Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


**Supplementary Information**

# Enantioselective Amino Acids Interactions in Solution

Natsuki Watanabe [1], Mitsuo Shoji [*2,3], Koichi Miyagawa [2], Yuta Hori [2],

Mauro Boero [4], Masayuki Umemura [2] and Yasuteru Shigeta [2]

[1] Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan.

[2] Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577, Japan.

[3] JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan

[4] University of Strasbourg, Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, UMR 7504, 23 rue du Loess, F-67034 France.

* Corresponding author: Mitsuo Shoji (*E-mail*: mshoji@ccs.tsukuba.ac.jp)

**Table of Contents**

**Supplementary Figure**

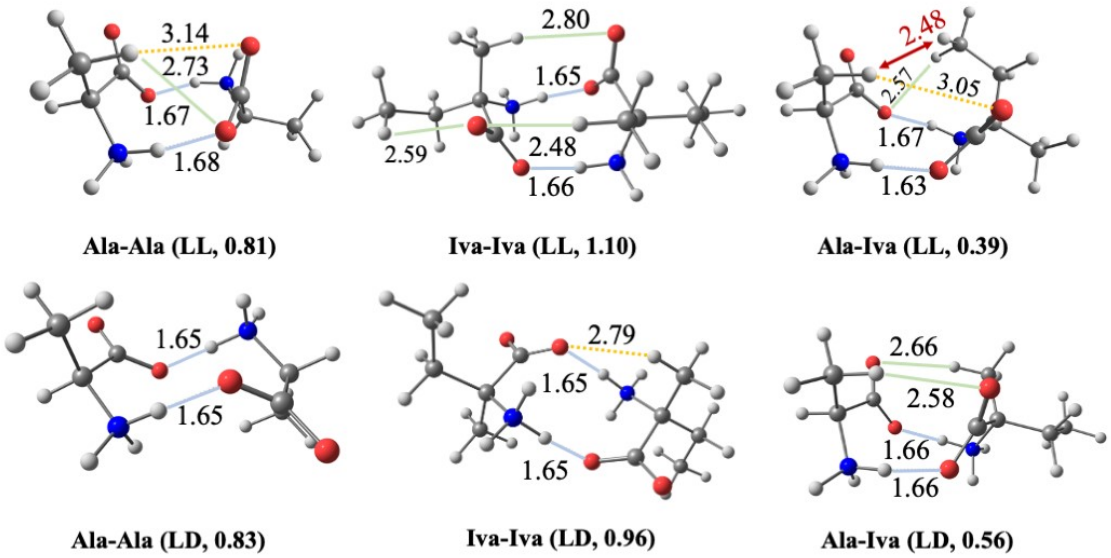


Figure S1. The third stable conformations of amino acid dimers in zwitterionic form. Color lines represent the electrostatic interactions (blue), hydrogen bonding (green), measurement (dashed yellow) and vdW contacts (dark red) along with their distances (Å). Relative energies (kcal $mol^{-1}$) to each of the most stable conformations of LL are given in parenthesis.

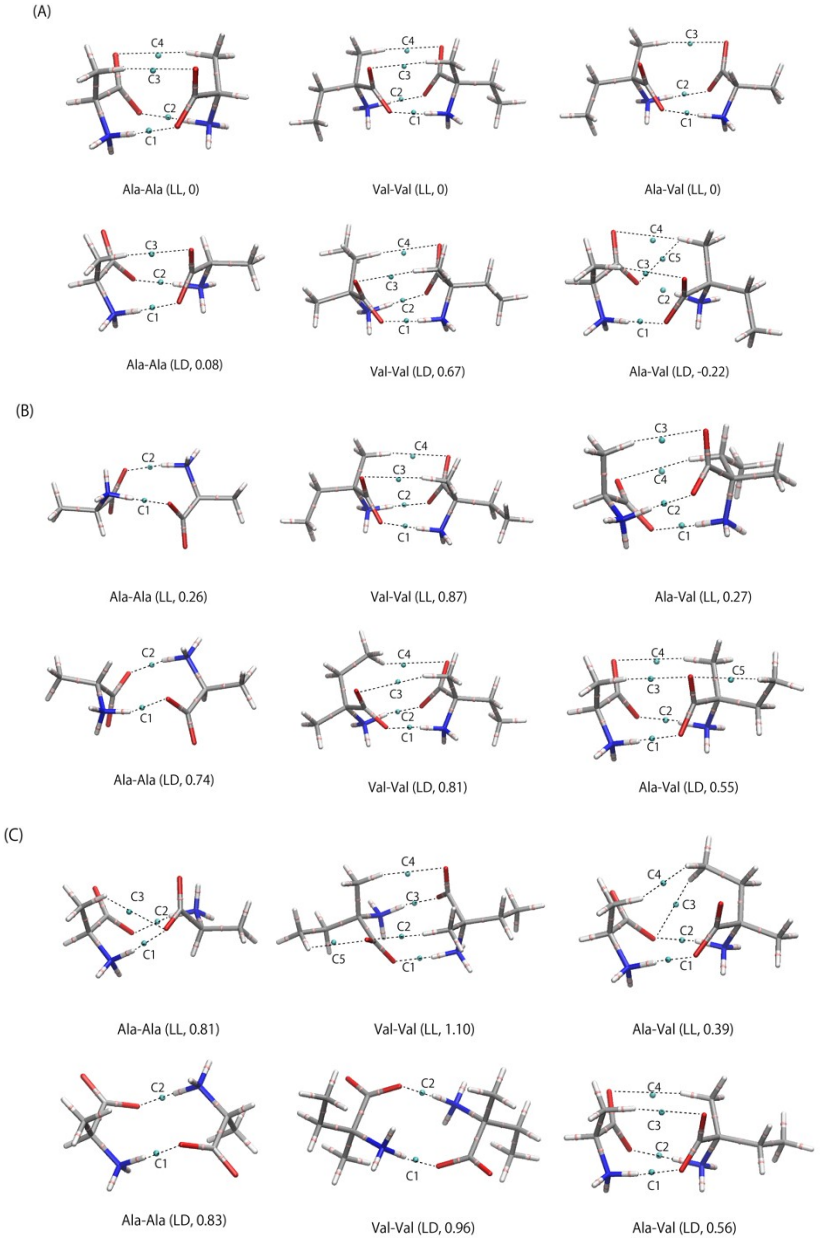


Figure S2. Molecular graphs of amino acid dimers obtained from Atoms in Molecules (AIM) analysis in the (A) most stable conformations, (B) second stable conformations and (C) third stable conformations. Attractors are colored according to the chemical element, and critical points along interaction lines are shown as small spheres, where the pink and cyan colors represent negative and positive signs of their Laplacian values, respectively. Detailed distances and positive values of the Laplacian are shown in Tables S2-S4.

**Supplementary Table**

Table S1. Relative energies (kcal $mol^{-1}$) of the stable conformations of amino acid dimers in zwitterionic forms. Energies were calculated at the B3LYP-D3//6-311++G(d,p) level within PCM. Zero-point vibrational energy corrections are included.

| Conformations | Ala-Ala | | Iva-Iva | | Ala-Iva | |
|---|---|---|---|---|---|---|
| | LL | LD | LL | LD | LL | LD |
| 1st stable | 0 | 0.08 | 0 | 0.67 | 0 | -0.22 |
| 2nd stable | 0.26 | 0.74 | 0.87 | 0.81 | 0.27 | 0.55 |
| 3rd stable | 0.81 | 0.83 | 1.10 | 0.96 | 0.39 | 0.56 |

Table S2. AIM analysis for the most stable conformations of amino acid dimers calculated at B3LYP/6-311+G(p,d) level of theory. Relevant distances and positive Laplacian values for critical points are reported. The corresponding molecular graphs are shown in Fig S3A.

| Molecule (chirality, $\Delta E$/kcal mol$^{-1}$) | Critical points | Atoms in interaction | Atomic distance/Å | Attractors distance/Å | Attractor-Critical point distance/Å | $\nabla^2\rho_{(r_c)}$ /a.u. |
|---|---|---|---|---|---|---|
| Ala-Ala(LL, 0) | C1 | N-H…O | 1.66 | 1.68 | 0.57 (H…C1) | 0.1442 |
| | C2 | N-H…O | 1.66 | 1.68 | 0.57 (H…C2) | 0.1442 |
| | C3 | C-H…O | 2.65 | 2.67 | 1.08 (H…C3) | 0.0205 |
| | C4 | C-H…O | 2.65 | 2.67 | 1.08 (H…C4) | 0.0205 |
| Ala-Ala(LD, 0.08) | C1 | N-H…O | 1.65 | 1.67 | 0.57 (H…C1) | 0.1443 |
| | C2 | N-H…O | 1.64 | 1.66 | 0.56 (H…C2) | 0.1485 |
| | C3 | C-H…O | 2.62 | 2.63 | 1.07 (H…C3) | 0.0212 |
| Val-Val(LL, 0) | C1 | N-H…O | 1.65 | 1.67 | 0.57 (H…C1) | 0.1450 |
| | C2 | N-H…O | 1.65 | 1.67 | 0.57 (H…C2) | 0.1450 |
| | C3 | C-H…O | 2.66 | 2.67 | 1.08 (H…C3) | 0.0211 |
| | C4 | C-H…O | 2.66 | 2.67 | 1.08 (H…C4) | 0.0211 |
| Val-Val(LD, 0.67) | C1 | N-H…O | 1.66 | 1.68 | 0.57 (H…C1) | 0.1437 |
| | C2 | N-H…O | 1.66 | 1.67 | 0.57 (H…C2) | 0.1461 |
| | C3 | C-H…O | 2.65 | 2.66 | 1.08 (H…C3) | 0.0215 |
| | C4 | C-H…O | 2.69 | 2.70 | 1.10 (H…C4) | 0.0210 |
| Ala-Val(LL, 0) | C1 | N-H…O | 1.63 | 1.65 | 0.56 (H…C1) | 0.1495 |
| | C2 | N-H…O | 1.66 | 1.68 | 0.57 (H…C2) | 0.1433 |
| | C3 | C-H…O | 2.61 | 2.62 | 1.06 (H…C3) | 0.0220 |
| Ala-Val(LD, -0.22) | C1 | N-H…O | 1.65 | 1.67 | 0.57 (H…C1) | 0.1462 |
| | C2 | N-H…O | 1.66 | 1.68 | 0.57 (H…C2) | 0.1442 |
| | C3 | C-H…O | 2.68 | 2.70 | 1.09 (H…C3) | 0.0197 |
| | C4 | C-H…O | 2.73 | 2.74 | 1.11 (H…C4) | 0.02011 |
| | C5 | C-H…O | 2.81 | 2.82 | 1.18 (H…C4) | 0.0214 |

