.115  1.00  0.00           C
ATOM     86  H   LEU A   6     -14.262  -1.897  -1.085  1.00  0.00           H
ATOM     87  HA  LEU A   6     -11.834  -3.039  -1.060  1.00  0.00           H
ATOM     88  HB2 LEU A   6     -14.017  -3.655  -2.737  1.00  0.00           H
ATOM     89  HB3 LEU A   6     -13.005  -2.845  -3.874  1.00  0.00           H
ATOM     90  HG  LEU A   6     -11.270  -4.344  -3.837  1.00  0.00           H
ATOM     91 HD11 LEU A   6     -12.672  -5.828  -1.539  1.00  0.00           H
ATOM     92 HD12 LEU A   6     -11.202  -6.458  -2.263  1.00  0.00           H
ATOM     93 HD13 LEU A   6     -11.103  -5.001  -1.256  1.00  0.00           H
ATOM     94 HD21 LEU A   6     -12.548  -6.549  -4.380  1.00  0.00           H
ATOM     95 HD22 LEU A   6     -13.872  -5.920  -3.620  1.00  0.00           H
ATOM     96 HD23 LEU A   6     -13.154  -5.056  -5.048  1.00  0.00           H
ATOM    135  N   LYS A   7     -11.328  -0.548  -2.861  1.00  0.00           N
ATOM    136  CA  LYS A   7     -10.429   0.423  -3.569  1.00  0.00           C
ATOM    137  C   LYS A   7      -9.638   1.346  -2.614  1.00  0.00           C
ATOM    138  O   LYS A   7      -8.678   2.016  -2.994  1.00  0.00           O
ATOM    139  CB  LYS A   7     -11.205   1.151  -4.684  1.00  0.00           C
ATOM    140  CG  LYS A   7     -11.228   0.538  -6.126  1.00  0.00           C
ATOM    141  CD  LYS A   7     -11.764  -0.886  -6.033  1.00  0.00           C
ATOM    142  CE  LYS A   7     -12.245  -1.418  -7.372  1.00  0.00           C
ATOM    143  NZ  LYS A   7     -13.545  -0.833  -7.748  1.00  0.00          N1+
ATOM    144  H   LYS A   7     -12.285  -0.194  -2.708  1.00  0.00           H
ATOM    145  HA  LYS A   7      -9.671  -0.289  -4.005  1.00  0.00           H
ATOM    146  HB2 LYS A   7     -12.204   1.308  -4.300  1.00  0.00           H
ATOM    147  HB3 LYS A   7     -10.784   2.147  -4.886  1.00  0.00           H
ATOM    148  HG2 LYS A   7     -10.156   0.574  -6.497  1.00  0.00           H
ATOM    149  HG3 LYS A   7     -11.809   1.106  -6.833  1.00  0.00           H
ATOM    150  HD2 LYS A   7     -10.935  -1.544  -5.738  1.00  0.00           H
ATOM    151  HD3 LYS A   7     -12.491  -1.038  -5.266  1.00  0.00           H
ATOM    152  HE2 LYS A   7     -12.355  -2.493  -7.413  1.00  0.00           H
ATOM    153  HE3 LYS A   7     -11.495  -1.137  -8.193  1.00  0.00           H
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ATOM    154  HZ1 LYS A   7     -13.694  -0.437  -8.742  1.00  0.00           H
ATOM    155  HZ2 LYS A   7     -13.902  -0.054  -7.170  1.00  0.00           H
ATOM    156  HZ3 LYS A   7     -14.254  -1.543  -7.584  1.00  0.00           H
ATOM    157  N   LYS A   8     -10.063   1.246  -1.243  1.00  0.00           N
ATOM    158  CA  LYS A   8      -9.281   1.885  -0.233  1.00  0.00           C
ATOM    159  C   LYS A   8      -8.315   0.777   0.308  1.00  0.00           C
ATOM    160  O   LYS A   8      -7.143   0.939   0.573  1.00  0.00           O
ATOM    161  CB  LYS A   8     -10.072   2.563   0.900  1.00  0.00           C
