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Supplementary Information

Impact of aza-substitutions on the preference of helix handedness for β-peptide oligomers: a DFT study

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Page	Contents
s1−s2	Table of Contents
s3	Table S1. Absolute electronic energies, single-point energies, and solvation free energies of (*M*)- and (*P*)-helices of pentamers for *c*-ACHC and their aza-analogues
s3	Table S2. Relative single-point energies, solvation free energies, conformational energies, and populations of (*M*)- and (*P*)-helices of pentamers for *c*-ACHC and their aza-analogues
s4	Table S3. Absolute electronic energies, single-point energies, and solvation free energies of (*M*)- and (*P*)-helices of pentamers for *c*-ACPC and their aza-analogues
s4	Table S4. Relative single-point energies, solvation free energies, conformational energies, and populations of (*M*)- and (*P*)-helices of pentamers for *c*-ACPC and their aza-analogues
s5	Fig. S1 The structures of (*M*)- and (*P*)-helices of *c*-ACHC pentamer analogues with the replacements by C^{β}-aza residues at (a) even and (b) positions optimized at the M06-2X/6-31+G(d) level of theory
s6	Fig. S2 The structures of (*M*)- and (*P*)-helices of *c*-ACHC pentamer analogues with the replacements by C^{α}-aza residues at (a) even and (b) positions optimized at the M06-2X/6-31+G(d) level of theory

s7 Fig. S3 The structures of (*M*)- and (*P*)-helices of *c*-ACPC pentamer analogues with the replacements by C^{β}-aza residues at (a) even and (b) positions optimized at the M06-2X/6-31+G(d) level of theory

s8 Fig. S4 The structures of (*M*)- and (*P*)-helices of *c*-ACPC pentamer analogues with the replacements by C^{α}-aza residues at (a) even and (b) positions optimized at the M06-2X/6-31+G(d) level of theory

s9−s20 Cartesian Coordinates of two helices of pentamers for *c*-ACHC and their aza-analogues optimized at the M06-2X/6-31+G(d) level of theory

s21−s30 Cartesian Coordinates of two helices of pentamers for *c*-ACPC and their aza-analogues optimized at the M06-2X/6-31+G(d) level of theory

Table S1 Absolute electronic energies, single-point energies, and solvation free energies of (*M*)- and (*P*)-helices of pentamers for *c*-ACHC and their aza-analogues[a]

Conf.	E_0[b]	E_{sp}[c]	E_{sp1}[d]	ΔG_s[e] (chloroform)	ΔG_s[e] (acetonitrile)	ΔG_s[e] (DMSO)	ΔG_s[e] (water)
Pentamer **1** (*M*)-helix	-2264.5737072	-2265.3813635	-2265.1487302	-2265.160474	-2265.165441	-2265.165653	-2265.165932
Pentamer **1** (*P*)-helix	-2264.5702782	-2265.3782809	-2265.1440748	-2265.157581	-2265.163197	-2265.163438	-2265.163755
Even C$^{\beta}$-aza (*M*)-helix	-2296.5621940	-2297.3818394	-2297.1437432	-2297.156992	-2297.163141	-2297.163414	-2297.163774
Even C$^{\beta}$-aza (*P*)-helix	-2296.5578607	-2297.3775213	-2297.1396311	-2297.152962	-2297.158364	-2297.158592	-2297.158891
Odd C$^{\beta}$-aza (*M*)-helix	-2312.5627813	-2313.3873564	-2313.1480031	-2313.160951	-2313.166351	-2313.166581	-2313.166882
Odd C$^{\beta}$-aza (*P*)-helix	-2312.5486500	-2313.3750018	-2313.1313362	-2313.148170	-2313.155744	-2313.156081	-2313.156525
Even C$^{\alpha}$-aza (*M*)-helix	-2296.6339171	-2297.4545343	-2297.2164211	-2297.229194	-2297.235207	-2297.235478	-2297.235836
Even C$^{\alpha}$-aza (*P*)-helix	-2296.6424117	-2297.4641814	-2297.2240429	-2297.237998	-2297.243849	-2297.244102	-2297.244433
Odd C$^{\alpha}$-aza (*M*)-helix	-2312.6812765	-2313.5104334	-2313.2674823	-2313.282040	-2313.288535	-2313.288821	-2313.289199
Odd C$^{\alpha}$-aza (*P*)-helix	-2312.6687285	-2313.4965679	-2313.2537826	-2313.268922	-2313.275669	-2313.275969	-2313.276365

