

Table 1. Atomic coordinates (Å) for each conformers.

Alanine				
atom	No.	X	Y	Z
C	1	0	0	2.151
O	2	-0.046	-1.098	-0.023
C	3	0	0	0.578
O	4	0	1.105	-0.021
N	5	0.01	1.367	2.737
C	6	1.194	-0.781	2.675
H	7	-0.938	-0.491	2.503
H	8	-0.842	1.82	2.474
H	9	0.773	1.878	2.34
H	10	2.147	-0.317	2.387
H	11	1.191	-0.865	3.771
H	12	1.192	-1.8	2.265
Val-1				
atom	No.	X	Y	Z
C	1	0	0	2.155
O	2	-0.053	-1.097	-0.025
C	3	0	0	0.578
O	4	0	1.105	-0.02
N	5	0.013	1.369	2.732
C	6	1.166	-0.848	2.69
C	7	1.031	-1.119	4.181
C	8	2.527	-0.243	2.389
H	9	2.732	0.652	2.993
H	10	2.6	0.046	1.332
H	11	3.333	-0.96	2.596
H	12	0.076	-1.607	4.416
H	13	1.079	-0.194	4.772

H	14	-0.952	-0.474	2.496
H	15	-0.839	1.819	2.463
H	16	0.777	1.878	2.334
H	17	1.103	-1.828	2.151
H	18	1.832	-1.778	4.541
Val-2				
atom	No.	X	Y	Z
C	1	0	0	2.155
O	2	-0.046	-1.098	-0.035
C	3	0	0	0.578
O	4	0	1.099	-0.026
N	5	0.027	1.379	2.71
C	6	1.186	-0.82	2.702
C	7	1.072	-2.26	2.226
C	8	1.267	-0.784	4.222
H	9	0.333	-1.132	4.684
H	10	1.461	0.228	4.602
H	11	2.074	-1.432	4.589
H	12	0.734	-2.248	1.156
H	13	0.33	-2.824	2.805
H	14	-0.949	-0.471	2.507
H	15	-0.819	1.836	2.436
H	16	0.798	1.872	2.306
H	17	2.13	-0.384	2.29
H	18	2.026	-2.793	2.304
Val-3				
atom	No.	X	Y	Z
C	1	0	0	2.152
O	2	-0.051	-1.104	-0.025
C	3	0	0	0.578
O	4	0	1.096	-0.03

N	5	0.031	1.364	2.738
C	6	1.149	-0.856	2.724
C	7	2.516	-0.388	2.25
C	8	0.92	-2.302	2.305
H	9	0.607	-2.297	1.226
H	10	0.116	-2.768	2.887
H	11	1.817	-2.92	2.424
H	12	2.75	0.626	2.602
H	13	2.573	-0.378	1.153
H	14	-0.961	-0.46	2.488
H	15	-0.814	1.829	2.475
H	16	0.802	1.867	2.346
H	17	1.131	-0.789	3.841
H	18	3.314	-1.048	2.618
Val-4				
atom	No.	X	Y	Z
C	1	0	0	2.154
O	2	-0.063	-1.088	-0.04
C	3	0	0	0.578
O	4	0	1.109	-0.014
N	5	0.004	1.377	2.72
C	6	1.172	-0.787	2.776
C	7	2.497	-0.493	2.091
C	8	0.891	-2.282	2.743
H	9	0.747	-2.636	1.712
H	10	-0.017	-2.533	3.307
H	11	1.718	-2.855	3.183
H	12	2.763	0.57	2.161
H	13	2.458	-0.751	1.023
H	14	-0.953	-0.474	2.493
H	15	-0.849	1.823	2.45

H	16	0.766	1.887	2.318
H	17	1.269	-0.488	3.852
H	18	3.318	-1.066	2.544
Leu-1				
atom	No.	X	Y	Z
C	1	-0.139	-2.908	3.143
C	2	0	0	2.149
O	3	-0.04	-1.109	-0.022
C	4	0	0	0.578
O	5	0	1.093	-0.034
N	6	0.038	1.362	2.737
C	7	1.174	-0.83	2.682
C	8	0.97	-2.299	2.306
C	9	2.252	-3.09	2.455
H	10	-0.418	-3.905	2.781
H	11	2.629	-3.075	3.488
H	12	3.046	-2.69	1.811
H	13	2.103	-4.142	2.178
H	14	0.632	-2.263	1.203
H	15	-0.947	-0.49	2.503
H	16	-0.804	1.833	2.476
H	17	0.812	1.858	2.342
H	18	2.127	-0.461	2.253
H	19	1.276	-0.72	3.781
H	20	-1.033	-2.264	3.095
H	21	0.142	-3.007	4.201
Leu-2				
atom	No.	X	Y	Z
C	1	2.296	-1.857	4.668
C	2	0	0	2.153
O	3	-0.049	-1.097	-0.025