Table S3. AIM analysis for the second stable conformations of amino acid dimers calculated at B3LYP/6-311+G(p,d) level of theory. Relevant distances and positive Laplacian values for critical points are given. Corresponding molecular graphs are shown in Fig S3B.

| Molecule (chirality, $\Delta E$/kcal mol$^{-1}$) | Critical points | Atoms in interaction | Atomic distance/Å | Attractors distance/Å | Attractor-Critical point distance/Å | $\nabla^2\rho(r_c)$/a.u. |
|---|---|---|---|---|---|---|
| Ala-Ala(LL, 0.26) | C1 | N-H…O | 1.64 | 1.66 | 0.56 (H…C1) | 0.1458 |
| | C2 | N-H…O | 1.64 | 1.66 | 0.56 (H…C2) | 0.1458 |
| Ala-Ala(LD, 0.74) | C1 | N-H…O | 1.66 | 1.68 | 0.57 (H…C1) | 0.1380 |
| | C2 | N-H…O | 1.67 | 1.69 | 0.58 (H…C2) | 0.1419 |
| Val-Val(LL, 0.87) | C1 | N-H…O | 1.65 | 1.67 | 0.57 (H…C1) | 0.1461 |
| | C2 | N-H…O | 1.65 | 1.67 | 0.57 (H…C2) | 0.1442 |
| | C3 | C-H…O | 2.69 | 2.70 | 1.10 (H…C3) | 0.0197 |
| | C4 | C-H…O | 2.61 | 2.62 | 1.06 (H…C4) | 0.0223 |
| Val-Val(LD, 0.81) | C1 | N-H…O | 1.64 | 1.66 | 0.56 (H…C1) | 0.1506 |
| | C2 | N-H…O | 1.67 | 1.69 | 0.58 (H…C2) | 0.1426 |
| | C3 | C-H…O | 2.56 | 2.57 | 1.06 (H…C3) | 0.0281 |
| | C4 | C-H…H | 2.53 | 2.55 | 1.27 (H…C4) | 0.0112 |
| Ala-Val(LL, 0.27) | C1 | N-H…O | 1.65 | 1.67 | 0.57 (H…C1) | 0.1447 |
| | C2 | N-H…O | 1.66 | 1.68 | 0.57 (H…C2) | 0.1449 |
| | C3 | C-H…O | 2.65 | 2.66 | 1.08 (H…C3) | 0.0204 |
| | C4 | C-H…O | 2.72 | 2.73 | 1.11 (H…C4) | 0.0206 |
| Ala-Val(LD, 0.55) | C1 | N-H…O | 1.66 | 1.68 | 0.57 (H…C1) | 0.1411 |
| | C2 | N-H…O | 1.66 | 1.67 | 0.57 (H…C2) | 0.1451 |
| | C3 | C-H…O | 2.48 | 2.49 | 1.00 (H…C3) | 0.0274 |
| | C4 | C-H…O | 2.70 | 2.71 | 1.10 (H…C4) | 0.0189 |
| | C5 | C-H…O | 2.61 | 2.61 | 1.12 (H…C5) | 0.0308 |

Table S4. AIM analysis for the third stable conformations of amino acid dimers calculated at B3LYP/6-311+G(p,d) level. Relevant distances and positive Laplacian values for critical points are given. Corresponding molecular graphs are shown in Fig S3C.

| Molecule (chirality, $\Delta E$/kcal mol$^{-1}$) | Critical points | Atoms in interaction | Atomic distance/Å | Attractors distance/Å | Attractor-Critical point distance/Å | $\nabla^2\rho(r_c)$/a.u. |
|---|---|---|---|---|---|---|
| Ala-Ala(LL, 0.81) | C1 | N-H…O | 1.67 | 1.69 | 0.58 (H…C1) | 0.1426 |
| | C2 | N-H…O | 1.68 | 1.70 | 0.58 (H…C2) | 0.1347 |
| | C3 | C-H…O | 2.73 | 2.74 | 1.15 (H…C3) | 0.0215 |
| Ala-Ala(LD, 0.83) | C1 | N-H…O | 1.65 | 1.67 | 0.56 (H…C1) | 0.1437 |
| | C2 | N-H…O | 1.65 | 1.66 | 0.56 (H…C2) | 0.1437 |
| Val-Val(LL, 1.10) | C1 | N-H…O | 1.66 | 1.68 | 0.57 (H…C1) | 0.1404 |
| | C2 | N-H…O | 1.65 | 1.67 | 0.57 (H…C2) | 0.1478 |
| | C3 | C-H…O | 2.48 | 2.50 | 1.00 (H…C3) | 0.0275 |
| | C4 | C-H…O | 2.80 | 2.81 | 1.15 (H…C4) | 0.0164 |
| | C5 | C-H…O | 2.59 | 2.60 | 1.12 (H…C4) | 0.0313 |
| Val-Val(LD, 0.96) | C1 | N-H…O | 1.65 | 1.67 | 0.57 (H…C1) | 0.1419 |
| | C2 | N-H…O | 1.65 | 1.67 | 0.57 (H…C2) | 0.1420 |
| Ala-Val(LL, 0.39) | C1 | N-H…O | 1.63 | 1.65 | 0.56 (H…C1) | 0.1508 |
| | C2 | N-H…O | 1.67 | 1.69 | 0.58 (H…C2) | 0.1425 |
| | C3 | C-H…O | 2.57 | 2.58 | 1.06 (H…C3) | 0.0279 |
| | C4 | C-H…H | 2.48 | 2.50 | 1.24 (H…C4) | 0.0121 |
| Ala-Val(LD, 0.56) | C1 | N-H…O | 1.66 | 1.67 | 0.57 (H…C1) | 0.1440 |
| | C2 | N-H…O | 1.66 | 1.68 | 0.57 (H…C2) | 0.1440 |
| | C3 | C-H…O | 2.58 | 2.60 | 1.05 (H…C3) | 0.0226 |
| | C4 | C-H…O | 2.66 | 2.68 | 1.08 (H…C4) | 0.0208 |

**Supplementary Text**

## S1. Details of the MM force field

The force fields used in our approach is composed of three terms accounting for bond ($V_{bond}$), angle bending ($V_{angle}$) and van der Waals ($V_{vdW}$) interactions,

$$V_{total} = V_{bond} + V_{angle} + V_{vdW} \quad \text{(S1)}$$

These terms are sufficient to provide a rapid and efficient initial optimization of the structures. Each term is explicitly reported here below.

### Bond term

$$V_{bond} = \frac{1}{2} \sum_{i,j \in bonds} k_B \left(r_{ij} - r_{ij}^0\right)^2 \quad \text{(S2)}$$

The term accounting for the bond stretching and labeled as '$bonds$' is the one reported in Eq. S1 is basically a sum of harmonic contributions for each atomic pairs $[i, j]$ forming a chemical bond in the molecule. For example, in the case of alanine shown in Figure S2, the pair list is

$$bonds = \{[1, 2], [1, 6], [1, 7], [1, 9], [2, 3], [2, 8], [2, 10], ...\}. \quad \text{(S3)}$$

The parameter $k_B$ is a force constant, set to $k_B = 1000$. $r_{ij}$ is the instantaneous interatomic distance $r_{ij} \equiv |r_i - r_j|$. $r_{ij}^0$ is the equilibrium distance depending on the type of atoms $i$ and $j$, written as

$$r_{ij}^0 = r_i^0 + r_j^0 \quad \text{(S4)}$$

The parameters of $r_i^0$ are listed in Table S1.

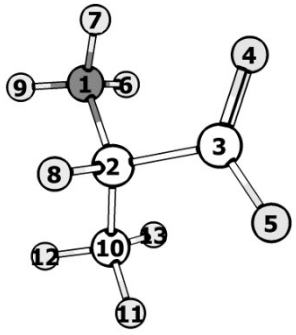

Figure S2. Molecular structure of alanine with atomic indexes.

