The GROMOS Software for (Bio)Molecular Simulation

Volume 3: Force Field and Topology Data Set

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Contents

CHAPTER 1

Introduction

In this volume the molecular model and the force field used in GROMOS are described. The GROMOS package comes with a number of standard data files. The ones involving the definition of a force field parameter set fall into two categories: interaction function parameter files (∗.ifp) and molecular topology building block files (∗.mtb). At least one of each of these types of files are required to build a molecular topology. This chapter continues with a short overview of the history of the GROMOS force field and a description of the background for its various versions. Chap. 2 summarizes the physical potential energy terms used in the GROMOS force fields. A detailed description of the Hamiltonian can be found in Vol. 2. The parameters contained in the interaction function parameter files of the 45A4 (45B4)[1–4] and 54A7 (54B7)[5–8] versions of the GROMOS force field are presented in Chap. 3. The corresponding molecular topology building blocks for the 54A7 force field are described in Chap. 4. Standard configurations of molecules or molecular systems are listed in Chap. 5.

1.1. GROMOS force fields

The GROMOS force field is continuously being tested and, if necessary, improved. From time to time a new version is brought out. The historic sequence of GROMOS force fields is the following:

- the 26C1 force field of June 1981
- the 37C2 (and 37D2) force field(s) of January 1983 (extended in November 1983)
- the 37C4 (and 37D4) force field(s) of November 1983 (revised in December 1985)
- the 43A1 (and 43B1) force field(s) of July 1996
- the 43A2 force field of October 2000
- the 45A3 (and 45B3) force field(s) of January 2001
- the 45A4 (and 45B4) force field(s) of July 2003
- the 53A5 (and 53B5) force field of July 2003
- the 53A6 (and 53B6) force field of July 2003
- the 54A7 (and 54B7) force field of April 2011
- the 54A8 force field of June 2012

The A-version of a force field is the basic force field designed for molecules in solution or in crystalline form. The B-version is derived from the A-version in order to be used for simulating molecules in vacuo, where the dielectric screening effect of the environment is neglected. The atomic charges and van der Waals parameters are changed such that atom charge groups with a non-zero total charge are neutralized while maintaining the hydrogen-bonding capacity of the individual atoms.

Since the functional form of the 43A1 and 43B1 force fields differs from that of the previous versions and the GROMOS file structure and formats were substantially changed in 1996, the force field versions older than 1996 have not been converted and have not been kept in the GROMOS package. For every force-field version, the complete set of interaction function parameters can be found in the corresponding file ∗.ifp. Building blocks of the 43A1 and 43A2, and the 43B1 and 43B2 force fields are given in the files 43a1.mtb and 43b1.mtb, respectively, and 45a3.mtb and 45b3.mtb present building blocks for the 45A3 and 45B3 force fields. In the newer versions of the GROMOS force field, building blocks are supplied via more than one file. These files contain building blocks that are categorized according to the kind of (sub)molecule they represent. For example, 45A4 building blocks can be found in: 45a4.mtb (α-amino acids, lipids, nucleotides and solvents), 45a4_carbo.mtb (carbohydrates and sugars), 45a4_beta.mtb (β-amino acids) and 45a4_cof.mtb (cofactors and other types of molecules).

Since the introduction of the 43A1 and 43B1 versions, the basic functional form of the GROMOS force field has been kept constant. It is described in Chap. 2-5 to Chap. 2-9 of Vol. 2. Chap. 3 and Chap. 4 of this Volume present the force field parameters and building blocks of the 54A7 force field. In the remaining of the current chapter, the events leading up to these force fields are sketched.

1.2. Development of the GROMOS force field

In the first GROMOS force field, 26C1, only 26 atom types were defined[9,10]. The molecular topology building block file contained only amino acid residues and a heme group. It was meant for simulation of proteins in aqueous solution or crystalline form.

The 37C2 force field was an extension of the 26C1 force field in order to allow for simulation of nucleotides, sugars, etc. Eleven new atom types were added. Some interaction function parameters were slightly changed, which made the version number change from 1 to 2. The molecular topology building block file contained many more building blocks. It was meant for simulation of proteins, DNA, sugars in aqueous solution or crystalline form.

The 37D2 force field was the one corresponding to the 37C2 one, but adapted in order to be used for simulations of molecules in vacuo.

In the previous force fields the repulsive part of the van der Waals interaction between third neighbour atoms (1-4 interaction) was too large, in case one or both of the atoms involved was an extended (CH1, CH2, CH3, CR1) carbon atom and the torsion angle 1-2-3-4 was in a cis-conformation. This effect was redressed by changing the programs such that for 1-4 or third-neighbour interactions, van der Waals parameters can be used which are different from the normal ones. These extra 1-4 van der Waals parameters had to be given on the interaction function parameter file. This change made the force field version number change from 2 to 4. It was meant for simulation of proteins, DNA, sugars, etc. in solution or crystalline form.

The 37D4 force field was the one corresponding to the 37C4 one, but adapted in order to be used for simulations of molecules in vacuo.

The 43A1 force field constitutes a significant change with respect to the 37C4 one, and differs from it in a number of aspects.

1. The non-polar solute atoms appeared to be slightly too hydrophilic[11]. Therefore, the C12(I,J) van der Waals parameter, where I denotes a non-polar atom type and J denotes a water oxygen, was enlarged.
2. The description of aromatic rings which was based on the use of united atoms, was improved by introducing explicit hydrogen atoms on some aromatic rings[11].
3. In order to reduce the rotational motion of the peptide plane, the dihedral angle torsional force constants for the φ, ψ dihedrals were slightly increased.
4. The force field parameters in the heme-group were slightly changed.
5. The functional forms of the covalent bond-stretching interaction and bond-angle bending interaction were changed in order to improve computational efficiency and to avoid singularities in the forces for (ideal) bond angles of 180° (see section Sec. 2.3).
6. The nomenclature (definition of improper dihedral angles) of the Leu and Val side chains was changed such that it corresponds to the IUPAC-IUB convention.
7. Due to the introduction of the distinction between mass atom types and non-bonded van der Waals atom types and by relinquishing the use of non-bonded atom types for the definition of bond, bond-angle and (improper) dihedral- angle types, the number of different (van der Waals) atom types could be reduced from 37 to 22.
8. New van der Waals atom types were added, especially to allow for the use of different solvents (apart from water). This brought the number of non-bonded (van der Waals) atom types to 43.

Shortly after the release of the 43A1 and 43B1 force fields, some small changes in the torsional-angle parameters and the third-neighbour-van der Waals interaction were introduced, in order to better reproduce the distribution of the torsional-angle values in short aliphatic chains. This modification resulted in the

43A2 parameter set.[12]. As it was then shown that the density for the longer alkanes was too high, a reparametrisation of the aliphatic united atoms followed, introducing two additional atom types for branched and cyclic alkanes. This resulted in the 45A3 and 45B3 set of parameters[1].
Several parametrisation efforts on different classes of molecular systems were subsequently collected in the 45A4 and 45B4 set of parameters. The most important changes involved

- Charges and torsional dihedral angles in nucleotides and common co-factors[3]
- Charges and torsional dihedral angles in carbohydrates[4]
- Charges and torsional dihedral angles in lipids[2]
- Modifications in the choice of polar/nonpolar C12 interaction parameters for atom type 6 (NT)
- Correction to the van der Waals interaction parameters for atom type 31 (BR)
- Modifications to the heme group covalent interactions
- A new definition of the molecular topology building block at the end of polypeptide, polynucleotide or polysaccharide chains

The 53A5 and 53A6 force fields[5] are the result of a complete reparametrisation of the non-bonded interaction parameters for condensed phase simulations of pure liquids of small molecules (53A5) and solutions of molecular systems in water or apolar solvents (53A6). All interaction types have been redefined in these force fields, which also include parameters for additional solvents. In addition, bond types, bond-angle types, dihedral-angle types and atom-types have been renumbered in 53A5 and 53A6.

In the 54A7 force field[6–8]

- The 53A6 helical propensities are corrected through new phi/psi torsional angle terms and a modification of the N-H, C=O repulsion.
- A new atom type for a charged -CH3 in the choline moiety is added.
- The Na+ and Cl- ions are modified to reproduce the free energy of hydration.
- Additional improper torsional angle types for free energy calculations involving a chirality change are introduced.
- For the cofactors the files 54c7_cof.mtb and 54d7_cof.mtb were introduced in which the partial charges were updated according to analogy of functional groups. Files 54a7_cof.mtb and 54b7_cof.mtb still contain the original charge distributions.

The 54A8 force field[13] involves a recalibration of the nonbonded interaction parameters for the charged amino-acid side chains, based on ionic side chain analogs. After a thorough analysis of the available experimental data, conventional hydration free energies for the ammonium; mono-, di-, tri-, and tetramethylammonium; formate; acetate; propanoate; imidazolium; and guanidinium ions were combined with a standard absolute intrinsic proton hydration free energy to yield absolute intrinsic single-ion hydration free energies serving as experimental target data. The raw hydration free energies calculated from atomistic simulations are affected by electrostatic and finite-size artifacts, and corrections were applied to reach methodological independence prior to comparison with these experimental values.

Solvent models that are consistent with the GROMOS biomolecular force fields are available for much used (co)-solvents[14]:

- water[15,16]
- methanol[17]
- DMSO[18]
- chloroform[19]
- carbontetrachloride[20]
- urea[21]
- acetonitrile[22]
- dimethylsulfone[23]

Polarisable (solvent) models consistent with the GROMOS biomolecular force field are available for:

- water[24]
- methanol[25]
- DMSO[26]

- chloroform[27]
- carbontetrachloride[28]
- urea[29]
- acetone[30]
- n-alkanes[31]

Supra-molecular polarisable coarse-grained solvent models compatible with the GROMOS biomolecular force fields are available for:

- water[32]
- methanol[33,34]
- DMSO[33]
- chloroform[33]

Supra-atomic polarisable coarse-grained models compatible with the GROMOS biomolecular force field are available for n-alkanes[35] and cyclohexane.[36]

CHAPTER 2

Physical forces: GROMOS force field

2.1. Introduction

This chapter summarizes the functional form of the GROMOS force field terms, which are described in detail in the following chapters of Vol. 2: The bonded interaction force-field terms are described in Chap. 2-5; van der Waals interactions are described in Chap. 2-6; electrostatic interactions are described in Chap. 2-7; forces between coarse-grained particles are described in Chap. 2-8; the special force-field terms are described in Chap. 2-9.

2.2. Bond stretching force-field terms

The potential energy (force-field) term associated with *bond stretching interactions* is the term $\mathcal{V}^{(b)}(\boldsymbol{r};\mathbf{s})$ in Eq. 2.1. It is given by

$$\mathcal{V}^{(b)}(\boldsymbol{r};\mathbf{s}) = \sum_{n=1}^{N^{(b)}} V^{(b)}(b_n; k_n^{(b)}, b_n^0) \ , \tag{2.1}$$

where $N^{(b)}$ is generally equal to the total number of all covalent bonds present in the system, *i.e.* each covalent bond is associated with one and only one stretching term in the GROMOS force-field, and $V^{(b)}$ is the function describing the potential energy associated with the stretching of a single bond. The quantity $b_n \doteq b_n(\boldsymbol{r})$ represents the length of bond n in the given system configuration, *i.e.* the distance between the two atoms $i \doteq i(n)$ and $j \doteq j(n)$ connected by the covalent bond n (minimum-image distance if PBC is applied). The quantities $k_n^{(b)}$ and b_n^0 represent force-field parameters, force constant and reference length, respectively characteristic for the specific bond n, as encoded by a corresponding *bond type code* $M_n^{(b)}$, *i.e.* one may write $k_n^{(b)} \doteq k^{(b)}(M_n^{(b)}, \mathbf{s})$ and $b_n^0 \doteq b^0(M_n^{(b)}, \mathbf{s})$. Two different expression can be used for the function $V^{(b)}$ in GROMOS (see Sec. 2-5.1), a quartic function with force constant $k^{(b)}$ and a harmonic function with force constant $k^{(b,h)}$. The coarse-grained (CG) model exploits yet another (quartic) interaction term for the bond between the central particle and the dipole particle of a CG bead.[32]

For reasons of ease of analysis, the list of $N^{(b)}$ covalent bonds is split into two lists, one of bonds involving hydrogen atoms (defined as having mass atom type code 1, see Tab. 3.1), and one involving the other bonds. These lists are kept in the molecular topology file (see Vol. 4). The first list contains NBONH bonds involving hydrogen atoms. Three items are stored: IBH, JBH[1..NBONH] are the atom sequence numbers of the atoms forming bond i-j as a function of the bond sequence number n, and ICBH[1..NBONH] is the bond-type code, denoting the parameters $k_n^{(b)}$, $k_n^{(b,h)}$ and b_n^0 , as a function of the bond sequence number n. The list for the bonds involving no hydrogen atoms contains corresponding items denoted by IB, JB, ICB[1..NBON]. The force field parameters $k_n^{(b)}$, $k_n^{(b,h)}$ and b_n^0 for the various types of covalent bonds are stored in CB[1..NBTY], HB[1..NBTY] and B0[1..NBTY], as a function of the bond-type code (ICBH or ICB). They can be found in the interaction function parameter files ∗.ifp. For the GROMOS force fields 45A4 and 45B4 they are listed in Tab. 3.2, for force fields 54A7 and 54B7 they are listed in Tab. 3.17.

Program MD++ reads values for $k_n^{(b)}$, $k_n^{(b,h)}$ and b_n^0 from the BONDSTRETCHTYPE block in the molecular topology file (∗.top). It can also read $k_n^{(b)}$ and b_n^0 from the BONDTYPE block and $k_n^{(b,h)}$ and b_n^0 from the HARMBONDTYPE block. If only BONDTYPE block or HARMBONDTYPEBLOCK are given, the missing force constant is calculated using equations Eq. 2-18.3 and Eq. 2-18.4.

2.3. Bond-angle bending force-field terms

The potential energy (force-field) term associated with *bond-angle bending interactions* is the term $\mathcal{V}^{(\theta)}(\boldsymbol{r};\mathbf{s})$ in Eq. 2.2. It is given by

$$\mathcal{V}^{(\theta)}(\boldsymbol{r};\mathbf{s}) = \sum_{n=1}^{N^{(\theta)}} V^{(\theta)}(\theta_n; k_n^{(\theta)}, \theta_n^0) \ , \tag{2.2}$$

where $N^{(\theta)}$ is generally equal to the total number of all covalent bond-angles present in the system, *i.e.* each definable covalent bond-angle is associated with one and only one bending term in the GROMOS force field, and $V^{(\theta)}$ is the function describing the potential energy associated with the bending of a single bond angle. The quantity $\theta_n \doteq \theta_n(\boldsymbol{r})$ represents the value of bond angle n in the given system configuration, *i.e.* the angle formed by the three atoms $i \doteq i(n)$, $j \doteq j(n)$ and $k \doteq k(n)$ defining the covalent bond angle n (minimum-image triplet if PBC is applied). The quantities $k_n^{(\theta)}$ and θ_n^0 represent force-field parameters, force constant and reference bond angle, respectively, characteristic for the specific bond angle n, as encoded by a corresponding *bond-angle type code* $M_n^{(\theta)}$*i.e.* one may write $k_n^{(\theta)} \doteq k^{(\theta)}(M_n^{(\theta)}, \mathbf{s})$ and $\theta_n^0 \doteq \theta^0(M_n^{(\theta)}, \mathbf{s})$. Two different expression can be used for the function $V^{(\theta)}$ in GROMOS (see Sec. 2-5.2), a cosine-harmonic function with force constant $k^{(\theta)}$ and a harmonic function with force constant $k^{(\theta,h)}$.

For reasons of ease of analysis, the list of $N^{(\theta)}$ bond angles is split into two lists, one of bond angles involving hydrogen atoms (defined as having mass atom type code 1, see Tab. 3.1), and one involving the other bond angles. These lists are kept in the molecular topology file (Volume 4). The first list contains NTHEH bond angles involving hydrogen atoms. Four items are stored: ITH, JTH, KTH[1...NTHEH] are the atom sequence numbers of the atoms forming bond angle i-j-k as a function of the bond-angle sequence number n, and ICTH [1...NTHEH] is the bond-angle type code, denoting the parameters $k_n^{(\theta)}$, $k_n^{(\theta,h)}$ and θ_n^0 as a function of the bond-angle sequence number n. The list for the bond angles involving no hydrogen atoms contains corresponding items denoted by IT, JT, KT, ICT[1...NTHE]. The force field parameters $k_n^{(\theta)}$, $k_n^{(\theta,h)}$ and θ_n^0 for the various types of bond angles are stored in CT[1...NTTY], CHT[1...NTTY] and T0[1 ... NTTY] as a function of the bond-angle type code (ICTH or ICT). They can be found in the interaction parameter files $*$.ifp. For the GROMOS force fields 45A4 and 45B4, they are listed in Tab. 3.3, for force fields 54A7 and 54B7 they are listed in Tab. 3.18.

Program MD++ reads values for $k_n^{(\theta)}$, $k_n^{(\theta,h)}$ and θ_n^0 from the BONDANGLEBENDTYPE block in the molecular topology file ($*$.top). If no BONDANGLEBENDTYPE is present $k_n^{(\theta)}$ can be read from the BONDANGLETYPE block and $k_n^{(\theta,h)}$ can be read from the HARMBONDANGLETYPE block.

2.4. Improper dihedral-angle bending force-field term

The potential energy (force-field) term associated with *improper dihedral-angle bending interactions*, *i.e.* typically controlling out-of-plane or out-of-tetrahedron distortions, is the term $\mathcal{V}^{(\xi)}(\boldsymbol{r};\mathbf{s})$ in Eq. 2.3. It is given by

$$\mathcal{V}^{(\xi)}(\boldsymbol{r};\mathbf{s}) = \sum_{n=1}^{N^{(\xi)}} V^{(\xi)}(\xi_n; k_n^{(\xi)}, \xi_n^0) \ , \tag{2.3}$$

where $N^{(\xi)}$ generally corresponds to a subset of all possibly definable improper dihedral angles in the system (see below; note, however, each definable covalent improper dihedral angle is associated with at most one bending term in the GROMOS force field), and $V^{(\xi)}$ is the function describing the potential energy associated with the bending of a single improper dihedral angle. The quantity $\xi_n \doteq \xi_n(\boldsymbol{r})$ represents the value of improper dihedral angle n in the given system configuration, *i.e.* the dihedral angle formed by the four atoms $i \doteq i(n)$, $j \doteq j(n)$, $k \doteq k(n)$ and $l \doteq l(n)$ defining the covalent improper dihedral angle n (minimum-image quadruplet if PBC is applied). The quantities $k_n^{(\xi)}$ and ξ_n^0 represent force-field parameters, force constant and reference improper dihedral-angle, respectively, characteristic for the specific improper dihedral angle n, as encoded by a corresponding *improper dihedral-angle type code* $M_n^{(\xi)}$*i.e.* one may write $k_n^{(\xi)} \doteq k^{(\xi)}(M_n^{(\xi)}, \mathbf{s})$ and $\xi_n^0 \doteq \xi^0(M_n^{(\xi)}, \mathbf{s})$. The function $V^{(\xi)}$ is always a *harmonic* function in GROMOS.
The improper dihedral angle definitions can be found in the molecular topology building block files $*$.mtb.

For reasons of ease of analysis, the list of $N^{(\xi)}$ improper dihedral angles is split into two lists, one of improper dihedrals involving hydrogen atoms (defined as having mass atom type code 1, see Tab. 3.1), and one involving the other one involving the other improper dihedrals. These lists are kept in the molecular topology file (Volume 4). The first list contains NQHIH improper dihedral angles involving hydrogen atoms. Five items are stored: IQH, JQH, KQH, LQH[1...NQHIH] are the atom sequence numbers of the atoms forming improper dihedral i-j-k-l as a function of the improper dihedral sequence number n, and ICQH[1...NQHIH] is the improper dihedral type code, denoting the parameters $k_n^{(\xi)}$ and ξ_n^0 , as a function of the improper dihedral sequence number n. The list for the improper dihedral angles involving no hydrogen atoms contains corresponding items denoted by IQ, JQ, KQ, LQ, ICQ[1...NQHI]. The force field parameters $k_n^{(\xi)}$ and ξ_n^0 for the various types of improper dihedrals are stored in CQ[1...NQTY] and Q0[1...NQTY] as a function of the improper dihedral type code (ICQH or ICQ). They can be found in the interaction parameter files $*$.ifp. For the GROMOS force fields 45A4, 45B4, 54A7 and 54B7 they are listed in Tab. 3.4 (and Tab. 3.19).

Program MD++ reads values for $k_n^{(\xi)}$, and ξ_n^0 from the IMPDIHEDRALTYPE block in the molecular topology file ($*$.top).

2.5. Proper dihedral-angle torsion force-field term

The potential energy (force-field) term associated with *proper dihedral-angle bending interactions*, *i.e.* typically controlling, in balance with non-bonded interactions, the rotational barriers around covalent bonds, is the term $\mathcal{V}^{(\varphi)}(\boldsymbol{r};\mathbf{s})$ in Eq. 2.4. It is given by

$$\mathcal{V}^{(\varphi)}(\boldsymbol{r};\mathbf{s}) = \sum_{n=1}^{N^{(\varphi)}} V^{(\varphi)}(\varphi_n; k_n^{(\varphi)}, \varphi_n^0, m_n^{(\varphi)}) \ , \tag{2.4}$$

where $N^{(\varphi)}$ generally corresponds to a subset of all possibly definable proper dihedral angles in the system and $V^{(\varphi)}$ is the function describing the potential energy contribution of the term to the torsion of the corresponding proper dihedral angle. The quantity $\varphi_n \doteq \varphi_n(\boldsymbol{r})$ represents the value of proper dihedral angle n in the given system configuration, *i.e.* the dihedral angle formed by the four atoms $i \doteq i(n)$, $j \doteq j(n)$, $k \doteq k(n)$ and $l \doteq l(n)$ defining the covalent proper dihedral angle n (minimum-image quadruplet if PBC is applied). Note that the sign of the dihedral angle as defined by Eq. 2-5.19 follows the IUPAC-IUB convention[37], and that the proper dihedral angle is undefined if either $r_{im'} = 0$ or $r_{in'} = 0$. The quantities $k_n^{(\varphi)}$, φ_n^0 and $m_n^{(\varphi)}$ represent force-field parameters (force constant, reference dihedral-angle, and multiplicity, respectively; the reference dihedral angle is also called the phase shift; the multiplicity is a positive non-zero integer) characteristic for the specific proper dihedral angle term n, as encoded by a corresponding *proper dihedral-angle type code* $M_n^{(\varphi)}$. Two different expression can be used for the function $V^{(\varphi)}$ in GROMOS (see Sec. 2-5.4).

The torsional dihedral angle definitions can be found in the molecular topology building block files $*$.mtb (see Vol. 4). Examples of the special definitions involving sugar or phosphor atoms can be found in the building blocks DADE or NADPH.

Program MD++ reads values for $k_n^{(\varphi)}$, φ_n^0 and $m_n^{(\varphi)}$ from the TORSDIHEDRALTYPE block in the molecular topology file ($*$.top), also if the DIHEDRALTYPE block is given as well. If the DIHEDRALTYPE is given in the topology instead of the TORSDIHEDRALTYPE, only cos φ_n values (instead of φ_n values) are read.

For reasons of ease of analysis, the list of $N^{(\varphi)}$ torsional dihedral angles is split into two lists, one of dihedrals involving hydrogen atoms (defined as having mass atom type code 1, see Table Tab. 3.1), and one involving the other dihedrals. These lists are kept in the molecular topology file (Vol. 4). The first list contains NPHIH dihedral angles involving hydrogen atoms. Five items are stored: IPH, JPH, KPH, LPH[1..NPHIH] are the atom sequence numbers of the atoms forming dihedral i-j-k-l as a function of the dihedral sequence number n, and ICPH[1..NPHIH] is the dihedral type code, denoting the parameters $k_n^{(\varphi)}$, φ_n^0 and $m_n^{(\varphi)}$, as a function of the dihedral sequence number n. The list for the dihedrals involving no hydrogen atoms contains corresponding items denoted by IP, JP, KP, LP, ICP[1..NPHI]. The force field parameters $k_n^{(\varphi)}$, φ_n^0 and $m_n^{(\varphi)}$ for the various types of torsional dihedrals are stored in CP[1..NPTY], NP[1..NPTY] and PD[1..NPTY] as a function of the torsional dihedral type code (ICPH or ICP). They can be found in the

interaction parameter files ∗.ifp. For the GROMOS force fields 45A4 and 45B4, they are listed in Tab. 3.5, for the GROMOS force fields 54A7 and 54B7, they are listed in Tab. 3.20.

As an additional feature, the specification at so-called cross-dihedral terms is supported. The corresponding expression for this type of interaction reads

$$\begin{aligned} V^{trig,cross}(\mathbf{r};s) &= \sum_{n=1}^{N_c} V_n^{trig,cross}\ (\varphi_n;\psi_n;K_{c_n};\delta_n;m_n) \\ &= \sum_{n=1}^{N_c} K_{c_n}\ [1+\cos\ (m_n(\varphi_n+\psi_n)-\delta_n)] \end{aligned} \tag{2.5}$$

The summation runs over the set of $n = 1, \ldots, N_c$ of coupled dihedral angles φ_n and ψ_n, as specified by atoms a-b-c-d and e-f-g-h, respectively, which are specified in the CROSSDIHEDRALH and CROSSDIHEDRAL blocks in the molecular topology file (∗.top). These blocks specify coupled dihedral angles that do involve hydrogens and do not involve hydrogens, respectively. In addition, the type of cross-dihedral term n is specified in the same blocks in the topology file, defining the force constant K_{c_n}, phase-shift δ_n and multiplicity m, as read from the TORSDIHEDRALTYPE block in the molecular topology file. Accordingly, the specification of cross-dihedral terms is only possible if the TORSDIHEDRALTYPE block is specified.

The forces on atoms a, b, c, d of dihedral φ_n and atoms e, f, g, h of dihedral ψ_n due to the n-th in (Eq. 2.5) are

$$\begin{aligned} \mathbf{f}_a &= -\frac{\partial V^{\ trig,cross}}{\partial\varphi_n}\frac{\partial\varphi_n}{\partial\mathbf{r}_a} \\ &= K_{c_n}m_n sin(m_n(\varphi_n+\psi_n)-\delta_n)\frac{r_{cb}}{r_{mb}^2}\ \mathbf{r}_{mj} \end{aligned} \tag{2.6}$$

$$\begin{aligned} \mathbf{f}_d &= -\frac{\partial V^{\ trig,cross}}{\partial\varphi_n}\frac{\partial\varphi_n}{\partial\mathbf{r}_d} \\ &= -K_{c_n}m_n sin(m_n(\varphi_n+\psi_n)-\delta_n)\frac{r_{cb}}{r_{mb}^2}\ \mathbf{r}_{nc} \end{aligned} \tag{2.7}$$

$$\begin{aligned} \mathbf{f}_b &= -\frac{\partial V^{\ trig,cross}}{\partial\varphi_n}\frac{\partial\varphi_n}{\partial\mathbf{r}_b} \\ &= \left[\frac{(\mathbf{r}_{ab}\ \cdot\ \mathbf{r}_{cb})}{r_{cb}^2}\ -1\right]\ \mathbf{f}_i\ -\frac{\mathbf{r}_{cd}\ \cdot\ \mathbf{r}_{cb}}{r_{cb}^2}\mathbf{f}_d \end{aligned} \tag{2.8}$$

$$\mathbf{f}_c = -\mathbf{f}_a\ -\mathbf{f}_b\ -\mathbf{f}_d \tag{2.9}$$

$$\begin{aligned} \mathbf{f}_e &= -\frac{\partial V^{\ trig,cross}}{\partial\psi_n}\frac{\partial\psi_n}{\partial\mathbf{r}_e} \\ &= K_{c_n}m_n sin(m_n(\varphi_n+\psi_n)-\delta_n)\frac{r_{gf}}{r_{mf}^2}\ \mathbf{r}_{mf} \end{aligned} \tag{2.10}$$

$$\begin{aligned} \mathbf{f}_h &= -\frac{\partial V^{\ trig,cross}}{\partial\psi_n}\frac{\partial\psi_n}{\partial\mathbf{r}_h} \\ &= -K_{c_n}m_n sin(m_n(\varphi_n+\psi_n)-\delta_n)\frac{r_{gf}}{r_{ng}^2}\ \mathbf{r}_{ng} \end{aligned} \tag{2.11}$$

$$\begin{aligned}\mathbf{f}_f &= -\frac{\partial V^{\,trig,cross}}{\partial \psi_n}\frac{\partial \psi_n}{\partial \mathbf{r}_f} \\ &= \left[\frac{(\mathbf{r}_{ef}\ \cdot\ \mathbf{r}_{gf})}{r_{gf}^2}\ -1\right]\ \mathbf{f}_e\ -\frac{(\mathbf{r}_{gh}\ \cdot\ \mathbf{r}_{gf})}{r_{gf}^2}\mathbf{f}_h\end{aligned} \tag{2.12}$$

$$\mathbf{f}_g = -\mathbf{f}_e\ -\mathbf{f}_f\ -\mathbf{f}_h \tag{2.13}$$

where

$$\mathbf{r}_{mb} = \mathbf{r}_{ab} \times \mathbf{r}_{cb} \tag{2.14}$$
$$\mathbf{r}_{nc} = \mathbf{r}_{cb} \times \mathbf{r}_{cd} \tag{2.15}$$
$$\mathbf{r}_{mf} = \mathbf{r}_{ef} \times \mathbf{r}_{gf} \tag{2.16}$$
$$\mathbf{r}_{ng} = \mathbf{r}_{gf} \times \mathbf{r}_{gh} \tag{2.17}$$

and

$$sin(m_n(\varphi_n + \psi_n) - \delta_n) = \sqrt{1 - cos^2(m_n(\varphi_n + \psi_n) - \delta_n)} \tag{2.18}$$

2.6. Non-bonded interactions

The term in the interaction function that represents the *non-bonded interaction* is a sum of contributions from van der Waals and electrostatic interactions,

$$\begin{aligned}&V^{nonb}(\mathbf{r}^{\mathbf{N}}; s) = \\ &\sum_{\substack{nonbonded\\ pairs(i,j)}} \big\{V^{LJ}(r_{ij}; C_{12}(i,j), C_6(i,j), R_{cp}, R_{cl}) \\ &\qquad +V^{CRF}(r_{ij}; q_i, q_j, R_{cp}, R_{cl}, R_{rf}, \varepsilon_1, \varepsilon_2, \kappa)\big\}\end{aligned} \tag{2.19}$$

with

$$V^{LJ} = \left[\frac{C_{12}(i,j)}{(r_{ij})^6} - C_6(i,j)\right]\frac{1}{(r_{ij})^6} \tag{2.20}$$

and

$$V^{CRF} = \frac{q_i q_j}{4\pi\varepsilon_0\varepsilon_{cs}}\left[\frac{1}{r_{ij}} - \frac{\frac{1}{2}C_{rf}(r_{ij})^2}{R_{rf}^3} - \frac{1-\frac{1}{2}C_{rf}}{R_{rf}}\right] \tag{2.21}$$

The van der Waals interactions are discussed in Chap. 2-6 and the electrostatic interactions are discussed in Chap. 2-7.

2.6.1. van der Waals parameters. The non-bonded interaction van der Waals parameters C_{12}(i,j) and C_6(i,j) in formula (Eq. 2.19) depend on the atom type or more specifically the integer atom codes I = IAC[i] and J = IAC[j] of the atoms with atom sequence numbers i and j. The integer atom codes of the various types of atoms in the GROMOS force fields 45A5 and 45B4 are listed in Tab. 3.6, for GROMOS force fields 54A7 and 54B7, they are listed in Tab. 3.21.

Lists of integer atom codes are kept in the molecular topology file (Volume 4). For the NRP atoms of the "solute" part of the molecular topology the integer atom codes are stored in IAC[1..NRP]. The integer atom codes of the NRAM solvent atoms are stored in IACS[1..NRAM]. The van der Waals parameters are kept in the molecular topology file (see Volume 4). For the NRATT atom types, C12[1 .. NRATT∗(NRATT+1)/2] contains the coefficient C_{12} in (Eq. 2.19) as a function of the occurring pair codes; the sequence of atom pairs with integer atom codes ranging from 1 to NRATT is:

1-1, 1-2, 2-2, ..., 1-NRATT, 2-NRATT, ..., NRATT-NRATT.

The coefficients C_6 in (Eq. 2.19) are kept likewise in C6[1 .. NRATT∗(NRATT+1)/2]. In this way it is possible to change the van der Waals interaction between each pair of atom types independently. Basically, the GROMOS van der Waals parameters for an atom pair with integer atom codes I and J are derived from single atom van der Waals parameters using the relations

$$C_6(I,J) = \sqrt{C_6^{\frac{1}{2}}(I,I)C_6^{\frac{1}{2}}(J,J)} \tag{2.22}$$

and

$$C_{12}(I,J) = \sqrt{C_{12}^{\frac{1}{2}}(I,I)C_{12}^{\frac{1}{2}}(J,J)} \tag{2.23}$$

For the GROMOS force fields 45A4 and 45B4, the single atom van der Waals parameters $(C6(I,I))^{1/2}$ and $(C_{12}(I,I))^{1/2}$ are given in the third and fourth column of Tables Tab. 3.7 and Tab. 3.8 as a function of integer atom code or non-bonded atom type. For the GROMOS force fields 54A7 and 54B7, they are given in the third and fourth column of Tables Tab. 3.22 and Tab. 3.23.

GROMOS also offers a possibility to specify the van der Waals parameters for a specific atom pair, thereby overruling the interaction parameters as derived from the normal (or third-neighbour) interaction parameters. This can be done by introducing a LJEXCEPTIONS block in the molecular topology file (see Vol. 4).

2.6.2. Atomic charges and charge groups. Lists of atomic charges are kept in the molecular topology file (see Volume 4). For the NRP atoms in the "solute" part of the molecular topology atomic charges are stored in CG[1..NRP] (multiplied by $(4\pi\varepsilon_0)^{-1/2}$). The atomic charges of the NRAM solvent atoms are stored in CGS[1..NRAM] (multiplied by $(4\pi\varepsilon_0)^{-1/2}$).

When the (partial) atomic charges of a group of atoms add up to exactly zero, the leading term of the electrostatic interaction between two such groups of atoms is of dipolar ($1/r^3$) character. The sum of the 1/r monopole contributions of the various atom pairs to the group-group interaction will be zero. Therefore, the range of the electrostatic interaction can be considerably reduced when atoms are assembled in so-called charge groups, which have a zero net charge, and for which the electrostatic interaction with other (groups of) atoms is either calculated for all atoms of the charge group or for none.

The GROMOS force fields make use of this *concept of charge groups*. The atoms that belong to a charge group are chosen such that their partial atomic charges add up to zero. For groups of atoms with a total charge of $+e$ or $-e$, like the sidechain atoms of Arg or Asp, the partial atomic charges of the charge group may add up to $+e$ or $-e$. In GROMOS, the non-bonded interactions are calculated between charge groups only. When a cut-off radius is used, the distance between two charge groups must be defined. The *position of a charge group* is defined differently for a charge group belonging to the "solute" part of the molecular topology and one in the "solvent" part of the molecular topology.

- The position of a "solute" charge group is taken to be its centre of geometry:

  $$R_{cg} = \sum_{i=1}^{N_{cg}} \mathbf{r}_i \; / N_{cg} \tag{2.24}$$

  where the number of atoms belonging to the charge group is denoted by N_{cg}.
- The position of a "solvent" charge group is taken to be the position of the first atom of a solvent molecule. A "solvent" molecule may only contain one charge group.

Since each solvent molecule consists of one charge group, the "solvent" part of the molecular topology file does not need to contain information on "solvent" charge groups. In the "solute" part of the molecular topology file the charge group information is kept in the following way. It is assumed that atoms belonging to one charge group have sequential atom sequence numbers. The last atom of any charge group is denoted by a charge group code value of 1. All other atoms have a charge group code value of 0. This requirement of

atoms of a charge group to have sequential atom sequence numbers is a less elegant restriction to choosing the atom sequence when defining molecular topology building blocks or molecular topologies (see Vol. 4).

The atomic charges and charge group definitions for the GROMOS force fields are given in the molecular topology building block files ∗.mtb (Chap. 3). The atomic charges and charge group definitions for amino acid residues, various solvents and nucleotides of the 45A4 and 45B4 GROMOS force fields are listed in Tables Tab. 3.12-Tab. 3.16. For the GROMOS force fields 54A7 and 54B7 they are listed in Tables Tab. 3.27-Tab. 3.31.

The charges for the B-versions of the force field are given between parentheses. The atoms for which no changes are listed have zero partial charge and form single atom or multiple atom charge groups.

CHAPTER 3

GROMOS interaction function parameters

mass atom type code	mass in a.m.u.	mass atom name
1	1.008	H
3	13.019	CH1
4	14.027	CH2
5	15.035	CH3
6	16.043	CH4
12	12.011	C
14	14.0067	N
16	15.9994	O
19	18.9984	F
23	22.9898	NA
24	24.305	MG
28	28.08	SI
31	30.9738	P
32	32.06	S
35	35.453	CL
39	39.948	AR
40	40.08	CA
56	55.847	FE
63	63.546	CU
65	65.37	ZN
80	79.904	BR

TABLE 3.1. GROMOS mass atom type codes, masses and names.

Bond-type code	Force constant	Ideal bond length	Examples of usage in terms of non-bonded atom types	
$M_n^{(b)}$	$k_n^{(b,q)}$	b_n^0		$k_n^{(b,h)}$
	[10^6 kJ·mol^{-1}·nm^{-4}]	[nm]		[10^6 kJ·mol^{-1}·nm^{-2}]
ICBH[N] ICB[N]	CB[N]	B0[N]		
1	15.7	0.100	H - OA	0.314
2	18.7	0.100	H - N (all)	0.374
3	12.3	0.109	HC - C	0.292
4	16.6	0.123	C - O	0.502
5	13.4	0.125	C - OM	0.419
6	12.0	0.132	CR1 - NR (6-ring)	0.418
7	8.87	0.133	H - S	0.314
8	10.6	0.133	C - NT, NL	0.375
9	11.8	0.133	C, CR1 - N, NR, CR1, C (peptide, 5-ring)	0.417
10	10.5	0.134	C - N, NZ, NE	0.377
11	11.7	0.134	C - NR (no H) (6-ring)	0.420
12	10.2	0.136	C - OA	0.377
13	11.0	0.138	C - NR (heme)	0.419
14	8.66	0.139	CH2 - C, CR1 (6-ring)	0.335
15	10.8	0.139	C, CR1 - CH2, C, CR1 (6-ring)	0.417
16	8.54	0.140	C, CR1, CH2 - NR (6-ring)	0.335
17	8.18	0.143	CHn - OA	0.335
18	9.21	0.143	CHn - OM	0.377
19	6.10	0.1435	CHn - OA (sugar)	0.251
20	8.71	0.147	CHn - N, NT, NL, NZ, NE	0.376
21	5.73	0.148	CHn - NR (5-ring)	0.251
22	7.64	0.148	CHn - NR (6-ring)	0.335
23	8.60	0.148	O, OM - P	0.377
24	8.37	0.150	O - S	0.377
25	5.43	0.152	CHn - CHn (sugar)	0.251
26	7.15	0.153	C, CHn - C, CHn	0.335
27	4.84	0.161	OA - P	0.251
28	4.72	0.163	OA - SI	0.251
29	5.94	0.178	CH3 - S	0.376
30	5.62	0.183	CH2 - S	0.376
31	3.59	0.187	CH1 - SI	0.251
32	0.640	0.198	NR - FE	0.0502
33	5.03	0.204	S - S	0.419
34	0.628	0.200	NR (heme) - FE	0.0502
35	23.2	0.100	HWat - OWat	0.464
36	12.1	0.110	HChl - CChl	0.293
37	8.12	0.1758	CChl - CLChl	0.502
38	8.04	0.153	ODmso - SDmso	0.376
39	4.95	0.195	SDmso - CDmso	0.376
40	8.10	0.176	CCl4 - CLCl4	0.502

TABLE 3.2: continues on next page.

Bond-type code	Force constant	Ideal bond length	Examples of usage in terms of non-bonded atom types	
$M_n^{(b)}$	$k_n^{(b,q)}$	b_n^0		$k_n^{(b,h)}$
	$[10^6$ kJ·mol^{-1}·nm$^{-4}]$	[nm]		$[10^6$ kJ·mol^{-1}·nm$^{-2}]$
ICBH[N] ICB[N]	CB[N]	B0[N]		
41	8.71	0.163299	HWat - HWat	0.465
42	2.68	0.233839	HChl - CLChl	0.293
43	2.98	0.290283	CLChl - CLChl	0.502
44	2.39	0.280412	ODmso - CDmso	0.376
45	2.19	0.292993	CDmso - CDmso	0.376
46	3.97	0.198842	HMet - CMet	0.314
47	3.04	0.287407	CLCl4 - CLCl4	0.502
48	0.540	0.221	NR (His) - FE	0.0527
49	2.72	0.178	FE - C (CO bound to heme)	0.172
50	37.0	0.112	C - O (CO bound to heme)	0.928

TABLE 3.2: GROMOS 45A4 and 45B4 bond-stretching parameters ($k_n^{(b,q)} = k_n^{(b,h)}/(2b_n^{0\,2})$).

Bond-angle type code	Force constant	Ideal bond angle	Example of usage in terms of non-bonded atom types	
$M_n^{(\theta)}$	$k_n^{(\theta,c)}$	θ_n^0		$k_n^{(\theta,h)}$
	[kJ·mol^{-1}]	[deg]		[kJ·mol^{-1}·deg^{-2}]
ICTH[N] ICT[N]	CT[N]	(T0[N])		
1	420	90.0	NR(heme) - FE - NR(heme)	0.128
2	405	96.0	H - S - CH2	0.122
3	475	100.0	CH2 - S - CH3	0.140
4	420	103.0	OA - P - OA	0.121
5	490	104.0	CH2 - S - S	0.140
6	465	108.0	NR, C, CR1(5-ring)	0.128
7	285	109.5	CHn - CHn - CHn, NR(6-ring) (sugar)	0.0769
8	320	109.5	CHn, OA - CHn - OA, NR(ring) (sugar)	0.0864
9	380	109.5	H - NL, NT - H, CHn - OA - CHn(sugar)	0.103
10	425	109.5	H - NL - C, CHn H - NT - CHn	0.115
11	450	109.5	X - OA, SI - X	0.122
12	520	109.5	CHn,C - CHn - C, CHn, OA, OM, N, NE	0.141
13	450	109.6	OM - P - OA	0.121
14	530	111.0	CHn - CHn - C, CHn, OA, NR, NT, NL	0.140
15	545	113.0	CHn - CH2 - S	0.140
16	50	115.0	NR(heme) - FE - NR	0.0123
17	460	115.0	H - N - CHn	0.115
18	610	115.0	CHn, C - C - OA, N, NT, NL	0.152
19	465	116.0	H - NE - CH2	0.114
20	620	116.0	CH2 - N - CH1	0.152
21	635	117.0	CH3 - N - C, CHn - C - OM	0.153
22	390	120.0	H - NT, NZ, NE - C	0.0889
23	445	120.0	H - NT, NZ - H	0.101
24	505	120.0	H - N - CH3, H, HC - 6-ring, H - NT - CHn	0.115
25	530	120.0	P, SI - OA - CHn, P	0.121
26	560	120.0	N, C, CR1 (6-ring, no H)	0.128
27	670	120.0	NZ - C - NZ, NE	0.153
28	780	120.0	OM - P - OM	0.178
29	685	121.0	O - C - CHn, C; CH3 - N - CHn	0.153
30	700	122.0	CH1, CH2 - N - C	0.153
31	415	123.0	H - N - C	0.0887
32	730	124.0	O - C - OA, N, NT, NL C - NE - CH2	0.153
33	375	125.0	FE - NR - CR1 (5-ring)	0.0765
34	750	125.0	-	0.153

TABLE 3.3: continues on next page.

Bond-angle type code	Force constant	Ideal bond angle	Example of usage in terms of non-bonded atom types	
$M_n^{(\theta)}$	$k_n^{(\theta,c)}$	θ_n^0		$k_n^{(\theta,h)}$
	[kJ·mol^{-1}]	[deg]		[kJ·mol^{-1}·deg^{-2}]
ICTH[N] ICT[N]	CT[N]	(T0[N])		
35	575	126.0	H, HC - 5-ring	0.114
36	640	126.0	X(noH) - 5-ring	0.127
37	770	126.0	OM - C - OM	0.153
38	760	132.0	5, 6 ring connnection	0.128
39	2215	155.0	SI - OA - SI	0.121
40	434	109.5	HWat - OWat - HWat	0.117
41	484	107.57	HChl - CChl - CLChl	0.134
42	632	111.30	CLChl - CChl - CLChl	0.167
43	469	97.4	CDmso - SDmso - CDmso	0.140
44	503	106.75	CDmso - SDmso - ODmso	0.140
45	443	108.53	HMet - OMet - CMet	0.121
46	618	109.5	CLCl4 - CCl4 - CLCl4	0.167
47	380	90.0	NR (heme) - FE - C (CO bound to heme)	0.116
48	91350	180.0	Fe - C - O (CO bound to heme)	0.0726

TABLE 3.3: GROMOS 45A4 and 45B4 bond-angle bending parameters ($k_n^{(\theta,c)} = g(k_n^{(\theta,h)}, \theta_n^0, E_{k_BT})$.

Improper dihedral-angle type code	Force constant	Ideal improper dihedral angle	Example of usage	
	$k_n^{(\xi)}$	ξ_n^0		$k_n^{(\xi)}$
	[kJmol^{-1}degree^{-2}]	[degree]		[kcalmol^{-1}rad^{-2}]
ICQH[N] ICQ[N]	CQ[N]	(Q0[N])		
1	0.0510	0.0	planar groups	40
2	0.102	35.26439	tetrahedral centres	80
3	0.204	0.0	heme iron	160

TABLE 3.4. GROMOS 45A4 and 45B4 improper (harmonic) dihedral angle parameters.

Dihedral-angle type code	Force constant	Phase shift	Multiplicity	Example of usage in terms of non-bonded atom types	
	$k_n^{(\varphi,s)}$	$\cos(\varphi_n^0)$	$m_n^{(\varphi)}$		$k_n^{(\varphi,s)}$
	[kJmol^{-1}]				[kcalmol^{-1}]
ICPH[N] ICP[N]	CP[N]	PD[N]	NP[N]		
1	5.86	-1.0	2	-C-C-	1.4
2	7.11	-1.0	2	-C-OA- (at ring)	1.7
3	16.7	-1.0	2	-C-OA- (carboxyl)	4.0
4	33.5	-1.0	2	-C-N, NT, NE, NZ,NR-	8.0
5	41.8	-1.0	2	-C-CR1- (6-ring)	10.0
6	0.0	+1.0	2	-CH1 (sugar)-NR(base)-	0.0
7	0.418	+1.0	2	O-CH1-CHn-no O	0.1
8	2.09	+1.0	2	O-CH1-CHn-O	0.5
9	3.14	+1.0	2	-OA-P-	0.75
10	16.7	+1.0	2	-S-S-	4.0
11	1.05	+1.0	3	-OA-P-; -P - O5* - C5* - C4* (dna)	0.25
12	1.26	+1.0	3	-CHn-OA(no sugar)-	0.3
13	2.93	+1.0	3	-CH2-S-	0.7
14	3.77	+1.0	3	-C,CHn,SI-NT,NL,OA(sugar)-	0.9
15	4.18	+1.0	3	HC-C-S-	1.0
16	5.44	+1.0	3	HC-C-C-	1.3
17	5.86	+1.0	3	-CHn,SI-CHn-	1.4
18	0.0	+1.0	4	-NR-FE-	0.0
19	1.0	-1.0	6	-CHn-N,NE-	0.24
20	1.0	+1.0	6	-CHn-C,NR (ring), CR1-	0.24
21	3.77	+1.0	6	-CHn-NT-	0.9
22	5.35	+1.0	1	O5* - C5* - C4* - O4* (dna)	1.3
23	2.53	+1.0	3	O5* - C5* - C4* - O4* (dna)	0.60
24	5.09	+1.0	2	CHn - O - P - O (dna, phosphodiester)	1.2
25	3.19	+1.0	3	CHn - O - P - O (dna, phosphodiester)	0.76
26	2.79	+1.0	1	P - O5* - C5* - C4* (dna)	0.67
27	5.86	-1.0	1	N - CHn - CHn - OA (lipid)	1.4
28	8.62	+1.0	3	N - CHn - CHn - OA (lipid)	2.1
29	24.0	-1.0	2	CHn - OA - C - CHn (ester lipid)	5.7
30	3.90	+1.0	3	CHn - CHn - OA - H (sugar)	0.93
31	9.35	-1.0	1	OA - CHn - CHn - OA (sugar) O5 - C5 - C6 - O6^b	2.2
32	9.50	+1.0	3	OA - CHn - CHn - OA (sugar) O5 - C5 - C6 - O6^b	2.3
33	9.45	-1.0	1	OA - CHn - OA - CHn,H (αsugar) O5 - C1 - O1 - C1′,H1	2.3
34	3.41	-1.0	1	OA - CHn - OA - CHn,H (βsugar) O5 - C1 - O1 - C1',H1	0.81
35	4.69	+1.0	3	OA - CHn - OA - CHn,H (βsugar) O5 - C1 - O1 - C1',H1	1.1
36	3.65	+1.0	3	OA - CHn - OA - CHn,H (αsugar) O5 - C1 - O1 - C1',H1	0.87

TABLE 3.5: continues on next page.

Dihedral-angle type code	Force constant	Phase shift	Multiplicity	Example of usage in terms of non-bonded atom types	
	$k_n^{(\varphi,s)}$	$\cos(\varphi_n^0)$	$m_n^{(\varphi)}$		$k_n^{(\varphi,s)}$
	[kJmol^{-1}]				[kcalmol^{-1}]
ICPH[N] ICP[N]	CP[N]	PD[N]	NP[N]		
37	6.66	-1.0	1	OA - CHn - CHn - OA (sugar) O5 - C5 - C6 - O6[a]	1.2
38	7.69	+1.0	3	OA - CHn - CHn - OA (sugar) O5 - C5 - C6 - O6[a]	1.8
39	2.67	-1.0	1	CHn - CHn - CHn - OA (sugar) O5 - C5 - C6 - O6[a]	0.64
40	1.53	-1.0	2	C1 - C2 - CAB - CBB (heme)	0.37

TABLE 3.5: GROMOS 45A4 and 45B4 (trigonometric) dihedral torsional angle parameters. a) To be used if - C5 - C6 - O6 and adjacent - C4 - O4 - are axial and the other equatorial, as in galactose; b) To be used if - C5 - C6 - O6 and adjacent - Cn - On - Hn are both simultaneously axial or equatorial, as in glucose.

integer atom code	atom type	description
IAC[N]	TYPE[N]	
1	O	carbonyl oxygen (C=O)
2	OM	carboxyl oxygen (CO^-)
3	OA	hydroxyl, sugar or ester oxygen
4	OW	water oxygen
5	N	peptide nitrogen (NH)
6	NT	terminal nitrogen (NH2)
7	NL	terminal nitrogen (NH3)
8	NR	aromatic nitrogen
9	NZ	Arg NH (NH2)
10	NE	Arg NE (NH)
11	C	bare carbon
12	CH1	aliphatic or sugar CH-group
13	CH2	aliphatic or sugar CH2-group
14	CH3	aliphatic CH3-group
15	CH4	methane
16	CR1	aromatic CH-group
17	HC	hydrogen bound to carbon
18	H	hydrogen not bound to carbon
19	DUM	dummy atom
20	S	sulphur
21	CU1+	copper (charge 1+)
22	CU2+	copper (charge 2+)
23	FE	iron (heme)
24	ZN2+	zinc (charge 2+)
25	MG2+	magnesium (charge 2+)
26	CA2+	calcium (charge 2+)
27	P, SI	phosphor or silicon
28	AR	argon
29	F	fluor (non-ionic)
30	CL	chlorine (non-ionic)
31	BR	bromine (non-ionic)
32	CMet	CH3-group in methanol (solvent)
33	OMet	oxygen in methanol (solvent)
34	NA+	sodium (charge 1+)
35	CL-	chloride (charge 1-)
36	CChl	carbon in chloroform (solvent)
37	CLChl	chloride in chloroform (solvent)
38	HChl	hydrogen in chloroform (solvent)
39	SDmso	sulphur in DMSO (solvent)
40	CDmso	CH3-group in DMSO (solvent)
41	ODmso	oxygen in DMSO (solvent)
42	CCl4	carbon in carbontetrachloride (solvent)
43	CLCl4	chloride in carbontetrachloride (solvent)
44	CH2r	aliphatic or sugar CH2 group in ring

TABLE 3.6: continues on next page.

integer atom code	atom type	description
IAC[N]	TYPE[N]	
45	CH0	bare sp3 carbon, 4 bound heavy atoms

TABLE 3.6: GROMOS 45A4 and 45B4 non-bonded atom types and integer atom codes.

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
1	O	0.04756	0.8611	1.125	-
2	OM	0.04756	0.8611	1.841	3.068
3	OA	0.04756	1.125	1.227	-
4	OW	0.05116	1.544	1.623	-
5	N	0.04936	1.301	1.943	-
6	NT	0.04936	1.301	2.250	-
7	NL	0.04936	1.301	3.068	-
8	NR	0.04936	1.301	1.841	-
9	NZ	0.04936	1.301	2.148	-
10	NE	0.04936	1.301	1.984	-
11	C	0.04838	1.837	-	-
12	CH1	0.07790	9.850	-	-
13	CH2	0.08642	5.828	-	-
14	CH3	0.09805	5.162	-	-
15	CH4	0.1148	5.862	-	-
16	CR1	0.07425	3.888	-	-
17	HC	0.0092	0.123	-	-
18	H	0.0	0.0	-	-
19	DUM	0.0	0.0	-	-
20	S	0.09992	3.616	-	-
21	CU1+	0.02045	0.07159	0.2250	-
22	CU2+	0.02045	0.07159	0.4091	-
23	FE	0.0	0.0	0.0	-
24	ZN2+	0.02045	0.09716	0.09716	-
25	MG2+	0.008080	0.05838	0.05838	-
26	CA2+	0.03170	0.7057	0.7057	-
27	P, SI	0.1214	4.711	-	-
28	AR	0.07915	3.138	-	-
29	F	0.03432	0.8722	1.227	-
30	CL	0.09362	3.911	-	-
31	BR	0.03434	8.092	-	-
32	CMet	0.09421	4.5665	-	-
33	OMet	0.04756	1.125	1.227	-
34	NA+	0.008489	0.1450	0.1450	-
35	CL-	0.1175	10.340	10.340	10.340
36	CChl	0.051292	2.0160	-	-
37	CLChl	0.091141	3.7101	-	-
38	HChl	0.0061400	0.065574	-	-
39	SDmso	0.10277	4.6366	-	-
40	CDmso	0.095139	4.6645	-	-
41	ODmso	0.047652	0.86686	1.125	-
42	CCl4	0.051292	2.7568		

TABLE 3.7: continues on next page.

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
43	CLCl4	0.087201	3.5732		
44	CH2r	0.08564	5.297	-	-
45	CH0	0.04896	14.33	-	-

TABLE 3.7: GROMOS 45A4 normal van der Waals parameters.

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
2	OM	0.04756	0.8611	1.125	1.125
7	NL	0.04936	1.301	1.943	-

TABLE 3.8. GROMOS 45B4 (vacuo) normal van der Waals parameters.

integer atom code	atom type	integer atom code	atom type	C_6 (I,J)	C_{12} (I,J)
I		J		$10^{-3}kJmol^{-1}nm^6$	$10^{-6}kJmol^{-1}nm^{12}$
36	CChl	37	CLChl	4.6754	7.4813
36	CChl	38	HChl	0.3622	0.1745
37	CLChl	38	HChl	0.6493	0.3266
39	SDmso	40	CDmso	9.7827	21.6523
39	SDmso	41	ODmso	5.2442	4.6094
40	CDmso	41	ODmso	4.9187	4.7597

TABLE 3.9. GROMOS 45A4 normal van der Waals parameters for mixed atom type pairs (I,J).

	J	1	2	3	4	5	6	7	8	9	10	21	22	23	24	25	26	27	29	30	31	33	34	35	41
I		O	OM	OA	OW	N	NT	NL	NR	NZ	NE	CU1+	CU2+	FE	ZN2+	MG2+	CA2+	P,SI	F	CL	BR	OMet	NA+	CL-	ODmso
1	O	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1
2	OM	1	1	2	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1
3	OA	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
4	OW	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
5	N	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
6	NT	2	2	2	2	2	2	2	2	2	2	1	1	1	1	1	1	1	2	2	2	2	1	2	2
7	NL	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
8	NR	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
9	NZ	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
10	NE	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
21	CU1+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
22	CU2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
23	FE	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
24	ZN2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
25	MG2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
26	CA2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
27	P,SI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
29	F	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1
30	CL	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
31	BR	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
33	OMet	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
34	NA+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
35	CL-	1	1	2	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1
41	ODmso	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1

TABLE 3.10. Selection of van der Waals (repulsive) $C_{12}^{1/2}(I,I)$ parameters (GROMOS 45A4 and 45B4).

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
12	CH1	0.05396	1.933	-	-
13	CH2	0.06873	2.178	-	-
14	CH3	0.08278	2.456	-	-
16	CR1	0.07435	2.886	-	-
44	CH2r	0.06873	2.178	-	-
45	CH0	0.04838	1.837	-	-

TABLE 3.11. GROMOS 45A4 and 45B4 third-neighbour van der Waals parameters.

atom name	charge in e	occurring in
N	-0.280	all residues
H	0.280	
C	0.380	all residues
O	-0.380	
CD	0.090 (0.0)	Arg (charge +1)
NE	-0.110 (-0.240)	
HE	0.240 (0.240)	
CZ	0.340 (0.0)	
NH1/2	-0.260 (-0.480)	
HH11/12/21/22	0.240 (0.240)	
NE	-0.280	Argn (neutral)
HE	0.280	
CZ	0.150	Argn (neutral)
NH1	-0.548	
HH1	0.398	
NH2	-0.830	Argn (neutral)
HH21/22	0.415	
CG, CD	0.380	Asn, Gln
OD1, OE1	-0.380	
ND2, NE2, NZ	-0.830	Asn, Gln, Lys
HD21/22, HE21/22, HZ1/2	0.415	
CG, CD	0.270 (0.720)	Asp, Glu (charge -1)
OD1/2, OE1/2	-0.635 (-0.360)	
CG, CD	0.530	Asph, Gluh
OD1, OE1	-0.380	
OD2, OE2	-0.548	
HD2, HE2	0.398	
CB	-0.100 (0.200)	Cys (charge -.5)
SG	-0.400 (-0.200)	
SG	-0.064	Cysh
HG	0.064	
CG	0.0	Hisa (proton at D1)
ND1	0.0	
HD1	0.190	
CD2	0.130	
CE1	0.260	
NE2	-0.580	
CG	0.130	Hisb (proton at E2)
ND1	-0.580	
CD2	0.0	
CE1	0.260	
NE2	0.0	
HE2	0.190	
CG	-0.050 (0.0)	Hish (charge +1)
ND1	0.380 (-0.300)	

TABLE 3.12: continues on next page.

atom name	charge in e	occurring in
HD1	0.300 (0.300)	
CD2	0.0 (0.0)	
CE1	-0.240 (0.0)	
NE2	0.310 (-0.300)	
HE2	0.300 (0.300)	
CG, CB, CB, CZ	0.150	Hypr, Ser, Thr, Tyr
OD1, OG, OG1, OH	-0.548	
HD1, HG, HG1, HH	0.398	
CE	0.127 (0.0)	Lysh (charge +1)
NZ	0.129 (-0.744)	
HZ1/2/3	0.248 (0.248)	
CG	-0.140	Trp
CD1	-0.100	
HD1	0.100	
CD2	0.0	
NE1	-0.050	
HE1	0.190	
CE2	0.0	
C	-0.100	all aromatic C-H groups in Phe, Tyr, Trp
H	0.100	

TABLE 3.12: GROMOS 45A4 (45B4) atomic charges and charge group definitions for amino acid residues. The charges for the 45B4 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

atom name	charge in e	occurring in
OW	-0.8200	H_2O (SPC model)
HW1/2	0.4100	
OW	-0.8476	H_2O (SPC/E model)
HW1/2	0.4238	
CChl	0.1790	Chloroform
CLChl	-0.0870	
HChl	0.0820	
SDmso	0.1390	DMSO
CDmso	0.1600	
ODmso	-0.4590	
CMet	0.1760	Methanol
OMet	-0.5740	
HMet	0.3980	
CCl4	0.0	Carbontetrachloride
CLCl4	0.0	

TABLE 3.13. GROMOS 45A4 atomic charges for various solvents.

atom name	charge in e	occurring in
O3/5*	-0.360 (-0.360)	all nucleotides
P	0.990 (1.440)	
O1/2P	-0.635 (-0.360)	
C4*	0.160	all nucleotides
O4*	-0.360	
C1*	0.200	
N9, N9, N1, N1, N1	-0.200	dAde, dGua, dCyt, dThy, Ura
C4, C4	0.200	dAde, dGua
C6, C6, C6	0.100	dCyt, dThy, Ura
H6, H6, H6	0.100	dCyt, dThy, Ura
N1, N3, N7, N3, N7, N3	-0.540	dAde, dAde, dAde, dGua, dGua, dGua, dCyt
C2, C8, C8	0.440	dAde, dAde, dGua
H2, H8, H8	0.100	dAde, dAde, dGua
C6, C2, C4	0.540	dAde, dGua, dCyt
N6, N2, N4	-0.830	dAde, dGua, dCyt
H61/62, H21/22, H41/42	0.415	dAde, dGua, dCyt
N1, N3, N3	-0.310	dGua, dThy, Ura
H1, H3, H3	0.310	dGua, dThy, Ura
C6, C2, C2, C4, C2, C4	0.450	dGua, dCyt, dThy, dThy, Ura, Ura
O6, O2, O2, O4, O2, O4	-0.450	dGua, dCyt, dThy, dThy, Ura, Ura
C5, C5	-0.100	dCyt, Ura
H5, H5	0.100	dCyt, Ura

TABLE 3.14. GROMOS 45A4 (45B4) atomic charges and charge group definitions for nucleotides. The charges for the 45B4 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

atom name	charge in e	occurring in
C32, C33, C34, C35	0.250 (0.0)	dppc
N	0.0	dppc
C31	0.0	dppc
O31, O32	-0.360 (-0.360)	dppc
O33, O34	-0.635 (-0.360)	dppc
P	0.990 (1.440)	dppc
C3	0.0	dppc
C1, C2	0.160	dppc
O11, O21	-0.360	dppc
O12, O22	-0.380	dppc
C11, C21	0.580	dppc
C12, ..., C22, ...	0.0	dppc

TABLE 3.15. GROMOS 45A4 (45B4) atomic charges and charge group definitions for lipids. The charges for the 45B4 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

atom name	charge in e	occurring in
C1, C2, C3, C4, C6	0.232	hexopyranose, uronate
O2, O3, O4, O6	-0.642	hexopyranose, uronate
HO2, HO3, HO4, HO6	0.410	hexopyranose, uronate
C5	0.376	hexopyranose, uronate
O5	-0.480	hexopyranose, uronate
O1	-0.360	hexopyranose, uronate
C6	0.360 (0.720)	uronate
O61, O62	-0.680 (-0.360)	uronate
C1	0.232	terminal C1 - O1 - HO1 group
O1	-0.538	terminal C1 - O1 - HO1 group
HO1	0.410	terminal C1 - O1 - HO1 group
C1	0.232	terminal C1 - O1 - CM group
O1	-0.360	terminal C1 - O1 - CM group
CM (methyl)	0.232	terminal C1 - O1 - CM group
C5, C5'	0.378	terminal C1 - O1 - C1'(sugar) group
O5, O5'	-0.450	terminal C1 - O1 - C1'(sugar) group
C1, C1'	0.242	terminal C1 - O1 - C1'(sugar) group
O1	-0.340	terminal C1 - O1 - C1'(sugar) group

TABLE 3.16. GROMOS 45A4 (45B4) atomic charges and charge group definitions for carbohydrates.

Bond-type code	Force constant	Ideal bond length	Examples of usage in terms of non-bonded atom types	
$M_n^{(b)}$	$k_n^{(b,q)}$	b_n^0		$k_n^{(b,h)}$
	[10^6 kJ·mol^{-1}·nm^{-4}]	[nm]		[10^6 kJ·mol^{-1}·nm^{-2}]
ICBH[N] ICB[N]	CB[N]	B0[N]		
1	15.7	0.100	H - OA	0.314
2	18.7	0.100	H - N (all)	0.374
3	12.3	0.109	HC - C	0.292
4	37.0	0.112	C - O (CO bound to heme)	0.928
5	16.6	0.123	C - O	0.502
6	13.4	0.125	C - OM	0.419
7	12.0	0.132	CR1 - NR (6-ring)	0.418
8	8.87	0.133	H - S	0.314
9	10.6	0.133	C - NT, NL	0.375
10	11.8	0.133	C, CR1 - N, NR, CR1, C (peptide, 5-ring)	0.417
11	10.5	0.134	C - N, NZ, NE	0.377
12	11.7	0.134	C - NR (no H) (6-ring)	0.420
13	10.2	0.136	C - OA, FTfe - CTfe	0.377
14	11.0	0.138	C - NR (heme)	0.419
15	8.66	0.139	CH2 - C, CR1 (6-ring)	0.335
16	10.8	0.139	C, CR1 - CH2, C, CR1 (6-ring)	0.417
17	8.54	0.140	C, CR1, CH2 - NR (6-ring)	0.335
18	8.18	0.143	CHn - OA	0.335
19	9.21	0.143	CHn - OM	0.377
20	6.10	0.1435	CHn - OA (sugar)	0.251
21	8.71	0.147	CHn - N, NT, NL, NZ, NE	0.376
22	5.73	0.148	CHn - NR (5-ring)	0.251
23	7.64	0.148	CHn - NR (6-ring)	0.335
24	8.60	0.148	O, OM - P	0.377
25	8.37	0.150	O - S	0.377
26	5.43	0.152	CHn - CHn (sugar)	0.251
27	7.15	0.153	C, CHn - C, CHn	0.335
28	4.84	0.161	OA - P	0.251
29	4.72	0.163	OA - SI	0.251
30	2.72	0.178	FE - C (CO bound to heme)	0.172
31	5.94	0.178	CH3 - S	0.376
32	5.62	0.183	CH2 - S	0.376
33	3.59	0.187	CH1 - SI	0.251
34	0.640	0.198	NR (His) - FE (43A1)	0.0502
35	0.628	0.200	NR (heme) - FE	0.0502
36	5.03	0.204	S - S	0.419
37	0.540	0.221	NR (His) - FE	0.0527
38	23.2	0.100	HWat - OWat	0.464
39	12.1	0.110	HChl - CChl	0.293
40	8.12	0.1758	CChl - CLChl	0.502

TABLE 3.17: continues on next page.

Bond-type code	Force constant	Ideal bond length	Examples of usage in terms of non-bonded atom types	
$M_n^{(b)}$	$k_n^{(b,q)}$	b_n^0		$k_n^{(b,h)}$
	[10^6 kJ·mol^{-1}·nm^{-4}]	[nm]		[10^6 kJ·mol^{-1}·nm^{-2}]
ICBH[N] ICB[N]	CB[N]	B0[N]		
41	8.04	0.153	ODmso - SDmso	0.376
42	4.95	0.193799	SDmso - CDmso	0.372
43	8.10	0.176	CCl4 - CLCl4	0.502
44	13.1	0.1265	CUrea - OUrea	0.419
45	10.3	0.135	CUrea - NUrea	0. 375
46	8.71	0.163299	HWat - HWat	0.465
47	2.68	0.233839	HChl - CLChl	0.293
48	2.98	0.290283	CLChl - CLChl	0.502
49	2.39	0.279388	ODmso - CDmso	0.373
50	2.19	0.291189	CDmso - CDmso	0.371
51	3.97	0.2077	HMet - CMet	0.343
52	3.04	0.287407	CLCl4 - CLCl4	0.502

TABLE 3.17: GROMOS 54A7 and 54B7 bond-stretching parameters ($k_n^{(b,q)} = k_n^{(b,h)}/(2{b_n^0}^2)$).