C	4	0	0	0.578
O	5	0	1.105	-0.019
N	6	0.012	1.37	2.73
C	7	1.191	-0.802	2.681
C	8	1.017	-1.226	4.143
C	9	-0.146	-2.193	4.283
H	10	2.184	-2.181	5.712
H	11	0.071	-3.162	3.813
H	12	-1.039	-1.779	3.784
H	13	-0.397	-2.383	5.334
H	14	0.796	-0.316	4.752
H	15	-0.941	-0.498	2.509
H	16	-0.84	1.821	2.465
H	17	0.775	1.879	2.33
H	18	1.321	-1.704	2.049
H	19	2.129	-0.221	2.574
H	20	3.137	-1.152	4.63
H	21	2.583	-2.739	4.08
Leu-3				
atom	No.	X	Y	Z
C	1	1.844	-2.777	4.086
C	2	0	0	2.149
O	3	-0.058	-1.092	-0.045
C	4	0	0	0.578
O	5	0	1.1	-0.024
N	6	0.004	1.379	2.712
C	7	1.2	-0.765	2.729
C	8	0.87	-2.227	3.054
C	9	0.892	-3.072	1.794
H	10	1.646	-3.837	4.292
H	11	1.917	-3.307	1.48

H	12	0.409	-2.499	0.953
H	13	0.365	-4.023	1.932
H	14	-0.158	-2.268	3.491
H	15	-0.948	-0.48	2.495
H	16	-0.851	1.824	2.445
H	17	0.764	1.888	2.308
H	18	2.052	-0.726	2.021
H	19	1.561	-0.27	3.655
H	20	1.775	-2.238	5.041
H	21	2.884	-2.701	3.742
Leu-4				
atom	No.	X	Y	Z
C	1	-0.154	-2.613	3.732
C	2	0	0	2.152
O	3	-0.05	-1.092	-0.035
C	4	0	0	0.578
O	5	0	1.107	-0.016
N	6	0.002	1.374	2.722
C	7	1.206	-0.764	2.713
C	8	0.96	-2.274	2.756
C	9	2.235	-3.008	3.136
H	10	-0.431	-3.673	3.68
H	11	2.606	-2.7	4.123
H	12	3.037	-2.817	2.411
H	13	2.075	-4.094	3.171
H	14	0.646	-2.594	1.729
H	15	-0.937	-0.501	2.514
H	16	-0.853	1.818	2.456
H	17	0.761	1.885	2.319
H	18	2.1	-0.558	2.091
H	19	1.461	-0.411	3.734

H	20	-1.05	-2.013	3.499
H	21	0.128	-2.395	4.771
Ile-1				
atom	No.	X	Y	Z
C	1	0	0	2.153
O	2	-0.052	-1.099	-0.035
C	3	0	0	0.578
O	4	0	1.097	-0.028
N	5	0.023	1.382	2.704
C	6	1.186	-0.812	2.719
C	7	1.103	-2.258	2.225
C	8	1.216	-0.776	4.241
C	9	2.428	-2.977	2.286
H	10	2.826	-3.04	3.309
H	11	3.189	-2.475	1.674
H	12	2.336	-4.005	1.911
H	13	0.275	-1.145	4.673
H	14	1.376	0.239	4.627
H	15	2.025	-1.407	4.638
H	16	0.709	-2.216	1.158
H	17	0.343	-2.814	2.806
H	18	-0.949	-0.472	2.503
H	19	-0.825	1.835	2.429
H	20	0.792	1.876	2.299
H	21	2.134	-0.36	2.335
Ile-2				
atom	No.	X	Y	Z
C	1	0	0	2.154
O	2	-0.053	-1.097	-0.025
C	3	0	0	0.578
O	4	0	1.105	-0.019

N	5	0.012	1.369	2.731
C	6	1.161	-0.854	2.694
C	7	0.966	-1.205	4.172
C	8	2.521	-0.207	2.486
C	9	-0.239	-2.096	4.377
H	10	-0.08	-3.099	3.959
H	11	-1.119	-1.668	3.867
H	12	-0.485	-2.215	5.439
H	13	2.688	0.646	3.158
H	14	2.626	0.156	1.455
H	15	3.333	-0.923	2.672
H	16	0.858	-0.278	4.769
H	17	1.875	-1.706	4.561
H	18	-0.951	-0.484	2.506
H	19	-0.841	1.817	2.463
H	20	0.775	1.879	2.332
H	21	1.142	-1.807	2.106
Ile-3				
atom	No.	X	Y	Z
C	1	0	0	2.156
O	2	-0.054	-1.097	-0.024
C	3	0	0	0.578
O	4	0	1.105	-0.019
N	5	0.014	1.369	2.733
C	6	1.161	-0.854	2.69
C	7	1.046	-1.095	4.198
C	8	2.529	-0.279	2.355
C	9	2.02	-2.157	4.663
H	10	3.034	-1.942	4.283
H	11	1.743	-3.153	4.294
H	12	2.073	-2.213	5.757



H	13	2.698	0.707	2.809
H	14	2.655	-0.171	1.27
H	15	3.322	-0.945	2.735
H	16	0.012	-1.397	4.455
H	17	1.227	-0.149	4.747
H	18	-0.955	-0.47	2.494
H	19	-0.837	1.819	2.465
H	20	0.778	1.879	2.335
H	21	1.074	-1.845	2.174
Ile-4				
atom	No.	X	Y	Z
C	1	0	0	2.152
O	2	-0.05	-1.105	-0.024
C	3	0	0	0.578
O	4	0	1.096	-0.03
N	5	0.027	1.363	2.74
C	6	1.149	-0.856	2.723
C	7	2.522	-0.386	2.233
C	8	0.914	-2.304	2.309
C	9	3.647	-1.159	2.886
H	10	3.487	-2.244	2.769
H	11	3.713	-0.954	3.963
H	12	4.62	-0.912	2.444
H	13	0.585	-2.301	1.236
H	14	0.128	-2.775	2.909
H	15	1.828	-2.907	2.415
H	16	2.653	0.696	2.433
H	17	2.57	-0.495	1.13
H	18	-0.959	-0.463	2.488
H	19	-0.819	1.827	2.476
H	20	0.798	1.869	2.349