ATOM    162  CG  LYS A   8      -9.320   3.838   1.283  1.00  0.00           C
ATOM    163  CD  LYS A   8     -10.050   4.601   2.495  1.00  0.00           C
ATOM    164  CE  LYS A   8      -9.500   5.975   2.705  1.00  0.00           C
ATOM    165  NZ  LYS A   8     -10.286   6.724   3.713  1.00  0.00           N1+
ATOM    166  H   LYS A   8     -10.598   0.428  -1.091  1.00  0.00           H
ATOM    167  HA  LYS A   8      -8.678   2.642  -0.762  1.00  0.00           H
ATOM    168  HB2 LYS A   8     -10.131   1.848   1.727  1.00  0.00           H
ATOM    169  HB3 LYS A   8     -11.025   2.844   0.518  1.00  0.00           H
ATOM    170  HG2 LYS A   8      -9.239   4.436   0.365  1.00  0.00           H
ATOM    171  HG3 LYS A   8      -8.328   3.530   1.628  1.00  0.00           H
ATOM    172  HD2 LYS A   8     -11.158   4.679   2.316  1.00  0.00           H
ATOM    173  HD3 LYS A   8      -9.940   3.906   3.348  1.00  0.00           H
ATOM    174  HE2 LYS A   8      -9.509   6.572   1.801  1.00  0.00           H
ATOM    175  HE3 LYS A   8      -8.518   5.860   3.102  1.00  0.00           H
ATOM    176  HZ1 LYS A   8     -11.294   6.886   3.410  1.00  0.00           H
ATOM    177  HZ2 LYS A   8      -9.871   7.620   3.953  1.00  0.00           H
ATOM    178  HZ3 LYS A   8     -10.291   6.245   4.662  1.00  0.00           H
ATOM    125  N   ALA A   9      -8.869  -0.450   0.486  1.00  0.00           N
ATOM    126  CA  ALA A   9      -8.123  -1.596   1.032  1.00  0.00           C
ATOM    127  C   ALA A   9      -6.878  -1.900   0.160  1.00  0.00           C
ATOM    128  O   ALA A   9      -5.845  -2.347   0.685  1.00  0.00           O
ATOM    129  CB  ALA A   9      -8.970  -2.837   1.237  1.00  0.00           C
ATOM    130  H   ALA A   9      -9.880  -0.515   0.658  1.00  0.00           H
ATOM    131  HA  ALA A   9      -7.651  -1.214   1.947  1.00  0.00           H
ATOM    132  HB1 ALA A   9      -9.925  -2.670   1.862  1.00  0.00           H
ATOM    133  HB2 ALA A   9      -9.298  -3.216   0.260  1.00  0.00           H
ATOM    134  HB3 ALA A   9      -8.481  -3.717   1.761  1.00  0.00           H
ATOM    135  N   LYS A  10      -7.149  -1.846  -1.263  1.00  0.00           N
ATOM    136  CA  LYS A  10      -6.061  -2.189  -2.129  1.00  0.00           C
ATOM    137  C   LYS A  10      -5.135  -0.945  -2.351  1.00  0.00           C
ATOM    138  O   LYS A  10      -4.127  -1.123  -3.050  1.00  0.00           O
ATOM    139  CB  LYS A  10      -6.553  -2.832  -3.418  1.00  0.00           C
ATOM    140  CG  LYS A  10      -7.032  -4.272  -3.101  1.00  0.00           C
ATOM    141  CD  LYS A  10      -7.816  -4.789  -4.280  1.00  0.00           C
ATOM    142  CE  LYS A  10      -8.188  -6.329  -4.193  1.00  0.00           C
ATOM    143  NZ  LYS A  10      -8.711  -6.659  -5.535  1.00  0.00           N1+
ATOM    144  H   LYS A  10      -8.148  -1.952  -1.489  1.00  0.00           H
ATOM    145  HA  LYS A  10      -5.467  -2.892  -1.586  1.00  0.00           H
ATOM    146  HB2 LYS A  10      -7.467  -2.202  -3.812  1.00  0.00           H
ATOM    147  HB3 LYS A  10      -5.792  -2.818  -4.238  1.00  0.00           H