Bond-angle type code	Force constant	Ideal bond angle	Example of usage in terms of non-bonded atom types	
$M_n^{(\theta)}$	$k_n^{(\theta,c)}$	θ_n^0		$k_n^{(\theta,h)}$
	[kJ·mol^{-1}]	[deg]		[kJ·mol^{-1}·deg^{-2}]
ICTH[N] ICT[N]	CT[N]	(T0[N])		
1	380	90.0	NR (heme) - FE - C (CO bound to heme)	0.116
2	420	90.0	NR(heme) - FE - NR(heme), NR (His)	0.128
3	405	96.0	H - S - CH2	0.122
4	475	100.0	CH2 - S - CH3	0.140
5	420	103.0	OA - P - OA	0.121
6	490	104.0	CH2 - S - S	0.140
7	465	108.0	NR, C, CR1(5-ring)	0.128
8	285	109.5	CHn - CHn - CHn, NR(6-ring) (sugar)	0.0769
9	320	109.5	CHn, OA - CHn - OA, NR(ring) (sugar)	0.0864
10	380	109.5	H - NL, NT - H; CHn - OA - CHn(sugar)	0.103
11	425	109.5	H - NL - C, CHn; H - NT - CHn	0.115
12	450	109.5	X - OA, SI - X	0.122
13	520	109.5	CH,C - CHn - C, CHn, OA, OM, N, NE	0.141
14	450	109.6	OM - P - OA	0.121
15	530	111.0	CHn - CHn - C, CHn, OA, NR, NT, NL	0.140
16	545	113.0	CHn - CH2 - S	0.140
17	50.0	115.0	NR(heme) - FE - NR (His) (43A1)	0.0123
18	460	115.0	H - N - CHn	0.115
19	610	115.0	CHn, C - C - OA, N, NT, NL	0.152
20	465	116.0	H - NE - CH2	0.114
21	620	116.0	CH2 - N - CH1	0.152
22	635	117.0	CH3 - N - C; CHn - C - OM	0.153
23	390	120.0	H - NT, NZ, NE - C	0.0889
24	445	120.0	H - NT, NZ - H	0.101
25	505	120.0	H - N - CH3, H; HC - 6-ring,; H - NT - CHn	0.115
26	530	120.0	P, SI - OA - CHn, P	0.121
27	560	120.0	N, C, CR1 (6-ring, no H)	0.128
28	670	120.0	NZ - C - NZ, NE	0.153
29	780	120.0	OM - P - OM	0.178
30	685	121.0	O - C - CHn, C; CH3 - N - CHn	0.153
31	700	122.0	CH1, CH2 - N - C	0.153
32	415	123.0	H - N - C	0.0887

TABLE 3.18: continues on next page.

Bond-angle type code	Force constant	Ideal bond angle	Example of usage in terms of non-bonded atom types	
$M_n^{(\theta)}$	$k_n^{(\theta,c)}$	θ_n^0		$k_n^{(\theta,h)}$
	[kJ·mol^{-1}]	[deg]		[kJ·mol^{-1}·deg^{-2}]
ICTH[N] ICT[N]	CT[N]	(T0[N])		
33	730	124.0	O - C - OA, N, NT, NL C - NE - CH2	0.153
34	375	125.0	FE - NR - CR1 (5-ring)	0.0765
35	750	125.0	-	0.153
36	575	126.0	H, HC - 5-ring	0.114
37	640	126.0	X(noH) - 5-ring	0.127
38	770	126.0	OM - C - OM	0.153
39	760	132.0	5, 6 ring connnection	0.128
40	2215	155.0	SI - OA - SI	0.121
41	91350	180.0	Fe - C - O (CO bound to heme)	0.0726
42	434	109.5	HWat - OWat - HWat	0.117
43	484	107.57	HChl - CChl - CLChl	0.134
44	632	111.30	CLChl - CChl - CLChl	0.167
45	469	97.4	CDmso - SDmso - CDmso	0.140
46	503	106.75	CDmso - SDmso - ODmso	0.140
47	443	108.53	HMet - OMet - CMet	0.121
48	618	109.5	CLCl4 - CCl4 - CLCl4	0.167
49	507	107.6	FTfe - CTfe - FTfe	0.140
50	448	109.5	HTfe - OTfe - CHTfe	0.121
51	524	110.3	OTfe - CHTfe - CTfe	0.140
52	532	111.4	CHTfe - CTfe - FTfe	0.140
53	636	117.2	NUrea - CUrea - NUrea	0.153
54	690	121.4	OUrea - CUrea - NUrea	0.153

TABLE 3.18: GROMOS 54A7 and 54B7 bond-angle bending parameters ($k_n^{(\theta,c)} = g(k_n^{(\theta,h)}, \theta_n^0, E_{k_BT})$).

Improper dihedral-angle type code	Force constant	Ideal improper dihedral angle	Example of usage	
	$k_n^{(\xi)}$	ξ_n^0		$k_n^{(\xi)}$
	[kJmol^{-1}degree^{-2}]	[degree]		[kcalmol^{-1}rad^{-2}]
ICQH[N] ICQ[N]	CQ[N]	(Q0[N])		
1	0.0510	0.0	planar groups	40
2	0.102	35.26439	tetrahedral centres	80
3	0.204	0.0	heme iron	160
4	0.0510	180.0	planar groups	40
5	0.102	-35.26439	tetrahedral centres	80

TABLE 3.19. GROMOS 54A7 and 54B7 improper (harmonic) dihedral angle parameters.

Dihedral-angle type code	Force constant	Phase shift	Multiplicity	Example of usage in terms of non-bonded atom types	
	$k_n^{(\varphi,s)}$	$\cos(\varphi_n^0)$	$m_n^{(\varphi)}$		$k_n^{(\varphi,s)}$
	[kJmol^{-1}]				[kcalmol^{-1}]
ICPH[N] ICP[N]	CP[N]	PD[N]	NP[N]		
1	2.67	-1.0	1	CHn-CHn-CHn-OA (sugar) C4-C5-C6-O6[a]	0.6
2	3.41	-1.0	1	OA-CHn-OA-CHn,H (βsugar) O5-C1-O1-C1',H1	0.8
3	4.97	-1.0	1	OA-CHn-CHn-OA (sugar) O5-C5-C6-O6[a]	1.2
4	5.86	-1.0	1	N-CHn-CHn-OA(lipid)	1.4
5	9.35	-1.0	1	OA-CHn-CHn-OA(sugar) O5-C5-C6-O6[b]	2.2
6	9.45	-1.0	1	OA-CHn-OA-CHn,H (α sugar) O5-C1-O1-C1$'$,H1	2.3
7	2.79	+1.0	1	P-O5*-C5*-C4* (dna)	0.7
8	5.35	+1.0	1	O5*-C5*-C4*-O4* (dna)	1.3
9	1.53	-1.0	2	C1-C2-CAB-CBB (heme)	0.4
10	5.86	-1.0	2	-C-C-	1.4
11	7.11	-1.0	2	-C-OA- (at ring)	1.7
12	16.7	-1.0	2	-C-OA- (carboxyl)	4.0
13	24.0	-1.0	2	CHn-OA-C-CHn (ester lipid)	5.7
14	33.5	-1.0	2	-C-N,NT,NE,NZ,NR-	8.0
15	41.8	-1.0	2	-C-CR1- (6-ring)	10.0
16	0.0	+1.0	2	-CH1(sugar)-NR(base)-	0.0
17	0.418	+1.0	2	O-CH1-CHn-no O	0.1
18	2.09	+1.0	2	O-CH1-CHn-O	0.5
19	3.14	+1.0	2	-OA-P-	0.75
20	5.09	+1.0	2	CHn-O-P-O (dna, phosphodiester)	1.2
21	16.7	+1.0	2	-S-S-	4.0
22	1.05	+1.0	3	-OA-P-	0.25
23	1.26	+1.0	3	-CHn-OA(no sugar)-	0.3
24	1.30	+1.0	3	HTfe-OTfe-CHTfe-CTfe	0.3
25	2.53	+1.0	3	O5*-C5*-C4*-O4* (dna)	0.6
26	2.93	+1.0	3	-CH2-S-	0.7
27	3.19	+1.0	3	CHn-O-P-O (dna, phosphodiester)	0.8
28	3.65	+1.0	3	OA-CHn-OA-CHn,H (α sugar) O5 - C1 - O1 - C1',H1	0.9
29	3.77	+1.0	3	-C,CHn,SI-NT,NL,OA(sugar)-	0.9
30	3.90	+1.0	3	CHn-CHn-OA-H (sugar)	0.9
31	4.18	+1.0	3	HC-C-S-	1.0
32	4.69	+1.0	3	OA-CHn-OA-CHn,H (β sugar) O5 - C1 - O1 - C1',H1	1.1
33	5.44	+1.0	3	HC-C-C-	1.3
34	5.92	+1.0	3	-CHn,SI-CHn-	1.4
35	7.69	+1.0	3	OA-CHn-CHn-OA (sugar) O5 - C5 - C6 - O6[a]	1.8
36	8.62	+1.0	3	N-CHn-CHn-OA (lipid)	2.1
37	9.50	+1.0	3	OA-CHn-CHn-OA (sugar) O5-C5-C6-O6[b]	2.3
38	0.0	+1.0	4	-NR-FE-	0.0
39	1.0	-1.0	6	-CHn-N,NE-	0.24
40	1.0	+1.0	6	-CHn-C,NR(ring),CR1-	0.24

TABLE 3.20: continues on next page.

Dihedral-angle type code	Force constant	Phase shift	Multiplicity	Example of usage in terms of non-bonded atom types	
	$k_n^{(\varphi,s)}$	$\cos(\varphi_n^0)$	$m_n^{(\varphi)}$		$k_n^{(\varphi,s)}$
	[kJmol^{-1}]				[kcalmol^{-1}]
ICPH[N] ICP[N]	CP[N]	PD[N]	NP[N]		
41	3.77	+1.0	6	-CHn-NT-	0.9
42	3.50	-1.0	2	-CHn-C-	0.84
43	2.80	+1.0	3	-CHn-N-	0.64
44	0.70	-1.0	6	-CHn-N-	0.17
45	0.49	+1.0	6	-CHn-C-	0.10

TABLE 3.20: GROMOS 54A7 and 54B7 (trigonometric) dihedral torsional angle parameters. a) To be used if – C5 – C6 – O6 and adjacent – C4 – O4 – are axial and the other equatorial, as in galactose; b) To be used if – C5 – C6 – O6 and adjacent – Cn – On – Hn are both simultaneously axial or equatorial, as in glucose.

integer atom code	atom type	description
IAC[N]	TYPE[N]	
1	O	carbonyl oxygen (C=O)
2	OM	carboxyl oxygen (CO^-)
3	OA	hydroxyl or sugar oxygen
4	OE	ether or ester oxygen
5	OW	water oxygen
6	N	peptide nitrogen (NH)
7	NT	terminal nitrogen (NH2)
8	NL	terminal nitrogen (NH3)
9	NR	aromatic nitrogen
10	NZ	Arg NH (NH2)
11	NE	Arg NE (NH)
12	C	bare carbon
13	CH0	bare sp3 carbon, 4 bound heavy atoms
14	CH1	aliphatic or sugar CH-group
15	CH2	aliphatic or sugar CH2-group
16	CH3	aliphatic CH3-group
17	CH4	methane
18	CH2r	aliphatic or sugar CH2 group in ring
19	CR1	aromatic CH-group
20	HC	hydrogen bound to carbon
21	H	hydrogen not bound to carbon
22	DUM	dummy atom
23	S	sulphur
24	CU1+	copper (charge 1+)
25	CU2+	copper (charge 2+)
26	FE	iron (heme)
27	ZN2+	zinc (charge 2+)
28	MG2+	magnesium (charge 2+)
29	CA2+	calcium (charge 2+)
30	P, SI	phosphor or silicon
31	AR	argon
32	F	fluor (non-ionic)
33	CL	chlorine (non-ionic)
34	BR	bromine (non-ionic)
35	CMet	CH3-group in methanol (solvent)
36	OMet	oxygen in methanol (solvent)
37	NA+	sodium (charge 1+)
38	CL-	chloride (charge 1-)
39	CChl	carbon in chloroform (solvent)
40	CLChl	chloride in chloroform (solvent)
41	HChl	hydrogen in chloroform (solvent)
42	SDmso	sulphur in DMSO (solvent)
43	CDmso	CH3-group in DMSO (solvent)
44	ODmso	oxygen in DMSO (solvent)

TABLE 3.21: continues on next page.

integer atom code	atom type	description
IAC[N]	TYPE[N]	
45	CCl4	carbon in carbontetrachloride (solvent)
46	CLCl4	chloride in carbontetrachloride (solvent)
47	FTfe	fluor in trifluorethanol
48	CTfe	carbon in trifluorethanol
49	CHTfe	CH2-group in trifluorethanol
50	OTfe	oxygen in trifluorethanol
51	CUrea	carbon in urea
52	OUrea	oxygen in urea
53	NUrea	nitrogen in urea
54	CH3p	positively charged methyl

TABLE 3.21: GROMOS 54A7 and 54B7 non-bonded atom types and integer atom codes.

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
1	O	0.04756	1.000	1.130	-
2	OM	0.04756	0.8611	1.841	3.068
3	OA	0.04756	1.100	1.227	-
4	OE	0.04756	1.100	1.227	-
5	OW	0.05116	1.623	1.623	-
6	N	0.04936	1.523	1.943	-
7	NT	0.04936	1.523	2.250	-
8	NL	0.04936	1.523	3.068	-
9	NR	0.04936	1.523	1.841	-
10	NZ	0.04936	1.523	2.148	-
11	NE	0.04936	1.523	1.984	-
12	C	0.04838	2.222	-	-
13	CH0	0.04896	14.33	-	-
14	CH1	0.07790	9.850	-	-
15	CH2	0.08642	5.828	-	-
16	CH3	0.09805	5.162	-	-
17	CH4	0.1148	5.862	-	-
18	CH2r	0.08564	5.297	-	-
19	CR1	0.07425	3.888	-	-
20	HC	0.0092	0.123	-	-
21	H	0.0	0.0	-	-
22	DUM	0.0	0.0	-	-
23	S	0.09992	3.616	-	-
24	CU1+	0.02045	0.07159	0.2250	-
25	CU2+	0.02045	0.07159	0.4091	-
26	FE	0.0	0.0	0.0	-
27	ZN2+	0.02045	0.09716	0.09716	-
28	MG2+	0.008080	0.05838	0.05838	-
29	CA2+	0.03170	0.7057	0.7057	-
30	P, SI	0.1214	4.711	4.711	-
31	AR	0.07915	3.138	-	-
32	F	0.03432	0.8722	1.227	-
33	CL	0.09362	3.911	-	-
34	BR	0.1663	8.092	-	-
35	CMet	0.09421	4.400	-	-
36	OMet	0.04756	1.525	1.525	-
37	NA+	0.0088792	0.2700	0.2700	-
38	CL-	0.11318	7.776	7.776	7.776
39	CChl	0.051292	2.0160	-	-
40	CLChl	0.091141	3.7101	-	-
41	HChl	0.006140	0.065574	-	-
42	SDmso	0.10277	4.6366	-	-

TABLE 3.22: continues on next page.

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
43	CDmso	0.098050	5.1620	-	-
44	ODmso	0.047652	0.86686	1.1250	-
45	CCl4	0.051292	2.7568	-	-
46	CLCl4	0.087201	3.5732	-	-
47	FTfe	0.034320	1.0000	1.0000	-
48	CTfe	0.048380	1.8370	-	-
49	CHTfe	0.084290	5.0770	-	-
50	OTfe	0.047560	1.2270	1.2270	-
51	CUrea	0.069906	3.6864	-	-
52	OUrea	0.048620	1.2609	1.2609	-
53	NUrea	0.057903	1.9877	1.9877	-
54	CH3p	0.09805	5.162	-	-

TABLE 3.22: GROMOS 54A7 normal van der Waals parameters.

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
2	OM	0.04756	0.8611	1.125	1.125
8	NL	0.04936	1.523	1.943	-

TABLE 3.23. GROMOS 54B7 (vacuo) normal van der Waals parameters. Only the changes relative to Tab. 3.22 are listed.

	J	1	2	3	4	5	6	7	8	9	10	11	24	25	26	27	28	29	30	32	33	34	36	37	38	44	47	50	52	53	54
I		O	OM	OA	OE	OW	N	NT	NL	NR	NZ	NE	CU1+	CU2+	FE	ZN2+	MG2+	CA2+	P,SI	F	CL	BR	OMet	NA+	CL-	ODmso	FTfe	OTfe	OUrea	NUrea	CH3p
1	O	1	1	2	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
2	OM	1	1	2	1	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1	1	1	1	2	3
3	OA	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
4	OE	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
5	OW	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
6	N	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
7	NT	2	2	2	2	2	2	2	2	2	2	2	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	2	2	2	1
8	NL	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
9	NR	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
10	NZ	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
11	NE	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
24	CU1+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
25	CU2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
26	FE	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
27	ZN2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
28	MG2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
29	CA2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
30	P,SI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
32	F	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
33	CL	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
34	BR	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
36	OMet	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
37	NA+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
38	CL-	1	1	2	1	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1	1	1	1	2	1
44	ODmso	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	2	1	2	1
47	FTfe	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
50	OTfe	1	1	2	1	2	1	2	1	2	1	1	1	1	1	1	1	1	1	1	1	1	2	1	1	2	1	2	2	2	1
52	OUrea	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	2	1	2	1
53	NUrea	2	2	2	2	2	2	2	2	2	2	2	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	2	2	2	1
54	CH3p	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

TABLE 3.24. Selection of van der Waals (repulsive) $C_{12}^{1/2}(I,I)$ parameters (GROMOS 54A7 and 54B7)

integer atom code	atom type	integer atom code	atom type	C_6 (I,J)	C_{12} (I,J)
I		J		10^{-3}kJmol^{-1}nm^6	10^{-6}kJmol^{-1}nm^{12}
39	CChl	40	CLChl	4.6754	7.4813
39	CChl	41	HChl	0.3622	0.1745
40	CLChl	41	HChl	0.6493	0.3266

TABLE 3.25. GROMOS 54A7 normal van der Waals parameters for mixed atom type pairs (I,J)

integer atom code	atom type	$C_6^{1/2}$(I,I)		$C_{12}^{1/2}$(I,I)	
		$[kJmol^{-1}\ nm^6]^{1/2}$		$10^{-3}[kJmol^{-1}\ nm^{12}]^{1/2}$	
I=IAC[N]	TYPE[N]		**1**	**2**	**3**
1	O	0.04756	0.8611	-	-
3	OA	0.04756	1.125	-	-
4	OE	0.04756	1.125	-	-
6	N	0.04936	1.301	-	-
7	NT	0.04936	1.301	-	-
8	NL	0.04936	1.301	-	-
9	NR	0.04936	1.301	-	-
10	NZ	0.04936	1.301	-	-
11	NE	0.04936	1.301	-	-
12	C	0.04838	1.837	-	-
13	CH0	0.04838	1.837	-	-
14	CH1	0.05396	1.933	-	-
15	CH2	0.06873	2.178	-	-
16	CH3	0.08278	2.456	-	-
18	CH2r	0.06873	2.178	-	-
19	CR1	0.07435	2.886	-	-
54	CH3p	0.08278	2.456	-	-

TABLE 3.26. GROMOS 54A7 and 54B7 third-neighbour van der Waals parameters

atom name	charge in e	occurring in
N	-0.310	all residues
H	0.310	
C	0.450	all residues
O	-0.450	
CD	0.090 (0.0)	Arg (charge +1)
NE	-0.110 (-0.240)	
HE	0.240 (0.240)	
CZ	0.340 (0.0)	
NH1/2	-0.260 (-0.480)	
HH11/12/21/22	0.240 (0.240)	
NE	-0.310	Argn (neutral)
HE	0.310	
CZ	0.266	Argn (neutral)
NH1	-0.674	
HH1	0.408	
NH2	-0.880	Argn (neutral)
HH21/22	0.440	
CG, CD	0.290	Asn, Gln
OD1, OE1	-0.450	
ND2, NE2, NZ	-0.720	Asn, Gln
HD21/22, HE21/22, HZ1/2	0.440	
CG, CD	0.270 (0.720)	Asp, Glu (charge -1)
OD1/2, OE1/2	-0.635 (-0.360)	
CG, CD	0.330	Asph, Gluh
OD1, OE1	-0.450	
OD2, OE2	-0.288	
HD2, HE2	0.408	
CB	-0.100 (0.200)	Cys (charge -.5)
SG	-0.400 (-0.200)	
CB	0.150	Cysh
SG	-0.370	
HG	0.220	
CG	0.0	Hisa (proton at D1)
ND1	-0.050	
HD1	0.310	
CD2	0.0	
HD2	0.140	
CE1	0.0	
HE1	0.140	
NE2	-0.540	
CG	0.0	Hisb (proton at E2)
ND1	-0.540	
CD2	0.0	
HD2	0.140	
CE1	0.0	

TABLE 3.27: continues on next page.

atom name	charge in e	occurring in
HE1	0.140	
NE2	-0.050	
HE2	0.310	
CG	-0.050 (0.0)	Hish (charge +1)
ND1	0.380 (-0.300)	
HD1	0.300 (0.300)	
CD2	-0.100 (-0.100)	
HD2	0.100 (0.100)	
CE1	-0.340 (-0.100)	
HE1	0.100 (0.100)	
NE2	0.310 (-0.300)	
HE2	0.300 (0.300)	
CG, CB, CB	0.266	Hypr, Ser, Thr
OD1, OG, OG1	-0.674	
HD1, HG, HG1	0.408	
CE	0.127 (0.0)	Lysh (charge +1)
NZ	0.129 (-0.744)	
HZ1/2/3	0.248 (0.248)	
CE	-0.240	Lys (neutral)
NZ	-0.640	
HZ1/2	0.440	
CG /CE	0.241	Met
SD	-0.482	
CG	-0.210	Trp
CD1	-0.140	
HD1	0.140	
CD2	0.0	
NE1	-0.100	
HE1	0.310	
CE2	0.0	
CZ	0.203	Tyr
OH	-0.611	
HH	0.408	
C	-0.140	all aromatic C-H groups in Phe, Tyr, Trp
H	0.140	
C	0.0	aromatic C connected to an aliphatic CHn in Phe, Tyr
CH2	0.0	aliphatic CHn connected to aromatic C in Phe, Tyr

TABLE 3.27: GROMOS 54A7 (54B7) atomic charges and charge group definitions for amino acid residues. The charges for the 54B7 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

atom name	charge in e	occurring in
OW	-0.82000	H_2O (SPC model)
HW1/2	0.41000	
OW	-0.84760	H_2O (SPC/E model)
HW1/2	0.42380	
OW	-0.68850	H_2O (SPC/L model)
HW1/2	0.34425	
CChl	0.17900	Chloroform
CLChl	-0.08700	
HChl	0.08200	
SDmso	0.12753	DMSO
CDmso	0.16000	
ODmso	-0.44753	
CMet	0.26600	Methanol
OMet	-0.67400	
HMet	0.40800	
CCl4	0.0	Carbontetrachloride
CLCl4	0.0	
FTfe	-0.17000	2,2,2- Trifluoroethanol
CTfe	0.45200	
CHTfe	0.27300	
OTfe	-0.62500	
HTfe	0.41000	
CUrea	0.14200	Urea
OUrea	-0.39000	
NUrea	-0.54200	
HUrea	0.33300	

TABLE 3.28. GROMOS 54A7 atomic charges for various (co)solvents.

atom name	charge in e	occurring in
O3/5*	-0.360 (-0.360)	all nucleotides
P	0.990 (1.440)	
O1/2P	-0.635 (-0.360)	
C4*	0.160	all nucleotides
O4*	-0.360	
C1*	0.200	
N9, N9, N1, N1, N1	-0.200	dAde, dGua, dCyt, dThy, Ura
C4, C4	0.200	dAde, dGua
C6, C6, C6	0.100	dCyt, dThy, Ura
H6, H6, H6	0.100	dCyt, dThy, Ura
N1, N3, N7, N3, N7, N3	-0.540	dAde, dAde, dAde, dGua, dGua, dCyt
C2, C8, C8	0.440	dAde, dAde, dGua
H2, H8, H8	0.100	dAde, dAde, dGua
C6, C2, C4	0.540	dAde, dGua, dCyt
N6, N2, N4	-0.830	dAde, dGua, dCyt
H61/62, H21/22, H41/42	0.415	dAde, dGua, dCyt
N1, N3, N3	-0.310	dGua, dThy, Ura
H1, H3, H3	0.310	dGua, dThy, Ura
C6, C2, C2, C4, C2, C4	0.450	dGua, dCyt, dThy, dThy, Ura, Ura
O6, O2, O2, O4, O2, O4	-0.450	dGua, dCyt, dThy, dThy, Ura, Ura
C5, C5	-0.100	dCyt, Ura
H5, H5	0.100	dCyt, Ura

TABLE 3.29. GROMOS 54A7 (54B7) atomic charges and charge group definitions for nucleotides. The charges for the 54B7 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

atom name	charge in e	occurring in
C31, C33, C34, C35	0.400	dppc
N	-0.500	dppc
C32	0.300	dppc
O31	-0.700	dppc
O32, O33, O34	-0.800	dppc
P	1.700	dppc
C3	0.400	dppc
C2	0.300	dppc
C1	0.500	dppc
O11, O21, O22	-0.700	dppc
O12	-0.600	dppc
C11	0.800	dppc
C21	0.700	dppc
C12, ..., C22, ...	0.000	dppc

TABLE 3.30. GROMOS 54A7 (54B7) atomic charges and charge group definitions for lipids. The charges for the 54B7 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

atom name	charge in e	occurring in
C1, C2, C3, C4, C6	0.232	hexopyranose, uronate
O2, O3, O4, O6	-0.642	hexopyranose, uronate
HO2, HO3, HO4, HO6	0.410	hexopyranose, uronate
C5	0.376	hexopyranose, uronate
O5	-0.480	hexopyranose, uronate
O1	-0.360	hexopyranose, uronate
C6	0.360 (0.720)	uronate
O61, O62	-0.680 (-0.360)	uronate
C1	0.232	terminal C1 - O1 - HO1 group
O1	-0.538	terminal C1 - O1 - HO1 group
HO1	0.410	terminal C1 - O1 - HO1 group
C1	0.232	terminal C1 - O1 - CM group
O1	-0.360	terminal C1 - O1 - CM group
CM (methyl)	0.232	terminal C1 - O1 - CM group
C5, C5'	0.378	terminal C1 - O1 - C1'(sugar) group
O5, O5'	-0.450	terminal C1 - O1 - C1'(sugar) group
C1, C1'	0.242	terminal C1 - O1 - C1'(sugar) group
O1	-0.340	terminal C1 - O1 - C1'(sugar) group

TABLE 3.31. GROMOS 54A7 (54B7) atomic charges and charge group definitions for carbohydrates.

CHAPTER 4

GROMOS molecular topology building blocks

4.1. Introduction

The GROMOS molecular topology building block files ∗.mtb contain the building blocks for a number of important types of molecules, such as proteins, DNA, RNA, sugars, etc. We note that three types of building blocks exist in the molecular topology building block file:

A. Solute building blocks with blockname MTBUILDBLSOLUTE
B. Solvent building blocks with blockname MTBUILDBLSOLVENT
C. Solute end-group building blocks with blockname MTBUILDBLEND

A solvent molecule may occur under the same name in types A and B of blocks, which contain partially different information. The solute block contains data on interaction function parameters for internal degrees of freedom and charge group information not present in the solvent block. The solvent block contains data on geometric constraints not present in the solute block. Examples of molecules that can be treated as solute molecule as well as solvent molecule are water (H2O, H2OE), chloroform (CHCL3), DMSO (DMSO), methanol (CH3OH) and carbontetrachloride (CCL4).

Below we list for each building block of the file 54a7.mtb (α-amino acids, lipids, nucleotides and solvents), 54a7_beta.mtb (β-amino acids), 54a7_cof.mtb (cofactors and other types of molecules) and 54a7_carbo.mtb (carbohydrates and sugars) the building block name and a description of the residue, nucleotide, glucose unit or molecule it is representing. The building blocks that are marked with a dagger are specified in the molecular topology building block files but are not presented in graphical and tabular form in this chapter. In the pictures of the building blocks the charged state is indicated for the simulation in solution. In the force field for in vacuo simulations (file 54b7.mtb), groups of atoms bear a total charge of zero, which is not indicated here. We note that the IUPAC-IUB nomenclature has been used throughout. When no IUPAC-IUB rules were defined (HEME group) Brookhaven protein data bank nomenclature has been used.

A. *Solute Building Blocks* (Blockname: MTBUILDBLSOLUTE)

Name	**Description** (charges in e)
α-Amino Acids and Analogues (L if not indicated otherwise)	
ALA	Alanine
ARG	Arginine (protonated; charge $+e$)
ARGN	Arginine (deprotonated; neutral)
ASN	Asparagine
ASN1	Asparagine (coordinated with ZN)
ASP	Aspartic acid (deprotonated; charge -e)
ASPH	Aspartic acid (protonated; neutral)
CYS	Cysteine (deprotonated; charge -1/2e)

CYSH	Cysteine (protonated; neutral)
CYS1	Cysteine (1st member of S-S bridge)
CYS2	Cysteine (2nd member of S-S bridge)
GLN	Glutamine
GLU	Glutamic acid (deprotonated; charge -e)
GLUH	Glutamic acid (protonated; neutral)
GLY	Glycine
HISA	Histidine (protonated at ND1; neutral)
HISB	Histidine (protonated at NE2; neutral)
HISH	Histidine (protonated at ND1 and NE2; charge +e)
HIS1	Histidine (coupled to HEME at NE2; neutral)
HIS2	Histidine (coupled to HEMC at NE2: neutral)
HYPR	Hydroxyproline (R-configuration at CG)
†HYPS	Hydroxyproline (S-configuration at CG)
ILE	Isoleucine
LEU	Leucine
LYS	Lysine (deprotonated; neutral)
LYSH	Lysine (protonated; charge +e)
MET	Methionine
PHE	Phenylalanine
PRO	Proline
SER	Serine
THR	Threonine
TRP	Tryptophan
TYR	Tyrosine
VAL	Valine
DALA	D-Alanine
ABU	L-2-amino-butanoic acid
AIB	2-aminoisobutyric acid
MEBMT	(4R)-4-[(E)-2-butanyl]-4, N-dimethyl-L-threonine
MELEU	N-methyl-L-leucine
MEVAL	N-methyl-L-valine
SAR	Sarcosine or N-methylglycine

β-Amino Acids

RAF	(R)-β^2-Phenylalanine
RAV	(R)-β^2-Valine
RBCH	(R)-β^3-Cysteine (protonated; neutral)
RBI	(R)-β^3-Isoleucine
RBKH	(R)-β^3-Lysine (protonated; charge $+e$)
RBM	(R)-β^3-Methionine
RBN	(R)-β^3-Asparagine
RBS	(R)-β^3-Serine
RBSP	(R)-β^3-Serine(propylated)
RBT	(R)-β^3-Threonine
RBV	(R)-β^3-Valine
SAA	(S)-β^2-Alanine
SAF	(S)-β^2-Phenylalanine
SAFF	(S)-β^2-Phenylalanine(Cα fluorinated)
SAL	(S)-β^2-Leucine
SAM	(S)-β^2-Methionine
SAV	(S)-β^2-Valine
SBA	(S)-β^3-Alanine
SBCH	(S)-β^3-Cysteine (protonated)
SBD	(S)-β^3-Aspartic acid (deprotonated; charge -e)
SBDH	(S)-β^3-Aspartic acid (protonated; neutral)
SBE	(S)-β^3-Glutamic acid (deprotonated; charge -e)
SBEH	(S)-β^3-Glutamic acid (protonated; neutral)
SBQ	(S)-β^3-Glutamine
SBF	(S)-β^3-Phenylalanine
BGL	β-Glycine
SBHA	(S)-β^3-Histidine (protonated at NE1; neutral)
SBHH	(S)-β^3-Histidine(protonated at NE1 and NZ2; charge $+e$)
SBI	(S)-β^3-Isoleucine
SBKH	(S)-β^3-Lysine (protonated; charge $+e$)
SBL	(S)-β^3-Leucine
SBM	(S)-β^3-Methionine

SBP	(S)-β^3-Proline
SBR	(S)-β^3-Arginine (protonated; charge $+e$)
SBS	(S)-β^3-Serine
SBT	(S)-β^3-Threonine
SBV	(S)-β^3-Valine
SBY	(S)-β^3-Tyrosine
SBW	(S)-β^3-Tryptophan
SRAM	(R,S)-$\beta^(2,3)$-Alanine(αMe)
SRLM	(R,S)-$\beta^(2,3)$-Leucine(αMe)
SRVM	(R,S)-$\beta^(2,3)$-Valine(αMe)
SSAM	(S,S)-$\beta^(2,3)$-Alanine(αMe)

Nucleotides

DADE	2'-deoxyadenosine 5'-phosphoric acid (DNA, charge -e)
DGUA	2'-deoxyguanosine 5'-phosphoric acid (DNA, charge -e)
DCYT	2'-deoxycitidine 5'-phosphoric acid (DNA, charge -e)
DTHY	2'-deoxythymidine 5'-phosphoric acid (DNA, charge -e)
ADE	adenosine 5'-phosphoric acid (RNA, charge -e)
GUA	guanosine 5'-phosphoric acid (RNA, charge -e)
CYT	cytidine 5'-phosphoric acid (RNA, charge -e)
URA	uridine 5'-phosphoric acid (RNA, charge -e)
FMNO	flavin mononucleotide (oxydized, deprotonated at FN5 and FN1; charge -e, $OPOHO_2^-$)
†FMNS	flavin mononucleotide (semi-reduced, protonated at FN5; charge -e, $OPOHO_2^-$)
†FMNR	flavin mononucleotide (reduced, protonated at FN5 and FN1; charge -e, $OPOHO_2^-$)
PFN	proflavin (protonated at FN5; charge $+e$)
NADP	nicotinamide adenine dinucleotide (NAD+; charge -e)
†NADH	nicotinamide adenine dinucleotide (NADH; charge -2e)
NDPH	nicotinamide adenine dinucleotide phosphate (NADPH; charge -3e, $OPOHO_2^-$)
†NDPP	nicotinamide adenine dinucleotide phosphate (NADP+; charge -2e, $OPOHO_2^-$)
†NDPHN	nicotinamide adenine dinucleotide phosphate (NADPH; neutral, $OPO(OH)_2$)

Carbohydrates

†NA2P	-2-D-allopyranose-α-1-

†NA3P	-3-D-allopyranose-α-1-
†NA4P	-4-D-allopyranose-α-1-
†NA6P	-6-D-allopyranose-α-1-
†NB2P	-2-D-allopyranose-β-1-
†NB3P	-3-D-allopyranose-β-1-
†NB4P	-4-D-allopyranose-β-1-
†NB6P	-6-D-allopyranose-β-1-
†EA2P	-2-D-altropyranose-α-1-
†EA3P	-3-D-altropyranose-α-1-
†EA4P	-4-D-altropyranose-α-1-
†EA6P	-6-D-altropyranose-α-1-
†EB2P	-2-D-altropyranose-β-1-
†EB3P	-3-D-altropyranose-β-1-
†EB4P	-4-D-altropyranose-β-1-
†EB6P	-6-D-altropyranose-β-1-
†GA2P	-2-D-glucopyranose-α-1-
†GA3P	-3-D-glucopyranose-α-1-
GA4P	-4-D-glucopyranose-α-1-
†GA6P	-6-D-glucopyranose-α-1-
GB2P	-2-D-glucopyranose-β-1-
GB3P	-3-D-glucopyranose-β-1-
GB4P	-4-D-glucopyranose-β-1-
GB6P	-6-D-glucopyranose-β-1-
†MA2P	-2-D-mannopyranose-α-1-
†MA3P	-3-D-mannopyranose-α-1-
†MA4P	-4-D-mannopyranose-α-1-
†MA6P	-6-D-mannopyranose-α-1-
†MB2P	-2-D-mannopyranose-β-1-
†MB3P	-3-D-mannopyranose-β-1-
†MB4P	-4-D-mannopyranose-β-1-
†MB6P	-6-D-mannopyranose-β-1-
†KA2P	-2-D-gulopyranose-α-1-
†KA3P	-3-D-gulopyranose-α-1-

†KA4P	-4-D-gulopyranose-α-1-
†KA6P	-6-D-gulopyranose-α-1-
†KB2P	-2-D-gulopyranose-β-1-
†KB3P	-3-D-gulopyranose-β-1-
†KB4P	-4-D-gulopyranose-β-1-
†KB6P	-6-D-gulopyranose-β-1-
†IA2P	-2-D-idopyranose-α-1-
†IA3P	-3-D-idopyranose-α-1-
†IA4P	-4-D-idopyranose-α-1-
†IA6P	-6-D-idopyranose-α-1-
†IB2P	-2-D-idopyranose-β-1-
†IB3P	-3-D-idopyranose-β-1-
†IB4P	-4-D-idopyranose-β-1-
†IB6P	-6-D-idopyranose-β-1-
†LA2P	-2-D-galactopyranose-α-1-
†LA3P	-3-D-galactopyranose-α-1-
†LA4P	-4-D-galactopyranose-α-1-
†LA6P	-6-D-galactopyranose-α-1-
†LB2P	-2-D-galactopyranose-β-1-
†LB3P	-3-D-galactopyranose-β-1-
LB4P	-4-D-galactopyranose-β-1-
†LB6P	-6-D-galactopyranose-β-1-
†TA2P	-2-D-talopyranose-α-1-
†TA3P	-3-D-talopyranose-α-1-
†TA4P	-4-D-talopyranose-α-1-
†TA6P	-6-D-talopyranose-α-1-
†TB2P	-2-D-talopyranose-β-1-
†TB3P	-3-D-talopyranose-β-1-
†TB4P	-4-D-talopyranose-β-1-
†TB6P	-6-D-talopyranose-β-1-
†nA2P	-2-L-allopyranose-α-1-
†nA3P	-3-L-allopyranose-α-1-
†nA4P	-4-L-allopyranose-α-1-

†nA6P	-6-L-allopyranose-α-1-
†nB2P	-2-L-allopyranose-β-1-
†nB3P	-3-L-allopyranose-β-1-
†nB4P	-4-L-allopyranose-β-1-
†nB6P	-6-L-allopyranose-β-1-
†eA2P	-2-L-altropyranose-α-1-
†eA3P	-3-L-altropyranose-α-1-
†eA4P	-4-L-altropyranose-α-1-
†eA6P	-6-L-altropyranose-α-1-
†eB2P	-2-L-altropyranose-β-1-
†eB3P	-3-L-altropyranose-β-1-
†eB4P	-4-L-altropyranose-β-1-
†eB6P	-6-L-altropyranose-β-1-
†gA2P	-2-L-glucopyranose-α-1-
†gA3P	-3-L-glucopyranose-α-1-
†gA4P	-4-L-glucopyranose-α-1-
†gA6P	-6-L-glucopyranose-α-1-
†gB2P	-2-L-glucopyranose-β-1-
†gB3P	-3-L-glucopyranose-β-1-
gB4P	-4-L-glucopyranose-β-1-
†gB6P	-6-L-glucopyranose-β-1-
†mA2P	-2-L-mannopyranose-α-1-
†mA3P	-3-L-mannopyranose-α-1-
†mA4P	-4-L-mannopyranose-α-1-
†mA6P	-6-L-mannopyranose-α-1-
†mB2P	-2-L-mannopyranose-β-1-
†mB3P	-3-L-mannopyranose-β-1-
†mB4P	-4-L-mannopyranose-β-1-
†mB6P	-6-L-mannopyranose-β-1-
†kA2P	-2-L-gulopyranose-α-1-
†kA3P	-3-L-gulopyranose-α-1-
†kA4P	-4-L-gulopyranose-α-1-
†kA6P	-6-L-gulopyranose-α-1-

†kB2P	-2-L-gulopyranose-β-1-
†kB3P	-3-L-gulopyranose-β-1-
†kB4P	-4-L-gulopyranose-β-1-
†kB6P	-6-L-gulopyranose-β-1-
†iA2P	-2-L-idopyranose-α-1-
†iA3P	-3-L-idopyranose-α-1-
†iA4P	-4-L-idopyranose-α-1-
†iA6P	-6-L-idopyranose-α-1-
†iB2P	-2-L-galactopyranose-β-1-
†iB3P	-3-L-galactopyranose-β-1-
†iB4P	-4-L-galactopyranose-β-1-
†iB6P	-6-L-galactopyranose-β-1-
†lA2P	-2-L-galactopyranose-α-1-
†lA3P	-3-L-galactopyranose-α-1-
†lA4P	-4-L-galactopyranose-α-1-
†lA6P	-6-L-galactopyranose-α-1-
†lB2P	-2-L-galactopyranose-β-1-
†lB3P	-3-L-galactopyranose-β-1-
†lB4P	-4-L-galactopyranose-β-1-
†lB6P	-6-L-galactopyranose-β-1-
†tA2P	-2-L-talopyranose-α-1-
†tA3P	-3-L-talopyranose-α-1-
†tA4P	-4-L-talopyranose-α-1-
†tA6P	-6-L-talopyranose-α-1-
†tB2P	-2-L-talopyranose-β-1-
†tB3P	-3-L-talopyranose-β-1-
†tB4P	-4-L-talopyranose-β-1-
†tB6P	-6-L-talopyranose-β-1-
GB4U	-4-D-glucuronate-β-1-
LA4U	-4-D-galacturonate-α-1-
MB4U	-4-D-mannuronate-β-1-
kA4U	-4-L-guluronate-α-1-
iA4U	-4-L-iduronate-α-1-

Other Molecules

†DPPC	dipalmitoylphosphatidylcholine
HEME	heme group (charge -2e, acidic groups deprotonated)
†HEMC	heme group (charge -2e, acidic groups deprotonated, CO coordinated)
†CYT*	3',5'-O-(tetra isopropyl-1,3-disiloxanediyl)cytidine (neutral)
†MTXH	methotrexate (protonated at N1; charge -2e)
FOL	folate (charge -2e)
†DHF	7,8-dihydrofolate (charge -2e)
†THF	5,6,7,8-tetrahydrofolate (charge -2e)
TMP	trimethoprim (deprotonated at N1; neutral)
†TMPH	trimethoprim (protonated at N1; neutral)
†TMPHP	trimethoprim (protonated at N1; charge +e)
PDG	3-phosopho-D-glycerate (charge -2e)
ATP	adenosine 5'-triphosphate (ATP; charge -3e)
PMB	p-methylbenzyl alcoholate (charge -e)
†PMBH	p-methylbenzyl alcohol (neutral)
BA	benzoic acid
RTOL	retinol (neutral)
†TEMP	tetramethyl pyrrolinyl (nitroxide spin label; neutral)
†CH4	methane (united atom)
†AR	argon
†ETH	ethanolate (obsolete: removed from 45A4 onward)
†ETHH	ethanol (obsolete: removed from 45A4 onward)
†GALB	β-galactose (obsolete: removed from 45A4 onward)
†GLCA	α-glucose (obsolete: removed from 45A4 onward)
†GLCB	β-glucose (obsolete: removed from 45A4 onward)

Ions

†SO42-	SO_4^{-2} ion (charge -2e)
†ZN2+	zinc ion (charge +2e)
†NA+	sodium ion (charge +e)
†CL-	chlorine ion (charge -e)
†CA2+	calcium ion (charge +2e)

†MG2+	magnesium ion (charge $+2e$)
†CU1+	copper ion (charge $+e$)
†CU2+	copper ion (charge $+2e$)

Solvents

(equivalent to the corresponding solvent building blocks)

†TFE	2,2,2-trifluoroethanol
†UREA	urea
†H2O	water (SPC model, rigid)[15]
†H2OE	water (SPC/E model, rigid)[38]
†CHCL3	chloroform (rigid)[19]
†DMSO	dimethylsulfoxide (rigid)[39]
†CH3OH	methanol (rigid)[17]
†CCL4	carbontetrachloride (rigid)[20]

B. *Solvent Building Blocks*(Blockname: MTBUILDBLSOLVENT)

Name	**Description**
†H2O	water (SPC model)[15]
†H2OE	water (SPC/E model)[38]
†CHCL3	chloroform[19]
†DMSO	dimethylsulfoxide[39]
†CH3OH	methanol[17]
†CCL4	carbontetrachloride[20]

C. *Solute End-Group Building Blocks* (Blockname: MTBUILDBLEND)

Name	**Description**
†NH3+	N-terminal α-peptide end-group (protonated, charge $+e$)
†NH2	N-terminal α-peptide end-group (deprotonated, neutral)
†NPRO	N-terminal α-peptide end-group for proline or hydroxy proline (protonated, charge $+e$)
†COO-	C-terminal α-peptide end-group (deprotonated, charge $-e$)
†COOH	C-terminal α-peptide end-group (protonated, neutral)
†BH3+	N-terminal β-peptide end-group (protonated, charge $+e$)
†BH2	N-terminal β-peptide end-group (deprotonated, neutral)
†BOO-	C-terminal β-peptide end-group (deprotonated, charge $-e$)

†BOOH	C-terminal β-peptide end-group (protonated, neutral)
†D5OH	5'-terminal DNA end-group
†D3OH	3'-terminal DNA end-group
†5OH	5'-terminal RNA end-group
†3OH	3'-terminal RNA end-group
†CNAP	terminal group for carbohydrates: -1-α-D-allopyranose
†CNBP	terminal group for carbohydrates: -1-β-D-allopyranose
†CEAP	terminal group for carbohydrates: -1-α-D-altropyranose
†CEBP	terminal group for carbohydrates: -1-β-D-altropyranose
†CGAP	terminal group for carbohydrates: -1-α-D-glucopyranose
CGBP	terminal group for carbohydrates: -1-β-D-glucopyranose
†CMAP	terminal group for carbohydrates: -1-α-D-mannopyranose
†CMBP	terminal group for carbohydrates: -1-β-D-mannopyranose
†CKAP	terminal group for carbohydrates: -1-α-D-gulopyranose
†CKBP	terminal group for carbohydrates: -1-β-D-gulopyranose
†CIAP	terminal group for carbohydrates: -1-α-D-idopyranose
†CIBP	terminal group for carbohydrates: -1-β-D-idopyranose
†CLAP	terminal group for carbohydrates: -1-α-D-galactopyranose
†CLBP	terminal group for carbohydrates: -1-β-D-galactopyranose
†CTAP	terminal group for carbohydrates: -1-α-D-talopyranose
†CTBP	terminal group for carbohydrates: -1-β-D-talopyranose
†CnAP	terminal group for carbohydrates: -1-α-L-allopyranose
†CnBP	terminal group for carbohydrates: -1-β-L-allopyranose
†CeAP	terminal group for carbohydrates: -1-α-L-altropyranose
†CeBP	terminal group for carbohydrates: -1-β-L-altropyranose
†CgAP	terminal group for carbohydrates: -1-α-L-glucopyranose
†CgBP	terminal group for carbohydrates: -1-β-L-glucopyranose
†CmAP	terminal group for carbohydrates: -1-α-L-mannopyranose
†CmBP	terminal group for carbohydrates: -1-β-L-mannopyranose
†CkAP	terminal group for carbohydrates: -1-α-L-gulopyranose
†CkBP	terminal group for carbohydrates: -1-β-L-gulopyranose
†CiAP	terminal group for carbohydrates: -1-α-L-idopyranose
†CiAP	terminal group for carbohydrates: -1-β-L-idopyranose

†ClAP	terminal group for carbohydrates: -1-α-L-galactopyranose
†ClBP	terminal group for carbohydrates: -1-β-L-galactopyranose
†CtAP	terminal group for carbohydrates: -1-α-L-talopyranose
†CtBP	terminal group for carbohydrates: -1-β-L-talopyranose
†CGBU	terminal group for carbohydrates: -1-β-D-glucuronate
†CLAU	terminal group for carbohydrates: -1-α-D-galacturonate
†CMBU	terminal group for carbohydrates: -1-β-D-mannuronate
†CkAU	terminal group for carbohydrates: -1-α-L-guluronate
†CiAU	terminal group for carbohydrates: -1-α-L-iduronate
†C1OC	terminal group for carbohydrates: -C1-O1-CH3
†C1OH	terminal group for carbohydrates: -C1-O1-HO1
†HO2C	initial group for carbohydrates: HO2-O2-C2-
†HO3C	initial group for carbohydrates: HO3-O3-C3-
†HO4C	initial group for carbohydrates: HO4-O4-C4-
†HO6C	initial group for carbohydrates: HO6-O6-C6-

4.2. Definition of molecular topology building block pictures

a. Figure 1, *atoms*

- names: X
- numbering ^{n}X
- integer atom code X^{IAC}
- charge: X_{charge}
- charge groups: color boundaries between different charge groups

b. Figure 2, *bonds and bond angles*

- bond type codes: thin, underlined
- bond-angle type codes: bold, italics

In both building block figures the stereochemical configuration is represented such that the solid wedges indicate bonds that project above the plane of the paper and hashed wedges indicate bonds that project below the plane of the paper. The wedges are always oriented with the narrow end at the stereogenic center.

4.3. α-amino acids and analogues

Solute building block: Alanine
Name: ALA

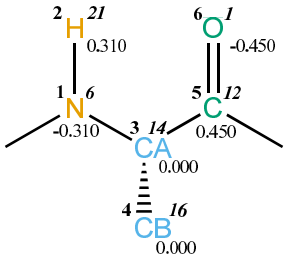

FIGURE 4.1. ALA non-bonded parameters.

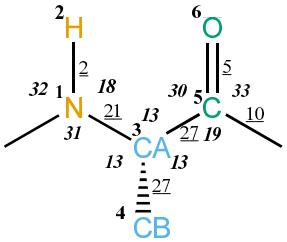

FIGURE 4.2. ALA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 5
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7
4	CB	16	5	0.00000	5
5	C	12	12	0.45000	
6	O	1	16	-0.45000	

TABLE 4.1. Atoms of building block ALA.

I	J	Type
1	2	2
1	3	21
3	4	27
3	5	27
5	6	5
5	7	10

TABLE 4.2. Bonds of building block ALA.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	5	13
4	3	5	13
3	5	6	30
3	5	7	19
6	5	7	33

TABLE 4.3. Bond angles of building block ALA.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	5	43
-1	1	3	5	44
1	3	5	7	42
1	3	5	7	45

TABLE 4.4. Dihedral angles of building block ALA.

I	J	K	L	Type
1	-1	3	2	1
3	1	5	4	2
5	3	7	6	1

TABLE 4.5. Improper dihedral angles of building block ALA.

Solute building block: Arginine (protonated; charge $+e$)
Name: ARG

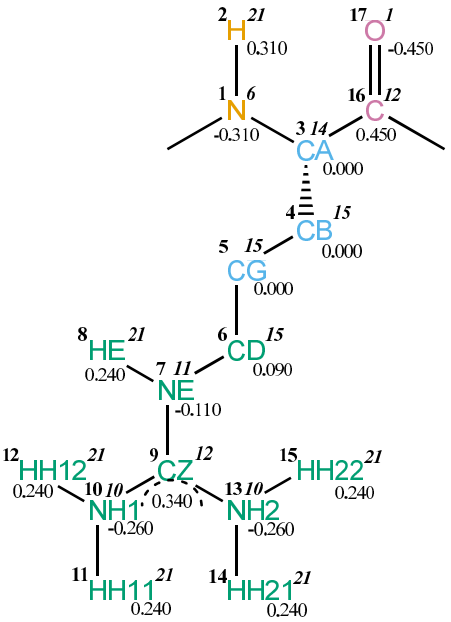

FIGURE 4.3. ARG non-bonded parameters.

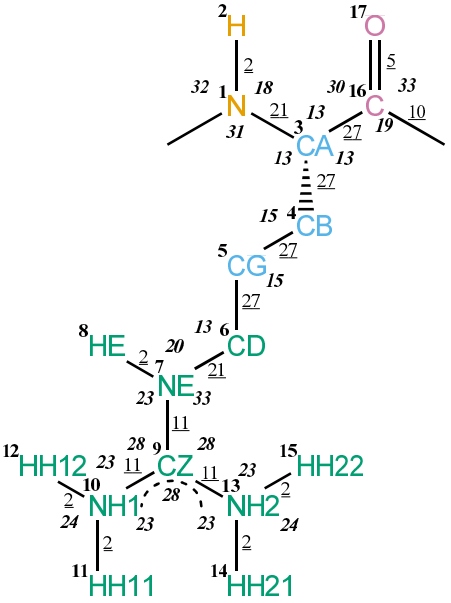

FIGURE 4.4. ARG bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 16
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 16 17 18
4	CB	15	4	0.00000	5 6 16
5	CG	15	4	0.00000	6 7
6	CD	15	4	0.09000	7 8 9
7	NE	11	14	-0.11000	8 9 10 13
8	HE	21	1	0.24000	9
9	CZ	12	12	0.34000	10 11 12 13 14 15
10	NH1	10	14	-0.26000	11 12 13
11	HH11	21	1	0.24000	12
12	HH12	21	1	0.24000	
13	NH2	10	14	-0.26000	14 15
14	HH21	21	1	0.24000	15
15	HH22	21	1	0.24000	
16	C	12	12	0.45000	
17	O	1	16	-0.45000	

TABLE 4.6. Atoms of building block ARG.

I	J	Type
1	2	2
1	3	21
3	4	27
3	16	27
4	5	27
5	6	27
6	7	21
7	8	2
7	9	11
9	10	11
9	13	11
10	11	2
10	12	2
13	14	2
13	15	2
16	17	5
16	18	10

TABLE 4.7. Bonds of building block ARG.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	16	13
4	3	16	13
3	4	5	15
4	5	6	15
5	6	7	13
6	7	8	20
6	7	9	33
8	7	9	23
7	9	10	28
7	9	13	28
10	9	13	28
9	10	11	23
9	10	12	23
11	10	12	24
9	13	14	23
9	13	15	23
14	13	15	24
3	16	17	30
3	16	18	19
17	16	18	33

TABLE 4.8. Bond angles of building block ARG.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	16	43
-1	1	3	16	44
1	3	4	5	34
1	3	16	18	42
1	3	16	18	45
3	4	5	6	34
4	5	6	7	34
5	6	7	9	39
6	7	9	10	14
7	9	10	11	14
7	9	13	14	14

TABLE 4.9. Dihedral angles of building block ARG.

I	J	K	L	Type
1	-1	3	2	1
3	1	16	4	2
7	6	9	8	1
9	10	13	7	1
10	11	12	9	1
13	14	15	9	1
16	3	18	17	1

TABLE 4.10. Improper dihedral angles of building block ARG.

Solute building block: Arginine (deprotonated; neutral)
Name: ARGN

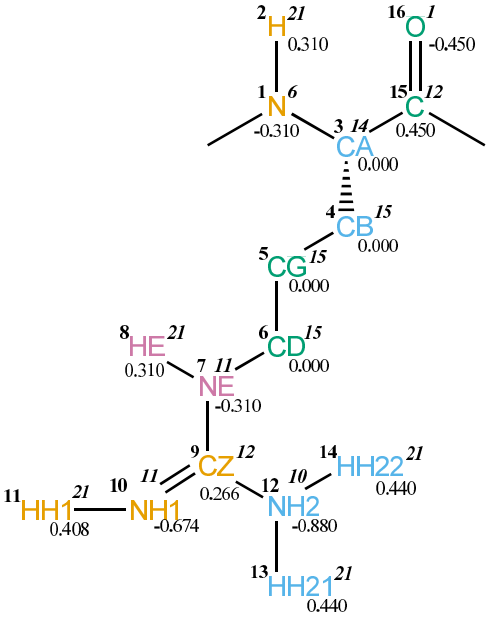

FIGURE 4.5. ARGN non-bonded parameters.

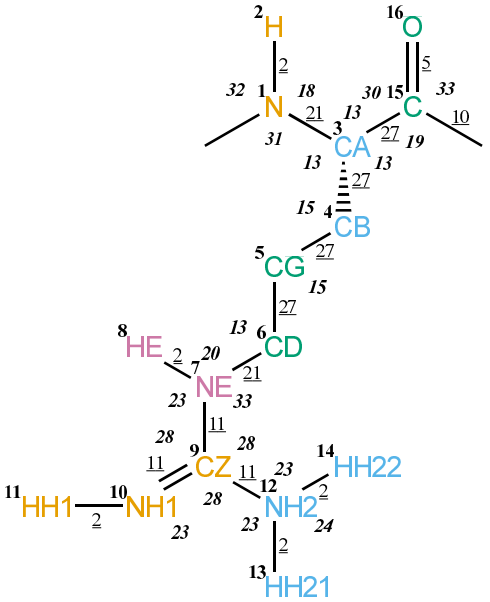

FIGURE 4.6. ARGN bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 15
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 15 16 17
4	CB	15	4	0.00000	5 6 15
5	CG	15	4	0.00000	6 7
6	CD	15	4	0.00000	7 8 9
7	NE	11	14	-0.31000	8 9 10 12
8	HE	21	1	0.31000	9
9	CZ	12	12	0.26600	10 11 12 13 14
10	NH1	11	14	-0.67400	11 12
11	HH1	21	1	0.40800	
12	NH2	10	14	-0.88000	13 14
13	HH21	21	1	0.44000	14
14	HH22	21	1	0.44000	
15	C	12	12	0.45000	
16	O	1	16	-0.45000	

TABLE 4.11. Atoms of building block ARGN.

I	J	Type
1	2	2
1	3	21
3	4	27
3	15	27
4	5	27
5	6	27
6	7	21
7	8	2
7	9	11
9	10	11
9	12	11
10	11	2
12	13	2
12	14	2
15	16	5
15	17	10

TABLE 4.12. Bonds of building block ARGN.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	15	13
4	3	15	13
3	4	5	15
4	5	6	15
5	6	7	13
6	7	8	20
6	7	9	33
8	7	9	23
7	9	10	28
7	9	12	28
10	9	12	28
9	10	11	23
9	12	13	23
9	12	14	23
13	12	14	24
3	15	16	30
3	15	17	19
16	15	17	33

TABLE 4.13. Bond angles of building block ARGN.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	15	43
-1	1	3	15	44
1	3	4	5	34
1	3	15	17	42
1	3	15	17	45
3	4	5	6	34
4	5	6	7	34
5	6	7	9	39
6	7	9	10	14
7	9	10	11	14
7	9	12	13	14

TABLE 4.14. Dihedral angles of building block ARGN.

I	J	K	L	Type
1	-1	3	2	1
3	1	15	4	2
7	6	9	8	1
9	10	12	7	1
12	13	14	9	1
15	3	17	16	1

TABLE 4.15. Improper dihedral angles of building block ARGN.

Solute building block: Asparagine
Name: ASN

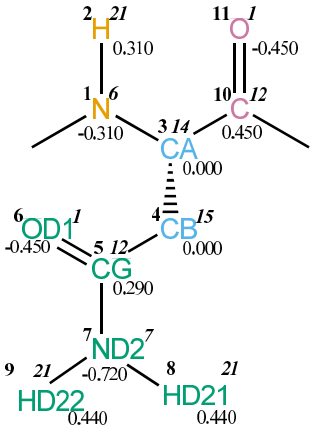

FIGURE 4.7. ASN non-bonded parameters.

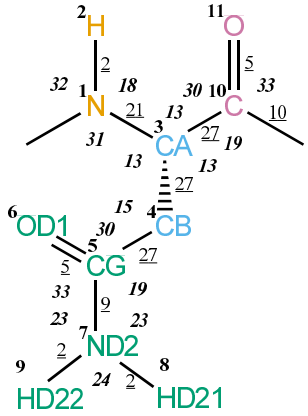

FIGURE 4.8. ASN bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 10
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 10 11 12
4	CB	15	4	0.00000	5 6 7 10
5	CG	12	12	0.29000	6 7 8 9
6	OD1	1	16	-0.45000	7
7	ND2	7	14	-0.72000	8 9
8	HD21	21	1	0.44000	9
9	HD22	21	1	0.44000	
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.16. Atoms of building block ASN.

I	J	Type
1	2	2
1	3	21
3	4	27
3	10	27
4	5	27
5	6	5
5	7	9
7	8	2
7	9	2
10	11	5
10	12	10

TABLE 4.17. Bonds of building block ASN.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	10	13
4	3	10	13
3	4	5	15
4	5	6	30
4	5	7	19
6	5	7	33
5	7	8	23
5	7	9	23
8	7	9	24
3	10	11	30
3	10	12	19
11	10	12	33

TABLE 4.18. Bond angles of building block ASN.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	10	43
-1	1	3	10	44
1	3	4	5	34
1	3	10	12	42
1	3	10	12	45
3	4	5	7	40
4	5	7	8	14

TABLE 4.19. Dihedral angles of building block ASN.

I	J	K	L	Type
1	-1	3	2	1
3	1	10	4	2
5	6	7	4	1
7	8	9	5	1
10	3	12	11	1

TABLE 4.20. Improper dihedral angles of building block ASN.

Solute building block: Asparagine (coordinated with ZN)
Name: ASN1

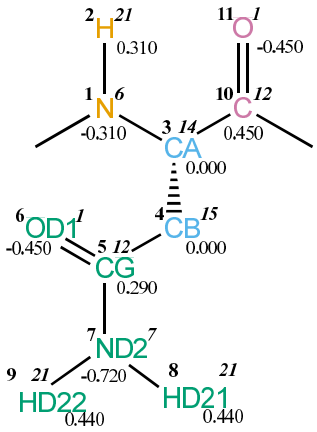

FIGURE 4.9. ASN1 non-bonded parameters.

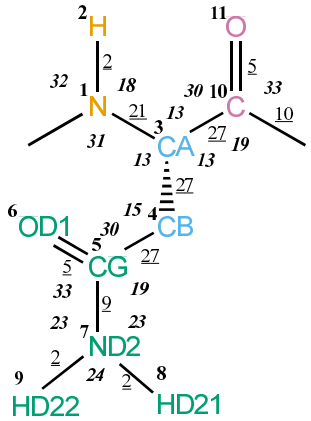

FIGURE 4.10. ASN1 bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 10
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 10 11 12
4	CB	15	4	0.00000	5 6 7 10
5	CG	12	12	0.29000	6 7 8 9
6	OD1	1	16	-0.45000	7
7	ND2	8	14	-0.72000	8 9
8	HD21	21	1	0.44000	9
9	HD22	21	1	0.44000	
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.21. Atoms of building block ASN1.

I	J	Type
1	2	2
1	3	21
3	4	27
3	10	27
4	5	27
5	6	5
5	7	9
7	8	2
7	9	2
10	11	5
10	12	10

TABLE 4.22. Bonds of building block ASN1.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	10	13
4	3	10	13
3	4	5	15
4	5	6	30
4	5	7	19
6	5	7	33
5	7	8	23
5	7	9	23
8	7	9	24
3	10	11	30
3	10	12	19
11	10	12	33

TABLE 4.23. Bond angles of building block ASN1.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	10	43
-1	1	3	10	44
1	3	4	5	34
1	3	10	12	42
1	3	10	12	45
3	4	5	7	40
4	5	7	8	14

TABLE 4.24. Dihedral angles of building block ASN1.

I	J	K	L	Type
1	-1	3	2	1
3	1	10	4	2
5	6	7	4	1
7	8	9	5	1
10	3	12	11	1

TABLE 4.25. Improper dihedral angles of building block ASN1.

Solute building block: Aspartic acid (deprotonated; charge -e)
Name: ASP

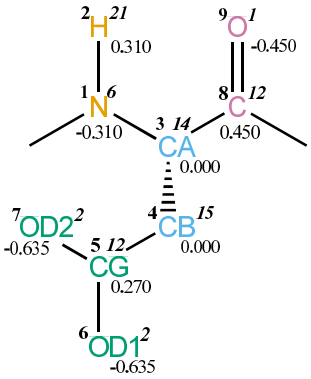

FIGURE 4.11. ASP non-bonded parameters.

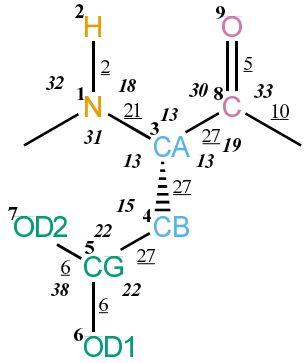

FIGURE 4.12. ASP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 8 9 10
4	CB	15	4	0.00000	5 6 7 8
5	CG	12	12	0.27000	6 7
6	OD1	2	16	-0.63500	7
7	OD2	2	16	-0.63500	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.26. Atoms of building block ASP.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	6
5	7	6
8	9	5
8	10	10

TABLE 4.27. Bonds of building block ASP.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	22
4	5	7	22
6	5	7	38
3	8	9	30
3	8	10	19
9	8	10	33

TABLE 4.28. Bond angles of building block ASP.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	42
1	3	8	10	45
3	4	5	6	40

TABLE 4.29. Dihedral angles of building block ASP.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
5	6	7	4	1
8	3	10	9	1

TABLE 4.30. Improper dihedral angles of building block ASP.

Solute building block: Aspartic acid (protonated; neutral)
Name: ASPH

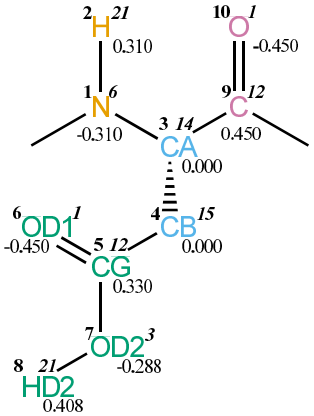

FIGURE 4.13. ASPH non-bonded parameters.

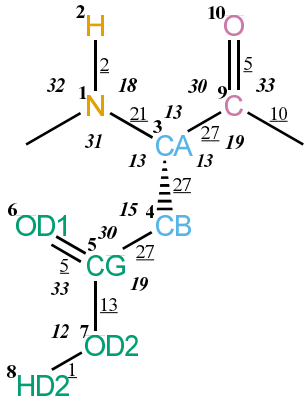

FIGURE 4.14. ASPH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 9
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 9 10 11
4	CB	15	4	0.00000	5 6 7 9
5	CG	12	12	0.33000	6 7 8
6	OD1	1	16	-0.45000	7
7	OD2	3	16	-0.28800	8
8	HD2	21	1	0.40800	
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.31. Atoms of building block ASPH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	9	27
4	5	27
5	6	5
5	7	13
7	8	1
9	10	5
9	11	10

TABLE 4.32. Bonds of building block ASPH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	9	13
4	3	9	13
3	4	5	15
4	5	6	30
4	5	7	19
6	5	7	33
5	7	8	12
3	9	10	30
3	9	11	19
10	9	11	33

TABLE 4.33. Bond angles of building block ASPH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	9	43
-1	1	3	9	44
1	3	4	5	34
1	3	9	11	42
1	3	9	11	45
3	4	5	7	40
4	5	7	8	12

TABLE 4.34. Dihedral angles of building block ASPH.

I	J	K	L	Type
1	-1	3	2	1
3	1	9	4	2
5	6	7	4	1
9	3	11	10	1

TABLE 4.35. Improper dihedral angles of building block ASPH.

Solute building block: Cysteine (deprotonated; charge -1/2e)
Name: CYS

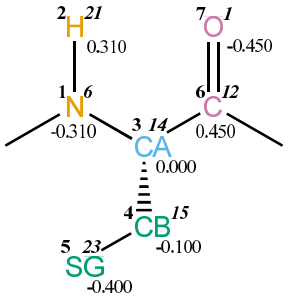

FIGURE 4.15. CYS non-bonded parameters.

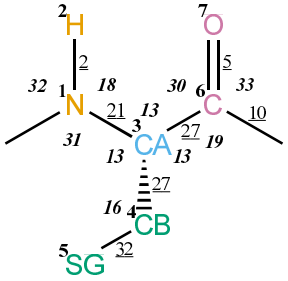

FIGURE 4.16. CYS bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 6
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7 8
4	CB	15	4	-0.10000	5 6
5	SG	23	32	-0.40000	
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.36. Atoms of building block CYS.