H	21	1.14	-0.782	3.839
Ile-5				
atom	No.	X	Y	Z
C	1	0	0	2.154
O	2	-0.061	-1.089	-0.04
C	3	0	0	0.578
O	4	0	1.108	-0.014
N	5	0.002	1.376	2.721
C	6	1.171	-0.789	2.775
C	7	2.494	-0.53	2.051
C	8	0.862	-2.28	2.782
C	9	3.664	-1.149	2.786
H	10	3.463	-2.21	3.009
H	11	3.858	-0.648	3.744
H	12	4.587	-1.097	2.196
H	13	0.583	-2.634	1.78
H	14	0.036	-2.519	3.463
H	15	1.745	-2.855	3.109
H	16	2.657	0.559	1.936
H	17	2.429	-0.932	1.019
H	18	-0.952	-0.476	2.493
H	19	-0.852	1.821	2.452
H	20	0.763	1.889	2.32
H	21	1.297	-0.465	3.84
Ile-6				
atom	No.	X	Y	Z
C	1	0	0	2.154
O	2	-0.039	-1.101	-0.032
C	3	0	0	0.578
O	4	0	1.097	-0.028
N	5	0.038	1.374	2.716

C	6	1.174	-0.854	2.677
C	7	0.914	-2.313	2.289
C	8	1.411	-0.703	4.171
C	9	-0.22	-2.943	3.062
H	10	-1.094	-2.269	3.059
H	11	0.04	-3.142	4.111
H	12	-0.528	-3.896	2.615
H	13	0.49	-0.86	4.749
H	14	1.788	0.296	4.426
H	15	2.15	-1.434	4.528
H	16	1.835	-2.912	2.4
H	17	0.643	-2.278	1.184
H	18	-0.949	-0.481	2.514
H	19	-0.804	1.838	2.443
H	20	0.814	1.862	2.316
H	21	2.105	-0.525	2.151

Table 2. The perturbation strength ( $\text{\AA}^{-1}$ ) calculated for each bond from four sets of bond polarizability values, together with their position ( $\text{\AA}$ ) and orientation (degree) parameters. Bonds with bold character are the most effective perturbors.

Bond	No. <sup>a</sup>	<i>X</i>	<i>Y</i>	<i>Z</i>	<i>R</i>	$\theta$	$\phi$	Debign	LeFevre	Allen	Amos
Ala1											
$\alpha$ CH	1-7	-	-0.25	2.33	2.39	108.35	27.65	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	0.60	-0.39	2.41	2.52	110.16	146.80	0.004	-0.001	-0.001	-0.003
$\beta$ CH	6-11	1.19	-0.82	3.22	3.53	175.62	88.27	-0.004	-0.003	-0.004	-0.004
<b><math>\beta</math>CH</b>	<b>6-12</b>	<b>1.19</b>	<b>-1.29</b>	<b>2.47</b>	<b>3.03</b>	<b>68.06</b>	<b>89.91</b>	<b>-0.010</b>	<b>-0.010</b>	<b>-0.011</b>	<b>-0.009</b>
$\beta$ CH	6-10	1.67	-0.55	2.53	3.08	74.78	205.98	-0.005	-0.006	-0.006	-0.004
Val1											