Table S1. Equilibrium interatomic distances ($r_i^0$) used in the bond term

| $i$ | $r_i^0$ (Å) |
|---|---|
| H | 0.354 |
| C | 0.729 |
| N | 0.699 |
| O | 0.680 |

**Angle bending term**

$$V_{angle} = \frac{1}{2} \sum_{l.m.n \in angles} k_A \left(\theta_{lmn} - \theta_{lmn}^0\right)^2 \quad \text{(S5)}$$

The three-body term accounting for the angles is labeled with '$angles$' in Eq. S5 is computed from three atomic pairs [$l$, $m$, $n$] that form an angle with their respective chemical bonds. For instance, for alanine shown in the Figure S2, the three-body list is

$$angles = \{[1, 2, 3], [1, 2, 8], [1, 2, 10], [3, 2, 8], [3, 2, 10], \cdots\} \quad \text{(S6)}$$

The pre-factor $k_A$ is the bending angle force constant, here set to $k_A = 2$. $\theta_{lmn}$ is the bond angle formed by the three atoms $l$, $m$ and $n$, and $\theta_{lmn}^0$ is the equilibrium angle, where $\theta_{lmn}^0 =$ 109.5 in this study.

**Van der Waals term**

$$V_{vw} = \sum_{p,q \in pairs} D_{pq} \left( \left( \frac{r_{pq}^{vdW}}{r_{pq}} \right)^{12} - 2 \left( \frac{r_{pq}^{vdW}}{r_{pq}} \right)^{6} \right) \quad \text{(S7)}$$

The long-range dispersion van der Waals interaction of Eq. (S7) is represented by a typical Lennard-Jones potential. The subscript '$pairs$' in reminds that this interaction pair-wise acting between atom pairs [p, q] in non-bonding conditions as in any classical force field. $r_{pq}$ is the interatomic distance $r_{pq} \equiv |r_p - r_q|$. $r_{pq}^{vdW}$ is the van der Waals radius depending on the type of atoms

$p$ and $q$, defined as

$$r_{pq}^{vdW} = \sqrt{r_p^{vdW} r_q^{vdW}} \quad \text{(S8)}$$

The parameters of $r_p^{vdW}$ are listed in Table S2.

$D_{pq}$ defines the potential depth that depends on the type of atoms $p$ and $q$, written as

$$D_{pq} = \sqrt{D_p^{vdW} D_q^{vdW}} \quad \text{(S9)}$$

and the resulting parameters of $D_p^{vdW}$ are listed in the same Table S2.

Table S2. Used vdW parameters for the interatomic distance ($r^{vdW}$) and potential depth ($D^{vdW}$)

| $p$ | $r_p^{vdW}$ (Å) | $D_p^{vdW}$ (kcal mol$^{-1}$) |
|---|---|---|
| H | 1.70 | 0.060 |
| C | 2.00 | 0.095 |
| N | 1.85 | 0.069 |
| O | 1.70 | 0.060 |

**Supplementary Data**

**Cartesian coordinates of amino acid dimers**

All the conformations are optimized at the B3LYP-D3/6-311++G(d,p) level. Atomic coordinates are provided in the standard XYZ format.

26
Ala-Ala (LL) _1st

| | | | |
|---|---|---|---|
| N | -1.79382100 | 0.86358900 | 1.30787500 |
| C | -2.25061800 | 0.18685500 | 0.04150000 |
| C | -1.46163700 | -1.14304900 | -0.12183800 |
| O | -0.79699900 | -1.51867900 | 0.89495400 |
| O | -1.57023400 | -1.72238700 | -1.21127600 |
| H | -0.80806800 | 1.21799900 | 1.18550200 |
| H | -1.76543600 | 0.17825700 | 2.06512600 |
| H | -3.29974200 | -0.07833900 | 0.19108400 |
| H | -2.40534100 | 1.63605100 | 1.57092100 |
| C | -2.10786400 | 1.13859400 | -1.14052300 |
| H | -2.45197300 | 0.63116600 | -2.04049200 |
| H | -2.71260100 | 2.03722900 | -0.99486000 |
| H | -1.06574400 | 1.43307300 | -1.28450600 |
| N | 1.79357300 | -0.86394500 | 1.30786000 |
| C | 2.25058200 | -0.18684100 | 0.04176400 |
| C | 1.46137200 | 1.14294400 | -0.12138000 |
| O | 0.79681200 | 1.51834100 | 0.89555000 |
| O | 1.57048100 | 1.72289100 | -1.21044200 |
| H | 2.40500700 | -1.63652300 | 1.57076400 |
| H | 0.80780900 | -1.21822800 | 1.18521300 |
| H | 3.29962600 | 0.07849000 | 0.19168100 |
| H | 1.76510300 | -0.17883500 | 2.06531300 |
| C | 2.10828200 | -1.13830200 | -1.14053800 |
| H | 2.45252900 | -0.63059000 | -2.04029200 |
| H | 1.06625100 | -1.43292600 | -1.28485700 |
| H | 2.71313700 | -2.03687100 | -0.99494500 |

26
Ala-Ala_(LL) 2nd

| | | | |
|---|---|---|---|
| N | 1.7021570157 | -1.1052400495 | -1.0702116706 |
| C | 2.2172125754 | -0.4480545908 | 0.181693135 |
| C | 1.5127120447 | 0.9235000019 | 0.3518349427 |
| O | 1.5909598656 | 1.4433648106 | 1.4737755523 |
| O | 0.945663318 | 1.386112439 | -0.6875840741 |
| H | 2.2086140996 | -1.9630996526 | -1.2900951225 |
| H | 0.6735263646 | -1.3197613391 | -0.9625094592 |
| H | 1.9270349695 | -1.0931337197 | 1.011079813 |
| H | 1.7866234915 | -0.4523710388 | -1.852483511 |
| C | 3.7346892892 | -0.2962427747 | 0.1242737711 |
| H | 4.0780115758 | 0.1783392035 | 1.0435763617 |
| H | 4.0334118364 | 0.3297540461 | -0.720926183 |
| H | 4.2262759248 | -1.2679110104 | 0.033708669 |
| N | -1.702107767 | 1.1052844905 | -1.0701757768 |
| C | -2.2172000986 | 0.4480451361 | 0.1816864781 |
| C | -1.5127393696 | -0.9235369649 | 0.3517788657 |
| O | -1.5910518335 | -1.4434626674 | 1.4736871769 |
| O | -0.9456159402 | -1.3860849761 | -0.6876268466 |
| H | -1.7865481566 | 0.4524505082 | -1.8524792802 |
| H | -0.6734808472 | 1.3198135236 | -0.9624373423 |
| H | -1.9270194988 | 1.0930767552 | 1.0111095782 |
| H | -2.2085641428 | 1.9631501719 | -1.2900372233 |
| C | -3.734680158 | 0.296279602 | 0.1242359526 |
| H | -4.0334078358 | -0.3296658534 | -0.721000348 |
| H | -4.2262373178 | 1.267966677 | 0.033712425 |
| H | -4.0780284049 | -0.1783397281 | 1.0435091163 |

26
Ala-Ala (LL) 3rd
N 1.871742 1.499361 -0.069435
C 2.080255 0.056466 -0.440831
C 1.231197 -0.786295 0.548775
O 1.227959 -0.40044 1.733279
O 0.640539 -1.791244 0.058651
H 2.517518 2.129798 -0.544551
H 0.875239 1.740695 -0.318502
H 1.693951 -0.060183 -1.451428
H 1.984433 1.5932 0.944513
C 3.55618 -0.318235 -0.365765
H 3.941955 -0.173298 0.646176
H 3.675411 -1.369447 -0.633507
H 4.150194 0.27949 -1.061497
N -1.541558 -1.026677 -1.381742
C -2.370231 -0.236536 -0.400477
C -1.632605 1.095783 -0.086506
O -0.666025 1.378238 -0.862655
O -2.063578 1.761943 0.86454
H -1.207757 -0.398369 -2.115685
H -2.070373 -1.790723 -1.801947
H -3.298212 0.021989 -0.915731
H -0.684242 -1.41419 -0.902406
C -2.662597 -1.079983 0.834051
H -1.733401 -1.360173 1.334515
H -3.210589 -1.987516 0.56911
H -3.269777 -0.495238 1.523174

26
Ala-Ala (LD) 1st
N 1.65656300 -1.39893700 0.64260500
C 2.10532200 -0.38153700 -0.37035500
C 1.37896100 0.95848700 -0.08524100
O 0.86529100 1.07481400 1.07117800
O 1.38681800 1.79207400 -1.00230100
H 1.77464600 -1.01362600 1.58232300
H 0.62662300 -1.59631500 0.52131000
H 1.78543800 -0.75234600 -1.34424500
H 2.17975800 -2.27165200 0.56828900
C 3.62162600 -0.21530500 -0.32805300
H 3.91869000 0.52255700 -1.07335000
H 4.12917000 -1.15641900 -0.55298500
H 3.94742300 0.13491100 0.65510400
N -1.72413800 0.48048100 1.56252400
C -2.39051200 0.24632600 0.23152600
C -1.77949400 -1.02523300 -0.42189000
O -2.13801600 -1.27246500 -1.58127300
O -0.99507100 -1.70502900 0.31235600
H -0.72576300 0.79188300 1.41946800
H -2.21850600 1.17767500 2.11899000
H -3.43953300 0.02775200 0.44296200
H -1.68236900 -0.39829200 2.08146500
C -2.27331600 1.49329400 -0.63796500
H -1.22674700 1.73572400 -0.83698400
H -2.75055900 2.35168300 -0.15901500
H -2.77295500 1.30431500 -1.58705100