I	J	Type
1	2	2
1	3	21
3	4	27
3	6	27
4	5	32
6	7	5
6	8	10

TABLE 4.37. Bonds of building block CYS.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	6	13
4	3	6	13
3	4	5	16
3	6	7	30
3	6	8	19
7	6	8	33

TABLE 4.38. Bond angles of building block CYS.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	6	43
-1	1	3	6	44
1	3	4	5	34
1	3	6	8	42
1	3	6	8	45

TABLE 4.39. Dihedral angles of building block CYS.

I	J	K	L	Type
1	-1	3	2	1
3	1	6	4	2
6	3	8	7	1

TABLE 4.40. Improper dihedral angles of building block CYS.

Solute building block: Cysteine (protonated; neutral)
Name: CYSH

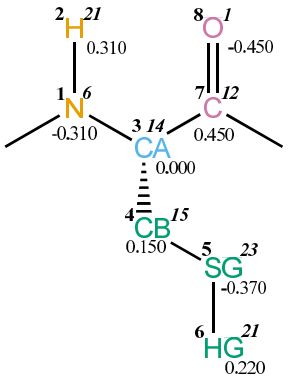

FIGURE 4.17. CYSH non-bonded parameters.

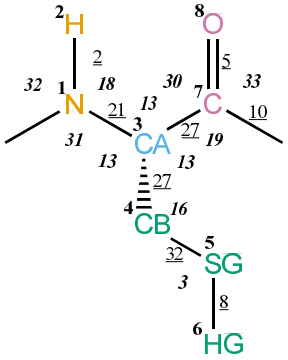

FIGURE 4.18. CYSH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 7 8 9
4	CB	15	4	0.15000	5 6 7
5	SG	23	32	-0.37000	6
6	HG	21	1	0.22000	
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.41. Atoms of building block CYSH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	32
5	6	8
7	8	5
7	9	10

TABLE 4.42. Bonds of building block CYSH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	16
4	5	6	3
3	7	8	30
3	7	9	19
8	7	9	33

TABLE 4.43. Bond angles of building block CYSH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	9	42
1	3	7	9	45
3	4	5	6	26

TABLE 4.44. Dihedral angles of building block CYSH.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
7	3	9	8	1

TABLE 4.45. Improper dihedral angles of building block CYSH.

Solute building block: Cysteine (1st member of S-S bridge)
Name: CYS1

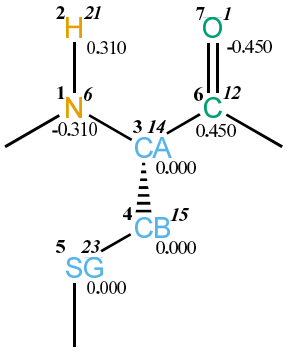

FIGURE 4.19. CYS1 non-bonded parameters.

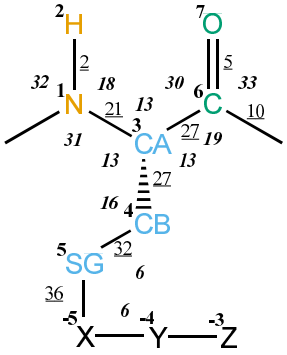

FIGURE 4.20. CYS1 bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 6
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7 8
4	CB	15	4	0.00000	-5 5 6
5	SG	23	32	0.00000	-5 -4
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.46. Atoms of building block CYS1.

I	J	Type
-5	5	36
1	2	2
1	3	21
3	4	27
3	6	27
4	5	32
6	7	5
6	8	10

TABLE 4.47. Bonds of building block CYS1.

I	J	K	Type
-4	-5	5	6
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	6	13
4	3	6	13
3	4	5	16
-5	5	4	6
3	6	7	30
3	6	8	19
7	6	8	33

TABLE 4.48. Bond angles of building block CYS1.

I	J	K	L	Type
5	-5	-4	-3	26
-4	-5	5	4	21
-2	-1	1	3	14
-1	1	3	6	43
-1	1	3	6	44
1	3	4	5	34
1	3	6	8	42
1	3	6	8	45
3	4	5	-5	26

TABLE 4.49. Dihedral angles of building block CYS1.

I	J	K	L	Type
1	-1	3	2	1
3	1	6	4	2
6	3	8	7	1

TABLE 4.50. Improper dihedral angles of building block CYS1.

Solute building block: Cysteine (2nd member of S-S bridge)
Name: CYS2

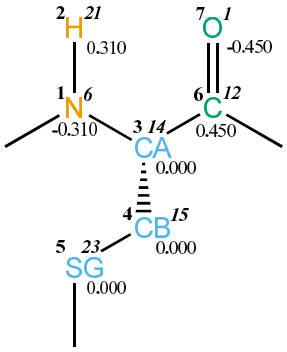

FIGURE 4.21. CYS2 non-bonded parameters.

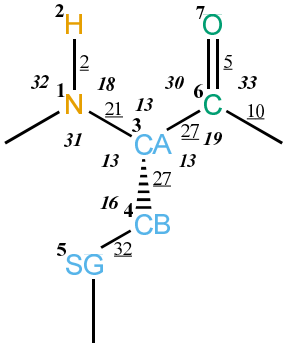

FIGURE 4.22. CYS2 bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 6
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7 8
4	CB	15	4	0.00000	5 6
5	SG	23	32	0.00000	
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.51. Atoms of building block CYS2.

I	J	Type
1	2	2
1	3	21
3	4	27
3	6	27
4	5	32
6	7	5
6	8	10

TABLE 4.52. Bonds of building block CYS2.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	6	13
4	3	6	13
3	4	5	16
3	6	7	30
3	6	8	19
7	6	8	33

TABLE 4.53. Bond angles of building block CYS2.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	6	43
-1	1	3	6	44
1	3	4	5	34
1	3	6	8	42
1	3	6	8	45

TABLE 4.54. Dihedral angles of building block CYS2.

I	J	K	L	Type
1	-1	3	2	1
3	1	6	4	2
6	3	8	7	1

TABLE 4.55. Improper dihedral angles of building block CYS2.

Solute building block: Glutamine
Name: GLN

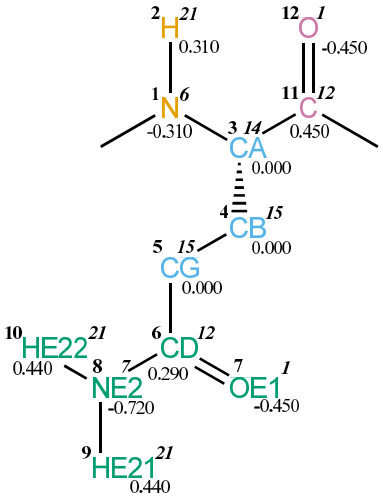

FIGURE 4.23. GLN non-bonded parameters.

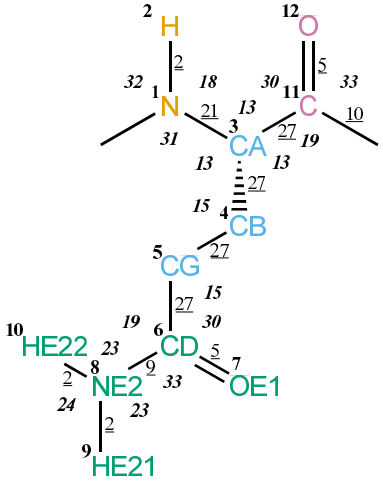

FIGURE 4.24. GLN bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 11
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 11 12 13
4	CB	15	4	0.00000	5 6 11
5	CG	15	4	0.00000	6 7 8
6	CD	12	12	0.29000	7 8 9 10
7	OE1	1	16	-0.45000	8
8	NE2	7	14	-0.72000	9 10
9	HE21	21	1	0.44000	10
10	HE22	21	1	0.44000	
11	C	12	12	0.45000	
12	O	1	16	-0.45000	

TABLE 4.56. Atoms of building block GLN.

I	J	Type
1	2	2
1	3	21
3	4	27
3	11	27
4	5	27
5	6	27
6	7	5
6	8	9
8	9	2
8	10	2
11	12	5
11	13	10

TABLE 4.57. Bonds of building block GLN.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	11	13
4	3	11	13
3	4	5	15
4	5	6	15
5	6	7	30
5	6	8	19
7	6	8	33
6	8	9	23
6	8	10	23
9	8	10	24
3	11	12	30
3	11	13	19
12	11	13	33

TABLE 4.58. Bond angles of building block GLN.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	11	43
-1	1	3	11	44
1	3	4	5	34
1	3	11	13	42
1	3	11	13	45
3	4	5	6	34
4	5	6	8	40
5	6	8	9	14

TABLE 4.59. Dihedral angles of building block GLN.

I	J	K	L	Type
1	-1	3	2	1
3	1	11	4	2
6	7	8	5	1
8	9	10	6	1
11	3	13	12	1

TABLE 4.60. Improper dihedral angles of building block GLN.

Solute building block: Glutamic acid (deprotonated; charge -e)
Name: GLU

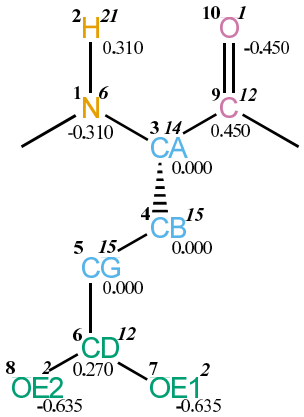

FIGURE 4.25. GLU non-bonded parameters.

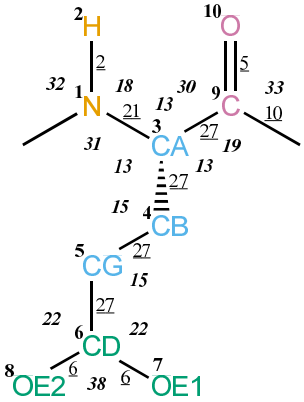

FIGURE 4.26. GLU bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 9
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 9 10 11
4	CB	15	4	0.00000	5 6 9
5	CG	15	4	0.00000	6 7 8
6	CD	12	12	0.27000	7 8
7	OE1	2	16	-0.63500	8
8	OE2	2	16	-0.63500	
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.61. Atoms of building block GLU.

I	J	Type
1	2	2
1	3	21
3	4	27
3	9	27
4	5	27
5	6	27
6	7	6
6	8	6
9	10	5
9	11	10

TABLE 4.62. Bonds of building block GLU.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	9	13
4	3	9	13
3	4	5	15
4	5	6	15
5	6	7	22
5	6	8	22
7	6	8	38
3	9	10	30
3	9	11	19
10	9	11	33

TABLE 4.63. Bond angles of building block GLU.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	9	43
-1	1	3	9	44
1	3	4	5	34
1	3	9	11	42
1	3	9	11	45
3	4	5	6	34
4	5	6	8	40

TABLE 4.64. Dihedral angles of building block GLU.

I	J	K	L	Type
1	-1	3	2	1
3	1	9	4	2
6	7	8	5	1
9	3	11	10	1

TABLE 4.65. Improper dihedral angles of building block GLU.

Solute building block: Glutamic acid (protonated; neutral)
Name: GLUH

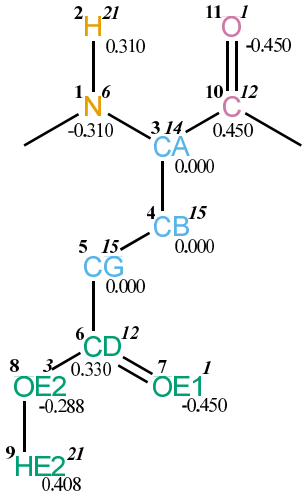

FIGURE 4.27. GLUH non-bonded parameters.

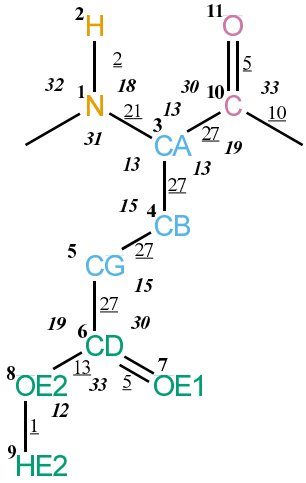

FIGURE 4.28. GLUH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 10
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 10 11 12
4	CB	15	4	0.00000	5 6 10
5	CG	15	4	0.00000	6 7 8
6	CD	12	12	0.33000	7 8 9
7	OE1	1	16	-0.45000	8
8	OE2	3	16	-0.28800	9
9	HE2	21	1	0.40800	
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.66. Atoms of building block GLUH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	10	27
4	5	27
5	6	27
6	7	5
6	8	13
8	9	1
10	11	5
10	12	10

TABLE 4.67. Bonds of building block GLUH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	10	13
4	3	10	13
3	4	5	15
4	5	6	15
5	6	7	30
5	6	8	19
7	6	8	33
6	8	9	12
3	10	11	30
3	10	12	19
11	10	12	33

TABLE 4.68. Bond angles of building block GLUH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	10	43
-1	1	3	10	44
1	3	4	5	34
1	3	10	12	42
1	3	10	12	45
3	4	5	6	34
4	5	6	8	40
5	6	8	9	12

TABLE 4.69. Dihedral angles of building block GLUH.

I	J	K	L	Type
1	-1	3	2	1
3	1	10	4	2
6	7	8	5	1
10	3	12	11	1

TABLE 4.70. Improper dihedral angles of building block GLUH.

Solute building block: Glycine
Name: GLY

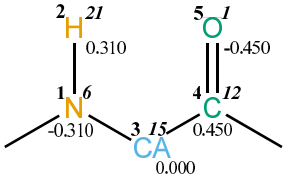

FIGURE 4.29. GLY non-bonded parameters.

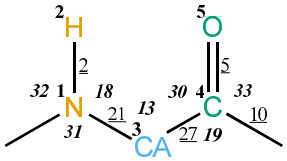

FIGURE 4.30. GLY bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CA	15	4	0.00000	4 5 6
4	C	12	12	0.45000	
5	O	1	16	-0.45000	

TABLE 4.71. Atoms of building block GLY.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	5
4	6	10

TABLE 4.72. Bonds of building block GLY.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	30
3	4	6	19
5	4	6	33

TABLE 4.73. Bond angles of building block GLY.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	6	42
1	3	4	6	45

TABLE 4.74. Dihedral angles of building block GLY.

I	J	K	L	Type
1	-1	3	2	1
4	3	6	5	1

TABLE 4.75. Improper dihedral angles of building block GLY.

Solute building block: Histidine (protonated at ND1; neutral)
Name: HISA

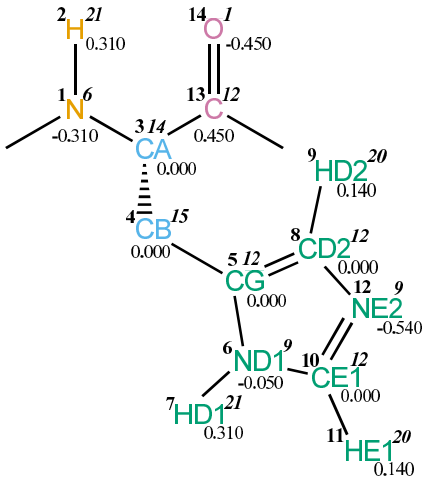

FIGURE 4.31. HISA non-bonded parameters.

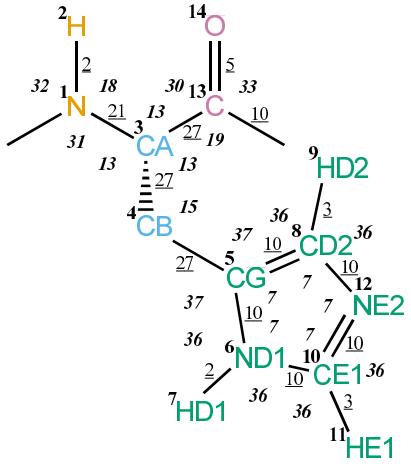

FIGURE 4.32. HISA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 13
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 13 14 15
4	CB	15	4	0.00000	5 6 7 8 9 10 12 13
5	CG	12	12	0.00000	6 7 8 9 10 11 12
6	ND1	9	14	-0.05000	7 8 9 10 11 12
7	HD1	21	1	0.31000	8 10 11 12
8	CD2	12	12	0.00000	9 10 11 12
9	HD2	20	1	0.14000	10 12
10	CE1	12	12	0.00000	11 12
11	HE1	20	1	0.14000	12
12	NE2	9	14	-0.54000	
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.76. Atoms of building block HISA.

I	J	Type
1	2	2
1	3	21
3	4	27
3	13	27
4	5	27
5	6	10
5	8	10
6	7	2
6	10	10
8	9	3
8	12	10
10	11	3
10	12	10
13	14	5
13	15	10

TABLE 4.77. Bonds of building block HISA.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	13	13
4	3	13	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	10	7
7	6	10	36
5	8	9	36
5	8	12	7
9	8	12	36
6	10	11	36
6	10	12	7
11	10	12	36
8	12	10	7
3	13	14	30
3	13	15	19
14	13	15	33

TABLE 4.78. Bond angles of building block HISA.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	13	43
-1	1	3	13	44
1	3	4	5	34
1	3	13	15	42
1	3	13	15	45
3	4	5	6	40

TABLE 4.79. Dihedral angles of building block HISA.

I	J	K	L	Type
1	-1	3	2	1
3	1	13	4	2
5	6	8	4	1
5	6	10	12	1
5	8	12	10	1
6	5	8	12	1
6	5	10	7	1
6	10	12	8	1
8	5	6	10	1
8	5	12	9	1
10	6	12	11	1
13	3	15	14	1

TABLE 4.80. Improper dihedral angles of building block HISA.

Solute building block: Histidine (protonated at NE2; neutral)
Name: HISB

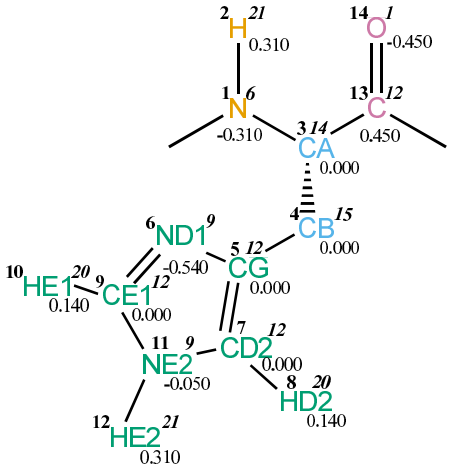

FIGURE 4.33. HISB non-bonded parameters.

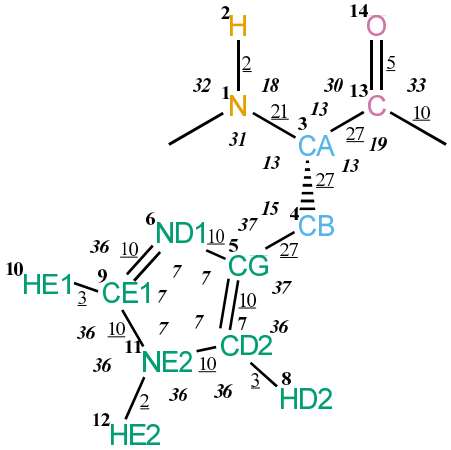

FIGURE 4.34. HISB bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 13
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 13 14 15
4	CB	15	4	0.00000	5 6 7 8 9 11 13
5	CG	12	12	0.00000	6 7 8 9 10 11 12
6	ND1	9	14	-0.54000	7 8 9 10 11 12
7	CD2	12	12	0.00000	8 9 10 11 12
8	HD2	20	1	0.14000	9 11 12
9	CE1	12	12	0.00000	10 11 12
10	HE1	20	1	0.14000	11 12
11	NE2	9	14	-0.05000	12
12	HE2	21	1	0.31000	
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.81. Atoms of building block HISB.

I	J	Type
1	2	2
1	3	21
3	4	27
3	13	27
4	5	27
5	6	10
5	7	10
6	9	10
7	8	3
7	11	10
9	10	3
9	11	10
11	12	2
13	14	5
13	15	10

TABLE 4.82. Bonds of building block HISB.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	13	13
4	3	13	13
3	4	5	15
4	5	6	37
4	5	7	37
6	5	7	7
5	6	9	7
5	7	8	36
5	7	11	7
8	7	11	36
6	9	10	36
6	9	11	7
10	9	11	36
7	11	9	7
7	11	12	36
9	11	12	36
3	13	14	30
3	13	15	19
14	13	15	33

TABLE 4.83. Bond angles of building block HISB.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	13	43
-1	1	3	13	44
1	3	4	5	34
1	3	13	15	42
1	3	13	15	45
3	4	5	6	40

TABLE 4.84. Dihedral angles of building block HISB.

I	J	K	L	Type
1	-1	3	2	1
3	1	13	4	2
5	6	7	4	1
5	6	9	11	1
5	7	11	9	1
6	5	7	11	1
6	9	11	7	1
7	5	6	9	1
7	5	11	8	1
9	6	11	10	1
11	7	9	12	1
13	3	15	14	1

TABLE 4.85. Improper dihedral angles of building block HISB.

Solute building block: Histidine (protonated at ND1 and NE2; charge $+e$)
Name: HISH

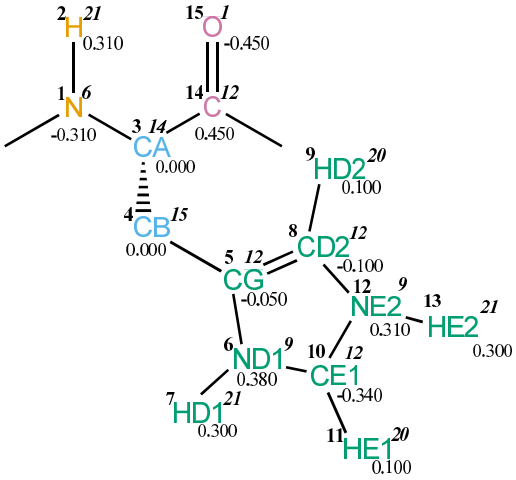

FIGURE 4.35. HISH non-bonded parameters.

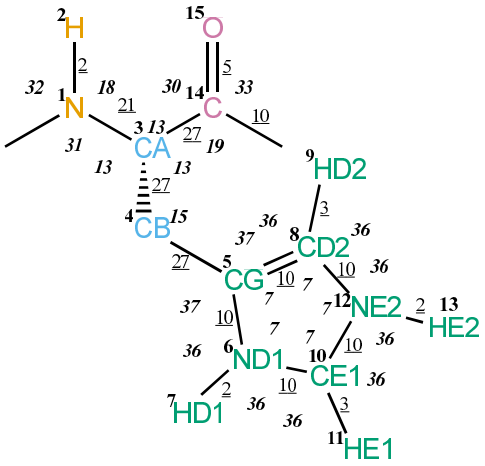

FIGURE 4.36. HISH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 14
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 14 15 16
4	CB	15	4	0.00000	5 6 7 8 9 10 12 14
5	CG	12	12	-0.05000	6 7 8 9 10 11 12 13
6	ND1	9	14	0.38000	7 8 9 10 11 12 13
7	HD1	21	1	0.30000	8 10 11 12
8	CD2	12	12	-0.10000	9 10 11 12 13
9	HD2	20	1	0.10000	10 12 13
10	CE1	12	12	-0.34000	11 12 13
11	HE1	20	1	0.10000	12 13
12	NE2	9	14	0.31000	13
13	HE2	21	1	0.30000	
14	C	12	12	0.45000	
15	O	1	16	-0.45000	

TABLE 4.86. Atoms of building block HISH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	14	27
4	5	27
5	6	10
5	8	10
6	7	2
6	10	10
8	9	3
8	12	10
10	11	3
10	12	10
12	13	2
14	15	5
14	16	10

TABLE 4.87. Bonds of building block HISH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	14	13
4	3	14	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	10	7
7	6	10	36
5	8	9	36
5	8	12	7
9	8	12	36
6	10	11	36
6	10	12	7
11	10	12	36
8	12	10	7
8	12	13	36
10	12	13	36
3	14	15	30
3	14	16	19
15	14	16	33

TABLE 4.88. Bond angles of building block HISH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	14	43
-1	1	3	14	44
1	3	4	5	34
1	3	14	16	42
1	3	14	16	45
3	4	5	6	40

TABLE 4.89. Dihedral angles of building block HISH.

I	J	K	L	Type
1	-1	3	2	1
3	1	14	4	2
5	6	8	4	1
5	6	10	12	1
5	8	12	10	1
6	5	8	12	1
6	5	10	7	1
6	10	12	8	1
8	5	6	10	1
8	5	12	9	1
10	6	12	11	1
12	8	10	13	1
14	3	16	15	1

TABLE 4.90. Improper dihedral angles of building block HISH.

Solute building block: Histidine (coupled to HEME at NE2; neutral)
Name: HIS1

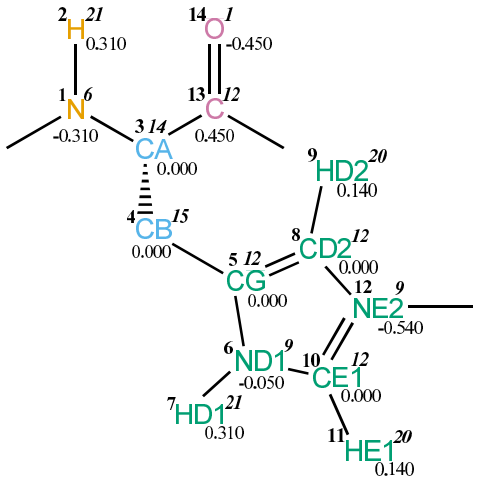

FIGURE 4.37. HIS1 non-bonded parameters.

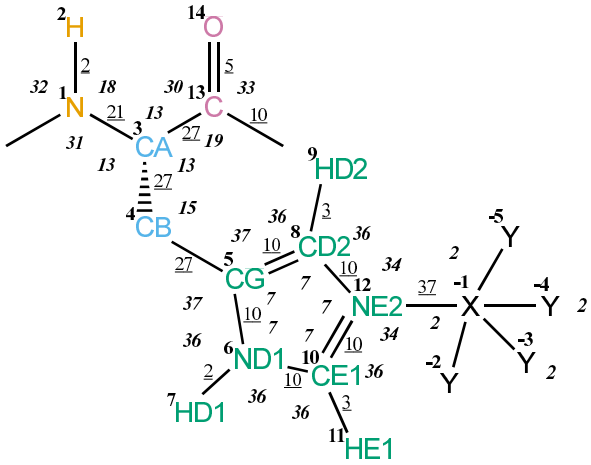

FIGURE 4.38. HIS1 bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 13
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 13 14 15
4	CB	15	4	0.00000	5 6 7 8 9 10 12 13
5	CG	12	12	0.00000	-1 6 7 8 9 10 11 12
6	ND1	9	14	-0.05000	-1 7 8 9 10 11 12
7	HD1	21	1	0.31000	8 10 11 12
8	CD2	12	12	0.00000	-1 9 10 11 12
9	HD2	20	1	0.14000	-1 10 12
10	CE1	12	12	0.00000	-1 11 12
11	HE1	20	1	0.14000	-1 12
12	NE2	9	14	-0.54000	-5 -4 -3 -2 -1
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.91. Atoms of building block HIS1.

I	J	Type
-1	12	37
1	2	2
1	3	21
3	4	27
3	13	27
4	5	27
5	6	10
5	8	10
6	7	2
6	10	10
8	9	3
8	12	10
10	11	3
10	12	10
13	14	5
13	15	10

TABLE 4.92. Bonds of building block HIS1.

I	J	K	Type
-5	-1	12	2
-4	-1	12	2
-3	-1	12	2
-2	-1	12	2
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	13	13
4	3	13	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	10	7
7	6	10	36
5	8	9	36
5	8	12	7
9	8	12	36
6	10	11	36
6	10	12	7
11	10	12	36
-1	12	8	34
-1	12	10	34
8	12	10	7
3	13	14	30
3	13	15	19
14	13	15	33

TABLE 4.93. Bond angles of building block HIS1.

I	J	K	L	Type
-2	-1	1	3	14
-2	-1	12	8	38
-1	1	3	13	43
-1	1	3	13	44
1	3	4	5	34
1	3	13	15	42
1	3	13	15	45
3	4	5	6	40

TABLE 4.94. Dihedral angles of building block HIS1.

I	J	K	L	Type
1	-1	3	2	1
3	1	13	4	2
5	6	8	4	1
5	6	10	12	1
5	8	12	10	1
6	5	8	12	1
6	5	10	7	1
6	10	12	8	1
8	5	6	10	1
8	5	12	9	1
10	6	12	11	1
13	3	15	14	1

TABLE 4.95. Improper dihedral angles of building block HIS1.

Solute building block: Histidine (coupled to HEMC at NE2: neutral)
Name: HIS2

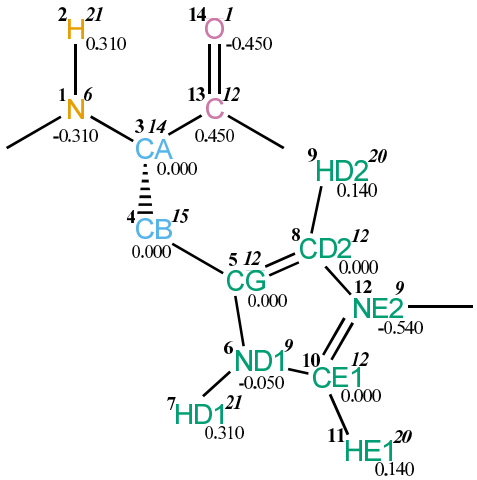

FIGURE 4.39. HIS2 non-bonded parameters.

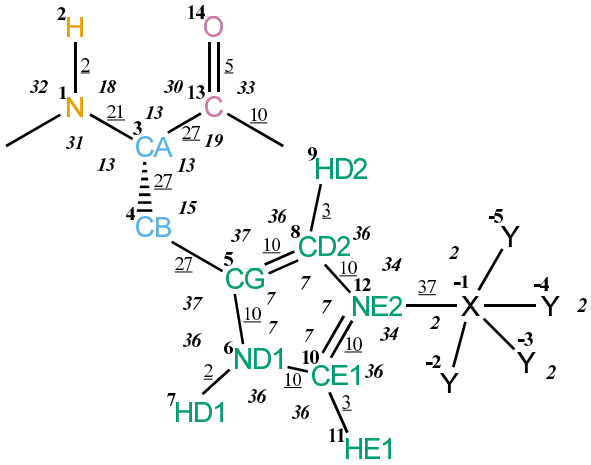

FIGURE 4.40. HIS2 bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 13
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 13 14 15
4	CB	15	4	0.00000	5 6 7 8 9 10 12 13
5	CG	12	12	0.00000	-1 6 7 8 9 10 11 12
6	ND1	9	14	-0.05000	-1 7 8 9 10 11 12
7	HD1	21	1	0.31000	8 10 11 12
8	CD2	12	12	0.00000	-1 9 10 11 12
9	HD2	20	1	0.14000	-1 10 12
10	CE1	12	12	0.00000	-1 11 12
11	HE1	20	1	0.14000	-1 12
12	NE2	9	14	-0.54000	-48 -5 -4 -3 -2 -1
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.96. Atoms of building block HIS2.

I	J	Type
-1	12	37
1	2	2
1	3	21
3	4	27
3	13	27
4	5	27
5	6	10
5	8	10
6	7	2
6	10	10
8	9	3
8	12	10
10	11	3
10	12	10
13	14	5
13	15	10

TABLE 4.97. Bonds of building block HIS2.

I	J	K	Type
-5	-1	12	2
-4	-1	12	2
-3	-1	12	2
-2	-1	12	2
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	13	13
4	3	13	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	10	7
7	6	10	36
5	8	9	36
5	8	12	7
9	8	12	36
6	10	11	36
6	10	12	7
11	10	12	36
-1	12	8	34
-1	12	10	34
8	12	10	7
3	13	14	30
3	13	15	19
14	13	15	33

TABLE 4.98. Bond angles of building block HIS2.

I	J	K	L	Type
-2	-1	1	3	14
-2	-1	12	8	38
-1	1	3	13	43
-1	1	3	13	44
1	3	4	5	34
1	3	13	15	42
1	3	13	15	45
3	4	5	6	40

TABLE 4.99. Dihedral angles of building block HIS2.

I	J	K	L	Type
1	-1	3	2	1
3	1	13	4	2
5	6	8	4	1
5	6	10	12	1
5	8	12	10	1
6	5	8	12	1
6	5	10	7	1
6	10	12	8	1
8	5	6	10	1
8	5	12	9	1
10	6	12	11	1
13	3	15	14	1

TABLE 4.100. Improper dihedral angles of building block HIS2.

Solute building block: Hydroxyproline (R-configuration at CG)
Name: HYPR

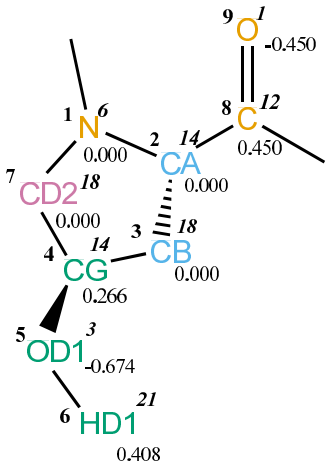

FIGURE 4.41. HYPR non-bonded parameters.

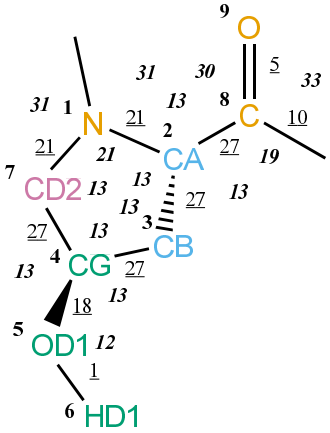

FIGURE 4.42. HYPR bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 7
0					1
1	N	6	14	0.00000	2 3 4 7 8
2	CA	14	3	0.00000	3 4 7 8 9 10
3	CB	18	4	0.00000	4 5 7 8
4	CG	14	3	0.26600	5 6 7
5	OD1	3	16	-0.67400	6 7
6	HD1	21	1	0.40800	
7	CD2	18	4	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.101. Atoms of building block HYPR.

I	J	Type
1	2	21
1	7	21
2	3	27
2	8	27
3	4	27
4	5	18
4	7	27
5	6	1
8	9	5
8	10	10

TABLE 4.102. Bonds of building block HYPR.

I	J	K	Type
-1	1	2	31
-1	1	7	31
2	1	7	21
1	2	3	13
1	2	8	13
3	2	8	13
2	3	4	13
3	4	5	13
3	4	7	13
5	4	7	13
4	5	6	12
1	7	4	13
2	8	9	30
2	8	10	19
9	8	10	33

TABLE 4.103. Bond angles of building block HYPR.

I	J	K	L	Type
-2	-1	1	2	14
-1	1	2	8	43
-1	1	2	8	44
2	1	7	4	39
1	2	3	4	34
1	2	8	10	42
1	2	8	10	45
2	3	4	7	34
3	4	5	6	23
3	4	7	1	34

TABLE 4.104. Dihedral angles of building block HYPR.

I	J	K	L	Type
1	-1	2	7	1
2	1	8	3	2
4	3	7	5	2
8	2	10	9	1

TABLE 4.105. Improper dihedral angles of building block HYPR.

Solute building block: Isoleucine
Name: ILE

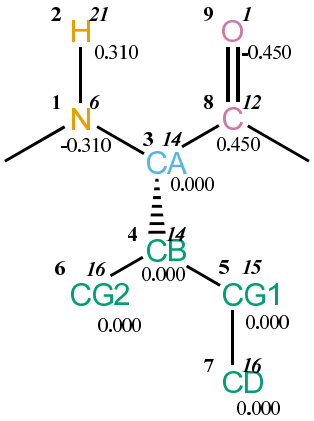

FIGURE 4.43. ILE non-bonded parameters.

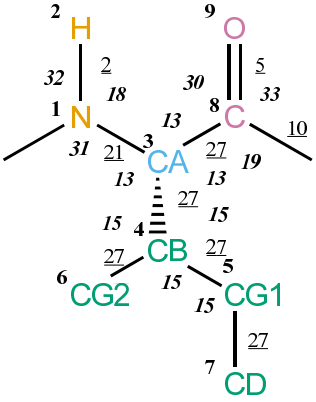

FIGURE 4.44. ILE bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 8 9 10
4	CB	14	3	0.00000	5 6 7 8
5	CG1	15	4	0.00000	6 7
6	CG2	16	5	0.00000	
7	CD	16	5	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.106. Atoms of building block ILE.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
4	6	27
5	7	27
8	9	5
8	10	10

TABLE 4.107. Bonds of building block ILE.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
3	4	6	15
5	4	6	15
4	5	7	15
3	8	9	30
3	8	10	19
9	8	10	33

TABLE 4.108. Bond angles of building block ILE.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	42
1	3	8	10	45
3	4	5	7	34

TABLE 4.109. Dihedral angles of building block ILE.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	5	6	3	2
8	3	10	9	1

TABLE 4.110. Improper dihedral angles of building block ILE.

Solute building block: Leucine
Name: LEU

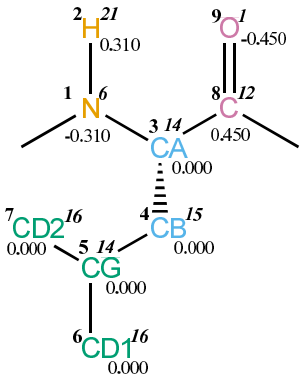

FIGURE 4.45. LEU non-bonded parameters.

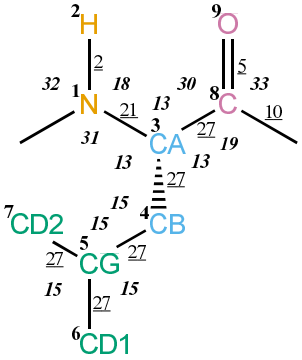

FIGURE 4.46. LEU bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 8 9 10
4	CB	15	4	0.00000	5 6 7 8
5	CG	14	3	0.00000	6 7
6	CD1	16	5	0.00000	7
7	CD2	16	5	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.111. Atoms of building block LEU.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	27
5	7	27
8	9	5
8	10	10

TABLE 4.112. Bonds of building block LEU.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	15
4	5	7	15
6	5	7	15
3	8	9	30
3	8	10	19
9	8	10	33

TABLE 4.113. Bond angles of building block LEU.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	42
1	3	8	10	45
3	4	5	6	34

TABLE 4.114. Dihedral angles of building block LEU.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	6	7	5	2
8	3	10	9	1

TABLE 4.115. Improper dihedral angles of building block LEU.

Solute building block: Lysine (deprotonated; neutral)
Name: LYS

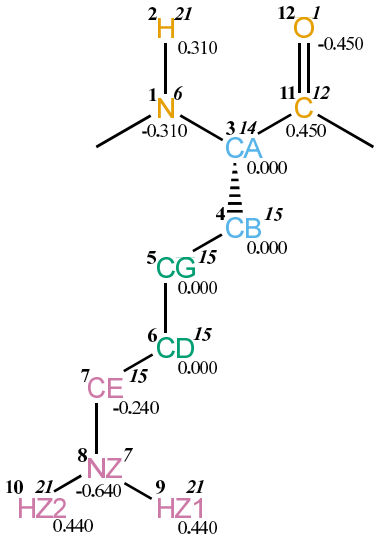

FIGURE 4.47. LYS non-bonded parameters.

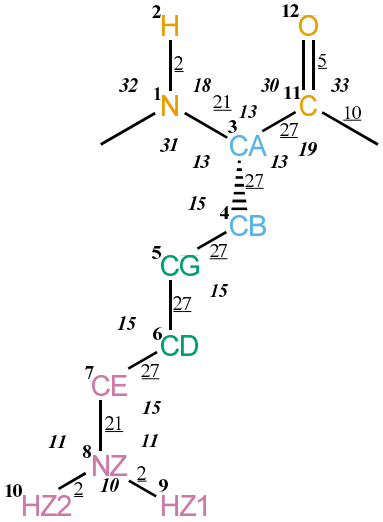

FIGURE 4.48. LYS bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 11
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 11 12 13
4	CB	15	4	0.00000	5 6 11
5	CG	15	4	0.00000	6 7
6	CD	15	4	0.00000	7 8
7	CE	15	4	-0.24000	8 9 10
8	NZ	7	14	-0.64000	9 10
9	HZ1	21	1	0.44000	10
10	HZ2	21	1	0.44000	
11	C	12	12	0.45000	
12	O	1	16	-0.45000	

TABLE 4.116. Atoms of building block LYS.

I	J	Type
1	2	2
1	3	21
3	4	27
3	11	27
4	5	27
5	6	27
6	7	27
7	8	21
8	9	2
8	10	2
11	12	5
11	13	10

TABLE 4.117. Bonds of building block LYS.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	11	13
4	3	11	13
3	4	5	15
4	5	6	15
5	6	7	15
6	7	8	15
7	8	9	11
7	8	10	11
9	8	10	10
3	11	12	30
3	11	13	19
12	11	13	33

TABLE 4.118. Bond angles of building block LYS.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	11	43
-1	1	3	11	44
1	3	4	5	34
1	3	11	13	42
1	3	11	13	45
3	4	5	6	34
4	5	6	7	34
5	6	7	8	34
6	7	8	9	29

TABLE 4.119. Dihedral angles of building block LYS.

I	J	K	L	Type
1	-1	3	2	1
3	1	11	4	2
11	3	13	12	1

TABLE 4.120. Improper dihedral angles of building block LYS.

Solute building block: Lysine (protonated; charge $+e$)
Name: LYSH

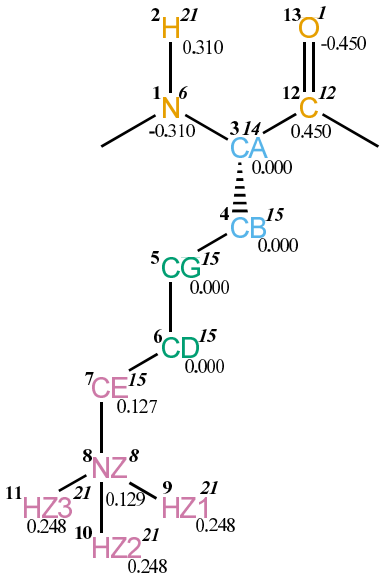

FIGURE 4.49. LYSH non-bonded parameters.

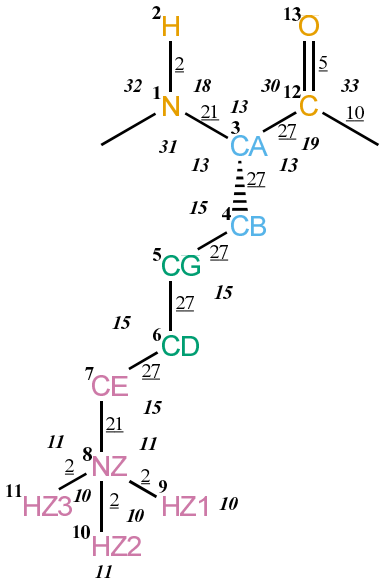

FIGURE 4.50. LYSH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 12
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 12 13 14
4	CB	15	4	0.00000	5 6 12
5	CG	15	4	0.00000	6 7
6	CD	15	4	0.00000	7 8
7	CE	15	4	0.12700	8 9 10 11
8	NZ	8	14	0.12900	9 10 11
9	HZ1	21	1	0.24800	10 11
10	HZ2	21	1	0.24800	11
11	HZ3	21	1	0.24800	
12	C	12	12	0.45000	
13	O	1	16	-0.45000	

TABLE 4.121. Atoms of building block LYSH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	12	27
4	5	27
5	6	27
6	7	27
7	8	21
8	9	2
8	10	2
8	11	2
12	13	5
12	14	10

TABLE 4.122. Bonds of building block LYSH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	12	13
4	3	12	13
3	4	5	15
4	5	6	15
5	6	7	15
6	7	8	15
7	8	9	11
7	8	10	11
7	8	11	11
9	8	10	10
9	8	11	10
10	8	11	10
3	12	13	30
3	12	14	19
13	12	14	33

TABLE 4.123. Bond angles of building block LYSH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	12	43
-1	1	3	12	44
1	3	4	5	34
1	3	12	14	42
1	3	12	14	45
3	4	5	6	34
4	5	6	7	34
5	6	7	8	34
6	7	8	9	29

TABLE 4.124. Dihedral angles of building block LYSH.

I	J	K	L	Type
1	-1	3	2	1
3	1	12	4	2
12	3	14	13	1

TABLE 4.125. Improper dihedral angles of building block LYSH.

Solute building block: Methionine
Name: MET

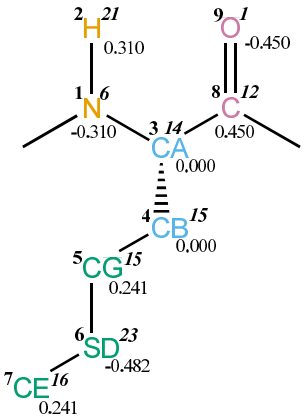

FIGURE 4.51. MET non-bonded parameters.

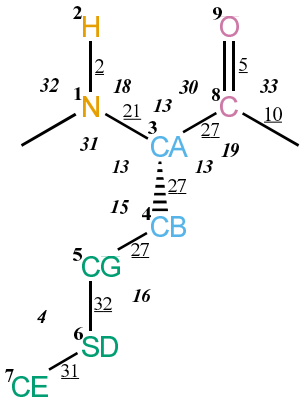

FIGURE 4.52. MET bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 8 9 10
4	CB	15	4	0.00000	5 6 8
5	CG	15	4	0.24100	6 7
6	SD	23	32	-0.48200	7
7	CE	16	5	0.24100	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.126. Atoms of building block MET.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	32
6	7	31
8	9	5
8	10	10

TABLE 4.127. Bonds of building block MET.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	16
5	6	7	4
3	8	9	30
3	8	10	19
9	8	10	33

TABLE 4.128. Bond angles of building block MET.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	42
1	3	8	10	45
3	4	5	6	34
4	5	6	7	26

TABLE 4.129. Dihedral angles of building block MET.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
8	3	10	9	1

TABLE 4.130. Improper dihedral angles of building block MET.

Solute building block: Phenylalanine
Name: PHE

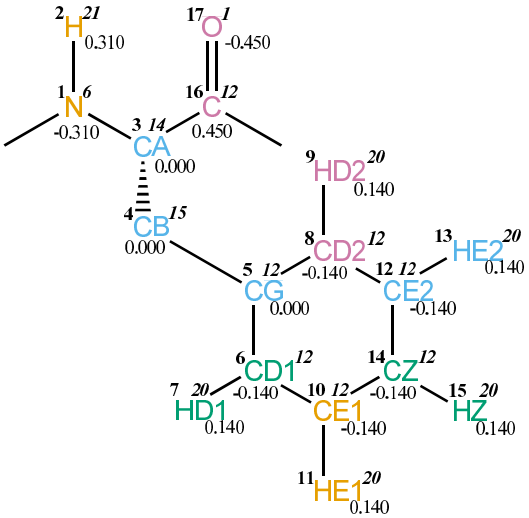

FIGURE 4.53. PHE non-bonded parameters.

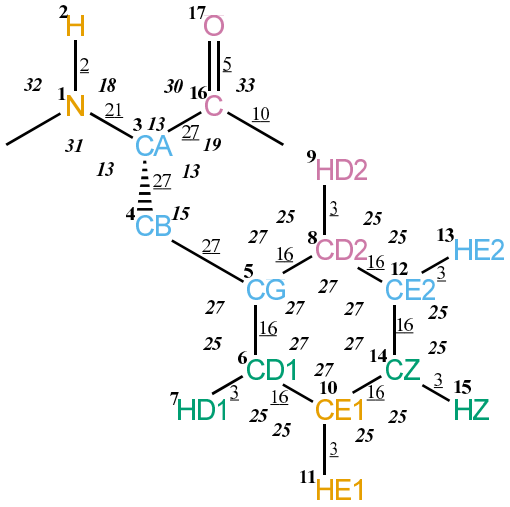

FIGURE 4.54. PHE bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 16
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 16 17 18
4	CB	15	4	0.00000	5 6 7 8 9 10 12 16
5	CG	12	12	0.00000	6 7 8 9 10 11 12 13 14
6	CD1	12	12	-0.14000	7 8 9 10 11 12 14 15
7	HD1	20	1	0.14000	8 10 11 14
8	CD2	12	12	-0.14000	9 10 12 13 14 15
9	HD2	20	1	0.14000	12 13 14
10	CE1	12	12	-0.14000	11 12 13 14 15
11	HE1	20	1	0.14000	12 14 15
12	CE2	12	12	-0.14000	13 14 15
13	HE2	20	1	0.14000	14 15
14	CZ	12	12	-0.14000	15
15	HZ	20	1	0.14000	
16	C	12	12	0.45000	
17	O	1	16	-0.45000	

TABLE 4.131. Atoms of building block PHE.

I	J	Type
1	2	2
1	3	21
3	4	27
3	16	27
4	5	27
5	6	16
5	8	16
6	7	3
6	10	16
8	9	3
8	12	16
10	11	3
10	14	16
12	13	3
12	14	16
14	15	3
16	17	5
16	18	10

TABLE 4.132. Bonds of building block PHE.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	16	13
4	3	16	13
3	4	5	15
4	5	6	27
4	5	8	27
6	5	8	27
5	6	7	25
5	6	10	27
7	6	10	25
5	8	9	25
5	8	12	27
9	8	12	25
6	10	11	25
6	10	14	27
11	10	14	25
8	12	13	25
8	12	14	27
13	12	14	25
10	14	12	27
10	14	15	25
12	14	15	25
3	16	17	30
3	16	18	19
17	16	18	33

TABLE 4.133. Bond angles of building block PHE.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	16	43
-1	1	3	16	44
1	3	4	5	34
1	3	16	18	42
1	3	16	18	45
3	4	5	6	40

TABLE 4.134. Dihedral angles of building block PHE.

I	J	K	L	Type
1	-1	3	2	1
3	1	16	4	2
5	6	8	4	1
5	6	10	14	1
5	8	12	14	1
6	5	8	12	1
6	5	10	7	1
6	10	14	12	1
8	5	6	10	1
8	5	12	9	1
8	12	14	10	1
11	6	14	10	1
13	8	14	12	1
14	10	12	15	1
16	3	18	17	1

TABLE 4.135. Improper dihedral angles of building block PHE.

Solute building block: Proline
Name: PRO

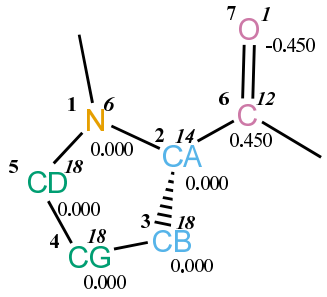

FIGURE 4.55. PRO non-bonded parameters.

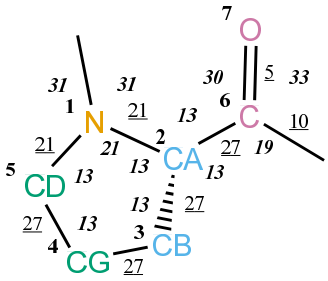

FIGURE 4.56. PRO bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 5
0					1
1	N	6	14	0.00000	2 3 4 5 6
2	CA	14	3	0.00000	3 4 5 6 7 8
3	CB	18	4	0.00000	4 5 6
4	CG	18	4	0.00000	5
5	CD	18	4	0.00000	
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.136. Atoms of building block PRO.

I	J	Type
1	2	21
1	5	21
2	3	27
2	6	27
3	4	27
4	5	27
6	7	5
6	8	10

TABLE 4.137. Bonds of building block PRO.

I	J	K	Type
-1	1	2	31
-1	1	5	31
2	1	5	21
1	2	3	13
1	2	6	13
3	2	6	13
2	3	4	13
3	4	5	13
1	5	4	13
2	6	7	30
2	6	8	19
7	6	8	33

TABLE 4.138. Bond angles of building block PRO.

I	J	K	L	Type
-2	-1	1	2	14
-1	1	2	6	43
-1	1	2	6	44
2	1	5	4	39
1	2	3	4	34
1	2	6	8	42
1	2	6	8	45
2	3	4	5	34
3	4	5	1	34

TABLE 4.139. Dihedral angles of building block PRO.

I	J	K	L	Type
1	-1	2	5	1
2	1	6	3	2
6	2	8	7	1

TABLE 4.140. Improper dihedral angles of building block PRO.

Solute building block: Serine
Name: SER

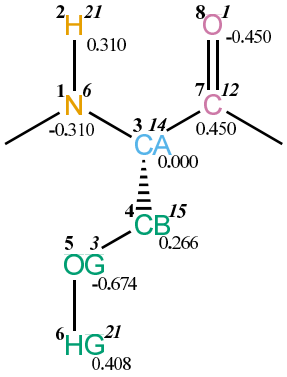

FIGURE 4.57. SER non-bonded parameters.

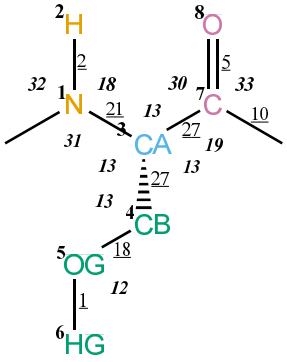

FIGURE 4.58. SER bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 7 8 9
4	CB	15	4	0.26600	5 6 7
5	OG	3	16	-0.67400	6
6	HG	21	1	0.40800	
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.141. Atoms of building block SER.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	18
5	6	1
7	8	5
7	9	10

TABLE 4.142. Bonds of building block SER.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	13
4	5	6	12
3	7	8	30
3	7	9	19
8	7	9	33

TABLE 4.143. Bond angles of building block SER.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	9	42
1	3	7	9	45
3	4	5	6	23

TABLE 4.144. Dihedral angles of building block SER.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
7	3	9	8	1

TABLE 4.145. Improper dihedral angles of building block SER.

Solute building block: Threonine
Name: THR

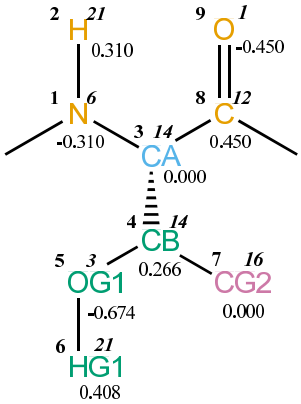

FIGURE 4.59. THR non-bonded parameters.

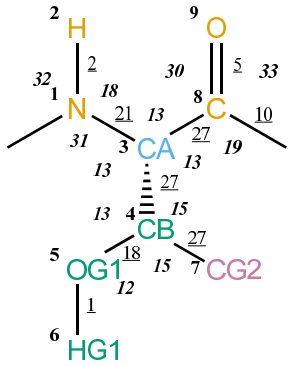

FIGURE 4.60. THR bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 7 8 9 10
4	CB	14	3	0.26600	5 6 7 8
5	OG1	3	16	-0.67400	6 7
6	HG1	21	1	0.40800	
7	CG2	16	5	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.146. Atoms of building block THR.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	18
4	7	27
5	6	1
8	9	5
8	10	10

TABLE 4.147. Bonds of building block THR.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	13
3	4	7	15
5	4	7	15
4	5	6	12
3	8	9	30
3	8	10	19
9	8	10	33

TABLE 4.148. Bond angles of building block THR.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	42
1	3	8	10	45
3	4	5	6	23

TABLE 4.149. Dihedral angles of building block THR.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	5	7	3	2
8	3	10	9	1

TABLE 4.150. Improper dihedral angles of building block THR.

Solute building block: Tryptophan
Name: TRP

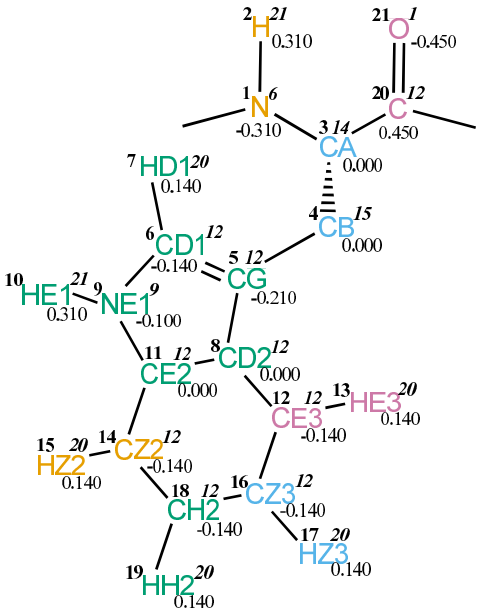

FIGURE 4.61. TRP non-bonded parameters.

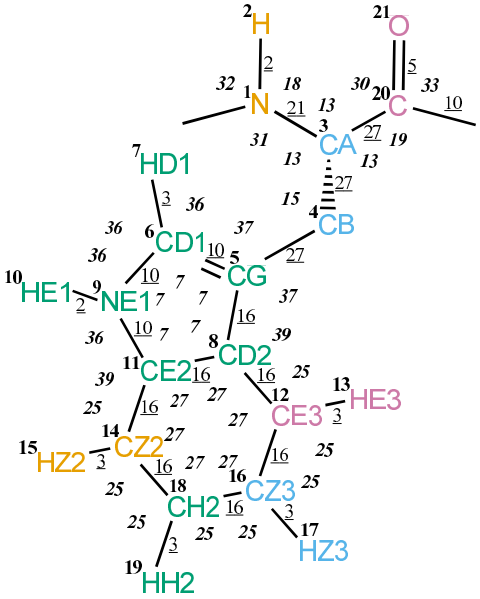

FIGURE 4.62. TRP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 20
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 20 21 22
4	CB	15	4	0.00000	5 6 7 8 9 11 12 20
5	CG	12	12	-0.21000	6 7 8 9 10 11 12 13 14 16
6	CD1	12	12	-0.14000	7 8 9 10 11 12 14
7	HD1	20	1	0.14000	8 9 10 11
8	CD2	12	12	0.00000	9 10 11 12 13 14 15 16 17 18
9	NE1	9	14	-0.10000	10 11 12 14 15 18
10	HE1	21	1	0.31000	11 14
11	CE2	12	12	0.00000	12 13 14 15 16 18 19
12	CE3	12	12	-0.14000	13 14 16 17 18 19
13	HE3	20	1	0.14000	16 17 18
14	CZ2	12	12	-0.14000	15 16 17 18 19
15	HZ2	20	1	0.14000	16 18 19
16	CZ3	12	12	-0.14000	17 18 19
17	HZ3	20	1	0.14000	18 19
18	CH2	12	12	-0.14000	19
19	HH2	20	1	0.14000	
20	C	12	12	0.45000	
21	O	1	16	-0.45000	

TABLE 4.151. Atoms of building block TRP.

I	J	Type
1	2	2
1	3	21
3	4	27
3	20	27
4	5	27
5	6	10
5	8	16
6	7	3
6	9	10
8	11	16
8	12	16
9	10	2
9	11	10
11	14	16
12	13	3
12	16	16
14	15	3
14	18	16
16	17	3
16	18	16
18	19	3
20	21	5
20	22	10

TABLE 4.152. Bonds of building block TRP.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	20	13
4	3	20	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	9	7
7	6	9	36
5	8	11	7
5	8	12	39
11	8	12	27
6	9	10	36
6	9	11	7
10	9	11	36
8	11	9	7
8	11	14	27
9	11	14	39
8	12	13	25
8	12	16	27
13	12	16	25
11	14	15	25
11	14	18	27
15	14	18	25
12	16	17	25
12	16	18	27
17	16	18	25
14	18	16	27
14	18	19	25
16	18	19	25
3	20	21	30
3	20	22	19
21	20	22	33

TABLE 4.153. Bond angles of building block TRP.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	20	43
-1	1	3	20	44
1	3	4	5	34
1	3	20	22	42
1	3	20	22	45
3	4	5	8	40

TABLE 4.154. Dihedral angles of building block TRP.

I	J	K	L	Type
1	-1	3	2	1
3	1	20	4	2
5	6	8	4	1
5	6	9	11	1
5	8	11	9	1
6	5	8	11	1
6	5	9	7	1
6	9	11	8	1
8	5	6	9	1
8	11	12	5	1
8	11	14	18	1
8	12	16	18	1
9	6	11	10	1
11	8	12	16	1
11	8	14	9	1
11	14	18	16	1
12	8	11	14	1
12	8	16	13	1
12	16	18	14	1
14	11	18	15	1
16	12	18	17	1
18	14	16	19	1
20	3	22	21	1

TABLE 4.155. Improper dihedral angles of building block TRP.

Solute building block: Tyrosine
Name: TYR

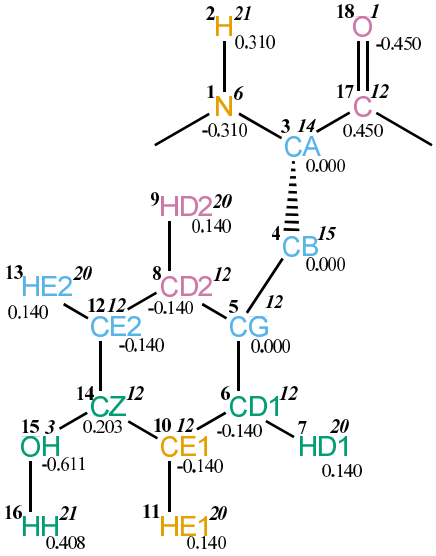

FIGURE 4.63. TYR non-bonded parameters.

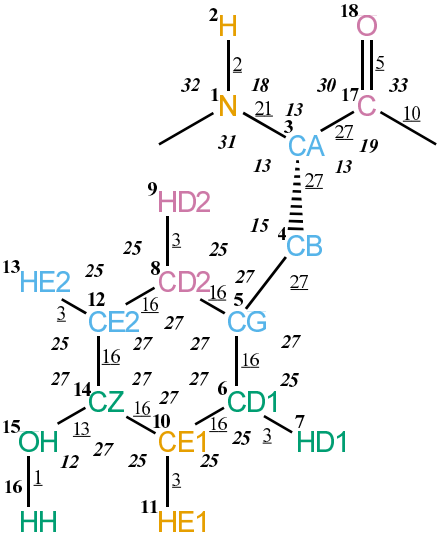

FIGURE 4.64. TYR bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 17
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 17 18 19
4	CB	15	4	0.00000	5 6 7 8 9 10 12 17
5	CG	12	12	0.00000	6 7 8 9 10 11 12 13 14
6	CD1	12	12	-0.14000	7 8 9 10 11 12 14 15
7	HD1	20	1	0.14000	8 10 11 14
8	CD2	12	12	-0.14000	9 10 12 13 14 15
9	HD2	20	1	0.14000	12 13 14
10	CE1	12	12	-0.14000	11 12 13 14 15
11	HE1	20	1	0.14000	12 14 15
12	CE2	12	12	-0.14000	13 14 15
13	HE2	20	1	0.14000	14 15
14	CZ	12	12	0.20300	15 16
15	OH	3	16	-0.61100	16
16	HH	21	1	0.40800	
17	C	12	12	0.45000	
18	O	1	16	-0.45000	

TABLE 4.156. Atoms of building block TYR.

I	J	Type
1	2	2
1	3	21
3	4	27
3	17	27
4	5	27
5	6	16
5	8	16
6	7	3
6	10	16
8	9	3
8	12	16
10	11	3
10	14	16
12	13	3
12	14	16
14	15	13
15	16	1
17	18	5
17	19	10

TABLE 4.157. Bonds of building block TYR.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	17	13
4	3	17	13
3	4	5	15
4	5	6	27
4	5	8	27
6	5	8	27
5	6	7	25
5	6	10	27
7	6	10	25
5	8	9	25
5	8	12	27
9	8	12	25
6	10	11	25
6	10	14	27
11	10	14	25
8	12	13	25
8	12	14	27
13	12	14	25
10	14	12	27
10	14	15	27
12	14	15	27
14	15	16	12
3	17	18	30
3	17	19	19
18	17	19	33

TABLE 4.158. Bond angles of building block TYR.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	17	43
-1	1	3	17	44
1	3	4	5	34
1	3	17	19	42
1	3	17	19	45
3	4	5	6	40
10	14	15	16	11

TABLE 4.159. Dihedral angles of building block TYR.

I	J	K	L	Type
1	-1	3	2	1
3	1	17	4	2
5	6	8	4	1
5	6	10	14	1
5	8	12	14	1
6	5	8	12	1
6	5	10	7	1
6	10	14	12	1
8	5	6	10	1
8	5	12	9	1
8	12	14	10	1
11	6	14	10	1
13	8	14	12	1
14	10	12	15	1
17	3	19	18	1

TABLE 4.160. Improper dihedral angles of building block TYR.

Solute building block: Valine
Name: VAL

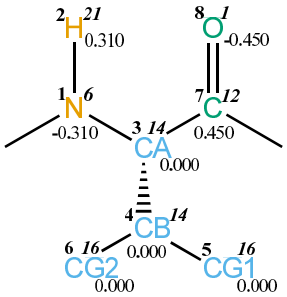

FIGURE 4.65. VAL non-bonded parameters.

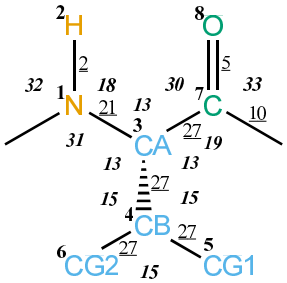

FIGURE 4.66. VAL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7 8 9
4	CB	14	3	0.00000	5 6 7
5	CG1	16	5	0.00000	6
6	CG2	16	5	0.00000	
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.161. Atoms of building block VAL.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	27
4	6	27
7	8	5
7	9	10

TABLE 4.162. Bonds of building block VAL.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	15
3	4	6	15
5	4	6	15
3	7	8	30
3	7	9	19
8	7	9	33

TABLE 4.163. Bond angles of building block VAL.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	9	42
1	3	7	9	45

TABLE 4.164. Dihedral angles of building block VAL.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
3	5	6	4	2
7	3	9	8	1

TABLE 4.165. Improper dihedral angles of building block VAL.

Solute building block: D-ALanine
Name: DALA

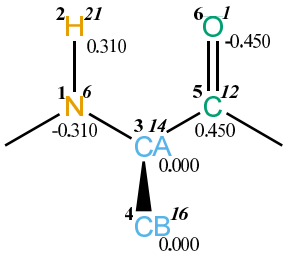

FIGURE 4.67. DALA non-bonded parameters.

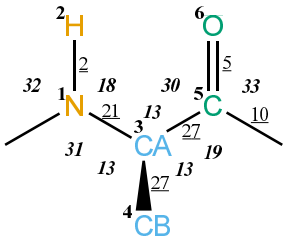

FIGURE 4.68. DALA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 5
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7
4	CB	16	5	0.00000	5
5	C	12	12	0.45000	
6	O	1	16	-0.45000	

TABLE 4.166. Atoms of building block DALA.

I	J	Type
1	2	2
1	3	21
3	4	27
3	5	27
5	6	5
5	7	10

TABLE 4.167. Bonds of building block DALA.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	5	13
4	3	5	13
3	5	6	30
3	5	7	19
6	5	7	33

TABLE 4.168. Bond angles of building block DALA.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	5	43
-1	1	3	5	44
1	3	5	7	42
1	3	5	7	45

TABLE 4.169. Dihedral angles of building block DALA.

I	J	K	L	Type
1	-1	3	2	1
4	1	5	3	2
5	3	7	6	1

TABLE 4.170. Improper dihedral angles of building block DALA.

Solute building block: L-2-amino-butanoic acid
Name: ABU

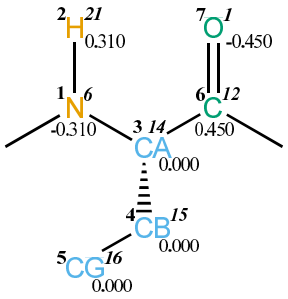

FIGURE 4.69. ABU non-bonded parameters.

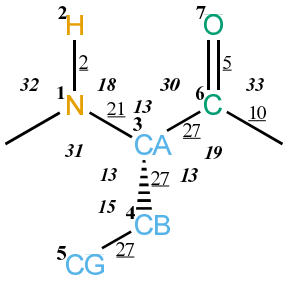

FIGURE 4.70. ABU bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 6
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7 8
4	CB	15	4	0.00000	5 6
5	CG	16	5	0.00000	
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.171. Atoms of building block ABU.

I	J	Type
1	2	2
1	3	21
3	4	27
3	6	27
4	5	27
6	7	5
6	8	10

TABLE 4.172. Bonds of building block ABU.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	6	13
4	3	6	13
3	4	5	15
3	6	7	30
3	6	8	19
7	6	8	33

TABLE 4.173. Bond angles of building block ABU.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	6	43
-1	1	3	6	44
1	3	4	5	34
1	3	6	8	42
1	3	6	8	45

TABLE 4.174. Dihedral angles of building block ABU.

