Supplementary material

I. STATIC AND MOLECULAR DYNAMICS CALCULATIONS

A. Static DFT and DFT+vdW calculations

All single-point DFT calculations and geometry relaxations were done with the FHI-aims code [1]. FHI-aims is an all-electron code which employs numeric atomic orbitals as a basis set. This choice allows accurate convergence of DFT energies with a relatively small basis set size.

The calculations for the data shown in Fig. 1 of the paper were consistently done at the convergence level designated as "really tight", i.e., essentially converged with respect to all numerical parameters and the basis set. The basis set level for "really tight" settings is "tier 2" as defined and explained in Ref. 1. In particular, Ref. 1 shows that DFT results based on this level are essentially free of basis set error. For the smaller benchmark molecules (Ala_2 and Ala_4) discussed in Sec. II of this supplementary material, we additionally verified the basis set convergence explicitly at the "tier 3" basis set level (again, see Ref. 1 for a definition and discussion). The vdW correction has been presented in Ref. [2].

In Fig. 1 of our paper, the fully extended and α-helical structures are not the most stable for short neutral alanine peptides [3], but our main point is studying the evolution of the α-helical stability with polypeptide length, and the influence of the ionic termination. For the ion-terminated peptides in Fig. 1 (which are locally stable in their respective conformations), we tested that geometry optimization does not influence our conclusions. On the other hand, the geometry of extended peptides in Table I has been fully optimized with all forces below 5×10^{-3} eV/Å.

B. CCSD(T) calculations on Ala_2 and Ala_4

For small alanine dipeptide and tetrapeptide cases, we have calculated the $\Delta_{\mathrm{MP2}}^{\mathrm{CCSD(T)}}$ correction to the relative stabilization energies as proposed by Hobza and co-workers [4]. CCSD(T) calculations are done with the Gaussian 03 code [5]. The 6-31G* basis set is used and the $\Delta_{\mathrm{MP2}}^{\mathrm{CCSD(T)}}$(6-31G*) correction is added to the MP2 energies from the literature

computed at the complete basis set limit. For selected cases we used a larger 6-311G** basis set with the largest observed deviation of 0.14 kcal/mol from the 6-31G* basis set.

C. *Ab initio* molecular dynamics simulations

The molecular dynamics simulations were performed with *ab initio* forces (at the Born-Oppenheimer surface) from DFT and DFT+vdW using the FHI-aims code [1, 6] without periodic boundary conditions. In PBE+vdW, the vdW parameters were updated at each time step. The basis set used was the "light" default of FHI-aims (tier1 basis set). The MD runs used a Nosé-Hoover thermostat. The time-step was 1 femtosecond, and the force convergence threshold was 5×10^{-4} eV/Å. For 500 K and 800 K, two different runs were performed, producing similar trajectories.

Each molecular dynamics step, with the basis sets we used in our simulation (tier 1 [9]), took around 30 seconds in 128 CPUs (IBM Power6), for our 180 atoms molecule. This means that the longest simulation presented in this work (70ps), with the 1 fs time-step, takes around 3 weeks to run in 128 CPUs. This simulation was only possible due to large (and continuous) efforts we made to improve the scalability of our code and the availability of state-of-the-art machines.

It is well known that even 70 ps is not enough for converged conformational changes in the sense of full folding [7], but local conformational changes without large barriers are captured in our simulations.

II. SMALL PEPTIDES (ALA_2 AND ALA_4)

Let us scrutinize the accuracy of DFT+vdW for polyalanine chains by studying the relative stabilization energies of different conformations of alanine dipeptide analog Ac-Ala-NMe (Ala_2) and alanine tetrapeptide analog Ac-Ala_3-NMe (Ala_4). All DFT calculations are performed as explained above. Reference geometries and energies for 5 conformations of Ala_2 [8] and 27 conformations of Ala_4 [9, 10] are available in the literature at the complete basis set limit of Møller-Plesset second-order perturbation theory (MP2). The relevant geometries are also included in this supplementary material. Since MP2 is known to significantly overestimate the dispersion interaction energy [4, 11], we have computed the $\Delta_{\mathrm{MP2}}^{\mathrm{CCSD(T)}}$ correction for

Ala_2 and Ala_4 as explained above. Figure 1 shows the comparison of different DFT+vdW methods to reference CCSD(T) stabilization energies. Compared to plain DFT-PBE (MAE of 1.2 kcal/mol; maximum error of 4.4 kcal/mol), the inclusion of vdW forces significantly reduces the MAE to 0.4 kcal/mol. For comparison, employing a typical classical force field (for example OPLS-AA [12]) results in a MAE of 2.4 kcal/mol, a factor of six larger than with PBE+vdW. The maximum error of 1.7 kcal/mol in PBE+vdW is for the left-handed 2_7-helical structure, whose stability is inherently overestimated by different DFT approximations (PBE, PBE0, and B3LYP). The effect of vdW interactions on the stabilization energies of Ala_2 is rather small with both PBE and PBE+vdW yielding similar results. However, the effect of vdW becomes more pronounced for the larger Ala_4 peptide. A noticeable challenge is reproducing the energy difference between globular and fully extended conformations of Ala_4 (both are shown in Fig. 1). The energy difference is 5.3 kcal/mol at the CCSD(T) level while PBE gives a negligible difference of 0.5 kcal/mol. The PBE+vdW method yields a value of 4.8 kcal/mol, in good agreement with CCSD(T). Different DFT functionals (PBE, PBE0, B3LYP) show very similar performance for Ala_2 and Ala_4 after applying the vdW correction. We should note that the employed Ala_2 and Ala_4 structures correspond to potential-energy minima. The performance of PBE+vdW for structures far from equilibrium (transition states, etc.) remains to be assessed should the reference data become available. It is encouraging that the accuracy of DFT+vdW for the relative energies of Ala_2 and Ala_4 is essentially the same as for the S22 database of intermolecular interactions. Thus, the DFT+vdW method is able to describe both intermolecular and intramolecular dispersion interactions with equal accuracy (MAE of 0.3 – 0.4 kcal/mol in comparison to CCSD(T)). We should remark that the DFT+vdW calculations have the computational cost of standard DFT, being faster by at least five orders of magnitude compared to CCSD(T). We choose the PBE+vdW approach for further discussion since it is suitable for MD simulations due to its lower computational cost and essentially the same accuracy for small peptides as vdW-corrected hybrid DFT functionals (PBE0+vdW or B3LYP+vdW).

The relative energies of different Ala_4 and Ala_2 conformers are shown in Tables I and II.

TABLE I. Relative energies (in kcal/mol) of Ala_4 conformers with PBE and PBE+vdW in comparison with CCSD(T).

