Supplementary Material for PCCP

Electronic Supplementary Information

The structure of the neutral gas-phase glycine tripeptide

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Fig. S1 The (N)H···O distance as a function of the ϕ_3 torsion angle in conformer 14.

Fig. S2 The ϕ_1 torsion angle as a function of ϕ_3 in conformer 14.

Fig. S3 Potential energy profiles for rotation around the N12-C17 bond in conformer 14.

Fig. S4 B3LYP and MP2 relative energies of the 97 conformers identified in the current work.

Fig. S5 Relative energies of the 20 most stable Gly-Gly-Gly conformers (based on the MP2+ZPE energies) computed at different levels of theory.

Table S1. BSSE values as a function of the ϕ_3 torsion angle in conformer 14.

Table S2. Cartesian coordinates (in Å) of the 20 conformers identified by the hierarchical selection and H-bond selection methods and the extra conformer obtained after MP2 geometry optimisations of all conformers.

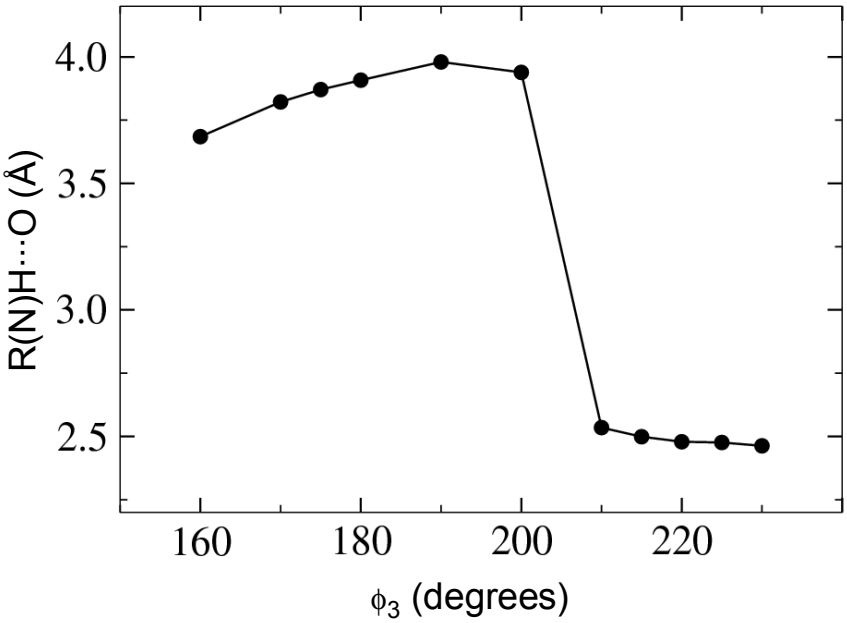

Fig. S1 The (N)H···O distance as a function of the ϕ_3 torsion angle in conformer 14, using structures optimised with M05-2X/6-31+G(d) at fixed ϕ_3 angles.

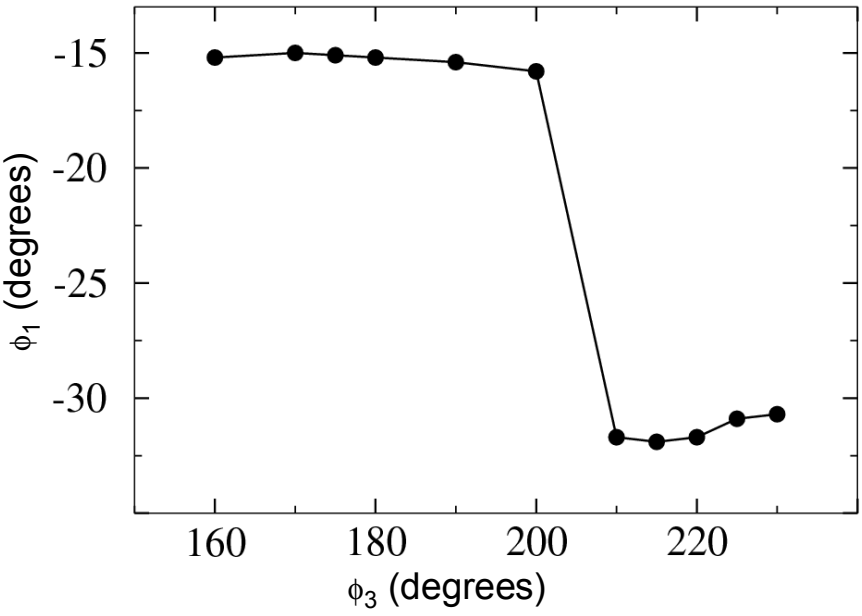

Fig. S2 The ϕ_1 torsion angle as a function of ϕ_3 in conformer 14, using structures optimised with M05-2X/6-31+G(d) at fixed ϕ_3 angles.