I	J	K	L	Type
1	-1	3	2	1
3	1	6	4	2
6	3	8	7	1

TABLE 4.175. Improper dihedral angles of building block ABU.

Solute building block: 2-aminoisobutyric acid
Name: AIB

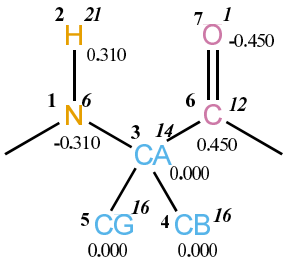

FIGURE 4.71. AIB non-bonded parameters.

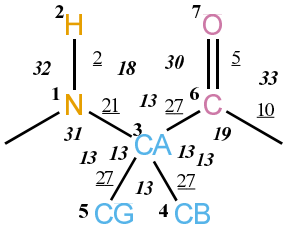

FIGURE 4.72. AIB bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 5 6
2	H	21	1	0.31000	3
3	CA	14	3	0.00000	4 5 6 7 8
4	CB	16	5	0.00000	5 6
5	CG	16	5	0.00000	6
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.176. Atoms of building block AIB.

I	J	Type
1	2	2
1	3	21
3	4	27
3	5	27
3	6	27
6	7	5
6	8	10

TABLE 4.177. Bonds of building block AIB.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	5	13
1	3	6	13
4	3	5	13
4	3	6	13
5	3	6	13
3	6	7	30
3	6	8	19
7	6	8	33

TABLE 4.178. Bond angles of building block AIB.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	6	43
-1	1	3	6	44
1	3	6	8	42
1	3	6	8	45

TABLE 4.179. Dihedral angles of building block AIB.

I	J	K	L	Type
1	-1	3	2	1
6	3	8	7	1

TABLE 4.180. Improper dihedral angles of building block AIB.

Solute building block: (4R)-4-[(E)-2-butanyl]-4, N-dimethyl-L-threonine
Name: MEBMT

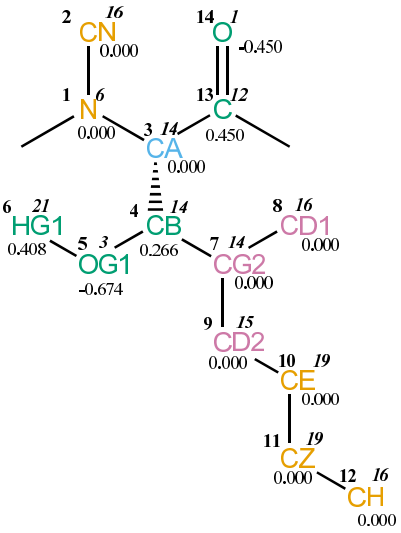

FIGURE 4.73. MEBMT non-bonded parameters.

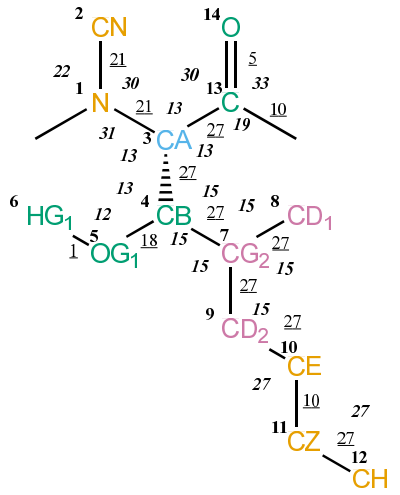

FIGURE 4.74. MEBMT bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	0.00000	2 3 4 13
2	CN	16	5	0.00000	3
3	CA	14	3	0.00000	4 5 7 13 14 15
4	CB	14	3	0.26600	5 6 7 8 9 13
5	OG1	3	16	-0.67400	6 7
6	HG1	21	1	0.40800	
7	CG2	14	3	0.00000	8 9 10
8	CD1	16	5	0.00000	9
9	CD2	15	4	0.00000	10 11
10	CE	19	3	0.00000	11 12
11	CZ	19	3	0.00000	12
12	CH	16	5	0.00000	
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.181. Atoms of building block MEBMT.

I	J	Type
1	2	21
1	3	21
3	4	27
3	13	27
4	5	18
4	7	27
5	6	1
7	8	27
7	9	27
9	10	27
10	11	10
11	12	27
13	14	5
13	15	10

TABLE 4.182. Bonds of building block MEBMT.

I	J	K	Type
-1	1	2	22
-1	1	3	31
2	1	3	30
1	3	4	13
1	3	13	13
4	3	13	13
3	4	5	13
3	4	7	15
5	4	7	15
4	5	6	12
4	7	8	15
4	7	9	15
8	7	9	15
7	9	10	15
9	10	11	27
10	11	12	27
3	13	14	30
3	13	15	19
14	13	15	33

TABLE 4.183. Bond angles of building block MEBMT.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	13	43
-1	1	3	13	44
1	3	4	7	34
1	3	13	15	42
1	3	13	15	45
3	4	5	6	23
3	4	7	9	34
4	7	9	10	34
7	9	10	11	40
9	10	11	12	14

TABLE 4.184. Dihedral angles of building block MEBMT.

I	J	K	L	Type
1	-1	3	2	1
3	1	13	4	2
4	5	7	3	2
7	8	9	4	2
13	3	15	14	1

TABLE 4.185. Improper dihedral angles of building block MEBMT.

Solute building block: N-methyl-L-leucine
Name: MELEU

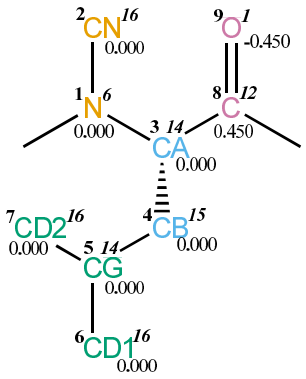

FIGURE 4.75. MELEU non-bonded parameters.

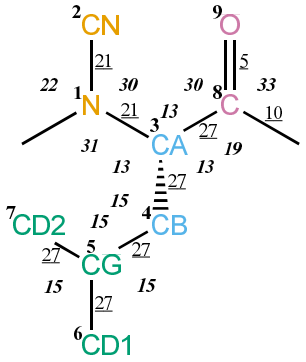

FIGURE 4.76. MELEU bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	0.00000	2 3 4 8
2	CN	16	5	0.00000	3
3	CA	14	3	0.00000	4 5 8 9 10
4	CB	15	4	0.00000	5 6 7 8
5	CG	14	3	0.00000	6 7
6	CD1	16	5	0.00000	7
7	CD2	16	5	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.186. Atoms of building block MELEU.

I	J	Type
1	2	21
1	3	21
3	4	27
3	8	27
4	5	27
5	6	27
5	7	27
8	9	5
8	10	10

TABLE 4.187. Bonds of building block MELEU.

I	J	K	Type
-1	1	2	22
-1	1	3	31
2	1	3	30
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	15
4	5	7	15
6	5	7	15
3	8	9	30
3	8	10	19
9	8	10	33

TABLE 4.188. Bond angles of building block MELEU.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	42
1	3	8	10	45
3	4	5	6	34

TABLE 4.189. Dihedral angles of building block MELEU.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	6	7	5	2
8	3	10	9	1

TABLE 4.190. Improper dihedral angles of building block MELEU.

Solute building block: N-methyl-L-valine
Name: MEVAL

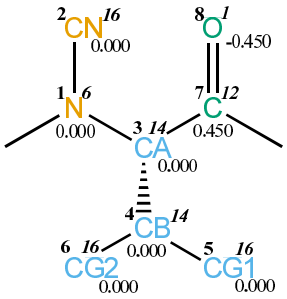

FIGURE 4.77. MEVAL non-bonded parameters.

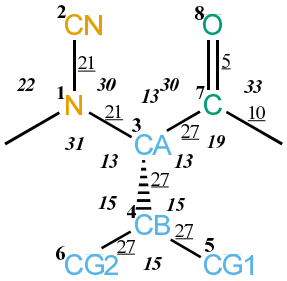

FIGURE 4.78. MEVAL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	0.00000	2 3 4 7
2	CN	16	5	0.00000	3
3	CA	14	3	0.00000	4 5 6 7 8 9
4	CB	14	3	0.00000	5 6 7
5	CG1	16	5	0.00000	6
6	CG2	16	5	0.00000	
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.191. Atoms of building block MEVAL.

I	J	Type
1	2	21
1	3	21
3	4	27
3	7	27
4	5	27
4	6	27
7	8	5
7	9	10

TABLE 4.192. Bonds of building block MEVAL.

I	J	K	Type
-1	1	2	22
-1	1	3	31
2	1	3	30
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	15
3	4	6	15
5	4	6	15
3	7	8	30
3	7	9	19
8	7	9	33

TABLE 4.193. Bond angles of building block MEVAL.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	9	42
1	3	7	9	45

TABLE 4.194. Dihedral angles of building block MEVAL.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
3	5	6	4	2
7	3	9	8	1

TABLE 4.195. Improper dihedral angles of building block MEVAL.

Solute building block: Sarcosine or N-methylglycine
Name: SAR

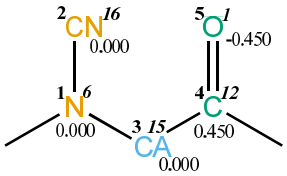

FIGURE 4.79. SAR non-bonded parameters.

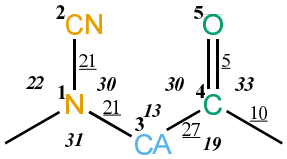

FIGURE 4.80. SAR bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	0.00000	2 3 4
2	CN	16	5	0.00000	3
3	CA	15	4	0.00000	4 5 6
4	C	12	12	0.45000	
5	O	1	16	-0.45000	

TABLE 4.196. Atoms of building block SAR.

I	J	Type
1	2	21
1	3	21
3	4	27
4	5	5
4	6	10

TABLE 4.197. Bonds of building block SAR.

I	J	K	Type
-1	1	2	22
-1	1	3	31
2	1	3	30
1	3	4	13
3	4	5	30
3	4	6	19
5	4	6	33

TABLE 4.198. Bond angles of building block SAR.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	6	42
1	3	4	6	45

TABLE 4.199. Dihedral angles of building block SAR.

I	J	K	L	Type
1	-1	3	2	1
4	3	6	5	1

TABLE 4.200. Improper dihedral angles of building block SAR.

4.4. β-amino acids

Solute building block: (R)-β^2-Phenylalanine
Name: RAF

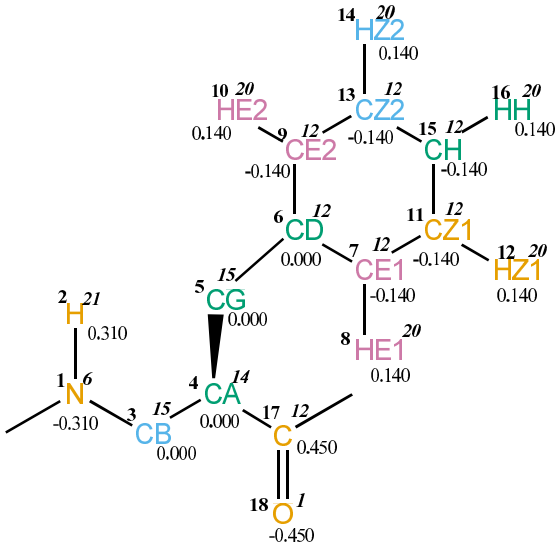

FIGURE 4.81. RAF non-bonded parameters.

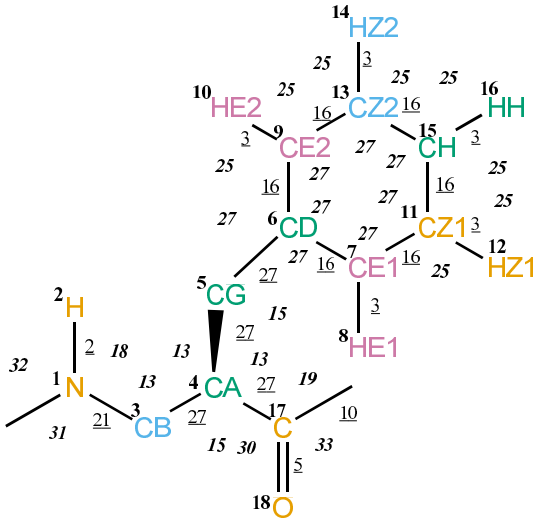

FIGURE 4.82. RAF bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 17
4	CA	14	3	0.00000	5 6 17 18 19
5	CG	15	4	0.00000	6 7 8 9 10 11 13 17
6	CD	12	12	0.00000	7 8 9 10 11 12 13 14 15
7	CE1	12	12	-0.14000	8 9 10 11 12 13 15 16
8	HE1	20	1	0.14000	9 11 12 15
9	CE2	12	12	-0.14000	10 11 13 14 15 16
10	HE2	20	1	0.14000	13 14 15
11	CZ1	12	12	-0.14000	12 13 14 15 16
12	HZ1	20	1	0.14000	13 15 16
13	CZ2	12	12	-0.14000	14 15 16
14	HZ2	20	1	0.14000	15 16
15	CH	12	12	-0.14000	16
16	HH	20	1	0.14000	
17	C	12	12	0.45000	
18	O	1	16	-0.45000	

TABLE 4.201. Atoms of building block RAF.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	17	27
5	6	27
6	7	16
6	9	16
7	8	3
7	11	16
9	10	3
9	13	16
11	12	3
11	15	16
13	14	3
13	15	16
15	16	3
17	18	5
17	19	10

TABLE 4.202. Bonds of building block RAF.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	13
3	4	17	15
5	4	17	13
4	5	6	15
5	6	7	27
5	6	9	27
7	6	9	27
6	7	8	25
6	7	11	27
8	7	11	25
6	9	10	25
6	9	13	27
10	9	13	25
7	11	12	25
7	11	15	27
12	11	15	25
9	13	14	25
9	13	15	27
14	13	15	25
11	15	13	27
11	15	16	25
13	15	16	25
4	17	18	30
4	17	19	19
18	17	19	33

TABLE 4.203. Bond angles of building block RAF.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	17	34
3	4	5	6	34
3	4	17	19	42
3	4	17	19	45
4	5	6	7	40

TABLE 4.204. Dihedral angles of building block RAF.

I	J	K	L	Type
1	-1	3	2	1
4	3	17	5	2
6	7	9	5	1
6	7	11	15	1
6	9	13	15	1
7	6	9	13	1
7	6	11	8	1
7	11	15	13	1
9	6	7	11	1
9	6	13	10	1
9	13	15	11	1
12	7	15	11	1
14	9	15	13	1
15	11	13	16	1
17	4	19	18	1

TABLE 4.205. Improper dihedral angles of building block RAF.

Solute building block: (R)-β^2-Valine
Name: RAV

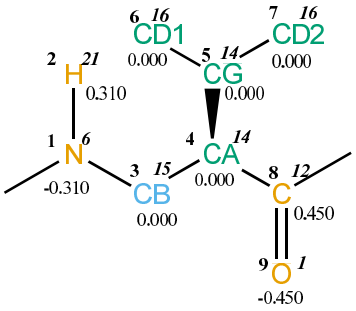

FIGURE 4.83. RAV non-bonded parameters.

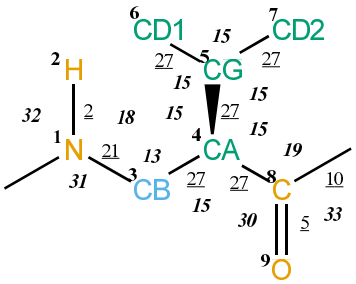

FIGURE 4.84. RAV bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 8
4	CA	14	3	0.00000	5 6 7 8 9 10
5	CG	14	3	0.00000	6 7 8
6	CD1	16	5	0.00000	7
7	CD2	16	5	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.206. Atoms of building block RAV.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	8	27
5	6	27
5	7	27
8	9	5
8	10	10

TABLE 4.207. Bonds of building block RAV.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
3	4	8	15
5	4	8	15
4	5	6	15
4	5	7	15
6	5	7	15
4	8	9	30
4	8	10	19
9	8	10	33

TABLE 4.208. Bond angles of building block RAV.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	8	34
3	4	5	6	34
3	4	8	10	42
3	4	8	10	45

TABLE 4.209. Dihedral angles of building block RAV.

I	J	K	L	Type
1	-1	3	2	1
4	3	8	5	2
4	6	7	5	2
8	4	10	9	1

TABLE 4.210. Improper dihedral angles of building block RAV.

Solute building block: (R)-β^3-Cysteine (protonated; neutral)
Name: RBCH

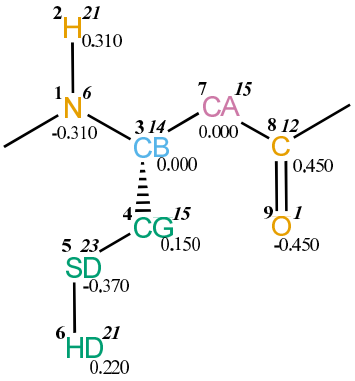

FIGURE 4.85. RBCH non-bonded parameters.

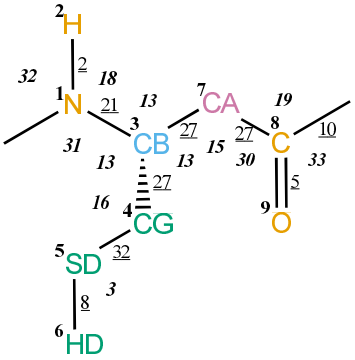

FIGURE 4.86. RBCH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 7 8
4	CG	15	4	0.15000	5 6 7
5	SD	23	32	-0.37000	6
6	HD	21	1	0.22000	
7	CA	15	4	0.00000	8 9 10
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.211. Atoms of building block RBCH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	32
5	6	8
7	8	27
8	9	5
8	10	10

TABLE 4.212. Bonds of building block RBCH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	16
4	5	6	3
3	7	8	15
7	8	9	30
7	8	10	19
9	8	10	33

TABLE 4.213. Bond angles of building block RBCH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	8	34
3	4	5	6	26
3	7	8	10	42
3	7	8	10	45

TABLE 4.214. Dihedral angles of building block RBCH.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
8	7	10	9	1

TABLE 4.215. Improper dihedral angles of building block RBCH.

Solute building block: (R)-β^3-Isoleucine
Name: RBI

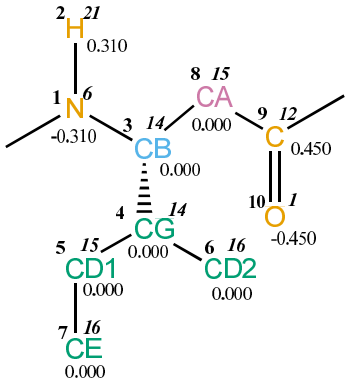

FIGURE 4.87. RBI non-bonded parameters.

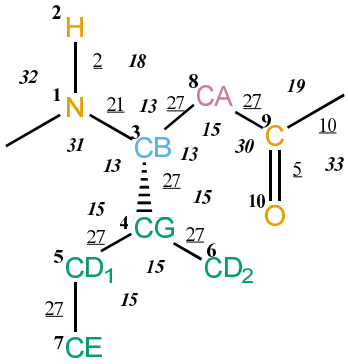

FIGURE 4.88. RBI bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 8 9
4	CG	14	3	0.00000	5 6 7 8
5	CD1	15	4	0.00000	6 7
6	CD2	16	5	0.00000	
7	CE	16	5	0.00000	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.216. Atoms of building block RBI.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
4	6	27
5	7	27
8	9	27
9	10	5
9	11	10

TABLE 4.217. Bonds of building block RBI.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
3	4	6	15
5	4	6	15
4	5	7	15
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.218. Bond angles of building block RBI.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	7	34
3	8	9	11	42
3	8	9	11	45

TABLE 4.219. Dihedral angles of building block RBI.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	5	6	3	2
9	8	11	10	1

TABLE 4.220. Improper dihedral angles of building block RBI.

Solute building block: (R)-β^3-Lysine (protonated; charge $+e$)
Name: RBKH

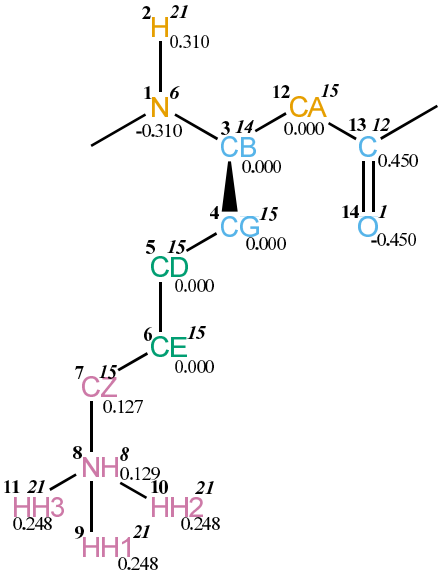

FIGURE 4.89. RBKH non-bonded parameters.

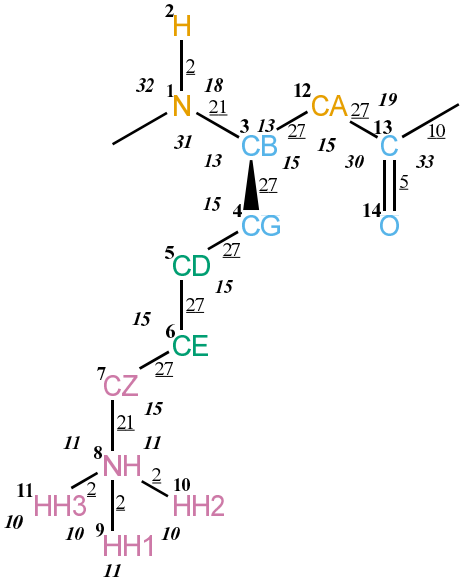

FIGURE 4.90. RBKH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 12
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 12 13
4	CG	15	4	0.00000	5 6 12
5	CD	15	4	0.00000	6 7
6	CE	15	4	0.00000	7 8
7	CZ	15	4	0.12700	8 9 10 11
8	NH	8	14	0.12900	9 10 11
9	HH1	21	1	0.24800	10 11
10	HH2	21	1	0.24800	11
11	HH3	21	1	0.24800	
12	CA	15	4	0.00000	13 14 15
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.221. Atoms of building block RBKH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	12	27
4	5	27
5	6	27
6	7	27
7	8	21
8	9	2
8	10	2
8	11	2
12	13	27
13	14	5
13	15	10

TABLE 4.222. Bonds of building block RBKH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	12	13
4	3	12	15
3	4	5	15
4	5	6	15
5	6	7	15
6	7	8	15
7	8	9	11
7	8	10	11
7	8	11	11
9	8	10	10
9	8	11	10
10	8	11	10
3	12	13	15
12	13	14	30
12	13	15	19
14	13	15	33

TABLE 4.223. Bond angles of building block RBKH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	12	43
-1	1	3	12	44
1	3	4	5	34
1	3	12	13	34
3	4	5	6	34
4	5	6	7	34
5	6	7	8	34
6	7	8	9	29
3	12	13	15	42
3	12	13	15	45

TABLE 4.224. Dihedral angles of building block RBKH.

I	J	K	L	Type
1	-1	3	2	1
4	1	12	3	2
13	12	15	14	1

TABLE 4.225. Improper dihedral angles of building block RBKH.

Solute building block: (R)-β^3-Methionine
Name: RBM

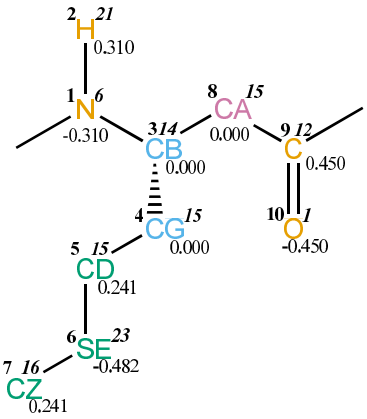

FIGURE 4.91. RBM non-bonded parameters.

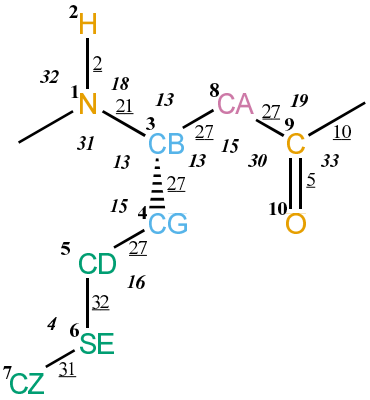

FIGURE 4.92. RBM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 8 9
4	CG	15	4	0.00000	5 6 8
5	CD	15	4	0.24100	6 7
6	SE	23	32	-0.48200	7
7	CZ	16	5	0.24100	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.226. Atoms of building block RBM.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	32
6	7	31
8	9	27
9	10	5
9	11	10

TABLE 4.227. Bonds of building block RBM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	16
5	6	7	4
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.228. Bond angles of building block RBM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	6	34
4	5	6	7	26
3	8	9	11	42
3	8	9	11	45

TABLE 4.229. Dihedral angles of building block RBM.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
9	8	11	10	1

TABLE 4.230. Improper dihedral angles of building block RBM.

Solute building block: (R)-β^3-Asparagine
Name: RBN

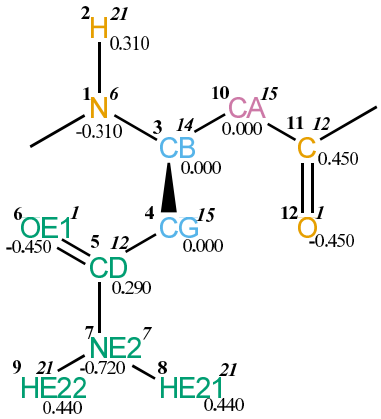

FIGURE 4.93. RBN non-bonded parameters.

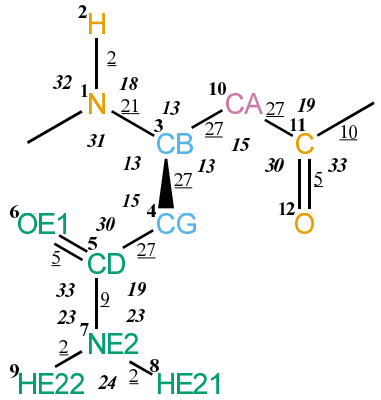

FIGURE 4.94. RBN bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 10
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 10 11
4	CG	15	4	0.00000	5 6 7 10
5	CD	12	12	0.29000	6 7 8 9
6	OE1	1	16	-0.45000	7
7	NE2	7	14	-0.72000	8 9
8	HE21	21	1	0.44000	9
9	HE22	21	1	0.44000	
10	CA	15	4	0.00000	11 12 13
11	C	12	12	0.45000	
12	O	1	16	-0.45000	

TABLE 4.231. Atoms of building block RBN.

I	J	Type
1	2	2
1	3	21
3	4	27
3	10	27
4	5	27
5	6	5
5	7	9
7	8	2
7	9	2
10	11	27
11	12	5
11	13	10

TABLE 4.232. Bonds of building block RBN.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	10	13
4	3	10	13
3	4	5	15
4	5	6	30
4	5	7	19
6	5	7	33
5	7	8	23
5	7	9	23
8	7	9	24
3	10	11	15
10	11	12	30
10	11	13	19
12	11	13	33

TABLE 4.233. Bond angles of building block RBN.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	10	43
-1	1	3	10	44
1	3	4	5	34
1	3	10	11	34
3	4	5	7	40
4	5	7	8	14
3	10	11	13	42
3	10	11	13	45

TABLE 4.234. Dihedral angles of building block RBN.

I	J	K	L	Type
1	-1	3	2	1
4	1	10	3	2
5	6	7	4	1
7	8	9	5	1
11	10	13	12	1

TABLE 4.235. Improper dihedral angles of building block RBN.

Solute building block: (R)-β^3-Serine
Name: RBS

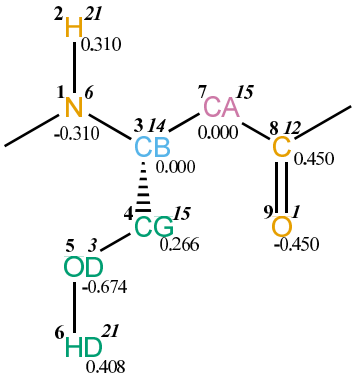

FIGURE 4.95. RBS non-bonded parameters.

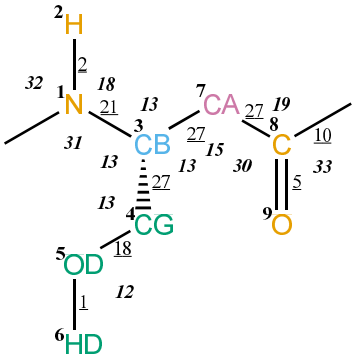

FIGURE 4.96. RBS bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 7 8
4	CG	15	4	0.26600	5 6 7
5	OD	3	16	-0.67400	6
6	HD	21	1	0.40800	
7	CA	15	4	0.00000	8 9 10
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.236. Atoms of building block RBS.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	18
5	6	1
7	8	27
8	9	5
8	10	10

TABLE 4.237. Bonds of building block RBS.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	13
4	5	6	12
3	7	8	15
7	8	9	30
7	8	10	19
9	8	10	33

TABLE 4.238. Bond angles of building block RBS.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	8	34
3	4	5	6	23
3	7	8	10	42
3	7	8	10	45

TABLE 4.239. Dihedral angles of building block RBS.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
8	7	10	9	1

TABLE 4.240. Improper dihedral angles of building block RBS.

Solute building block: (R)-β^3-Serine(propylated)
Name: RBSP

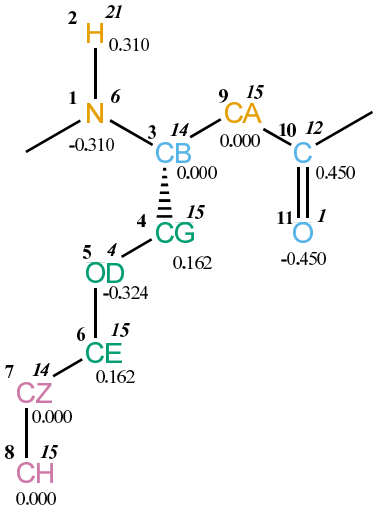

FIGURE 4.97. RBSP non-bonded parameters.

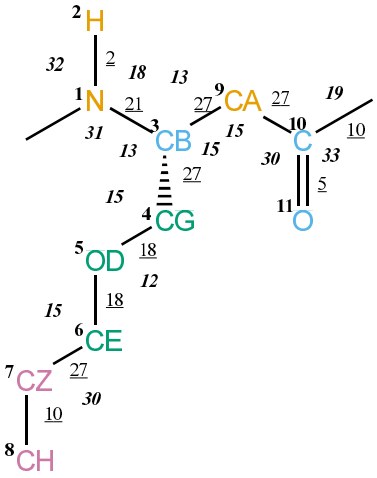

FIGURE 4.98. RBSP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 9
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 9 10
4	CG	15	4	0.16200	5 6 9
5	OD	4	16	-0.32400	6 7
6	CE	15	4	0.16200	7 8
7	CZ	14	3	0.00000	8
8	CH	15	4	0.00000	
9	CA	15	4	0.00000	10 11 12
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.241. Atoms of building block RBSP.

I	J	Type
1	2	2
1	3	21
3	4	27
3	9	27
4	5	18
5	6	18
6	7	27
7	8	10
9	10	27
10	11	5
10	12	10

TABLE 4.242. Bonds of building block RBSP.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	9	13
4	3	9	15
3	4	5	15
4	5	6	12
5	6	7	15
6	7	8	30
3	9	10	15
9	10	11	30
9	10	12	19
11	10	12	33

TABLE 4.243. Bond angles of building block RBSP.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	9	43
-1	1	3	9	44
1	3	4	5	34
1	3	9	10	34
3	4	5	6	23
4	5	6	7	23
5	6	7	8	40
3	9	10	12	42
3	9	10	12	45

TABLE 4.244. Dihedral angles of building block RBSP.

I	J	K	L	Type
1	-1	3	2	1
3	1	9	4	2
10	9	12	11	1

TABLE 4.245. Improper dihedral angles of building block RBSP.

Solute building block: (R)-β^3-Threonine
Name: RBT

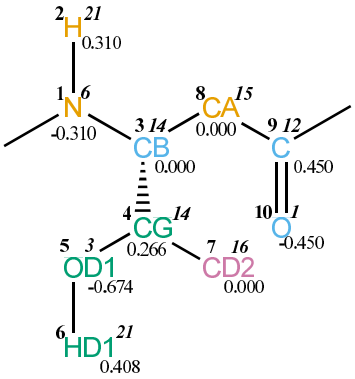

FIGURE 4.99. RBT non-bonded parameters.

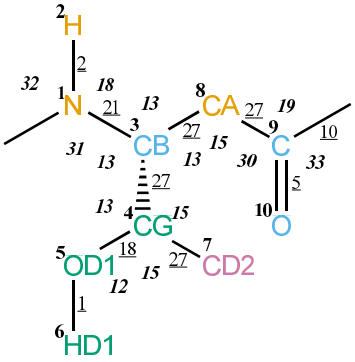

FIGURE 4.100. RBT bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 7 8 9
4	CG	14	3	0.26600	5 6 7 8
5	OD1	3	16	-0.67400	6 7
6	HD1	21	1	0.40800	
7	CD2	16	5	0.00000	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.246. Atoms of building block RBT.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	18
4	7	27
5	6	1
8	9	27
9	10	5
9	11	10

TABLE 4.247. Bonds of building block RBT.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	13
3	4	7	15
5	4	7	15
4	5	6	12
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.248. Bond angles of building block RBT.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	6	23
3	8	9	11	42
3	8	9	11	45

TABLE 4.249. Dihedral angles of building block RBT.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	5	7	3	2
9	8	11	10	1

TABLE 4.250. Improper dihedral angles of building block RBT.

Solute building block: (R)-β^3-Valine
Name: RBV

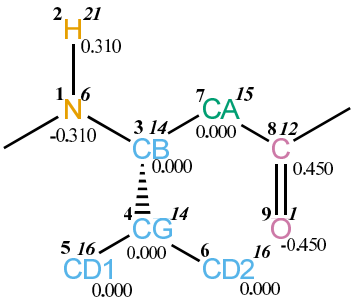

FIGURE 4.101. RBV non-bonded parameters.

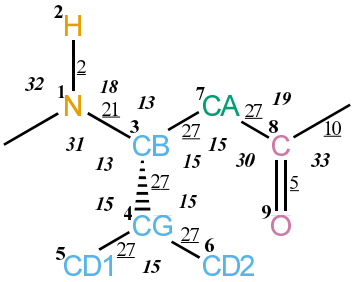

FIGURE 4.102. RBV bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 7 8
4	CG	14	3	0.00000	5 6 7
5	CD1	16	5	0.00000	6
6	CD2	16	5	0.00000	
7	CA	15	4	0.00000	8 9 10
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.251. Atoms of building block RBV.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	27
4	6	27
7	8	27
8	9	5
8	10	10

TABLE 4.252. Bonds of building block RBV.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	15
3	4	5	15
3	4	6	15
5	4	6	15
3	7	8	15
7	8	9	30
7	8	10	19
9	8	10	33

TABLE 4.253. Bond angles of building block RBV.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	8	34
3	7	8	10	42
3	7	8	10	45

TABLE 4.254. Dihedral angles of building block RBV.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
3	5	6	4	2
8	7	10	9	1

TABLE 4.255. Improper dihedral angles of building block RBV.

Solute building block: (S)-β^2-Alanine
Name: SAA

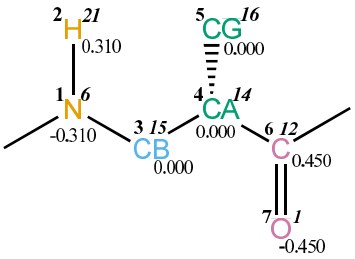

FIGURE 4.103. SAA non-bonded parameters.

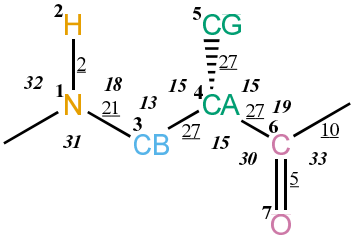

FIGURE 4.104. SAA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 6
4	CA	14	3	0.00000	5 6 7 8
5	CG	16	5	0.00000	6
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.256. Atoms of building block SAA.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	6	27
6	7	5
6	8	10

TABLE 4.257. Bonds of building block SAA.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
3	4	6	15
5	4	6	15
4	6	7	30
4	6	8	19
7	6	8	33

TABLE 4.258. Bond angles of building block SAA.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	6	34
3	4	6	8	42
3	4	6	8	45

TABLE 4.259. Dihedral angles of building block SAA.

I	J	K	L	Type
1	-1	3	2	1
5	3	6	4	2
6	4	8	7	1

TABLE 4.260. Improper dihedral angles of building block SAA.

Solute building block: (S)-β^2-Phenylalanine
Name: SAF

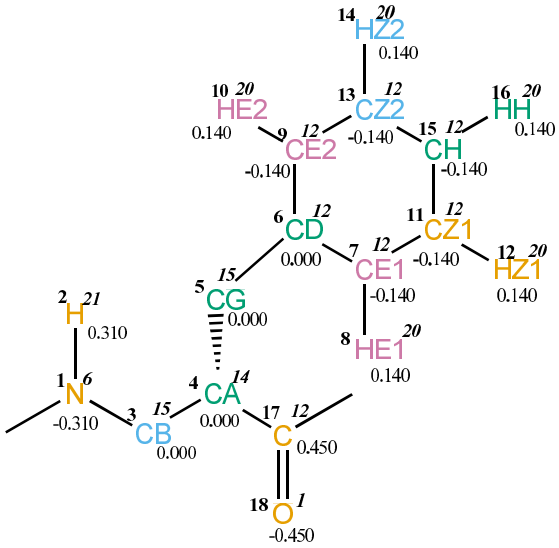

FIGURE 4.105. SAF non-bonded parameters.

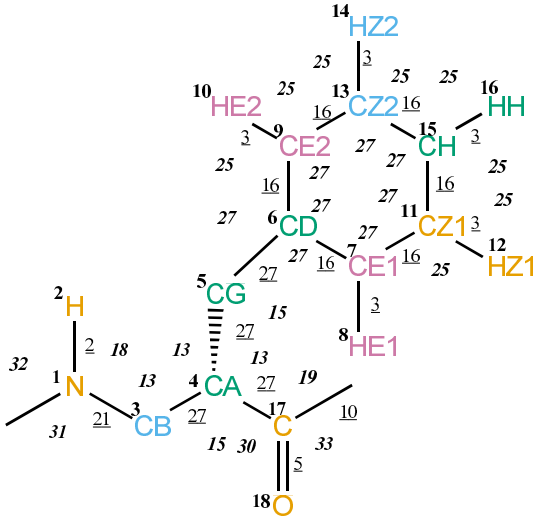

FIGURE 4.106. SAF bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 17
4	CA	14	3	0.00000	5 6 17 18 19
5	CG	15	4	0.00000	6 7 8 9 10 11 13 17
6	CD	12	12	0.00000	7 8 9 10 11 12 13 14 15
7	CE1	12	12	-0.14000	8 9 10 11 12 13 15 16
8	HE1	20	1	0.14000	9 11 12 15
9	CE2	12	12	-0.14000	10 11 13 14 15 16
10	HE2	20	1	0.14000	13 14 15
11	CZ1	12	12	-0.14000	12 13 14 15 16
12	HZ1	20	1	0.14000	13 15 16
13	CZ2	12	12	-0.14000	14 15 16
14	HZ2	20	1	0.14000	15 16
15	CH	12	12	-0.14000	16
16	HH	20	1	0.14000	
17	C	12	12	0.45000	
18	O	1	16	-0.45000	

TABLE 4.261. Atoms of building block SAF.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	17	27
5	6	27
6	7	16
6	9	16
7	8	3
7	11	16
9	10	3
9	13	16
11	12	3
11	15	16
13	14	3
13	15	16
15	16	3
17	18	5
17	19	10

TABLE 4.262. Bonds of building block SAF.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	13
3	4	17	15
5	4	17	13
4	5	6	15
5	6	7	27
5	6	9	27
7	6	9	27
6	7	8	25
6	7	11	27
8	7	11	25
6	9	10	25
6	9	13	27
10	9	13	25
7	11	12	25
7	11	15	27
12	11	15	25
9	13	14	25
9	13	15	27
14	13	15	25
11	15	13	27
11	15	16	25
13	15	16	25
4	17	18	30
4	17	19	19
18	17	19	33

TABLE 4.263. Bond angles of building block SAF.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	17	34
3	4	5	6	34
3	4	17	19	42
3	4	17	19	45
4	5	6	7	40

TABLE 4.264. Dihedral angles of building block SAF.

I	J	K	L	Type
1	-1	3	2	1
5	3	17	4	2
6	7	9	5	1
6	7	11	15	1
6	9	13	15	1
7	6	9	13	1
7	6	11	8	1
7	11	15	13	1
9	6	7	11	1
9	6	13	10	1
9	13	15	11	1
12	7	15	11	1
14	9	15	13	1
15	11	13	16	1
17	4	19	18	1

TABLE 4.265. Improper dihedral angles of building block SAF.

Solute building block: (S)-β^2-Phenylalanine(Cα fluorinated)
Name: SAFF

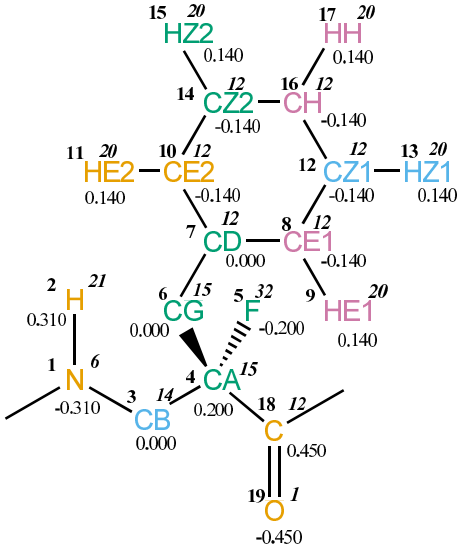

FIGURE 4.107. SAFF non-bonded parameters.

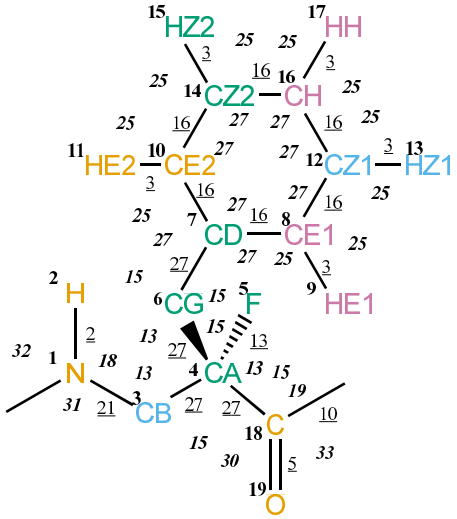

FIGURE 4.108. SAFF bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 18
4	CA	15	4	0.20000	5 6 7 18 19 20
5	F	32	19	-0.20000	6 18 19 20
6	CG	15	4	0.00000	7 8 9 10 11 12 14 18
7	CD	12	12	0.00000	8 9 10 11 12 13 14 15 16
8	CE1	12	12	-0.14000	9 10 11 12 13 14 16 17
9	HE1	20	1	0.14000	10 12 13 16
10	CE2	12	12	-0.14000	11 12 14 15 16 17
11	HE2	20	1	0.14000	14 15 16
12	CZ1	12	12	-0.14000	13 14 15 16 17
13	HZ1	20	1	0.14000	14 16 17
14	CZ2	12	12	-0.14000	15 16 17
15	HZ2	20	1	0.14000	16 17
16	CH	12	12	-0.14000	17
17	HH	20	1	0.14000	
18	C	12	12	0.45000	
19	O	1	16	-0.45000	

TABLE 4.266. Atoms of building block SAFF.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	13
4	6	27
4	18	27
6	7	27
7	8	16
7	10	16
8	9	3
8	12	16
10	11	3
10	14	16
12	13	3
12	16	16
14	15	3
14	16	16
16	17	3
18	19	5
18	20	10

TABLE 4.267. Bonds of building block SAFF.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
3	4	6	13
3	4	18	15
5	4	6	15
5	4	18	15
6	4	18	13
4	6	7	15
6	7	8	27
6	7	10	27
8	7	10	27
7	8	9	25
7	8	12	27
9	8	12	25
7	10	11	25
7	10	14	27
11	10	14	25
8	12	13	25
8	12	16	27
13	12	16	25
10	14	15	25
10	14	16	27
15	14	16	25
12	16	14	27
12	16	17	25
14	16	17	25
4	18	19	30
4	18	20	19
19	18	20	33

TABLE 4.268. Bond angles of building block SAFF.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	18	34
3	4	6	7	34
3	4	18	20	42
3	4	18	20	45
4	6	7	8	40

TABLE 4.269. Dihedral angles of building block SAFF.

I	J	K	L	Type
1	-1	3	2	1
4	3	18	6	2
7	8	10	6	1
7	8	12	16	1
7	10	14	16	1
8	7	10	14	1
8	7	12	9	1
8	12	16	14	1
10	7	8	12	1
10	7	14	11	1
10	14	16	12	1
13	8	16	12	1
15	10	16	14	1
16	12	14	17	1
18	4	20	19	1

TABLE 4.270. Improper dihedral angles of building block SAFF.

Solute building block: (S)-β^2-Leucine
Name: SAL

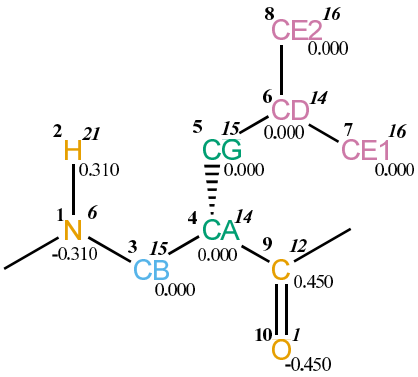

FIGURE 4.109. SAL non-bonded parameters.

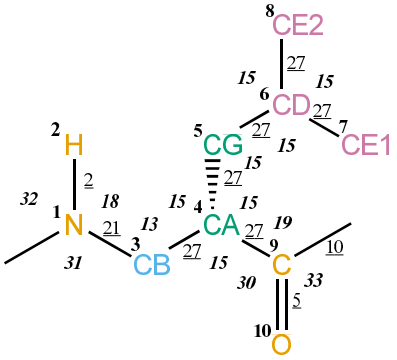

FIGURE 4.110. SAL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 9
4	CA	14	3	0.00000	5 6 9 10 11
5	CG	15	4	0.00000	6 7 8 9
6	CD	14	3	0.00000	7 8
7	CE1	16	5	0.00000	8
8	CE2	16	5	0.00000	
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.271. Atoms of building block SAL.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	9	27
5	6	27
6	7	27
6	8	27
9	10	5
9	11	10

TABLE 4.272. Bonds of building block SAL.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
3	4	9	15
5	4	9	15
4	5	6	15
5	6	7	15
5	6	8	15
7	6	8	15
4	9	10	30
4	9	11	19
10	9	11	33

TABLE 4.273. Bond angles of building block SAL.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	9	34
3	4	5	6	34
3	4	9	11	42
3	4	9	11	45
4	5	6	7	34

TABLE 4.274. Dihedral angles of building block SAL.

I	J	K	L	Type
1	-1	3	2	1
5	3	9	4	2
5	7	8	6	2
9	4	11	10	1

TABLE 4.275. Improper dihedral angles of building block SAL.

Solute building block: (S)-β^2-Methionine
Name: SAM

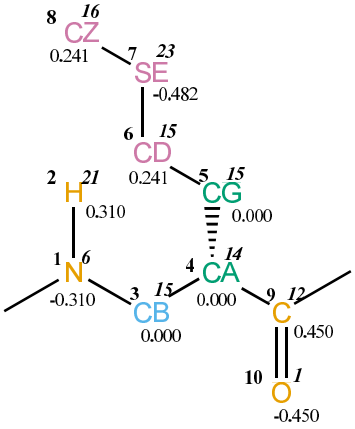

FIGURE 4.111. SAM non-bonded parameters.

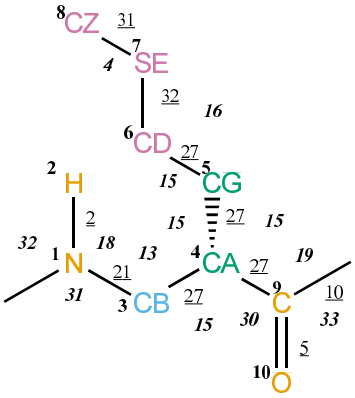

FIGURE 4.112. SAM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 9
4	CA	14	3	0.00000	5 6 9 10 11
5	CG	15	4	0.00000	6 7 9
6	CD	15	4	0.24100	7 8
7	SE	23	32	-0.48200	8
8	CZ	16	5	0.24100	
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.276. Atoms of building block SAM.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	9	27
5	6	27
6	7	32
7	8	31
9	10	5
9	11	10

TABLE 4.277. Bonds of building block SAM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
3	4	9	15
5	4	9	15
4	5	6	15
5	6	7	16
6	7	8	4
4	9	10	30
4	9	11	19
10	9	11	33

TABLE 4.278. Bond angles of building block SAM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	9	34
3	4	5	6	34
3	4	9	11	42
3	4	9	11	45
4	5	6	7	34
5	6	7	8	26

TABLE 4.279. Dihedral angles of building block SAM.

I	J	K	L	Type
1	-1	3	2	1
5	3	9	4	2
9	4	11	10	1

TABLE 4.280. Improper dihedral angles of building block SAM.

Solute building block: (S)-β^2-Valine
Name: SAV

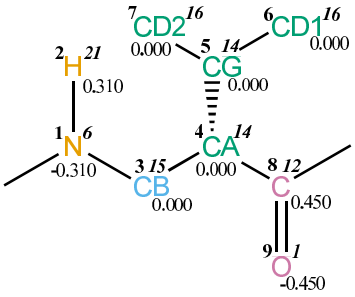

FIGURE 4.113. SAV non-bonded parameters.

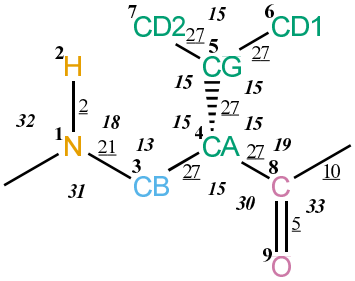

FIGURE 4.114. SAV bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5 8
4	CA	14	3	0.00000	5 6 7 8 9 10
5	CG	14	3	0.00000	6 7 8
6	CD1	16	5	0.00000	7
7	CD2	16	5	0.00000	
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.281. Atoms of building block SAV.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
4	8	27
5	6	27
5	7	27
8	9	5
8	10	10

TABLE 4.282. Bonds of building block SAV.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
3	4	8	15
5	4	8	15
4	5	6	15
4	5	7	15
6	5	7	15
4	8	9	30
4	8	10	19
9	8	10	33

TABLE 4.283. Bond angles of building block SAV.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	8	34
3	4	5	6	34
3	4	8	10	42
3	4	8	10	45

TABLE 4.284. Dihedral angles of building block SAV.

I	J	K	L	Type
1	-1	3	2	1
4	6	7	5	2
5	3	8	4	2
8	4	10	9	1

TABLE 4.285. Improper dihedral angles of building block SAV.

Solute building block: (S)-β^3-Alanine
Name: SBA

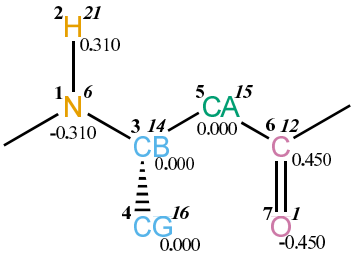

FIGURE 4.115. SBA non-bonded parameters.

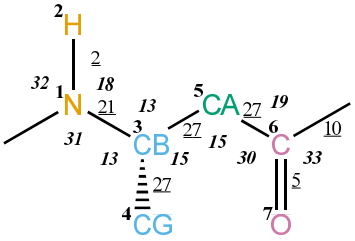

FIGURE 4.116. SBA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 5
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6
4	CG	16	5	0.00000	5
5	CA	15	4	0.00000	6 7 8
6	C	12	12	0.45000	
7	O	1	16	-0.45000	

TABLE 4.286. Atoms of building block SBA.

I	J	Type
1	2	2
1	3	21
3	4	27
3	5	27
5	6	27
6	7	5
6	8	10

TABLE 4.287. Bonds of building block SBA.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	5	13
4	3	5	15
3	5	6	15
5	6	7	30
5	6	8	19
7	6	8	33

TABLE 4.288. Bond angles of building block SBA.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	5	43
-1	1	3	5	44
1	3	5	6	34
3	5	6	8	42
3	5	6	8	45

TABLE 4.289. Dihedral angles of building block SBA.

I	J	K	L	Type
1	-1	3	2	1
3	1	5	4	2
6	5	8	7	1

TABLE 4.290. Improper dihedral angles of building block SBA.

Solute building block: (S)-β^3-Cysteine (protonated)
Name: SBCH

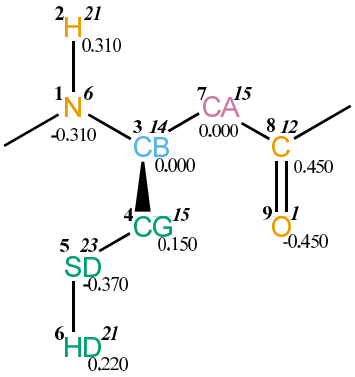

FIGURE 4.117. SBCH non-bonded parameters.

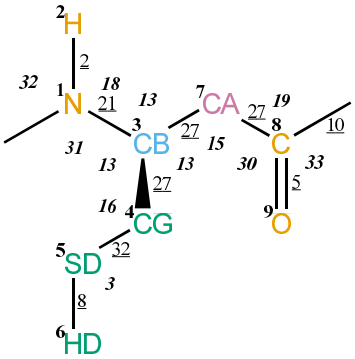

FIGURE 4.118. SBCH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 7 8
4	CG	15	4	0.15000	5 6 7
5	SD	23	32	-0.37000	6
6	HD	21	1	0.22000	
7	CA	15	4	0.00000	8 9 10
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.291. Atoms of building block SBCH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	32
5	6	8
7	8	27
8	9	5
8	10	10

TABLE 4.292. Bonds of building block SBCH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	16
4	5	6	3
3	7	8	15
7	8	9	30
7	8	10	19
9	8	10	33

TABLE 4.293. Bond angles of building block SBCH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	8	34
3	4	5	6	26
3	7	8	10	42
3	7	8	10	45

TABLE 4.294. Dihedral angles of building block SBCH.

I	J	K	L	Type
1	-1	3	2	1
4	1	7	3	2
8	7	10	9	1

TABLE 4.295. Improper dihedral angles of building block SBCH.

Solute building block: (S)-β^3-Aspartic acid (deprotonated; charge -e)
Name: SBD

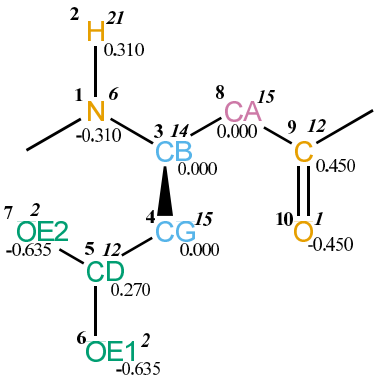

FIGURE 4.119. SBD non-bonded parameters.

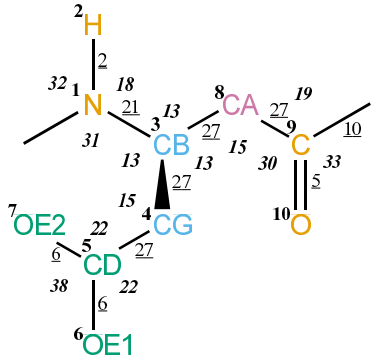

FIGURE 4.120. SBD bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 8 9
4	CG	15	4	0.00000	5 6 7 8
5	CD	12	12	0.27000	6 7
6	OE1	2	16	-0.63500	7
7	OE2	2	16	-0.63500	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.296. Atoms of building block SBD.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	6
5	7	6
8	9	27
9	10	5
9	11	10

TABLE 4.297. Bonds of building block SBD.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	22
4	5	7	22
6	5	7	38
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.298. Bond angles of building block SBD.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	6	40
3	8	9	11	42
3	8	9	11	45

TABLE 4.299. Dihedral angles of building block SBD.

I	J	K	L	Type
1	-1	3	2	1
4	1	8	3	2
5	6	7	4	1
9	8	11	10	1

TABLE 4.300. Improper dihedral angles of building block SBD.

Solute building block: (S)-β^3-Aspartic acid (protonated; neutral)
Name: SBDH

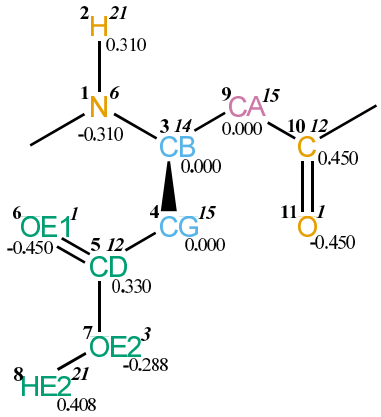

FIGURE 4.121. SBDH non-bonded parameters.

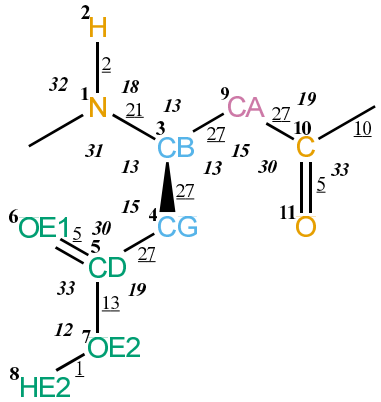

FIGURE 4.122. SBDH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 9
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 9 10
4	CG	15	4	0.00000	5 6 7 9
5	CD	12	12	0.33000	6 7 8
6	OE1	1	16	-0.45000	7
7	OE2	3	16	-0.28800	8
8	HE2	21	1	0.40800	
9	CA	15	4	0.00000	10 11 12
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.301. Atoms of building block SBDH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	9	27
4	5	27
5	6	5
5	7	13
7	8	1
9	10	27
10	11	5
10	12	10

TABLE 4.302. Bonds of building block SBDH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	9	13
4	3	9	13
3	4	5	15
4	5	6	30
4	5	7	19
6	5	7	33
5	7	8	12
3	9	10	15
9	10	11	30
9	10	12	19
11	10	12	33

TABLE 4.303. Bond angles of building block SBDH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	9	43
-1	1	3	9	44
1	3	4	5	34
1	3	9	10	34
3	4	5	7	40
4	5	7	8	12
3	9	10	12	42
3	9	10	12	45

TABLE 4.304. Dihedral angles of building block SBDH.

I	J	K	L	Type
1	-1	3	2	1
4	1	9	3	2
5	6	7	4	1
10	9	12	11	1

TABLE 4.305. Improper dihedral angles of building block SBDH.

Solute building block: (S)-β^3-Glutamic acid (deprotonated; charge -e)
Name: SBE

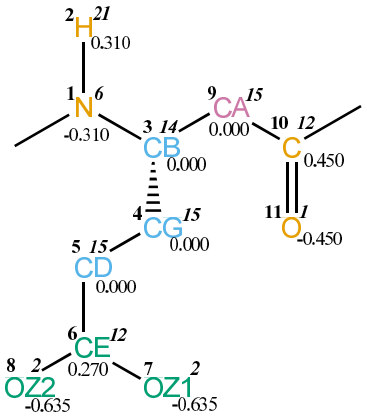

FIGURE 4.123. SBE non-bonded parameters.

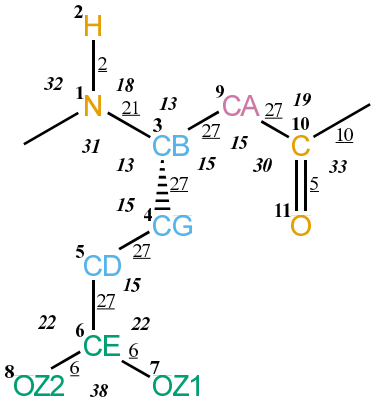

FIGURE 4.124. SBE bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 9
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 9 10
4	CG	15	4	0.00000	5 6 9
5	CD	15	4	0.00000	6 7 8
6	CE	12	12	0.27000	7 8
7	OZ1	2	16	-0.63500	8
8	OZ2	2	16	-0.63500	
9	CA	15	4	0.00000	10 11 12
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.306. Atoms of building block SBE.

I	J	Type
1	2	2
1	3	21
3	4	27
3	9	27
4	5	27
5	6	27
6	7	6
6	8	6
9	10	27
10	11	5
10	12	10

TABLE 4.307. Bonds of building block SBE.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	9	13
4	3	9	15
3	4	5	15
4	5	6	15
5	6	7	22
5	6	8	22
7	6	8	38
3	9	10	15
9	10	11	30
9	10	12	19
11	10	12	33

TABLE 4.308. Bond angles of building block SBE.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	9	43
-1	1	3	9	44
1	3	4	5	34
1	3	9	10	34
3	4	5	6	34
4	5	6	8	40
3	9	10	12	42
3	9	10	12	45

TABLE 4.309. Dihedral angles of building block SBE.

I	J	K	L	Type
1	-1	3	2	1
3	1	9	4	2
6	7	8	5	1
10	9	12	11	1

TABLE 4.310. Improper dihedral angles of building block SBE.

Solute building block: (S)-β^3-Glutamic acid (protonated; neutral)
Name: SBEH

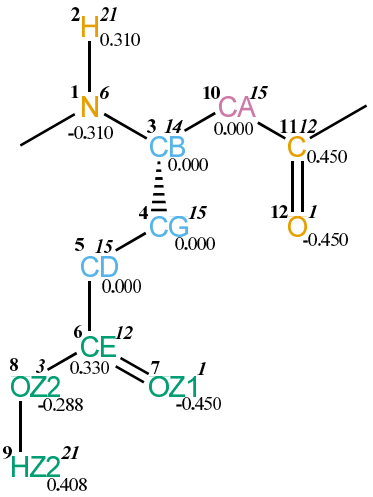

FIGURE 4.125. SBEH non-bonded parameters.

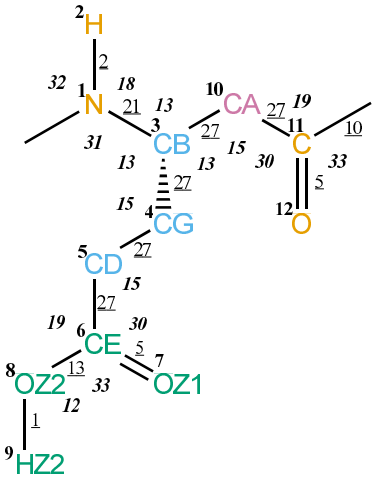

FIGURE 4.126. SBEH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 10
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 10 11
4	CG	15	4	0.00000	5 6 10
5	CD	15	4	0.00000	6 7 8
6	CE	12	12	0.33000	7 8 9
7	OZ1	1	16	-0.45000	8
8	OZ2	3	16	-0.28800	9
9	HZ2	21	1	0.40800	
10	CA	15	4	0.00000	11 12 13
11	C	12	12	0.45000	
12	O	1	16	-0.45000	

TABLE 4.311. Atoms of building block SBEH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	10	27
4	5	27
5	6	27
6	7	5
6	8	13
8	9	1
10	11	27
11	12	5
11	13	10

TABLE 4.312. Bonds of building block SBEH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	10	13
4	3	10	13
3	4	5	15
4	5	6	15
5	6	7	30
5	6	8	19
7	6	8	33
6	8	9	12
3	10	11	15
10	11	12	30
10	11	13	19
12	11	13	33

TABLE 4.313. Bond angles of building block SBEH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	10	43
-1	1	3	10	44
1	3	4	5	34
1	3	10	11	34
3	4	5	6	34
4	5	6	8	40
5	6	8	9	12
3	10	11	13	42
3	10	11	13	45

TABLE 4.314. Dihedral angles of building block SBEH.

I	J	K	L	Type
1	-1	3	2	1
3	1	10	4	2
6	7	8	5	1
11	10	13	12	1

TABLE 4.315. Improper dihedral angles of building block SBEH.

Solute building block: (S)-β^3-Glutamine
Name: SBQ

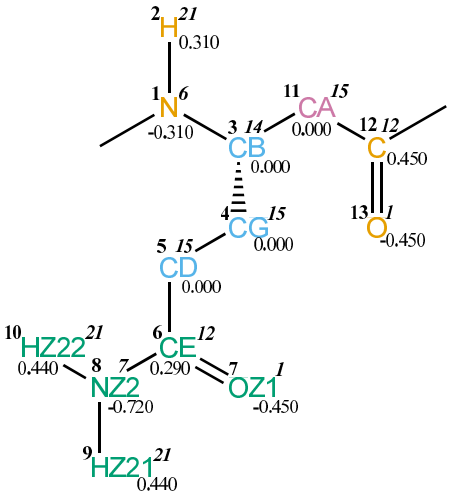

FIGURE 4.127. SBQ non-bonded parameters.

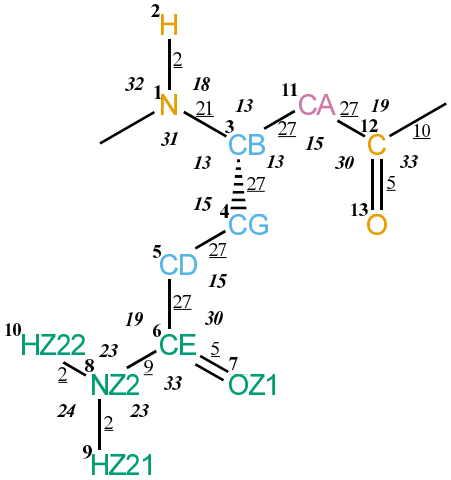

FIGURE 4.128. SBQ bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 11
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 11 12
4	CG	15	4	0.00000	5 6 11
5	CD	15	4	0.00000	6 7 8
6	CE	12	12	0.29000	7 8 9 10
7	OZ1	1	16	-0.45000	8
8	NZ2	7	14	-0.72000	9 10
9	HZ21	21	1	0.44000	10
10	HZ22	21	1	0.44000	
11	CA	15	4	0.00000	12 13 14
12	C	12	12	0.45000	
13	O	1	16	-0.45000	

TABLE 4.316. Atoms of building block SBQ.

I	J	Type
1	2	2
1	3	21
3	4	27
3	11	27
4	5	27
5	6	27
6	7	5
6	8	9
8	9	2
8	10	2
11	12	27
12	13	5
12	14	10

TABLE 4.317. Bonds of building block SBQ.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	11	13
4	3	11	13
3	4	5	15
4	5	6	15
5	6	7	30
5	6	8	19
7	6	8	33
6	8	9	23
6	8	10	23
9	8	10	24
3	11	12	15
11	12	13	30
11	12	14	19
13	12	14	33

TABLE 4.318. Bond angles of building block SBQ.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	11	43
-1	1	3	11	44
1	3	4	5	34
1	3	11	12	34
3	4	5	6	34
4	5	6	8	40
5	6	8	9	14
3	11	12	14	42
3	11	12	14	45

TABLE 4.319. Dihedral angles of building block SBQ.

I	J	K	L	Type
1	-1	3	2	1
3	1	11	4	2
6	7	8	5	1
8	9	10	6	1
12	11	14	13	1

TABLE 4.320. Improper dihedral angles of building block SBQ.