ATOM    148  HG2 LYS A  10      -6.136  -4.968  -2.911  1.00  0.00           H
ATOM    149  HG3 LYS A  10      -7.740  -4.332  -2.211  1.00  0.00           H
ATOM    150  HD2 LYS A  10      -8.740  -4.137  -4.457  1.00  0.00           H
ATOM    151  HD3 LYS A  10      -7.173  -4.673  -5.187  1.00  0.00           H
ATOM    152  HE2 LYS A  10      -7.321  -7.021  -3.983  1.00  0.00           H
ATOM    153  HE3 LYS A  10      -8.967  -6.383  -3.435  1.00  0.00           H
ATOM    154  HZ1 LYS A  10      -8.008  -6.941  -6.332  1.00  0.00           H
ATOM    155  HZ2 LYS A  10      -9.292  -7.532  -5.559  1.00  0.00           H
ATOM    156  HZ3 LYS A  10      -9.415  -6.082  -5.882  1.00  0.00           H
ATOM    157  N   LYS A  11      -5.537   0.343  -1.912  1.00  0.00           N
ATOM    158  CA  LYS A  11      -4.577   1.419  -1.917  1.00  0.00           C
ATOM    159  C   LYS A  11      -3.605   1.125  -0.746  1.00  0.00           C
ATOM    160  O   LYS A  11      -2.376   1.178  -0.763  1.00  0.00           O
ATOM    161  CB  LYS A  11      -5.157   2.894  -1.678  1.00  0.00           C
ATOM    162  CG  LYS A  11      -4.082   3.968  -1.975  1.00  0.00           C
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ATOM    163  CD  LYS A  11      -4.754   5.383  -1.978  1.00  0.00           C
ATOM    164  CE  LYS A  11      -3.801   6.528  -1.951  1.00  0.00           C
ATOM    165  NZ  LYS A  11      -3.132   6.720  -3.226  1.00  0.00           N1+
ATOM    166  H   LYS A  11      -6.459   0.447  -1.401  1.00  0.00           H
ATOM    167  HA  LYS A  11      -4.014   1.372  -2.918  1.00  0.00           H
ATOM    168  HB2 LYS A  11      -5.988   2.955  -2.396  1.00  0.00           H
ATOM    169  HB3 LYS A  11      -5.590   2.937  -0.656  1.00  0.00           H
ATOM    170  HG2 LYS A  11      -3.389   3.936  -1.125  1.00  0.00           H
ATOM    171  HG3 LYS A  11      -3.553   3.805  -2.887  1.00  0.00           H
ATOM    172  HD2 LYS A  11      -5.460   5.492  -2.828  1.00  0.00           H
ATOM    173  HD3 LYS A  11      -5.332   5.508  -0.956  1.00  0.00           H
ATOM    174  HE2 LYS A  11      -4.264   7.479  -1.802  1.00  0.00           H
ATOM    175  HE3 LYS A  11      -2.987   6.469  -1.211  1.00  0.00           H
ATOM    176  HZ1 LYS A  11      -2.368   6.054  -3.512  1.00  0.00           H
ATOM    177  HZ2 LYS A  11      -3.909   6.716  -3.969  1.00  0.00           H
ATOM    178  HZ3 LYS A  11      -2.640   7.671  -3.207  1.00  0.00           H
ATOM    179  N   PHE A  12      -4.203   0.711   0.463  1.00  0.00           N
ATOM    180  CA  PHE A  12      -3.460   0.643   1.719  1.00  0.00           C
ATOM    181  C   PHE A  12      -2.332  -0.370   1.688  1.00  0.00           C
ATOM    182  O   PHE A  12      -1.237  -0.115   2.184  1.00  0.00           O
ATOM    183  CB  PHE A  12      -4.371   0.517   2.902  1.00  0.00           C
ATOM    184  CG  PHE A  12      -3.692   0.729   4.263  1.00  0.00           C
ATOM    185  CD1 PHE A  12      -3.003  -0.312   4.977  1.00  0.00           C
ATOM    186  CD2 PHE A  12      -3.656   1.992   4.891  1.00  0.00           C