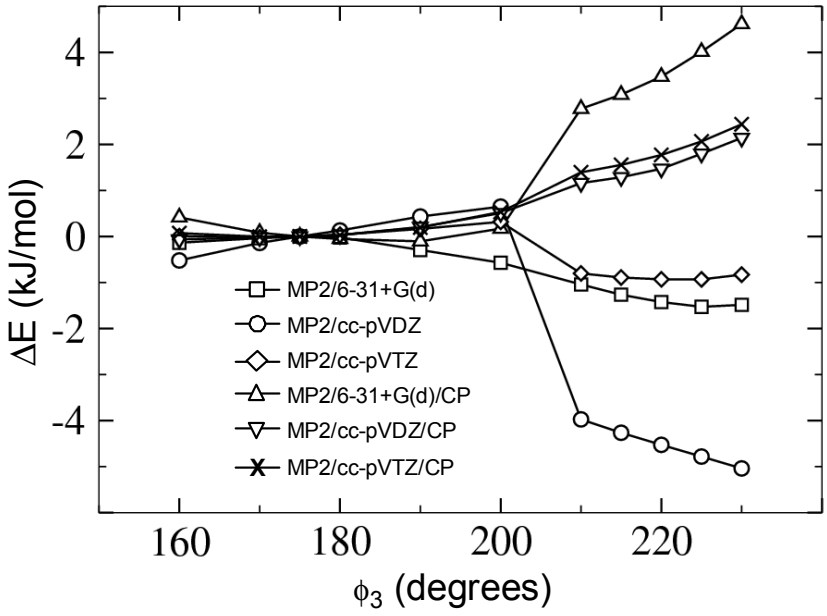

Fig. S3 Potential energy profiles for rotation around the N12-C17 bond in conformer 14, computed using structures optimised with M05-2X/6-31+G(d) at fixed ϕ_3 values. The energy at ϕ_3 = 175° was taken as the reference point for the relative energies.

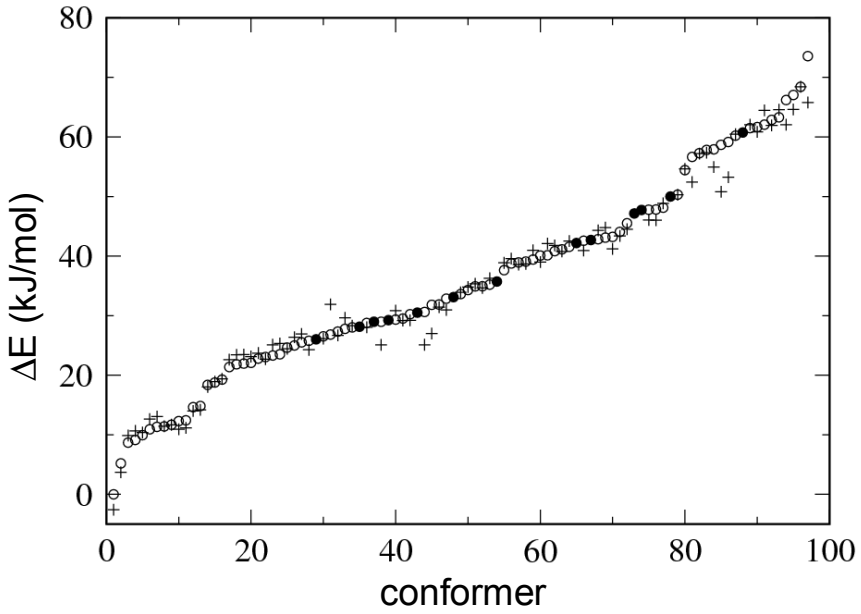

Fig. S4 Relative energies of the 97 conformers identified in the current work. Circles: Relative energies computed using MP2/6-31+G(d) single-point energies using the B3LYP/6-31+G(d) geometries. The solid circles indicate conformers that converged to other structures upon MP2 geometry optimisation. Plusses: Relative energies from MP2/6-31+G(d) geometry optimisations. The curves were made to overlap at conformer 9.