Solute building block: (S)-β^3-Phenylalanine
Name: SBF

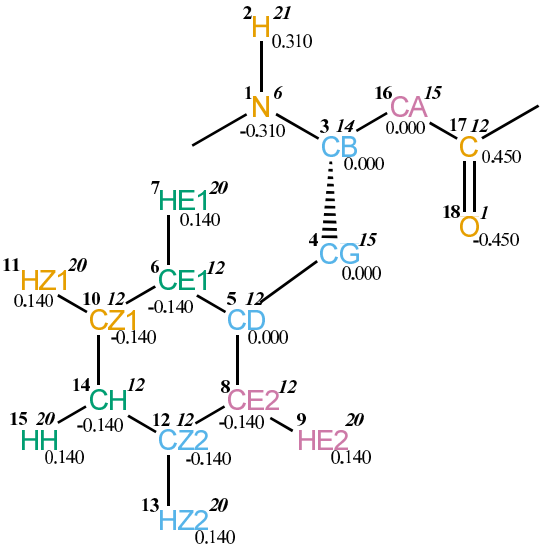

FIGURE 4.129. SBF non-bonded parameters.

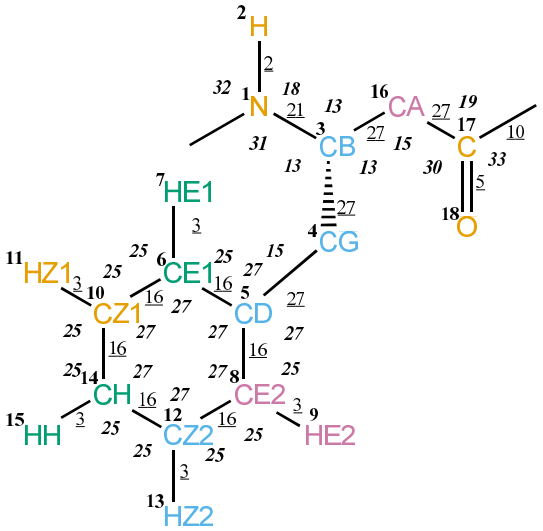

FIGURE 4.130. SBF bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 16
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 16 17
4	CG	15	4	0.00000	5 6 7 8 9 10 12 16
5	CD	12	12	0.00000	6 7 8 9 10 11 12 13 14
6	CE1	12	12	-0.14000	7 8 9 10 11 12 14 15
7	HE1	20	1	0.14000	8 10 11 14
8	CE2	12	12	-0.14000	9 10 12 13 14 15
9	HE2	20	1	0.14000	12 13 14
10	CZ1	12	12	-0.14000	11 12 13 14 15
11	HZ1	20	1	0.14000	12 14 15
12	CZ2	12	12	-0.14000	13 14 15
13	HZ2	20	1	0.14000	14 15
14	CH	12	12	-0.14000	15
15	HH	20	1	0.14000	
16	CA	15	4	0.00000	17 18 19
17	C	12	12	0.45000	
18	O	1	16	-0.45000	

TABLE 4.321. Atoms of building block SBF.

I	J	Type
1	2	2
1	3	21
3	4	27
3	16	27
4	5	27
5	6	16
5	8	16
6	7	3
6	10	16
8	9	3
8	12	16
10	11	3
10	14	16
12	13	3
12	14	16
14	15	3
16	17	27
17	18	5
17	19	10

TABLE 4.322. Bonds of building block SBF.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	16	13
4	3	16	13
3	4	5	15
4	5	6	27
4	5	8	27
6	5	8	27
5	6	7	25
5	6	10	27
7	6	10	25
5	8	9	25
5	8	12	27
9	8	12	25
6	10	11	25
6	10	14	27
11	10	14	25
8	12	13	25
8	12	14	27
13	12	14	25
10	14	12	27
10	14	15	25
12	14	15	25
3	16	17	15
16	17	18	30
16	17	19	19
18	17	19	33

TABLE 4.323. Bond angles of building block SBF.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	16	43
-1	1	3	16	44
1	3	4	5	34
1	3	16	17	34
3	4	5	6	40
3	16	17	19	42
3	16	17	19	45

TABLE 4.324. Dihedral angles of building block SBF.

I	J	K	L	Type
1	-1	3	2	1
3	1	16	4	2
5	6	8	4	1
5	6	10	14	1
5	8	12	14	1
6	5	8	12	1
6	5	10	7	1
6	10	14	12	1
8	5	6	10	1
8	5	12	9	1
8	12	14	10	1
11	6	14	10	1
13	8	14	12	1
14	10	12	15	1
17	16	19	18	1

TABLE 4.325. Improper dihedral angles of building block SBF.

Solute building block: β-Glycine
Name: BGL

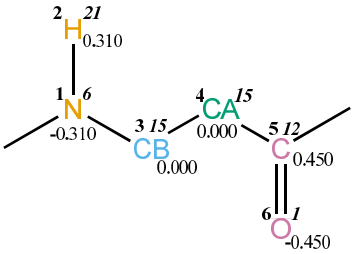

FIGURE 4.131. BGL non-bonded parameters.

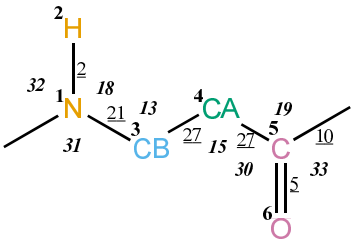

FIGURE 4.132. BGL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4
2	H	21	1	0.31000	3
3	CB	15	4	0.00000	4 5
4	CA	15	4	0.00000	5 6 7
5	C	12	12	0.45000	
6	O	1	16	-0.45000	

TABLE 4.326. Atoms of building block BGL.

I	J	Type
1	2	2
1	3	21
3	4	27
4	5	27
5	6	5
5	7	10

TABLE 4.327. Bonds of building block BGL.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
3	4	5	15
4	5	6	30
4	5	7	19
6	5	7	33

TABLE 4.328. Bond angles of building block BGL.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	4	43
-1	1	3	4	44
1	3	4	5	34
3	4	5	7	42
3	4	5	7	45

TABLE 4.329. Dihedral angles of building block BGL.

I	J	K	L	Type
1	-1	3	2	1
5	4	7	6	1

TABLE 4.330. Improper dihedral angles of building block BGL.

Solute building block: (S)-β^3-Histidine (protonated at NE1; neutral)
Name: SBHA

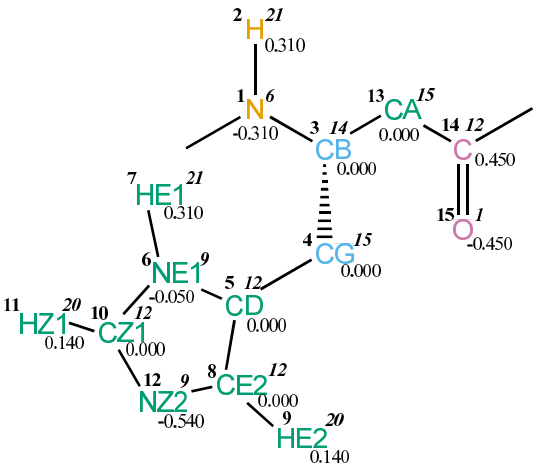

FIGURE 4.133. SBHA non-bonded parameters.

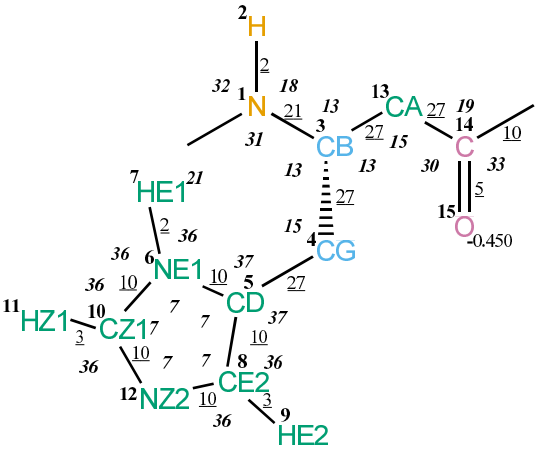

FIGURE 4.134. SBHA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 13
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 13 14
4	CG	15	4	0.00000	5 6 7 8 9 10 12 13
5	CD	12	12	0.00000	6 7 8 9 10 11 12
6	NE1	9	14	-0.05000	7 8 9 10 11 12
7	HE1	21	1	0.31000	8 10 11 12
8	CE2	12	12	0.00000	9 10 11 12
9	HE2	20	1	0.14000	10 12
10	CZ1	12	12	0.00000	11 12
11	HZ1	20	1	0.14000	12
12	NZ2	9	14	-0.54000	
13	CA	15	4	0.00000	14 15 16
14	C	12	12	0.45000	
15	O	1	16	-0.45000	

TABLE 4.331. Atoms of building block SBHA.

I	J	Type
1	2	2
1	3	21
3	4	27
3	13	27
4	5	27
5	6	10
5	8	10
6	7	2
6	10	10
8	9	3
8	12	10
10	11	3
10	12	10
13	14	27
14	15	5
14	16	10

TABLE 4.332. Bonds of building block SBHA.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	13	13
4	3	13	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	10	7
7	6	10	36
5	8	9	36
5	8	12	7
9	8	12	36
6	10	11	36
6	10	12	7
11	10	12	36
8	12	10	7
3	13	14	15
13	14	15	30
13	14	16	19
15	14	16	33

TABLE 4.333. Bond angles of building block SBHA.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	13	43
-1	1	3	13	44
1	3	4	5	34
1	3	13	14	34
3	4	5	6	40
3	13	14	16	42
3	13	14	16	45

TABLE 4.334. Dihedral angles of building block SBHA.

I	J	K	L	Type
1	-1	3	2	1
3	1	13	4	2
5	6	8	4	1
5	6	10	12	1
5	8	12	10	1
6	5	8	12	1
6	5	10	7	1
6	10	12	8	1
8	5	6	10	1
8	5	12	9	1
10	6	12	11	1
14	13	16	15	1

TABLE 4.335. Improper dihedral angles of building block SBHA.

Solute building block: (S)-β^3-Histidine(protonated at NE1 and NZ2; charge $+e$)
Name: SBHH

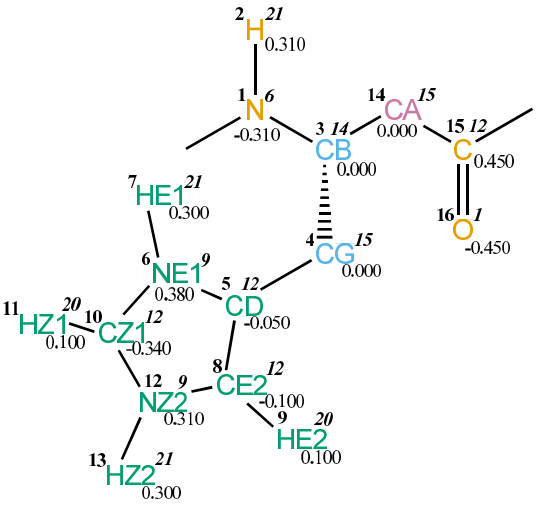

FIGURE 4.135. SBHH non-bonded parameters.

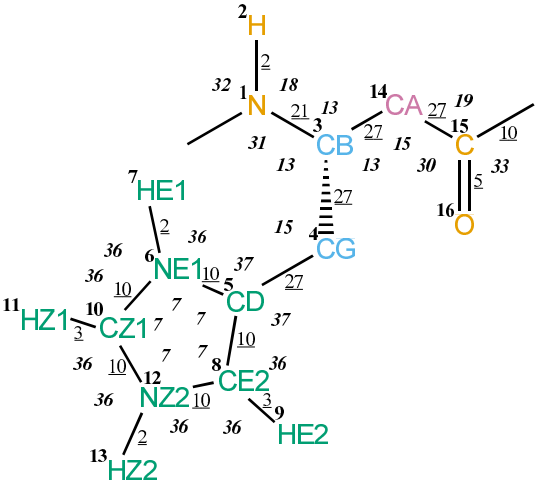

FIGURE 4.136. SBHH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 14
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 14 15
4	CG	15	4	0.00000	5 6 7 8 9 10 12 14
5	CD	12	12	-0.05000	6 7 8 9 10 11 12 13
6	NE1	9	14	0.38000	7 8 9 10 11 12 13
7	HE1	21	1	0.30000	8 10 11 12
8	CE2	12	12	-0.10000	9 10 11 12 13
9	HE2	20	1	0.10000	10 12 13
10	CZ1	12	12	-0.34000	11 12 13
11	HZ1	20	1	0.10000	12 13
12	NZ2	9	14	0.31000	13
13	HZ2	21	1	0.30000	
14	CA	15	4	0.00000	15 16 17
15	C	12	12	0.45000	
16	O	1	16	-0.45000	

TABLE 4.336. Atoms of building block SBHH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	14	27
4	5	27
5	6	10
5	8	10
6	7	2
6	10	10
8	9	3
8	12	10
10	11	3
10	12	10
12	13	2
14	15	27
15	16	5
15	17	10

TABLE 4.337. Bonds of building block SBHH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	14	13
4	3	14	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	10	7
7	6	10	36
5	8	9	36
5	8	12	7
9	8	12	36
6	10	11	36
6	10	12	7
11	10	12	36
8	12	10	7
8	12	13	36
10	12	13	36
3	14	15	15
14	15	16	30
14	15	17	19
16	15	17	33

TABLE 4.338. Bond angles of building block SBHH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	14	43
-1	1	3	14	44
1	3	4	5	34
1	3	14	15	34
3	4	5	6	40
3	14	15	17	42
3	14	15	17	45

TABLE 4.339. Dihedral angles of building block SBHH.

I	J	K	L	Type
1	-1	3	2	1
3	1	14	4	2
5	6	8	4	1
5	6	10	12	1
5	8	12	10	1
6	5	8	12	1
6	5	10	7	1
6	10	12	8	1
8	5	6	10	1
8	5	12	9	1
10	6	12	11	1
12	8	10	13	1
15	14	17	16	1

TABLE 4.340. Improper dihedral angles of building block SBHH.

Solute building block: (S)-β^3-Isoleucine
Name: SBI

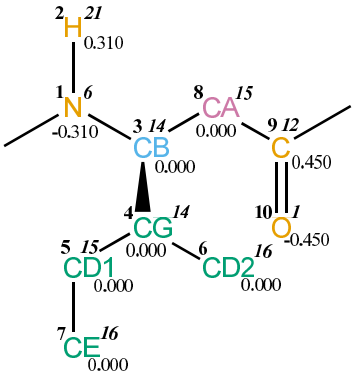

FIGURE 4.137. SBI non-bonded parameters.

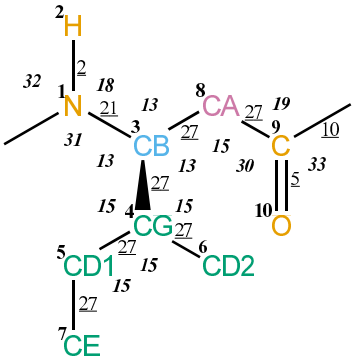

FIGURE 4.138. SBI bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 8 9
4	CG	14	3	0.00000	5 6 7 8
5	CD1	15	4	0.00000	6 7
6	CD2	16	5	0.00000	
7	CE	16	5	0.00000	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.341. Atoms of building block SBI.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
4	6	27
5	7	27
8	9	27
9	10	5
9	11	10

TABLE 4.342. Bonds of building block SBI.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
3	4	6	15
5	4	6	15
4	5	7	15
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.343. Bond angles of building block SBI.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	7	34
3	8	9	11	42
3	8	9	11	45

TABLE 4.344. Dihedral angles of building block SBI.

I	J	K	L	Type
1	-1	3	2	1
4	1	8	3	2
4	5	6	3	2
9	8	11	10	1

TABLE 4.345. Improper dihedral angles of building block SBI.

Solute building block: (S)-β^3-Lysine (protonated; charge $+e$)
Name: SBKH

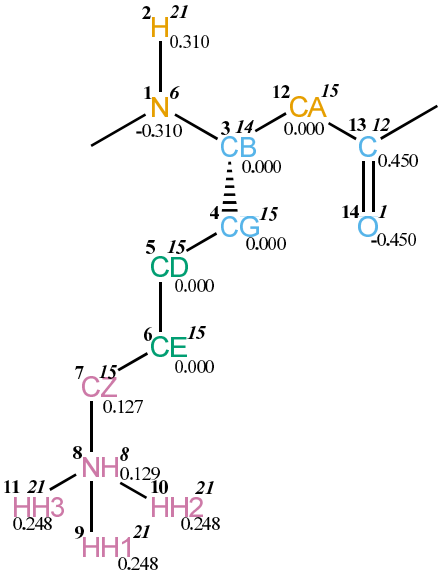

FIGURE 4.139. SBKH non-bonded parameters.

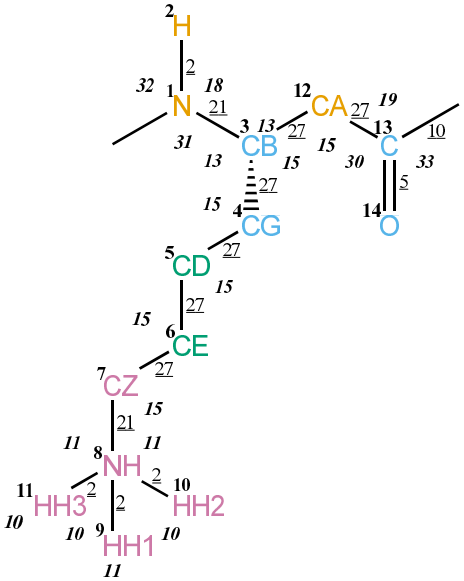

FIGURE 4.140. SBKH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 12
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 12 13
4	CG	15	4	0.00000	5 6 12
5	CD	15	4	0.00000	6 7
6	CE	15	4	0.00000	7 8
7	CZ	15	4	0.12700	8 9 10 11
8	NH	8	14	0.12900	9 10 11
9	HH1	21	1	0.24800	10 11
10	HH2	21	1	0.24800	11
11	HH3	21	1	0.24800	
12	CA	15	4	0.00000	13 14 15
13	C	12	12	0.45000	
14	O	1	16	-0.45000	

TABLE 4.346. Atoms of building block SBKH.

I	J	Type
1	2	2
1	3	21
3	4	27
3	12	27
4	5	27
5	6	27
6	7	27
7	8	21
8	9	2
8	10	2
8	11	2
12	13	27
13	14	5
13	15	10

TABLE 4.347. Bonds of building block SBKH.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	12	13
4	3	12	15
3	4	5	15
4	5	6	15
5	6	7	15
6	7	8	15
7	8	9	11
7	8	10	11
7	8	11	11
9	8	10	10
9	8	11	10
10	8	11	10
3	12	13	15
12	13	14	30
12	13	15	19
14	13	15	33

TABLE 4.348. Bond angles of building block SBKH.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	12	43
-1	1	3	12	44
1	3	4	5	34
1	3	12	13	34
3	4	5	6	34
4	5	6	7	34
5	6	7	8	34
6	7	8	9	29
3	12	13	15	42
3	12	13	15	45

TABLE 4.349. Dihedral angles of building block SBKH.

I	J	K	L	Type
1	-1	3	2	1
3	1	12	4	2
13	12	15	14	1

TABLE 4.350. Improper dihedral angles of building block SBKH.

Solute building block: (S)-β^3-Leucine
Name: SBL

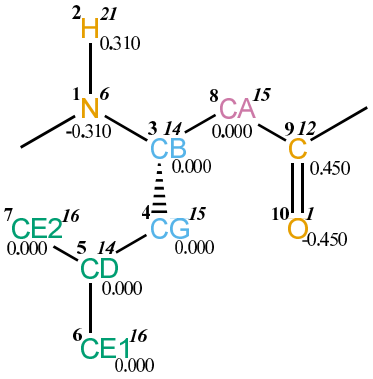

FIGURE 4.141. SBL non-bonded parameters.

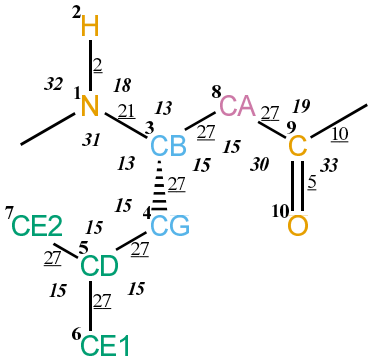

FIGURE 4.142. SBL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 8 9
4	CG	15	4	0.00000	5 6 7 8
5	CD	14	3	0.00000	6 7
6	CE1	16	5	0.00000	7
7	CE2	16	5	0.00000	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.351. Atoms of building block SBL.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	27
5	7	27
8	9	27
9	10	5
9	11	10

TABLE 4.352. Bonds of building block SBL.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	15
3	4	5	15
4	5	6	15
4	5	7	15
6	5	7	15
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.353. Bond angles of building block SBL.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	6	34
3	8	9	11	42
3	8	9	11	45

TABLE 4.354. Dihedral angles of building block SBL.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	6	7	5	2
9	8	11	10	1

TABLE 4.355. Improper dihedral angles of building block SBL.

Solute building block: (S)-β^3-Methionine
Name: SBM

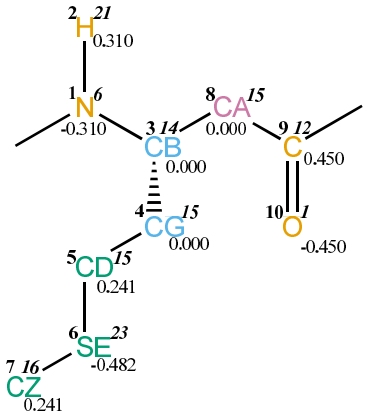

FIGURE 4.143. SBM non-bonded parameters.

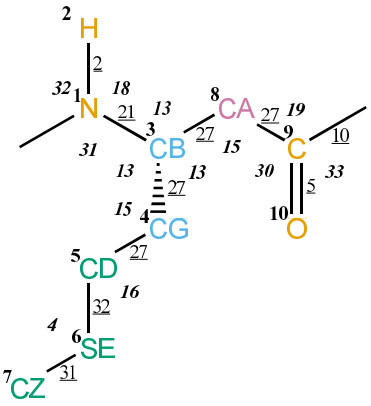

FIGURE 4.144. SBM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 8 9
4	CG	15	4	0.00000	5 6 8
5	CD	15	4	0.24100	6 7
6	SE	23	32	-0.48200	7
7	CZ	16	5	0.24100	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.356. Atoms of building block SBM.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	32
6	7	31
8	9	27
9	10	5
9	11	10

TABLE 4.357. Bonds of building block SBM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	15
4	5	6	16
5	6	7	4
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.358. Bond angles of building block SBM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	6	34
4	5	6	7	26
3	8	9	11	42
3	8	9	11	45

TABLE 4.359. Dihedral angles of building block SBM.

I	J	K	L	Type
1	-1	3	2	1
4	1	8	3	2
9	8	11	10	1

TABLE 4.360. Improper dihedral angles of building block SBM.

Solute building block: (S)-β^3-Proline
Name: SBP

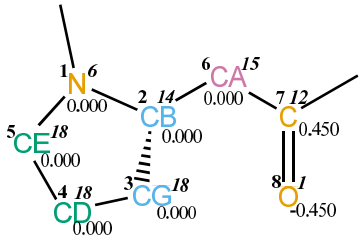

FIGURE 4.145. SBP non-bonded parameters.

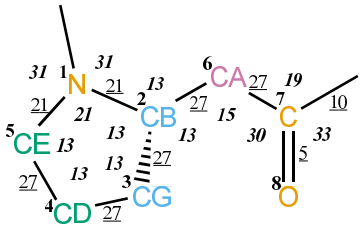

FIGURE 4.146. SBP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 5
0					1
1	N	6	14	0.00000	2 3 4 5 6
2	CB	14	3	0.00000	3 4 5 6 7
3	CG	18	4	0.00000	4 5 6
4	CD	18	4	0.00000	5
5	CE	18	4	0.00000	
6	CA	15	4	0.00000	7 8 9
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.361. Atoms of building block SBP.

I	J	Type
1	2	21
1	5	21
2	3	27
2	6	27
3	4	27
4	5	27
6	7	27
7	8	5
7	9	10

TABLE 4.362. Bonds of building block SBP.

I	J	K	Type
-1	1	2	31
-1	1	5	31
2	1	5	21
1	2	3	13
1	2	6	13
3	2	6	13
2	3	4	13
3	4	5	13
1	5	4	13
2	6	7	15
6	7	8	30
6	7	9	19
8	7	9	33

TABLE 4.363. Bond angles of building block SBP.

I	J	K	L	Type
-2	-1	1	2	14
-1	1	2	6	43
-1	1	2	6	44
2	1	5	4	39
1	2	3	4	34
1	2	6	7	34
2	3	4	5	34
3	4	5	1	34
2	6	7	9	42
2	6	7	9	45

TABLE 4.364. Dihedral angles of building block SBP.

I	J	K	L	Type
1	-1	2	5	1
2	1	6	3	2
7	6	9	8	1

TABLE 4.365. Improper dihedral angles of building block SBP.

Solute building block: (S)-β^3-Arginine (protonated; charge $+e$)
Name: SBR

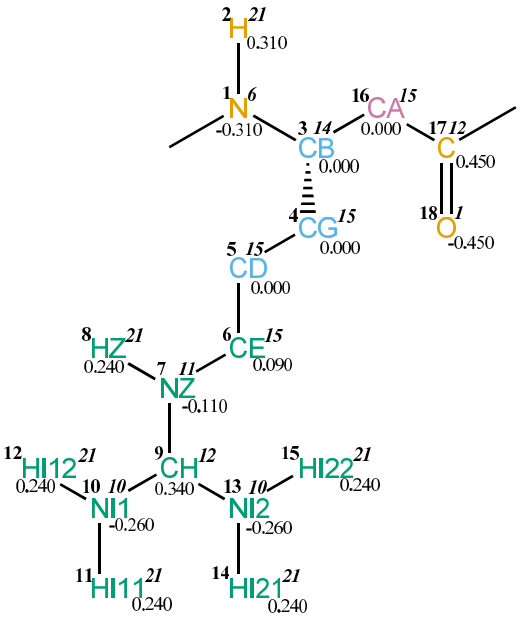

FIGURE 4.147. SBR non-bonded parameters.

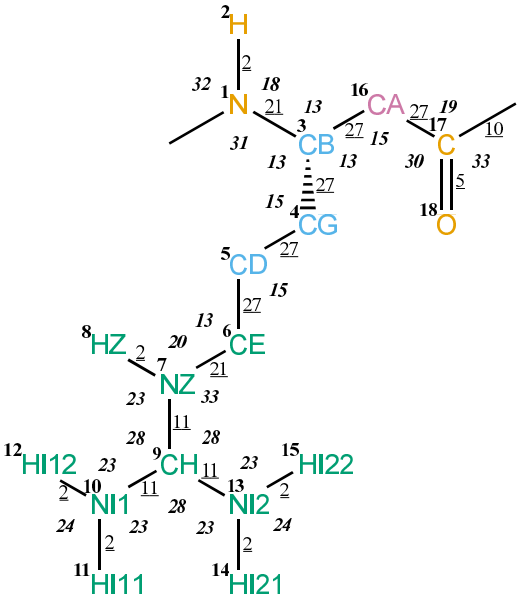

FIGURE 4.148. SBR bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 16
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 16 17
4	CG	15	4	0.00000	5 6 16
5	CD	15	4	0.00000	6 7
6	CE	15	4	0.09000	7 8 9
7	NZ	11	14	-0.11000	8 9 10 13
8	HZ	21	1	0.24000	9
9	CH	12	12	0.34000	10 11 12 13 14 15
10	NI1	10	14	-0.26000	11 12 13
11	HI11	21	1	0.24000	12
12	HI12	21	1	0.24000	
13	NI2	10	14	-0.26000	14 15
14	HI21	21	1	0.24000	15
15	HI22	21	1	0.24000	
16	CA	15	4	0.00000	17 18 19
17	C	12	12	0.45000	
18	O	1	16	-0.45000	

TABLE 4.366. Atoms of building block SBR.

I	J	Type
1	2	2
1	3	21
3	4	27
3	16	27
4	5	27
5	6	27
6	7	21
7	8	2
7	9	11
9	10	11
9	13	11
10	11	2
10	12	2
13	14	2
13	15	2
16	17	27
17	18	5
17	19	10

TABLE 4.367. Bonds of building block SBR.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	16	13
4	3	16	13
3	4	5	15
4	5	6	15
5	6	7	13
6	7	8	20
6	7	9	33
8	7	9	23
7	9	10	28
7	9	13	28
10	9	13	28
9	10	11	23
9	10	12	23
11	10	12	24
9	13	14	23
9	13	15	23
14	13	15	24
3	16	17	15
16	17	18	30
16	17	19	19
18	17	19	33

TABLE 4.368. Bond angles of building block SBR.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	16	43
-1	1	3	16	44
1	3	4	5	34
1	3	16	17	34
3	4	5	6	34
4	5	6	7	34
5	6	7	9	39
6	7	9	10	14
7	9	10	11	14
7	9	13	14	14
3	16	17	19	42
3	16	17	19	45

TABLE 4.369. Dihedral angles of building block SBR.

I	J	K	L	Type
1	-1	3	2	1
3	1	16	4	2
7	6	9	8	1
9	10	13	7	1
10	11	12	9	1
13	14	15	9	1
17	16	19	18	1

TABLE 4.370. Improper dihedral angles of building block SBR.

Solute building block: (S)-β^3-Serine
Name: SBS

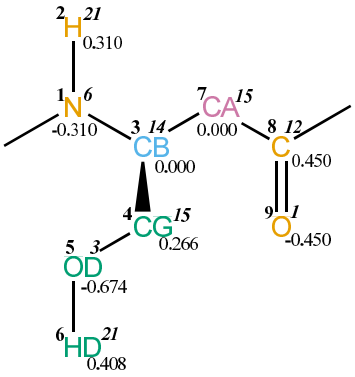

FIGURE 4.149. SBS non-bonded parameters.

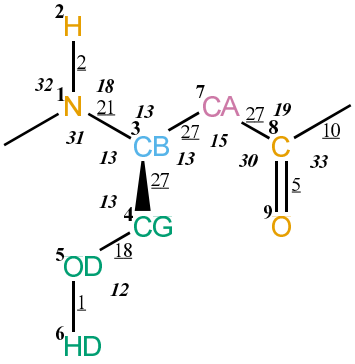

FIGURE 4.150. SBS bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 7 8
4	CG	15	4	0.26600	5 6 7
5	OD	3	16	-0.67400	6
6	HD	21	1	0.40800	
7	CA	15	4	0.00000	8 9 10
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.371. Atoms of building block SBS.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	18
5	6	1
7	8	27
8	9	5
8	10	10

TABLE 4.372. Bonds of building block SBS.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	13
3	4	5	13
4	5	6	12
3	7	8	15
7	8	9	30
7	8	10	19
9	8	10	33

TABLE 4.373. Bond angles of building block SBS.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	8	34
3	4	5	6	23
3	7	8	10	42
3	7	8	10	45

TABLE 4.374. Dihedral angles of building block SBS.

I	J	K	L	Type
1	-1	3	2	1
4	1	7	3	2
8	7	10	9	1

TABLE 4.375. Improper dihedral angles of building block SBS.

Solute building block: (S)-β^3-Threonine
Name: SBT

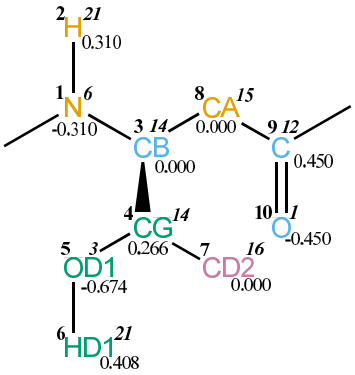

FIGURE 4.151. SBT non-bonded parameters.

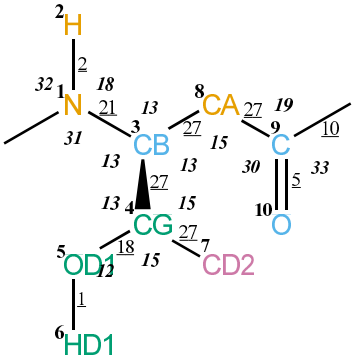

FIGURE 4.152. SBT bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 7 8 9
4	CG	14	3	0.26600	5 6 7 8
5	OD1	3	16	-0.67400	6 7
6	HD1	21	1	0.40800	
7	CD2	16	5	0.00000	
8	CA	15	4	0.00000	9 10 11
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.376. Atoms of building block SBT.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	18
4	7	27
5	6	1
8	9	27
9	10	5
9	11	10

TABLE 4.377. Bonds of building block SBT.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	13
3	4	5	13
3	4	7	15
5	4	7	15
4	5	6	12
3	8	9	15
8	9	10	30
8	9	11	19
10	9	11	33

TABLE 4.378. Bond angles of building block SBT.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	9	34
3	4	5	6	23
3	8	9	11	42
3	8	9	11	45

TABLE 4.379. Dihedral angles of building block SBT.

I	J	K	L	Type
1	-1	3	2	1
4	1	8	3	2
4	5	7	3	2
9	8	11	10	1

TABLE 4.380. Improper dihedral angles of building block SBT.

Solute building block: (S)-β^3-Valine
Name: SBV

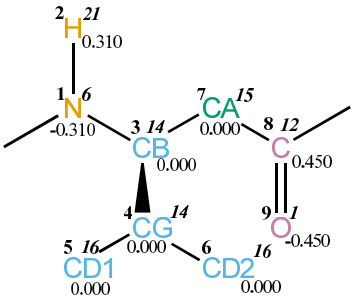

FIGURE 4.153. SBV non-bonded parameters.

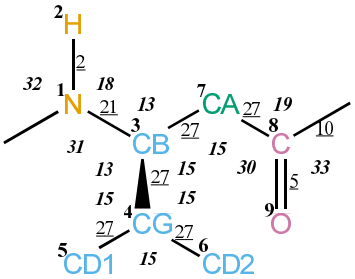

FIGURE 4.154. SBV bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 7 8
4	CG	14	3	0.00000	5 6 7
5	CD1	16	5	0.00000	6
6	CD2	16	5	0.00000	
7	CA	15	4	0.00000	8 9 10
8	C	12	12	0.45000	
9	O	1	16	-0.45000	

TABLE 4.381. Atoms of building block SBV.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	27
4	6	27
7	8	27
8	9	5
8	10	10

TABLE 4.382. Bonds of building block SBV.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	15
3	4	5	15
3	4	6	15
5	4	6	15
3	7	8	15
7	8	9	30
7	8	10	19
9	8	10	33

TABLE 4.383. Bond angles of building block SBV.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	8	34
3	7	8	10	42
3	7	8	10	45

TABLE 4.384. Dihedral angles of building block SBV.

I	J	K	L	Type
1	-1	3	2	1
3	5	6	4	2
4	1	7	3	2
8	7	10	9	1

TABLE 4.385. Improper dihedral angles of building block SBV.

Solute building block: (S)-β^3-Tyrosine
Name: SBY

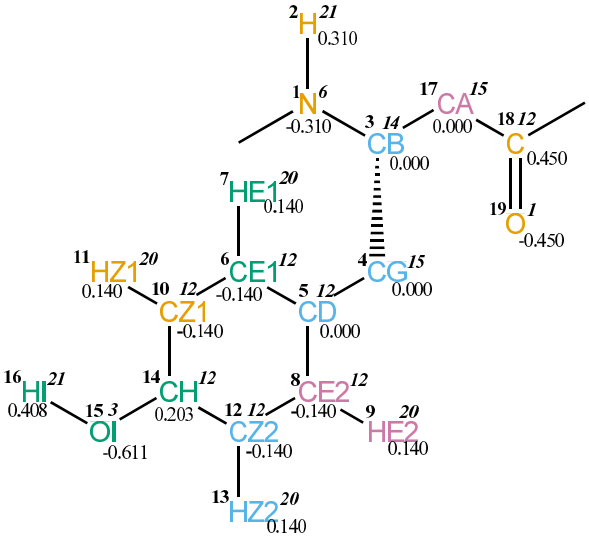

FIGURE 4.155. SBY non-bonded parameters.

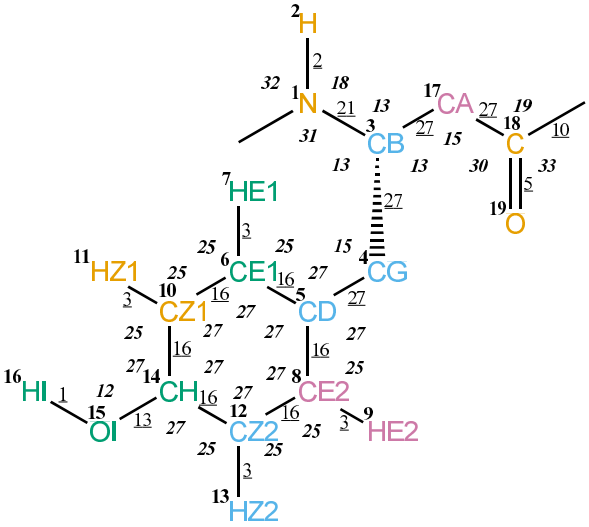

FIGURE 4.156. SBY bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 17
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 17 18
4	CG	15	4	0.00000	5 6 7 8 9 10 12 17
5	CD	12	12	0.00000	6 7 8 9 10 11 12 13 14
6	CE1	12	12	-0.14000	7 8 9 10 11 12 14 15
7	HE1	20	1	0.14000	8 10 11 14
8	CE2	12	12	-0.14000	9 10 12 13 14 15
9	HE2	20	1	0.14000	12 13 14
10	CZ1	12	12	-0.14000	11 12 13 14 15
11	HZ1	20	1	0.14000	12 14 15
12	CZ2	12	12	-0.14000	13 14 15
13	HZ2	20	1	0.14000	14 15
14	CH	12	12	0.20300	15 16
15	OI	3	16	-0.61100	16
16	HI	21	1	0.40800	
17	CA	15	4	0.00000	18 19 20
18	C	12	12	0.45000	
19	O	1	16	-0.45000	

TABLE 4.386. Atoms of building block SBY.

I	J	Type
1	2	2
1	3	21
3	4	27
3	17	27
4	5	27
5	6	16
5	8	16
6	7	3
6	10	16
8	9	3
8	12	16
10	11	3
10	14	16
12	13	3
12	14	16
14	15	13
15	16	1
17	18	27
18	19	5
18	20	10

TABLE 4.387. Bonds of building block SBY.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	17	13
4	3	17	13
3	4	5	15
4	5	6	27
4	5	8	27
6	5	8	27
5	6	7	25
5	6	10	27
7	6	10	25
5	8	9	25
5	8	12	27
9	8	12	25
6	10	11	25
6	10	14	27
11	10	14	25
8	12	13	25
8	12	14	27
13	12	14	25
10	14	12	27
10	14	15	27
12	14	15	27
14	15	16	12
3	17	18	15
17	18	19	30
17	18	20	19
19	18	20	33

TABLE 4.388. Bond angles of building block SBY.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	17	43
-1	1	3	17	44
1	3	4	5	34
1	3	17	18	34
3	4	5	6	40
10	14	15	16	11
3	17	18	20	42
3	17	18	20	45

TABLE 4.389. Dihedral angles of building block SBY.

I	J	K	L	Type
1	-1	3	2	1
3	1	17	4	2
5	6	8	4	1
5	6	10	14	1
5	8	12	14	1
6	5	8	12	1
6	5	10	7	1
6	10	14	12	1
8	5	6	10	1
8	5	12	9	1
8	12	14	10	1
11	6	14	10	1
13	8	14	12	1
14	10	12	15	1
18	17	20	19	1

TABLE 4.390. Improper dihedral angles of building block SBY.

Solute building block: (S)-β^3-Tryptophan
Name: SBW

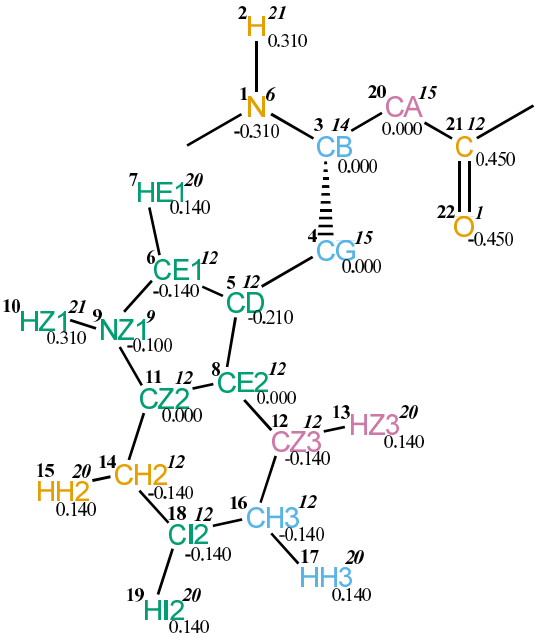

FIGURE 4.157. SBW non-bonded parameters.

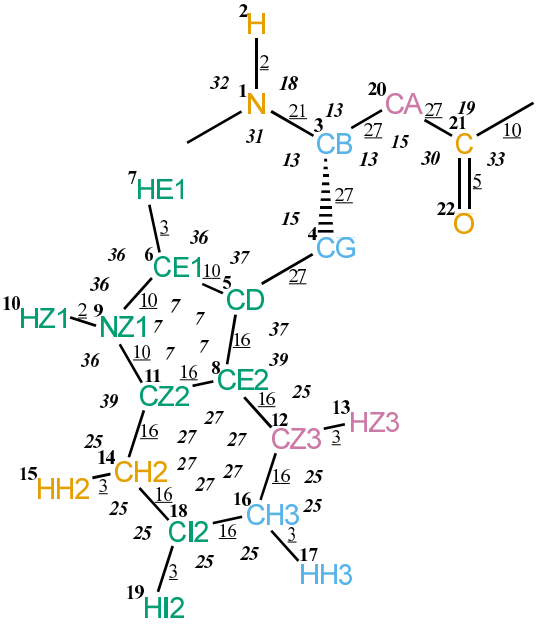

FIGURE 4.158. SBW bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 20
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 20 21
4	CG	15	4	0.00000	5 6 7 8 9 11 12 20
5	CD	12	12	-0.21000	6 7 8 9 10 11 12 13 14 16
6	CE1	12	12	-0.14000	7 8 9 10 11 12 14
7	HE1	20	1	0.14000	8 9 10 11
8	CE2	12	12	0.00000	9 10 11 12 13 14 15 16 17 18
9	NZ1	9	14	-0.10000	10 11 12 14 15 18
10	HZ1	21	1	0.31000	11 14
11	CZ2	12	12	0.00000	12 13 14 15 16 18 19
12	CZ3	12	12	-0.14000	13 14 16 17 18 19
13	HZ3	20	1	0.14000	16 17 18
14	CH2	12	12	-0.14000	15 16 17 18 19
15	HH2	20	1	0.14000	16 18 19
16	CH3	12	12	-0.14000	17 18 19
17	HH3	20	1	0.14000	18 19
18	CI2	12	12	-0.14000	19
19	HI2	20	1	0.14000	
20	CA	15	4	0.00000	21 22 23
21	C	12	12	0.45000	
22	O	1	16	-0.45000	

TABLE 4.391. Atoms of building block SBW.

I	J	Type
1	2	2
1	3	21
3	4	27
3	20	27
4	5	27
5	6	10
5	8	16
6	7	3
6	9	10
8	11	16
8	12	16
9	10	2
9	11	10
11	14	16
12	13	3
12	16	16
14	15	3
14	18	16
16	17	3
16	18	16
18	19	3
20	21	27
21	22	5
21	23	10

TABLE 4.392. Bonds of building block SBW.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	20	13
4	3	20	13
3	4	5	15
4	5	6	37
4	5	8	37
6	5	8	7
5	6	7	36
5	6	9	7
7	6	9	36
5	8	11	7
5	8	12	39
11	8	12	27
6	9	10	36
6	9	11	7
10	9	11	36
8	11	9	7
8	11	14	27
9	11	14	39
8	12	13	25
8	12	16	27
13	12	16	25
11	14	15	25
11	14	18	27
15	14	18	25
12	16	17	25
12	16	18	27
17	16	18	25
14	18	16	27
14	18	19	25
16	18	19	25
3	20	21	15
20	21	22	30
20	21	23	19
22	21	23	33

TABLE 4.393. Bond angles of building block SBW.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	20	43
-1	1	3	20	44
1	3	4	5	34
1	3	20	21	34
3	4	5	8	40
3	20	21	22	42
3	20	21	22	45

TABLE 4.394. Dihedral angles of building block SBW.

I	J	K	L	Type
1	-1	3	2	1
3	1	20	4	2
5	6	8	4	1
5	6	9	11	1
5	8	11	9	1
6	5	8	11	1
6	5	9	7	1
6	9	11	8	1
8	5	6	9	1
8	11	12	5	1
8	11	14	18	1
8	12	16	18	1
9	6	11	10	1
11	8	12	16	1
11	8	14	9	1
11	14	18	16	1
12	8	11	14	1
12	8	16	13	1
12	16	18	14	1
14	11	18	15	1
16	12	18	17	1
18	14	16	19	1
21	20	23	22	1

TABLE 4.395. Improper dihedral angles of building block SBW.

Solute building block: (R,S)-$\beta^{(}2,3$)-Alanine(αMe)
Name: SRAM

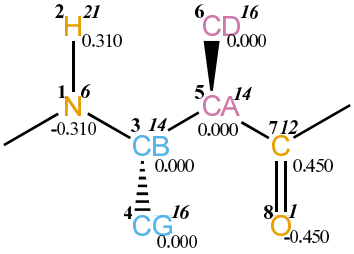

FIGURE 4.159. SRAM non-bonded parameters.

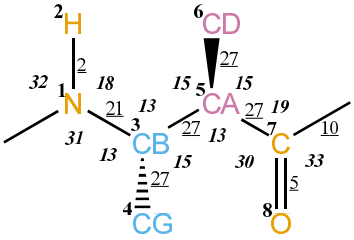

FIGURE 4.160. SRAM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 5
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 7
4	CG	16	5	0.00000	5
5	CA	14	3	0.00000	6 7 8 9
6	CD	16	5	0.00000	7
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.396. Atoms of building block SRAM.

I	J	Type
1	2	2
1	3	21
3	4	27
3	5	27
5	6	27
5	7	27
7	8	5
7	9	10

TABLE 4.397. Bonds of building block SRAM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	5	13
4	3	5	15
3	5	6	15
3	5	7	13
6	5	7	15
5	7	8	30
5	7	9	19
8	7	9	33

TABLE 4.398. Bond angles of building block SRAM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	5	43
-1	1	3	5	44
1	3	5	7	34
3	5	7	9	42
3	5	7	9	45

TABLE 4.399. Dihedral angles of building block SRAM.

I	J	K	L	Type
1	-1	3	2	1
3	1	5	4	2
5	3	7	6	2
7	5	9	8	1

TABLE 4.400. Improper dihedral angles of building block SRAM.

Solute building block: (R,S)-$\beta^{(}2,3$)-Leucine(αMe)
Name: SRLM

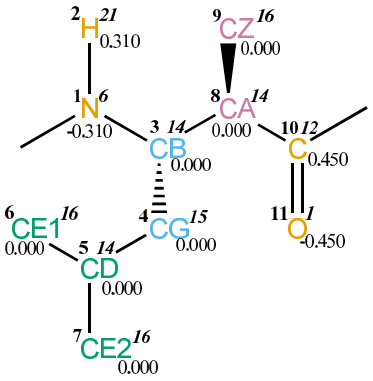

FIGURE 4.161. SRLM non-bonded parameters.

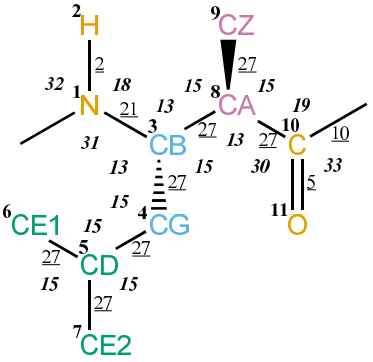

FIGURE 4.162. SRLM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 8
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 8 9 10
4	CG	15	4	0.00000	5 6 7 8
5	CD	14	3	0.00000	6 7
6	CE1	16	5	0.00000	7
7	CE2	16	5	0.00000	
8	CA	14	3	0.00000	9 10 11 12
9	CZ	16	5	0.00000	10
10	C	12	12	0.45000	
11	O	1	16	-0.45000	

TABLE 4.401. Atoms of building block SRLM.

I	J	Type
1	2	2
1	3	21
3	4	27
3	8	27
4	5	27
5	6	27
5	7	27
8	9	27
8	10	27
10	11	5
10	12	10

TABLE 4.402. Bonds of building block SRLM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	8	13
4	3	8	15
3	4	5	15
4	5	6	15
4	5	7	15
6	5	7	15
3	8	9	15
3	8	10	13
9	8	10	15
8	10	11	30
8	10	12	19
11	10	12	33

TABLE 4.403. Bond angles of building block SRLM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	8	43
-1	1	3	8	44
1	3	4	5	34
1	3	8	10	34
3	4	5	6	34
3	8	10	12	42
3	8	10	12	45

TABLE 4.404. Dihedral angles of building block SRLM.

I	J	K	L	Type
1	-1	3	2	1
3	1	8	4	2
4	6	7	5	2
8	3	10	9	2
10	8	12	11	1

TABLE 4.405. Improper dihedral angles of building block SRLM.

Solute building block: (R,S)-$\beta^{(}2,3$)-Valine(αMe)
Name: SRVM

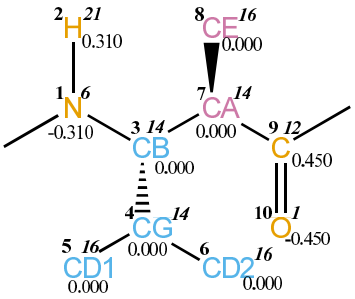

FIGURE 4.163. SRVM non-bonded parameters.

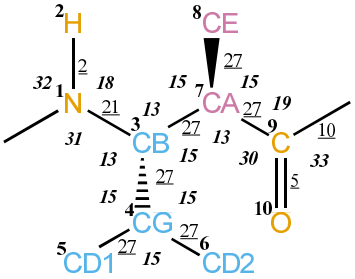

FIGURE 4.164. SRVM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 7
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 7 8 9
4	CG	14	3	0.00000	5 6 7
5	CD1	16	5	0.00000	6
6	CD2	16	5	0.00000	
7	CA	14	3	0.00000	8 9 10 11
8	CE	16	5	0.00000	9
9	C	12	12	0.45000	
10	O	1	16	-0.45000	

TABLE 4.406. Atoms of building block SRVM.

I	J	Type
1	2	2
1	3	21
3	4	27
3	7	27
4	5	27
4	6	27
7	8	27
7	9	27
9	10	5
9	11	10

TABLE 4.407. Bonds of building block SRVM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	7	13
4	3	7	15
3	4	5	15
3	4	6	15
5	4	6	15
3	7	8	15
3	7	9	13
8	7	9	15
7	9	10	30
7	9	11	19
10	9	11	33

TABLE 4.408. Bond angles of building block SRVM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	7	43
-1	1	3	7	44
1	3	4	5	34
1	3	7	9	34
3	7	9	11	42
3	7	9	11	45

TABLE 4.409. Dihedral angles of building block SRVM.

I	J	K	L	Type
1	-1	3	2	1
3	1	7	4	2
3	5	6	4	2
7	3	9	8	2
9	7	11	10	1

TABLE 4.410. Improper dihedral angles of building block SRVM.

Solute building block: (S,S)-$\beta^{(}2,3$)-Alanine(αMe)
Name: SSAM

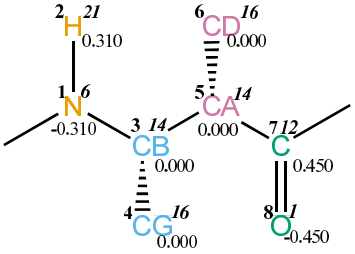

FIGURE 4.165. SSAM non-bonded parameters.

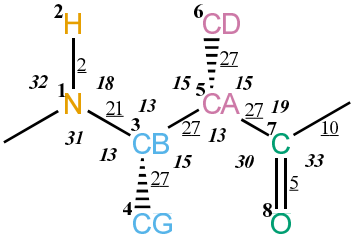

FIGURE 4.166. SSAM bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1 2 3
0					1
1	N	6	14	-0.31000	2 3 4 5
2	H	21	1	0.31000	3
3	CB	14	3	0.00000	4 5 6 7
4	CG	16	5	0.00000	5
5	CA	14	3	0.00000	6 7 8 9
6	CD	16	5	0.00000	7
7	C	12	12	0.45000	
8	O	1	16	-0.45000	

TABLE 4.411. Atoms of building block SSAM.

I	J	Type
1	2	2
1	3	21
3	4	27
3	5	27
5	6	27
5	7	27
7	8	5
7	9	10

TABLE 4.412. Bonds of building block SSAM.

I	J	K	Type
-1	1	2	32
-1	1	3	31
2	1	3	18
1	3	4	13
1	3	5	13
4	3	5	15
3	5	6	15
3	5	7	13
6	5	7	15
5	7	8	30
5	7	9	19
8	7	9	33

TABLE 4.413. Bond angles of building block SSAM.

I	J	K	L	Type
-2	-1	1	3	14
-1	1	3	5	43
-1	1	3	5	44
1	3	5	7	34
3	5	7	9	42
3	5	7	9	45

TABLE 4.414. Dihedral angles of building block SSAM.

I	J	K	L	Type
1	-1	3	2	1
3	1	5	4	2
6	3	7	5	2
7	5	9	8	1

TABLE 4.415. Improper dihedral angles of building block SSAM.

4.5. Nucleotides

Solute building block: 2'-deoxyadenosine 5'-phosphoric acid (DNA, charge -e)
Name: DADE

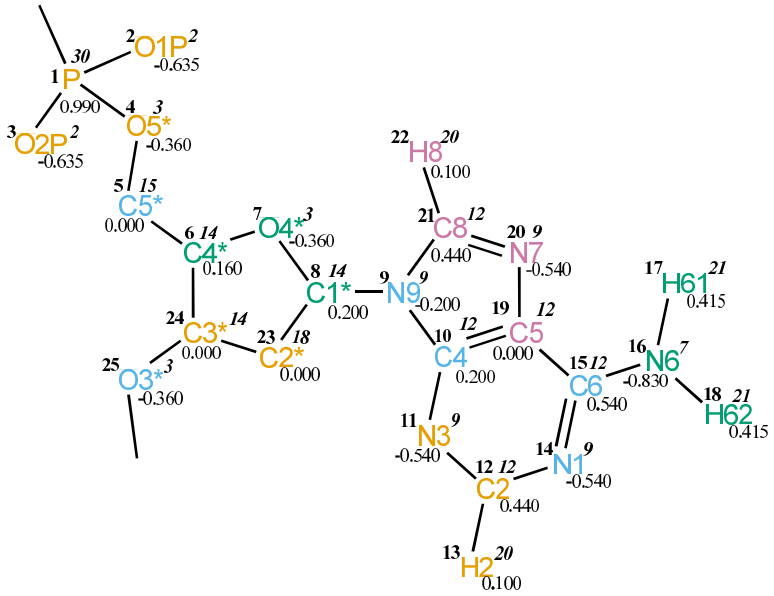

FIGURE 4.167. DADE non-bonded parameters.

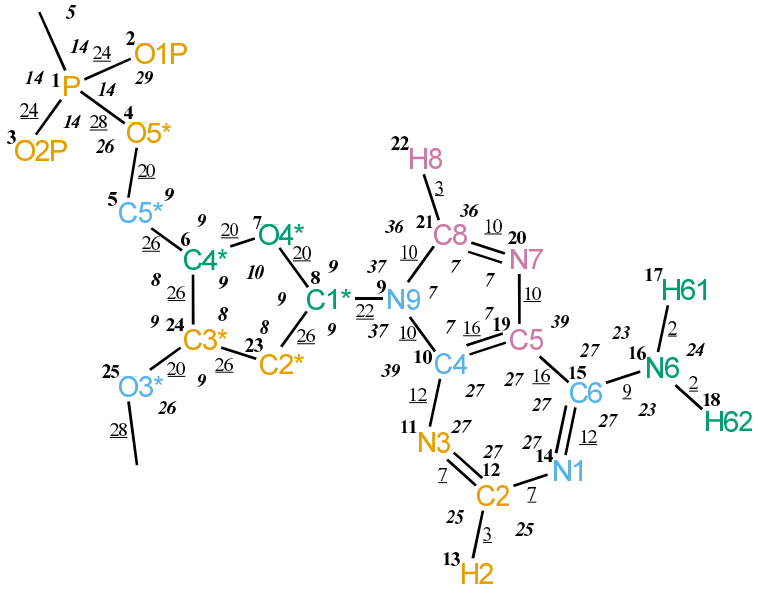

FIGURE 4.168. DADE bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 24
6	C4*	14	3	0.16000	7 8 23 24 25
7	O4*	3	16	-0.36000	8 9 23 24
8	C1*	14	3	0.20000	9 10 11 19 20 21 22 23 24
9	N9	9	14	-0.20000	10 11 12 15 19 20 21 22 23
10	C4	12	12	0.20000	11 12 13 14 15 16 19 20 21 22
11	N3	9	14	-0.54000	12 13 14 15 19 20 21
12	C2	12	12	0.44000	13 14 15 16 19
13	H2	20	1	0.10000	14 15
14	N1	9	14	-0.54000	15 16 19 20
15	C6	12	12	0.54000	16 17 18 19 20 21
16	N6	7	14	-0.83000	17 18 19 20
17	H61	21	1	0.41500	18 20
18	H62	21	1	0.41500	20
19	C5	12	12	0.00000	20 21 22
20	N7	9	14	-0.54000	21 22
21	C8	12	12	0.44000	22
22	H8	20	1	0.10000	
23	C2*	18	4	0.00000	24 25
24	C3*	14	3	0.00000	
25	O3*	3	16	-0.36000	

TABLE 4.416. Atoms of building block DADE.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	24	26
7	8	20
8	9	22
8	23	26
9	10	10
9	21	10
10	11	12
10	19	16
11	12	7
12	13	3
12	14	7
14	15	12
15	16	9
15	19	16
16	17	2
16	18	2
19	20	10
20	21	10
21	22	3
23	24	26
24	25	20
25	26	28

TABLE 4.417. Bonds of building block DADE.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	24	8
7	6	24	9
6	7	8	10
7	8	9	9
7	8	23	9
9	8	23	9
8	9	10	37
8	9	21	37
10	9	21	7
9	10	11	39
9	10	19	7
11	10	19	27
10	11	12	27
11	12	13	25
11	12	14	27
13	12	14	25
12	14	15	27
14	15	16	27
14	15	19	27
16	15	19	27
15	16	17	23
15	16	18	23
17	16	18	24
10	19	15	27
10	19	20	7
15	19	20	39
19	20	21	7
9	21	20	7
9	21	22	36
20	21	22	36
8	23	24	8
6	24	23	8
6	24	25	9
23	24	25	9
24	25	26	26

TABLE 4.418. Bond angles of building block DADE.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	24	17
4	5	6	24	34
24	6	7	8	29
5	6	24	23	34
5	6	24	25	17
7	6	24	23	17
7	6	24	25	18
6	7	8	23	29
7	8	9	10	16
7	8	23	24	17
7	8	23	24	34
19	15	16	17	14
8	23	24	6	34
8	23	24	25	17
6	24	25	26	29

TABLE 4.419. Dihedral angles of building block DADE.

I	J	K	L	Type
8	10	21	9	1
9	10	19	20	1
10	9	11	19	1
10	9	21	20	1
10	11	12	14	1
10	19	20	21	1
11	10	19	15	1
11	12	14	15	1
12	11	13	14	1
12	14	15	19	1
14	15	19	10	1
16	14	19	15	1
16	17	18	15	1
19	10	11	12	1
19	15	20	10	1
19	20	21	9	1
21	9	10	19	1
21	9	20	22	1
23	7	9	8	2
24	5	7	6	2
24	23	25	6	2

TABLE 4.420. Improper dihedral angles of building block DADE.

Solute building block: 2'-deoxyguanosine 5'-phosphoric acid (DNA, charge -*e*)
Name: DGUA

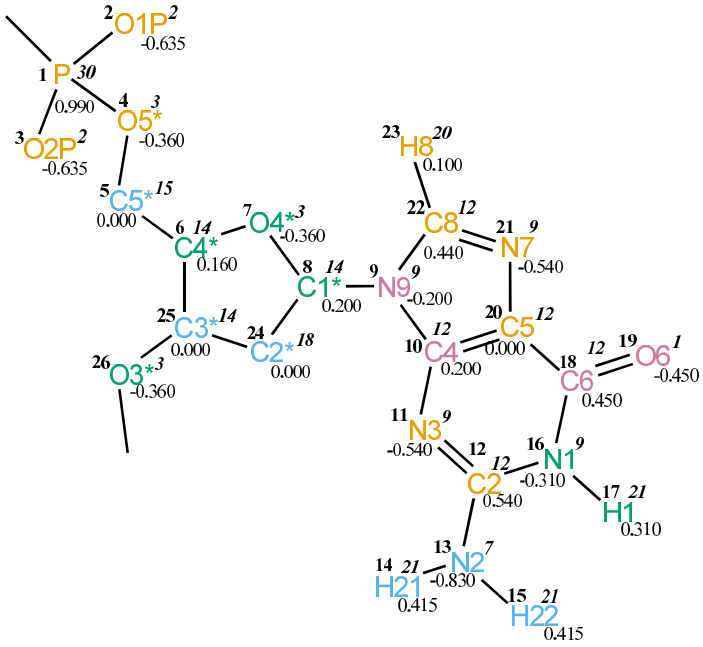

FIGURE 4.169. DGUA non-bonded parameters.

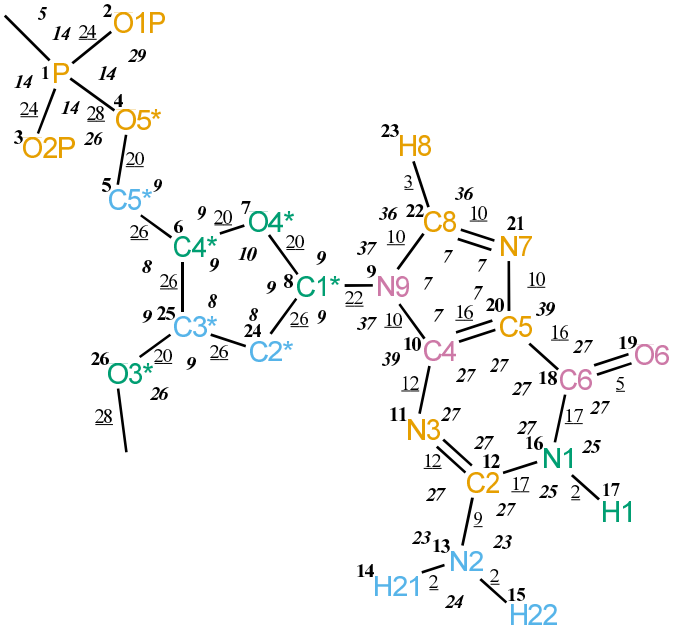

FIGURE 4.170. DGUA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 25
6	C4*	14	3	0.16000	7 8 24 25 26
7	O4*	3	16	-0.36000	8 9 24 25
8	C1*	14	3	0.20000	9 10 11 20 21 22 23 24 25
9	N9	9	14	-0.20000	10 11 12 18 20 21 22 23 24
10	C4	12	12	0.20000	11 12 13 16 18 19 20 21 22 23
11	N3	9	14	-0.54000	12 13 16 17 18 20 21 22
12	C2	12	12	0.54000	13 14 15 16 17 18 19 20
13	N2	7	14	-0.83000	14 15 16 17 18
14	H21	21	1	0.41500	15
15	H22	21	1	0.41500	
16	N1	9	14	-0.31000	17 18 19 20 21
17	H1	21	1	0.31000	18 19 20
18	C6	12	12	0.45000	19 20 21 22
19	O6	1	16	-0.45000	20 21
20	C5	12	12	0.00000	21 22 23
21	N7	9	14	-0.54000	22 23
22	C8	12	12	0.44000	23
23	H8	20	1	0.10000	
24	C2*	18	4	0.00000	25 26
25	C3*	14	3	0.00000	
26	O3*	3	16	-0.36000	

TABLE 4.421. Atoms of building block DGUA.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	25	26
7	8	20
8	9	22
8	24	26
9	10	10
9	22	10
10	11	12
10	20	16
11	12	12
12	13	9
12	16	17
13	14	2
13	15	2
16	17	2
16	18	17
18	19	5
18	20	16
20	21	10
21	22	10
22	23	3
24	25	26
25	26	20
26	27	28

TABLE 4.422. Bonds of building block DGUA.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	25	8
7	6	25	9
6	7	8	10
7	8	9	9
7	8	24	9
9	8	24	9
8	9	10	37
8	9	22	37
10	9	22	7
9	10	11	39
9	10	20	7
11	10	20	27
10	11	12	27
11	12	13	27
11	12	16	27
13	12	16	27
12	13	14	23
12	13	15	23
14	13	15	24
12	16	17	25
12	16	18	27
17	16	18	25
16	18	19	27
16	18	20	27
19	18	20	27
10	20	18	27
10	20	21	7
18	20	21	39
20	21	22	7
9	22	21	7
9	22	23	36
21	22	23	36
8	24	25	8
6	25	24	8
6	25	26	9
24	25	26	9
25	26	27	26

TABLE 4.423. Bond angles of building block DGUA.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	25	17
4	5	6	25	34
25	6	7	8	29
5	6	25	24	34
5	6	25	26	17
7	6	25	24	17
7	6	25	26	18
6	7	8	24	29
7	8	9	10	16
7	8	24	25	17
7	8	24	25	34
11	12	13	14	14
8	24	25	6	34
8	24	25	26	17
6	25	26	27	29

TABLE 4.424. Dihedral angles of building block DGUA.

I	J	K	L	Type
8	10	22	9	1
9	10	20	21	1
10	9	11	20	1
10	9	22	21	1
10	11	12	16	1
10	20	21	22	1
11	10	20	18	1
11	12	16	18	1
12	16	18	20	1
13	11	16	12	1
13	14	15	12	1
16	18	20	10	1
17	12	18	16	1
19	16	20	18	1
20	10	11	12	1
20	18	21	10	1
20	21	22	9	1
22	9	10	20	1
22	9	21	23	1
24	7	9	8	2
25	5	7	6	2
25	24	26	6	2

TABLE 4.425. Improper dihedral angles of building block DGUA.

Solute building block: 2'-deoxycytidine 5'-phosphoric acid (DNA, charge -e)
Name: DCYT

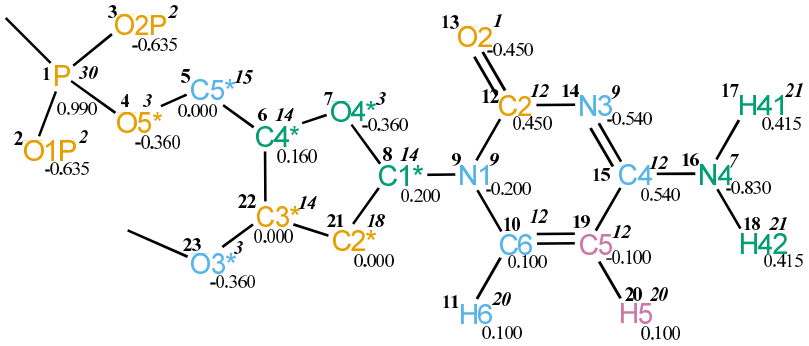

FIGURE 4.171. DCYT non-bonded parameters.