Conformer	PBE	PBE+vdW	CCSD(T)
1	1.30	3.75	4.13
2	1.54	3.73	4.19
3	0.69	0.00	0.57
4	3.39	5.23	5.73
5	3.83	5.09	5.26
6	3.32	3.38	2.90
7	7.42	7.04	6.67
8	6.23	5.58	4.64
9	5.83	6.31	7.92
10	8.29	8.18	7.79
11	1.86	0.51	0.00
12	2.70	0.91	0.29
13	1.47	3.30	3.66
14	3.96	4.59	4.68
15	5.03	3.66	2.19
16	3.87	3.19	3.55
17	4.22	3.10	3.42
18	0.00	1.76	1.91
19	1.87	3.18	3.82
20	1.24	1.95	1.76
21	3.39	2.87	2.92
22	6.10	5.72	5.82
23	6.20	5.81	5.82
24	4.61	4.62	3.98
25	2.34	2.96	2.50
26	1.72	1.55	0.67
27	3.72	4.01	4.02

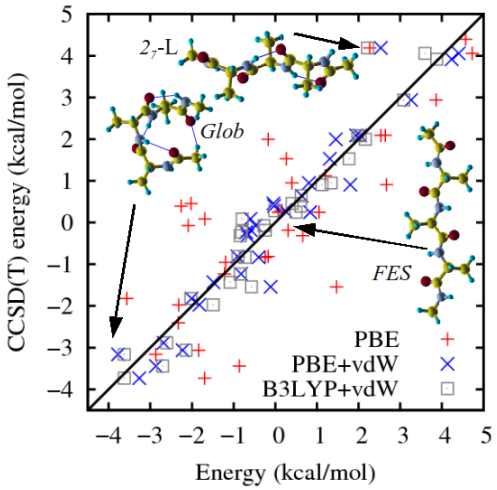

FIG. 1. Stabilization energies of Ala_2 and Ala_4 conformers as obtained by PBE, PBE+vdW, and B3LYP+vdW methods in comparison to CCSD(T) results. The left-handed 2_7-helical, globular (Glob) and fully extended (FES) structures are shown for illustration. For every method, the mean energy was subtracted.

TABLE II. Relative energies (in kcal/mol) of Ala_2 conformers with PBE and PBE+vdW in comparison with CCSD(T).

Conformer	PBE	PBE+vdW	CCSD(T)
$C7_{eq}$	0.00	0.00	0.00
C5	1.13	1.20	1.45
$C7_{ax}$	2.40	1.98	2.65
β_2	3.53	3.32	3.53
α'	6.90	6.92	6.80

III. GEOMETRIES OF ALA_2 AND ALA_4

All values are reported in Å.