ATOM    187  CE1 PHE A  12      -2.215  -0.134   6.106  1.00  0.00           C
ATOM    188  CE2 PHE A  12      -2.807   2.233   6.014  1.00  0.00           C
ATOM    189  CZ  PHE A  12      -2.142   1.164   6.607  1.00  0.00           C
ATOM    190  H   PHE A  12      -5.180   0.827   0.669  1.00  0.00           H
ATOM    191  HA  PHE A  12      -3.006   1.646   1.734  1.00  0.00           H
ATOM    192  HB2 PHE A  12      -5.336   1.072   2.711  1.00  0.00           H
ATOM    193  HB3 PHE A  12      -4.709  -0.495   3.016  1.00  0.00           H
ATOM    194  HD1 PHE A  12      -2.828  -1.242   4.439  1.00  0.00           H
ATOM    195  HD2 PHE A  12      -4.260   2.851   4.501  1.00  0.00           H
ATOM    196  HE1 PHE A  12      -1.476  -0.980   6.329  1.00  0.00           H
ATOM    197  HE2 PHE A  12      -2.756   3.170   6.479  1.00  0.00           H
ATOM    198  HZ  PHE A  12      -1.551   1.456   7.459  1.00  0.00           H
ATOM    199  N   GLY A  13      -2.563  -1.462   0.952  1.00  0.00           N
ATOM    200  CA  GLY A  13      -1.714  -2.638   1.097  1.00  0.00           C
ATOM    201  C   GLY A  13      -0.384  -2.301   0.276  1.00  0.00           C
ATOM    202  O   GLY A  13       0.694  -2.775   0.457  1.00  0.00           O
ATOM    203  H   GLY A  13      -3.577  -1.701   0.788  1.00  0.00           H
ATOM    204  HA2 GLY A  13      -1.467  -2.826   2.152  1.00  0.00           H
ATOM    205  HA3 GLY A  13      -2.246  -3.519   0.676  1.00  0.00           H
ATOM    206  N   LYS A  14      -0.526  -1.400  -0.780  1.00  0.00           N
ATOM    207  CA  LYS A  14       0.646  -0.842  -1.571  1.00  0.00           C
ATOM    208  C   LYS A  14       1.290   0.339  -0.756  1.00  0.00           C
ATOM    209  O   LYS A  14       2.486   0.595  -0.534  1.00  0.00           O
ATOM    210  CB  LYS A  14       0.089  -0.455  -2.985  1.00  0.00           C
ATOM    211  CG  LYS A  14       1.168   0.019  -4.011  1.00  0.00           C
ATOM    212  CD  LYS A  14       2.278  -1.035  -4.254  1.00  0.00           C
ATOM    213  CE  LYS A  14       3.197  -0.557  -5.414  1.00  0.00           C
ATOM    214  NZ  LYS A  14       4.297  -1.507  -5.724  1.00  0.00           N1+
ATOM    215  H   LYS A  14      -1.420  -0.917  -0.834  1.00  0.00           H
ATOM    216  HA  LYS A  14       1.470  -1.478  -1.704  1.00  0.00           H
ATOM    217  HB2 LYS A  14      -0.415  -1.369  -3.263  1.00  0.00           H
ATOM    218  HB3 LYS A  14      -0.719   0.389  -2.898  1.00  0.00           H
ATOM    219  HG2 LYS A  14       0.788   0.252  -5.032  1.00  0.00           H
ATOM    220  HG3 LYS A  14       1.677   0.897  -3.529  1.00  0.00           H
ATOM    221  HD2 LYS A  14       2.903  -1.276  -3.433  1.00  0.00           H
ATOM    222  HD3 LYS A  14       1.781  -1.944  -4.669  1.00  0.00           H
ATOM    223  HE2 LYS A  14       2.690  -0.421  -6.359  1.00  0.00           H
ATOM    224  HE3 LYS A  14       3.554   0.391  -5.132  1.00  0.00           H
ATOM    225  HZ1 LYS A  14       4.015  -2.363  -6.260  1.00  0.00           H