$\alpha$ CH	1-14	1.58	-0.48	-0.24	1.66	72.43	140.50	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.58	-0.42	1.30	70.90	208.41	0.004	-0.001	-0.001	-0.003
<b><math>\beta</math>CH</b>	<b>6-17</b>	<b>1.85</b>	<b>1.13</b>	<b>-1.34</b>	<b>2.55</b>	<b>59.93</b>	<b>177.86</b>	<b>-0.011</b>	<b>-0.011</b>	<b>-0.012</b>	<b>-0.010</b>
$\beta$ CC1	6-8	1.35	1.85	-0.55	2.35	101.36	206.84	0.001	-0.001	-0.002	-0.003
$\beta$ CC2	6-7	1.35	1.10	-0.98	2.00	84.27	177.13	-0.006	-0.003	-0.003	-0.002
$\gamma$ 1CH	8-9	1.66	2.63	0.19	3.12	124.63	188.61	0.000	0.001	0.001	-0.000
$\gamma$ 1CH	8-10	1.66	2.57	-0.11	3.06	103.50	182.92	-0.000	-0.001	-0.001	0.000
$\gamma$ 1CH	8-11	1.66	2.93	-0.62	3.43	66.01	211.22	-0.002	-0.002	-0.002	-0.002
$\gamma$ 2CH	7-18	2.59	1.43	-1.45	3.30	78.63	194.14	-0.001	-0.001	-0.001	-0.001
$\gamma$ 2CH	7-12	2.59	0.55	-1.36	2.98	81.65	163.29	-0.001	-0.001	-0.001	-0.000
$\gamma$ 2CH	7-13	2.59	1.06	-0.66	2.87	106.20	180.87	-0.001	-0.000	-0.001	-0.001
Val2											
$\alpha$ CH	1-14	1.58	-0.47	-0.24	1.66	72.50	140.59	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.59	-0.41	1.30	71.57	208.84	0.004	-0.001	-0.001	-0.003
$\beta$ CH	6-17	1.85	1.66	-0.60	2.56	102.60	208.99	-0.006	-0.006	-0.007	-0.005
$\beta$ CC1	6-8	1.35	1.23	-0.80	1.99	90.76	181.70	-0.006	-0.003	-0.003	-0.002
$\beta$ CC2	6-7	1.35	1.13	-1.54	2.34	61.96	177.59	-0.002	-0.005	-0.006	-0.006
$\gamma$ 1CH	8-9	2.61	0.80	-0.96	2.89	84.06	163.84	-0.001	-0.000	-0.001	-0.000
$\gamma$ 1CH	8-10	2.61	1.36	-0.28	2.96	107.39	183.45	-0.000	-0.000	-0.000	-0.000
$\gamma$ 1CH	8-11	2.61	1.67	-1.11	3.29	78.95	194.07	-0.001	-0.001	-0.001	-0.001
$\gamma$ 2CH	7-18	1.61	1.55	-2.53	3.37	71.06	217.90	-0.005	-0.006	-0.006	-0.004
<b><math>\gamma</math>2CH</b>	<b>7-12</b>	<b>1.61</b>	<b>0.90</b>	<b>-2.25</b>	<b>2.91</b>	<b>90.55</b>	<b>164.57</b>	<b>-0.013</b>	<b>-0.011</b>	<b>-0.013</b>	<b>-0.013</b>
$\gamma$ 2CH	7-13	1.61	0.70	-2.54	3.09	68.50	148.81	-0.004	-0.003	-0.004	-0.004
Val3											
$\alpha$ CH	1-14	1.58	-0.48	-0.23	1.66	72.95	140.16	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.57	-0.43	1.29	70.65	208.09	0.004	-0.001	-0.001	-0.003
$\beta$ CH	6-17	1.86	1.14	-0.82	2.33	92.25	179.40	-0.003	-0.003	-0.003	-0.004
$\beta$ CC1	6-8	1.36	1.03	-1.58	2.33	62.13	175.19	-0.001	-0.004	-0.005	-0.005
$\beta$ CC2	6-7	1.36	1.83	-0.62	2.37	98.74	206.65	0.001	-0.002	-0.003	-0.003
<b><math>\gamma</math>1CH</b>	<b>8-9</b>	<b>1.65</b>	<b>0.76</b>	<b>-2.30</b>	<b>2.93</b>	<b>90.23</b>	<b>166.51</b>	<b>-0.010</b>	<b>-0.009</b>	<b>-0.011</b>	<b>-0.011</b>
$\gamma$ 1CH	8-10	1.65	0.52	-2.54	3.07	73.07	148.38	-0.003	-0.002	-0.003	-0.003

$\gamma$ 1CH	8-11	1.65	1.37	-2.61	3.38	68.69	214.51	-0.004	-0.005	-0.005	-0.004
$\gamma$ 2CH	7-18	1.62	2.91	-0.72	3.41	66.01	212.55	-0.002	-0.003	-0.003	-0.002
$\gamma$ 2CH	7-12	1.62	2.63	0.12	3.10	128.56	190.59	0.000	0.001	0.001	-0.000
$\gamma$ 2CH	7-13	1.62	2.54	-0.38	3.04	90.45	182.61	-0.005	-0.004	-0.005	-0.005
Val4											
$\alpha$ CH	1-14	1.58	-0.48	-0.24	1.66	72.42	140.46	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.59	-0.39	1.29	72.20	208.54	0.004	-0.000	-0.001	-0.002
$\beta$ CH	6-17	1.89	1.22	-0.64	2.34	99.54	183.13	-0.003	-0.002	-0.003	-0.003
$\beta$ CC1	6-8	1.39	1.03	-1.53	2.31	61.82	174.22	-0.000	-0.003	-0.003	-0.004
$\beta$ CC2	6-7	1.39	1.83	-0.64	2.39	95.47	205.51	-0.000	-0.003	-0.003	-0.004
$\gamma$ 1CH	8-9	1.87	0.82	-2.46	3.20	78.56	175.27	-0.006	-0.005	-0.006	-0.006
$\gamma$ 1CH	8-10	1.87	0.44	-2.41	3.08	82.73	152.49	-0.002	-0.002	-0.002	-0.002
$\gamma$ 1CH	8-11	1.87	1.30	-2.57	3.44	73.45	205.39	-0.003	-0.003	-0.003	-0.003
$\gamma$ 2CH	7-18	1.55	2.91	-0.78	3.38	67.23	216.96	-0.003	-0.003	-0.003	-0.003
$\gamma$ 2CH	7-12	1.55	2.63	0.04	3.05	133.43	193.71	0.000	0.000	0.000	-0.000
<b><math>\gamma</math>2CH</b>	<b>7-13</b>	<b>1.55</b>	<b>2.48</b>	<b>-0.62</b>	<b>2.99</b>	<b>76.68</b>	<b>177.95</b>	<b>-0.010</b>	<b>-0.007</b>	<b>-0.009</b>	<b>-0.011</b>
Leu1											
$\alpha$ CH	2-15	1.57	-0.47	-0.24	1.66	71.79	140.51	0.003	0.004	0.004	0.002
$\alpha$ CC	2-7	1.07	0.59	-0.41	1.29	71.28	208.65	0.004	-0.001	-0.001	-0.003
$\beta$ CH	7-18	1.84	1.65	-0.65	2.56	100.79	209.55	-0.006	-0.007	-0.008	-0.005
$\beta$ CH	7-19	1.84	1.22	-0.77	2.34	93.74	183.46	-0.003	-0.003	-0.003	-0.004
$\beta$ CC	7-8	1.34	1.07	-1.56	2.32	61.36	175.65	-0.001	-0.004	-0.005	-0.005
<b><math>\gamma</math> CH</b>	<b>8-14</b>	<b>1.65</b>	<b>0.80</b>	<b>-2.28</b>	<b>2.93</b>	<b>91.51</b>	<b>165.48</b>	<b>-0.011</b>	<b>-0.010</b>	<b>-0.011</b>	<b>-0.011</b>
$\gamma$ CC1	8-1	1.15	0.42	-2.60	2.88	76.61	154.32	-0.007	-0.003	-0.003	-0.002
$\gamma$ CC2	8-9	1.15	1.61	-2.69	3.34	73.31	209.07	-0.001	-0.002	-0.002	-0.003
$\delta$ 1CH	1-20	2.07	-0.59	-2.59	3.36	105.51	157.36	0.001	0.002	0.002	0.001
$\delta$ 1CH	1-21	2.07	0.00	-2.96	3.61	87.37	187.47	0.000	-0.000	0.000	0.000
$\delta$ 2CH	1-10	2.07	-0.28	-3.41	4.00	65.24	172.59	0.000	0.000	0.001	0.000
$\delta$ 2CH	9-11	1.73	2.44	-3.08	4.29	90.57	194.52	-0.002	-0.002	-0.002	-0.003
$\delta$ 2CH	9-12	1.73	2.65	-2.89	4.28	103.58	208.60	-0.003	-0.003	-0.003	-0.003
$\delta$ 2CH	9-13	1.73	2.18	-3.62	4.56	54.29	174.14	-0.002	-0.002	-0.002	-0.001