[a] Absolute electronic energies, single-point energies, and solvation free energies are in hartrees. [b] Conformational energies calculated at the M06-2X/6-31+G(d) level of theory. [c] Single-point energies calculated at the M06-2X/def2-TZVP level of theory. [d] Single-point energies calculated at the M06-2X/6-311G(d,p) level of theory. [e] Solvation free energies calculated at the PCM M06-2X/6-311G(d,p) level of theory.

Table S2 Relative single-point energies, solvation free energies, conformational energies, and populations of (*M*)- and (*P*)-helices of pentamers for *c*-ACHC and their aza-analogues[a]

	Chloroform				Acetonitrile			DMSO			Water		
Conf.	ΔE_{sp}[b]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]
Pentamer **1** (*M*)-helix	0.00	0.00	0.00	80	0.00	0.00	67	0.00	0.00	66	0.00	0.00	65
Pentamer **1** (*P*)-helix	1.93	-1.11	0.83	20	-1.51	0.42	33	-1.53	0.40	34	-1.56	0.38	35
Even C$^{\beta}$-aza (*M*)-helix	0.00	0.00	0.00	99	0.00	0.00	99	0.00	0.00	100	0.00	0.00	100
Even C$^{\beta}$-aza (*P*)-helix	2.71	-0.05	2.66	1	0.42	3.13	1	0.45	3.16	0	0.48	3.19	0
Odd C$^{\beta}$-aza (*M*)-helix	0.00	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100
Odd C$^{\beta}$-aza (*P*)-helix	7.75	-2.44	5.31	0	-3.80	3.95	0	-3.87	3.88	0	-3.96	3.79	0
Even C$^{\alpha}$-aza (*M*)-helix	6.05	0.74	6.80	0	0.64	6.69	0	0.63	6.68	0	0.61	6.67	0
Even C$^{\alpha}$-aza (*P*)-helix	0.00	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100
Odd C$^{\alpha}$-aza (*M*)-helix	0.00	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100
Odd C$^{\alpha}$-aza (*P*)-helix	8.70	-0.36	8.34	0	-0.52	8.18	0	-0.53	8.17	0	-0.54	8.16	0

[a] All energies are in kcal mol^{-1}. Populations are in %. [b] Relative single-point energies calculated at the M06-2X/def2-TZVP level of theory. [c] Relative solvation free energies calculated at the PCM M06-2X/6-311G(d,p) level of theory; calculated using the values of ΔG_s and E_{sp1} listed in Table S1. [d] Relative conformational energies calculated by the sum of ΔE_{sp} and $\Delta\Delta G_s$. [e] Populations were calculated by ΔE_s for each pair of (*M*)- and (*P*)-helices at 25 °C.

Table S3 Absolute electronic energies, single-point energies, and solvation free energies of (*M*)- and (*P*)-helices of pentamers for *c*-ACPC and their aza-analogues[a]