26
Ala-Ala_(LD)_2nd
N -1.86878 1.41289 -0.600117
C -2.108285 -0.07239 -0.573099
C -1.467718 -0.600786 0.739223
O -0.834097 -1.692608 0.652975
O -1.655537 0.09451 1.754947
H -2.391464 1.884637 -1.33811
H -0.831983 1.55657 -0.738934
H -1.586647 -0.483398 -1.435109
H -2.134212 1.803048 0.309045
C -3.599752 -0.382616 -0.629984

H -4.118639 0.053174 0.227005
H -4.046325 0.002621 -1.550039
H -3.745055 -1.464046 -0.608584
N 1.526571 -1.466457 -0.6487
C 2.273379 -0.452004 0.175748
C 1.542635 0.911536 0.068099
O 0.746997 1.029157 -0.915546
O 1.817801 1.754602 0.933712
H 2.037618 -2.345314 -0.734958
H 1.359825 -1.078995 -1.580516
H 2.220887 -0.794185 1.209022
H 0.579393 -1.653337 -0.216003
C 3.724421 -0.346292 -0.284992
H 4.245889 -1.300246 -0.174826
H 4.236664 0.397304 0.32583
H 3.780127 -0.032834 -1.33078

26
Ala-Ala_LD_3rd
N 1.143609 -1.256542 -1.090969
C 2.344503 -0.641239 -0.421738
C 2.108682 0.881191 -0.240369
O 0.968822 1.319381 -0.593345
O 3.058002 1.524011 0.230314
H 0.848266 -0.676885 -1.877965
H 1.343059 -2.197445 -1.43146
H 3.18784 -0.77217 -1.101659
H 0.320734 -1.302755 -0.428973
C 2.610473 -1.347507 0.904517
H 1.757364 -1.234383 1.578067
H 2.80075 -2.412851 0.754642
H 3.487084 -0.900685 1.371907
N -1.143596 1.256709 1.090691
C -2.344557 0.64122 0.421762
C -2.108606 -0.881201 0.24052
O -0.968596 -1.319166 0.593251
O -3.057934 -1.524185 -0.229938
H -0.320772 1.30276 0.428616
H -1.343034 2.19772 1.430893
H -3.187791 0.772189 1.101793
H -0.848135 0.677324 1.877843
C -2.61076 1.347291 -0.904563
H -2.800999 2.41266 -0.754806
H -1.757769 1.234077 -1.578248
H -3.48746 0.900417 -1.371735

38
Iva-Iva (LL) 1st
N -1.67010300 1.11370900 -1.06288900
H -1.74524900 0.46345500 -1.84651700
C -2.25893500 0.48306000 0.18371300
C -3.78838400 0.38766300 0.03190300
C -1.64472700 -0.94843800 0.30882100
H -4.16134800 -0.03013300 0.96946200
C -4.28452900 -0.46100700 -1.14293100
O -0.99679800 -1.36647300 -0.70153000
H -5.37594200 -0.49890400 -1.13870000
H -3.91314000 -1.48692700 -1.08135600
H -3.98278100 -0.04934600 -2.11058900
C -1.87460900 1.35884000 1.37783600
H -0.79098500 1.44128900 1.48262100
H -2.27594800 0.90951900 2.28493900
H -2.29289400 2.36363900 1.27005500
H -4.19197400 1.40391300 -0.04245500
H -2.13779800 1.98911700 -1.30020300
O -1.86314300 -1.55234000 1.36831100
H -0.63937400 1.29349400 -0.92970400
N 1.66986700 -1.11426500 -1.06243700
H 1.74509000 -0.46450900 -1.84646700
C 2.25883400 -0.48296300 0.18376600
C 3.78830200 -0.38795400 0.03191400

| | | | |
|---|---|---|---|
| C | 1.64491600 | 0.94873100 | 0.30800800 |
| H | 4.16134200 | 0.03019100 | 0.96928600 |
| C | 4.28461800 | 0.46011300 | -1.14328800 |
| O | 1.86391600 | 1.55344200 | 1.36691500 |
| H | 5.37603600 | 0.49785000 | -1.13903700 |
| H | 3.91338100 | 1.48611800 | -1.08219200 |
| H | 3.98284900 | 0.04805900 | -2.11077100 |
| C | 1.87430900 | -1.35792300 | 1.37842700 |
| H | 0.79066300 | -1.44001700 | 1.48328400 |
| H | 2.29232200 | -2.36289900 | 1.27124100 |
| H | 2.27578700 | -0.90815700 | 2.28524800 |
| H | 4.19170200 | -1.40431300 | -0.04198600 |
| H | 0.63910400 | -1.29384600 | -0.92914600 |
| O | 0.99660200 | 1.36605200 | -0.70238400 |
| H | 2.13743300 | -1.98988400 | -1.29923400 |

38
Iva-Iva_(LL)_2nd

| | | | |
|---|---|---|---|
| N | 1.6978672461 | -1.0731334931 | -0.9528113852 |
| H | 0.6987801759 | -1.3023209849 | -0.7026748201 |
| C | 2.2725319554 | -0.080716125 | 0.0379184784 |
| C | 3.7489284612 | 0.1930184565 | -0.3159166266 |
| C | 1.4769179976 | 1.2530558892 | -0.1456495419 |
| H | 4.0754253444 | 0.9959887742 | 0.348418198 |
| C | 4.7057155914 | -0.9978820167 | -0.1945764968 |
| O | 1.6262636769 | 2.1136909348 | 0.7328009824 |
| H | 5.7145712549 | -0.6851628604 | -0.4731746036 |
| H | 4.436867068 | -1.8239512867 | -0.8603146392 |
| H | 4.7495868505 | -1.3839806286 | 0.8256168825 |
| C | 2.0781287905 | -0.6490657258 | 1.444447545 |
| H | 1.017936578 | -0.7701576655 | 1.6756098046 |
| H | 2.5662915046 | -1.6200171961 | 1.5527394384 |
| H | 2.5121443895 | 0.0420887095 | 2.1655182093 |
| H | 3.7899075545 | 0.5954341639 | -1.3342434827 |
| H | 1.6744784366 | -0.6498420341 | -1.882353893 |
| O | 0.7685137888 | 1.3362131923 | -1.1981540146 |
| H | 2.2382858817 | -1.9371799271 | -0.9870895812 |
| N | -1.8656607371 | 0.734247651 | -1.2981683393 |
| H | -0.8581784894 | 1.0470158242 | -1.2862879416 |
| C | -2.3327061476 | 0.4102739657 | 0.1075867201 |
| C | -3.8433479336 | 0.1099203798 | 0.0882119119 |
| C | -1.5441914458 | -0.856416523 | 0.5730476493 |
| H | -4.1307419683 | -0.0613080089 | 1.127887546 |
| C | -4.2739039602 | -1.0867985583 | -0.7660529015 |
| O | -0.8979310441 | -1.4724498392 | -0.3317249204 |
| H | -4.0715499523 | -0.9354555499 | -1.8304512143 |
| H | -5.3499424782 | -1.24467035 | -0.6659423955 |
| H | -3.7701973884 | -2.0046448637 | -0.4529107286 |
| C | -2.0220195845 | 1.6170694228 | 0.994842522 |
| H | -2.5765419301 | 2.497173606 | 0.6571144867 |
| H | -0.9557791742 | 1.8524615156 | 0.9937267011 |
| H | -2.323292483 | 1.3865532485 | 2.0155963134 |
| H | -4.3705290001 | 1.0137120885 | -0.2379970718 |
| H | -2.4384565793 | 1.4602692927 | -1.7297520392 |
| O | -1.6413610198 | -1.1590872248 | 1.7703028046 |
| H | -1.8930282302 | -0.1086242533 | -1.8738255567 |