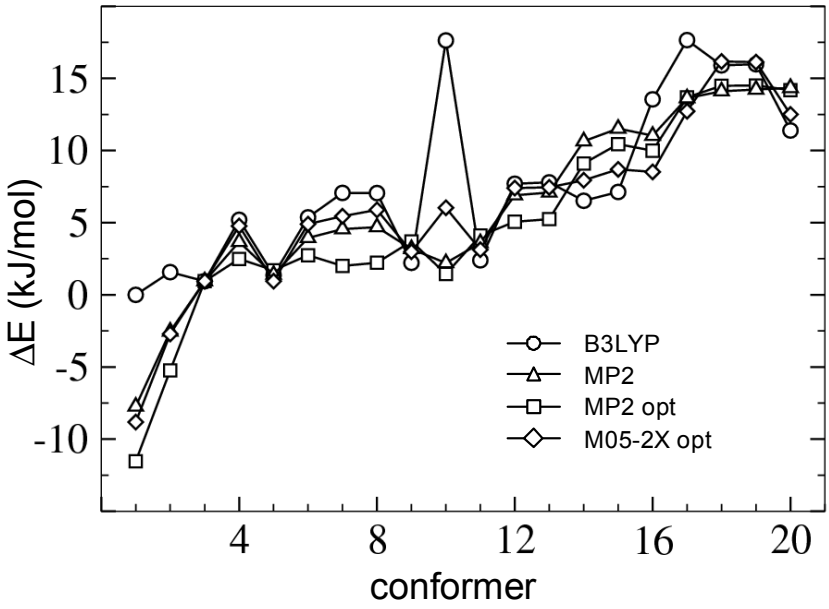

Fig. S5 Relative energies of the 20 most stable Gly-Gly-Gly conformers (based on the MP2+ZPE energies) computed at different levels of theory. The profiles labelled "B3LYP" and "MP2" were computed using the B3LYP/6-31+G(d) geometries. The "MP2 opt" and M05-2X opt" profiles were computed using MP2/6-31+G(d) and M05-2X/6-31+G(d) geometries, respectively. All calculations employed the 6-31+G(d) basis set. In the B3LYP curve, the energy of conformer 1 was taken as the reference point for the relative energies. The other curves were shifted to coincide with the B3LYP curve at conformer 3.

Table S1. BSSE values (in kJ/mol) as a function of the ϕ_3 torsion angle in conformer 14

ϕ_3 (degrees)	MP2/6-31+G*	MP2/cc-pVDZ	MP2/cc-pVTZ	M05-2X/6-31+G*	B3LYP/6-31+G*
160	49.135	54.519	25.783	7.880	7.431
170	48.701	54.181	25.733	7.760	7.357
175	48.583	54.063	25.718	7.744	7.356
180	48.551	53.966	25.711	7.765	7.389
190	48.770	53.835	25.750	7.921	7.557
200	49.325	53.922	25.932	8.192	7.816
210	52.401	59.195	27.913	9.368	8.920
215	52.929	59.613	28.166	9.524	9.059
220	53.479	60.060	28.418	9.669	9.184
225	54.124	60.642	28.714	9.828	9.321
230	54.685	61.243	28.982	9.960	9.431

Table S2. Cartesian coordinates (in Å) of the 20 conformers identified by the hierarchical selection and H-bond selection methods and the extra conformer obtained after the MP2 geometry optimisations of all 97 conformers. The structures are optimised with B3LYP/6-31+G(d).

Conf. 1	x	y	z
N	-2.677785	-1.599283	-1.183280
C	-2.754050	-1.317111	0.254229
C	-1.982977	-0.050382	0.627908
N	-1.773022	0.815465	-0.390356
O	-1.596451	0.150366	1.786383
H	-3.432390	-2.211426	-1.481579
H	-2.372266	-2.117347	0.901876
H	-3.803697	-1.152429	0.526601
H	-1.798643	-2.060703	-1.412184
C	-0.958553	2.015933	-0.250259
C	0.541023	1.686028	-0.336418
N	1.020672	0.986130	0.737297
O	1.229322	2.011139	-1.298841
H	-2.031946	0.477497	-1.313608
H	-1.196288	2.486728	0.709299
H	-1.197931	2.704977	-1.061132
C	2.297656	0.324005	0.669496
C	2.216877	-1.053461	0.015947
O	1.211960	-1.595788	-0.389692
O	3.442582	-1.624674	-0.048230
H	0.332174	0.652702	1.411660
H	2.718995	0.205691	1.673778
H	2.994090	0.937312	0.089983
H	3.339687	-2.497605	-0.472705