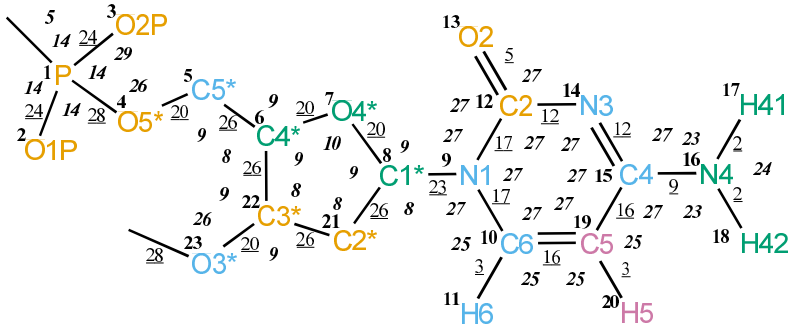

FIGURE 4.172. DCYT bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 22
6	C4*	14	3	0.16000	7 8 21 22 23
7	O4*	3	16	-0.36000	8 9 21 22
8	C1*	14	3	0.20000	9 10 11 12 13 14 19 21 22
9	N1	9	14	-0.20000	10 11 12 13 14 15 19 20 21
10	C6	12	12	0.10000	11 12 13 14 15 16 19 20
11	H6	20	1	0.10000	12 15 19 20
12	C2	12	12	0.45000	13 14 15 16 19
13	O2	1	16	-0.45000	14 15
14	N3	9	14	-0.54000	15 16 19 20
15	C4	12	12	0.54000	16 17 18 19 20
16	N4	7	14	-0.83000	17 18 19 20
17	H41	21	1	0.41500	18
18	H42	21	1	0.41500	
19	C5	12	12	-0.10000	20
20	H5	20	1	0.10000	
21	C2*	18	4	0.00000	22 23
22	C3*	14	3	0.00000	
23	O3*	3	16	-0.36000	

TABLE 4.426. Atoms of building block DCYT.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	22	26
7	8	20
8	9	23
8	21	26
9	10	17
9	12	17
10	11	3
10	19	16
12	13	5
12	14	12
14	15	12
15	16	9
15	19	16
16	17	2
16	18	2
19	20	3
21	22	26
22	23	20
23	24	28

TABLE 4.427. Bonds of building block DCYT.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	22	8
7	6	22	9
6	7	8	10
7	8	9	9
7	8	21	9
9	8	21	8
8	9	10	27
8	9	12	27
10	9	12	27
9	10	11	25
9	10	19	27
11	10	19	25
9	12	13	27
9	12	14	27
13	12	14	27
12	14	15	27
14	15	16	27
14	15	19	27
16	15	19	27
15	16	17	23
15	16	18	23
17	16	18	24
10	19	15	27
10	19	20	25
15	19	20	25
8	21	22	8
6	22	21	8
6	22	23	9
21	22	23	9
22	23	24	26

TABLE 4.428. Bond angles of building block DCYT.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	22	17
4	5	6	22	34
22	6	7	8	29
5	6	22	21	34
5	6	22	23	17
7	6	22	21	17
7	6	22	23	18
6	7	8	21	29
7	8	9	12	16
7	8	21	22	17
7	8	21	22	34
14	15	16	17	14
8	21	22	6	34
8	21	22	23	17
6	22	23	24	29

TABLE 4.429. Dihedral angles of building block DCYT.

I	J	K	L	Type
9	10	12	8	1
9	10	19	15	1
9	12	14	15	1
10	9	12	14	1
10	9	19	11	1
12	9	10	19	1
12	14	15	19	1
13	9	14	12	1
14	15	19	10	1
16	14	19	15	1
16	17	18	15	1
19	10	15	20	1
21	7	9	8	2
22	5	7	6	2
22	21	23	6	2

TABLE 4.430. Improper dihedral angles of building block DCYT.

Solute building block: 2'-deoxythymidine 5'-phosphoric acid (DNA, charge -*e*)
Name: DTHY

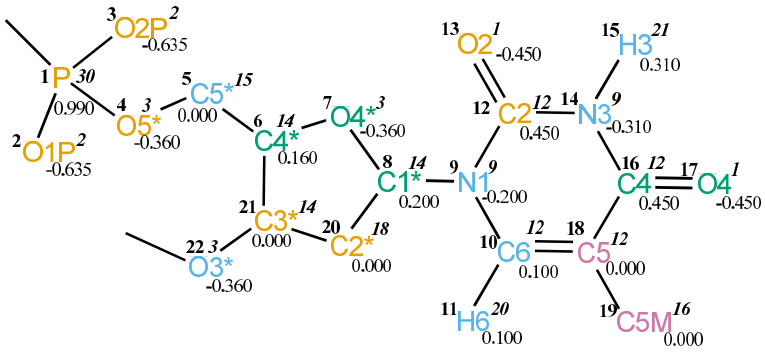

FIGURE 4.173. DTHY non-bonded parameters.

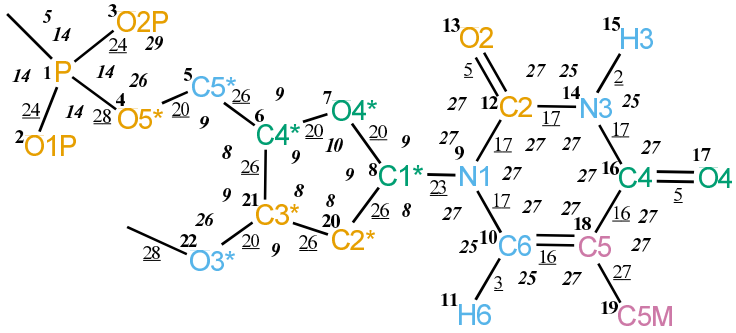

FIGURE 4.174. DTHY bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 21
6	C4*	14	3	0.16000	7 8 20 21 22
7	O4*	3	16	-0.36000	8 9 20 21
8	C1*	14	3	0.20000	9 10 11 12 13 14 18 20 21
9	N1	9	14	-0.20000	10 11 12 13 14 15 16 18 19 20
10	C6	12	12	0.10000	11 12 13 14 16 17 18 19
11	H6	20	1	0.10000	12 16 18 19
12	C2	12	12	0.45000	13 14 15 16 17 18
13	O2	1	16	-0.45000	14 15 16
14	N3	9	14	-0.31000	15 16 17 18 19
15	H3	21	1	0.31000	16 17 18
16	C4	12	12	0.45000	17 18 19
17	O4	1	16	-0.45000	18 19
18	C5	12	12	0.00000	19
19	C5M	16	5	0.00000	
20	C2*	18	4	0.00000	21 22
21	C3*	14	3	0.00000	
22	O3*	3	16	-0.36000	

TABLE 4.431. Atoms of building block DTHY.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	21	26
7	8	20
8	9	23
8	20	26
9	10	17
9	12	17
10	11	3
10	18	16
12	13	5
12	14	17
14	15	2
14	16	17
16	17	5
16	18	16
18	19	27
20	21	26
21	22	20
22	23	28

TABLE 4.432. Bonds of building block DTHY.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	21	8
7	6	21	9
6	7	8	10
7	8	9	9
7	8	20	9
9	8	20	8
8	9	10	27
8	9	12	27
10	9	12	27
9	10	11	25
9	10	18	27
11	10	18	25
9	12	13	27
9	12	14	27
13	12	14	27
12	14	15	25
12	14	16	27
15	14	16	25
14	16	17	27
14	16	18	27
17	16	18	27
10	18	16	27
10	18	19	27
16	18	19	27
8	20	21	8
6	21	20	8
6	21	22	9
20	21	22	9
21	22	23	26

TABLE 4.433. Bond angles of building block DTHY.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	21	17
4	5	6	21	34
21	6	7	8	29
5	6	21	20	34
5	6	21	22	17
7	6	21	20	17
7	6	21	22	18
6	7	8	20	29
7	8	9	12	16
7	8	20	21	17
7	8	20	21	34
8	20	21	6	34
8	20	21	22	17
6	21	22	23	29

TABLE 4.434. Dihedral angles of building block DTHY.

I	J	K	L	Type
9	10	12	8	1
9	10	18	16	1
9	12	14	16	1
10	9	12	14	1
10	9	18	11	1
12	9	10	18	1
12	14	16	18	1
13	9	14	12	1
14	16	18	10	1
15	12	16	14	1
17	14	18	16	1
18	10	16	19	1
20	7	9	8	2
21	5	7	6	2
21	20	22	6	2

TABLE 4.435. Improper dihedral angles of building block DTHY.

Solute building block: adenosine 5'-phosphoric acid (RNA, charge -e)
Name: ADE

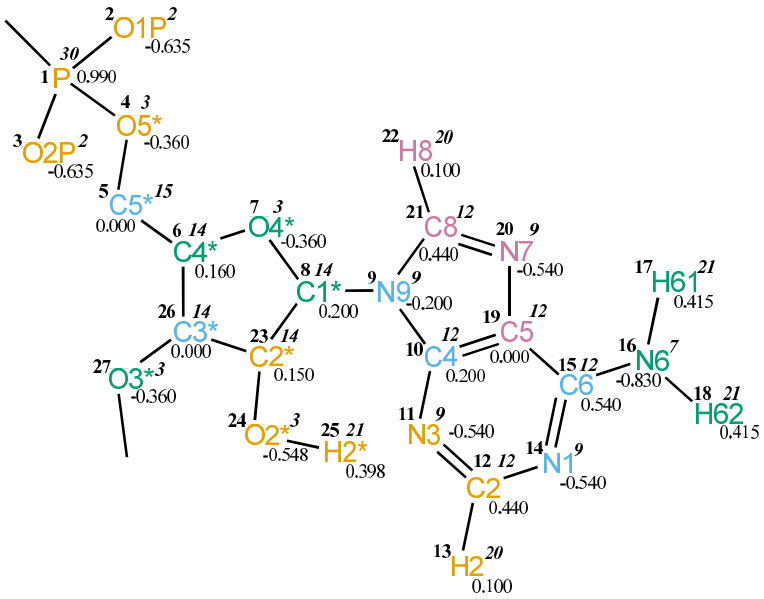

FIGURE 4.175. ADE non-bonded parameters.

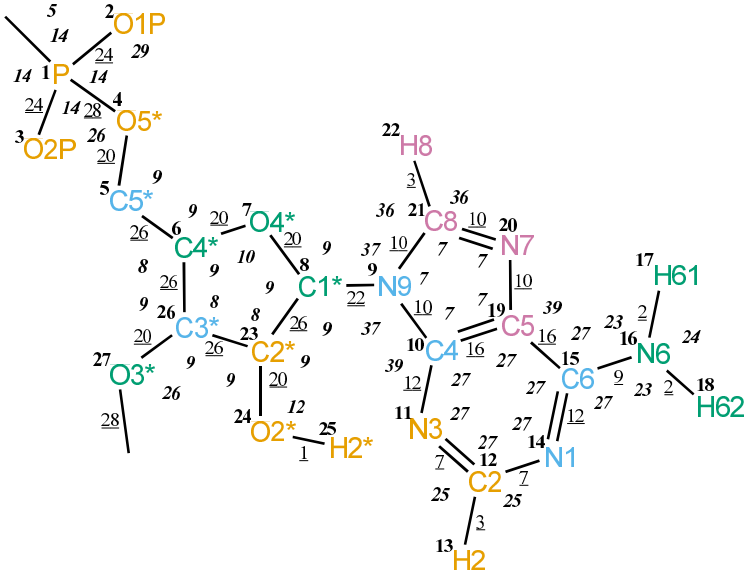

FIGURE 4.176. ADE bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 26
6	C4*	14	3	0.16000	7 8 23 26 27
7	O4*	3	16	-0.36000	8 9 23 26
8	C1*	14	3	0.20000	9 10 11 19 20 21 22 23 24 26
9	N9	9	14	-0.20000	10 11 12 15 19 20 21 22 23
10	C4	12	12	0.20000	11 12 13 14 15 16 19 20 21 22
11	N3	9	14	-0.54000	12 13 14 15 19 20 21
12	C2	12	12	0.44000	13 14 15 16 19
13	H2	20	1	0.10000	14 15
14	N1	9	14	-0.54000	15 16 19 20
15	C6	12	12	0.54000	16 17 18 19 20 21
16	N6	7	14	-0.83000	17 18 19 20
17	H61	21	1	0.41500	18 20
18	H62	21	1	0.41500	20
19	C5	12	12	0.00000	20 21 22
20	N7	9	14	-0.54000	21 22
21	C8	12	12	0.44000	22
22	H8	20	1	0.10000	
23	C2*	14	3	0.15000	24 25 26 27
24	O2*	3	16	-0.54800	25 26
25	H2*	21	1	0.39800	
26	C3*	14	3	0.00000	
27	O3*	3	16	-0.36000	

TABLE 4.436. Atoms of building block ADE.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	26	26
7	8	20
8	9	22
8	23	26
9	10	10
9	21	10
10	11	12
10	19	16
11	12	7
12	13	3
12	14	7
14	15	12
15	16	9
15	19	16
16	17	2
16	18	2
19	20	10
20	21	10
21	22	3
23	24	20
23	26	26
24	25	1
26	27	20
27	28	28

TABLE 4.437. Bonds of building block ADE.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	26	8
7	6	26	9
6	7	8	10
7	8	9	9
7	8	23	9
9	8	23	9
8	9	10	37
8	9	21	37
10	9	21	7
9	10	11	39
9	10	19	7
11	10	19	27
10	11	12	27
11	12	13	25
11	12	14	27
13	12	14	25
12	14	15	27
14	15	16	27
14	15	19	27
16	15	19	27
15	16	17	23
15	16	18	23
17	16	18	24
10	19	15	27
10	19	20	7
15	19	20	39
19	20	21	7
9	21	20	7
9	21	22	36
20	21	22	36
8	23	24	9
8	23	26	8
24	23	26	9
23	24	25	12
6	26	23	8
6	26	27	9
23	26	27	9
26	27	28	26

TABLE 4.438. Bond angles of building block ADE.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	26	17
4	5	6	26	34
26	6	7	8	29
5	6	26	23	34
5	6	26	27	17
7	6	26	23	17
7	6	26	27	18
6	7	8	23	29
7	8	9	10	16
7	8	23	24	18
7	8	23	26	17
7	8	23	26	34
9	8	23	24	17
19	15	16	17	14
8	23	24	25	23
8	23	26	6	34
8	23	26	27	17
24	23	26	6	17
24	23	26	27	18
6	26	27	28	29

TABLE 4.439. Dihedral angles of building block ADE.

I	J	K	L	Type
8	10	21	9	1
9	10	19	20	1
10	9	11	19	1
10	9	21	20	1
10	11	12	14	1
10	19	20	21	1
11	10	19	15	1
11	12	14	15	1
12	11	13	14	1
12	14	15	19	1
14	15	19	10	1
16	14	19	15	1
16	17	18	15	1
19	10	11	12	1
19	15	20	10	1
19	20	21	9	1
21	9	10	19	1
21	9	20	22	1
23	7	9	8	2
23	24	26	8	2
26	5	7	6	2
26	23	27	6	2

TABLE 4.440. Improper dihedral angles of building block ADE.

Solute building block: guanosine 5'-phosphoric acid (RNA, charge -*e*)
Name: GUA

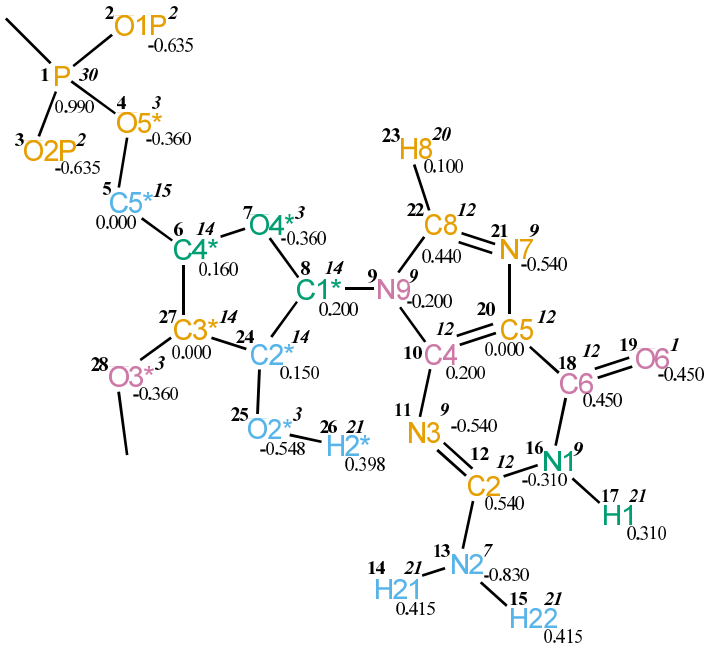

FIGURE 4.177. GUA non-bonded parameters.

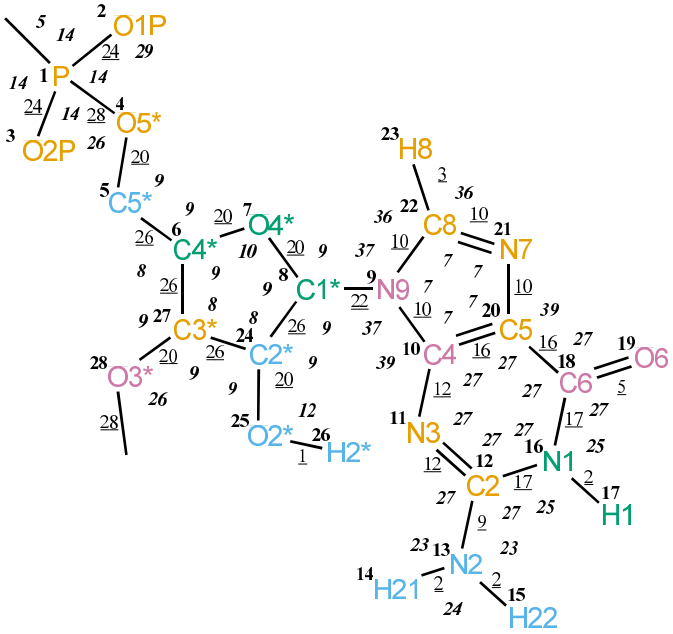

FIGURE 4.178. GUA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 27
6	C4*	14	3	0.16000	7 8 24 27 28
7	O4*	3	16	-0.36000	8 9 24 27
8	C1*	14	3	0.20000	9 10 11 20 21 22 23 24 25 27
9	N9	9	14	-0.20000	10 11 12 18 20 21 22 23 24
10	C4	12	12	0.20000	11 12 13 16 18 19 20 21 22 23
11	N3	9	14	-0.54000	12 13 16 17 18 20 21 22
12	C2	12	12	0.54000	13 14 15 16 17 18 19 20
13	N2	7	14	-0.83000	14 15 16 17 18
14	H21	21	1	0.41500	15
15	H22	21	1	0.41500	
16	N1	9	14	-0.31000	17 18 19 20 21
17	H1	21	1	0.31000	18 19 20
18	C6	12	12	0.45000	19 20 21 22
19	O6	1	16	-0.45000	20 21
20	C5	12	12	0.00000	21 22 23
21	N7	9	14	-0.54000	22 23
22	C8	12	12	0.44000	23
23	H8	20	1	0.10000	
24	C2*	14	3	0.15000	25 26 27 28
25	O2*	3	16	-0.54800	26 27
26	H2*	21	1	0.39800	
27	C3*	14	3	0.00000	
28	O3*	3	16	-0.36000	

TABLE 4.441. Atoms of building block GUA.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26

TABLE 4.443: continues on next page.

I	J	K	Type
4	5	6	9
5	6	7	9
5	6	27	8
7	6	27	9
6	7	8	10
7	8	9	9
7	8	24	9
9	8	24	9
8	9	10	37
8	9	22	37
10	9	22	7
9	10	11	39
9	10	20	7
11	10	20	27
10	11	12	27
11	12	13	27
11	12	16	27
13	12	16	27
12	13	14	23
12	13	15	23
14	13	15	24
12	16	17	25
12	16	18	27
17	16	18	25
16	18	19	27
16	18	20	27
19	18	20	27
10	20	18	27
10	20	21	7
18	20	21	39
20	21	22	7
9	22	21	7
9	22	23	36
21	22	23	36
8	24	25	9
8	24	27	8
25	24	27	9
24	25	26	12
6	27	24	8
6	27	28	9
24	27	28	9
27	28	29	26

TABLE 4.443: Bond angles of building block GUA.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	27	26
7	8	20
8	9	22
8	24	26
9	10	10
9	22	10
10	11	12
10	20	16
11	12	12
12	13	9
12	16	17
13	14	2
13	15	2
16	17	2
16	18	17
18	19	5
18	20	16
20	21	10
21	22	10
22	23	3
24	25	20
24	27	26
25	26	1
27	28	20
28	29	28

TABLE 4.442. Bonds of building block GUA.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	27	17
4	5	6	27	34
27	6	7	8	29
5	6	27	24	34
5	6	27	28	17
7	6	27	24	17
7	6	27	28	18
6	7	8	24	29
7	8	9	10	16
7	8	24	25	18
7	8	24	27	17
7	8	24	27	34
9	8	24	25	17
11	12	13	14	14
8	24	25	26	23
8	24	27	6	34
8	24	27	28	17
25	24	27	6	17
25	24	27	28	18
6	27	28	29	29

TABLE 4.444. Dihedral angles of building block GUA.

I	J	K	L	Type
8	10	22	9	1
9	10	20	21	1
10	9	11	20	1
10	9	22	21	1
10	11	12	16	1
10	20	21	22	1
11	10	20	18	1
11	12	16	18	1
12	16	18	20	1
13	11	16	12	1
13	14	15	12	1
16	18	20	10	1
17	12	18	16	1
19	16	20	18	1
20	10	11	12	1
20	18	21	10	1
20	21	22	9	1
22	9	10	20	1
22	9	21	23	1
24	7	9	8	2
24	25	27	8	2
27	5	7	6	2
27	24	28	6	2

TABLE 4.445. Improper dihedral angles of building block GUA.

Solute building block: cytidine 5'-phosphoric acid (RNA, charge -e)
Name: CYT

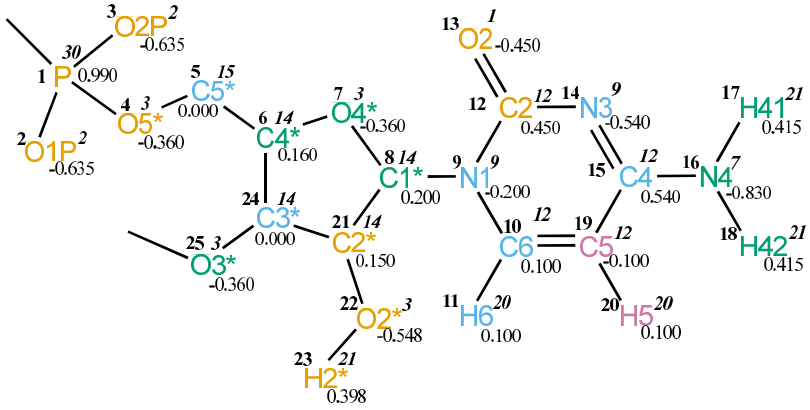

FIGURE 4.179. CYT non-bonded parameters.

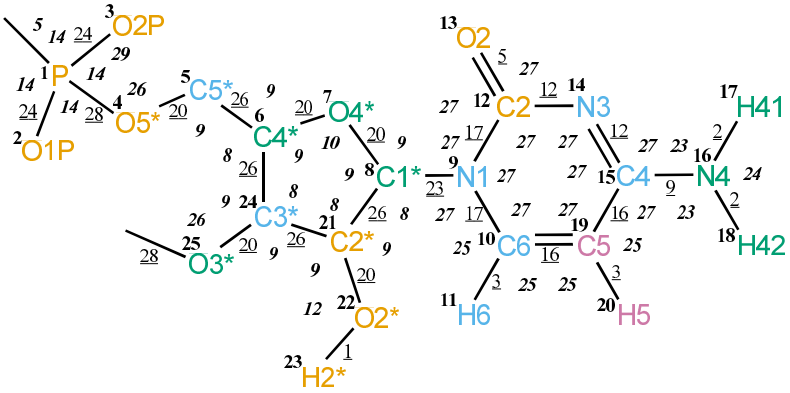

FIGURE 4.180. CYT bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 24
6	C4*	14	3	0.16000	7 8 21 24 25
7	O4*	3	16	-0.36000	8 9 21 24
8	C1*	14	3	0.20000	9 10 11 12 13 14 19 21 22 24
9	N1	9	14	-0.20000	10 11 12 13 14 15 19 20 21
10	C6	12	12	0.10000	11 12 13 14 15 16 19 20
11	H6	20	1	0.10000	12 15 19 20
12	C2	12	12	0.45000	13 14 15 16 19
13	O2	1	16	-0.45000	14 15
14	N3	9	14	-0.54000	15 16 19 20
15	C4	12	12	0.54000	16 17 18 19 20
16	N4	7	14	-0.83000	17 18 19 20
17	H41	21	1	0.41500	18
18	H42	21	1	0.41500	
19	C5	12	12	-0.10000	20
20	H5	20	1	0.10000	
21	C2*	14	3	0.15000	22 23 24 25
22	O2*	3	16	-0.54800	23 24
23	H2*	21	1	0.39800	
24	C3*	14	3	0.00000	
25	O3*	3	16	-0.36000	

TABLE 4.446. Atoms of building block CYT.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	24	26
7	8	20
8	9	23
8	21	26
9	10	17
9	12	17
10	11	3
10	19	16
12	13	5
12	14	12
14	15	12
15	16	9
15	19	16
16	17	2
16	18	2
19	20	3
21	22	20
21	24	26
22	23	1
24	25	20
25	26	28

TABLE 4.447. Bonds of building block CYT.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	24	8
7	6	24	9
6	7	8	10
7	8	9	9
7	8	21	9
9	8	21	8
8	9	10	27
8	9	12	27
10	9	12	27
9	10	11	25
9	10	19	27
11	10	19	25
9	12	13	27
9	12	14	27
13	12	14	27
12	14	15	27
14	15	16	27
14	15	19	27
16	15	19	27
15	16	17	23
15	16	18	23
17	16	18	24
10	19	15	27
10	19	20	25
15	19	20	25
8	21	22	9
8	21	24	8
22	21	24	9
21	22	23	12
6	24	21	8
6	24	25	9
21	24	25	9
24	25	26	26

TABLE 4.448. Bond angles of building block CYT.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	24	17
4	5	6	24	34
24	6	7	8	29
5	6	24	21	34
5	6	24	25	17
7	6	24	21	17
7	6	24	25	18
6	7	8	21	29
7	8	9	12	16
7	8	21	22	18
7	8	21	24	17
7	8	21	24	34
9	8	21	22	17
14	15	16	17	14
8	21	22	23	23
8	21	24	6	34
8	21	24	25	17
22	21	24	6	17
22	21	24	25	18
6	24	25	26	29

TABLE 4.449. Dihedral angles of building block CYT.

I	J	K	L	Type
9	10	12	8	1
9	10	19	15	1
9	12	14	15	1
10	9	12	14	1
10	9	19	11	1
12	9	10	19	1
12	14	15	19	1
13	9	14	12	1
14	15	19	10	1
16	14	19	15	1
16	17	18	15	1
19	10	15	20	1
21	7	9	8	2
21	22	24	8	2
24	5	7	6	2
24	21	25	6	2

TABLE 4.450. Improper dihedral angles of building block CYT.

Solute building block: uridine 5'-phosphoric acid (RNA, charge -e)
Name: URA

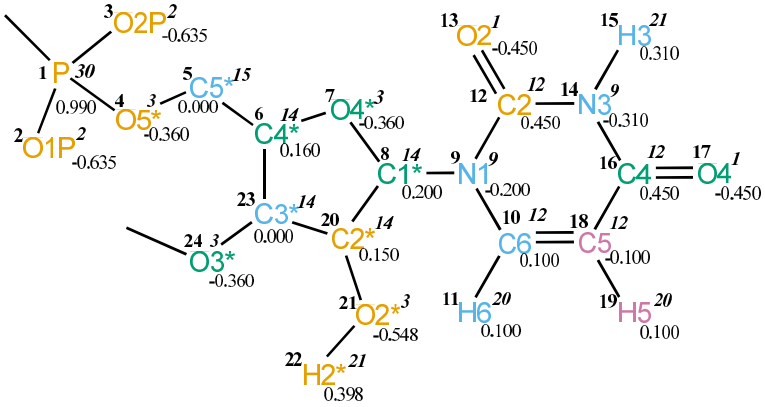

FIGURE 4.181. URA non-bonded parameters.

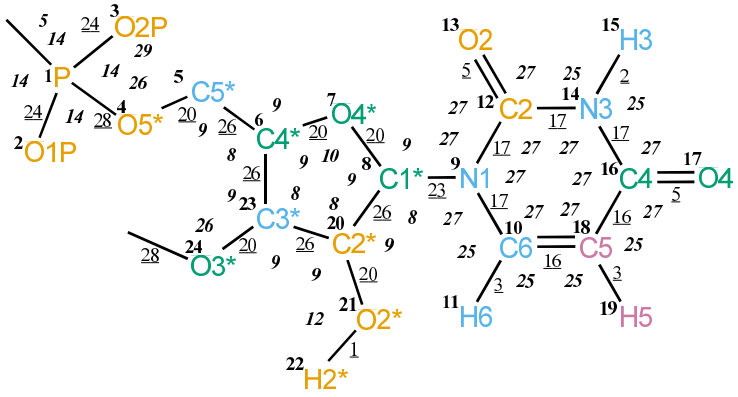

FIGURE 4.182. URA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 3 4
1	P	30	31	0.99000	2 3 4 5
2	O1P	2	16	-0.63500	3 4
3	O2P	2	16	-0.63500	4
4	O5*	3	16	-0.36000	5 6
5	C5*	15	4	0.00000	6 7 23
6	C4*	14	3	0.16000	7 8 20 23 24
7	O4*	3	16	-0.36000	8 9 20 23
8	C1*	14	3	0.20000	9 10 11 12 13 14 18 20 21 23
9	N1	9	14	-0.20000	10 11 12 13 14 15 16 18 19 20
10	C6	12	12	0.10000	11 12 13 14 16 17 18 19
11	H6	20	1	0.10000	12 16 18 19
12	C2	12	12	0.45000	13 14 15 16 17 18
13	O2	1	16	-0.45000	14 15 16
14	N3	9	14	-0.31000	15 16 17 18 19
15	H3	21	1	0.31000	16 17 18
16	C4	12	12	0.45000	17 18 19
17	O4	1	16	-0.45000	18 19
18	C5	12	12	-0.10000	19
19	H5	20	1	0.10000	
20	C2*	14	3	0.15000	21 22 23 24
21	O2*	3	16	-0.54800	22 23
22	H2*	21	1	0.39800	
23	C3*	14	3	0.00000	
24	O3*	3	16	-0.36000	

TABLE 4.451. Atoms of building block URA.

I	J	Type
1	2	24
1	3	24
1	4	28
4	5	20
5	6	26
6	7	20
6	23	26
7	8	20
8	9	23
8	20	26
9	10	17
9	12	17
10	11	3
10	18	16
12	13	5
12	14	17
14	15	2
14	16	17
16	17	5
16	18	16
18	19	3
20	21	20
20	23	26
21	22	1
23	24	20
24	25	28

TABLE 4.452. Bonds of building block URA.

I	J	K	Type
0	1	2	14
0	1	3	14
0	1	4	5
2	1	3	29
2	1	4	14
3	1	4	14
1	4	5	26
4	5	6	9
5	6	7	9
5	6	23	8
7	6	23	9
6	7	8	10
7	8	9	9
7	8	20	9
9	8	20	8
8	9	10	27
8	9	12	27
10	9	12	27
9	10	11	25
9	10	18	27
11	10	18	25
9	12	13	27
9	12	14	27
13	12	14	27
12	14	15	25
12	14	16	27
15	14	16	25
14	16	17	27
14	16	18	27
17	16	18	27
10	18	16	27
10	18	19	25
16	18	19	25
8	20	21	9
8	20	23	8
21	20	23	9
20	21	22	12
6	23	20	8
6	23	24	9
20	23	24	9
23	24	25	26

TABLE 4.453. Bond angles of building block URA.

I	J	K	L	Type
-1	0	1	4	20
-1	0	1	4	27
0	1	4	5	20
0	1	4	5	27
1	4	5	6	7
1	4	5	6	22
4	5	6	7	8
4	5	6	7	25
4	5	6	23	17
4	5	6	23	34
23	6	7	8	29
5	6	23	20	34
5	6	23	24	17
7	6	23	20	17
7	6	23	24	18
6	7	8	20	29
7	8	9	12	16
7	8	20	21	18
7	8	20	23	17
7	8	20	23	34
9	8	20	21	17
8	20	21	22	23
8	20	23	6	34
8	20	23	24	17
21	20	23	6	17
21	20	23	24	18
6	23	24	25	29

TABLE 4.454. Dihedral angles of building block URA.

I	J	K	L	Type
9	10	12	8	1
9	10	18	16	1
9	12	14	16	1
10	9	12	14	1
10	9	18	11	1
12	9	10	18	1
12	14	16	18	1
13	9	14	12	1
14	16	18	10	1
15	12	16	14	1
17	14	18	16	1
18	10	16	19	1
20	7	9	8	2
20	21	23	8	2
23	5	7	6	2
23	20	24	6	2

TABLE 4.455. Improper dihedral angles of building block URA.

Solute building block: flavin mononucleotide (oxydized,deprotonated at FN5 and FN1;charge -e, $OPOHO_2^-$)
Name: FMNO

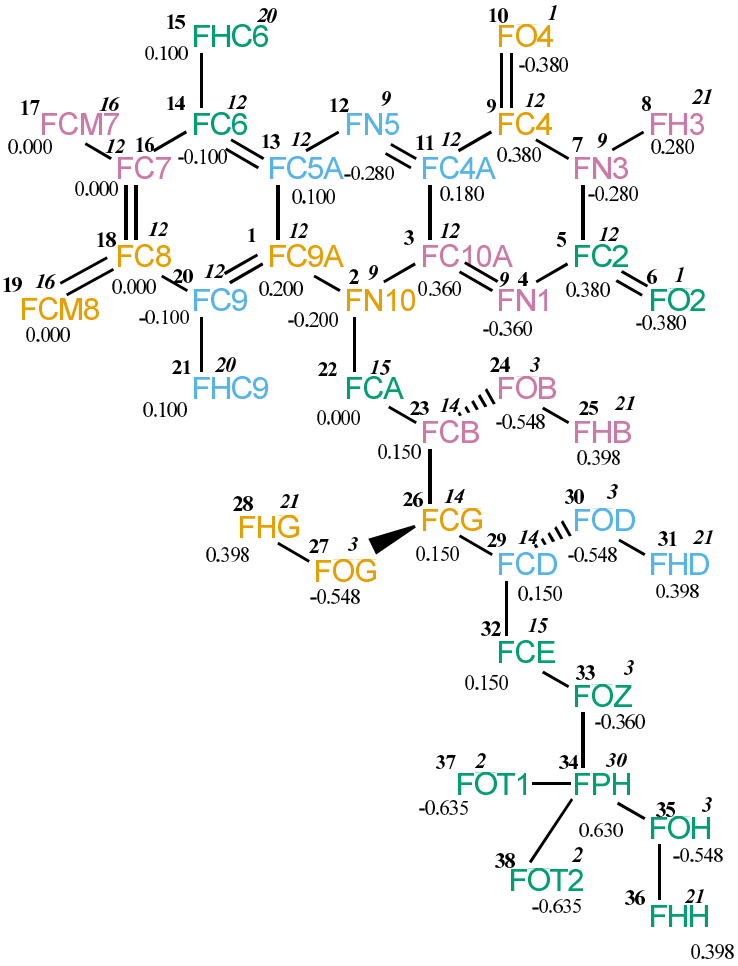

FIGURE 4.183. FMNO non-bonded parameters.

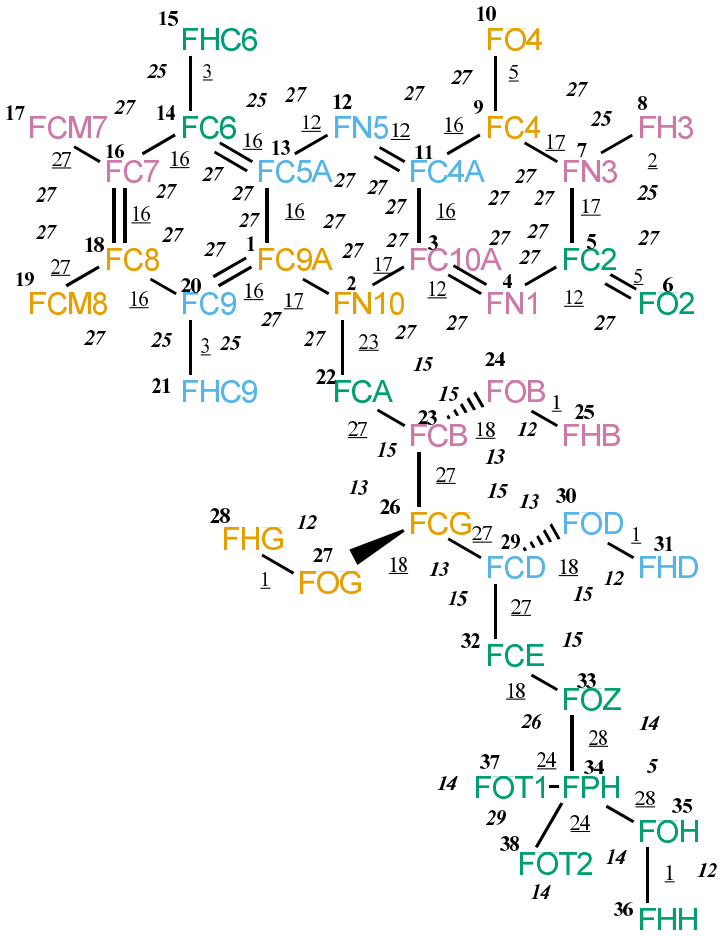

FIGURE 4.184. FMNO bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	FC9A	12	12	0.20000	2 3 4 11 12 13 14 15 16 18 19 20 21 22
2	FN10	9	14	-0.20000	3 4 5 9 11 12 13 14 18 20 21 22 23
3	FC10A	12	12	0.36000	4 5 6 7 9 10 11 12 13 20 22
4	FN1	9	14	-0.36000	5 6 7 8 9 11 12 22
5	FC2	12	12	0.38000	6 7 8 9 10 11
6	FO2	1	16	-0.38000	7 8 9
7	FN3	9	14	-0.28000	8 9 10 11 12
8	FH3	21	1	0.28000	9 10 11
9	FC4	12	12	0.38000	10 11 12 13
10	FO4	1	16	-0.38000	11 12
11	FC4A	12	12	0.18000	12 13 14 22
12	FN5	9	14	-0.28000	13 14 15 16 20
13	FC5A	12	12	0.10000	14 15 16 17 18 20 21 22
14	FC6	12	12	-0.10000	15 16 17 18 19 20
15	FHC6	20	1	0.10000	16 17 18
16	FC7	12	12	0.00000	17 18 19 20 21
17	FCM7	16	5	0.00000	18 19 20
18	FC8	12	12	0.00000	19 20 21
19	FCM8	16	5	0.00000	20 21
20	FC9	12	12	-0.10000	21 22
21	FHC9	20	1	0.10000	
22	FCA	15	4	0.00000	23 24 26
23	FCB	14	3	0.15000	24 25 26 27 29
24	FOB	3	16	-0.54800	25 26
25	FHB	21	1	0.39800	
26	FCG	14	3	0.15000	27 28 29 30 32
27	FOG	3	16	-0.54800	28 29
28	FHG	21	1	0.39800	
29	FCD	14	3	0.15000	30 31 32 33
30	FOD	3	16	-0.54800	31 32
31	FHD	21	1	0.39800	
32	FCE	15	4	0.15000	33 34
33	FOZ	3	16	-0.36000	34 35 36 37 38
34	FPH	30	31	0.63000	35 36 37 38
35	FOH	3	16	-0.54800	36 37 38
36	FHH	21	1	0.39800	37 38
37	FOT1	2	16	-0.63500	38
38	FOT2	2	16	-0.63500	

TABLE 4.456: Atoms of building block FMNO.

I	J	Type
1	2	17
1	13	16
1	20	16
2	3	17
2	22	23
3	4	12
3	11	16
4	5	12
5	6	5
5	7	17
7	8	2
7	9	17
9	10	5
9	11	16
11	12	12
12	13	12
13	14	16
14	15	3
14	16	16
16	17	27
16	18	16
18	19	27
18	20	16
20	21	3
22	23	27
23	24	18
23	26	27
24	25	1
26	27	18
26	29	27
27	28	1
29	30	18
29	32	27
30	31	1
32	33	18
33	34	28
34	35	28
34	37	24
34	38	24
35	36	1

TABLE 4.457: Bonds of building block FMNO.

I	J	K	Type
2	1	13	27
2	1	20	27
13	1	20	27
1	2	3	27
1	2	22	27
3	2	22	27
2	3	4	27
2	3	11	27
4	3	11	27
3	4	5	27
4	5	6	27
4	5	7	27
6	5	7	27
5	7	8	25
5	7	9	27
8	7	9	25
7	9	10	27
7	9	11	27
10	9	11	27
3	11	9	27
3	11	12	27
9	11	12	27
11	12	13	27
1	13	12	27
1	13	14	27
12	13	14	27
13	14	15	25
13	14	16	27
15	14	16	25
14	16	17	27
14	16	18	27
17	16	18	27
16	18	19	27
16	18	20	27
19	18	20	27
1	20	18	27
1	20	21	25
18	20	21	25
2	22	23	15
22	23	24	15
22	23	26	15
24	23	26	13
23	24	25	12
23	26	27	13
23	26	29	15
27	26	29	13

TABLE 4.458: continues on next page.

I	J	K	Type
26	27	28	12
26	29	30	13
26	29	32	15
30	29	32	15
29	30	31	12
29	32	33	15
32	33	34	26
33	34	35	5
33	34	37	14
33	34	38	14
35	34	37	14
35	34	38	14
37	34	38	29
34	35	36	12

TABLE 4.458: Bond angles of building block FMNO.

I	J	K	L	Type
13	1	2	3	14
1	2	3	11	14
1	2	22	23	40
3	11	12	13	14
11	12	13	1	14
2	22	23	26	34
22	23	24	25	23
22	23	26	29	34
23	26	27	28	23
23	26	29	32	34
26	29	30	31	23
26	29	32	33	34
29	32	33	34	7
29	32	33	34	22
32	33	34	35	20
32	33	34	35	27
33	34	35	36	20
33	34	35	36	27

TABLE 4.459: Dihedral angles of building block FMNO.

I	J	K	L	Type
1	2	20	13	1
1	13	14	16	1
2	1	13	12	1
2	3	11	12	1
3	4	5	7	1
4	3	11	9	1
4	5	7	9	1
5	4	7	6	1
5	7	9	11	1
7	5	9	8	1
7	9	11	3	1
9	7	11	10	1
11	2	4	3	1
11	3	4	5	1
11	9	12	3	1
13	1	20	18	1
13	12	14	1	1
13	14	16	18	1
14	16	18	20	1
15	13	16	14	1
16	14	18	17	1
16	18	20	1	1
18	16	20	19	1
20	1	13	14	1
20	1	18	21	1
23	24	26	22	2
26	27	29	23	2
29	30	32	26	2

TABLE 4.460: Improper dihedral angles of building block FMNO.

Solute building block: proflavin (protonated at FN5; charge $+e$)
Name: PFN

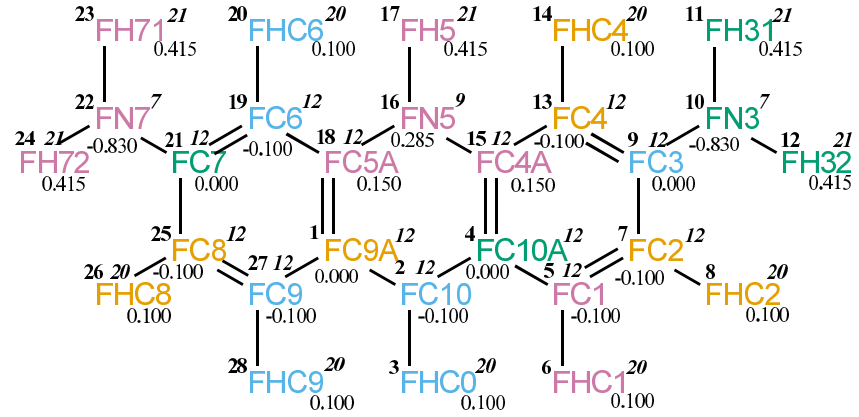

FIGURE 4.185. PFN non-bonded parameters.

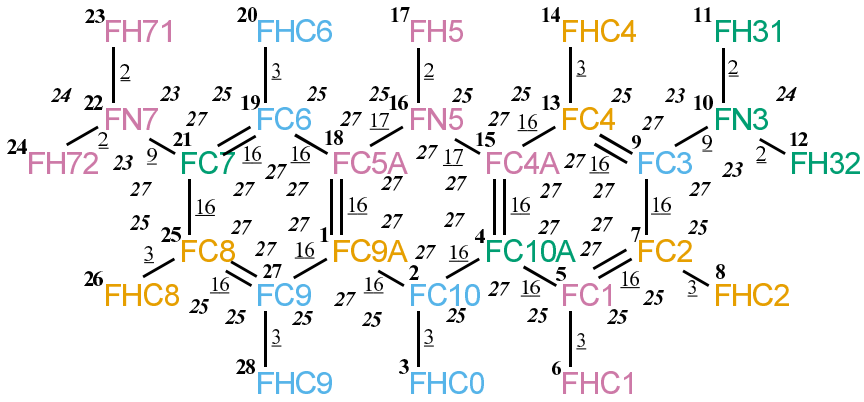

FIGURE 4.186. PFN bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	FC9A	12	12	0.00000	2 3 4 5 15 16 17 18 19 20 21 25 26 27 28
2	FC10	12	12	-0.10000	3 4 5 6 7 13 15 16 18 19 25 27 28
3	FHC0	20	1	0.10000	4 5 15 18 27
4	FC10A	12	12	0.00000	5 6 7 8 9 13 14 15 16 17 18 27
5	FC1	12	12	-0.10000	6 7 8 9 10 13 15 16
6	FHC1	20	1	0.10000	7 8 9 15
7	FC2	12	12	-0.10000	8 9 10 13 14 15
8	FHC2	20	1	0.10000	9 10 13
9	FC3	12	12	0.00000	10 11 12 13 14 15 16
10	FN3	7	14	-0.83000	11 12 13 14 15
11	FH31	21	1	0.41500	12
12	FH32	21	1	0.41500	
13	FC4	12	12	-0.10000	14 15 16 17 18
14	FHC4	20	1	0.10000	15 16
15	FC4A	12	12	0.15000	16 17 18 19
16	FN5	9	14	0.28500	17 18 19 20 21 27
17	FH5	21	1	0.41500	18 19
18	FC5A	12	12	0.15000	19 20 21 22 25 27 28
19	FC6	12	12	-0.10000	20 21 22 25 26 27
20	FHC6	20	1	0.10000	21 22 25
21	FC7	12	12	0.00000	22 23 24 25 26 27 28
22	FN7	7	14	-0.83000	23 24 25 26 27
23	FH71	21	1	0.41500	24
24	FH72	21	1	0.41500	
25	FC8	12	12	-0.10000	26 27 28
26	FHC8	20	1	0.10000	27 28
27	FC9	12	12	-0.10000	28
28	FHC9	20	1	0.10000	

TABLE 4.461: Atoms of building block PFN.

I	J	Type
1	2	16
1	18	16
1	27	16
2	3	3
2	4	16
4	5	16
4	15	16
5	6	3
5	7	16
7	8	3
7	9	16
9	10	9
9	13	16
10	11	2
10	12	2
13	14	3
13	15	16
15	16	17
16	17	2
16	18	17
18	19	16
19	20	3
19	21	16
21	22	9
21	25	16
22	23	2
22	24	2
25	26	3
25	27	16
27	28	3

TABLE 4.462: Bonds of building block PFN.

I	J	K	Type
2	1	18	27
2	1	27	27
18	1	27	27
1	2	3	25
1	2	4	27
3	2	4	25
2	4	5	27
2	4	15	27
5	4	15	27
4	5	6	25
4	5	7	27
6	5	7	25
5	7	8	25
5	7	9	27
8	7	9	25
7	9	10	27
7	9	13	27
10	9	13	27
9	10	11	23
9	10	12	23
11	10	12	24
9	13	14	25
9	13	15	27
14	13	15	25
4	15	13	27
4	15	16	27
13	15	16	27
15	16	17	25
15	16	18	27
17	16	18	25
1	18	16	27
1	18	19	27
16	18	19	27
18	19	20	25
18	19	21	27
20	19	21	25
19	21	22	27
19	21	25	27
22	21	25	27
21	22	23	23
21	22	24	23
23	22	24	24
21	25	26	25
21	25	27	27
26	25	27	25
1	27	25	27

TABLE 4.463: continues on next page.

I	J	K	Type
1	27	28	25
25	27	28	25

TABLE 4.463: Bond angles of building block PFN.

I	J	K	L	Type
7	9	10	11	14
25	21	22	23	14

TABLE 4.464: Dihedral angles of building block PFN.

I	J	K	L	Type
1	2	4	15	1
1	2	27	18	1
1	18	19	21	1
2	1	4	3	1
2	1	18	16	1
2	4	15	16	1
4	5	7	9	1
4	15	16	18	1
5	4	7	6	1
5	4	15	13	1
5	7	9	13	1
7	5	9	8	1
7	9	13	15	1
9	7	13	10	1
9	13	15	4	1
10	11	12	9	1
13	9	15	14	1
15	2	5	4	1
15	4	5	7	1
15	13	16	4	1
15	16	18	1	1
16	15	18	17	1
18	1	2	4	1
18	1	27	25	1
18	16	19	1	1
18	19	21	25	1
19	18	21	20	1
19	21	25	27	1
21	25	27	1	1
22	19	25	21	1
22	23	24	21	1
25	21	27	26	1
27	1	18	19	1
27	1	25	28	1

TABLE 4.465: Improper dihedral angles of building block PFN.

Solute building block: nicotinamide adenine dinucleotide (NAD+; charge -*e*)
Name: NADP

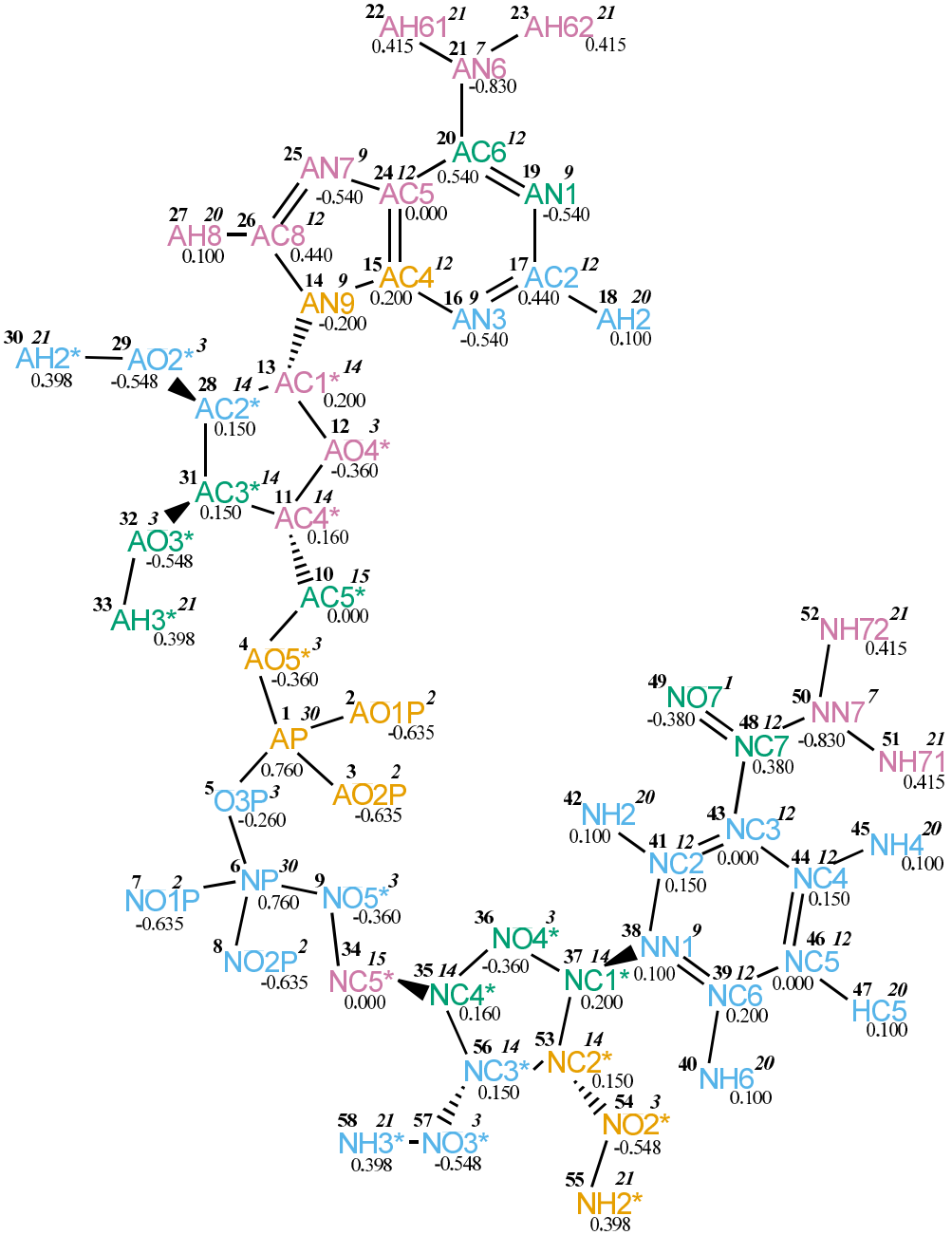

FIGURE 4.187. NADP non-bonded parameters.

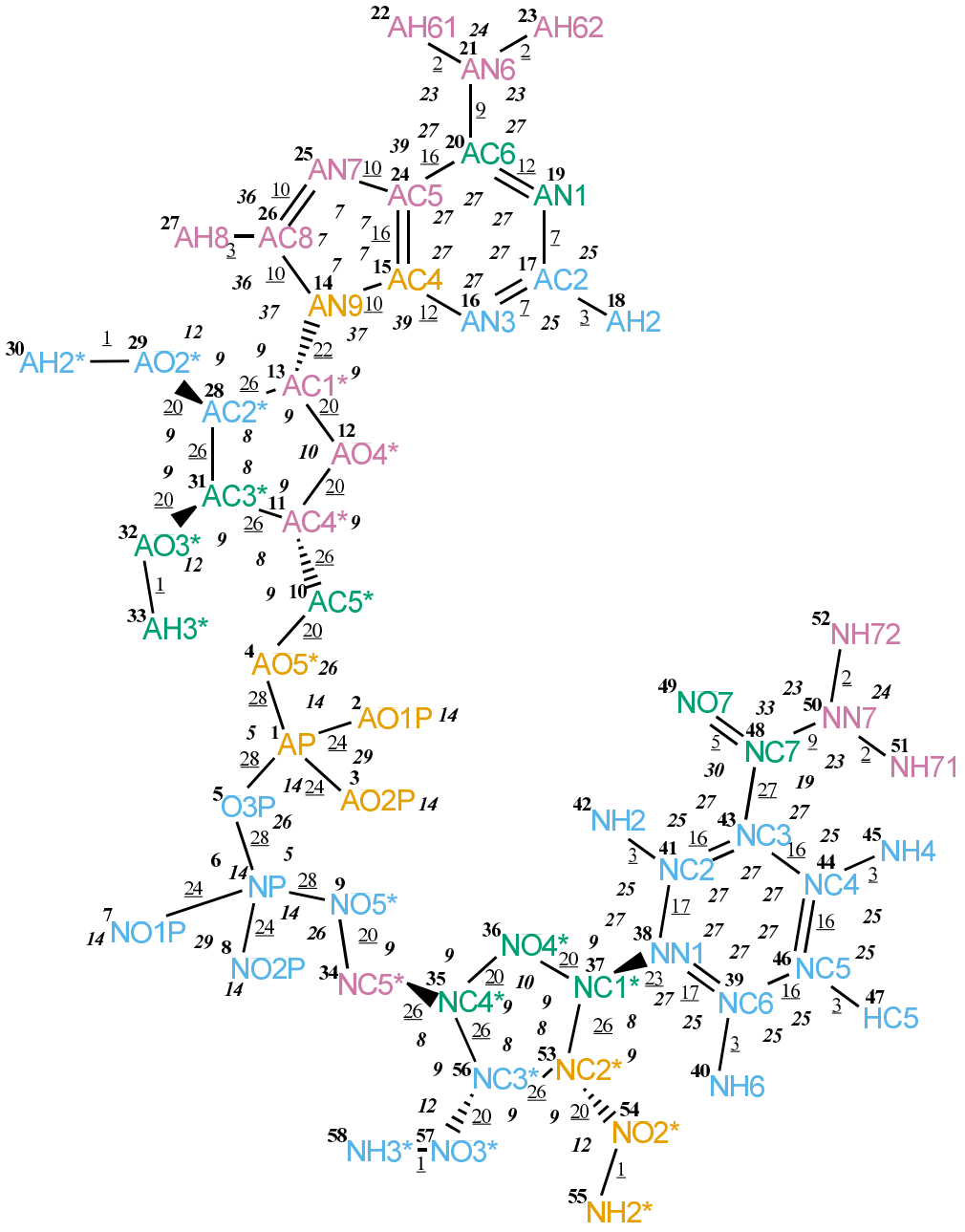

FIGURE 4.188. NADP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	AP	30	31	0.76000	2 3 4 5 6 10
2	AO1P	2	16	-0.63500	3 4 5
3	AO2P	2	16	-0.63500	4 5
4	AO5*	3	16	-0.36000	5 10 11
5	O3P	3	16	-0.26000	6 7 8 9
6	NP	30	31	0.76000	7 8 9 34
7	NO1P	2	16	-0.63500	8 9
8	NO2P	2	16	-0.63500	9
9	NO5*	3	16	-0.36000	34 35
10	AC5*	15	4	0.00000	11 12 31
11	AC4*	14	3	0.16000	12 13 28 31 32
12	AO4*	3	16	-0.36000	13 14 28 31
13	AC1*	14	3	0.20000	14 15 16 24 25 26 27 28 29 31
14	AN9	9	14	-0.20000	15 16 17 20 24 25 26 27 28
15	AC4	12	12	0.20000	16 17 18 19 20 21 24 25 26 27
16	AN3	9	14	-0.54000	17 18 19 20 24 25 26
17	AC2	12	12	0.44000	18 19 20 21 24
18	AH2	20	1	0.10000	19 20
19	AN1	9	14	-0.54000	20 21 24 25
20	AC6	12	12	0.54000	21 22 23 24 25 26
21	AN6	7	14	-0.83000	22 23 24 25
22	AH61	21	1	0.41500	23 25
23	AH62	21	1	0.41500	25
24	AC5	12	12	0.00000	25 26 27
25	AN7	9	14	-0.54000	26 27
26	AC8	12	12	0.44000	27
27	AH8	20	1	0.10000	
28	AC2*	14	3	0.15000	29 30 31 32
29	AO2*	3	16	-0.54800	30 31
30	AH2*	21	1	0.39800	
31	AC3*	14	3	0.15000	32 33
32	AO3*	3	16	-0.54800	33
33	AH3*	21	1	0.39800	
34	NC5*	15	4	0.00000	35 36 56
35	NC4*	14	3	0.16000	36 37 53 56 57
36	NO4*	3	16	-0.36000	37 38 53 56
37	NC1*	14	3	0.20000	38 39 40 41 42 43 46 53 54 56
38	NN1	9	14	0.10000	39 40 41 42 43 44 46 47 48 53
39	NC6	12	12	0.20000	40 41 42 43 44 45 46 47
40	NH6	20	1	0.10000	41 44 46 47
41	NC2	12	12	0.15000	42 43 44 45 46 48
42	NH2	20	1	0.10000	43 44 48
43	NC3	12	12	0.00000	44 45 46 47 48 49 50
44	NC4	12	12	0.15000	45 46 47 48
45	NH4	20	1	0.10000	46 47 48
46	NC5	12	12	0.00000	47 48

TABLE 4.466: continues on next page.

Seq.	Name	IAC	Mass	Charge	Exclusions
47	HC5	20	1	0.10000	
48	NC7	12	12	0.38000	49 50 51 52
49	NO7	1	16	-0.38000	50
50	NN7	7	14	-0.83000	51 52
51	NH71	21	1	0.41500	52
52	NH72	21	1	0.41500	
53	NC2*	14	3	0.15000	54 55 56 57
54	NO2*	3	16	-0.54800	55 56
55	NH2*	21	1	0.39800	
56	NC3*	14	3	0.15000	57 58
57	NO3*	3	16	-0.54800	58
58	NH3*	21	1	0.39800	

TABLE 4.466: Atoms of building block NADP.

I	J	Type
1	2	24
1	3	24
1	4	28
1	5	28
4	10	20
5	6	28
6	7	24
6	8	24
6	9	28
9	34	20
10	11	26
11	12	20
11	31	26
12	13	20
13	14	22
13	28	26
14	15	10
14	26	10
15	16	12
15	24	16
16	17	7
17	18	3
17	19	7
19	20	12
20	21	9
20	24	16
21	22	2
21	23	2
24	25	10
25	26	10
26	27	3
28	29	20
28	31	26
29	30	1
31	32	20
32	33	1
34	35	26
35	36	20
35	56	26
36	37	20
37	38	23
37	53	26
38	39	17
38	41	17
39	40	3
39	46	16

TABLE 4.467: continues on next page.

I	J	Type
41	42	3
41	43	16
43	44	16
43	48	27
44	45	3
44	46	16
46	47	3
48	49	5
48	50	9
50	51	2
50	52	2
53	54	20
53	56	26
54	55	1
56	57	20
57	58	1

TABLE 4.467: Bonds of building block NADP.

I	J	K	Type
2	1	3	29
2	1	4	14
2	1	5	14
3	1	4	14
3	1	5	14
4	1	5	5
1	4	10	26
1	5	6	26
5	6	7	14
5	6	8	14
5	6	9	5
7	6	8	29
7	6	9	14
8	6	9	14
6	9	34	26
4	10	11	9
10	11	12	9
10	11	31	8
12	11	31	9
11	12	13	10
12	13	14	9
12	13	28	9
14	13	28	9
13	14	15	37
13	14	26	37
15	14	26	7
14	15	16	39
14	15	24	7
16	15	24	27
15	16	17	27
16	17	18	25
16	17	19	27
18	17	19	25
17	19	20	27
19	20	21	27
19	20	24	27
21	20	24	27
20	21	22	23
20	21	23	23
22	21	23	24
15	24	20	27
15	24	25	7
20	24	25	39
24	25	26	7
14	26	25	7
14	26	27	36

TABLE 4.468: continues on next page.

I	J	K	Type
25	26	27	36
13	28	29	9
13	28	31	8
29	28	31	9
28	29	30	12
11	31	28	8
11	31	32	9
28	31	32	9
31	32	33	12
9	34	35	9
34	35	36	9
34	35	56	8
36	35	56	9
35	36	37	10
36	37	38	9
36	37	53	9
38	37	53	8
37	38	39	27
37	38	41	27
39	38	41	27
38	39	40	25
38	39	46	27
40	39	46	25
38	41	42	25
38	41	43	27
42	41	43	25
41	43	44	27
41	43	48	27
44	43	48	27
43	44	45	25
43	44	46	27
45	44	46	25
39	46	44	27
39	46	47	25
44	46	47	25
43	48	49	30
43	48	50	19
49	48	50	33
48	50	51	23
48	50	52	23
51	50	52	24
37	53	54	9
37	53	56	8
54	53	56	9
53	54	55	12
35	56	53	8
35	56	57	9

TABLE 4.468: continues on next page.

I	J	K	Type
53	56	57	9
56	57	58	12

TABLE 4.468: Bond angles of building block NADP.

I	J	K	L	Type
5	1	4	10	20
5	1	4	10	27
4	1	5	6	20
4	1	5	6	27
1	4	10	11	7
1	4	10	11	22
1	5	6	9	20
1	5	6	9	27
5	6	9	34	20
5	6	9	34	27
6	9	34	35	7
6	9	34	35	22
4	10	11	12	8
4	10	11	12	25
4	10	11	31	17
4	10	11	31	34
31	11	12	13	29
10	11	31	28	34
10	11	31	32	17
12	11	31	28	17
12	11	31	32	18
11	12	13	28	29
12	13	14	15	16
12	13	28	29	18
12	13	28	31	17
12	13	28	31	34
14	13	28	29	17
24	20	21	22	14
13	28	29	30	23
13	28	31	11	34
13	28	31	32	17
29	28	31	11	17
29	28	31	32	18
11	31	32	33	23
9	34	35	36	8
9	34	35	36	25
9	34	35	56	17
9	34	35	56	34
56	35	36	37	29
34	35	56	53	34
34	35	56	57	17
36	35	56	53	17
36	35	56	57	18
35	36	37	53	29
36	37	38	41	16
36	37	53	54	18

TABLE 4.469: continues on next page.

I	J	K	L	Type
36	37	53	56	17
36	37	53	56	34
38	37	53	54	17
41	43	48	50	10
43	48	50	51	14
37	53	54	55	23
37	53	56	35	34
37	53	56	57	17
54	53	56	35	17
54	53	56	57	18
35	56	57	58	23

TABLE 4.469: Dihedral angles of building block NADP.

I	J	K	L	Type
14	13	15	26	1
14	15	24	25	1
15	14	16	24	1
15	14	26	25	1
15	16	17	19	1
15	24	25	26	1
16	15	24	20	1
16	17	19	20	1
17	16	18	19	1
17	19	20	24	1
19	20	24	15	1
20	19	21	24	1
21	20	22	23	1
24	15	16	17	1
24	15	20	25	1
24	25	26	14	1
26	14	15	24	1
26	14	25	27	1
28	12	14	13	2
28	29	31	13	2
31	10	12	11	2
31	28	32	11	2
38	37	39	41	1
38	39	46	44	1
38	41	43	44	1
39	38	40	46	1
39	38	41	43	1
41	38	39	46	1
41	38	42	43	1
41	43	44	46	1
43	41	44	48	1
43	44	46	39	1
44	43	46	45	1
46	39	44	47	1
48	43	49	50	1
50	48	51	52	1
53	36	38	37	2
53	54	56	37	2
56	34	36	35	2
56	53	57	35	2

TABLE 4.470: Improper dihedral angles of building block NADP.

Solute building block: nicotinamide adenine dinucleotide phosphate(NADPH;charge -3e, $OPOHO_2^-$)
Name: NDPH

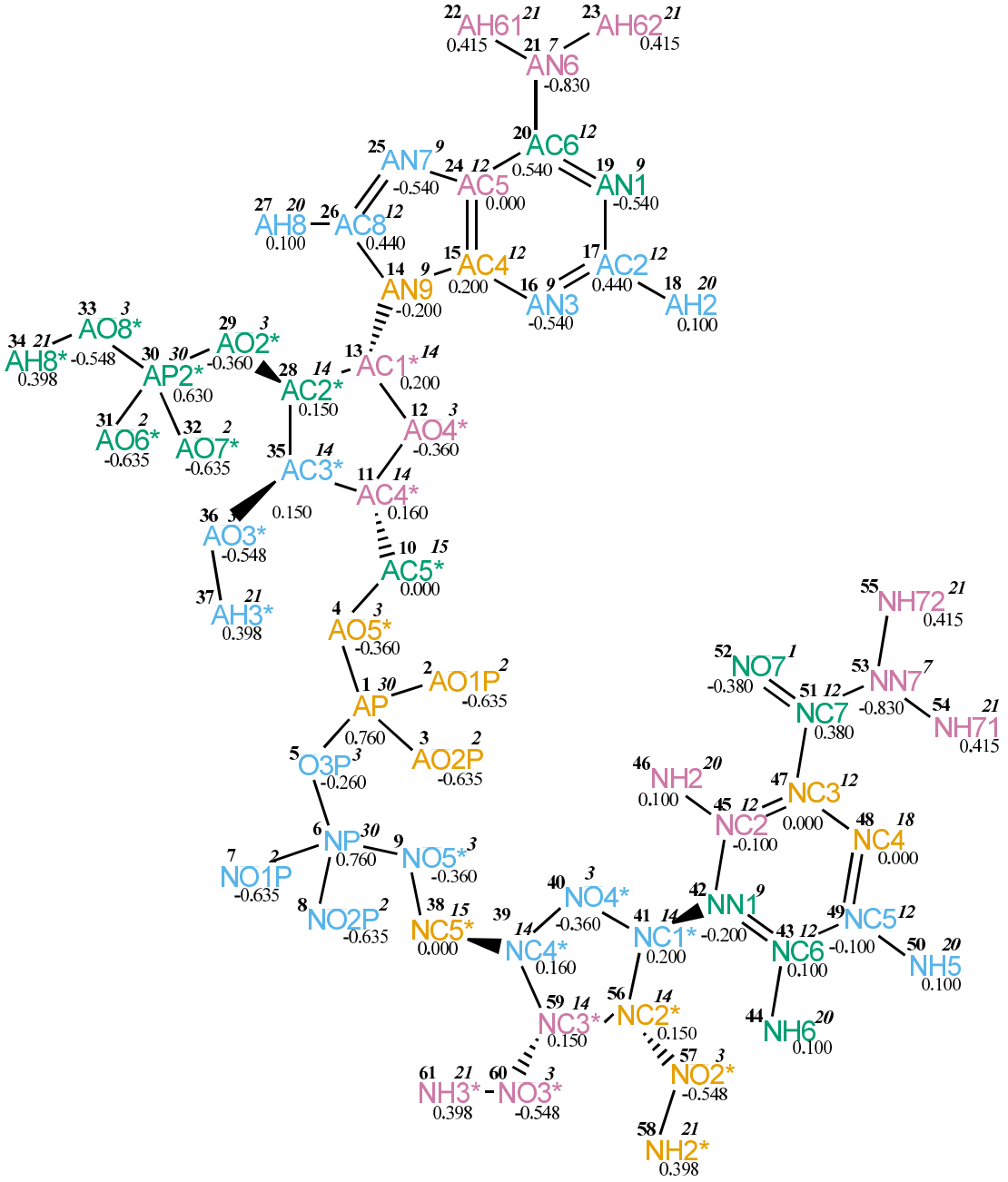

FIGURE 4.189. NDPH non-bonded parameters.