Ala_4 1

C -5.590 2.831 -0.065

H -6.199 3.410 0.619

H -5.148 3.518 -0.776

H -6.219 2.124 -0.593

C -4.478 2.174 0.723

O -3.701 2.825 1.373

N -4.415 0.830 0.649

H -5.037 0.313 0.071

C -3.380 0.072 1.310

H -2.439 0.599 1.200

C -3.669 -0.121 2.804

H -2.869 -0.665 3.295

H -3.763 0.850 3.273

H -4.595 -0.670 2.940

C -3.287 -1.278 0.602

O -4.179 -1.683 -0.102

N -2.171 -1.984 0.838

H -1.453 -1.640 1.437

C -1.976 -3.311 0.301

H -2.915 -3.849 0.363

C -1.515 -3.277 -1.162

H -1.403 -4.279 -1.564

H -2.252 -2.751 -1.754

H -0.564 -2.762 -1.245

C -0.937 -4.007 1.175

O -0.205 -3.381 1.901

N -0.878 -5.341 1.052

H -1.482 -5.836 0.433

C 0.117 -6.134 1.738

H 1.051 -5.583 1.736

C -0.286 -6.431 3.188

H 0.481 -7.003 3.700

H -0.429 -5.498 3.716

H -1.212 -6.996 3.212

C 0.282 -7.431 0.951

O -0.574 -7.821 0.199

N 1.415 -8.116 1.179

H 2.111 -7.724 1.769

C 1.673 -9.387 0.531

H 2.614 -9.775 0.897

H 0.886 -10.095 0.755

H 1.733 -9.270 -0.545

Ala_4 2

C -2.242 1.735 4.097

H -1.480 1.402 4.792

H -2.069 1.279 3.130

H -2.157 2.811 4.005

C -3.598 1.409 4.682

O -3.934 1.824 5.761

N -4.399 0.634 3.923

H -4.090 0.262 3.054

C -5.704 0.214 4.371

H -5.642 -0.046 5.422

C -6.760 1.315 4.194

H -7.729 0.998 4.567

H -6.449 2.191 4.747

H -6.860 1.575 3.146

C -6.083 -1.025 3.567

O -5.520 -1.311 2.539

N -7.098 -1.754 4.062

H -7.557 -1.499 4.908

C -7.619 -2.904 3.362

H -7.593 -2.694 2.299

C -6.801 -4.171 3.644

H -7.187 -5.023 3.094

H -5.775 -4.004 3.341

H -6.822 -4.405 4.703

C -9.062 -3.097 3.812

O -9.449 -2.666 4.873

N -9.848 -3.795 2.977

H -9.459 -4.163 2.138

C -11.244 -4.104 3.272

H -11.626 -3.280 3.860

C -12.033 -4.235 1.978

H -13.075 -4.433 2.194

H -11.963 -3.316 1.406

H -11.663 -5.061 1.384

C -11.319 -5.391 4.106

O -11.590 -6.450 3.606

N -11.049 -5.232 5.414

H -10.706 -4.348 5.718

C -10.963 -6.370 6.305

H -10.067 -6.957 6.129

H -10.954 -6.012 7.326

H -11.821 -7.012 6.163

Ala_4 3

C -5.414 2.763 5.172

H -6.458 2.846 4.890

H -5.286 1.939 5.859

H -5.110 3.684 5.660

C -4.528 2.534 3.973

O -3.549 1.830 4.011

N -4.894 3.184 2.840

H -5.615 3.867 2.888

C -4.117 3.098 1.616

H -3.736 2.088 1.554

C -4.995 3.398 0.409

H -4.424 3.300 -0.507

H -5.825 2.701 0.376

H -5.375 4.411 0.454

C -2.947 4.084 1.699

O -3.094 5.244 1.393

N -1.798 3.564 2.165

H -1.881 2.673 2.608

C -0.561 4.296 2.427

H 0.181 3.538 2.637

C -0.069 5.128 1.241

H 0.905 5.542 1.482

H 0.036 4.491 0.370

H -0.746 5.933 1.000

C -0.616 5.116 3.720

O 0.245 4.977 4.555

N -1.644 5.970 3.863

H -2.316 6.042 3.129

C -1.877 6.700 5.102

H -0.911 6.975 5.505

C -2.706 7.946 4.829

H -2.865 8.500 5.746

H -2.191 8.584 4.119

H -3.678 7.679 4.432

C -2.586 5.758 6.084

O -3.789 5.727 6.175

N -1.765 4.965 6.795

H -0.814 4.923 6.500

C -2.277 3.887 7.615

H -1.506 3.580 8.310

H -3.135 4.233 8.172

H -2.572 3.029 7.017

Ala_4 4

C -2.282 1.880 5.887

H -2.687 2.073 6.872

H -1.916 0.861 5.842

H -1.457 2.564 5.730

C -3.353 2.179 4.862

O -3.873 3.263 4.791

N -3.686 1.164 4.039

H -3.278 0.262 4.135

C -4.721 1.299 3.044

H -5.528 1.888 3.465

C -4.211 1.990 1.771

H -5.004 2.114 1.040

H -3.831 2.969 2.032

H -3.414 1.409 1.320

C -5.227 -0.102 2.721

O -4.569 -1.082 2.971

N -6.432 -0.170 2.125

H -6.915 0.669 1.899

C -7.034 -1.436 1.724

H -6.660 -2.186 2.407

C -8.550 -1.350 1.814

H -8.996 -2.300 1.546

H -8.846 -1.099 2.827

H -8.935 -0.604 1.129

C -6.583 -1.782 0.300

O -7.259 -1.507 -0.659

N -5.388 -2.389 0.211

H -4.825 -2.526 1.024

C -4.802 -2.715 -1.069

H -5.604 -3.022 -1.729

C -4.070 -1.520 -1.694

H -3.652 -1.780 -2.662

H -4.767 -0.703 -1.828

H -3.262 -1.196 -1.046

C -3.826 -3.867 -0.855

O -3.244 -4.009 0.187

N -3.623 -4.664 -1.922

H -4.216 -4.571 -2.713

C -2.705 -5.784 -1.864

H -3.109 -6.604 -1.279

H -2.512 -6.129 -2.871

H -1.775 -5.470 -1.412

Ala_4 5

C -5.670 0.471 4.418

H -6.653 0.788 4.747

H -5.771 -0.366 3.739

H -5.115 0.156 5.294

C -4.963 1.660 3.806

O -4.800 2.681 4.422

N -4.527 1.501 2.540

H -4.741 0.681 2.019

C -3.885 2.570 1.817

H -4.398 3.498 2.046

C -2.403 2.717 2.192

H -1.952 3.575 1.703

H -2.327 2.859 3.261

H -1.843 1.833 1.908

C -4.046 2.269 0.330

O -4.430 1.202 -0.068

N -3.692 3.263 -0.518

H -3.487 4.162 -0.147

C -3.893 3.132 -1.951

H -4.848 2.655 -2.128

C -3.878 4.511 -2.610
H -4.031 4.403 -3.675
H -4.668 5.133 -2.205
H -2.925 5.009 -2.449
C -2.874 2.229 -2.645
O -3.115 1.812 -3.748
N -1.719 1.992 -2.004
H -1.584 2.294 -1.067
C -0.727 1.092 -2.542
H -1.242 0.277 -3.039
C 0.194 1.788 -3.551
H 0.916 1.095 -3.970
H -0.406 2.190 -4.357
H 0.732 2.599 -3.071
C 0.080 0.548 -1.367
O 0.124 1.126 -0.311
N 0.767 -0.583 -1.606
H 0.604 -1.075 -2.453
C 1.580 -1.207 -0.580
H 2.206 -1.959 -1.043
H 2.209 -0.464 -0.109
H 0.970 -1.675 0.185

Ala_4 6
C -2.871 -2.474 2.219
H -1.841 -2.483 2.560
H -3.480 -2.976 2.963
H -2.949 -2.992 1.275
C -3.328 -1.048 2.028
O -3.585 -0.588 0.942
N -3.421 -0.308 3.158
H -3.085 -0.695 4.011