38
Iva-Iva_(LL)_3rd

| | | | |
|---|---|---|---|
| N | -1.7973457773 | 0.7577722045 | -1.3048459253 |
| H | -1.9170401666 | -0.1050043139 | -1.8378159461 |
| C | -2.2745832574 | 0.5458910284 | 0.1192290578 |
| C | -3.8073301628 | 0.3875716544 | 0.1233084489 |
| C | -1.6049927809 | -0.7687385787 | 0.6367067363 |
| H | -4.0982685669 | 0.2854173564 | 1.171141542 |
| C | -4.3573973981 | -0.7951621745 | -0.680111512 |
| O | -1.6936834836 | -0.9951490273 | 1.8511774794 |
| H | -5.4433737823 | -0.84169455 | -0.5738076234 |
| H | -3.9449371601 | -1.7445206373 | -0.3300174362 |
| H | -4.1446779509 | -0.707492286 | -1.749744417 |
| C | -1.8433230085 | 1.7578038552 | 0.9460758973 |

| | | | |
|---|---|---|---|
| H | -2.1549175277 | 1.6043358035 | 1.978291324 |
| H | -2.3169003017 | 2.669503493 | 0.5708100884 |
| H | -0.7595559915 | 1.8885912162 | 0.9279941389 |
| H | -4.2511799665 | 1.3233595124 | -0.2353814026 |
| H | -2.3032350232 | 1.5151913799 | -1.7651622565 |
| O | -1.0603113155 | -1.4988243848 | -0.2499816347 |
| H | -0.7632663568 | 0.9689977071 | -1.3249162893 |
| N | 1.524568938 | -1.4474918281 | -0.999690381 |
| H | 1.482484202 | -1.0395359945 | -1.935830666 |
| C | 2.256657269 | -0.493422555 | -0.0751636105 |
| C | 3.7149968652 | -0.4149048308 | -0.5785000824 |
| C | 1.5534268171 | 0.8948210791 | -0.2309679725 |
| H | 4.1282097266 | -1.4306578615 | -0.5658946016 |
| C | 4.6319319056 | 0.510911701 | 0.2240156475 |
| O | 1.7051973808 | 1.7143781564 | 0.6850223372 |
| H | 5.628277116 | 0.5166577288 | -0.224073889 |
| H | 4.7344490537 | 0.1768037514 | 1.2587940042 |
| H | 4.2526940095 | 1.5336659266 | 0.2349723402 |
| C | 2.1376536297 | -1.038179125 | 1.34653508 |
| H | 2.5864930524 | -0.3316772166 | 2.0410594522 |
| H | 2.6528901848 | -1.9986612178 | 1.4378940576 |
| H | 1.0900974324 | -1.1690776291 | 1.627288664 |
| H | 3.6992245431 | -0.0924520109 | -1.6255077525 |
| H | 1.9824604657 | -2.3581613938 | -1.0455573365 |
| O | 0.8988016678 | 1.0557262935 | -1.3107598114 |
| H | 0.5254767187 | -1.5688622322 | -0.6841397494 |

38
Iva-Iva (LD) 1st

| | | | |
|---|---|---|---|
| N | -1.73746100 | 0.40778500 | -1.51263500 |
| H | -1.61682500 | -0.36917700 | -2.16540400 |
| C | -2.38413200 | -0.11252900 | -0.24385100 |
| C | -2.26457100 | 0.96229300 | 0.85237700 |
| C | -1.59725000 | -1.40043800 | 0.16910800 |
| H | -1.20513000 | 1.11694700 | 1.07655300 |
| C | -2.91465500 | 2.31286800 | 0.53365300 |
| O | -0.79143000 | -1.86217400 | -0.69947300 |
| H | -3.98580300 | 2.22180100 | 0.34038500 |
| H | -2.79074800 | 2.98774800 | 1.38363700 |
| H | -2.45202700 | 2.80252900 | -0.32866800 |
| C | -3.83179100 | -0.49958500 | -0.56280400 |
| H | -4.41035500 | 0.35644400 | -0.91664600 |
| H | -3.86798200 | -1.27900300 | -1.32837900 |
| H | -4.30218500 | -0.88457000 | 0.34198900 |
| H | -2.71224800 | 0.53107200 | 1.74874600 |
| H | -2.29464600 | 1.13731700 | -1.95656900 |
| O | -1.84348200 | -1.86471400 | 1.29075400 |
| H | -0.77068200 | 0.77753800 | -1.30984600 |
| N | 1.83312400 | -1.21665200 | -0.87249200 |
| H | 1.89004800 | -0.66420600 | -1.72962300 |
| C | 2.19285200 | -0.35002900 | 0.31911900 |
| C | 3.70292100 | -0.04975200 | 0.29204900 |
| C | 1.38157200 | 0.97903300 | 0.18281100 |
| H | 3.91428900 | 0.52798900 | 1.19435400 |
| C | 4.20310300 | 0.71565800 | -0.93696800 |
| O | 1.40880100 | 1.74435900 | 1.15636800 |
| H | 5.27339800 | 0.91112400 | -0.84255200 |
| H | 4.06109400 | 0.15314700 | -1.86430000 |
| H | 3.69491800 | 1.67724500 | -1.04367400 |
| C | 1.80240500 | -1.10961800 | 1.58860600 |
| H | 0.73645300 | -1.34524900 | 1.60368000 |
| H | 2.03024400 | -0.48680400 | 2.45236000 |
| H | 2.36791000 | -2.04206300 | 1.67172800 |
| H | 4.24451900 | -0.99748300 | 0.39151100 |
| H | 0.83301700 | -1.54237800 | -0.80070100 |
| O | 0.78912200 | 1.15921000 | -0.92724200 |
| H | 2.44630100 | -2.02874500 | -0.95055800 |

38
Iva-Iva_(LD)_2nd

| | | | |
|---|---|---|---|
| N | 1.5937119414 | -1.4313424154 | -0.4983084453 |
| H | 1.6889392029 | -1.1704419477 | -1.4804053774 |
| C | 2.181205606 | -0.3490995877 | 0.3865860442 |
| C | 3.7157073354 | -0.3892105817 | 0.2824016177 |
| C | 1.6360213085 | 1.024389835 | -0.1233788408 |
| H | 4.0881276654 | 0.3696882674 | 0.9730472685 |
| C | 4.2828799726 | -0.1327926584 | -1.1173986484 |
| O | 2.0105084797 | 2.0251548615 | 0.5030623067 |
| H | 3.9812647404 | -0.8995116464 | -1.8371420147 |
| H | 5.3744440627 | -0.1380050391 | -1.0845127731 |
| H | 3.9650863441 | 0.8390290761 | -1.5039441108 |
| C | 1.7128681525 | -0.6127104124 | 1.8196199207 |
| H | 2.1019489094 | -1.5661435419 | 2.1875376221 |
| H | 2.0822408955 | 0.1860581672 | 2.4613727435 |
| H | 0.6229114951 | -0.6346501255 | 1.8828234898 |
| H | 4.0640268842 | -1.3579098908 | 0.6591249478 |
| H | 0.5600336387 | -1.5472303786 | -0.3238324763 |
| O | 0.8752747722 | 0.9855946189 | -1.1394109651 |
| H | 2.051720742 | -2.3304985314 | -0.3452925853 |
| N | -1.7154100607 | 0.3143309028 | -1.5799395755 |
| H | -1.5741296043 | -0.5519193804 | -2.1023976942 |
| C | -2.6316865375 | 0.0418811589 | -0.4007953812 |
| C | -2.833751926 | 1.3364327991 | 0.3997548582 |
| C | -1.9794330227 | -1.0974371046 | 0.4470581808 |
| H | -3.2949792711 | 2.0809323774 | -0.2595818188 |
| C | -1.5779655868 | 1.9172865617 | 1.0535879351 |
| O | -2.4570231366 | -1.2919576458 | 1.5730952867 |
| H | -1.1146460713 | 1.1910653566 | 1.7257994239 |
| H | -0.8284376612 | 2.2227792815 | 0.3221148336 |
| H | -1.840806295 | 2.797374254 | 1.6451129323 |
| C | -3.9651562054 | -0.4690251044 | -0.960774516 |
| H | -3.8260881704 | -1.3750509854 | -1.556294977 |
| H | -4.6325580085 | -0.7033310868 | -0.1316873404 |
| H | -4.4419605956 | 0.2915024875 | -1.5853836953 |
| H | -3.5710503357 | 1.1016119976 | 1.1691685849 |
| H | -0.7497575694 | 0.6301403521 | -1.303825813 |
| O | -1.0511082951 | -1.7500204837 | -0.1234134953 |
| H | -2.1190197954 | 1.0110301924 | -2.207772453 |

38

Iva-Iva_(LD)_3rd

| | | | |
|---|---|---|---|
| N | 1.560686 | -1.322785 | 0.176061 |
| H | 0.58273 | -1.305895 | -0.222578 |
| C | 2.434873 | -0.284501 | -0.498193 |
| C | 3.894426 | -0.476665 | -0.052312 |
| C | 1.910774 | 1.121865 | -0.063501 |
| H | 4.237107 | -1.459672 | -0.395199 |
| C | 4.145379 | -0.325317 | 1.451433 |
| O | 0.9625 | 1.129378 | 0.783493 |
| H | 3.822703 | 0.654475 | 1.813324 |
| H | 5.212157 | -0.424184 | 1.663126 |
| H | 3.630917 | -1.090746 | 2.039796 |
| C | 2.281711 | -0.465492 | -2.010211 |
| H | 2.634864 | -1.452364 | -2.321962 |
| H | 1.238081 | -0.354065 | -2.313093 |
| H | 2.87504 | 0.293464 | -2.518109 |
| H | 4.47805 | 0.26768 | -0.597555 |
| H | 1.462016 | -1.106169 | 1.168715 |
| O | 2.472108 | 2.098089 | -0.580325 |
| H | 1.943825 | -2.263288 | 0.074344 |
| N | -1.559472 | 1.321966 | -0.176365 |
| H | -1.942259 | 2.262812 | -0.076756 |
| C | -2.435334 | 0.285088 | 0.497888 |
| C | -3.893999 | 0.477327 | 0.049034 |
| C | -1.911213 | -1.122129 | 0.065952 |
| H | -4.236722 | 1.46109 | 0.389721 |
| C | -4.142385 | 0.323651 | -1.454899 |
| O | -2.473449 | -2.097334 | 0.583638 |
| H | -5.208686 | 0.423226 | -1.66866 |
| H | -3.626091 | 1.087516 | -2.043685 |
| H | -3.820045 | -0.657089 | -1.814497 |

| | | | |
|---|---|---|---|
| C | -2.284885 | 0.468227 | 2.009894 |
| H | -1.241817 | 0.357146 | 2.314826 |
| H | -2.63855 | 1.455568 | 2.319606 |
| H | -2.879196 | -0.289956 | 2.517792 |
| H | -4.479007 | -0.2658 | 0.594451 |
| H | -0.5823 | 1.305043 | 0.223951 |
| O | -0.962185 | -1.131262 | -0.780235 |
| H | -1.459195 | 1.103643 | -1.168501 |