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ATOM    226  HZ2 LYS A  14       5.026  -1.075  -6.346  1.00  0.00           H
ATOM    227  HZ3 LYS A  14       4.827  -1.747  -4.864  1.00  0.00           H
ATOM    228  N   ALA A  15       0.302   1.195  -0.181  1.00  0.00           N
ATOM    229  CA  ALA A  15       0.750   2.336   0.628  1.00  0.00           C
ATOM    230  C   ALA A  15       1.605   1.977   1.883  1.00  0.00           C
ATOM    231  O   ALA A  15       2.362   2.747   2.467  1.00  0.00           O
ATOM    232  CB  ALA A  15      -0.320   3.356   0.966  1.00  0.00           C
ATOM    233  H   ALA A  15      -0.673   1.140  -0.599  1.00  0.00           H
ATOM    234  HA  ALA A  15       1.484   2.894  -0.008  1.00  0.00           H
ATOM    235  HB1 ALA A  15      -0.995   2.990   1.806  1.00  0.00           H
ATOM    236  HB2 ALA A  15       0.114   4.391   1.220  1.00  0.00           H
ATOM    237  HB3 ALA A  15      -0.992   3.513   0.111  1.00  0.00           H
ATOM    238  N   PHE A  16       1.256   0.781   2.383  1.00  0.00           N
ATOM    239  CA  PHE A  16       1.819   0.189   3.580  1.00  0.00           C
ATOM    240  C   PHE A  16       3.414   0.136   3.219  1.00  0.00           C
ATOM    241  O   PHE A  16       4.299   0.435   4.032  1.00  0.00           O
ATOM    242  CB  PHE A  16       1.412  -1.258   3.805  1.00  0.00           C
ATOM    243  CG  PHE A  16       1.893  -1.809   5.168  1.00  0.00           C
ATOM    244  CD1 PHE A  16       2.480  -3.063   5.246  1.00  0.00           C
ATOM    245  CD2 PHE A  16       1.642  -1.132   6.318  1.00  0.00           C
ATOM    246  CE1 PHE A  16       2.895  -3.587   6.448  1.00  0.00           C
ATOM    247  CE2 PHE A  16       2.040  -1.642   7.565  1.00  0.00           C
ATOM    248  CZ  PHE A  16       2.652  -2.923   7.605  1.00  0.00           C
ATOM    249  H   PHE A  16       0.340   0.363   2.112  1.00  0.00           H
ATOM    250  HA  PHE A  16       1.825   0.853   4.390  1.00  0.00           H
ATOM    251  HB2 PHE A  16       0.297  -1.254   3.940  1.00  0.00           H
ATOM    252  HB3 PHE A  16       1.841  -1.928   3.016  1.00  0.00           H
ATOM    253  HD1 PHE A  16       2.734  -3.682   4.413  1.00  0.00           H
ATOM    254  HD2 PHE A  16       1.098  -0.199   6.247  1.00  0.00           H
ATOM    255  HE1 PHE A  16       3.205  -4.678   6.430  1.00  0.00           H
ATOM    256  HE2 PHE A  16       1.924  -1.004   8.518  1.00  0.00           H
ATOM    257  HZ  PHE A  16       2.767  -3.483   8.520  1.00  0.00           H
ATOM    258  N   VAL A  17       3.784  -0.204   1.969  1.00  0.00           N
ATOM    259  CA  VAL A  17       5.228  -0.399   1.683  1.00  0.00           C
ATOM    260  C   VAL A  17       6.043   0.855   1.875  1.00  0.00           C
ATOM    261  O   VAL A  17       7.249   0.860   2.058  1.00  0.00           O
ATOM    262  CB  VAL A  17       5.463  -0.981   0.262  1.00  0.00           C
ATOM    263  CG1 VAL A  17       6.941  -1.427   0.021  1.00  0.00           C
ATOM    264  CG2 VAL A  17       4.425  -2.064  -0.093  1.00  0.00           C