C -3.896 1.069 3.168

H -4.573 1.168 2.329

C -4.625 1.371 4.468

H -4.990 2.391 4.467

H -5.466 0.696 4.583

H -3.962 1.267 5.318

C -2.716 2.027 2.952

O -2.301 2.738 3.828

N -2.158 1.956 1.724

H -2.567 1.327 1.066

C -0.975 2.705 1.337

H -0.748 2.383 0.324

C -1.189 4.218 1.321

H -0.298 4.710 0.955

H -2.022 4.455 0.667

H -1.406 4.584 2.314

C 0.274 2.328 2.143

O 1.222 3.067 2.194

N 0.284 1.097 2.692

H -0.545 0.551 2.712

C 1.381 0.632 3.503

H 2.307 0.878 2.996

C 1.389 1.264 4.902

H 2.224 0.896 5.491

H 1.477 2.338 4.806

H 0.465 1.034 5.420

C 1.234 -0.880 3.627

O 0.147 -1.407 3.645

N 2.374 -1.575 3.763

H 3.242 -1.101 3.681

C 2.370 -3.013 3.943

H 1.755 -3.287 4.790

H 1.987 -3.517 3.064

H 3.385 -3.341 4.123

Ala_4 7

C -2.585 1.042 -0.995

H -2.678 0.376 -1.848

H -2.117 1.960 -1.319

H -1.968 0.560 -0.247

C -3.972 1.349 -0.484

O -4.610 2.290 -0.885

N -4.452 0.495 0.453

H -3.970 -0.369 0.548

C -5.855 0.488 0.819

H -6.001 -0.406 1.418

C -6.229 1.699 1.677

H -7.205 1.571 2.134

H -5.508 1.795 2.480

H -6.220 2.611 1.097

C -6.711 0.265 -0.439

O -6.247 -0.302 -1.396

N -7.996 0.662 -0.384

H -8.294 1.244 0.364

C -8.902 0.528 -1.520

H -8.507 -0.270 -2.132

C -10.306 0.182 -1.047

H -10.971 0.076 -1.894

H -10.286 -0.750 -0.492

H -10.710 0.965 -0.416

C -8.889 1.827 -2.340

O -9.866 2.522 -2.431

N -7.707 2.130 -2.909

H -6.954 1.483 -2.826

C -7.520 3.368 -3.656

H -8.346 3.483 -4.341

C -7.453 4.596 -2.739

H -7.290 5.491 -3.331

H -8.389 4.702 -2.207

H -6.648 4.502 -2.018

C -6.270 3.287 -4.526

O -6.310 3.597 -5.686

N -5.135 2.878 -3.920

H -5.091 2.811 -2.925

C -3.885 2.876 -4.648

H -3.136 2.377 -4.048

H -4.001 2.345 -5.583

H -3.544 3.883 -4.872

Ala_4 8

C -5.869 0.567 2.326

H -5.998 -0.013 1.423

H -6.432 0.120 3.137

H -6.243 1.572 2.151

C -4.395 0.671 2.630

O -3.563 0.617 1.759

N -4.083 0.854 3.937

H -4.842 1.036 4.553

C -2.756 1.168 4.465

H -2.866 1.163 5.540

C -1.678 0.151 4.089

H -0.753 0.411 4.594

H -1.984 -0.835 4.420

H -1.501 0.115 3.025

C -2.392 2.617 4.135

O -2.376 3.456 5.005

N -2.130 2.911 2.848

H -2.380 2.225 2.166

C -2.126 4.297 2.435

H -1.353 4.816 2.989

C -1.845 4.393 0.938

H -1.824 5.431 0.622

H -0.885 3.944 0.708

H -2.618 3.881 0.377

C -3.494 4.918 2.746

O -4.510 4.338 2.468

N -3.469 6.133 3.329

H -2.592 6.480 3.640

C -4.668 6.860 3.727

H -4.308 7.754 4.228

C -5.522 7.291 2.537

H -6.354 7.886 2.885

H -4.919 7.881 1.855

H -5.909 6.429 2.011

C -5.508 6.137 4.791

O -6.666 6.426 4.935

N -4.868 5.274 5.599

H -3.959 4.944 5.366

C -5.599 4.557 6.620

H -4.895 3.961 7.186

H -6.098 5.248 7.287

H -6.353 3.905 6.189

Ala_4 9

C -3.611 2.415 1.346

H -2.713 3.002 1.491

H -3.639 2.043 0.329

H -4.462 3.065 1.510

C -3.636 1.324 2.392

O -3.461 1.584 3.558

N -3.884 0.076 1.944

H -4.063 -0.034 0.974

C -3.880 -1.153 2.735

H -3.975 -1.955 2.016

C -2.586 -1.371 3.526

H -2.629 -2.335 4.022

H -1.741 -1.375 2.845

H -2.428 -0.601 4.266

C -5.120 -1.326 3.621

O -5.795 -2.322 3.488

N -5.355 -0.375 4.534

H -4.718 0.395 4.554

C -6.523 -0.277 5.406

H -6.438 0.688 5.883

C -7.857 -0.327 4.654

H -8.670 -0.172 5.356

H -7.888 0.466 3.915

H -8.003 -1.273 4.153

C -6.522 -1.256 6.589

O -6.692 -0.813 7.703

N -6.391 -2.557 6.307

H -6.315 -2.802 5.342

C -6.299 -3.653 7.270

H -6.052 -4.525 6.681

C -5.199 -3.453 8.316

H -5.134 -4.339 8.939

H -4.244 -3.311 7.821

H -5.393 -2.595 8.944

C -7.627 -4.038 7.936

O -7.969 -5.193 7.947

N -8.333 -3.060 8.524

H -7.961 -2.136 8.532

C -9.563 -3.355 9.224

H -10.269 -3.852 8.569

H -9.389 -3.998 10.080

H -9.996 -2.424 9.566

Ala_4 10

C -0.620 -1.578 1.316

H -0.889 -2.573 1.640

H -0.609 -1.562 0.230

H 0.372 -1.328 1.673

C -1.669 -0.606 1.803

O -2.803 -0.945 2.015

N -1.248 0.673 1.998

H -0.337 0.900 1.671

C -2.175 1.794 2.141

H -1.551 2.659 2.348

C -2.987 2.064 0.876

H -3.605 2.940 1.014

H -2.314 2.232 0.041

H -3.632 1.226 0.649

C -3.087 1.671 3.367

O -4.156 2.212 3.381

N -2.592 0.991 4.424

H -1.708 0.553 4.323

C -3.312 0.819 5.675

H -2.664 0.207 6.297

C -3.566 2.135 6.410

H -4.013 1.934 7.373

H -2.622 2.651 6.556

H -4.229 2.771 5.842

C -4.597 -0.016 5.558

O -5.400 0.034 6.463

N -4.709 -0.827 4.502

H -4.050 -0.735 3.761

C -5.755 -1.825 4.278

H -5.442 -2.358 3.393

C -5.885 -2.832 5.425

H -6.610 -3.591 5.151

H -4.930 -3.316 5.599

H -6.204 -2.355 6.342

C -7.131 -1.266 3.890

O -7.708 -1.741 2.944

N -7.659 -0.308 4.663

H -7.146 0.011 5.455

C -8.964 0.241 4.373

H -9.168 1.033 5.082

H -8.997 0.650 3.371

H -9.738 -0.514 4.455

Ala_4 11

C 9.449 -0.424 7.133

H 9.129 -1.430 7.372

H 10.520 -0.412 6.972

H 9.198 0.221 7.969

C 8.670 0.051 5.935

O 7.480 -0.150 5.828

N 9.359 0.728 4.992

H 10.286 1.011 5.207

C 8.722 1.352 3.839

H 9.501 1.926 3.355

C 8.191 0.325 2.841

H 7.736 0.823 1.991

H 9.017 -0.276 2.478

H 7.469 -0.343 3.291

C 7.736 2.431 4.316

O 8.165 3.442 4.801

N 6.413 2.210 4.156

H 6.110 1.286 3.948

C 5.442 3.165 4.650

H 5.757 4.152 4.343

C 4.060 2.861 4.073

H 3.345 3.588 4.437

H 4.088 2.908 2.990

H 3.722 1.872 4.369