32
Ala-Iva (LL) 1st

| | | | |
|---|---|---|---|
| N | 2.06446400 | -1.59347700 | -0.44843700 |
| C | 2.71224200 | -0.46850600 | 0.31143100 |
| C | 2.08058700 | 0.87052200 | -0.15037500 |
| O | 2.27207100 | 1.84979900 | 0.58516800 |
| O | 1.44464600 | 0.83337100 | -1.24961200 |
| H | 2.51482700 | -2.49051300 | -0.26579800 |
| H | 2.10710600 | -1.39168800 | -1.44984500 |
| H | 2.46903000 | -0.62469100 | 1.36258000 |
| H | 1.04094600 | -1.65469700 | -0.19529300 |
| C | 4.22400600 | -0.47698600 | 0.10167000 |
| H | 4.47296800 | -0.34448600 | -0.95473900 |
| H | 4.66736400 | -1.41179600 | 0.45302500 |
| H | 4.66454300 | 0.34527200 | 0.66560100 |
| N | -1.22876500 | 0.43273400 | -1.39768300 |
| H | -1.70591600 | 1.06510500 | -2.04107300 |
| C | -1.80409800 | 0.51502900 | 0.00337000 |
| C | -3.33464300 | 0.35491700 | -0.06580400 |
| C | -1.18408900 | -0.65999600 | 0.82742900 |
| H | -3.69955600 | 0.48199300 | 0.95563600 |
| C | -3.83809400 | -0.97834600 | -0.62774700 |
| O | -1.39745600 | -0.64976100 | 2.04700200 |
| H | -3.46720600 | -1.82424400 | -0.04375700 |
| H | -4.92953000 | -1.00418400 | -0.59903600 |
| H | -3.54195200 | -1.13139200 | -1.66961400 |
| C | -1.41625400 | 1.87340000 | 0.59014700 |
| H | -0.33212300 | 2.00013400 | 0.62266800 |
| H | -1.84857800 | 2.68604300 | -0.00057900 |
| H | -1.80262400 | 1.93851100 | 1.60624100 |
| H | -3.74206300 | 1.18784300 | -0.65029400 |
| H | -1.30200700 | -0.52515300 | -1.74392500 |
| O | -0.55095300 | -1.53564000 | 0.15702800 |
| H | -0.19952400 | 0.66078100 | -1.38636300 |

32
Ala-Iva_LL_2nd

| | | | |
|---|---|---|---|
| N | 2.43758593 | -1.0367562635 | 1.0089196226 |
| C | 2.7550701031 | 0.0061280835 | -0.0312350073 |
| C | 1.8390965923 | 1.2408732568 | 0.1970995724 |
| O | 1.8900285603 | 2.1300957472 | -0.6641019584 |
| O | 1.1402589829 | 1.2260261969 | 1.2583811218 |
| H | 1.4847620181 | -1.4545685051 | 0.8282427916 |
| H | 3.1349678327 | -1.7808559938 | 1.0249068794 |
| H | 3.7827043153 | 0.327067107 | 0.1530827426 |
| H | 2.3922752968 | -0.5971536095 | 1.9297248633 |
| C | 2.6297068644 | -0.5948514363 | -1.427121983 |
| H | 3.3215684219 | -1.4306751791 | -1.5572034474 |
| H | 1.6128400735 | -0.9480966467 | -1.614577312 |
| H | 2.8712149661 | 0.1730465745 | -2.1606592439 |
| N | -1.3378237282 | 0.1677861485 | 1.4899380697 |
| H | -2.0104627047 | 0.7843334562 | 1.9449409089 |
| C | -1.8016260093 | -0.27073629 | 0.1142106752 |
| C | -1.7082908904 | 0.9266260183 | -0.8492836693 |
| C | -0.837163542 | -1.4155194159 | -0.3417529622 |
| H | -2.0092892575 | 0.5511555424 | -1.8281616137 |
| C | -2.5494309537 | 2.1509693668 | -0.4727906754 |
| O | -0.9080263117 | -1.7636465411 | -1.5279741351 |
| H | -2.243383788 | 2.5874610292 | 0.4828474927 |
| H | -3.6150525423 | 1.91854427 | -0.4159049466 |
| H | -2.4228289191 | 2.9283010085 | -1.2297368585 |
| C | -3.2179801402 | -0.8411755388 | 0.2400362914 |

H -3.9205699363 -0.0968614483 0.6209202019
H -3.234392803 -1.7041763776 0.91050519
H -3.5568443098 -1.1647320479 -0.7442257833
H -0.658954507 1.2225487608 -0.9390598457
H -1.1928791818 -0.6610449138 2.0700841716
O -0.0836454354 -1.8975559069 0.5625919207
H -0.4029479971 0.6511255475 1.4292849258

32
Ala-Iva_LL_3rd
N -2.0198771222 -1.5634520863 -0.8658612084
C -2.6930274653 -0.543806734 0.0158429111
C -2.2422535515 0.8801163302 -0.4059111467
O -1.3693063261 0.9473190117 -1.3250100431
O -2.7900786821 1.8178594598 0.1915386305
H -2.4561233769 -2.4817888474 -0.7803302173
H -0.9952388049 -1.6504044077 -0.6238881361
H -3.7647412622 -0.6204810624 -0.1749578963
H -2.0674427508 -1.2649920139 -1.8410014571
C -2.3907706818 -0.846887755 1.4807392357
H -2.875603624 -0.0939394775 2.1009074386
H -1.315540496 -0.8186929944 1.6717213084
H -2.7687874649 -1.831189326 1.767452487
N 1.2911776729 0.4443623339 -1.5017763219
H 1.7223575306 1.2044793934 -2.0297181525
C 2.0710683752 0.1400363595 -0.2356362037
C 2.1110238778 1.3879363485 0.6576096142
C 1.3800591591 -1.0808214776 0.4535717215
H 2.7493401877 1.129606196 1.5041500832
C 0.7581218083 1.8860806762 1.1710776726
O 1.6941280081 -1.3073325889 1.6295746337
H 0.2437392898 1.1076595165 1.7391939551
H 0.096728764 2.2063990914 0.3644101931
H 0.9059256694 2.7401520334 1.8360840732
C 3.4859102274 -0.2786039412 -0.6549388748
H 3.4625024538 -1.1477785935 -1.3174009565
H 3.9988776657 0.5395558646 -1.1680822532
H 4.0583108114 -0.5406425686 0.2348605522
H 2.623915459 2.187815531 0.1111500995
H 1.2715612725 -0.3909752929 -2.0892125273
O 0.596425795 -1.7568354772 -0.2837620389
H 0.2803715811 0.6835624987 -1.3286411759

32
Ala-Iva (LD) 1st
N -2.10756800 -1.26553200 -1.24339800
C -2.80229400 -0.46300600 -0.17436100
C -2.24656600 0.98827000 -0.19561200
O -2.62941700 1.73672900 0.71480300
O -1.46591900 1.27136400 -1.15741200
H -2.09438900 -0.73406900 -2.11557500
H -2.56426300 -2.16336100 -1.40316000
H -3.85615100 -0.41203000 -0.45665500
H -1.09954000 -1.42855500 -0.97485800
C -2.64721600 -1.15109300 1.17771100
H -3.08580500 -2.15182300 1.16182200
H -3.16301000 -0.55828200 1.93169900
H -1.59465100 -1.23274900 1.45900500
N 1.22111300 0.93821600 -1.17195700
H 0.18692500 1.14026400 -1.18782800
C 1.65080200 0.50562600 0.21647300
C 3.18598100 0.39218200 0.26293100
C 1.00524900 -0.89368200 0.47918400
H 3.61083400 1.38863100 0.09611500
C 3.80466800 -0.61380800 -0.71274200
O 1.07920900 -1.32830400 1.63646700
H 3.41321800 -1.62127700 -0.55158500
H 4.88725400 -0.64847300 -0.57351200
H 3.62486600 -0.34418900 -1.75765400
C 1.14370800 1.54878300 1.21394700
H 0.05709200 1.64662100 1.17444100

| | | | |
|---|---|---|---|
| H | 1.42541500 | 1.23801400 | 2.21894300 |
| H | 1.59057700 | 2.52634200 | 1.01177800 |
| H | 3.43858600 | 0.11216100 | 1.28791700 |
| H | 1.73092100 | 1.76320000 | -1.48931200 |
| O | 0.48636000 | -1.46482800 | -0.53127200 |
| H | 1.36945800 | 0.17145500 | -1.82997200 |