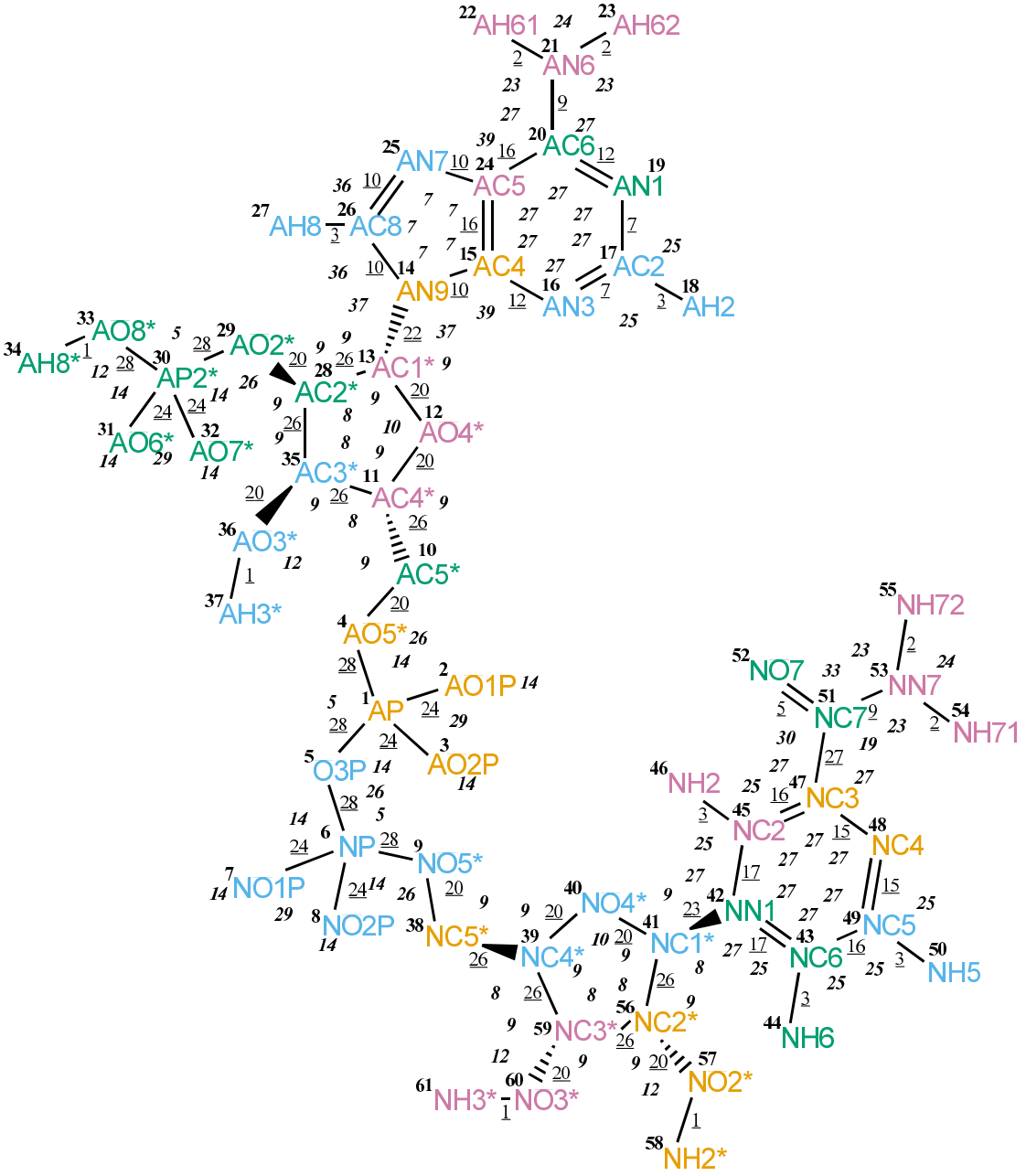

FIGURE 4.190. NDPH bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	AP	30	31	0.76000	2 3 4 5 6 10
2	AO1P	2	16	-0.63500	3 4 5
3	AO2P	2	16	-0.63500	4 5
4	AO5*	3	16	-0.36000	5 10 11
5	O3P	3	16	-0.26000	6 7 8 9
6	NP	30	31	0.76000	7 8 9 38
7	NO1P	2	16	-0.63500	8 9
8	NO2P	2	16	-0.63500	9
9	NO5*	3	16	-0.36000	38 39
10	AC5*	15	4	0.00000	11 12 35
11	AC4*	14	3	0.16000	12 13 28 35 36
12	AO4*	3	16	-0.36000	13 14 28 35
13	AC1*	14	3	0.20000	14 15 16 24 25 26 27 28 29 35
14	AN9	9	14	-0.20000	15 16 17 20 24 25 26 27 28
15	AC4	12	12	0.20000	16 17 18 19 20 21 24 25 26 27
16	AN3	9	14	-0.54000	17 18 19 20 24 25 26
17	AC2	12	12	0.44000	18 19 20 21 24
18	AH2	20	1	0.10000	19 20
19	AN1	9	14	-0.54000	20 21 24 25
20	AC6	12	12	0.54000	21 22 23 24 25 26
21	AN6	7	14	-0.83000	22 23 24 25
22	AH61	21	1	0.41500	23 25
23	AH62	21	1	0.41500	25
24	AC5	12	12	0.00000	25 26 27
25	AN7	9	14	-0.54000	26 27
26	AC8	12	12	0.44000	27
27	AH8	20	1	0.10000	
28	AC2*	14	3	0.15000	29 30 35 36
29	AO2*	3	16	-0.36000	30 31 32 33 34 35
30	AP2*	30	31	0.63000	31 32 33 34
31	AO6*	2	16	-0.63500	32 33 34
32	AO7*	2	16	-0.63500	33 34
33	AO8*	3	16	-0.54800	34
34	AH8*	21	1	0.39800	
35	AC3*	14	3	0.15000	36 37
36	AO3*	3	16	-0.54800	37
37	AH3*	21	1	0.39800	
38	NC5*	15	4	0.00000	39 40 59
39	NC4*	14	3	0.16000	40 41 56 59 60
40	NO4*	3	16	-0.36000	41 42 56 59
41	NC1*	14	3	0.20000	42 43 44 45 46 47 49 56 57 59
42	NN1	9	14	-0.20000	43 44 45 46 47 48 49 50 51 56
43	NC6	12	12	0.10000	44 45 46 47 48 49 50
44	NH6	20	1	0.10000	45 48 49 50
45	NC2	12	12	-0.10000	46 47 48 49 51
46	NH2	20	1	0.10000	47 48 51

TABLE 4.471: continues on next page.

Seq.	Name	IAC	Mass	Charge	Exclusions
47	NC3	12	12	0.00000	48 49 50 51 52 53
48	NC4	18	4	0.00000	49 50 51
49	NC5	12	12	-0.10000	50 51
50	NH5	20	1	0.10000	
51	NC7	12	12	0.38000	52 53 54 55
52	NO7	1	16	-0.38000	53
53	NN7	7	14	-0.83000	54 55
54	NH71	21	1	0.41500	55
55	NH72	21	1	0.41500	
56	NC2*	14	3	0.15000	57 58 59 60
57	NO2*	3	16	-0.54800	58 59
58	NH2*	21	1	0.39800	
59	NC3*	14	3	0.15000	60 61
60	NO3*	3	16	-0.54800	61
61	NH3*	21	1	0.39800	

TABLE 4.471: Atoms of building block NDPH.

I	J	Type
1	2	24
1	3	24
1	4	28
1	5	28
4	10	20
5	6	28
6	7	24
6	8	24
6	9	28
9	38	20
10	11	26
11	12	20
11	35	26
12	13	20
13	14	22
13	28	26
14	15	10
14	26	10
15	16	12
15	24	16
16	17	7
17	18	3
17	19	7
19	20	12
20	21	9
20	24	16
21	22	2
21	23	2
24	25	10
25	26	10
26	27	3
28	29	20
28	35	26
29	30	28
30	31	24
30	32	24
30	33	28
33	34	1
35	36	20
36	37	1
38	39	26
39	40	20
39	59	26
40	41	20
41	42	23
41	56	26

TABLE 4.472: continues on next page.

I	J	Type
42	43	17
42	45	17
43	44	3
43	49	16
45	46	3
45	47	16
47	48	15
47	51	27
48	49	15
49	50	3
51	52	5
51	53	9
53	54	2
53	55	2
56	57	20
56	59	26
57	58	1
59	60	20
60	61	1

TABLE 4.472: Bonds of building block NDPH.

I	J	K	Type
2	1	3	29
2	1	4	14
2	1	5	14
3	1	4	14
3	1	5	14
4	1	5	5
1	4	10	26
1	5	6	26
5	6	7	14
5	6	8	14
5	6	9	5
7	6	8	29
7	6	9	14
8	6	9	14
6	9	38	26
4	10	11	9
10	11	12	9
10	11	35	8
12	11	35	9
11	12	13	10
12	13	14	9
12	13	28	9
14	13	28	9
13	14	15	37
13	14	26	37
15	14	26	7
14	15	16	39
14	15	24	7
16	15	24	27
15	16	17	27
16	17	18	25
16	17	19	27
18	17	19	25
17	19	20	27
19	20	21	27
19	20	24	27
21	20	24	27
20	21	22	23
20	21	23	23
22	21	23	24
15	24	20	27
15	24	25	7
20	24	25	39
24	25	26	7
14	26	25	7
14	26	27	36

TABLE 4.473: continues on next page.

I	J	K	Type
25	26	27	36
13	28	29	9
13	28	35	8
29	28	35	9
28	29	30	26
29	30	31	14
29	30	32	14
29	30	33	5
31	30	32	29
31	30	33	14
32	30	33	14
30	33	34	12
11	35	28	8
11	35	36	9
28	35	36	9
35	36	37	12
9	38	39	9
38	39	40	9
38	39	59	8
40	39	59	9
39	40	41	10
40	41	42	9
40	41	56	9
42	41	56	8
41	42	43	27
41	42	45	27
43	42	45	27
42	43	44	25
42	43	49	27
44	43	49	25
42	45	46	25
42	45	47	27
46	45	47	25
45	47	48	27
45	47	51	27
48	47	51	27
47	48	49	27
43	49	48	27
43	49	50	25
48	49	50	25
47	51	52	30
47	51	53	19
52	51	53	33
51	53	54	23
51	53	55	23
54	53	55	24
41	56	57	9

TABLE 4.473: continues on next page.

I	J	K	Type
41	56	59	8
57	56	59	9
56	57	58	12
39	59	56	8
39	59	60	9
56	59	60	9
59	60	61	12

TABLE 4.473: Bond angles of building block NDPH.

I	J	K	L	Type
5	1	4	10	20
5	1	4	10	27
4	1	5	6	20
4	1	5	6	27
1	4	10	11	7
1	4	10	11	22
1	5	6	9	20
1	5	6	9	27
5	6	9	38	20
5	6	9	38	27
6	9	38	39	7
6	9	38	39	22
4	10	11	12	8
4	10	11	12	25
4	10	11	35	17
4	10	11	35	34
35	11	12	13	29
10	11	35	28	34
10	11	35	36	17
12	11	35	28	17
12	11	35	36	18
11	12	13	28	29
12	13	14	15	16
12	13	28	29	18
12	13	28	35	17
12	13	28	35	34
14	13	28	29	17
24	20	21	22	14
13	28	29	30	23
13	28	35	11	34
13	28	35	36	17
29	28	35	11	17
29	28	35	36	18
28	29	30	33	20
28	29	30	33	27
29	30	33	34	20
29	30	33	34	27
11	35	36	37	23
9	38	39	40	8
9	38	39	40	25
9	38	39	59	17
9	38	39	59	34
59	39	40	41	29
38	39	59	56	34
38	39	59	60	17
40	39	59	56	17

TABLE 4.474: continues on next page.

I	J	K	L	Type
40	39	59	60	18
39	40	41	56	29
40	41	42	45	16
40	41	56	57	18
40	41	56	59	17
40	41	56	59	34
42	41	56	57	17
45	47	51	53	10
47	51	53	54	14
41	56	57	58	23
41	56	59	39	34
41	56	59	60	17
57	56	59	39	17
57	56	59	60	18
39	59	60	61	23

TABLE 4.474: Dihedral angles of building block NDPH.

I	J	K	L	Type
14	13	15	26	1
14	15	24	25	1
15	14	16	24	1
15	14	26	25	1
15	16	17	19	1
15	24	25	26	1
16	15	24	20	1
16	17	19	20	1
17	16	18	19	1
17	19	20	24	1
19	20	24	15	1
20	19	21	24	1
21	20	22	23	1
24	15	16	17	1
24	15	20	25	1
24	25	26	14	1
26	14	15	24	1
26	14	25	27	1
28	12	14	13	2
28	29	35	13	2
35	10	12	11	2
35	28	36	11	2
42	41	43	45	1
42	43	49	48	1
42	45	47	48	1
43	42	44	49	1
43	42	45	47	1
45	42	43	49	1
45	42	46	47	1
45	47	48	49	1
47	45	48	51	1
47	48	49	43	1
49	43	48	50	1
51	47	52	53	1
53	51	54	55	1
56	40	42	41	2
56	57	59	41	2
59	38	40	39	2
59	56	60	39	2

TABLE 4.475: Improper dihedral angles of building block NDPH.

4.6. Carbohydrates

Solute building block: -2-D-glucopyranose-β-1-
Name: GB2P

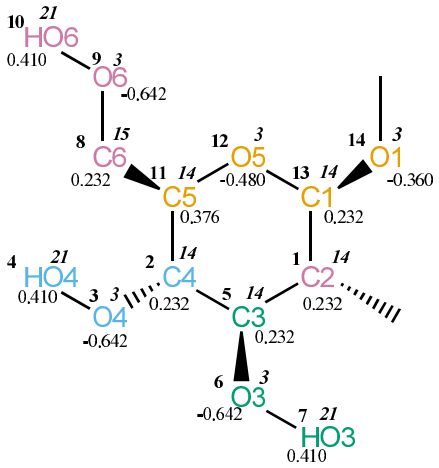

FIGURE 4.191. GB2P non-bonded parameters.

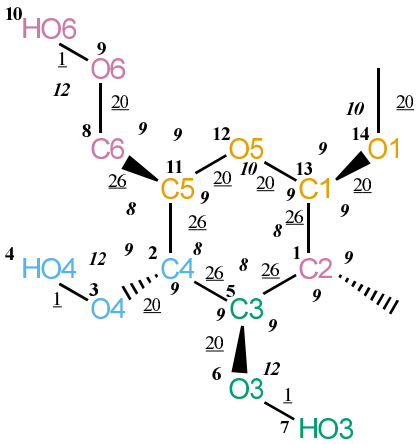

FIGURE 4.192. GB2P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 5 13
1	C2	14	3	0.23200	2 5 6 12 13 14
2	C4	14	3	0.23200	3 4 5 6 8 11 12
3	O4	3	16	-0.64200	4 5 11
4	HO4	21	1	0.41000	
5	C3	14	3	0.23200	6 7 11 13
6	O3	3	16	-0.64200	7
7	HO3	21	1	0.41000	
8	C6	15	4	0.23200	9 10 11 12
9	O6	3	16	-0.64200	10 11
10	HO6	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.476. Atoms of building block GB2P.

I	J	Type
1	5	26
1	13	26
2	3	20
2	5	26
2	11	26
3	4	1
5	6	20
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.477. Bonds of building block GB2P.

I	J	K	Type
0	1	5	9
0	1	13	9
5	1	13	8
3	2	5	9
3	2	11	9
5	2	11	8
2	3	4	12
1	5	2	8
1	5	6	9
2	5	6	9
5	6	7	12
9	8	11	9
8	9	10	12
2	11	8	8
2	11	12	9
8	11	12	9
11	12	13	10
1	13	12	9
1	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.478. Bond angles of building block GB2P.

I	J	K	L	Type
-1	0	1	13	30
0	1	5	2	17
0	1	5	6	18
13	1	5	2	34
13	1	5	6	17
0	1	13	14	18
5	1	13	12	17
5	1	13	12	34
5	1	13	14	17
5	2	3	4	30
3	2	5	1	17
3	2	5	6	18
11	2	5	1	34
11	2	5	6	17
3	2	11	8	17
5	2	11	12	17
5	2	11	12	34
1	5	6	7	30
11	8	9	10	30
9	8	11	12	5
9	8	11	12	37
2	11	12	13	29
11	12	13	1	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.479. Dihedral angles of building block GB2P.

I	J	K	L	Type
1	0	5	13	2
1	12	14	13	2
2	1	6	5	2
2	8	12	11	2
11	3	5	2	2

TABLE 4.480. Improper dihedral angles of building block GB2P.

Solute building block: -3-D-glucopyranose-β-1-
Name: GB3P

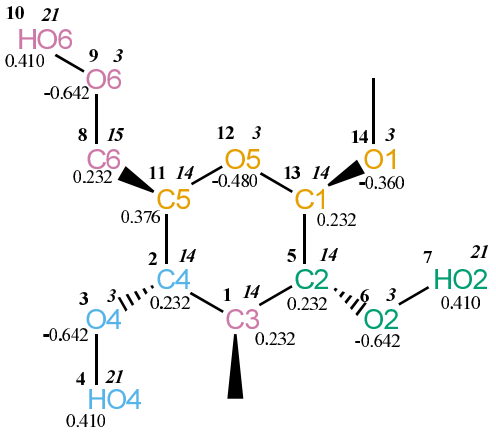

FIGURE 4.193. GB3P non-bonded parameters.

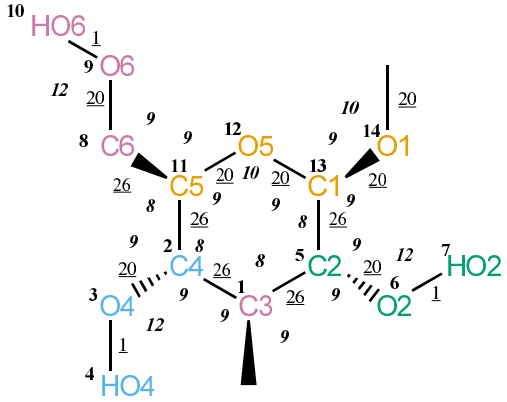

FIGURE 4.194. GB3P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 5
1	C3	14	3	0.23200	2 3 5 6 11 13
2	C4	14	3	0.23200	3 4 5 8 11 12
3	O4	3	16	-0.64200	4 11
4	HO4	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	15	4	0.23200	9 10 11 12
9	O6	3	16	-0.64200	10 11
10	HO6	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.481. Atoms of building block GB3P.

I	J	Type
1	2	26
1	5	26
2	3	20
2	11	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.482. Bonds of building block GB3P.

I	J	K	Type
0	1	2	9
0	1	5	9
2	1	5	8
1	2	3	9
1	2	11	8
3	2	11	9
2	3	4	12
1	5	6	9
1	5	13	8
6	5	13	9
5	6	7	12
9	8	11	9
8	9	10	12
2	11	8	8
2	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.483. Bond angles of building block GB3P.

I	J	K	L	Type
-1	0	1	5	30
0	1	2	3	18
0	1	2	11	17
5	1	2	3	17
5	1	2	11	34
0	1	5	6	18
0	1	5	13	17
2	1	5	6	17
2	1	5	13	34
1	2	3	4	30
1	2	11	12	17
1	2	11	12	34
3	2	11	8	17
13	5	6	7	30
1	5	13	12	17
1	5	13	12	34
1	5	13	14	17
6	5	13	14	18
11	8	9	10	30
9	8	11	12	5
9	8	11	12	37
2	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.484. Dihedral angles of building block GB3P.

I	J	K	L	Type
1	0	5	2	2
2	1	3	11	2
2	8	12	11	2
5	12	14	13	2
13	1	6	5	2

TABLE 4.485. Improper dihedral angles of building block GB3P.

Solute building block: -6-D-glucopyranose-β-1-
Name: GB6P

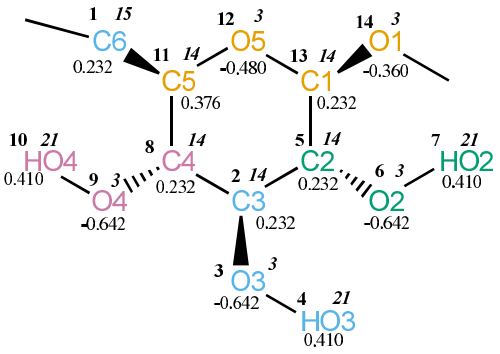

FIGURE 4.195. GB6P non-bonded parameters.

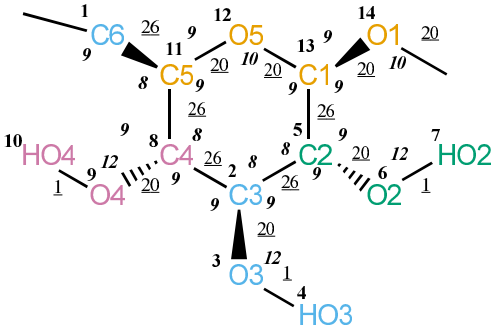

FIGURE 4.196. GB6P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 11
1	C6	15	4	0.23200	8 11 12
2	C3	14	3	0.23200	3 4 5 6 8 9 11 13
3	O3	3	16	-0.64200	4 5 8
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 8 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C4	14	3	0.23200	9 10 11 12
9	O4	3	16	-0.64200	10 11
10	HO4	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.486. Atoms of building block GB6P.

I	J	Type
1	11	26
2	3	20
2	5	26
2	8	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.487. Bonds of building block GB6P.

I	J	K	Type
0	1	11	9
3	2	5	9
3	2	8	9
5	2	8	8
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
2	8	9	9
2	8	11	8
9	8	11	9
8	9	10	12
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.488. Bond angles of building block GB6P.

I	J	K	L	Type
-1	0	1	11	30
0	1	11	12	5
0	1	11	12	37
5	2	3	4	30
3	2	5	6	18
3	2	5	13	17
8	2	5	6	17
8	2	5	13	34
3	2	8	9	18
3	2	8	11	17
5	2	8	9	17
5	2	8	11	34
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
2	8	9	10	30
2	8	11	12	17
2	8	11	12	34
9	8	11	1	17
8	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.489. Dihedral angles of building block GB6P.

I	J	K	L	Type
2	3	5	8	2
5	12	14	13	2
8	1	12	11	2
8	2	9	11	2
13	2	6	5	2

TABLE 4.490. Improper dihedral angles of building block GB6P.

Solute building block: -4-D-glucopyranose-β-1-
Name: GB4P

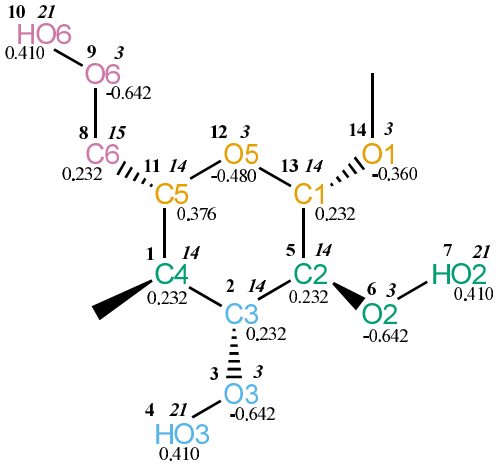

FIGURE 4.197. GB4P non-bonded parameters.

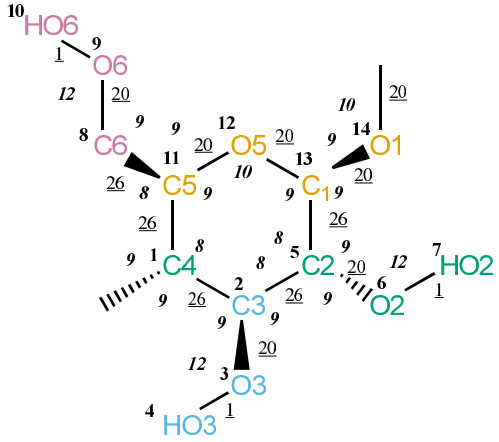

FIGURE 4.198. GB4P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	15	4	0.23200	9 10 11 12
9	O6	3	16	-0.64200	10 11
10	HO6	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.491. Atoms of building block GB4P.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.492. Bonds of building block GB4P.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	11	9
8	9	10	12
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.493. Bond angles of building block GB4P.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
11	8	9	10	30
9	8	11	12	5
9	8	11	12	37
1	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.494. Dihedral angles of building block GB4P.

I	J	K	L	Type
1	8	12	11	2
2	3	5	1	2
5	12	14	13	2
11	0	2	1	2
13	2	6	5	2

TABLE 4.495. Improper dihedral angles of building block GB4P.

Solute building block: -4-D-glucopyranose-α-1-
Name: GA4P

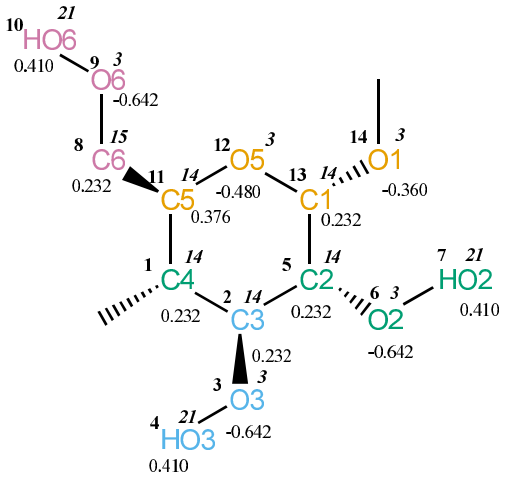

FIGURE 4.199. GA4P non-bonded parameters.

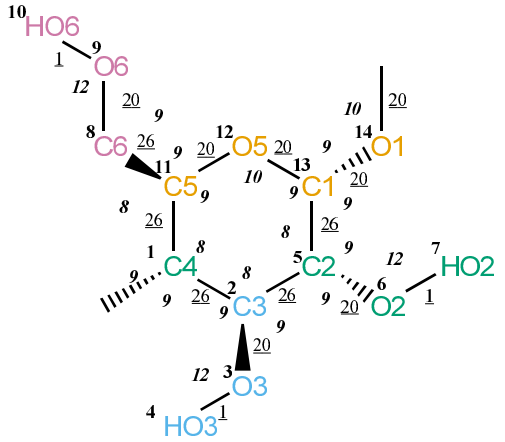

FIGURE 4.200. GA4P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	15	4	0.23200	9 10 11 12
9	O6	3	16	-0.64200	10 11
10	HO6	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.496. Atoms of building block GA4P.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.497. Bonds of building block GA4P.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	11	9
8	9	10	12
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.498. Bond angles of building block GA4P.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
11	8	9	10	30
9	8	11	12	5
9	8	11	12	37
1	11	12	13	29
11	12	13	5	29
12	13	14	15	6
12	13	14	15	28

TABLE 4.499. Dihedral angles of building block GA4P.

I	J	K	L	Type
1	8	12	11	2
2	3	5	1	2
11	0	2	1	2
13	2	6	5	2
13	12	14	5	2

TABLE 4.500. Improper dihedral angles of building block GA4P.

Solute building block: -4-L-glucopyranose-β-1-
Name: gB4P

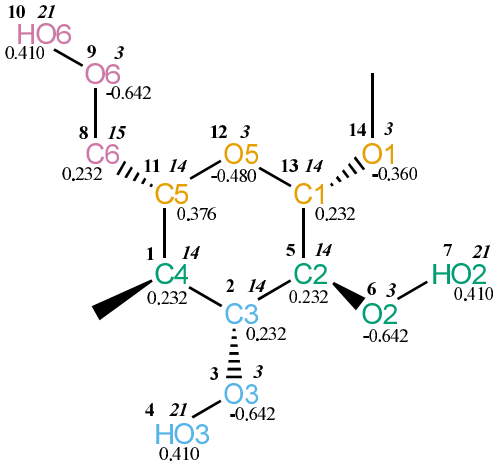

FIGURE 4.201. gB4P non-bonded parameters.

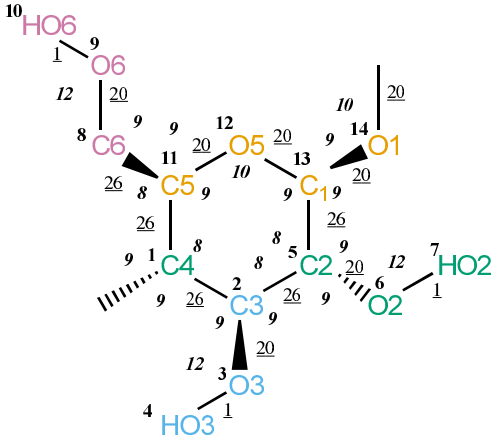

FIGURE 4.202. gB4P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	15	4	0.23200	9 10 11 12
9	O6	3	16	-0.64200	10 11
10	HO6	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.501. Atoms of building block gB4P.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.502. Bonds of building block gB4P.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	11	9
8	9	10	12
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.503. Bond angles of building block gB4P.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
11	8	9	10	30
9	8	11	12	5
9	8	11	12	37
1	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.504. Dihedral angles of building block gB4P.

I	J	K	L	Type
1	0	2	11	2
1	3	5	2	2
5	2	6	13	2
11	8	12	1	2
13	12	14	5	2

TABLE 4.505. Improper dihedral angles of building block gB4P.

Solute building block: -4-D-galactopyranose-β-1-
Name: LB4P

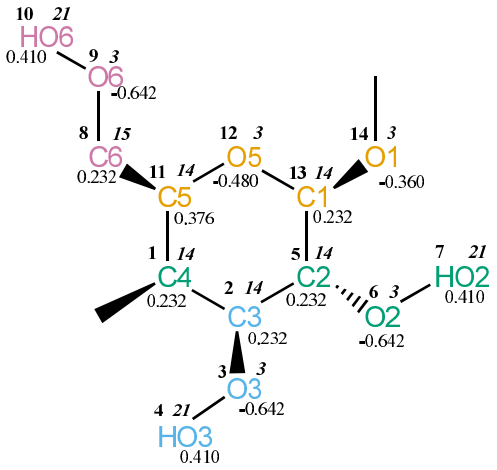

FIGURE 4.203. LB4P non-bonded parameters.

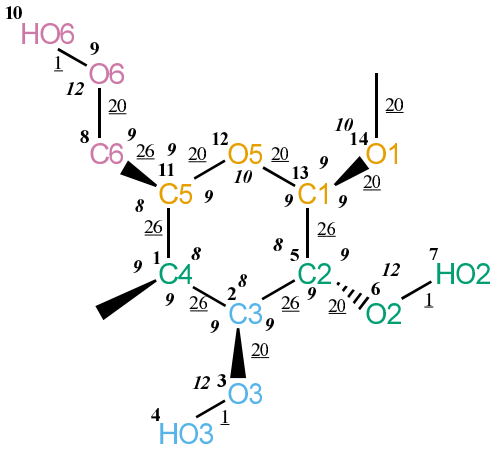

FIGURE 4.204. LB4P bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	15	4	0.23200	9 10 11 12
9	O6	3	16	-0.64200	10 11
10	HO6	21	1	0.41000	
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.506. Atoms of building block LB4P.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	20
8	11	26
9	10	1
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.507. Bonds of building block LB4P.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	11	9
8	9	10	12
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.508. Bond angles of building block LB4P.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
11	8	9	10	30
9	8	11	1	1
9	8	11	12	3
9	8	11	12	35
1	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.509. Dihedral angles of building block LB4P.

I	J	K	L	Type
1	0	2	11	2
1	8	12	11	2
2	3	5	1	2
5	12	14	13	2
13	2	6	5	2

TABLE 4.510. Improper dihedral angles of building block LB4P.

Solute building block: -4-D-glucuronate-β-1-
Name: GB4U

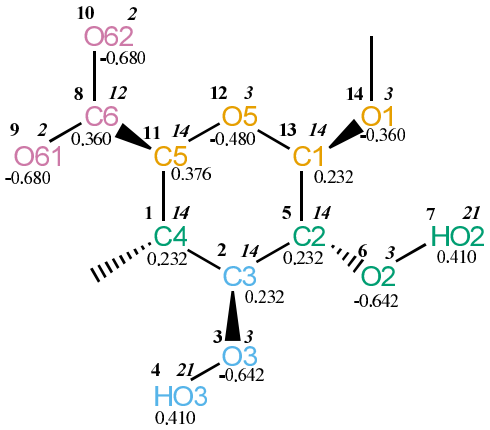

FIGURE 4.205. GB4U non-bonded parameters.

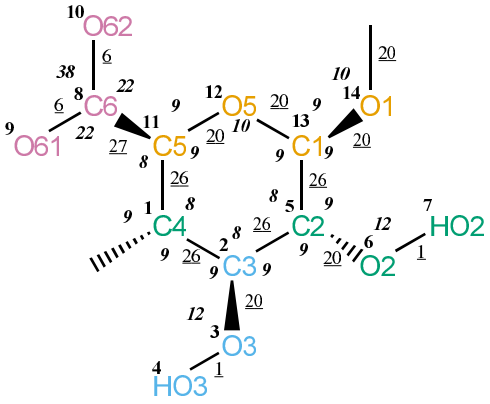

FIGURE 4.206. GB4U bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	12	12	0.36000	9 10 11 12
9	O61	2	16	-0.68000	10 11
10	O62	2	16	-0.68000	11
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.511. Atoms of building block GB4U.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	6
8	10	6
8	11	27
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.512. Bonds of building block GB4U.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	10	38
9	8	11	22
10	8	11	22
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.513. Bond angles of building block GB4U.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
9	8	11	12	40
1	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.514. Dihedral angles of building block GB4U.

I	J	K	L	Type
1	8	12	11	2
2	3	5	1	2
5	12	14	13	2
8	9	10	11	1
11	0	2	1	2
13	2	6	5	2

TABLE 4.515. Improper dihedral angles of building block GB4U.

Solute building block: -4-D-mannuronate-β-1-
Name: MB4U

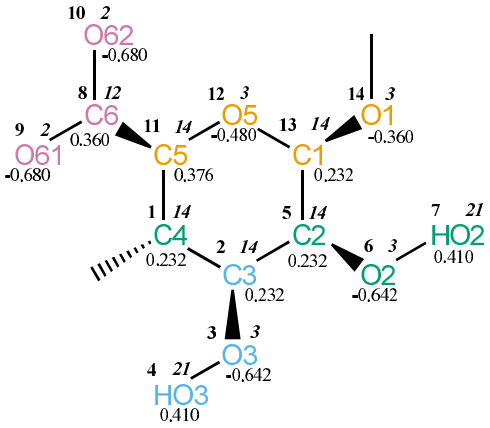

FIGURE 4.207. MB4U non-bonded parameters.

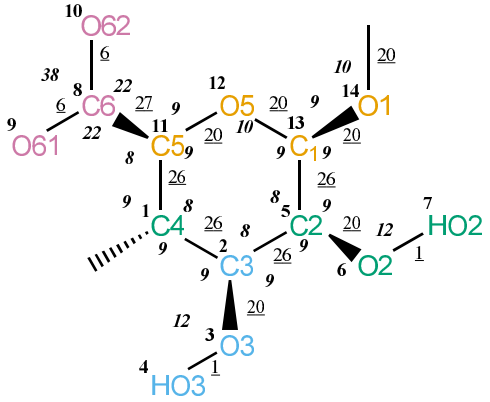

FIGURE 4.208. MB4U bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	12	12	0.36000	9 10 11 12
9	O61	2	16	-0.68000	10 11
10	O62	2	16	-0.68000	11
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.516. Atoms of building block MB4U.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	6
8	10	6
8	11	27
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.517. Bonds of building block MB4U.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	10	38
9	8	11	22
10	8	11	22
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.518. Bond angles of building block MB4U.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
9	8	11	12	40
1	11	12	13	29
11	12	13	5	29
12	13	14	15	2
12	13	14	15	32

TABLE 4.519. Dihedral angles of building block MB4U.

I	J	K	L	Type
1	8	12	11	2
2	3	5	1	2
5	2	6	13	2
5	12	14	13	2
8	9	10	11	1
11	0	2	1	2

TABLE 4.520. Improper dihedral angles of building block MB4U.

Solute building block: -4-D-galacturonate-α-1-
Name: LA4U

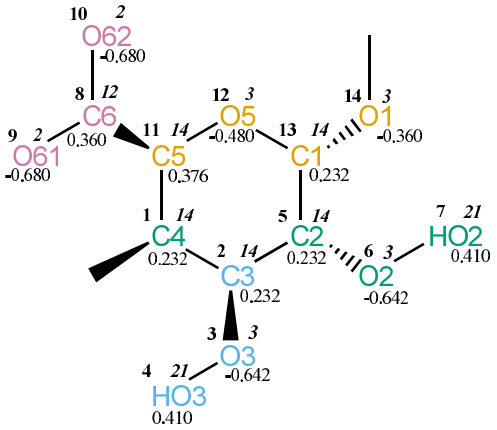

FIGURE 4.209. LA4U non-bonded parameters.

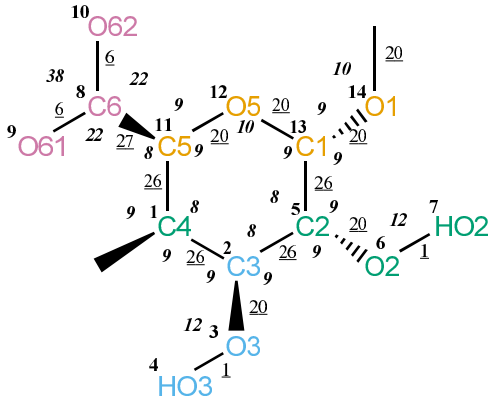

FIGURE 4.210. LA4U bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	12	12	0.36000	9 10 11 12
9	O61	2	16	-0.68000	10 11
10	O62	2	16	-0.68000	11
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.521. Atoms of building block LA4U.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	6
8	10	6
8	11	27
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.522. Bonds of building block LA4U.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	10	38
9	8	11	22
10	8	11	22
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.523. Bond angles of building block LA4U.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
9	8	11	12	40
1	11	12	13	29
11	12	13	5	29
12	13	14	15	6
12	13	14	15	28

TABLE 4.524. Dihedral angles of building block LA4U.

I	J	K	L	Type
1	0	2	11	2
1	8	12	11	2
2	3	5	1	2
8	9	10	11	1
13	2	6	5	2
13	12	14	5	2

TABLE 4.525. Improper dihedral angles of building block LA4U.

Solute building block: -4-L-guluronate-α-1-
Name: kA4U

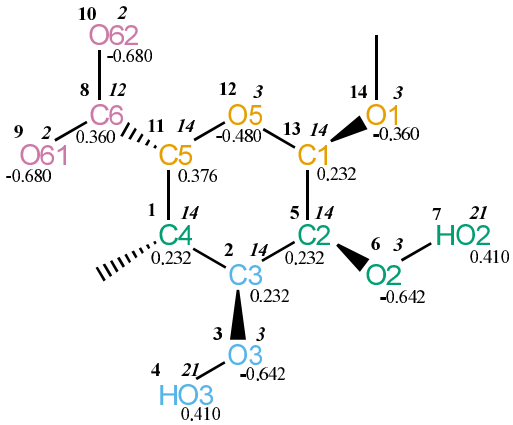

FIGURE 4.211. kA4U non-bonded parameters.

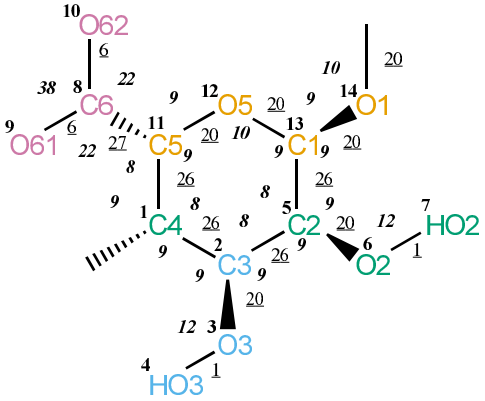

FIGURE 4.212. kA4U bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	12	12	0.36000	9 10 11 12
9	O61	2	16	-0.68000	10 11
10	O62	2	16	-0.68000	11
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.526. Atoms of building block kA4U.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	6
8	10	6
8	11	27
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.527. Bonds of building block kA4U.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	10	38
9	8	11	22
10	8	11	22
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.528. Bond angles of building block kA4U.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
9	8	11	12	40
1	11	12	13	29
11	12	13	5	29
12	13	14	15	6
12	13	14	15	28

TABLE 4.529. Dihedral angles of building block kA4U.

I	J	K	L	Type
2	3	5	1	2
5	2	6	13	2
5	12	14	13	2
8	9	10	11	1
11	0	2	1	2
11	8	12	1	2

TABLE 4.530. Improper dihedral angles of building block kA4U.

Solute building block: -4-L-iduronate-α-1-
Name: iA4U

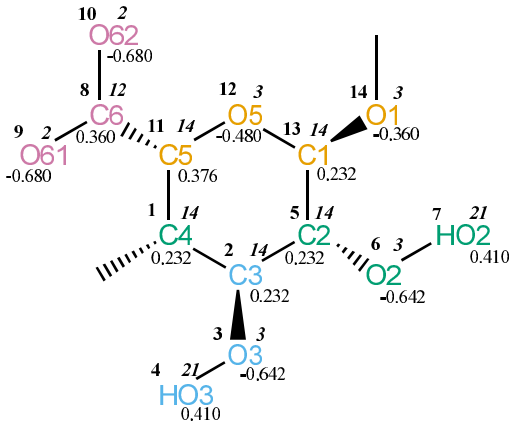

FIGURE 4.213. iA4U non-bonded parameters.

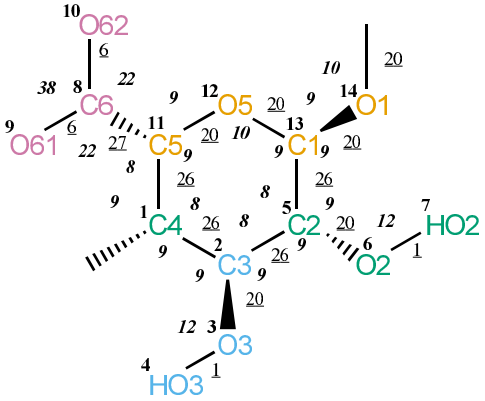

FIGURE 4.214. iA4U bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
-1					0 1
0					1 2 11
1	C4	14	3	0.23200	2 3 5 8 11 12
2	C3	14	3	0.23200	3 4 5 6 11 13
3	O3	3	16	-0.64200	4 5
4	HO3	21	1	0.41000	
5	C2	14	3	0.23200	6 7 12 13 14
6	O2	3	16	-0.64200	7 13
7	HO2	21	1	0.41000	
8	C6	12	12	0.36000	9 10 11 12
9	O61	2	16	-0.68000	10 11
10	O62	2	16	-0.68000	11
11	C5	14	3	0.37600	12 13
12	O5	3	16	-0.48000	13 14
13	C1	14	3	0.23200	
14	O1	3	16	-0.36000	

TABLE 4.531. Atoms of building block iA4U.

I	J	Type
1	2	26
1	11	26
2	3	20
2	5	26
3	4	1
5	6	20
5	13	26
6	7	1
8	9	6
8	10	6
8	11	27
11	12	20
12	13	20
13	14	20
14	15	20

TABLE 4.532. Bonds of building block iA4U.

I	J	K	Type
0	1	2	9
0	1	11	9
2	1	11	8
1	2	3	9
1	2	5	8
3	2	5	9
2	3	4	12
2	5	6	9
2	5	13	8
6	5	13	9
5	6	7	12
9	8	10	38
9	8	11	22
10	8	11	22
1	11	8	8
1	11	12	9
8	11	12	9
11	12	13	10
5	13	12	9
5	13	14	9
12	13	14	9
13	14	15	10

TABLE 4.533. Bond angles of building block iA4U.

I	J	K	L	Type
-1	0	1	2	30
0	1	2	3	18
0	1	2	5	17
11	1	2	3	17
11	1	2	5	34
0	1	11	8	17
2	1	11	12	17
2	1	11	12	34
5	2	3	4	30
1	2	5	6	17
1	2	5	13	34
3	2	5	6	18
3	2	5	13	17
13	5	6	7	30
2	5	13	12	17
2	5	13	12	34
2	5	13	14	17
6	5	13	14	18
9	8	11	12	40
1	11	12	13	29
11	12	13	5	29
12	13	14	15	6
12	13	14	15	28

TABLE 4.534. Dihedral angles of building block iA4U.

I	J	K	L	Type
2	3	5	1	2
5	12	14	13	2
8	9	10	11	1
11	0	2	1	2
11	8	12	1	2
13	2	6	5	2

TABLE 4.535. Improper dihedral angles of building block iA4U.

Solute building block: -1-β-D-glucopyranose
Name: CGBP

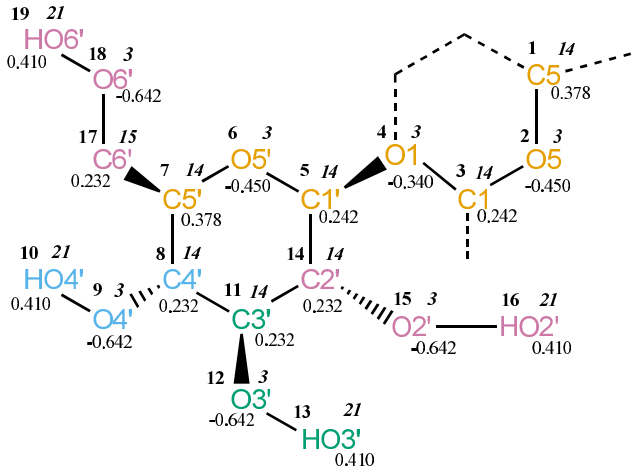

FIGURE 4.215. CGBP non-bonded parameters.

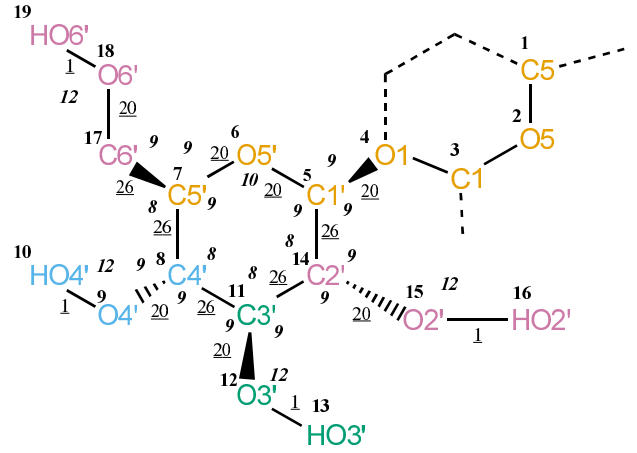

FIGURE 4.216. CGBP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	C5	14	3	0.37800	2 3
2	O5	3	16	-0.45000	3 4
3	C1	14	3	0.24200	4 5
4	O1	3	16	-0.34000	5 6 14
5	C1'	14	3	0.24200	6 7 11 14 15
6	O5'	3	16	-0.45000	7 8 14 17
7	C5'	14	3	0.37800	8 9 11 17 18
8	C4'	14	3	0.23200	9 10 11 12 14 17
9	O4'	3	16	-0.64200	10 11
10	HO4'	21	1	0.41000	
11	C3'	14	3	0.23200	12 13 14 15
12	O3'	3	16	-0.64200	13 14
13	HO3'	21	1	0.41000	
14	C2'	14	3	0.23200	15 16
15	O2'	3	16	-0.64200	16
16	HO2'	21	1	0.41000	
17	C6'	15	4	0.23200	18 19
18	O6'	3	16	-0.64200	19
19	HO6'	21	1	0.41000	

TABLE 4.536. Atoms of building block CGBP.

I	J	Type
5	6	20
5	14	26
6	7	20
7	8	26
7	17	26
8	9	20
8	11	26
9	10	1
11	12	20
11	14	26
12	13	1
14	15	20
15	16	1
17	18	20
18	19	1

TABLE 4.537. Bonds of building block CGBP.

I	J	K	Type
4	5	6	9
4	5	14	9
6	5	14	9
5	6	7	10
6	7	8	9
6	7	17	9
8	7	17	8
7	8	9	9
7	8	11	8
9	8	11	9
8	9	10	12
8	11	12	9
8	11	14	8
12	11	14	9
11	12	13	12
5	14	11	8
5	14	15	9
11	14	15	9
14	15	16	12
7	17	18	9
17	18	19	12

TABLE 4.538. Bond angles of building block CGBP.

I	J	K	L	Type
3	4	5	6	2
3	4	5	6	32
14	5	6	7	29
4	5	14	11	17
4	5	14	15	18
6	5	14	11	17
6	5	14	11	34
5	6	7	8	29
6	7	8	11	17
6	7	8	11	34
17	7	8	9	17
6	7	17	18	5
6	7	17	18	37
11	8	9	10	30
7	8	11	12	17
7	8	11	14	34
9	8	11	12	18
9	8	11	14	17
14	11	12	13	30
8	11	14	5	34
8	11	14	15	17
12	11	14	5	17
12	11	14	15	18
5	14	15	16	30
7	17	18	19	30

TABLE 4.539. Dihedral angles of building block CGBP.

I	J	K	L	Type
5	4	6	14	2
5	11	15	14	2
7	6	17	8	2
7	9	11	8	2
11	12	14	8	2

TABLE 4.540. Improper dihedral angles of building block CGBP.

4.7. Other molecules

Solute building block: heme group (charge -2, acidic groups deprotonated)
Name: HEME

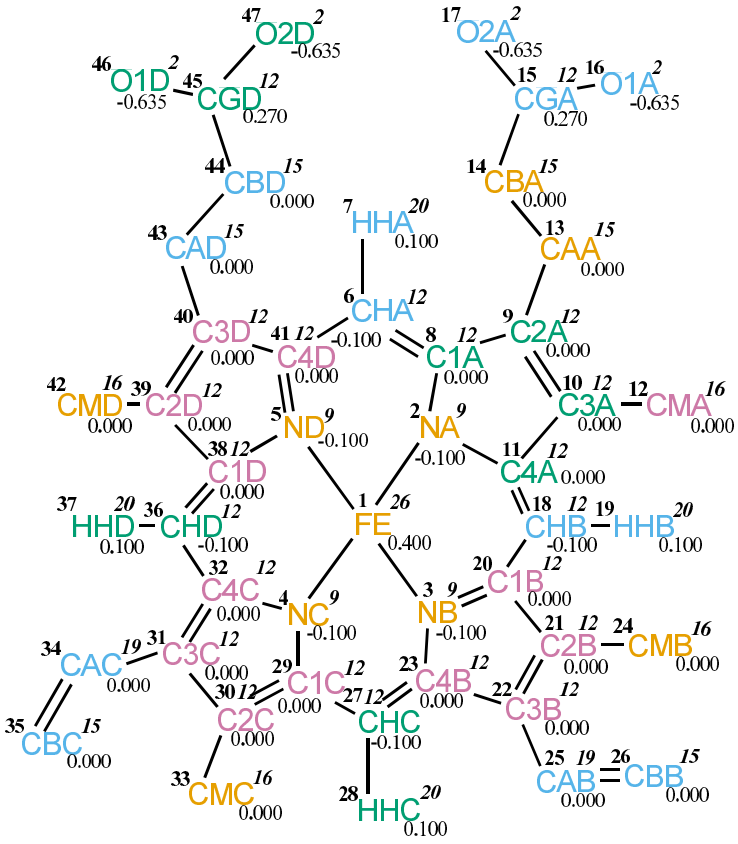

FIGURE 4.217. HEME non-bonded parameters.

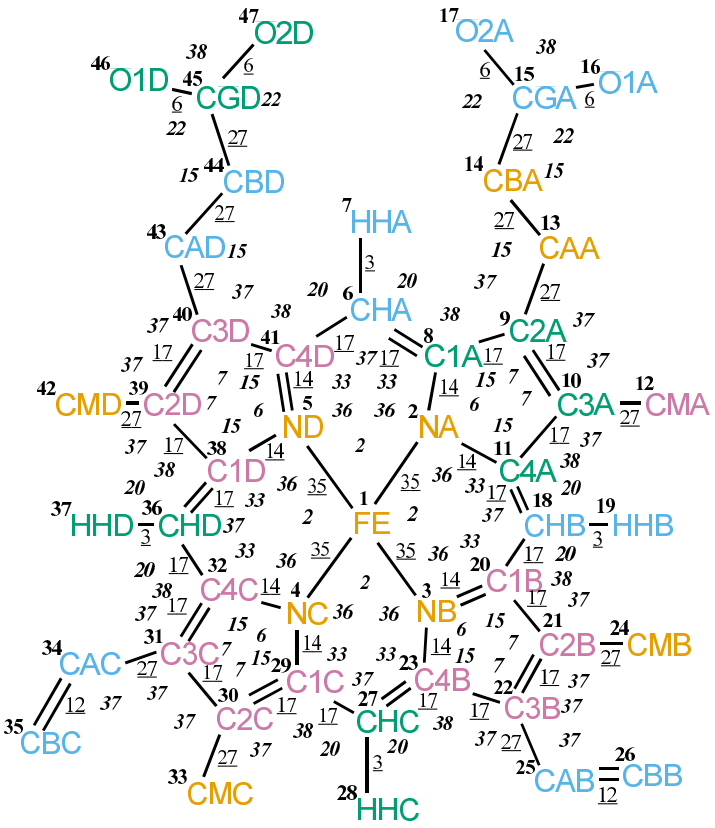

FIGURE 4.218. HEME bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	FE	26	56	0.40000	2 3 4 5 6 8 9 10 11 18 20 21 22 23 27 29 30 31 32 36 38 39 40 41
2	NA	9	14	-0.10000	3 4 5 6 7 8 9 10 11 12 13 18 19 20 23 29 32 38 41
3	NB	9	14	-0.10000	4 5 8 11 18 19 20 21 22 23 24 25 27 28 29 32 38 41
4	NC	9	14	-0.10000	5 8 11 20 23 27 28 29 30 31 32 33 34 36 37 38 41
5	ND	9	14	-0.10000	6 7 8 11 20 23 29 32 36 37 38 39 40 41 42 43
6	CHA	12	12	-0.10000	7 8 9 10 11 13 38 39 40 41 43
7	HHA	20	1	0.10000	8 9 40 41
8	C1A	12	12	0.00000	9 10 11 12 13 18 40 41
9	C2A	12	12	0.00000	10 11 12 13 14 18 41
10	C3A	12	12	0.00000	11 12 13 18 19 20
11	C4A	12	12	0.00000	12 13 18 19 20 21
12	CMA	16	5	0.00000	13 18
13	CAA	15	4	0.00000	14 15
14	CBA	15	4	0.00000	15 16 17
15	CGA	12	12	0.27000	16 17
16	O1A	2	16	-0.63500	17
17	O2A	2	16	-0.63500	
18	CHB	12	12	-0.10000	19 20 21 22 23 24
19	HHB	20	1	0.10000	20 21
20	C1B	12	12	0.00000	21 22 23 24 25 27
21	C2B	12	12	0.00000	22 23 24 25 27
22	C3B	12	12	0.00000	23 24 25 26 27 28 29
23	C4B	12	12	0.00000	24 25 27 28 29 30
24	CMB	16	5	0.00000	25
25	CAB	19	3	0.00000	26 27
26	CBB	15	4	0.00000	
27	CHC	12	12	-0.10000	28 29 30 31 32 33
28	HHC	20	1	0.10000	29 30
29	C1C	12	12	0.00000	30 31 32 33 34 36
30	C2C	12	12	0.00000	31 32 33 34 36
31	C3C	12	12	0.00000	32 33 34 35 36 37 38
32	C4C	12	12	0.00000	33 34 36 37 38 39
33	CMC	16	5	0.00000	34
34	CAC	19	3	0.00000	35 36
35	CBC	15	4	0.00000	
36	CHD	12	12	-0.10000	37 38 39 40 41 42
37	HHD	20	1	0.10000	38 39
38	C1D	12	12	0.00000	39 40 41 42 43
39	C2D	12	12	0.00000	40 41 42 43
40	C3D	12	12	0.00000	41 42 43 44
41	C4D	12	12	0.00000	42 43
42	CMD	16	5	0.00000	43
43	CAD	15	4	0.00000	44 45
44	CBD	15	4	0.00000	45 46 47
45	CGD	12	12	0.27000	46 47
46	O1D	2	16	-0.63500	47

TABLE 4.541: continues on next page.

Seq.	Name	IAC	Mass	Charge	Exclusions
47	O2D	2	16	-0.63500	

TABLE 4.541: Atoms of building block HEME.

I	J	Type
1	2	35
1	3	35
1	4	35
1	5	35
2	8	14
2	11	14
3	20	14
3	23	14
4	29	14
4	32	14
5	38	14
5	41	14
6	7	3
6	8	17
6	41	17
8	9	17
9	10	17
9	13	27
10	11	17
10	12	27
11	18	17
13	14	27
14	15	27
15	16	6
15	17	6
18	19	3
18	20	17
20	21	17
21	22	17
21	24	27
22	23	17
22	25	27
23	27	17
25	26	12
27	28	3
27	29	17
29	30	17
30	31	17
30	33	27
31	32	17
31	34	27
32	36	17
34	35	12
36	37	3
36	38	17
38	39	17

TABLE 4.542: continues on next page.

I	J	Type
39	40	17
39	42	27
40	41	17
40	43	27
43	44	27
44	45	27
45	46	6
45	47	6

TABLE 4.542: Bonds of building block HEME.

I	J	K	Type
2	1	3	2
2	1	5	2
3	1	4	2
4	1	5	2
1	2	8	36
1	2	11	36
8	2	11	6
1	3	20	36
1	3	23	36
20	3	23	6
1	4	29	36
1	4	32	36
29	4	32	6
1	5	38	36
1	5	41	36
38	5	41	6
7	6	8	20
7	6	41	20
8	6	41	37
2	8	6	33
2	8	9	15
6	8	9	38
8	9	10	7
8	9	13	37
10	9	13	37
9	10	11	7
9	10	12	37
11	10	12	37
2	11	10	15
2	11	18	33
10	11	18	38
9	13	14	15
13	14	15	15
14	15	16	22
14	15	17	22
16	15	17	38
11	18	19	20
11	18	20	37
19	18	20	20
3	20	18	33
3	20	21	15
18	20	21	38
20	21	22	7
20	21	24	37
22	21	24	37
21	22	23	7

TABLE 4.543: continues on next page.

I	J	K	Type
21	22	25	37
23	22	25	37
3	23	22	15
3	23	27	33
22	23	27	38
22	25	26	37
23	27	28	20
23	27	29	37
28	27	29	20
4	29	27	33
4	29	30	15
27	29	30	38
29	30	31	7
29	30	33	37
31	30	33	37
30	31	32	7
30	31	34	37
32	31	34	37
4	32	31	15
4	32	36	33
31	32	36	38
31	34	35	37
32	36	37	20
32	36	38	37
37	36	38	20
5	38	36	33
5	38	39	15
36	38	39	38
38	39	40	7
38	39	42	37
40	39	42	37
39	40	41	7
39	40	43	37
41	40	43	37
5	41	6	33
5	41	40	15
6	41	40	38
40	43	44	15
43	44	45	15
44	45	46	22
44	45	47	22
46	45	47	38

TABLE 4.543: Bond angles of building block HEME.

I	J	K	L	Type
41	6	8	2	15
8	6	41	5	15
8	9	13	14	40
2	11	18	20	15
9	13	14	15	34
13	14	15	16	40
11	18	20	3	15
21	22	25	26	9
3	23	27	29	15
23	27	29	4	15
30	31	34	35	9
4	32	36	38	15
32	36	38	5	15
39	40	43	44	40
40	43	44	45	34
43	44	45	46	40

TABLE 4.544: Dihedral angles of building block HEME.

I	J	K	L	Type
1	8	11	2	3
1	20	23	3	3
1	29	32	4	3
1	38	41	5	3
2	8	9	10	1
3	20	21	22	1
4	29	30	31	1
5	38	39	40	1
6	2	9	8	1
6	5	40	41	1
7	8	41	6	1
8	2	11	10	1
8	9	10	11	1
9	8	10	13	1
9	10	11	2	1
10	9	11	12	1
11	2	8	9	1
14	16	17	15	1
18	2	10	11	1
18	3	21	20	1
18	11	20	19	1
20	3	23	22	1
20	21	22	23	1
21	20	22	24	1
21	22	23	3	1
22	21	23	25	1
23	3	20	21	1
27	3	22	23	1
27	4	30	29	1
27	23	29	28	1
29	4	32	31	1
29	30	31	32	1
30	29	31	33	1
30	31	32	4	1
31	30	32	34	1
32	4	29	30	1
36	4	31	32	1
36	5	39	38	1
36	32	38	37	1
38	5	41	40	1
38	39	40	41	1
39	38	40	42	1
39	40	41	5	1
40	39	41	43	1
41	5	38	39	1
44	46	47	45	1

TABLE 4.545: Improper dihedral angles of building block HEME.

Solute building block: folate (charge -2e)
Name: FOL

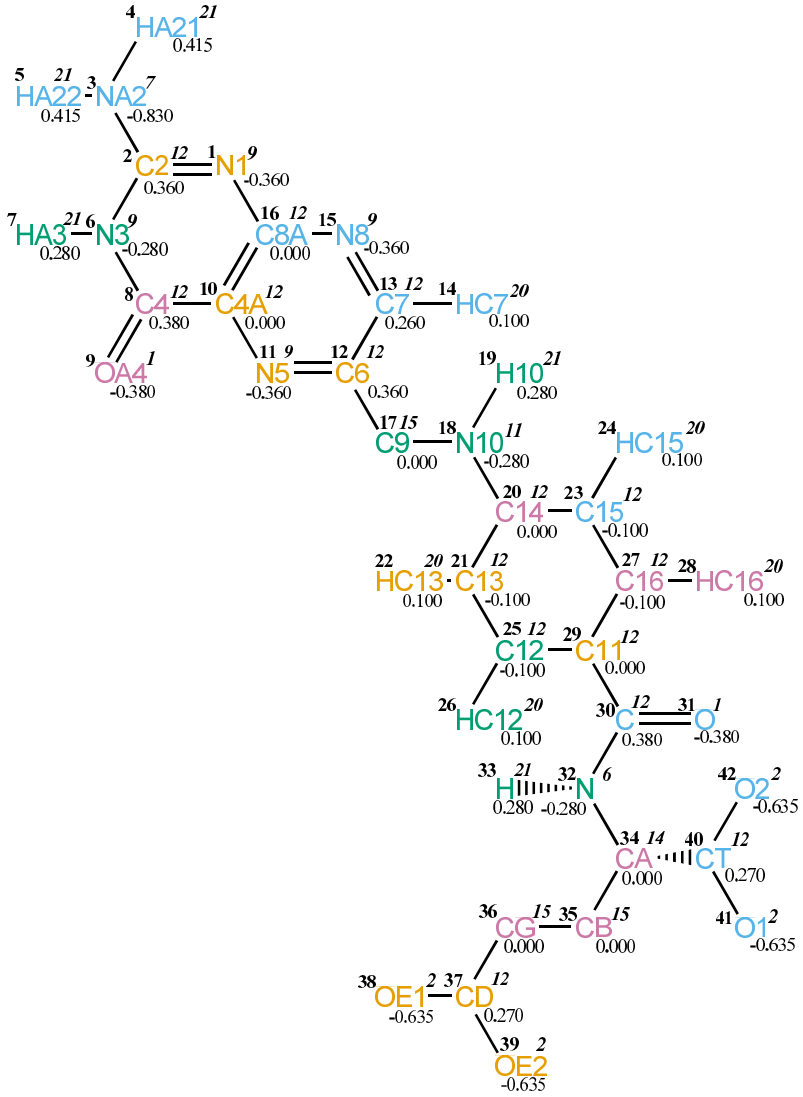

FIGURE 4.219. FOL non-bonded parameters.

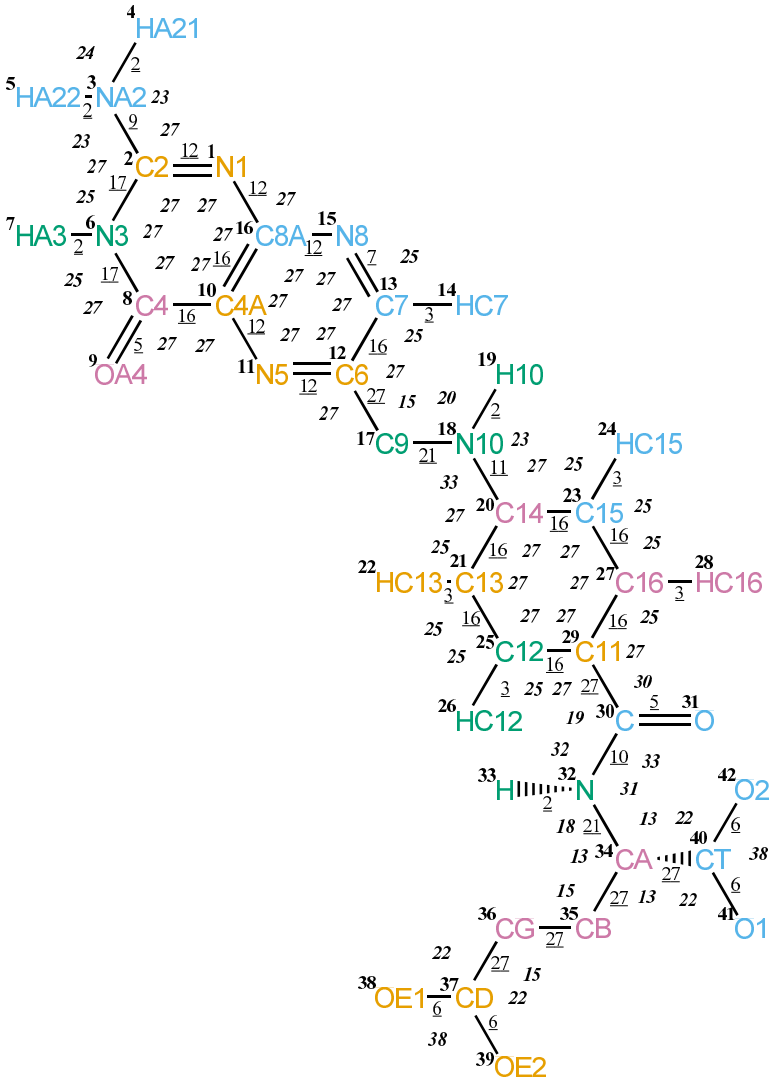

FIGURE 4.220. FOL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	N1	9	14	-0.36000	2 3 6 7 8 10 11 13 15 16
2	C2	12	12	0.36000	3 4 5 6 7 8 9 10 15 16
3	NA2	7	14	-0.83000	4 5 6 7 8 16
4	HA21	21	1	0.41500	5
5	HA22	21	1	0.41500	
6	N3	9	14	-0.28000	7 8 9 10 11 16
7	HA3	21	1	0.28000	8 9 10
8	C4	12	12	0.38000	9 10 11 12 15 16
9	OA4	1	16	-0.38000	10 11 16
10	C4A	12	12	0.00000	11 12 13 15 16 17
11	N5	9	14	-0.36000	12 13 14 15 16 17
12	C6	12	12	0.36000	13 14 15 16 17 18
13	C7	12	12	0.26000	14 15 16 17
14	HC7	20	1	0.10000	15 16 17
15	N8	9	14	-0.36000	16 17
16	C8A	12	12	0.00000	
17	C9	15	4	0.00000	18 19 20
18	N10	11	14	-0.28000	19 20 21 22 23 24 25 27
19	H10	21	1	0.28000	20
20	C14	12	12	0.00000	21 22 23 24 25 26 27 28 29
21	C13	12	12	-0.10000	22 23 24 25 26 27 29 30
22	HC13	20	1	0.10000	23 25 26 29
23	C15	12	12	-0.10000	24 25 27 28 29 30
24	HC15	20	1	0.10000	27 28 29
25	C12	12	12	-0.10000	26 27 28 29 30
26	HC12	20	1	0.10000	27 29 30
27	C16	12	12	-0.10000	28 29 30
28	HC16	20	1	0.10000	29 30
29	C11	12	12	0.00000	30 31 32
30	C	12	12	0.38000	31 32 33 34
31	O	1	16	-0.38000	32
32	N	6	14	-0.28000	33 34 35 40
33	H	21	1	0.28000	34
34	CA	14	3	0.00000	35 36 40 41 42
35	CB	15	4	0.00000	36 37 40
36	CG	15	4	0.00000	37 38 39
37	CD	12	12	0.27000	38 39
38	OE1	2	16	-0.63500	39
39	OE2	2	16	-0.63500	
40	CT	12	12	0.27000	41 42
41	O1	2	16	-0.63500	42
42	O2	2	16	-0.63500	

TABLE 4.546: Atoms of building block FOL.