C 5.353 3.242 6.175

O 4.929 4.251 6.688

N 5.696 2.147 6.873

H 6.153 1.388 6.414

C 5.695 2.132 8.330

H 4.915 2.808 8.653

C 5.422 0.727 8.845

H 5.440 0.713 9.928

H 4.446 0.398 8.506

H 6.171 0.033 8.487

C 7.048 2.665 8.819

O 7.938 1.928 9.166

N 7.161 4.004 8.802

H 6.443 4.517 8.337

C 8.437 4.651 9.023

H 9.100 4.537 8.170

H 8.268 5.706 9.197

H 8.916 4.223 9.892

Ala_4 12

C 5.196 1.404 1.648

H 5.838 1.576 0.795

H 4.481 0.624 1.418

H 4.664 2.325 1.861

C 6.059 1.080 2.841

O 7.090 1.673 3.059

N 5.618 0.106 3.664

H 4.691 -0.228 3.544

C 6.290 -0.206 4.917

H 5.619 -0.865 5.454

C 7.609 -0.943 4.693

H 8.065 -1.211 5.640

H 7.415 -1.858 4.145

H 8.305 -0.349 4.114

C 6.334 1.054 5.796

O 5.296 1.580 6.112

N 7.529 1.514 6.204

H 8.353 1.143 5.793

C 7.643 2.683 7.058

H 6.953 2.566 7.882

C 9.068 2.795 7.598

H 9.140 3.657 8.246

H 9.328 1.906 8.163

H 9.784 2.915 6.789

C 7.234 4.007 6.405

O 7.044 4.957 7.119

N 7.132 4.041 5.064

H 7.305 3.216 4.532

C 6.689 5.218 4.346

H 6.785 6.057 5.023

C 7.556 5.455 3.110

H 7.200 6.322 2.571

H 8.585 5.616 3.411

H 7.523 4.596 2.448

C 5.206 5.184 3.956

O 4.757 6.052 3.252

N 4.453 4.172 4.426

H 4.830 3.543 5.098

C 3.020 4.177 4.229

H 2.542 4.991 4.765

H 2.784 4.285 3.179

H 2.623 3.237 4.591

Ala_4 13

C 9.901 1.840 0.455

H 9.032 2.282 -0.011

H 10.513 2.614 0.904

H 10.484 1.344 -0.315

C 9.440 0.804 1.455

O 8.448 0.147 1.283

N 10.231 0.644 2.538

H 11.037 1.209 2.681

C 9.922 -0.319 3.566

H 8.849 -0.317 3.723

C 10.368 -1.739 3.189

H 10.107 -2.456 3.960

H 9.875 -2.028 2.270

H 11.442 -1.768 3.038

C 10.626 0.131 4.840

O 11.590 0.859 4.803

N 10.134 -0.359 5.991

H 9.346 -0.966 5.963

C 10.687 -0.019 7.297

H 11.088 0.984 7.215

C 9.595 -0.058 8.355

H 9.998 0.218 9.320

H 8.804 0.637 8.094

H 9.183 -1.056 8.450

C 11.842 -0.967 7.648

O 11.729 -1.810 8.505

N 12.963 -0.786 6.933

H 12.974 -0.066 6.242

C 14.122 -1.666 7.044

H 13.752 -2.644 7.323

C 14.849 -1.741 5.709

H 15.698 -2.409 5.783

H 14.177 -2.111 4.942

H 15.224 -0.767 5.420

C 15.052 -1.164 8.158

O 16.090 -0.609 7.916

N 14.610 -1.398 9.408

H 13.690 -1.761 9.520

C 15.322 -0.888 10.560

H 15.234 0.190 10.647

H 14.913 -1.347 11.451

H 16.372 -1.137 10.485

Ala_4 14

C 7.557 -0.968 1.285

H 6.777 -1.482 0.743

H 7.201 0.005 1.607

H 8.407 -0.813 0.627

C 7.970 -1.816 2.466

O 7.585 -2.943 2.624

N 8.823 -1.222 3.333

H 9.104 -0.274 3.216

C 9.289 -1.900 4.516

H 8.465 -2.468 4.932

C 10.452 -2.858 4.218

H 10.758 -3.400 5.107

H 10.132 -3.577 3.475

H 11.305 -2.309 3.833

C 9.731 -0.836 5.513

O 10.011 0.284 5.164

N 9.856 -1.237 6.797

H 9.478 -2.122 7.052

C 10.128 -0.281 7.861

H 9.475 0.575 7.745

C 9.880 -0.933 9.220

H 10.082 -0.216 10.004

H 8.847 -1.256 9.304

H 10.527 -1.793 9.364

C 11.539 0.309 7.829

O 11.750 1.327 8.429

N 12.481 -0.377 7.152

H 12.218 -1.227 6.711

C 13.854 0.074 7.022

H 13.952 0.937 7.668

C 14.835 -1.008 7.469

H 15.850 -0.655 7.360

H 14.650 -1.265 8.506

H 14.725 -1.906 6.866

C 14.200 0.567 5.612

O 15.352 0.727 5.303

N 13.179 0.816 4.773

H 12.244 0.789 5.108

C 13.426 1.402 3.473

H 13.785 2.423 3.554

H 14.168 0.825 2.938

H 12.499 1.397 2.915

Ala_4 15

C 5.648 2.691 5.860

H 5.685 2.923 4.805

H 5.686 1.612 5.976

H 4.722 3.057 6.286

C 6.866 3.273 6.530

O 7.933 3.348 5.970

N 6.713 3.689 7.808

H 5.896 3.411 8.302

C 7.870 4.075 8.590

H 8.388 4.857 8.049

C 7.431 4.594 9.956

H 8.291 4.915 10.532

H 6.762 5.440 9.837

H 6.926 3.813 10.512

C 8.789 2.864 8.768

O 8.352 1.829 9.206

N 10.075 3.029 8.413

H 10.320 3.866 7.937

C 11.055 1.948 8.452

H 11.936 2.339 7.950

C 11.440 1.554 9.875

H 12.213 0.800 9.849

H 11.808 2.427 10.404

H 10.587 1.152 10.403

C 10.629 0.724 7.624

O 11.012 -0.372 7.928

N 9.873 0.975 6.536

H 9.539 1.898 6.375

C 9.411 -0.052 5.616

H 8.841 0.488 4.865

C 10.547 -0.788 4.908

H 10.136 -1.465 4.172

H 11.187 -0.066 4.410

H 11.138 -1.356 5.612

C 8.397 -1.035 6.216

O 8.158 -2.066 5.645

N 7.717 -0.639 7.312

H 8.074 0.108 7.864

C 6.796 -1.554 7.952

H 7.306 -2.420 8.362

H 6.294 -1.028 8.754

H 6.061 -1.903 7.239

Ala_4 16

C 5.187 1.690 2.433

H 5.026 0.827 1.801

H 4.254 2.239 2.493

H 5.947 2.325 1.995

C 5.543 1.212 3.819

O 4.930 0.330 4.368

N 6.584 1.826 4.427

H 6.915 2.686 4.054

C 6.881 1.532 5.812

H 6.967 0.458 5.907

C 8.197 2.193 6.218

H 8.437 1.951 7.248

H 9.002 1.840 5.585

H 8.121 3.271 6.135

C 5.756 2.051 6.711

O 5.380 3.194 6.605

N 5.278 1.176 7.611
H 5.503 0.219 7.456
C 4.251 1.427 8.621
H 4.243 0.545 9.245
C 4.559 2.635 9.510
H 3.809 2.696 10.291
H 5.530 2.510 9.975
H 4.561 3.559 8.951
C 2.821 1.494 8.069
O 1.961 0.841 8.595
N 2.602 2.321 7.026
H 3.352 2.908 6.728
C 1.268 2.572 6.511
H 0.564 2.274 7.274
C 1.087 4.058 6.203
H 0.092 4.234 5.820
H 1.234 4.646 7.102
H 1.805 4.392 5.457
C 0.888 1.744 5.279
O -0.226 1.849 4.831
N 1.820 0.950 4.734
H 2.711 0.852 5.161
C 1.498 0.092 3.614
H 0.742 -0.637 3.881
H 1.120 0.675 2.783
H 2.401 -0.420 3.314

Ala_4 17
C -5.054 -1.962 2.044
H -5.585 -1.308 2.729
H -5.755 -2.338 1.312
H -4.621 -2.779 2.607