Conf. 2	x	y	z
N	-3.519538	-1.123656	-1.097856
C	-2.824212	-1.369638	0.170570
C	-1.969418	-0.186209	0.625171
N	-1.775463	0.778902	-0.299831
O	-1.476436	-0.157204	1.760698
H	-3.619958	-1.976262	-1.641037
H	-2.129741	-2.207602	0.041240
H	-3.483367	-1.630647	1.009394
H	-4.451653	-0.745209	-0.948129
C	-0.939895	1.949600	-0.066799
C	0.562152	1.654792	-0.227182
N	1.075930	0.830615	0.732937
O	1.225271	2.140078	-1.139331
H	-2.163178	0.593042	-1.220713
H	-1.141949	2.323060	0.943350
H	-1.202436	2.719127	-0.793762
C	2.404773	0.289089	0.616695
C	2.444130	-1.048667	-0.115312
O	1.492366	-1.654263	-0.554074
O	3.718250	-1.502858	-0.207501
H	0.411085	0.389443	1.368981
H	2.849880	0.151210	1.608643
H	3.032810	0.998624	0.069527
H	3.691226	-2.355636	-0.681443

Table S2 continued

Conf. 3	x	y	z
N	3.527827	-1.000893	-1.366683
C	3.275403	-1.141097	0.071712
C	2.183650	-0.194842	0.575261
N	1.818320	0.780659	-0.285762
O	1.692615	-0.326629	1.703879
H	2.967566	-1.654135	-1.909475
H	4.185469	-0.883245	0.625766
H	2.991614	-2.153582	0.387053
H	4.502041	-1.175647	-1.595582
C	0.874841	1.834727	0.062200
C	-0.592087	1.386297	-0.007769
N	-0.959524	0.437533	0.877576
O	-1.375813	1.877868	-0.836343
H	2.280781	0.768892	-1.191217
H	0.994104	2.657072	-0.643778
H	1.101581	2.192887	1.073409
C	-2.333614	-0.044367	1.003500
C	-2.805825	-0.949371	-0.150940
O	-3.219530	-2.071151	0.035947
O	-2.759309	-0.402825	-1.376487
H	-0.229894	0.042456	1.474001
H	-3.009343	0.818297	1.071383
H	-2.407333	-0.620927	1.925270
H	-2.400871	0.520642	-1.332503

Conf. 4	x	y	z
N	-4.490365	0.040907	-0.637699
C	-3.587366	-1.076292	-0.337359
C	-2.268337	-0.627827	0.297475
N	-2.020107	0.698540	0.243651
O	-1.491893	-1.453892	0.793258
H	-5.075714	-0.158481	-1.444016
H	-3.324032	-1.582021	-1.273564
H	-4.012418	-1.842945	0.324391
H	-5.110309	0.239968	0.144110
C	-0.845499	1.324875	0.837962
C	0.439426	1.217684	-0.002537
N	0.844303	-0.057604	-0.260673
O	1.037262	2.217756	-0.390792
H	-2.718747	1.259893	-0.235080
H	-0.665505	0.868287	1.818759
H	-1.050137	2.387336	0.974498
C	2.089306	-0.329244	-0.929513
C	3.261075	-0.507716	0.031137
O	3.212819	-0.461695	1.238134
O	4.405020	-0.746437	-0.659347
H	0.331404	-0.815446	0.188553
H	2.323805	0.502277	-1.601147
H	2.005114	-1.235244	-1.540445
H	5.122416	-0.851243	-0.006030

Table S2 continued

Conf. 5	x	y	z
N	3.801467	-0.720514	-1.294407
C	3.187524	-1.243784	-0.069225
C	2.157682	-0.289479	0.537594
N	1.806699	0.758813	-0.239583
O	1.671567	-0.501822	1.656239
H	4.688095	-0.259860	-1.105050
H	3.902202	-1.488874	0.727437
H	2.648408	-2.170011	-0.298669
H	3.979863	-1.457112	-1.970724
C	0.874190	1.790681	0.192639
C	-0.598560	1.368069	0.089807
N	-0.976653	0.353559	0.894149
O	-1.377744	1.938129	-0.691120
H	2.243334	0.796774	-1.157089
H	1.002940	2.667403	-0.442862
H	1.105706	2.060874	1.229608
C	-2.358181	-0.114511	0.986930
C	-2.850408	-0.914531	-0.234696
O	-3.280547	-2.041442	-0.137054
O	-2.803998	-0.269988	-1.411523
H	-0.251813	-0.098638	1.454712
H	-3.018834	0.751004	1.127534
H	-2.438494	-0.762883	1.859096
H	-2.429711	0.640626	-1.295740