ATOM    265  H   VAL A  17       3.082  -0.149   1.267  1.00  0.00           H
ATOM    266  HA  VAL A  17       5.552  -1.152   2.435  1.00  0.00           H
ATOM    267  HB  VAL A  17       5.352  -0.122  -0.496  1.00  0.00           H
ATOM    268 HG11 VAL A  17       7.576  -0.493   0.155  1.00  0.00           H
ATOM    269 HG12 VAL A  17       7.213  -2.017   0.869  1.00  0.00           H
ATOM    270 HG13 VAL A  17       7.153  -1.918  -0.906  1.00  0.00           H
ATOM    271 HG21 VAL A  17       3.429  -1.671  -0.412  1.00  0.00           H
ATOM    272 HG22 VAL A  17       4.797  -2.522  -0.931  1.00  0.00           H
ATOM    273 HG23 VAL A  17       4.309  -2.695   0.777  1.00  0.00           H
ATOM    206  N   LYS A  18       5.340   2.044   1.701  1.00  0.00           N
ATOM    207  CA  LYS A  18       5.985   3.328   1.842  1.00  0.00           C
ATOM    208  C   LYS A  18       6.255   3.648   3.338  1.00  0.00           C
ATOM    209  O   LYS A  18       6.760   4.702   3.761  1.00  0.00           O
ATOM    210  CB  LYS A  18       5.259   4.427   1.071  1.00  0.00           C
ATOM    211  CG  LYS A  18       6.204   5.031   0.030  1.00  0.00           C
ATOM    212  CD  LYS A  18       7.422   5.787   0.665  1.00  0.00           C
ATOM    213  CE  LYS A  18       7.189   7.004   1.531  1.00  0.00           C
ATOM    214  NZ  LYS A  18       8.410   7.647   1.970  1.00  0.00          N1+
ATOM    215  H   LYS A  18       4.307   2.072   1.877  1.00  0.00           H
ATOM    216  HA  LYS A  18       6.990   3.090   1.441  1.00  0.00           H
ATOM    217  HB2 LYS A  18       4.455   4.005   0.508  1.00  0.00           H
ATOM    218  HB3 LYS A  18       4.851   5.172   1.787  1.00  0.00           H
ATOM    219  HG2 LYS A  18       6.592   4.286  -0.683  1.00  0.00           H
ATOM    220  HG3 LYS A  18       5.642   5.815  -0.463  1.00  0.00           H
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ATOM    221  HD2 LYS A  18       7.900   5.042   1.317  1.00  0.00           H
ATOM    222  HD3 LYS A  18       8.063   6.053  -0.214  1.00  0.00           H
ATOM    223  HE2 LYS A  18       6.681   6.724   2.463  1.00  0.00           H
ATOM    224  HE3 LYS A  18       6.514   7.726   0.974  1.00  0.00           H
ATOM    225  HZ1 LYS A  18       8.305   8.349   2.692  1.00  0.00           H
ATOM    226  HZ2 LYS A  18       8.940   8.208   1.273  1.00  0.00           H
ATOM    227  HZ3 LYS A  18       9.042   6.914   2.249  1.00  0.00           H
ATOM     10  N   ILE A  19       5.869   2.676   4.238  1.00  0.00           N
ATOM     11  CA  ILE A  19       6.291   2.634   5.665  1.00  0.00           C
ATOM     12  C   ILE A  19       7.604   1.849   5.829  1.00  0.00           C
ATOM     13  O   ILE A  19       8.501   2.055   6.601  1.00  0.00           O
ATOM     14  CB  ILE A  19       5.163   2.046   6.585  1.00  0.00           C
ATOM     15  CG1 ILE A  19       5.492   1.998   8.054  1.00  0.00           C
ATOM     16  CG2 ILE A  19       5.914   3.313   8.535  1.00  0.00           C