Conf.	E_0[b]	E_{sp}[c]	E_{sp1}[d]	ΔG_s[e] (chloroform)	ΔG_s[e] (acetonitrile)	ΔG_s[e] (DMSO)	ΔG_s[e] (water)
Pentamer **2** (*M*)-helix	-2068.0577746	-2068.7994888	-2068.5817951	-2068.593325	-2068.598160	-2068.598367	-2068.598637
Pentamer **2** (*P*)-helix	-2068.0567683	-2068.7990881	-2068.5806579	-2068.593546	-2068.598961	-2068.599193	-2068.599497
Even C$^{\beta}$-aza (*M*)-helix	-2100.0486447	-2100.8025417	-2100.5784469	-2100.592521	-2100.598734	-2100.599005	-2100.599361
Even C$^{\beta}$-aza (*P*)-helix	-2100.0423209	-2100.7959373	-2100.5732755	-2100.586903	-2100.592478	-2100.592715	-2100.593024
Odd C$^{\beta}$-aza (*M*)-helix	-2116.0431250	-2116.8022791	-2116.5783913	-2116.591724	-2116.597289	-2116.597526	-2116.597837
Odd C$^{\beta}$-aza (*P*)-helix	-2116.0384757	-2116.7989290	-2116.5704551	-2116.586851	-2116.594053	-2116.594367	-2116.594780
Even C$^{\alpha}$-aza (*M*)-helix	-2100.1257907	-2100.8803501	-2100.6571152	-2100.670110	-2100.676052	-2100.676317	-2100.676666
Even C$^{\alpha}$-aza (*P*)-helix	-2100.1423698	-2100.8991219	-2100.6734202	-2100.690060	-2100.697107	-2100.697409	-2100.697805
Odd C$^{\alpha}$-aza (*M*)-helix	-2116.1935675	-2116.9554110	-2116.7286519	-2116.745466	-2116.752477	-2116.752778	-2116.753171
Odd C$^{\alpha}$-aza (*P*)-helix	-2116.1582465	-2116.9199098	-2116.6923305	-2116.705952	-2116.711733	-2116.711983	-2116.712310

[a] Absolute electronic energies, single-point energies, and solvation free energies are in hartrees. [b] Conformational energies calculated at the M06-2X/6-31+G(d) level of theory. [c] Single-point energies calculated at the M06-2X/def2-TZVP level of theory. [d] Single-point energies calculated at the M06-2X/6-311G(d,p) level of theory. [e] Solvation free energies calculated at the PCM M06-2X/6-311G(d,p) level of theory.

Table S4 Relative single-point energies, solvation free energies, conformational energies, and populations of (*M*)- and (*P*)-helices of pentamers for *c*-ACPC and their aza-analogues[a]

	Chloroform				Acetonitrile			DMSO			Water		
Conf.	ΔE_{sp}[b]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]	$\Delta\Delta G_s$[c]	ΔE_s[d]	w[e]
Pentamer **2** (*M*)-helix	0.00	0.60	0.60	27	0.96	0.96	16	0.98	0.98	16	1.00	1.00	16
Pentamer **2** (*P*)-helix	0.25	-0.25	0.00	73	-0.25	0.00	84	-0.25	0.00	84	-0.25	0.00	84
Even C$^{\beta}$-aza (*M*)-helix	0.00	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100
Even C$^{\beta}$-aza (*P*)-helix	4.14	0.28	4.42	0	0.68	4.82	0	0.70	4.85	0	0.73	4.88	0
Odd C$^{\beta}$-aza (*M*)-helix	0.00	0.00	0.00	58	0.85	0.85	19	0.90	0.90	18	0.96	0.96	17
Odd C$^{\beta}$-aza (*P*)-helix	2.10	-1.92	0.18	42	-2.10	0.00	81	-2.10	0.00	82	-2.10	0.00	83
Even C$^{\alpha}$-aza (*M*)-helix	11.78	2.29	14.07	0	2.98	14.76	0	3.00	14.78	0	3.03	14.81	0
Even C$^{\alpha}$-aza (*P*)-helix	0.00	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100
Odd C$^{\alpha}$-aza (*M*)-helix	0.00	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100	0.00	0.00	100
Odd C$^{\alpha}$-aza (*P*)-helix	22.28	2.00	24.28	0	2.78	25.05	0	2.81	25.08	0	2.85	25.13	0