Conf. 6	x	y	z
N	-4.331765	0.036864	-0.912896
C	-3.656775	-1.035764	-0.172465
C	-2.285459	-0.619119	0.368180
N	-2.025038	0.705228	0.326179
O	-1.500284	-1.461345	0.820875
H	-5.341550	-0.017823	-0.815415
H	-3.507949	-1.959599	-0.746895
H	-4.261854	-1.304123	0.701314
H	-4.120739	-0.005275	-1.907190
C	-0.833803	1.312925	0.907504
C	0.431717	1.210693	0.037888
N	0.822889	-0.062887	-0.248352
O	1.027971	2.212577	-0.348339
H	-2.751506	1.284129	-0.085549
H	-0.635425	0.840605	1.877460
H	-1.028258	2.374425	1.064066
C	2.054754	-0.331038	-0.942430
C	3.245349	-0.511837	-0.005368
O	3.219475	-0.475646	1.202598
O	4.377098	-0.740223	-0.719059
H	0.314049	-0.824381	0.199390
H	2.276062	0.502331	-1.616224
H	1.958809	-1.235491	-1.553846
H	5.106974	-0.847293	-0.080081

Table S2 continued

Conf. 7	x	y	z
N	3.681480	-0.992941	-1.053866
C	2.947785	-1.328917	0.171707
C	1.993122	-0.220916	0.621319
N	1.778179	0.761437	-0.279608
O	1.451373	-0.263546	1.733760
H	4.565993	-0.535146	-0.846314
H	3.584038	-1.569335	1.034169
H	2.326276	-2.212130	-0.015133
H	3.891399	-1.821685	-1.602964
C	0.919389	1.911018	-0.024182
C	-0.582912	1.621948	-0.199835
N	-1.092181	0.727195	0.693563
O	-1.249836	2.185294	-1.063536
H	2.233840	0.644719	-1.180287
H	1.179289	2.702696	-0.727773
H	1.107087	2.263037	0.996949
C	-2.461923	0.280699	0.627341
C	-2.716217	-1.029887	-0.109911
O	-3.801173	-1.569648	-0.145132
O	-1.622749	-1.536492	-0.725146
H	-0.436764	0.269630	1.327177
H	-3.052456	1.048178	0.116619
H	-2.874711	0.163963	1.634821
H	-1.912711	-2.352296	-1.176085

Conf. 8	x	y	z
N	-3.384031	-1.219203	-1.158812
C	-3.060514	-1.217736	0.272584
C	-2.031008	-0.149329	0.649141
N	-1.800719	0.790434	-0.292400
O	-1.478804	-0.161096	1.757049
H	-4.340362	-1.518407	-1.326598
H	-2.682107	-2.174946	0.654768
H	-3.967137	-0.987073	0.844084
H	-2.774348	-1.846881	-1.677840
C	-0.928138	1.939294	-0.084015
C	0.569443	1.624550	-0.253600
N	1.070378	0.757033	0.670834
O	1.240933	2.146506	-1.139581
H	-2.293547	0.666950	-1.172274
H	-1.106850	2.335203	0.922749
H	-1.180958	2.704819	-0.818302
C	2.436914	0.299155	0.623736
C	2.684416	-1.042503	-0.057371
O	3.765484	-1.590954	-0.065279
O	1.590581	-1.568227	-0.657058
H	0.412176	0.333507	1.324905
H	2.849166	0.221985	1.635258
H	3.032314	1.040941	0.081534
H	1.880030	-2.404364	-1.069515

Table S2 continued

Conf. 9	x	y	z
N	4.452888	0.197782	0.745803
C	3.669681	-0.951078	0.277426
C	2.338262	-0.545847	-0.358331
N	1.974796	0.742767	-0.175549
O	1.647124	-1.370794	-0.969629
H	4.989717	-0.028528	1.578140
H	3.422742	-1.591929	1.131629
H	4.186916	-1.588999	-0.451473
H	5.111309	0.515762	0.038594
C	0.787050	1.333034	-0.777641
C	-0.528143	0.996622	-0.061932
N	-0.852453	-0.310573	-0.001689
O	-1.252399	1.894803	0.397340
H	2.616322	1.309219	0.373202
H	0.715906	0.999172	-1.820320
H	0.890406	2.418450	-0.762954
C	-1.992034	-0.811101	0.765329
C	-3.371449	-0.545670	0.130891
O	-4.157565	-1.438871	-0.089679
O	-3.662488	0.739465	-0.120650
H	-0.208848	-0.974949	-0.435684
H	-1.979172	-0.356354	1.765045
H	-1.882775	-1.890340	0.869498
H	-2.906729	1.326080	0.140853