ATOM     17  CD1 ILE A  19       3.859   2.818   6.400  1.00  0.00           C
ATOM     18  H   ILE A  19       5.214   1.945   3.895  1.00  0.00           H
ATOM     19  HA  ILE A  19       6.533   3.690   5.867  1.00  0.00           H
ATOM     20  HB  ILE A  19       5.039   0.980   6.244  1.00  0.00           H
ATOM     21 HG12 ILE A  19       4.621   1.742   8.618  1.00  0.00           H
ATOM     22 HG13 ILE A  19       6.315   1.230   8.304  1.00  0.00           H
ATOM     23 HG21 ILE A  19       3.945   3.816   6.781  1.00  0.00           H
ATOM     24 HG22 ILE A  19       3.476   2.901   5.328  1.00  0.00           H
ATOM     25 HG23 ILE A  19       3.090   2.347   6.992  1.00  0.00           H
ATOM     26 HD11 ILE A  19       6.864   3.629   8.062  1.00  0.00           H
ATOM     27 HD12 ILE A  19       5.191   4.101   8.369  1.00  0.00           H
ATOM     28 HD13 ILE A  19       6.094   3.253   9.613  1.00  0.00           H
ATOM     78  N   LEU A  20       7.662   0.722   4.975  1.00  0.00           N
ATOM     79  CA  LEU A  20       8.735  -0.115   5.309  1.00  0.00           C
ATOM     80  C   LEU A  20       9.999   0.308   4.573  1.00  0.00           C
ATOM     81  O   LEU A  20      11.128   0.190   5.039  1.00  0.00           O
ATOM     82  CB  LEU A  20       8.491  -1.602   4.841  1.00  0.00           C
ATOM     83  CG  LEU A  20       7.260  -2.256   5.480  1.00  0.00           C
ATOM     84  CD1 LEU A  20       6.991  -2.141   6.956  1.00  0.00           C
ATOM     85  CD2 LEU A  20       7.253  -3.706   4.997  1.00  0.00           C
ATOM     86  H   LEU A  20       7.326   0.828   4.010  1.00  0.00           H
ATOM     87  HA  LEU A  20       8.889  -0.191   6.421  1.00  0.00           H
ATOM     88  HB2 LEU A  20       8.436  -1.794   3.738  1.00  0.00           H
ATOM     89  HB3 LEU A  20       9.475  -2.084   5.072  1.00  0.00           H
ATOM     90  HG  LEU A  20       6.507  -1.664   5.054  1.00  0.00           H
ATOM     91 HD11 LEU A  20       7.730  -2.725   7.575  1.00  0.00           H
ATOM     92 HD12 LEU A  20       6.931  -1.176   7.343  1.00  0.00           H
ATOM     93 HD13 LEU A  20       5.984  -2.528   7.201  1.00  0.00           H
ATOM     94 HD21 LEU A  20       7.249  -3.655   3.881  1.00  0.00           H
ATOM     95 HD22 LEU A  20       6.381  -4.288   5.323  1.00  0.00           H
ATOM     96 HD23 LEU A  20       8.220  -4.216   5.249  1.00  0.00           H
ATOM    135  N   LYS A  21       9.820   0.664   3.246  1.00  0.00           N
ATOM    136  CA  LYS A  21      10.975   0.955   2.372  1.00  0.00           C
ATOM    137  C   LYS A  21      11.304   2.464   2.404  1.00  0.00           C
ATOM    138  O   LYS A  21      10.924   3.166   1.434  1.00  0.00           O
ATOM    139  CB  LYS A  21      10.710   0.505   0.896  1.00  0.00           C
ATOM    140  CG  LYS A  21      10.529  -1.031   0.801  1.00  0.00           C
ATOM    141  CD  LYS A  21      10.227  -2.960  -0.740  1.00  0.00           C
ATOM    142  CE  LYS A  21      10.560  -1.466  -0.702  1.00  0.00           C
ATOM    143  NZ  LYS A  21       9.968  -3.392  -2.125  1.00  0.00          N1+