I	J	Type
1	2	12
1	16	12
2	3	9
2	6	17
3	4	2
3	5	2
6	7	2
6	8	17
8	9	5
8	10	16
10	11	12
10	16	16
11	12	12
12	13	16
12	17	27
13	14	3
13	15	7
15	16	12
17	18	21
18	19	2
18	20	11
20	21	16
20	23	16
21	22	3
21	25	16
23	24	3
23	27	16
25	26	3
25	29	16
27	28	3
27	29	16
29	30	27
30	31	5
30	32	10
32	33	2
32	34	21
34	35	27
34	40	27
35	36	27
36	37	27
37	38	6
37	39	6
40	41	6
40	42	6

TABLE 4.547: Bonds of building block FOL.

I	J	K	Type
2	1	16	27
1	2	3	27
1	2	6	27
3	2	6	27
2	3	4	23
2	3	5	23
4	3	5	24
2	6	7	25
2	6	8	27
7	6	8	25
6	8	9	27
6	8	10	27
9	8	10	27
8	10	11	27
8	10	16	27
11	10	16	27
10	11	12	27
11	12	13	27
11	12	17	27
13	12	17	27
12	13	14	25
12	13	15	27
14	13	15	25
13	15	16	27
1	16	10	27
1	16	15	27
10	16	15	27
12	17	18	15
17	18	19	20
17	18	20	33
19	18	20	23
18	20	21	27
18	20	23	27
21	20	23	27
20	21	22	25
20	21	25	27
22	21	25	25
20	23	24	25
20	23	27	27
24	23	27	25
21	25	26	25
21	25	29	27
26	25	29	25
23	27	28	25
23	27	29	27
28	27	29	25

TABLE 4.548: continues on next page.

I	J	K	Type
25	29	27	27
25	29	30	27
27	29	30	27
29	30	31	30
29	30	32	19
31	30	32	33
30	32	33	32
30	32	34	31
33	32	34	18
32	34	35	13
32	34	40	13
35	34	40	13
34	35	36	15
35	36	37	15
36	37	38	22
36	37	39	22
38	37	39	38
34	40	41	22
34	40	42	22
41	40	42	38

TABLE 4.548: Bond angles of building block FOL.

I	J	K	L	Type
1	2	3	4	14
11	12	17	18	40
12	17	18	20	39
17	18	20	21	14
25	29	30	32	10
29	30	32	34	14
30	32	34	40	39
32	34	35	36	34
32	34	40	41	40
34	35	36	37	34
35	36	37	38	40

TABLE 4.549: Dihedral angles of building block FOL.

I	J	K	L	Type
1	2	6	8	1
2	1	6	3	1
2	1	16	10	1
2	6	8	10	1
3	4	5	2	1
6	2	8	7	1
6	8	10	16	1
8	6	10	9	1
8	10	16	1	1
10	8	11	16	1
10	11	12	13	1
11	10	16	15	1
11	12	13	15	1
12	11	13	17	1
12	13	15	16	1
13	12	15	14	1
13	15	16	10	1
16	1	2	6	1
16	1	15	10	1
16	10	11	12	1
18	17	20	19	1
20	21	23	18	1
20	21	25	29	1
20	23	27	29	1
21	20	23	27	1
21	20	25	22	1
21	25	29	27	1
23	20	21	25	1
23	20	27	24	1
23	27	29	25	1
25	21	29	26	1
27	23	29	28	1
29	25	27	30	1
30	29	32	31	1
32	30	34	33	1
34	32	40	35	2
37	38	39	36	1
40	34	42	41	1

TABLE 4.550: Improper dihedral angles of building block FOL.

Solute building block: trimethoprim (deprotonated at N1; neutral)
Name: TMP

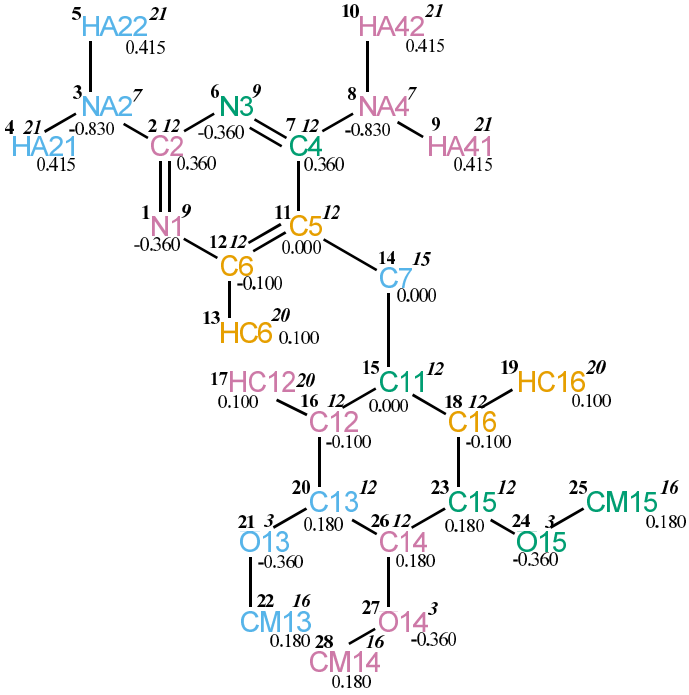

FIGURE 4.221. TMP non-bonded parameters.

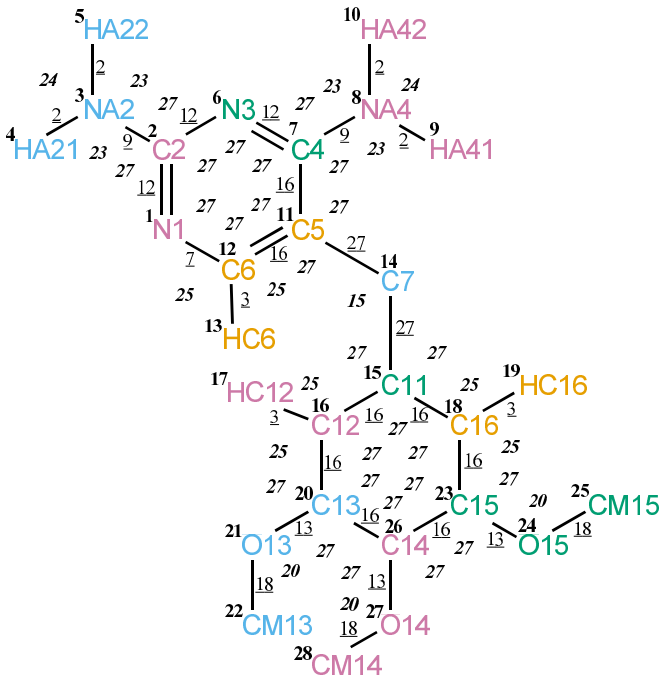

FIGURE 4.222. TMP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	N1	9	14	-0.36000	2 3 6 7 11 12 13 14
2	C2	12	12	0.36000	3 4 5 6 7 8 11 12 13
3	NA2	7	14	-0.83000	4 5 6 7 12
4	HA21	21	1	0.41500	5
5	HA22	21	1	0.41500	
6	N3	9	14	-0.36000	7 8 11 12 14
7	C4	12	12	0.36000	8 9 10 11 12 13 14
8	NA4	7	14	-0.83000	9 10 11 12 14
9	HA41	21	1	0.41500	10
10	HA42	21	1	0.41500	
11	C5	12	12	0.00000	12 13 14 15
12	C6	12	12	-0.10000	13 14
13	HC6	20	1	0.10000	14
14	C7	15	4	0.00000	15 16 17 18 19 20 23
15	C11	12	12	0.00000	16 17 18 19 20 21 23 24 26
16	C12	12	12	-0.10000	17 18 19 20 21 23 26 27
17	HC12	20	1	0.10000	18 20 21 26
18	C16	12	12	-0.10000	19 20 23 24 26 27
19	HC16	20	1	0.10000	23 24 26
20	C13	12	12	0.18000	21 22 23 24 26 27
21	O13	3	16	-0.36000	22 23 26 27
22	CM13	16	5	0.18000	
23	C15	12	12	0.18000	24 25 26 27
24	O15	3	16	-0.36000	25 26 27
25	CM15	16	5	0.18000	
26	C14	12	12	0.18000	27 28
27	O14	3	16	-0.36000	28
28	CM14	16	5	0.18000	

TABLE 4.551. Atoms of building block TMP.

I	J	Type
1	2	12
1	12	7
2	3	9
2	6	12
3	4	2
3	5	2
6	7	12
7	8	9
7	11	16
8	9	2
8	10	2
11	12	16
11	14	27
12	13	3
14	15	27
15	16	16
15	18	16
16	17	3
16	20	16
18	19	3
18	23	16
20	21	13
20	26	16
21	22	18
23	24	13
23	26	16
24	25	18
26	27	13
27	28	18

TABLE 4.552. Bonds of building block TMP.

I	J	K	Type
2	1	12	27
1	2	3	27
1	2	6	27
3	2	6	27
2	3	4	23
2	3	5	23
4	3	5	24
2	6	7	27
6	7	8	27
6	7	11	27
8	7	11	27
7	8	9	23
7	8	10	23
9	8	10	24
7	11	12	27
7	11	14	27
12	11	14	27
1	12	11	27
1	12	13	25
11	12	13	25
11	14	15	15
14	15	16	27
14	15	18	27
16	15	18	27
15	16	17	25
15	16	20	27
17	16	20	25
15	18	19	25
15	18	23	27
19	18	23	25
16	20	21	27
16	20	26	27
21	20	26	27
20	21	22	20
18	23	24	27
18	23	26	27
24	23	26	27
23	24	25	20
20	26	23	27
20	26	27	27
23	26	27	27
26	27	28	20

TABLE 4.553. Bond angles of building block TMP.

I	J	K	L	Type
1	2	3	4	14
11	7	8	9	14
7	11	14	15	40
11	14	15	16	40
16	20	21	22	11
16	20	21	22	12
18	23	24	25	11
18	23	24	25	12
20	26	27	28	11

TABLE 4.554. Dihedral angles of building block TMP.

I	J	K	L	Type
1	2	6	7	1
2	1	6	3	1
2	1	12	11	1
2	6	7	11	1
3	4	5	2	1
6	7	11	12	1
7	6	11	8	1
7	11	12	1	1
8	9	10	7	1
11	7	12	14	1
12	1	2	6	1
12	1	11	13	1
15	16	18	14	1
15	16	20	26	1
15	18	23	26	1
16	15	18	23	1
16	15	20	17	1
16	20	26	23	1
18	15	16	20	1
18	15	23	19	1
18	23	26	20	1
20	16	21	26	1
23	18	24	26	1
26	20	27	23	1

TABLE 4.555. Improper dihedral angles of building block TMP.

Solute building block: 3-phospho-D-glycerate (charge -2e)
Name: PDG

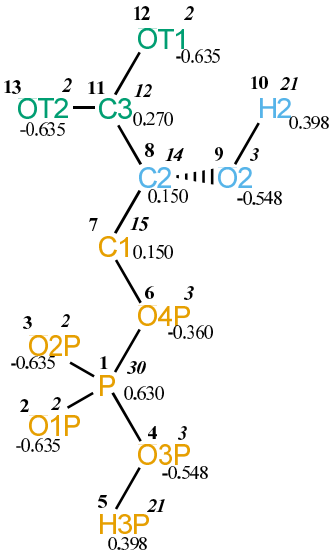

FIGURE 4.223. PDG non-bonded parameters.

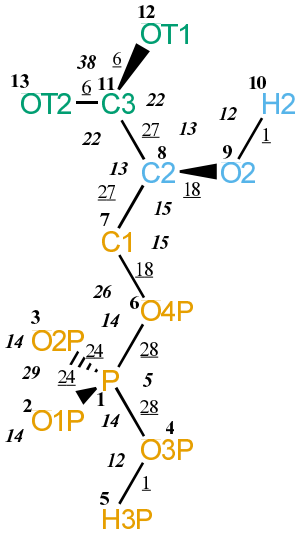

FIGURE 4.224. PDG bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	P	30	31	0.63000	2 3 4 5 6 7
2	O1P	2	16	-0.63500	3 4 5 6
3	O2P	2	16	-0.63500	4 5 6
4	O3P	3	16	-0.54800	5 6
5	H3P	21	1	0.39800	6
6	O4P	3	16	-0.36000	7 8
7	C1	15	4	0.15000	8 9 11
8	C2	14	3	0.15000	9 10 11 12 13
9	O2	3	16	-0.54800	10 11
10	H2	21	1	0.39800	
11	C3	12	12	0.27000	12 13
12	OT1	2	16	-0.63500	13
13	OT2	2	16	-0.63500	

TABLE 4.556. Atoms of building block PDG.

I	J	Type
1	2	24
1	3	24
1	4	28
1	6	28
4	5	1
6	7	18
7	8	27
8	9	18
8	11	27
9	10	1
11	12	6
11	13	6

TABLE 4.557. Bonds of building block PDG.

I	J	K	Type
2	1	3	29
2	1	4	14
2	1	6	14
3	1	4	14
3	1	6	14
4	1	6	5
1	4	5	12
1	6	7	26
6	7	8	15
7	8	9	15
7	8	11	13
9	8	11	13
8	9	10	12
8	11	12	22
8	11	13	22
12	11	13	38

TABLE 4.558. Bond angles of building block PDG.

I	J	K	L	Type
6	1	4	5	20
6	1	4	5	27
4	1	6	7	20
4	1	6	7	27
1	6	7	8	7
1	6	7	8	22
6	7	8	11	34
7	8	9	10	23
7	8	11	12	40

TABLE 4.559. Dihedral angles of building block PDG.

I	J	K	L	Type
8	7	11	9	2
11	8	13	12	1

TABLE 4.560. Improper dihedral angles of building block PDG.

Solute building block: adenosine-5'-triphosphate (ATP; charge -3e)
Name: ATP

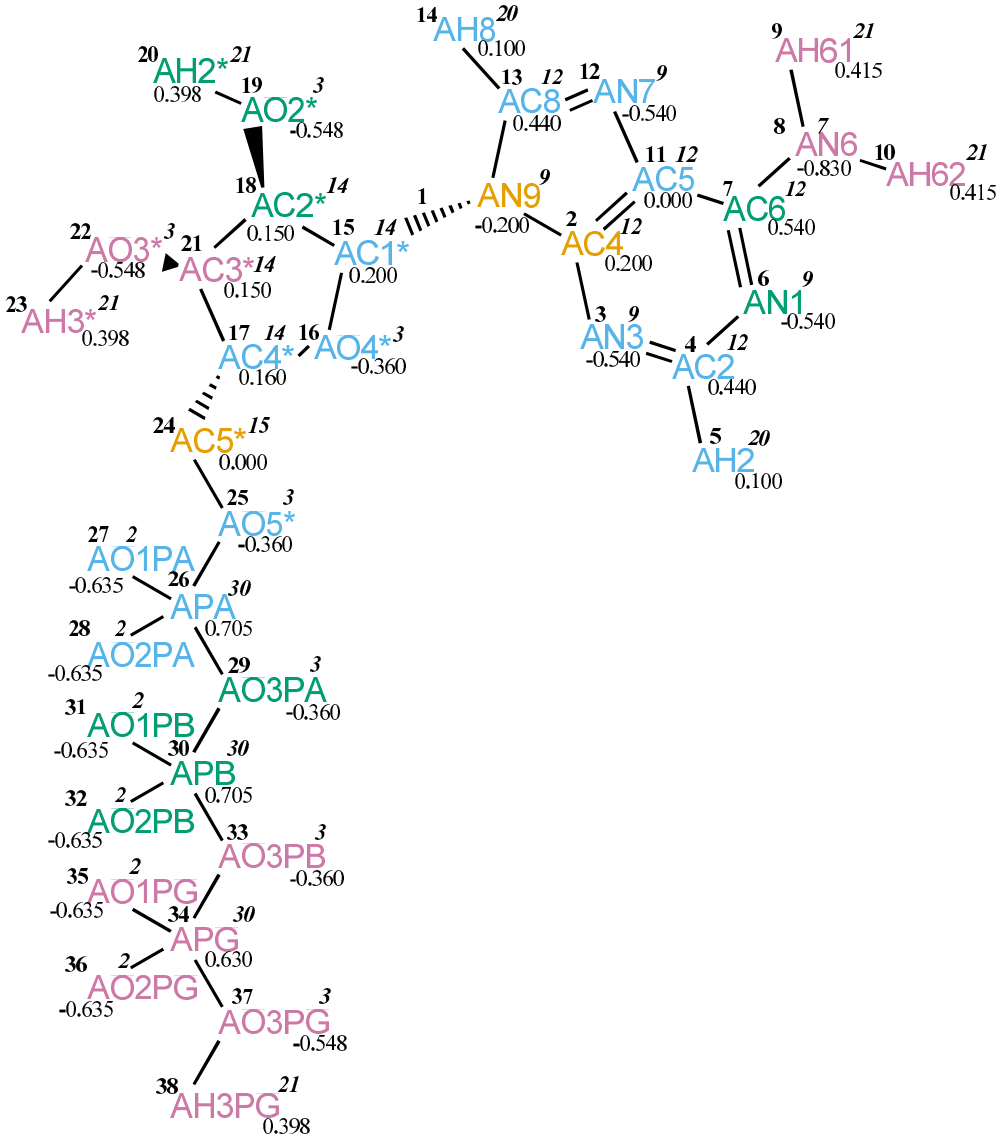

FIGURE 4.225. ATP non-bonded parameters.

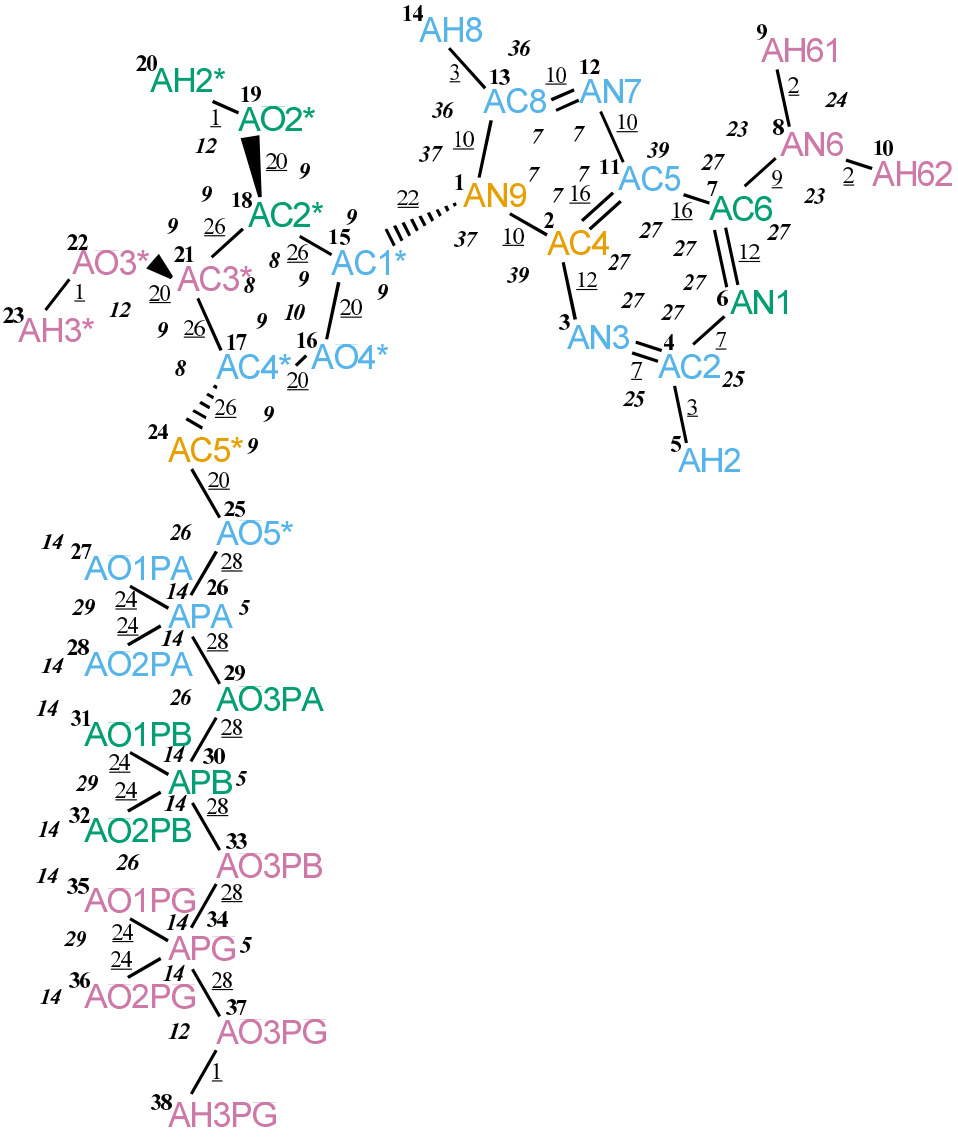

FIGURE 4.226. ATP bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	AN9	9	14	-0.20000	2 3 4 7 11 12 13 14 15 16 18
2	AC4	12	12	0.20000	3 4 5 6 7 8 11 12 13 14 15
3	AN3	9	14	-0.54000	4 5 6 7 11 12 13 15
4	AC2	12	12	0.44000	5 6 7 8 11
5	AH2	20	1	0.10000	6 7
6	AN1	9	14	-0.54000	7 8 11 12
7	AC6	12	12	0.54000	8 9 10 11 12 13
8	AN6	7	14	-0.83000	9 10 11 12
9	AH61	21	1	0.41500	10 12
10	AH62	21	1	0.41500	12
11	AC5	12	12	0.00000	12 13 14 15
12	AN7	9	14	-0.54000	13 14 15
13	AC8	12	12	0.44000	14 15
14	AH8	20	1	0.10000	15
15	AC1*	14	3	0.20000	16 17 18 19 21
16	AO4*	3	16	-0.36000	17 18 21 24
17	AC4*	14	3	0.16000	18 21 22 24 25
18	AC2*	14	3	0.15000	19 20 21 22
19	AO2*	3	16	-0.54800	20 21
20	AH2*	21	1	0.39800	
21	AC3*	14	3	0.15000	22 23 24
22	AO3*	3	16	-0.54800	23
23	AH3*	21	1	0.39800	
24	AC5*	15	4	0.00000	25 26
25	AO5*	3	16	-0.36000	26 27 28 29
26	APA	30	31	0.70500	27 28 29 30
27	AO1PA	2	16	-0.63500	28 29
28	AO2PA	2	16	-0.63500	29
29	AO3PA	3	16	-0.36000	30 31 32 33
30	APB	30	31	0.70500	31 32 33 34
31	AO1PB	2	16	-0.63500	32 33
32	AO2PB	2	16	-0.63500	33
33	AO3PB	3	16	-0.36000	34 35 36 37
34	APG	30	31	0.63000	35 36 37 38
35	AO1PG	2	16	-0.63500	36 37 38
36	AO2PG	2	16	-0.63500	37 38
37	AO3PG	3	16	-0.54800	38
38	AH3PG	21	1	0.39800	

TABLE 4.561: Atoms of building block ATP.

I	J	Type
1	2	10
1	13	10
1	15	22
2	3	12
2	11	16
3	4	7
4	5	3
4	6	7
6	7	12
7	8	9
7	11	16
8	9	2
8	10	2
11	12	10
12	13	10
13	14	3
15	16	20
15	18	26
16	17	20
17	21	26
17	24	26
18	19	20
18	21	26
19	20	1
21	22	20
22	23	1
24	25	20
25	26	28
26	27	24
26	28	24
26	29	28
29	30	28
30	31	24
30	32	24
30	33	28
33	34	28
34	35	24
34	36	24
34	37	28
37	38	1

TABLE 4.562: Bonds of building block ATP.

I	J	K	Type
2	1	13	7
2	1	15	37
13	1	15	37
1	2	3	39
1	2	11	7
3	2	11	27
2	3	4	27
3	4	5	25
3	4	6	27
5	4	6	25
4	6	7	27
6	7	8	27
6	7	11	27
8	7	11	27
7	8	9	23
7	8	10	23
9	8	10	24
2	11	7	27
2	11	12	7
7	11	12	39
11	12	13	7
1	13	12	7
1	13	14	36
12	13	14	36
1	15	16	9
1	15	18	9
16	15	18	9
15	16	17	10
16	17	21	9
16	17	24	9
21	17	24	8
15	18	19	9
15	18	21	8
19	18	21	9
18	19	20	12
17	21	18	8
17	21	22	9
18	21	22	9
21	22	23	12
17	24	25	9
24	25	26	26
25	26	27	14
25	26	28	14
25	26	29	5
27	26	28	29
27	26	29	14

TABLE 4.563: continues on next page.

I	J	K	Type
28	26	29	14
26	29	30	26
29	30	31	14
29	30	32	14
29	30	33	5
31	30	32	29
31	30	33	14
32	30	33	14
30	33	34	26
33	34	35	14
33	34	36	14
33	34	37	5
35	34	36	29
35	34	37	14
36	34	37	14
34	37	38	12

TABLE 4.563: Bond angles of building block ATP.

I	J	K	L	Type
2	1	15	16	16
11	7	8	9	14
18	15	16	17	29
1	15	18	19	17
16	15	18	19	18
16	15	18	21	17
16	15	18	21	34
15	16	17	21	29
16	17	21	18	17
16	17	21	22	18
24	17	21	18	34
24	17	21	22	17
16	17	24	25	8
16	17	24	25	25
21	17	24	25	17
21	17	24	25	34
15	18	19	20	23
15	18	21	17	34
15	18	21	22	17
19	18	21	17	17
19	18	21	22	18
17	21	22	23	23
17	24	25	26	7
17	24	25	26	22
24	25	26	29	20
24	25	26	29	27
25	26	29	30	20
25	26	29	30	27
26	29	30	33	20
26	29	30	33	27
29	30	33	34	20
29	30	33	34	27
30	33	34	37	20
30	33	34	37	27
33	34	37	38	20
33	34	37	38	27

TABLE 4.564: Dihedral angles of building block ATP.

I	J	K	L	Type
1	2	11	12	1
1	2	13	15	1
2	1	3	11	1
2	1	13	12	1
2	3	4	6	1
2	11	12	13	1
3	2	11	7	1
3	4	6	7	1
4	3	5	6	1
4	6	7	11	1
6	7	11	2	1
7	6	8	11	1
8	7	9	10	1
11	2	3	4	1
11	2	7	12	1
11	12	13	1	1
13	1	2	11	1
13	1	12	14	1
15	1	16	18	2
17	16	24	21	2
18	19	21	15	2
21	18	22	17	2

TABLE 4.565: Improper dihedral angles of building block ATP.

Solute building block: p-methylbenzyl alcoholate (charge -e)
Name: PMB

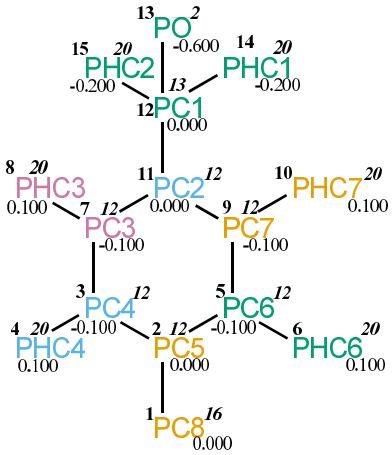

FIGURE 4.227. PMB non-bonded parameters.

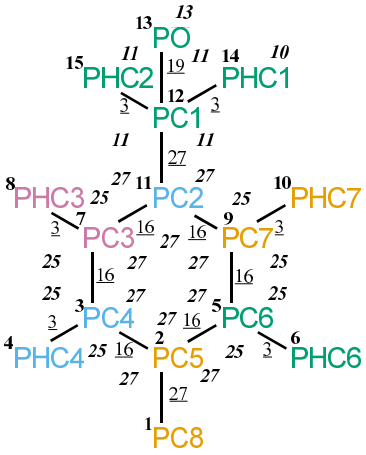

FIGURE 4.228. PMB bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	PC8	16	5	0.00000	2 3 4 5 6 7 9
2	PC5	12	12	0.00000	3 4 5 6 7 8 9 10 11
3	PC4	12	12	-0.10000	4 5 6 7 8 9 11 12
4	PHC4	20	1	0.10000	5 7 8 11
5	PC6	12	12	-0.10000	6 7 9 10 11 12
6	PHC6	20	1	0.10000	9 10 11
7	PC3	12	12	-0.10000	8 9 10 11 12
8	PHC3	20	1	0.10000	9 11 12
9	PC7	12	12	-0.10000	10 11 12
10	PHC7	20	1	0.10000	11 12
11	PC2	12	12	0.00000	12 13 14 15
12	PC1	13	12	0.00000	13 14 15
13	PO	2	16	-0.60000	14 15
14	PHC1	20	1	-0.20000	15
15	PHC2	20	1	-0.20000	

TABLE 4.566. Atoms of building block PMB.

I	J	Type
1	2	27
2	3	16
2	5	16
3	4	3
3	7	16
5	6	3
5	9	16
7	8	3
7	11	16
9	10	3
9	11	16
11	12	27
12	13	19
12	14	3
12	15	3

TABLE 4.567. Bonds of building block PMB.

I	J	K	Type
1	2	3	27
1	2	5	27
3	2	5	27
2	3	4	25
2	3	7	27
4	3	7	25
2	5	6	25
2	5	9	27
6	5	9	25
3	7	8	25
3	7	11	27
8	7	11	25
5	9	10	25
5	9	11	27
10	9	11	25
7	11	9	27
7	11	12	27
9	11	12	27
11	12	13	13
11	12	14	11
11	12	15	11
13	12	14	11
13	12	15	11
14	12	15	10

TABLE 4.568. Bond angles of building block PMB.

I	J	K	L	Type
7	11	12	13	40

TABLE 4.569. Dihedral angles of building block PMB.

I	J	K	L	Type
2	3	5	1	1
2	3	7	11	1
2	5	9	11	1
3	2	5	9	1
3	2	7	4	1
3	7	11	9	1
5	2	3	7	1
5	2	9	6	1
5	9	11	7	1
7	3	11	8	1
9	5	11	10	1
11	7	9	12	1

TABLE 4.570. Improper dihedral angles of building block PMB.

Solute building block: benzoic acid
Name: BA

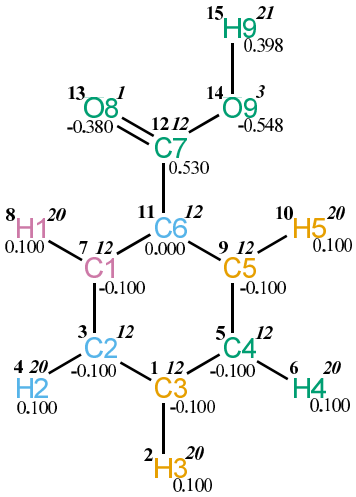

FIGURE 4.229. BA non-bonded parameters.

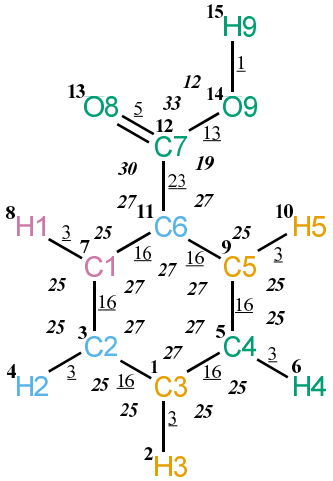

FIGURE 4.230. BA bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	C3	12	12	-0.10000	2 3 4 5 6 7 8 9 10 11
2	H3	20	1	0.10000	3 4 5 6 7 9
3	C2	12	12	-0.10000	4 5 6 7 8 9 11 12
4	H2	20	1	0.10000	5 7 8 11
5	C4	12	12	-0.10000	6 7 9 10 11 12
6	H4	20	1	0.10000	9 10 11
7	C1	12	12	-0.10000	8 9 10 11 12
8	H1	20	1	0.10000	9 11 12
9	C5	12	12	-0.10000	10 11 12
10	H5	20	1	0.10000	11 12
11	C6	12	12	0.00000	12 13 14
12	C7	12	12	0.53000	13 14 15
13	O8	1	16	-0.38000	14
14	O9	3	16	-0.54800	15
15	H9	21	1	0.39800	

TABLE 4.571. Atoms of building block BA.

I	J	Type
1	2	3
1	3	16
1	5	16
3	4	3
3	7	16
5	6	3
5	9	16
7	8	3
7	11	16
9	10	3
9	11	16
11	12	23
12	13	5
12	14	13
14	15	1

TABLE 4.572. Bonds of building block BA.

I	J	K	Type
2	1	3	25
2	1	5	25
3	1	5	27
1	3	4	25
1	3	7	27
4	3	7	25
1	5	6	25
1	5	9	27
6	5	9	25
3	7	8	25
3	7	11	27
8	7	11	25
5	9	10	25
5	9	11	27
10	9	11	25
7	11	9	27
7	11	12	27
9	11	12	27
11	12	13	30
11	12	14	19
13	12	14	33
12	14	15	12

TABLE 4.573. Bond angles of building block BA.

I	J	K	L	Type
7	11	12	14	10
11	12	14	15	12

TABLE 4.574. Dihedral angles of building block BA.

I	J	K	L	Type
1	3	5	2	1
1	3	7	11	1
1	5	9	11	1
3	1	5	9	1
3	7	11	9	1
4	1	7	3	1
5	1	3	7	1
5	9	11	7	1
6	1	9	5	1
7	3	11	8	1
9	5	11	10	1
11	7	9	12	1
12	13	14	11	1

TABLE 4.575. Improper dihedral angles of building block BA.

Solute building block: retinol(neutral)
Name: RTOL

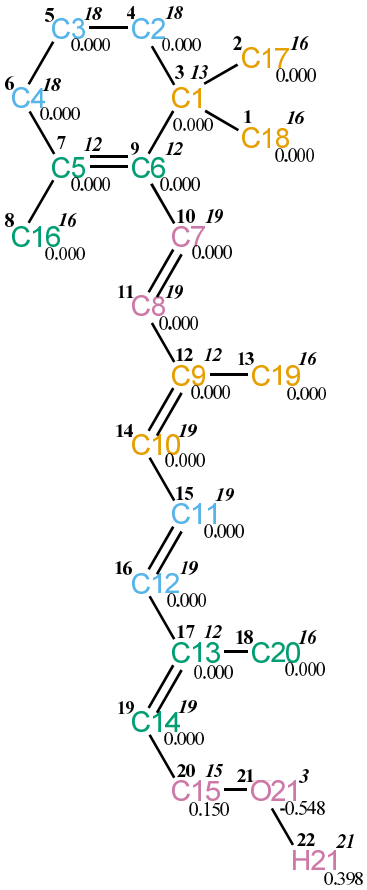

FIGURE 4.231. RTOL non-bonded parameters.

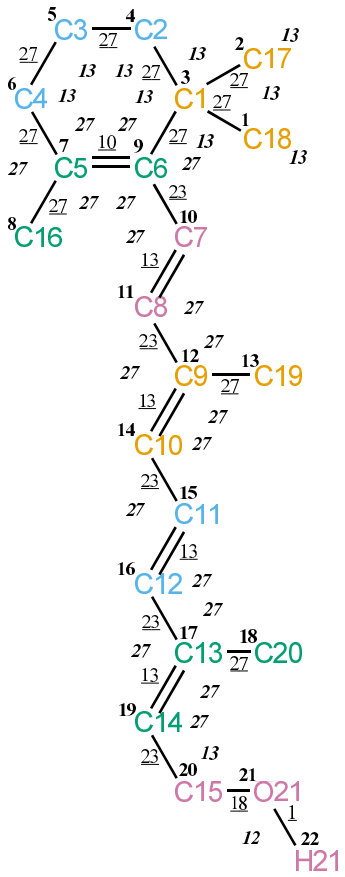

FIGURE 4.232. RTOL bonded parameters.

Seq.	Name	IAC	Mass	Charge	Exclusions
1	C18	16	5	0.00000	2 3 4 9
2	C17	16	5	0.00000	3 4 9
3	C1	13	12	0.00000	4 5 7 9 10
4	C2	18	4	0.00000	5 6 9
5	C3	18	4	0.00000	6 7
6	C4	18	4	0.00000	7 8 9
7	C5	12	12	0.00000	8 9 10
8	C16	16	5	0.00000	9
9	C6	12	12	0.00000	10 11
10	C7	19	3	0.00000	11 12
11	C8	19	3	0.00000	12 13 14
12	C9	12	12	0.00000	13 14 15
13	C19	16	5	0.00000	14
14	C10	19	3	0.00000	15 16
15	C11	19	3	0.00000	16 17
16	C12	19	3	0.00000	17 18 19
17	C13	12	12	0.00000	18 19 20
18	C20	16	5	0.00000	19
19	C14	19	3	0.00000	20 21
20	C15	15	4	0.15000	21 22
21	O21	3	16	-0.54800	22
22	H21	21	1	0.39800	

TABLE 4.576. Atoms of building block RTOL.

I	J	Type
1	3	27
2	3	27
3	4	27
3	9	27
4	5	27
5	6	27
6	7	27
7	8	27
7	9	10
9	10	23
10	11	13
11	12	23
12	13	27
12	14	13
14	15	23
15	16	13
16	17	23
17	18	27
17	19	13
19	20	23
20	21	18
21	22	1

TABLE 4.577. Bonds of building block RTOL.

I	J	K	Type
1	3	2	13
1	3	4	13
1	3	9	13
2	3	4	13
2	3	9	13
4	3	9	13
3	4	5	13
4	5	6	13
5	6	7	13
6	7	8	27
6	7	9	27
8	7	9	27
3	9	7	27
3	9	10	27
7	9	10	27
9	10	11	27
10	11	12	27
11	12	13	27
11	12	14	27
13	12	14	27
12	14	15	27
14	15	16	27
15	16	17	27
16	17	18	27
16	17	19	27
18	17	19	27
17	19	20	27
19	20	21	13
20	21	22	12

TABLE 4.578. Bond angles of building block RTOL.

I	J	K	L	Type
9	3	4	5	34
4	3	9	7	34
3	4	5	6	34
4	5	6	7	34
5	6	7	9	34
6	7	9	3	14
7	9	10	11	34
9	10	11	12	14
10	11	12	14	12
11	12	14	15	14
12	14	15	16	12
14	15	16	17	14
15	16	17	19	12
16	17	19	20	14
17	19	20	21	40
19	20	21	22	23

TABLE 4.579. Dihedral angles of building block RTOL.

I	J	K	L	Type
7	6	9	8	1
9	3	10	7	1
12	11	14	13	1
17	16	19	18	1

TABLE 4.580. Improper dihedral angles of building block RTOL.

CHAPTER 5

GROMOS standard configurations

When simulating a molecule in solution or in crystalline form, the initial positions of solvent molecules surrounding it are to be generated in some way. The GROMOS package comes with files with *standard configurations* of a box with *solvent* molecules. This can be done using the GROMOS++ program sim_box, which requires a standard GROMOS atomic coordinate file containing a number of solvent molecules. Data on the solvent configuration files are given in Tab. 5.1. The configurations are taken from MD simulations at the indicated temperature at constant volume. The atomic coordinates are in nm.

5.1. Water

See Tab. 5.1.

5.2. Chloroform

See Tab. 5.1.

5.3. DMSO

See Tab. 5.1.

5.4. Methanol

See Tab. 5.1.

5.5. Carbontetrachloride

See Tab. 5.1.

solvent	number of molecules	temperature	periodic box type	length of box edge	cut-off radius	file name
		(K)		(nm)	(nm)	
water	5384	300	cubic	5.4937	1.4	spc.cnf
chloroform	1000	293	cubic	5.0816	1.4	chcl3.cnf
DMSO	1024	298	cubic	4.9505	1.4	dmso.cnf
methanol	1000	300	cubic	4.0669	1.4	ch3oh.cnf
CCl4	1000	293	cubic	5.4260	1.4	ccl4.cnf

TABLE 5.1. Standard Solvent Configuration Files.

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Symbols

Symbol	Meaning
	Common names and abbreviations
GROMOS	The GROMOS software package
MD++	The MD++ simulation engine in C++
GROMOS++	The GROMOS++ analysis package in C++
GROMOS96	The GROMOS96 simulation package (1996)
3D	abbreviation for three dimensions
AA	Atomistic (All Atom) models
BD	Brownian Dynamics simulation
B&S – LEUS	Ball and stick local elevation umbrella sampling
CG	Coarse Grained models
CGEM	Conjugate gradient method for energy minimization
FRCG	Fletcher-Reeves conjugate gradient method for energy minimization
PRCG	Polak-Ribiére conjugate gradient method for energy minimization
COG	Center of geometry
COS	Charge On Spring approach
CP	Car Parrinello approach
DF	Distancefield
DOF	Degrees of freedom (abbreviation)
DPD	Diffusive Particle Dynamics simulation
`doxygen`	Documentation platform
EM	Energy minimisation
EDS	Enveloping distribution sampling
FBC	Fixed boundary conditions
HBC	Hyper-spherical boundary conditions
LE	Local elevation
LEUS	Local elevation umbrella sampling
LS	Lattice-sum method
MC	Monte Carlo sampling
MD	Molecular Dynamics simulation
NOE	Nuclear Overhauser Effect
PBC	Periodic boundary conditions
PPPM	Particle-particle–particle-mesh (P^3M) method
QM	Quantum Mechanical models
QMD	Quantum Molecular Dynamics simulation
RDF	Radial distribution function
RE	Replica Exchange
REMD	Replica Exchange Molecular Dynamics simulation
RF	Reaction-field method
RMSD	Root-mean-square difference
RMSF	Root-mean-square fluctuation
SD	Stochastic Dynamics simulation
SDEM	Steepest descent method for energy minimization
TI	Thermodynamic integration
US	Umbrella sampling

Symbol	Meaning
VBC	Vacuum boundary conditions
Physical constants	
h	Planck's constant [0.3990313 kJ mol^{-1} ps]
$\hbar$	Planck's constant divided by 2π [0.06350780 kJ mol^{-1} ps]
$N_{\rm Av}$	Avogadro's number [6.02214 $\times 10^{23}$]
k_B	Boltzmann's constant [1.380662 $\times 10^{-26}$ kJ K^{-1})]
R	Ideal gas constant ($N_{\rm Av} \times k_B$)
c	Speed of light [2.99792458 $\times 10^5$ nm ps^{-1}]
Degrees of freedom and system configuration	
$\mathcal{N}_d$	Number of degrees of freedom of a system
$\mathcal{N}_a$	Number of particles in a system of particles ($\mathcal{N}_d$ =3$\mathcal{N}_a$)
$\mathcal{N}_a^{solu}$	Number of particles the solute consists of
$\boldsymbol{q}$	$3\mathcal{N}_a$-dimensional generalized coordinate vector of a system of particles
$\boldsymbol{p_q}$	$3\mathcal{N}_a$-dimensional generalized momentum vector of a system of particles
$\boldsymbol{r}$	$3\mathcal{N}_a$-dimensional Cartesian coordinate vector of a system of particles
$\boldsymbol{p}$	$3\mathcal{N}_a$-dimensional Cartesian momentum vector of a system of particles
$\boldsymbol{f}$	$3\mathcal{N}_a$-dimensional Cartesian force vector of a system of particles
$\overline{\boldsymbol{f}}$	$3\mathcal{N}_a$-dimensional Cartesian mean force vector of a system of particles
$\boldsymbol{f}^{st}$	$3\mathcal{N}_a$-dimensional Cartesian stochastic force vector of a system of particles
$\mathbf{f}_i^{st}$	$3\mathcal{N}_a$-dimensional Cartesian stochastic force vector of a system of particles
$\boldsymbol{v}$	$3\mathcal{N}_a$-dimensional Cartesian velocity vector of a system of particles
$\mathbf{r}$	3-dimensional Cartesian coordinate vector of a particle
$\mathbf{p}$	3-dimensional Cartesian momentum vector of a particle
$\mathbf{f}$	3-dimensional Cartesian force vector of a particle
$\mathbf{v}$	3-dimensional Cartesian velocity vector of a particle
Ψ $[\Psi(\boldsymbol{r})]$	Wavefunction (position representation; configuration of a quantum-mechanical system of $\mathcal{N}_a$ particles)
$\{$ $\boldsymbol{r}$,$\boldsymbol{p}$ $\}$	Phase-space point (Cartesian coordinates; configuration of a classical system of $\mathcal{N}_a$ particles)
(Statistical) thermodynamics	
$\mathcal{F}$	Free energy
G	Gibbs free energy
H	Enthalpy
$\mathcal{U}$	Energy of a system
$\mathcal{S}$	Entropy of a system
$\mathcal{Z}$	Partition function
$\mathcal{T}$	Instantaneous temperature
$\mathcal{T}_o$	Reference temperature
$\mathcal{K}$	Instantaneous kinetic energy of a system
$\mathcal{K}_{tr}$	Instantaneous translational kinetic energy
$\mathcal{K}_{ir}$	Instantaneous internal+rotational kinetic energy
$\mathcal{U}$	Instantaneous total potential energy of a system
$\mathcal{W}$	Instantaneous virial of a system
$\mathcal{P}$	Instantaneous pressure of a system
$\mathcal{V}$	Instantaneous volume of a system
ρ_J	Number particle density of particles J
Miscellaneous	

Symbol	Meaning
t	Time
Δt	discrete time step
$\mathcal{N}_t$	Number of MD steps
P	Probability
m	Mass of a particle
M	Mass of the whole system
$\underline{\mathbf{m}}$	Diagonal mass matrix of a system of $\mathcal{N}_a$ particles
γ	Friction coefficient of a particle
$\underline{\gamma}$	Diagonal friction coefficient matrix of a system of $\mathcal{N}_a$ particles
T	Absolute temperature
β	prefactor: $1/k_BT$
τ_T	relaxation time for the coupling to a temperature bath
$\mathbf{s}$	Vector denoting the collection of all force-field parameters
λ	Coupling parameter Lambda for a lambda dependent Hamiltonian
$\mathcal{N}_\lambda$	Number of λ-values in a TI simulation
H	Heaviside function defined as $H(x) = 0 \; \forall \; x < 0$ and $H(x) = 1 \; \forall \; x > 0$
sign	Sign function: $\text{sign}(x) = 1 \; \forall \; x > 0$ and $\text{sign}(x) = -1 \; \forall \; x < 0$
i	imaginary number, $i^2 = -1$
δ_{ij}	general Kronecker delta
σ	Standard deviation
σ^2	Variance
$\mathcal{N}_{conf}$	Number of configurations in an ensemble
D	Diffusion constant
R_{gyr}	radius of gyration
η	the viscosity of a system
$g(r)$	radial distribution function
s	Smoothness parameter in EDS simulations
E^R	Energy offset parameter in EDS simulations
$\mathcal{N}^{(s)}$	Number of states in EDS simulations
Spatial boundary conditions	
$\underline{\mathcal{B}}$	3×3-matrix of the box-edge vectors (columns) in the reference Cartesian coordinate system (PBC)
$\hat{\mathbf{e}}$	Unit vector
$\mathbf{a}$	First edge vector of a (triclinic) box (in the reference coordinate system)
$\mathbf{b}$	Second edge vector of a (triclinic) box (in the reference coordinate system)
$\mathbf{c}$	Third edge vector of a (triclinic) box (in the reference coordinate system)
a	length of first edge of a (triclinic) box
b	length of second edge of a (triclinic) box
c	length of third edge of a (triclinic) box
$\mathbf{T}$	Position vector of the reference corner of a triclinic box (components in the reference coordinate system and vector relative to the origin of this system)
$\underline{\mathbf{L}}$	Computational box matrix (columns defined by the components of edge vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ in the reference coordinate system)
$\underline{\mathbf{B}}$	Edge length matrix (diagonal, elements a, b and c)
α	First edge angle a triclinic box (between $\mathbf{b}$ and $\mathbf{c}$)
β	Second edge angle a triclinic box (between $\mathbf{a}$ and $\mathbf{c}$)
γ	Third edge angle a triclinic box (between $\mathbf{a}$ and $\mathbf{b}$)
ϕ	First Euler angle of a triclinic box

Symbol	Meaning
θ	Second Euler angle of a triclinic box
ψ	Third Euler angle of a triclinic box
$\check{\mathbf{r}}$	Oblique coordinates of a real-space vector (with reference to the box-edge vectors)
$\check{\mathbf{r}}$	Oblique fractional coordinates of a real-space vector (with reference to the box-edge vectors)
$\check{\mathbf{k}}$	Oblique coordinates of a reciprocal-space vector
$\check{\mathbf{k}}$	Oblique fractional coordinates of a reciprocal-space vector
$\mathbf{l}$	Lattice vector (three-dimensional vector with integer components)
$\mathbf{k}$	Reciprocal-lattice vector ($\mathbf{k} = 2\pi\underline{\mathbf{L}}^{-1}\mathbf{l}$)
$\underline{\mathbf{S}}$	Transformation matrix
$\underline{\mathbf{R}}$	Transformation matrix
$\underline{\mathbf{T}}$	Transformation matrix
Representation of the interaction	
$\hat{\mathcal{H}}$	Hamiltonian operator describing the interaction for quantum-mechanical degrees of freedom
$\hat{\mathcal{K}}$	Kinetic energy operator (kinetic energy contribution to the quantum-mechanical Hamiltonian operator)
$\hat{\mathcal{V}}$	Potential energy operator (potential energy contribution to the quantum-mechanical Hamiltonian operator)
$\mathcal{H}$ $[\mathcal{H}(\boldsymbol{r},\boldsymbol{p})]$	Hamiltonian function describing the interaction for classical degrees of freedom
$\mathcal{K}$ $[\mathcal{K}(\boldsymbol{p})]$	Kinetic energy contribution to the classical Hamiltonian function
$\mathcal{V}$ $[\mathcal{V}(\boldsymbol{r})]$	Potential energy contribution to the classical Hamiltonian function
$\overline{\mathcal{V}}$ $[\overline{\mathcal{V}}(\boldsymbol{r})]$	Potential of mean force contribution to the classical Hamiltonian function
Physical interactions	
φ [Proper dihedral-angle term]	
$\mathcal{V}^{(phys)}$ $[\mathcal{V}^{(phys)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Physical potential energy contribution to $\mathcal{V}$
$\mathcal{V}^{(cov)}$ $[\mathcal{V}^{(cov)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Covalent potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathcal{V}^{(nbd)}$ $[\mathcal{V}^{(nbd)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Non-bonded potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathcal{V}^{(b)}$ $[\mathcal{V}^{(b)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Bond stretching potential energy contribution to $\mathcal{V}^{(cov)}$
$\mathcal{V}^{(\theta)}$ $[\mathcal{V}^{(\theta)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Bond-angle bending potential energy contribution to $\mathcal{V}^{(cov)}$
$\mathcal{V}^{(\xi)}$ $[\mathcal{V}^{(\xi)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Improper dihedral-angle bending potential energy contribution to $\mathcal{V}^{(cov)}$
$\mathcal{V}^{(\varphi)}$ $[\mathcal{V}^{(\varphi)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Proper dihedral-angle torsion potential energy contribution to $\mathcal{V}^{(cov)}$
$\mathcal{V}^{(vdw)}$ $[\mathcal{V}^{(vdw)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Van der Waals potential energy contribution to $\mathcal{V}^{(nbd)}$
$\mathcal{V}^{(ele)}$ $[\mathcal{V}^{(ele)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Electrostatic potential energy contribution to $\mathcal{V}^{(nbd)}$
$\mathcal{V}^{(LJCRF)}$	Sum of the non-bonded potentials $\mathcal{V}^{(vdw)}$ and $\mathcal{V}^{(ele)}$
Physical force-field terms	
$V^{(b)}$ $[V^{(b)}(b;k^{(b)},b^0)]$	Potential energy function associated with the stretching of a single covalent bond (quartic: $V^{(b,q)}$; harmonic: $V^{(b,h)}$; soft harmonic: $V^{(bs,h)}$)
$V_n^{(b)}$ $[V^{(b)}(b_n;k_n^{(b)},b_n^0)]$	Potential energy function associated with the stretching of the nth single covalent bond (quartic: $V_n^{(b,q)}$; harmonic: $V_n^{(b,h)}$; soft harmonic: $V_n^{(bs,h)}$)
$\mathbf{f}^{(b,q)}$	Force due to the bond stretching potential (quartic)
$\mathbf{f}^{(b,h)}$	Force due to the bond stretching potential (harmonic)
$\mathbf{f}^{(bs,h)}$	Force due to the bond stretching potential (soft harmonic)
$N^{(b)}$	Number of covalent bonds in the molecular system
$N^{(bs)}$	Number of soft covalent bonds in the molecular system
$M_n^{(b)}$	Bond type code associated with covalent bond term n

Symbol	Meaning
b_n $[b_n(\boldsymbol{r}, \underline{\mathcal{B}})]$	Length of covalent bond n in the considered configuration
b_n^0 $[b^0(M_n^{(b)}, \mathbf{s})]$	Reference length of covalent bond term n
$k_n^{(b,q)}$	Force constant of stretching for covalent bond term n (quartic potential)
$k_n^{(b,h)}$	Force constant of stretching for covalent bond term n (harmonic potential)
$V^{(\theta)}$ $[V^{(\theta)}(\theta; k^{(\theta)}, \theta^0)]$	Potential energy function associated with the bending of a single covalent bond angle (cosine-harmonic: $V^{(\theta,c)}$; soft cosine-harmonic: $V^{(\theta s,c)}$; angle-harmonic: $V^{(\theta,h)}$)
$V_n^{(\theta)}$ $[V_n^{(\theta)}(\theta_n; k_n^{(\theta)}, \theta_n^0)]$	Potential energy function associated with the bending of the nth covalent bond angle (cosine-harmonic: $V_n^{(\theta,c)}$; soft cosine-harmonic: $V_n^{(\theta s,c)}$; angle-harmonic: $V_n^{(\theta,h)}$)
$\mathbf{f}^{(\theta,c)}$	Force due to the bond angle potential (cosine-harmonic)
$\mathbf{f}^{(\theta s,c)}$	Force due to the bond angle potential (soft cosine-harmonic)
$\mathbf{f}^{(\theta,h)}$	Force due to the bond angle potential (angle-harmonic)
$N^{(\theta)}$	Number of covalent bond angles in the molecular system
$M_n^{(\theta)}$	Bond-angle type code associated with covalent bond-angle term n
θ_n $[\theta_n(\boldsymbol{r}, \underline{\mathcal{B}})]$	Value of covalent bond angle n in the considered configuration
θ_n^0 $[\theta^0(M_n^{(\theta)}, \mathbf{s})]$	Reference angle of covalent bond-angle term n
$k_n^{(\theta,c)}$	Force constant of bending for covalent bond-angle term n (cosine-harmonic potential)
$k_n^{(\theta s,c)}$	Force constant of bending for covalent bond-angle term n (soft cosine-harmonic potential)
$k_n^{(\theta,h)}$	Force constant of bending for covalent bond-angle term n (angle-harmonic potential)
$V^{(\xi)}$ $[V^{(\xi)}(\xi; k^{(\xi)}, \xi^0)]$	Potential energy function associated with the bending of a single covalent improper dihedral angle
$V^{(\xi s)}$ $[V^{(\xi s)}(\xi; k^{(\xi)}, \xi^0)]$	Potential energy function associated with the bending of a single covalent improper dihedral angle
$\mathbf{f}^{(\xi)}$	Force due to the improper dihedral-angle potential
$\mathbf{f}^{(\xi s)}$	Force due to the soft improper dihedral-angle potential
$N^{(\xi)}$	Number of covalent improper dihedral angles in the molecular system
$N^{(\xi s)}$	Number of covalent improper dihedral angles in the molecular system
$M_n^{(\xi)}$	Improper dihedral-angle type code associated with covalent improper dihedral-angle term n
ξ_n $[\xi_n(\boldsymbol{r}, \underline{\mathcal{B}})]$	Value of covalent improper dihedral angle n in the considered configuration
ξ_n^0 $[\xi^0(M_n^{(\xi)}, \mathbf{s})]$	Reference angle of covalent improper dihedral-angle term n
$k_n^{(\xi)}$	Force constant of bending for covalent improper dihedral-angle term n
$V^{(\varphi)}$ $[V^{(\varphi)}(\varphi; k^{(\varphi)}, \varphi^0)]$	Potential energy function associated with the torsion of a single covalent proper dihedral angle (symmetric potential: $V^{(\varphi,s)}$; generalized: $V^{(\varphi,g)}$)
$\mathbf{f}^{(\varphi,s)}$	Force due to the symmetric proper dihedral-angle potential
$\mathbf{f}^{(\varphi,g)}$	Force due to the generalized proper dihedral-angle potential
$N^{(\varphi)}$	Number of covalent proper dihedral angles in the molecular system
$M_n^{(\varphi)}$	Proper dihedral-angle type code associated with covalent proper dihedral-angle term n
φ_n $[\varphi_n(\boldsymbol{r}, \underline{\mathcal{B}})]$	Value of covalent proper dihedral angle n in the considered configuration
φ_n^0 $[\varphi^0(M_n^{(\varphi)}, \mathbf{s})]$	Reference angle (phase shift) of covalent proper dihedral-angle term n
$m_n^{(\varphi)}$ $[m_n^{(\varphi)}(M_n^{(\varphi)}, \mathbf{s})]$	Multiplicity of covalent proper dihedral-angle term n
$k_n^{(\varphi,s)}$	Force constant of torsion for covalent proper dihedral-angle term n (symmetric potential; $\varphi_n^0 = 0, \pi$; $m_n^{(\varphi)} \leq 6$)

Symbol	Meaning
$k_n^{(\varphi,g)}$	Force constant of torsion for covalent proper dihedral-angle term n (generalized potential; $\varphi_n^0 \in [0, 2\pi[$)
q	Partial charge of an atom or site
C_{12}	Van der Waals (Pauli) repulsion coefficient of an atom or site (Lennard-Jones function)
C_6	Van der Waals (London) dispersion coefficient of an atom or site (Lennard-Jones function)
C_{126}	Ratio of Van der Waals coefficients $\frac{C_{12}}{C_6}$ (Lennard-Jones function)
α_{LJ}	Lennard-Jones soft-core switching parameter
α_C	Coulomb soft-core switching parameter
$\mathcal{V}^{(ele,pws)}$ $[\mathcal{V}^{(ele,pws)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Pairwise potential energy contribution to $\mathcal{V}^{(ele)}$
$\mathcal{V}^{(ele,slf)}$ $[\mathcal{V}^{(ele,slf)}(\underline{\mathcal{B}};\mathbf{s})]$	Self potential energy contribution to $\mathcal{V}^{(ele)}$
$\mathcal{V}^{(ele,srf)}$ $[\mathcal{V}^{(ele,srf)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Surface potential energy contribution to $\mathcal{V}^{(ele)}$
$\mathbf{f}^{(nbd)}$	Force due to the non-bonded forces
$\Psi_{ij}^{(ele)}$ $[\Psi_{ij}^{(ele)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Electrostatic influence function associated with the particle pair $i-j$
$\delta_{ij}^{(exc)}$ $[\delta_{ij}^{(exc)}(\mathbf{s})]$	Indicator of non-bonded exclusion for the particle pair $i-j$
$\Psi^{(ele,slf)}$ $[\Psi^{(ele,slf)}(\underline{\mathcal{B}})]$	Electrostatic self influence function
$\psi^{(RF)}$ $[\psi^{(RF)}(\mathrm{x})]$	Influence function at distance x of a particle in RF electrostatics
H $[H(\mathrm{x})]$	Heaviside step function (one if x is positive, zero otherwise)
R_C	Cutoff distance (truncation)
R_{cp}	Short-range cut-off
R_{cl}	Long-range cut-off
R^{cg}	radius of a charge group
N_{cg}	number of atoms belonging to a charge group
R_{RF}	Cutoff distance (onset of the RF continuum; usually set equal to R_C)
ϵ_{RF}	Relative dielectric permittivity of the RF continuum (usually set equal to that of the solvent)
κ_{RF}	Inverse Debye screening length of the RF continuum (usually set to zero)
C_{RF}	Constant characterizing the effect of the RF continuum
$\overline{\mathbf{R}}_{ij}$ $[\overline{\mathbf{R}}_{ij}(\boldsymbol{r})]$	Vector (FBC) or minimum-image vector (PBC) connecting the center of the CG containing particle j to the center of the CG containing particle i (norm $\overline{R}_{ij}$)
$\mathcal{V}^{(ele,pws,RF-CB)}$ $[\mathcal{V}^{(ele,pws,RF-CB)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Coulombic pairwise potential energy contribution to $\mathcal{V}^{(ele,pws)}$ (RF electrostatics)
$\mathcal{V}^{(ele,pws,RF-RF)}$ $[\mathcal{V}^{(ele,pws,RF-RF)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Distance-dependent pairwise potential energy contribution to $\mathcal{V}^{(ele,pws)}$ (RF electrostatics)
$\mathcal{V}^{(ele,pws,RF-RC)}$ $[\mathcal{V}^{(ele,pws,RF-RC)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Distance-independent pairwise potential energy contribution to $\mathcal{V}^{(ele,pws)}$ (RF electrostatics)
$\Psi_{ij}^{(ele,LS-RS)}$ $[\Psi_{ij}^{(ele,LS-RS)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Real-space component of electrostatic influence function $\Psi_{ij}^{(ele)}$ (LS electrostatics)
$\Psi_{ij}^{(ele,LS-KS)}$ $[\Psi_{ij}^{(ele,LS-KS)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Reciprocal-space component of the electrostatic influence function $\Psi_{ij}^{(ele)}$ (LS electrostatics)
$\mathcal{V}^{(ele,pws,LS-RS)}$ $[\mathcal{V}^{(ele,pws,LS-RS)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Real-space pairwise potential energy contribution to $\mathcal{V}^{(ele,pws)}$ (LS electrostatics)
$\mathcal{V}^{(ele,pws,LS-KS)}$ $[\mathcal{V}^{(ele,pws,LS-KS)}(\boldsymbol{r};\underline{\mathcal{B}};\mathbf{s})]$	Reciprocal-space pairwise potential energy contribution to $\mathcal{V}^{(ele,pws)}$ (LS electrostatics)
$\psi^{(LS)}$ $[\psi^{(LS)}(\mathbf{x})]$	Influence function at position $\mathbf{x}$ relative to a particle in LS electrostatics
a	Width of the charge-shaping function
γ $[\gamma(\mathrm{x})]$	Charge-shaping function

Symbol	Meaning
$\hat{\gamma}$ $[\hat{\gamma}\ (\mathrm{x})]$	Fourier transformed charge-shaping function
$\mathbf{E}$	Electric field
$\boldsymbol{\mu}$	Dipole
$\boldsymbol{J}$	
α	Electronic polarisability
$\mathbf{P}$	Polarisation
ϵ	Dielectric permittivity
γ^{pol}	γ to calculate position of off site charge
k^{ho}	harmonic force constant in the COS model
ϕ	Electrostatic potential
Unphysical force-field terms	
$\mathcal{V}^{(spec)}$	Unphysical potential energy
$\mathcal{V}^{(res)}$	Restraint energy
$\mathcal{V}^{(pr)}$	Position restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathbf{f}^{(c)}$	Force due to the position constraints
$k^{(pr)}$	Force constant of an unphysical position-restraining term
$\mathcal{N}^{(pr)}$	number of positionally restrained atoms
l	Lagrange multiplier for position constraints
$\mathcal{V}^{(dr)}$	Distance restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathbf{f}^{(dir)}$	Force due to the atom-atom distance restraints
$k^{(dr)}$	Force constant of an unphysical distance-restraining term
$\mathbf{r}^0$	Equilibrium distance of distance restraint
$N^{(dir)}$	Number of atom-atom distance restraints
d_{CH}	carbon-hydrogen distance
d_{CC}	carbon-carbon distance
τ_{dr}	decay time for time-averaged distance restraining
$\mathcal{V}^{(tr)}$	Dihedral-angle restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$k^{(tr)}$	Force constant of an unphysical dihedral-angle restraining term
$\mathcal{N}^{(tr)}$	number of restrained dihedral angles
$\mathcal{V}^{(Jr)}$	^3J-restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$k^{(Jr)}$	Force constant of an unphysical ^3J-value restraining term
^3J	J-value or J-coupling constant
$^3J^0$	experimental J-value
J	general representation of a J-value
J^0	experimental J-value
ΔJ^0	width of flat-bottom for J-value restraining
a	a in Karplus relation
b	b in Karplus relation
c	c in Karplus relation
τ^s_{Jr}	period of scaling in periodically-scaled J-value restraining
Δt_ω	time period for which scaling is suspended in periodically-scaled J-value restraining
N_{le}	number of bins in J-value local elevation biasing
$w_{\zeta ni}$	weight of gaussian in J-value LE
$\mathcal{V}^{(Fxr)}$	$\mid F \mid$-restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathcal{V}^{(exr)}$	ρ-restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathcal{V}^{(sxr)}$	symmetry restraining potential energy contribution to $\mathcal{V}^{(phys)}$

Symbol	Meaning
k^{xr}	(harmonic) force constant for the crystallographic restraining
k^{sym}	harmonic force constant for the crystallographic symmetry restraining
F	Structure factor amplitude
ρ	Electron density
S	space group of a crystal
N_{sym}	Number of symmetry operations of a space group
$\mathbb{S}$	Symmetry operator $\mathbb{S} = \mathbf{R}\mathbf{r} + \mathbf{t}$
$\mathbf{R}$	Rotation matrix of a symmetry operator
$\mathbf{t}$	Translation vector of a symmetry operator
$\mathcal{V}^{(Sr)}$	S^2-restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$k^{(Sr)}$	Force constant of an unphysical S^2-value restraining term
S^2	S^2-order parameter
$S^{2,0}$	experimental S^2-value
S	general representation of a S^2-value
S^0	experimental S^2-value
$\mathcal{V}^{(df)}$	Distancefield restraining potential energy contribution to $\mathcal{V}^{(phys)}$
$\mathbf{f}^{(df)}$	Force due to the atom-atom distance restraints
$k^{(df)}$	Force constant of an unphysical distance-restraining term
l^0	Equilibrium distance of distance restraint
g_s	Distancefield grid distance
$\mathcal{V}^{(le)}$	Local elevation (LE) energy
$\mathcal{V}^{(bias)}$	bias energy
γ	LE basis function
$k^{(le)}$	LE force constant
$\mathbf{r}^{uc}$	unconstrained atomic positions
N_c	Number of constraints
N_{sh}	number of iterations of the SHAKE algorithm
d^0	constraint length
$\mathbf{f}^{uc}$	unconstrained atomic forces