Conf. 10	x	y	z
N	-2.695429	0.965037	-0.358841
C	-2.641745	-0.504192	-0.469088
C	-1.442528	-1.002582	0.339425
N	-0.632290	-1.915614	-0.263888
O	-1.255524	-0.591801	1.486778
H	-3.544435	1.324768	-0.790970
H	-2.553305	-0.774032	-1.526649
H	-3.538864	-1.001545	-0.068084
H	-2.722141	1.222100	0.628818
C	0.669121	-2.280742	0.306623
C	1.684952	-1.186777	-0.070789
N	1.643470	-0.085698	0.742065
O	2.391702	-1.288318	-1.066609
H	-0.721070	-2.027094	-1.266559
H	0.990776	-3.228988	-0.126041
H	0.550019	-2.391164	1.387174
C	2.006234	1.238329	0.244662
C	0.729540	2.008858	-0.110519
O	0.415803	3.072701	0.383655
O	-0.029383	1.321410	-0.981696
H	0.917159	-0.101385	1.453428
H	2.635028	1.100371	-0.639348
H	2.555475	1.804419	0.999776
H	-0.993140	1.577178	-0.905798

Table S2 continued

Conf. 11	x	y	z
N	4.300256	0.147868	0.992581
C	3.732156	-0.894207	0.129758
C	2.352734	-0.525183	-0.421490
N	1.980261	0.761160	-0.240479
O	1.652718	-1.364606	-1.001930
H	4.098201	-0.026142	1.974159
H	3.634619	-1.876461	0.610090
H	4.380259	-1.036692	-0.742653
H	5.309957	0.205836	0.897516
C	0.779386	1.337659	-0.830832
C	-0.521493	0.999243	-0.090700
N	-0.836412	-0.309306	-0.013981
O	-1.244046	1.896744	0.372813
H	2.646702	1.346342	0.256597
H	0.693051	0.995280	-1.869788
H	0.875945	2.423705	-0.826126
C	-1.960986	-0.810515	0.774337
C	-3.351833	-0.558545	0.159546
O	-4.135698	-1.458295	-0.041516
O	-3.654853	0.722753	-0.097155
H	-0.194288	-0.973279	-0.450952
H	-1.935867	-0.347826	1.770212
H	-1.843495	-1.888235	0.885128
H	-2.898581	1.315923	0.147561

Conf. 12	x	y	z
N	4.467903	-0.003452	-0.618573
C	3.546911	-1.105087	-0.316112
C	2.230838	-0.632304	0.306629
N	2.003969	0.697284	0.244632
O	1.436716	-1.443107	0.800713
H	5.048599	-0.212498	-1.425753
H	3.956611	-1.872776	0.354013
H	3.281789	-1.614452	-1.249814
H	5.092050	0.186659	0.162042
C	0.834908	1.344462	0.827385
C	-0.445707	1.252871	-0.022358
N	-0.871361	-0.016947	-0.270780
O	-1.023680	2.261332	-0.419478
H	2.715598	1.245204	-0.230783
H	1.054887	2.404352	0.959887
H	0.642305	0.895465	1.809387
C	-2.092334	-0.285306	-0.989894
C	-3.327995	-0.566447	-0.140401
O	-4.389424	-0.913988	-0.612585
O	-3.129717	-0.391652	1.184379
H	-0.353797	-0.781579	0.161667
H	-1.964457	-1.143287	-1.658367
H	-2.328194	0.585237	-1.610328
H	-3.979869	-0.580332	1.625358

Table S2 continued

Conf. 13	x	y	z
N	4.313133	-0.009687	-0.890462
C	3.614780	-1.066867	-0.149775
C	2.247537	-0.623343	0.379091
N	2.008860	0.704457	0.325241
O	1.444834	-1.448650	0.833365
H	5.320885	-0.077599	-0.781281
H	4.208746	-1.342095	0.729472
H	3.453622	-1.990563	-0.721050
H	4.112613	-0.056020	-1.886725
C	0.823360	1.335129	0.893557
C	-0.437424	1.246355	0.014789
N	-0.850387	-0.022813	-0.257219
O	-1.012515	2.255803	-0.384233
H	2.747253	1.268317	-0.086428
H	1.033482	2.394594	1.043466
H	0.612182	0.872993	1.865801
C	-2.056244	-0.289209	-1.002027
C	-3.310338	-0.568557	-0.179057
O	-4.363838	-0.907501	-0.674666
O	-3.137514	-0.403215	1.150378
H	-0.337354	-0.789502	0.177056
H	-1.914868	-1.147767	-1.666991
H	-2.278318	0.581106	-1.627782
H	-3.997253	-0.589705	1.573320