Leu2											
$\alpha$ CH	2-15	1.58	-0.47	-0.25	1.66	71.50	140.79	0.003	0.004	0.004	0.002
$\alpha$ CC	2-7	1.08	0.60	-0.40	1.29	71.95	208.94	0.004	-0.001	-0.001	-0.003
<b><math>\beta</math>CH</b>	<b>7-18</b>	<b>1.84</b>	<b>1.26</b>	<b>-1.25</b>	<b>2.56</b>	<b>61.84</b>	<b>184.43</b>	<b>-0.012</b>	<b>-0.012</b>	<b>-0.014</b>	<b>-0.012</b>
$\beta$ CH	7-19	1.84	1.66	-0.51	2.53	106.77	209.18	-0.004	-0.005	-0.005	-0.003
$\beta$ CC	7-8	1.34	1.10	-1.01	2.01	81.03	176.30	-0.006	-0.003	-0.003	-0.003
$\gamma$ CH	8-14	2.57	0.91	-0.77	2.83	106.11	175.97	-0.001	-0.000	-0.001	-0.001
$\gamma$ CC1	8-1	2.07	1.66	-1.54	3.07	81.71	197.15	0.000	-0.000	-0.000	-0.001
$\gamma$ CC2	8-9	2.07	0.44	-1.71	2.72	77.33	164.31	-0.000	-0.000	-0.000	-0.000
$\delta$ 1CH	1-20	2.83	2.72	-1.50	4.20	100.61	192.91	-0.001	-0.001	-0.001	-0.001
$\delta$ 1CH	1-21	2.83	2.44	-2.30	4.39	76.52	184.47	-0.001	-0.001	-0.001	-0.001
$\delta$ 2CH	1-10	2.83	2.24	-2.02	4.14	84.96	178.26	-0.001	-0.001	-0.001	-0.001
$\delta$ 2CH	9-11	2.64	-0.04	-2.68	3.76	73.60	183.79	0.000	0.000	0.000	-0.000
$\delta$ 2CH	9-12	2.64	-0.59	-1.99	3.36	96.94	164.79	0.001	0.001	0.001	0.001
$\delta$ 2CH	9-13	2.64	-0.27	-2.29	3.51	86.71	175.64	0.000	0.000	0.000	0.000
Leu3											
$\alpha$ CH	2-15	1.57	-0.47	-0.24	1.66	72.15	140.50	0.003	0.004	0.004	0.002
$\alpha$ CC	2-7	1.07	0.60	-0.38	1.29	72.74	209.17	0.004	-0.001	-0.001	-0.002
<b><math>\beta</math>CH</b>	<b>7-18</b>	<b>1.86</b>	<b>1.63</b>	<b>-0.75</b>	<b>2.58</b>	<b>91.16</b>	<b>206.23</b>	<b>-0.009</b>	<b>-0.009</b>	<b>-0.010</b>	<b>-0.008</b>
$\beta$ CH	7-19	1.86	1.38	-0.52	2.38	105.65	191.80	-0.003	-0.002	-0.003	-0.003
$\beta$ CC	7-8	1.36	1.04	-1.50	2.27	61.99	173.11	-0.001	-0.003	-0.003	-0.003
$\gamma$ CH	8-14	2.03	0.36	-2.25	3.05	88.97	153.40	-0.001	-0.001	-0.001	-0.001
$\gamma$ CC1	8-1	1.53	1.36	-2.50	3.23	80.25	197.68	-0.002	-0.001	-0.002	-0.001
$\gamma$ CC2	8-9	1.53	0.88	-2.65	3.18	74.52	180.40	-0.004	-0.003	-0.004	-0.003
$\delta$ 1CH	1-20	2.54	1.81	-2.51	4.00	99.90	178.73	-0.001	-0.001	-0.001	-0.001
$\delta$ 1CH	1-21	2.54	2.36	-2.74	4.42	91.35	198.63	-0.001	-0.001	-0.001	-0.001
$\delta$ 2CH	1-10	2.54	1.74	-3.31	4.52	71.08	176.33	-0.001	-0.001	-0.001	-0.001
$\delta$ 2CH	9-11	1.40	1.40	-3.19	3.75	79.74	232.24	-0.004	-0.004	-0.004	-0.003
$\delta$ 2CH	9-12	1.40	0.65	-2.79	3.18	121.67	148.71	-0.005	-0.005	-0.006	-0.005
$\delta$ 2CH	9-13	1.40	0.63	-3.55	3.86	45.06	146.44	-0.001	-0.001	-0.002	-0.001
Leu4											