[a] All energies are in kcal mol^{-1}. Populations are in %. [b] Relative single-point energies calculated at the M06-2X/def2-TZVP level of theory. [c] Relative solvation free energies calculated at the PCM M06-2X/6-311G(d,p) level of theory; calculated using the values of ΔG_s and E_{sp1} listed in Table S3. [d] Relative conformational energies calculated by the sum of ΔE_{sp} and $\Delta\Delta G_s$. [e] Populations were calculated by ΔE_s for each pair of (*M*)- and (*P*)-helices at 25 °C.

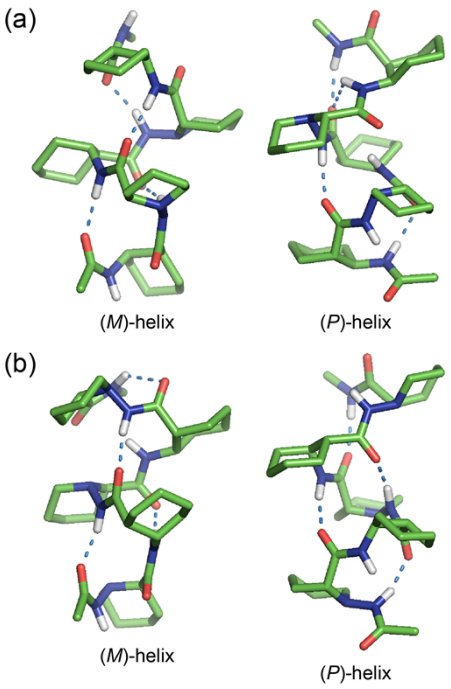

Fig. S1 The structures of (*M*)- and (*P*)-helices of *c*-ACHC pentamer analogues with the replacements by C^{β}-aza residues at (a) even and (b) odd positions optimized at the M06-2X/6-31+G(d) level of theory. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

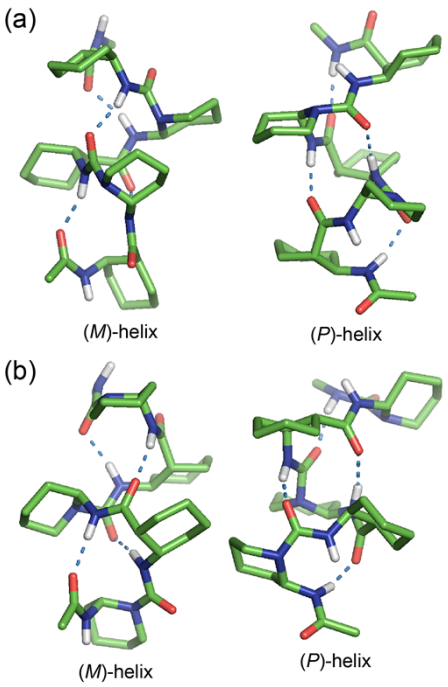

Fig. S2 The structures of (*M*)- and (*P*)-helices of *c*-ACHC pentamer analogues with the replacements by C^{α}-aza residues at (a) even and (b) odd positions optimized at the M06-2X/6-31+G(d) level of theory. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