Conf. 14	x	y	z
N	2.734909	-1.909626	-1.122470
C	3.183276	-1.355384	0.161492
C	2.466692	-0.053712	0.543646
N	1.728890	0.506409	-0.459390
O	2.579263	0.424585	1.668265
H	3.476553	-2.431090	-1.581554
H	4.248387	-1.107051	0.088290
H	3.077466	-2.039344	1.014032
H	1.950966	-2.547015	-0.999244
C	1.088024	1.802044	-0.341279
C	-0.443953	1.785770	-0.268752
N	-1.021304	0.572368	-0.078939
O	-1.088297	2.827233	-0.370045
H	1.795581	0.036313	-1.358498
H	1.361816	2.445677	-1.183705
H	1.454678	2.275985	0.574865
C	-2.450734	0.422627	0.049857
C	-2.802032	-1.046452	0.123721
O	-2.002517	-1.960074	0.094097
O	-4.133633	-1.230065	0.234453
H	-0.445243	-0.255890	0.012581
H	-2.972271	0.879946	-0.800334
H	-2.834111	0.926654	0.947762
H	-4.297466	-2.191019	0.285129

Table S2 continued

Conf. 15	x	y	z
N	-3.213584	-1.597591	-1.228824
C	-3.097962	-1.407082	0.223355
C	-2.403114	-0.093889	0.607577
N	-1.714992	0.502903	-0.408806
O	-2.451462	0.336736	1.756021
H	-3.163255	-2.580149	-1.482973
H	-2.485761	-2.214889	0.640933
H	-4.054725	-1.427019	0.760834
H	-4.097980	-1.239463	-1.581790
C	-1.056403	1.787096	-0.271390
C	0.476746	1.758806	-0.242789
N	1.056421	0.538209	-0.119826
O	1.121833	2.802221	-0.319555
H	-1.826102	0.065475	-1.319869
H	-1.390722	2.237058	0.668904
H	-1.347875	2.458069	-1.086131
C	2.489368	0.391904	-0.022018
C	2.846643	-1.074293	0.072271
O	2.050507	-1.990579	0.078353
O	4.181941	-1.251115	0.154174
H	0.485160	-0.294619	-0.035383
H	2.889623	0.915371	0.856838
H	2.992741	0.832662	-0.891926
H	4.349754	-2.210508	0.218777

Conf. 16	x	y	z
N	-4.010294	-0.563222	0.797711
C	-3.022390	-1.359471	0.061260
C	-1.834151	-0.522268	-0.409729
N	-2.006206	0.813774	-0.371715
O	-0.794217	-1.057786	-0.819000
H	-4.948008	-0.939603	0.691303
H	-3.492400	-1.772902	-0.838713
H	-2.609339	-2.208977	0.620882
H	-3.802003	-0.545117	1.793745
C	-0.934408	1.722343	-0.735223
C	0.309208	1.467804	0.135230
N	1.446037	1.151689	-0.553280
O	0.253494	1.544564	1.356338
H	-2.868263	1.144245	0.051507
H	-1.276417	2.743826	-0.551278
H	-0.706470	1.620570	-1.803280
C	2.657895	0.708807	0.108651
C	2.899220	-0.812040	0.129954
O	3.993406	-1.240874	0.422139
O	1.885134	-1.634485	-0.170300
H	1.368558	1.001272	-1.550979
H	2.610627	1.049489	1.146891
H	3.536722	1.165420	-0.354813
H	1.025456	-1.196313	-0.368545

Table S2 continued

Conf. 17	x	y	z
N	-3.989708	-0.725695	-0.757223
C	-2.917876	-1.378938	0.003381
C	-1.798511	-0.413721	0.403026
N	-1.802845	0.784823	-0.234786
O	-0.934071	-0.745068	1.219616
H	-4.750354	-0.428833	-0.150397
H	-2.455619	-2.157732	-0.614356
H	-3.250212	-1.872632	0.925644
H	-4.387800	-1.347989	-1.454803
C	-0.957850	1.894517	0.188453
C	0.555535	1.692921	0.036404
N	0.956643	0.678301	-0.783905
O	1.326993	2.430102	0.636487
H	-2.606601	0.944533	-0.837791
H	-1.117734	2.118641	1.248526
H	-1.243832	2.779826	-0.387104
C	2.336666	0.246835	-0.875399
C	2.683005	-1.043046	-0.110026
O	3.737892	-1.601384	-0.312060
O	1.801048	-1.518350	0.782235
H	0.241257	0.142659	-1.257667
H	2.961773	1.047943	-0.469937
H	2.627416	0.092161	-1.918372
H	0.972362	-0.994380	0.862403