$\alpha$ CH	2-15	1.58	-0.47	-0.25	1.66	71.35	140.89	0.003	0.004	0.004	0.002
$\alpha$ CC	2-7	1.08	0.60	-0.38	1.29	72.79	209.26	0.004	-0.001	-0.001	-0.002
<b><math>\beta</math>CH</b>	<b>7-18</b>	<b>1.86</b>	<b>1.65</b>	<b>-0.66</b>	<b>2.57</b>	<b>96.10</b>	<b>207.57</b>	<b>-0.007</b>	<b>-0.008</b>	<b>-0.009</b>	<b>-0.007</b>
$\beta$ CH	7-19	1.86	1.33	-0.59	2.36	101.54	188.47	-0.003	-0.002	-0.003	-0.003
$\beta$ CC	7-8	1.36	1.08	-1.52	2.31	61.00	174.83	-0.000	-0.003	-0.003	-0.004
$\gamma$ CH	8-14	1.88	0.80	-2.43	3.18	79.82	169.87	-0.006	-0.005	-0.006	-0.005
$\gamma$ CC1	8-1	1.38	0.40	-2.44	2.83	83.50	157.99	-0.005	-0.002	-0.002	-0.002
$\gamma$ CC2	8-9	1.38	1.60	-2.64	3.38	76.41	204.83	-0.001	-0.002	-0.002	-0.002
$\delta$ 1CH	1-20	2.37	-0.60	-2.31	3.36	101.79	161.85	0.001	0.001	0.001	0.001
$\delta$ 1CH	1-21	2.37	-0.01	-2.50	3.45	94.53	185.90	0.000	0.000	0.000	0.000
$\delta$ 2CH	1-10	2.37	-0.29	-3.14	3.94	68.89	174.20	0.000	0.000	0.000	0.000
$\delta$ 2CH	9-11	2.07	2.42	-2.85	4.28	98.08	189.85	-0.002	-0.002	-0.002	-0.002
$\delta$ 2CH	9-12	2.07	2.64	-2.91	4.44	94.78	200.58	-0.002	-0.002	-0.003	-0.002
$\delta$ 2CH	9-13	2.07	2.15	-3.55	4.64	63.12	175.71	-0.001	-0.001	-0.002	-0.001
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Ile1											
$\alpha$ CH	1-18	1.58	-0.47	-0.24	1.66	72.46	140.54	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.59	-0.41	1.29	71.72	208.84	0.004	-0.001	-0.001	-0.002
$\beta$ CH	6-21	1.86	1.66	-0.59	2.56	102.95	208.88	-0.005	-0.006	-0.006	-0.004
$\beta$ CC1	6-8	1.36	1.20	-0.79	1.98	90.75	180.63	-0.006	-0.003	-0.003	-0.002
$\beta$ CC2	6-7	1.36	1.14	-1.54	2.35	62.00	178.26	-0.002	-0.005	-0.006	-0.006
$\gamma$ 1CH	8-13	2.62	0.75	-0.96	2.89	83.76	163.82	-0.000	-0.000	-0.001	-0.000
$\gamma$ 1CH	8-14	2.62	1.30	-0.27	2.94	107.37	182.83	-0.000	-0.000	-0.000	-0.000
$\gamma$ 1CH	8-15	2.62	1.62	-1.09	3.27	79.32	194.01	-0.001	-0.001	-0.001	-0.001
<b><math>\gamma</math>2CH</b>	<b>7-16</b>	<b>1.61</b>	<b>0.91</b>	<b>-2.24</b>	<b>2.90</b>	<b>91.89</b>	<b>162.18</b>	<b>-0.013</b>	<b>-0.011</b>	<b>-0.013</b>	<b>-0.013</b>
$\gamma$ 2CH	7-17	1.61	0.72	-2.54	3.09	68.92	148.16	-0.004	-0.003	-0.004	-0.004
$\gamma$ 2CC	7-9	1.11	1.77	-2.62	3.35	74.48	210.78	-0.000	-0.002	-0.003	-0.003
$\delta$ CH	9-10	1.64	2.63	-3.01	4.32	87.36	197.19	-0.003	-0.002	-0.003	-0.003
$\delta$ CH	9-11	1.64	2.81	-2.73	4.24	108.59	210.62	-0.003	-0.003	-0.003	-0.003
$\delta$ CH	9-12	1.64	2.38	-3.49	4.53	51.43	175.92	-0.002	-0.002	-0.002	-0.001
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Ile2											
$\alpha$ CH	1-18	1.58	-0.48	-0.24	1.66	72.07	140.52	0.003	0.004	0.004	0.002