C -3.994 -1.156 1.334

O -4.194 -0.636 0.263

N -2.823 -1.017 2.001

H -2.611 -1.698 2.700

C -1.710 -0.260 1.451

H -2.136 0.479 0.786

C -0.922 0.421 2.560

H -0.096 0.987 2.146

H -1.573 1.095 3.105

H -0.509 -0.308 3.246

C -0.826 -1.210 0.635

O 0.257 -1.566 1.034

N -1.385 -1.645 -0.512

H -2.321 -1.343 -0.687

C -0.907 -2.764 -1.322

H -1.561 -2.796 -2.182

C 0.533 -2.610 -1.815

H 0.774 -3.435 -2.477

H 0.624 -1.685 -2.374

H 1.243 -2.590 -1.003

C -1.170 -4.095 -0.608

O -1.973 -4.879 -1.048

N -0.477 -4.332 0.527

H 0.030 -3.574 0.933

C -0.859 -5.432 1.382

H -0.942 -6.313 0.766

C 0.206 -5.653 2.455

H -0.062 -6.489 3.093

H 1.161 -5.866 1.989

H 0.304 -4.771 3.077

C -2.196 -5.126 2.069

O -2.353 -4.075 2.648

N -3.149 -6.074 2.064

H -3.980 -5.801 2.540

C -3.213 -7.259 1.223

H -4.194 -7.698 1.347

H -3.074 -7.009 0.179

H -2.480 -8.001 1.520

Ala_4 18

C 5.407 5.617 6.017

H 4.680 6.391 6.215

H 6.315 6.058 5.622

H 4.995 4.946 5.270

C 5.640 4.834 7.288

O 4.753 4.631 8.079

N 6.889 4.349 7.467

H 7.602 4.586 6.817

C 7.243 3.479 8.580

H 6.357 2.907 8.826

C 8.373 2.543 8.178

H 8.623 1.881 8.997

H 8.070 1.945 7.326

H 9.268 3.101 7.928

C 7.625 4.322 9.803

O 8.773 4.450 10.154

N 6.592 4.902 10.436

H 5.681 4.795 10.042

C 6.776 5.875 11.505

H 7.718 6.380 11.325

C 5.635 6.882 11.497

H 5.778 7.620 12.276

H 5.597 7.386 10.538

H 4.686 6.391 11.680

C 6.880 5.164 12.861

O 6.000 5.237 13.686

N 8.014 4.472 13.055

H 8.682 4.447 12.313

C 8.235 3.630 14.224

H 7.267 3.264 14.542

C 9.142 2.464 13.860

H 9.292 1.823 14.720

H 8.693 1.882 13.062

H 10.115 2.817 13.542

C 8.833 4.462 15.369

O 9.987 4.364 15.692

N 7.964 5.293 15.973

H 7.059 5.398 15.570

C 8.402 6.218 16.995

H 8.999 7.027 16.582

H 7.530 6.638 17.480

H 9.000 5.700 17.731

Ala_4 19

C 11.746 -1.166 2.725

H 11.969 -2.060 2.159

H 11.994 -0.289 2.140

H 12.358 -1.169 3.621

C 10.293 -1.204 3.137

O 9.737 -2.240 3.407

N 9.666 -0.010 3.217

H 10.147 0.814 2.938

C 8.305 0.132 3.714

H 8.153 -0.650 4.446

C 8.116 1.496 4.359

H 7.110 1.592 4.749

H 8.819 1.617 5.176

H 8.262 2.290 3.636

C 7.309 -0.083 2.567

O 6.744 0.842 2.033

N 7.124 -1.364 2.205

H 7.691 -2.058 2.645

C 6.357 -1.742 1.025

H 6.447 -0.934 0.307

C 6.913 -3.029 0.434

H 6.360 -3.306 -0.454

H 7.956 -2.892 0.171

H 6.829 -3.846 1.140

C 4.868 -1.891 1.378

O 4.334 -2.975 1.391

N 4.244 -0.737 1.660

H 4.814 0.082 1.683

C 2.830 -0.560 1.982

H 2.683 0.509 2.030

C 1.890 -1.127 0.914

H 0.865 -0.889 1.177

H 2.112 -0.672 -0.046

H 1.988 -2.199 0.819

C 2.430 -1.038 3.385

O 1.858 -0.283 4.128

N 2.703 -2.312 3.707

H 3.155 -2.893 3.036

C 2.318 -2.850 4.993

H 1.242 -2.827 5.123

H 2.659 -3.875 5.052

H 2.766 -2.283 5.801

Ala_4 20

C 8.504 -1.545 1.342

H 8.511 -1.389 0.272

H 9.493 -1.365 1.745

H 8.235 -2.580 1.530

C 7.448 -0.658 1.955

O 6.405 -0.430 1.393

N 7.725 -0.161 3.181

H 8.620 -0.323 3.583

C 6.765 0.621 3.948

H 5.781 0.249 3.695

C 7.020 0.459 5.439

H 6.293 1.024 6.008

H 6.942 -0.586 5.715

H 8.002 0.832 5.705

C 6.856 2.092 3.522

O 7.456 2.909 4.172

N 6.214 2.397 2.373

H 5.900 1.624 1.822

C 6.468 3.656 1.691

H 7.535 3.840 1.654

C 5.912 3.592 0.268

H 6.112 4.525 -0.240

H 6.381 2.784 -0.284

H 4.840 3.424 0.279

C 5.899 4.883 2.401

O 6.329 5.968 2.119

N 4.903 4.680 3.287

H 4.605 3.746 3.449

C 4.291 5.754 4.044

H 4.526 6.673 3.524

C 2.775 5.577 4.104

H 2.334 6.382 4.674

H 2.362 5.575 3.101

H 2.511 4.639 4.586

C 4.859 5.929 5.458

O 4.335 6.713 6.208

N 5.928 5.195 5.800

H 6.391 4.633 5.123

C 6.570 5.387 7.082

H 5.851 5.282 7.884

H 7.341 4.636 7.193

H 7.020 6.371 7.160

Ala_4 21

C -0.517 0.228 -0.294

H 0.016 0.999 0.247

H 0.031 -0.704 -0.255

H -0.599 0.543 -1.329

C -1.911 0.110 0.280

O -2.552 1.075 0.598

N -2.379 -1.156 0.403

H -1.828 -1.913 0.053

C -3.749 -1.433 0.796

H -4.071 -0.599 1.407

C -4.687 -1.582 -0.396

H -5.698 -1.789 -0.066

H -4.684 -0.659 -0.964

H -4.369 -2.395 -1.037

C -3.741 -2.692 1.668

O -4.355 -3.683 1.362

N -2.985 -2.599 2.785

H -2.405 -1.791 2.842

C -2.583 -3.712 3.643

H -2.062 -3.262 4.476

C -3.748 -4.534 4.194

H -3.362 -5.265 4.899

H -4.433 -3.879 4.721

H -4.295 -5.047 3.419

C -1.509 -4.545 2.937

O -0.372 -4.550 3.332

N -1.888 -5.229 1.834

H -2.795 -5.046 1.459

C -0.874 -5.737 0.942

H -0.215 -6.383 1.509

C -1.525 -6.530 -0.190

H -0.771 -6.931 -0.857

H -2.099 -7.354 0.218

H -2.187 -5.893 -0.766

C -0.064 -4.580 0.345

O -0.612 -3.602 -0.107

N 1.264 -4.760 0.291

H 1.656 -5.456 0.882

C 2.146 -3.726 -0.212

H 2.226 -2.893 0.480

H 3.129 -4.151 -0.367

H 1.770 -3.358 -1.155