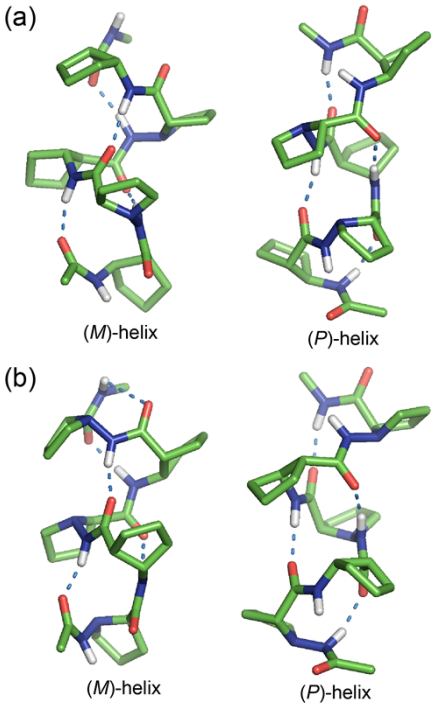

Fig. S3 The structures of (*M*)- and (*P*)-helices of *c*-ACPC pentamer analogues with the replacements by C^{β}-aza residues at (a) even and (b) odd positions optimized at the M06-2X/6-31+G(d) level of theory. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

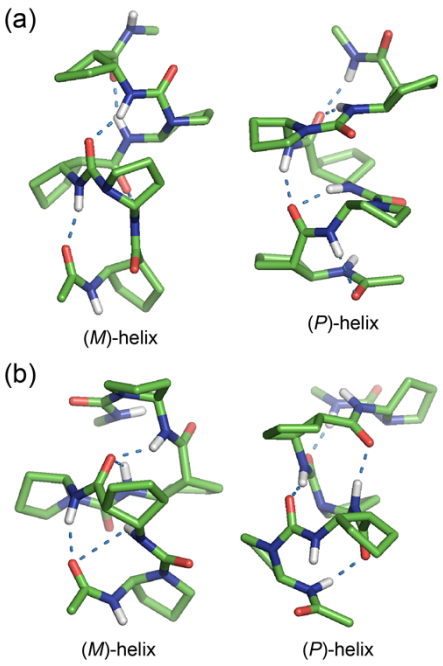

Fig. S4 The structures of (*M*)- and (*P*)-helices of *c*-ACPC pentamer analogues with the replacements by C^{α}-aza residues at (a) even and (b) odd positions optimized at the M06-2X/6-31+G(d) level of theory. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

Cartesian Coordinates of two helices of *c*-ACHC pentamer **1** and its aza-analogues optimized at the M06-2X/6-31+G(d) level of theory**:**