$\alpha$ CC	1-6	1.08	0.58	-0.43	1.30	70.77	208.33	0.004	-0.001	-0.001	-0.003
<b><math>\beta</math>CH</b>	<b>6-21</b>	<b>1.85</b>	<b>1.15</b>	<b>-1.33</b>	<b>2.55</b>	<b>60.63</b>	<b>179.36</b>	<b>-0.011</b>	<b>-0.011</b>	<b>-0.013</b>	<b>-0.011</b>
$\beta$ CC1	6-8	1.35	1.84	-0.53	2.34	102.09	206.78	0.001	-0.001	-0.002	-0.002
$\beta$ CC2	6-7	1.35	1.06	-1.03	2.00	82.59	175.86	-0.006	-0.003	-0.003	-0.002
$\gamma$ 1CH	8-13	1.74	2.60	0.22	3.14	119.69	186.42	0.000	0.001	0.001	-0.000
$\gamma$ 1CH	8-14	1.74	2.57	-0.03	3.11	103.68	184.04	0.001	-0.000	0.000	0.001
$\gamma$ 1CH	8-15	1.74	2.93	-0.57	3.45	67.08	208.66	-0.002	-0.002	-0.002	-0.001
$\gamma$ 2CH	7-16	2.59	0.91	-0.74	2.84	106.28	178.05	-0.001	-0.000	-0.001	-0.001
$\gamma$ 2CH	7-17	2.59	1.42	-1.46	3.29	81.37	195.99	-0.001	-0.001	-0.001	-0.001
$\gamma$ 2CC	7-9	2.09	0.36	-1.65	2.68	78.40	163.89	-0.000	-0.000	-0.000	-0.000
$\delta$ CH	9-10	2.69	-0.16	-2.60	3.74	73.48	182.70	0.000	0.000	0.000	0.000
$\delta$ CH	9-11	2.69	-0.68	-1.88	3.35	96.99	165.39	0.001	0.001	0.001	0.001
$\delta$ CH	9-12	2.69	-0.36	-2.16	3.46	87.99	175.84	0.000	0.000	0.000	0.000
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Ile3											
$\alpha$ CH	1-18	1.58	-0.48	-0.24	1.67	72.59	140.42	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.58	-0.43	1.30	70.77	208.31	0.004	-7.6E-4	-0.001	-0.003
<b><math>\beta</math>CH</b>	<b>6-21</b>	<b>1.84</b>	<b>1.12</b>	<b>-1.35</b>	<b>2.54</b>	<b>59.64</b>	<b>177.04</b>	<b>-0.011</b>	<b>-0.011</b>	<b>-0.012</b>	<b>-0.010</b>
$\beta$ CC1	6-8	1.34	1.84	-0.57	2.35	100.79	206.95	0.001	-0.002	-0.002	-0.003
$\beta$ CC2	6-7	1.34	1.10	-0.97	1.99	84.89	177.55	-0.006	-0.003	-0.003	-0.002
$\gamma$ 1CH	8-13	1.68	2.61	0.21	3.11	125.82	187.11	0.000	0.001	0.001	-0.000
$\gamma$ 1CH	8-14	1.68	2.59	-0.23	3.10	94.51	185.33	-0.002	-0.002	-0.002	-0.002
$\gamma$ 1CH	8-15	1.68	2.93	-0.61	3.43	67.02	210.37	-0.002	-0.002	-0.002	-0.001
$\gamma$ 2CH	7-16	2.60	0.53	-1.25	2.93	84.87	162.07	-0.000	-0.000	-0.001	-0.000
$\gamma$ 2CH	7-17	2.60	1.14	-0.62	2.90	106.44	183.23	-0.000	-0.000	-0.001	-0.001
$\gamma$ 2CC	7-9	2.10	1.53	-1.63	3.07	76.16	193.07	0.000	-0.000	-0.000	-0.001
$\delta$ CH	9-10	2.83	2.53	-2.05	4.31	93.24	195.46	-0.001	-0.001	-0.001	-0.001
$\delta$ CH	9-11	2.83	1.88	-2.65	4.31	74.83	175.67	-0.001	-0.001	-0.001	-0.001
$\delta$ CH	9-12	2.83	2.05	-2.18	4.12	89.12	180.83	-0.001	-0.001	-0.001	-0.001
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Ile4											
$\alpha$ CH	1-18	1.58	-0.48	-0.23	1.66	72.84	140.20	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.57	-0.43	1.29	70.66	208.11	0.004	-0.001	-0.001	-0.003