ATOM    144  H   LYS A  21       8.942   0.992   2.869  1.00  0.00           H
ATOM    145  HA  LYS A  21      11.743   0.333   2.848  1.00  0.00           H
ATOM    146  HB2 LYS A  21      11.576   0.881   0.402  1.00  0.00           H
ATOM    147  HB3 LYS A  21       9.836   0.996   0.487  1.00  0.00           H
ATOM    148  HG2 LYS A  21      11.280  -1.515   1.394  1.00  0.00           H
ATOM    149  HG3 LYS A  21       9.594  -1.356   1.205  1.00  0.00           H
ATOM    150  HD2 LYS A  21       9.737  -0.890  -1.158  1.00  0.00           H
ATOM    151  HD3 LYS A  21      11.512  -1.175  -1.049  1.00  0.00           H
ATOM    152  HE2 LYS A  21      11.067  -3.517  -0.382  1.00  0.00           H
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ATOM    153  HE3 LYS A  21       9.383  -3.343  -0.240  1.00  0.00           H
ATOM    154  HZ1 LYS A  21       9.189  -2.889  -2.560  1.00  0.00           H
ATOM    155  HZ2 LYS A  21       9.911  -4.495  -2.254  1.00  0.00           H
ATOM    156  HZ3 LYS A  21      10.772  -3.208  -2.783  1.00  0.00           H
ATOM    157  N   LYS A  22      11.791   2.998   3.600  1.00  0.00           N
ATOM    158  CA  LYS A  22      12.039   4.454   3.802  1.00  0.00           C
ATOM    159  C   LYS A  22      10.607   5.044   3.702  1.00  0.00           C
ATOM    160  O   LYS A  22      10.339   5.902   2.845  1.00  0.00           O
ATOM    161  CB  LYS A  22      12.952   5.063   2.637  1.00  0.00           C
ATOM    162  CG  LYS A  22      14.274   4.373   2.639  1.00  0.00           C
ATOM    163  CD  LYS A  22      15.051   4.894   3.888  1.00  0.00           C
ATOM    164  CE  LYS A  22      16.510   4.490   3.758  1.00  0.00           C
ATOM    165  NZ  LYS A  22      17.224   5.014   4.915  1.00  0.00           N1+
ATOM    166  H   LYS A  22      11.555   2.391   4.423  1.00  0.00           H
ATOM    167  HA  LYS A  22      12.477   4.538   4.794  1.00  0.00           H
ATOM    168  HB2 LYS A  22      12.518   4.953   1.649  1.00  0.00           H
ATOM    169  HB3 LYS A  22      13.051   6.186   2.715  1.00  0.00           H
ATOM    170  HG2 LYS A  22      14.231   3.327   2.611  1.00  0.00           H
ATOM    171  HG3 LYS A  22      14.778   4.760   1.792  1.00  0.00           H
ATOM    172  HD2 LYS A  22      15.053   5.977   4.001  1.00  0.00           H
ATOM    173  HD3 LYS A  22      14.588   4.539   4.848  1.00  0.00           H
ATOM    174  HE2 LYS A  22      17.032   4.841   2.903  1.00  0.00           H
ATOM    175  HE3 LYS A  22      16.518   3.387   3.793  1.00  0.00           H
ATOM    176  HZ1 LYS A  22      17.155   6.062   4.999  1.00  0.00           H
ATOM    177  HZ2 LYS A  22      18.313   4.839   4.858  1.00  0.00           H
ATOM    178  HZ3 LYS A  22      16.949   4.578   5.862  1.00  0.00           H
HETATM  358  N   NH2 A  23       9.733   4.558   4.652  1.00  0.00           N
HETATM  359  HN1 NH2 A  23       8.807   5.068   4.793  1.00  0.00           H
HETATM  360  HN2 NH2 A  23      10.040   4.137   5.484  1.00  0.00           H
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