Ala_4 22

C 9.090 1.754 1.134

H 10.031 1.283 1.378

H 8.550 1.108 0.448

H 9.269 2.703 0.642

C 8.278 1.906 2.398

O 8.419 1.178 3.342

N 7.377 2.926 2.408

H 7.207 3.392 1.546

C 6.331 3.025 3.421

H 5.808 3.954 3.208

C 5.327 1.876 3.369

H 4.535 2.043 4.086

H 4.896 1.817 2.375

H 5.806 0.935 3.604

C 6.895 3.216 4.835

O 6.283 2.800 5.787

N 8.025 3.936 4.928

H 8.496 4.135 4.077

C 8.711 4.331 6.156

H 9.492 5.007 5.839

C 7.812 5.077 7.147

H 8.416 5.423 7.979

H 7.369 5.940 6.661

H 7.018 4.450 7.524

C 9.480 3.202 6.855

O 10.625 3.394 7.171

N 8.809 2.060 7.110

H 7.827 2.049 6.928

C 9.377 0.995 7.917

H 10.425 1.231 8.039

C 8.718 0.925 9.295

H 9.157 0.128 9.878

H 8.855 1.868 9.813

H 7.652 0.735 9.205

C 9.338 -0.375 7.235

O 9.561 -1.367 7.883

N 9.087 -0.411 5.919

H 8.945 0.428 5.406

C 9.106 -1.665 5.200

H 10.083 -2.133 5.253

H 8.381 -2.357 5.612

H 8.862 -1.463 4.167

Ala_4 23

C 8.473 -1.386 5.296

H 9.075 -2.004 4.645

H 9.127 -0.676 5.794

H 7.995 -2.001 6.049

C 7.479 -0.620 4.457

O 7.710 -0.296 3.324

N 6.295 -0.320 5.058

H 6.224 -0.483 6.036

C 5.358 0.642 4.484

H 4.490 0.625 5.137

C 5.907 2.065 4.434

H 5.146 2.744 4.075

H 6.210 2.371 5.431

H 6.759 2.126 3.771

C 4.822 0.196 3.118

O 4.515 1.020 2.293

N 4.638 -1.126 2.961

H 5.024 -1.715 3.660

C 4.062 -1.796 1.796

H 3.956 -2.830 2.090

C 2.678 -1.267 1.410

H 2.280 -1.875 0.605

H 2.007 -1.341 2.259

H 2.713 -0.237 1.088

C 4.992 -1.866 0.578

O 5.202 -2.933 0.067

N 5.493 -0.703 0.112

H 5.210 0.144 0.557

C 6.247 -0.636 -1.126

H 5.992 -1.507 -1.712

C 5.875 0.628 -1.903

H 6.437 0.667 -2.825

H 4.814 0.627 -2.131

H 6.100 1.520 -1.325

C 7.768 -0.699 -0.965

O 8.452 -0.786 -1.954

N 8.278 -0.625 0.270

H 7.683 -0.568 1.063

C 9.708 -0.672 0.482

H 10.122 -1.616 0.147

H 10.205 0.123 -0.060

H 9.894 -0.554 1.540

Ala_4 24

C 11.139 -1.055 3.447

H 12.127 -1.423 3.214

H 10.465 -1.269 2.625

H 11.198 0.021 3.575

C 10.682 -1.669 4.748

O 11.446 -1.935 5.637

N 9.349 -1.905 4.868

H 8.742 -1.548 4.166

C 8.771 -2.242 6.159

H 9.220 -1.622 6.923

C 7.260 -2.012 6.133

H 6.838 -2.267 7.096

H 7.040 -0.970 5.924

H 6.785 -2.628 5.375

C 9.050 -3.674 6.609

O 8.919 -3.953 7.776

N 9.372 -4.574 5.668

H 9.556 -4.250 4.747

C 9.634 -5.975 5.972

H 9.016 -6.227 6.824

C 9.263 -6.846 4.782

H 9.436 -7.890 5.012

H 8.215 -6.708 4.536

H 9.871 -6.602 3.919

C 11.106 -6.173 6.370

O 11.872 -6.774 5.667

N 11.454 -5.607 7.544

H 10.740 -5.156 8.072

C 12.774 -5.758 8.141

H 12.749 -5.151 9.042

C 13.087 -7.199 8.539

H 14.038 -7.242 9.050

H 12.309 -7.567 9.201

H 13.140 -7.834 7.665

C 13.903 -5.152 7.296

O 15.012 -5.617 7.339

N 13.611 -4.034 6.613

H 12.680 -3.691 6.571

C 14.625 -3.362 5.831

H 14.949 -3.972 4.994

H 14.204 -2.438 5.460

H 15.493 -3.142 6.441

Ala_4 25

C 11.912 0.416 4.874

H 12.569 1.239 4.633

H 11.659 0.442 5.928

H 12.437 -0.513 4.671

C 10.691 0.486 3.989

O 10.712 1.006 2.905

N 9.556 -0.071 4.488

H 9.628 -0.590 5.334

C 8.422 -0.367 3.623

H 8.781 -0.810 2.702

C 7.477 -1.342 4.323

H 6.637 -1.555 3.677

H 7.989 -2.273 4.545

H 7.101 -0.921 5.251

C 7.633 0.860 3.167

O 6.836 0.737 2.278

N 7.849 2.025 3.810

H 8.528 2.050 4.534

C 7.179 3.249 3.426

H 6.210 2.979 3.030

C 7.000 4.161 4.640

H 6.493 5.068 4.345

H 6.416 3.656 5.401

H 7.962 4.434 5.068

C 7.865 4.029 2.301

O 7.309 5.014 1.869

N 9.058 3.608 1.864

H 9.432 2.742 2.187

C 9.808 4.326 0.838

H 9.551 5.373 0.942

C 11.301 4.127 1.052

H 11.861 4.667 0.298

H 11.584 4.498 2.032

H 11.566 3.081 0.978

C 9.379 3.868 -0.564

O 10.099 3.210 -1.267

N 8.151 4.274 -0.939

H 7.581 4.732 -0.262

C 7.562 3.818 -2.178

H 7.315 2.762 -2.144

H 6.657 4.384 -2.359

H 8.249 3.979 -2.998

Ala_4 26

C 6.079 0.648 3.885

H 5.045 0.952 3.950

H 6.619 1.311 3.219

H 6.115 -0.357 3.474

C 6.671 0.625 5.274

O 6.003 0.441 6.256

N 8.014 0.828 5.359

H 8.537 0.837 4.512

C 8.734 0.515 6.584

H 8.437 -0.464 6.940

C 10.240 0.530 6.324

H 10.767 0.300 7.240

H 10.504 -0.214 5.579

H 10.565 1.505 5.973

C 8.413 1.453 7.744

O 8.644 1.090 8.869

N 7.916 2.666 7.454

H 7.728 2.889 6.505

C 7.592 3.628 8.492

H 8.423 3.679 9.183

C 7.361 5.004 7.871

H 7.128 5.716 8.651

H 8.249 5.336 7.344

H 6.529 4.982 7.172

C 6.391 3.249 9.365

O 6.204 3.879 10.372

N 5.597 2.247 8.946

H 5.806 1.771 8.096

C 4.475 1.768 9.729

H 4.206 2.559 10.416

C 3.286 1.453 8.822

H 2.463 1.079 9.415

H 2.973 2.350 8.299

H 3.551 0.701 8.084

C 4.797 0.559 10.614

O 3.913 0.055 11.261

N 6.060 0.110 10.636

H 6.771 0.575 10.121

C 6.435 -0.990 11.496

H 6.285 -0.742 12.541

H 5.848 -1.872 11.271