32
Ala-Iva_(LD)_2nd

| | | | |
|---|---|---|---|
| N | 2.3582254145 | -0.8235567738 | 1.3654297449 |
| C | 2.8441718282 | -0.3279076342 | 0.0278064897 |
| C | 2.1219214965 | 1.0118551523 | -0.2938714036 |
| O | 2.2056986048 | 1.4265545306 | -1.4579378131 |
| O | 1.5350993334 | 1.5671688824 | 0.6882013771 |
| H | 2.9203365797 | -1.600445532 | 1.7124380852 |
| H | 2.3880769256 | -0.0552840244 | 2.0385953797 |
| H | 3.9051290866 | -0.0972632328 | 0.1509156506 |
| H | 1.3456704704 | -1.1188033744 | 1.2991283741 |
| C | 2.6545319118 | -1.4052919175 | -1.0323209131 |
| H | 3.2101770419 | -2.3106013159 | -0.7747122457 |
| H | 3.0286117624 | -1.027984678 | -1.9830310087 |
| H | 1.5975428801 | -1.6548812592 | -1.1494774374 |
| N | -1.0823631864 | 1.2247158072 | 1.25052699 |
| H | -1.6144844638 | 2.0755947711 | 1.4347966083 |
| C | -1.6804415257 | 0.4202841686 | 0.1115495465 |
| C | -3.1511247208 | 0.1355740566 | 0.4878572974 |
| C | -0.8734262903 | -0.9183934291 | 0.0507347333 |
| H | -3.6499081189 | 1.0993626359 | 0.6449428822 |
| C | -3.9373493486 | -0.6771335891 | -0.5434529731 |
| O | -0.8766111232 | -1.5372594327 | -1.02157634 |
| H | -3.4649944453 | -1.6422684963 | -0.7326349102 |
| H | -4.9501104857 | -0.8550424315 | -0.1745779155 |
| H | -4.0182625027 | -0.1476561242 | -1.4952610273 |
| C | -1.5330087627 | 1.2414348009 | -1.1672982892 |
| H | -0.4865231582 | 1.4968465776 | -1.3480592716 |
| H | -2.1198811352 | 2.1625616883 | -1.1061177359 |
| H | -1.8870924109 | 0.6567419732 | -2.0133716616 |
| H | -3.1636249839 | -0.388203305 | 1.4499736741 |
| H | -0.0806291622 | 1.4725321345 | 1.0346971711 |
| O | -0.3018608434 | -1.2568052608 | 1.1370308128 |
| H | -1.0607246681 | 0.6464726319 | 2.0932181292 |

32
Ala-Iva_(LD)_3rd

| | | | |
|---|---|---|---|
| N | -2.4210822913 | -0.7635344056 | -1.3644696536 |
| C | -2.8898569906 | -0.0566501461 | -0.1191816049 |
| C | -2.0351554805 | 1.2267139571 | 0.0774600686 |
| O | -2.1782226147 | 1.8264719446 | 1.1522307863 |
| O | -1.2851861104 | 1.5477595198 | -0.8971671511 |
| H | -2.3265882627 | -0.0864346943 | -2.1235592246 |
| H | -3.0637927439 | -1.5027757382 | -1.6482928963 |
| H | -3.9158687907 | 0.2652618709 | -0.3113121022 |
| H | -1.4602482658 | -1.1716329255 | -1.2068410933 |
| C | -2.846934338 | -1.0090991926 | 1.0705266766 |
| H | -3.205613274 | -0.4809066715 | 1.9527615578 |
| H | -1.8280569613 | -1.3538290924 | 1.2618506923 |
| H | -3.4882634518 | -1.8775084083 | 0.9003278633 |
| N | 1.2857094374 | 0.7498310008 | -1.1804440685 |
| H | 1.2561598012 | 0.09088585 | -1.9608234646 |
| C | 1.6729992029 | 0.0069837019 | 0.0831620664 |
| C | 3.1275817844 | -0.4896454929 | -0.0483218737 |
| C | 0.7411767863 | -1.2461296889 | 0.1703629029 |
| H | 3.3086848796 | -1.1318752947 | 0.816354913 |
| C | 4.2061178446 | 0.5967368507 | -0.1169103821 |
| O | 0.7096816576 | -1.8418596182 | 1.2557637568 |
| H | 4.0717209421 | 1.2719627853 | -0.9677203299 |
| H | 4.2337504212 | 1.2001471218 | 0.7923963748 |
| H | 5.1871295746 | 0.1313225555 | -0.2355405804 |
| C | 1.4552855621 | 0.9450446893 | 1.2712841416 |
| H | 0.401098807 | 1.2083133452 | 1.3762521726 |
| H | 2.0297630619 | 1.867157224 | 1.1593951125 |

| | | | |
|---|---|---|---|
| H | 1.7778942324 | 0.4418115503 | 2.1816863871 |
| H | 3.1935964388 | -1.1325214229 | -0.9332700102 |
| H | 0.3127660124 | 1.1439180174 | -1.0866732952 |
| O | 0.121221986 | -1.5495868432 | -0.8979517262 |
| H | 1.9348761433 | 1.5062296505 | -1.3957680156 |

26
Ala-Ala (LL) non-ion

| | | | |
|---|---|---|---|
| N | -4.06321400 | -0.94075600 | -0.66083200 |
| H | -3.74418400 | -1.74578500 | -0.12819400 |
| C | -3.43055700 | 0.27543300 | -0.14966700 |
| H | -3.71873800 | 1.11098200 | -0.79296200 |
| C | -3.79040500 | 0.63404400 | 1.31014100 |
| C | -1.92348500 | 0.13944500 | -0.24522400 |
| H | -3.49105900 | -0.17268800 | 1.98488400 |
| H | -3.30194200 | 1.55910900 | 1.62495300 |
| H | -4.87121900 | 0.76863900 | 1.38992700 |
| O | -1.35034400 | -0.94503200 | -0.24074000 |
| H | -5.06826800 | -0.87795300 | -0.52947100 |
| O | -1.29514800 | 1.30081900 | -0.27757300 |
| H | -0.30506500 | 1.16550100 | -0.26817700 |
| N | 4.06318500 | 0.94077200 | -0.66085200 |
| H | 3.74414800 | 1.74579500 | -0.12820900 |
| C | 3.43056000 | -0.27543000 | -0.14968000 |
| H | 3.71874000 | -1.11097800 | -0.79297700 |
| C | 3.79042900 | -0.63402800 | 1.31012600 |
| C | 1.92348600 | -0.13945600 | -0.24521200 |
| H | 3.49111100 | 0.17271600 | 1.98486900 |
| H | 3.30195700 | -1.55908100 | 1.62495700 |
| H | 4.87124200 | -0.76864000 | 1.38989200 |
| O | 1.35033900 | 0.94501700 | -0.24073400 |
| H | 5.06824200 | 0.87798600 | -0.52950300 |
| O | 1.29515200 | -1.30083200 | -0.27756900 |
| H | 0.30506500 | -1.16553600 | -0.26817700 |

26
Ala-Ala (LD) non-ion

| | | | |
|---|---|---|---|
| N | -3.98825500 | 1.23846800 | 0.34257200 |
| H | -3.72707500 | 1.70474900 | -0.52227100 |
| C | -3.42197000 | -0.11046400 | 0.37050400 |
| H | -3.63919200 | -0.55603000 | 1.34471900 |
| C | -3.94450000 | -1.06074900 | -0.73095300 |
| C | -1.91327600 | -0.02676700 | 0.24440100 |
| H | -3.71765500 | -0.65690900 | -1.72155800 |
| H | -3.49972200 | -2.05476000 | -0.64316400 |
| H | -5.02824400 | -1.15695700 | -0.63636100 |
| O | -1.34298000 | 0.90299000 | -0.31697100 |
| H | -5.00190800 | 1.17801800 | 0.35194200 |
| O | -1.28655900 | -1.07500900 | 0.74711500 |
| H | -0.30293100 | -1.00921400 | 0.58257700 |
| N | 3.98806400 | -1.23858400 | -0.34285800 |
| H | 3.72702300 | -1.70486300 | 0.52202700 |
| C | 3.42191900 | 0.11041000 | -0.37062300 |
| H | 3.63899800 | 0.55599000 | -1.34486400 |
| C | 3.94477300 | 1.06059300 | 0.73076700 |
| C | 1.91324100 | 0.02687500 | -0.24421300 |
| H | 3.71806400 | 0.65674700 | 1.72140000 |
| H | 3.50010300 | 2.05466200 | 0.64309500 |
| H | 5.02851100 | 1.15666600 | 0.63597200 |
| O | 1.34295300 | -0.90287600 | 0.31717800 |
| H | 5.00172200 | -1.17824300 | -0.35244900 |
| O | 1.28653500 | 1.07516100 | -0.74684700 |
| H | 0.30293300 | 1.00943600 | -0.58215500 |