$\beta$ CH	6-21	1.86	1.14	-0.82	2.33	92.48	179.70	-0.003	-0.003	-0.003	-0.004
$\beta$ CC1	6-8	1.36	1.03	-1.58	2.33	62.10	175.05	-0.001	-0.004	-0.005	-0.005
$\beta$ CC2	6-7	1.36	1.84	-0.62	2.37	98.78	206.75	0.001	-0.002	-0.003	-0.003
<b><math>\gamma</math>1CH</b>	<b>8-13</b>	<b>1.65</b>	<b>0.75</b>	<b>-2.30</b>	<b>2.93</b>	<b>90.09</b>	<b>165.89</b>	<b>-0.010</b>	<b>-0.009</b>	<b>-0.010</b>	<b>-0.010</b>
$\gamma$ 1CH	8-14	1.65	0.52	-2.54	3.08	72.84	149.02	-0.003	-0.002	-0.003	-0.003
$\gamma$ 1CH	8-15	1.65	1.37	-2.61	3.38	69.30	214.92	-0.005	-0.005	-0.005	-0.004
$\gamma$ 2CH	7-16	1.62	2.59	0.16	3.05	131.11	186.06	0.001	0.001	0.001	0.001
$\gamma$ 2CH	7-17	1.62	2.55	-0.44	3.05	84.91	182.26	-0.006	-0.005	-0.006	-0.007
$\gamma$ 2CC	7-9	1.12	3.08	-0.77	3.37	72.82	206.74	-0.001	-0.001	-0.001	-0.001
$\delta$ CH	9-10	1.94	3.57	-1.70	4.40	60.18	175.14	-0.002	-0.002	-0.002	-0.001
$\delta$ CH	9-11	1.94	3.68	-1.06	4.29	96.17	182.01	-0.001	-0.001	-0.001	-0.001
$\delta$ CH	9-12	1.94	4.13	-1.04	4.68	96.63	207.28	-0.001	-0.001	-0.001	-0.000
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Ile5											
$\alpha$ CH	1-18	1.58	-0.48	-0.24	1.66	72.37	140.48	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.59	-0.39	1.29	72.15	208.52	0.004	-0.000	-0.001	-0.002
$\beta$ CH	6-21	1.89	1.23	-0.63	2.34	100.34	184.07	-0.003	-0.002	-0.003	-0.003
$\beta$ CC1	6-8	1.39	1.02	-1.53	2.31	61.90	173.66	-0.000	-0.003	-0.003	-0.004
$\beta$ CC2	6-7	1.39	1.83	-0.66	2.39	94.82	205.50	-0.001	-0.003	-0.004	-0.004
$\gamma$ 1CH	8-13	1.89	0.72	-2.46	3.18	78.90	171.11	-0.005	-0.005	-0.005	-0.005
$\gamma$ 1CH	8-14	1.89	0.45	-2.40	3.09	83.06	155.12	-0.002	-0.001	-0.002	-0.002
$\gamma$ 1CH	8-15	1.89	1.30	-2.57	3.45	73.87	206.36	-0.003	-0.003	-0.003	-0.002
$\gamma$ 2CH	7-16	1.53	2.58	0.01	2.99	135.68	188.82	0.000	0.000	0.000	0.001
<b><math>\gamma</math>2CH</b>	<b>7-17</b>	<b>1.53</b>	<b>2.46</b>	<b>-0.73</b>	<b>2.99</b>	<b>69.12</b>	<b>176.47</b>	<b>-0.011</b>	<b>-0.008</b>	<b>-0.010</b>	<b>-0.013</b>
$\gamma$ 2CC	7-9	1.03	3.08	-0.84	3.35	75.33	209.70	-0.002	-0.002	-0.002	-0.002
$\delta$ CH	9-10	1.89	3.56	-1.68	4.37	59.43	173.58	-0.001	-0.002	-0.002	-0.001
$\delta$ CH	9-11	1.89	3.76	-0.90	4.31	105.56	186.18	-0.001	-0.001	-0.001	-0.001
$\delta$ CH	9-12	1.89	4.13	-1.12	4.68	91.46	207.32	-0.001	-0.001	-0.001	-0.001
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Ile6											
$\alpha$ CH	1-18	1.58	-0.47	-0.24	1.66	72.17	140.57	0.003	0.004	0.004	0.002
$\alpha$ CC	1-6	1.08	0.59	-0.43	1.30	70.82	208.60	0.004	-0.001	-0.002	-0.003
$\beta$ CH	6-21	1.84	1.64	-0.69	2.56	99.71	209.03	-0.007	-0.008	-0.009	-0.006

$\beta$ CC1	6-8	1.34	1.29	-0.78	2.02	93.21	185.05	-0.006	-0.003	-0.003	-0.002
$\beta$ CC2	6-7	1.34	1.04	-1.58	2.32	61.52	174.44	-0.001	-0.004	-0.005	-0.005
$\gamma$ 1CH	8-13	2.59	0.95	-0.78	2.86	87.27	163.81	-0.001	-0.000	-0.001	-0.001
$\gamma$ 1CH	8-14	2.59	1.60	-0.20	3.05	107.37	186.77	-0.000	-0.000	-0.000	-0.000
$\gamma$ 1CH	8-15	2.59	1.78	-1.07	3.32	77.35	193.12	-0.001	-0.001	-0.001	-0.001
$\gamma$ 2CH	7-16	1.64	1.37	-2.61	3.38	69.28	215.56	-0.005	-0.005	-0.005	-0.004
<b><math>\gamma</math>2CH</b>	<b>7-17</b>	<b>1.64</b>	<b>0.78</b>	<b>-2.30</b>	<b>2.93</b>	<b>91.50</b>	<b>168.16</b>	<b>-0.011</b>	<b>-0.009</b>	<b>-0.011</b>	<b>-0.012</b>
$\gamma$ 2CC	7-9	1.14	0.35	-2.63	2.89	76.14	153.64	-0.006	-0.003	-0.003	-0.002
$\delta$ CH	9-10	2.03	-0.66	-2.61	3.37	106.76	157.04	0.002	0.002	0.002	0.001
$\delta$ CH	9-11	2.03	-0.09	-3.04	3.66	84.53	187.21	0.000	0.000	0.000	0.000
$\delta$ CH	9-12	2.03	-0.37	-3.42	3.99	65.43	171.51	0.001	0.001	0.001	0.001

<sup>a</sup>Bonds as defined by numbers given to individual atoms in Table 1.