01 *c*-ACHC pentamer: (*M*)-helix

O	-3.4434	-1.849164	1.529501
O	-4.526673	-0.369894	-2.406918
O	0.913154	-1.551393	-0.780508
O	-1.182381	1.56891	0.485725
O	4.177746	1.97832	-0.752805
O	3.221221	0.474811	2.099162
N	-5.031135	-0.473068	0.655414
H	-5.861262	-0.467463	0.073998
N	-2.418288	-0.186696	-1.56223
H	-1.820403	0.346343	-0.927736
N	-0.593377	-1.43846	0.918436
H	-1.565856	-1.595193	1.189711
N	1.048472	1.956824	0.69658
H	1.890522	1.692929	1.211297
N	3.453785	-0.161961	-0.968769
H	2.621774	-0.750756	-1.010224
N	5.37514	1.140758	1.963072
H	6.235018	1.003239	1.448614
C	-4.535307	-1.689758	0.977908
C	-4.21266	0.739743	0.675163
H	-3.212691	0.42239	0.968218
C	-4.727924	1.770736	1.679899
H	-3.955967	2.546472	1.778791
H	-4.834453	1.289357	2.659307
C	-6.043138	2.409185	1.229007
H	-6.834664	1.645079	1.20296
H	-6.363986	3.162949	1.956876
C	-5.893353	3.033662	-0.160988
H	-5.15803	3.849658	-0.109572
H	-6.840794	3.479941	-0.484025
C	-5.430431	1.994171	-1.184519
H	-5.296473	2.448307	-2.172356
H	-6.205752	1.227817	-1.318654
C	-4.121531	1.333426	-0.74905
H	-3.320089	2.083121	-0.713191
C	-3.713791	0.197999	-1.681273
C	-1.898011	-1.365294	-2.23105
H	-2.771409	-1.849193	-2.685029
C	-0.920198	-1.019086	-3.356494
H	-0.039115	-0.512202	-2.941668
H	-1.417406	-0.319597	-4.038406
C	-0.492267	-2.289467	-4.094957
H	-1.377557	-2.740049	-4.568124
H	0.205766	-2.041841	-4.902753
C	0.143588	-3.297779	-3.135955
H	1.085613	-2.891633	-2.755682
H	0.376011	-4.228211	-3.66817
C	-0.785977	-3.616371	-1.958788
H	-0.285956	-4.285565	-1.248043
H	-1.663431	-4.15877	-2.339055
C	-1.312811	-2.3729	-1.21471
H	-2.136103	-2.675251	-0.556702
C	-0.230748	-1.748402	-0.341626
C	0.343178	-0.889824	1.894885
H	1.307391	-0.826721	1.391371
C	0.457707	-1.800604	3.122151
H	0.692543	-2.819009	2.789029
H	1.311485	-1.446152	3.716773
C	-0.814313	-1.7796	3.975006
H	-0.679721	-2.41731	4.856386
H	-1.654901	-2.200601	3.405692
C	-1.165091	-0.350383	4.399861
H	-2.094509	-0.346712	4.980417
H	-0.374366	0.040305	5.057418
C	-1.312602	0.55943	3.177305
H	-1.548028	1.587654	3.477646
H	-2.154251	0.205114	2.572409
C	-0.034351	0.543591	2.339277
H	0.808727	0.887909	2.953693
C	-0.118882	1.41482	1.100707
C	1.203232	2.588307	-0.605687
H	0.186069	2.716931	-0.993931
C	1.852859	3.968503	-0.50614
H	2.851194	3.875567	-0.064573
H	1.242778	4.591449	0.158307
C	1.958304	4.602374	-1.896829
H	0.945334	4.775811	-2.290446
H	2.441114	5.583513	-1.825134
C	2.728957	3.701693	-2.865891
H	3.76526	3.60571	-2.525244
H	2.749327	4.154601	-3.864406
C	2.089501	2.312497	-2.954454
H	2.668259	1.659926	-3.61952
H	1.08599	2.403817	-3.394573
C	1.928698	1.636463	-1.577832
H	1.296372	0.747008	-1.68591
C	3.282733	1.182271	-1.047031
C	4.721303	-0.733036	-0.544529
H	5.475095	0.025046	-0.781381
C	5.032265	-2.015256	-1.325795
H	4.947934	-1.800611	-2.396913

H	6.079256	-2.286161	-1.129391
C	4.132328	-3.186805	-0.924958
H	3.085697	-2.965904	-1.17891
H	4.41459	-4.079431	-1.494551
C	4.233746	-3.448624	0.579057
H	5.25931	-3.756713	0.832143
H	3.572892	-4.273415	0.868327
C	3.858495	-2.188389	1.359535
H	3.902222	-2.360217	2.441382
H	2.822883	-1.926118	1.120107
C	4.762095	-1.011184	0.985475
H	5.80409	-1.26534	1.23285
C	4.378417	0.255056	1.734866
C	5.057815	2.496738	2.376399
H	4.526758	3.026537	1.57721
H	5.985608	3.020152	2.612216
H	4.428352	2.462501	3.267157
C	-5.394976	-2.875088	0.600027
H	-5.262433	-3.6621	1.343707
H	-6.453871	-2.620239	0.51105
H	-5.048444	-3.25005	-0.369394