38
Iva-Iva (LL) non-ion

| | | | |
|---|---|---|---|
| N | 3.94170500 | -0.60210700 | -1.34556600 |
| H | 3.46098300 | -0.02022300 | -2.02400700 |
| C | 3.45432400 | -0.33191800 | 0.01312100 |
| C | 3.82061800 | 1.09021000 | 0.54279200 |
| C | 1.93092700 | -0.42905800 | -0.00581100 |

| | | | |
|---|---|---|---|
| H | 3.46742000 | 1.17775100 | 1.57397700 |
| H | 4.91445300 | 1.13477100 | 0.57630900 |
| O | 1.27344700 | -0.44216100 | -1.04198800 |
| H | 4.93009500 | -0.37342300 | -1.39847300 |
| O | 1.38649400 | -0.44230300 | 1.19729000 |
| H | 0.38941400 | -0.45025900 | 1.12957300 |
| N | -3.94173600 | -0.60213600 | 1.34552400 |
| H | -3.46094500 | -0.02035000 | 2.02399900 |
| C | -3.45434400 | -0.33190400 | -0.01315200 |
| C | -3.82051100 | 1.09029500 | -0.54272300 |
| C | -1.93095500 | -0.42919600 | 0.00576300 |
| H | -3.46724300 | 1.17790100 | -1.57387900 |
| H | -4.91434100 | 1.13493700 | -0.57630700 |
| O | -1.27347700 | -0.44238200 | 1.04194000 |
| H | -4.93010100 | -0.37335100 | 1.39845800 |
| O | -1.38650700 | -0.44205000 | -1.19733400 |
| H | -0.38942400 | -0.45000000 | -1.12961400 |
| C | 3.27863300 | 2.25207300 | -0.29244100 |
| H | 2.18470300 | 2.26198700 | -0.31266400 |
| H | 3.60851000 | 3.20500500 | 0.12793000 |
| H | 3.63395900 | 2.20718100 | -1.32527600 |
| C | -3.27850200 | 2.25205200 | 0.29264200 |
| H | -2.18457200 | 2.26189700 | 0.31292900 |
| H | -3.60829600 | 3.20504200 | -0.12766400 |
| H | -3.63388800 | 2.20709100 | 1.32545300 |
| C | -4.04024000 | -1.39534600 | -0.95860200 |
| H | -3.73906700 | -2.39687400 | -0.64477500 |
| H | -5.13136400 | -1.33873800 | -0.92564400 |
| H | -3.71586900 | -1.23187400 | -1.98636500 |
| C | 4.04010500 | -1.39548000 | 0.95851100 |
| H | 3.73885400 | -2.39696000 | 0.64460300 |
| H | 5.13123400 | -1.33896600 | 0.92559300 |
| H | 3.71571500 | -1.23205300 | 1.98627600 |

38

Iva-Iva (LD) non-ion

| | | | |
|---|---|---|---|
| N | 3.86294800 | -0.42823100 | -1.50336600 |
| H | 3.48997000 | 0.38274900 | -1.98616700 |
| C | 3.42565400 | -0.44939400 | -0.10153900 |
| C | 4.02652500 | 0.70235500 | 0.76371400 |
| C | 1.90756400 | -0.28835600 | -0.08012500 |
| H | 3.69479600 | 0.56890500 | 1.79708900 |
| H | 5.11236300 | 0.55932200 | 0.75715500 |
| O | 1.25799000 | 0.07143100 | -1.05713600 |
| H | 4.87594000 | -0.36051900 | -1.53738600 |
| O | 1.36765800 | -0.52095100 | 1.10250200 |
| H | 0.38318700 | -0.35014000 | 1.07692300 |
| N | -3.86296500 | 0.42822100 | 1.50336300 |
| H | -3.48996700 | -0.38273700 | 1.98618300 |
| C | -3.42566700 | 0.44936600 | 0.10153600 |
| C | -4.02650500 | -0.70241800 | -0.76369400 |
| C | -1.90757200 | 0.28838000 | 0.08011400 |
| H | -3.69479300 | -0.56896800 | -1.79707400 |
| H | -5.11234800 | -0.55942300 | -0.75712500 |
| O | -1.25797400 | -0.07138000 | 1.05711900 |
| H | -4.87595600 | 0.36048500 | 1.53738500 |
| O | -1.36767200 | 0.52107400 | -1.10249800 |
| H | -0.38319800 | 0.35031900 | -1.07690600 |
| C | 3.82101200 | -1.80599700 | 0.50830300 |
| H | 3.35867900 | -2.62567100 | -0.04537400 |
| H | 4.90645700 | -1.92047700 | 0.44846700 |
| H | 3.52329900 | -1.87048200 | 1.55492600 |
| C | 3.68584000 | 2.11609000 | 0.28773300 |
| H | 2.60928500 | 2.30837900 | 0.32434100 |
| H | 4.17391000 | 2.85677600 | 0.92552900 |
| H | 4.02419900 | 2.28993900 | -0.73710900 |
| C | -3.68576500 | -2.11613500 | -0.28770000 |
| H | -4.17380900 | -2.85684400 | -0.92548900 |
| H | -2.60920400 | -2.30838400 | -0.32430900 |
| H | -4.02411600 | -2.28998800 | 0.73714400 |
| C | -3.82107400 | 1.80594300 | -0.50833200 |

| | | | |
|---|---|---|---|
| H | -4.90652300 | 1.92038700 | -0.44849500 |
| H | -3.35876600 | 2.62564400 | 0.04532500 |
| H | -3.52336800 | 1.87041300 | -1.55495800 |

32
Ala-Iva (LL) non-ion

| | | | |
|---|---|---|---|
| N | -3.45718800 | 0.17270200 | 1.40922800 |
| H | -3.01259300 | 1.04451600 | 1.67798000 |
| C | -2.92696000 | -0.31074300 | 0.12788400 |
| C | -3.30711100 | 0.58941000 | -1.08941200 |
| C | -1.40337900 | -0.32410800 | 0.22353000 |
| H | -2.92335900 | 0.12178100 | -2.00031600 |
| H | -4.40009400 | 0.56956400 | -1.15738700 |
| O | -0.78284200 | 0.24332100 | 1.11720100 |
| H | -4.45104000 | 0.35888600 | 1.31084300 |
| O | -0.81689700 | -0.95714700 | -0.77654000 |
| H | 0.17648900 | -0.88559400 | -0.70190100 |
| N | 4.56278800 | -1.09824900 | -0.50070000 |
| H | 4.20057600 | -1.09991500 | -1.45064000 |
| C | 3.96171200 | -0.00106500 | 0.25832200 |
| H | 4.30215400 | -0.07148100 | 1.29460800 |
| C | 4.28814400 | 1.41415400 | -0.27048400 |
| C | 2.45427600 | -0.16364700 | 0.27194700 |
| H | 3.93664900 | 1.52609000 | -1.29988200 |
| H | 3.82554500 | 2.18696800 | 0.34784000 |
| H | 5.37017700 | 1.56141500 | -0.25654400 |
| O | 1.83971200 | -0.75040700 | -0.61280200 |
| H | 5.56568100 | -0.95235500 | -0.56611200 |
| O | 1.87208900 | 0.43385400 | 1.29581600 |
| H | 0.87765100 | 0.35716800 | 1.22747600 |
| C | -2.81821300 | 2.03679700 | -1.00295500 |
| H | -1.72591800 | 2.09557900 | -0.97752200 |
| H | -3.15771900 | 2.60225100 | -1.87392900 |
| H | -3.20325500 | 2.54082100 | -0.11258800 |
| C | -3.45386200 | -1.73739100 | -0.10697800 |
| H | -3.14297700 | -2.40012400 | 0.70316900 |
| H | -4.54637700 | -1.71402600 | -0.13114600 |
| H | -3.09493700 | -2.14013100 | -1.05418900 |

32
Ala -Iva (LD) non-ion

| | | | |
|---|---|---|---|
| N | -4.45356800 | 1.15143700 | -0.74354900 |
| H | -4.18151900 | 0.81621400 | -1.66399400 |
| C | -3.95448400 | 0.23781000 | 0.28472300 |
| H | -4.18211700 | 0.66407200 | 1.26520400 |
| C | -4.53676600 | -1.19261900 | 0.22458600 |
| C | -2.44499200 | 0.13867900 | 0.18149500 |
| H | -4.30440900 | -1.65753400 | -0.73749000 |
| H | -4.13859700 | -1.81889500 | 1.02632300 |
| H | -5.62250600 | -1.14236800 | 0.33136400 |
| O | -1.83460600 | 0.33549500 | -0.86427500 |
| H | -5.46878600 | 1.16176600 | -0.72039100 |
| O | -1.86592300 | -0.23096900 | 1.30935400 |
| H | -0.88129500 | -0.34440400 | 1.17746900 |
| N | 3.39158400 | -1.09227200 | 1.03586000 |
| H | 3.02306800 | -0.65383300 | 1.87367000 |
| C | 2.90079300 | -0.41178300 | -0.16933500 |
| C | 3.44856700 | 1.03998800 | -0.33965800 |
| C | 1.38057100 | -0.31458100 | -0.06880500 |
| H | 3.07740800 | 1.44206500 | -1.28635400 |
| H | 4.53578200 | 0.94962000 | -0.43653100 |
| O | 0.76292000 | -0.52331500 | 0.97077600 |
| H | 4.40372100 | -1.01423000 | 1.07506300 |
| O | 0.80017800 | 0.06685900 | -1.19233200 |
| H | -0.18509600 | 0.16614600 | -1.06151100 |
| C | 3.10653800 | 1.99963400 | 0.80199500 |
| H | 3.55609400 | 2.97850100 | 0.61949500 |
| H | 2.02661800 | 2.14620300 | 0.89940100 |
| H | 3.48497700 | 1.63728300 | 1.76141600 |
| C | 3.29587300 | -1.25390300 | -1.39531500 |
| H | 4.38444800 | -1.34830300 | -1.42629800 |

| | | | |
|---|---|---|---|
| H | 2.86656300 | -2.25561500 | -1.32831200 |
| H | 2.96237300 | -0.78475000 | -2.32100600 |