H 7.482 -1.208 11.331

Ala_4 27

C 8.007 0.379 1.631

H 8.120 -0.219 0.739

H 7.693 1.383 1.366

H 8.971 0.440 2.127

C 7.029 -0.303 2.557

O 6.869 -1.494 2.558

N 6.329 0.506 3.397

H 6.596 1.463 3.449

C 5.609 -0.049 4.535

H 6.245 -0.755 5.055

C 5.203 1.073 5.490

H 4.666 0.653 6.329

H 6.080 1.590 5.865

H 4.559 1.793 4.993

C 4.372 -0.862 4.158

O 3.913 -1.626 4.960

N 3.825 -0.643 2.943

H 4.265 0.008 2.335

C 2.667 -1.375 2.477

H 2.078 -1.639 3.344

C 1.832 -0.506 1.537

H 0.963 -1.055 1.204

H 1.511 0.393 2.050

H 2.407 -0.217 0.660

C 2.983 -2.712 1.794

O 2.050 -3.393 1.429

N 4.268 -3.033 1.615

H 4.961 -2.421 1.986

C 4.785 -4.303 1.104

H 5.854 -4.241 1.243

C 4.266 -5.524 1.870

H 4.757 -6.416 1.494

H 4.502 -5.419 2.924

H 3.197 -5.639 1.765

C 4.628 -4.490 -0.410

O 5.588 -4.796 -1.072

N 3.401 -4.343 -0.931

H 2.640 -4.144 -0.319

C 3.161 -4.574 -2.338

H 3.346 -5.608 -2.609

H 2.129 -4.333 -2.555

H 3.804 -3.950 -2.946

Ala_2 $C7_{eq}$

C -3.042 0.811 0.708

C -1.530 0.773 0.765

O -0.849 1.814 0.802

N -0.957 -0.464 0.785

C 0.494 -0.654 0.855

C 1.094 -0.527 -0.558

O 1.451 -1.511 -1.220

N 1.175 0.754 -1.005

C 1.583 1.029 -2.376

C 0.813 -2.008 1.472

H -3.345 1.385 -0.178

H -3.409 1.342 1.597

H -3.497 -0.189 0.669

H -1.544 -1.282 0.669

H 0.880 0.167 1.480

H 0.695 1.464 -0.453

H 1.705 2.112 -2.495

H 0.839 0.660 -3.101

H 2.537 0.528 -2.583

H 1.901 -2.139 1.542

H 0.425 -2.819 0.840

H 0.377 -2.076 2.480

Ala_2 C5

C -3.097 1.715 0.315

C -1.583 1.678 0.286

O -0.893 2.708 0.329

N -1.019 0.438 0.210

C 0.421 0.271 0.193

C 0.705 -1.122 -0.365

O -0.117 -2.042 -0.251

N 1.933 -1.271 -0.935

C 2.421 -2.551 -1.430

C 1.022 0.401 1.602

H -3.447 2.348 -0.513

H -3.417 2.185 1.256

H -3.552 0.719 0.232

H -1.576 -0.410 0.176

H 0.846 1.050 -0.461

H 2.520 -0.451 -1.013

H 3.327 -2.860 -0.889

H 2.641 -2.496 -2.505

H 1.629 -3.290 -1.262

H 2.119 0.312 1.572

H 0.619 -0.391 2.250

H 0.757 1.384 2.014

Ala_2 $C7_{ax}$

C -3.195 0.524 -0.588

C -1.680 0.490 -0.606

O -1.013 1.538 -0.679

N -1.113 -0.748 -0.539

C 0.322 -1.057 -0.637

C 1.136 -0.681 0.612

O 1.881 -1.516 1.150

N 1.019 0.600 1.037

C 1.787 1.066 2.182

C 0.966 -0.484 -1.906

H -3.539 0.977 -1.529

H -3.519 1.173 0.237

H -3.653 -0.468 -0.476

H -1.740 -1.533 -0.419

H 0.383 -2.154 -0.672

H 0.411 1.226 0.508

H 1.565 0.455 3.068

H 1.517 2.110 2.379

H 2.867 0.996 1.983

H 2.017 -0.807 -1.945

H 0.926 0.612 -1.912

H 0.447 -0.866 -2.798

$\mathrm{Ala}_2\beta_2$

C -2.867 1.637 -0.009

C -1.381 1.356 -0.123

O -0.670 1.870 -0.992

N -0.863 0.474 0.799

C 0.580 0.287 0.929

C 1.178 -0.684 -0.097

O 2.405 -0.830 -0.166

N 0.296 -1.391 -0.854

C 0.779 -2.239 -1.936

C 0.914 -0.207 2.338

H -3.322 1.539 -1.003

H -2.999 2.677 0.321

H -3.378 0.969 0.698

H -1.457 0.169 1.561

H 1.069 1.253 0.734

H -0.665 -1.074 -0.855

H 1.173 -1.640 -2.772

H -0.046 -2.868 -2.290

H 1.588 -2.875 -1.557

H 1.996 -0.372 2.416

H 0.402 -1.161 2.543

H 0.608 0.534 3.091

$\mathrm{Ala}_2\ \alpha'$

C -2.876 1.830 0.007

C -1.360 1.798 0.038

O -0.679 2.826 0.080

N -0.792 0.540 0.043

C 0.658 0.395 -0.139

C 1.005 -1.052 -0.476

O 1.897 -1.341 -1.279

N 0.276 -2.005 0.191

C 0.663 -3.409 0.085

C 1.430 0.814 1.120

H -3.195 2.384 -0.887

H -3.231 2.380 0.889

H -3.330 0.829 -0.002

H -1.376 -0.217 -0.298

H 0.990 1.010 -0.990

H -0.242 -1.705 1.010

H -0.100 -4.024 0.578

H 1.645 -3.596 0.546

H 0.724 -3.683 -0.975

H 2.507 0.668 0.951

H 1.119 0.205 1.982

H 1.239 1.872 1.338

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[1] V. Blum *et al.*, Comput. Phys. Comm. **180**, 2175 (2009).

[2] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).

[3] M. Rossi *et al.*, J. Phys. Chem. Lett. **1**, 3465 (2010).

[4] P. Jurecka, J. Sponer, J. Cerny, and P. Hobza, Phys. Chem. Chem. Phys. **8**, 1985 (2006).

[5] M. J. Frisch et al., "Computer code Gaussian 03, Revision B.05," (2003).

[6] V. Havu, V. Blum, P. Havu, and M. Scheffler, J. Comp. Phys. **228**, 8367 (2009).

[7] W. A. Hegefeld, S. E. Chen, K. Y. Deleon, K. Kuczera, and G. S. Jas, J. Phys. Chem. A. **114**, 12391 (2010).

[8] R. Vargas, J. Garza, B. P. Hay, and D. A. Dixon, J. Phys. Chem. A **106**, 3213 (2002).

[9] R. A. DiStasio Jr., Y. Jung, and M. Head-Gordon, J. Chem. Theory Comput. **1**, 862 (2005).

[10] R. A. DiStasio Jr., Y. Jung, and M. Head-Gordon, J. Comp. Chem. **28**, 839 (2007).

[11] A. Tkatchenko, R. A. DiStasio Jr., M. Head-Gordon, and M. Scheffler, J. Chem. Phys. **131**, 094106 (2009).

[12] W. L. Jorgensen, D. S. Maxwell, and J. Tirado-Rives, J. Am. Chem. Soc. **118**, 11225 (1996).