Conf. 18	x	y	z
N	-3.838147	-0.918392	-1.036193
C	-3.088268	-1.334021	0.154554
C	-2.056963	-0.295624	0.602825
N	-1.828678	0.711323	-0.269470
O	-1.461921	-0.412513	1.682006
H	-4.722325	-0.480202	-0.789982
H	-2.529886	-2.250469	-0.068143
H	-3.713126	-1.556730	1.029460
H	-4.049026	-1.705948	-1.642234
C	-0.975284	1.855513	0.024412
C	0.535334	1.614584	-0.145393
N	1.021375	0.512948	0.518778
O	1.230142	2.367405	-0.814755
H	-2.372270	0.677242	-1.128383
H	-1.159291	2.175144	1.058312
H	-1.242799	2.672477	-0.646588
C	2.448662	0.245854	0.616871
C	2.912469	-1.002156	-0.146888
O	4.022749	-1.458561	-0.022800
O	2.002579	-1.552351	-0.980810
H	0.386695	0.073901	1.189966
H	2.747649	0.124087	1.662296
H	2.990546	1.103758	0.206566
H	1.177887	-1.031157	-0.910505

Table S2 continued

Conf. 19	x	y	z
N	-3.605282	-1.105299	-1.139838
C	-3.174526	-1.229980	0.257382
C	-2.079266	-0.229441	0.635248
N	-1.838387	0.740376	-0.275428
O	-1.475065	-0.320478	1.711619
H	-3.121071	-1.766137	-1.742692
H	-2.807219	-2.228065	0.529023
H	-4.020884	-1.018792	0.921142
H	-4.601142	-1.276477	-1.243646
C	-0.972441	1.885530	-0.021910
C	0.534184	1.621250	-0.189934
N	1.011235	0.540650	0.514273
O	1.234003	2.338358	-0.892499
H	-2.409846	0.700830	-1.115922
H	-1.148645	2.243039	1.000995
H	-1.233653	2.681210	-0.720261
C	2.435256	0.256492	0.610646
C	2.872718	-1.026429	-0.109806
O	3.977745	-1.494163	0.017819
O	1.943657	-1.594545	-0.910521
H	0.374947	0.134137	1.204281
H	2.741880	0.169673	1.657348
H	2.985895	1.090014	0.163488
H	1.128498	-1.057433	-0.847906

Conf. 20	x	y	z
N	-3.652995	1.537000	-1.071965
C	-3.693096	0.935230	0.266879
C	-2.688306	-0.211004	0.440380
N	-1.711260	-0.264166	-0.517291
O	-2.755590	-0.981580	1.391519
H	-3.868180	2.529738	-1.044681
H	-4.674398	0.539243	0.558091
H	-3.431132	1.696936	1.010632
H	-4.327559	1.100940	-1.696442
C	-0.779647	-1.370794	-0.612724
C	0.652299	-1.074172	-0.170863
N	0.883775	0.108831	0.434998
O	1.547867	-1.908026	-0.371038
H	-1.841603	0.375950	-1.297351
H	-0.729946	-1.743132	-1.640923
H	-1.146352	-2.184562	0.022441
C	2.160428	0.444136	1.064725
C	3.288753	0.786664	0.072516
O	3.878480	1.842774	0.113860
O	3.596520	-0.170576	-0.814034
H	0.100800	0.741251	0.541670
H	2.481462	-0.400874	1.687630
H	2.009274	1.313646	1.703922
H	3.010185	-0.961893	-0.693126

Table S2 continued

Extra	x	y	z
N	-2.326547	-1.715165	-1.170434
C	-2.618974	-1.345959	0.218107
C	-1.966368	-0.013694	0.587327
N	-1.736730	0.819958	-0.456599
O	-1.674184	0.265328	1.757026
H	-2.966633	-2.430601	-1.504878
H	-2.285660	-2.072872	0.970542
H	-3.703887	-1.229330	0.333007
H	-1.379251	-2.085838	-1.242913
C	-0.947584	2.038223	-0.322859
C	0.553126	1.709117	-0.341268
N	0.992078	1.031260	0.768200
O	1.280920	1.993249	-1.286846
H	-1.872365	0.405575	-1.375940
H	-1.228624	2.533230	0.611922
H	-1.160608	2.699780	-1.163537
C	2.224583	0.291264	0.709060
C	2.054784	-1.089458	0.051286
O	0.996667	-1.568565	-0.274826
O	3.204724	-1.788565	-0.126478
H	0.276256	0.720716	1.425299
H	2.620706	0.148304	1.722356
H	2.955080	0.874768	0.137412
H	3.980962	-1.264649	0.137636