02 *c*-ACHC pentamer: (*P*)-helix

O	7.001484	0.936544	-0.161607
O	2.024946	-0.933219	1.507748
O	2.432664	1.095489	-2.256524
O	-2.173941	-1.858431	-0.768085
O	-1.430152	1.208552	0.686979
O	-6.653112	-0.086405	0.057104
N	4.985701	0.419284	-1.062224
H	4.209269	0.710042	-1.658467
N	2.929489	1.062894	0.928307
H	3.775797	1.508454	0.594637
N	0.38733	0.461891	-1.491346
H	-0.360802	0.67843	-0.829523
N	-0.739424	-1.743719	0.990752
H	0.230483	-1.567651	1.256226
N	-3.619519	0.977348	1.218898
H	-4.291933	0.511211	1.817949
N	-5.018682	-1.606175	-0.28856
H	-4.045269	-1.762723	-0.541688
C	6.071608	1.222766	-0.907173
C	4.915987	-0.890156	-0.438251
H	5.94864	-1.258308	-0.382997
C	4.087543	-1.846145	-1.294082
H	4.453065	-1.811494	-2.326966
H	3.044057	-1.497447	-1.315067
C	4.1689	-3.268701	-0.734803
H	5.208583	-3.617491	-0.815249
C	3.719768	-3.325411	0.727126
H	3.890769	-4.330285	1.13095
H	2.642944	-3.134052	0.787981
C	4.459718	-2.29931	1.594423
H	5.518498	-2.583322	1.66557
H	4.054567	-2.307958	2.61161
C	4.404998	-0.872051	1.02949
H	5.096705	-0.232312	1.593888
C	3.008773	-0.264798	1.16989
C	1.681376	1.818282	0.90751
H	0.889261	1.102748	1.123893
C	1.676354	2.925354	1.965281
H	0.656986	3.332837	2.01594
H	1.900502	2.48406	2.943772
C	2.662499	4.04632	1.627299
H	3.691382	3.657659	1.662479
H	2.606959	4.834562	2.386137
C	2.382785	4.622293	0.236127
H	3.114288	5.401147	-0.007394
H	1.394382	5.104157	0.2381
C	2.409712	3.526209	-0.831889
H	3.421309	3.104371	-0.907207
H	2.185742	3.935528	-1.823177
C	1.420257	2.410624	-0.497644
H	0.400449	2.819248	-0.467896
C	1.461279	1.276793	-1.51381
C	0.332485	-0.794013	-2.221647
H	1.311584	-0.898082	-2.70531
C	-0.733403	-0.788266	-3.319496
H	-0.52997	0.054693	-3.989858
H	-1.722373	-0.633148	-2.87246
C	-0.705741	-2.112183	-4.08879
H	0.262788	-2.205876	-4.602416
C	-0.899508	-3.30712	-3.151928
H	-0.816437	-4.244283	-3.714812
H	-1.904051	-3.270498	-2.718504
C	0.142328	-3.302659	-2.0284
H	1.140103	-3.452607	-2.466383
H	-0.026896	-4.136317	-1.335883
C	0.191342	-1.977553	-1.241996
H	1.083134	-1.977897	-0.604414
C	-1.017644	-1.840993	-0.326522
C	-1.775934	-1.667843	2.010112
H	-2.701585	-1.993057	1.523855
C	-1.447975	-2.612129	3.174916
H	-2.328302	-2.662381	3.830613
H	-1.282312	-3.618266	2.774336
C	-0.240061	-2.13783	3.987434
H	-0.067783	-2.825734	4.822725

H	0.666939	-2.162774	3.36761
C	-0.456316	-0.712721	4.502774
H	0.429387	-0.368917	5.048234
H	-1.294843	-0.702329	5.214887
C	-0.752148	0.24176	3.343463
H	-0.915249	1.263674	3.70676
H	0.11839	0.270507	2.680255
C	-1.975548	-0.225007	2.548264
H	-2.83886	-0.269989	3.228892
C	-2.308743	0.71836	1.404084
C	-4.148284	1.688164	0.059862
H	-3.304714	2.248595	-0.358301
C	-5.240297	2.669249	0.486158
H	-4.811143	3.379708	1.202605
H	-6.04557	2.121328	0.990789
C	-5.812063	3.399236	-0.73089
H	-5.019369	4.002356	-1.199005
C	-6.369336	2.405856	-1.751961
H	-6.74461	2.940745	-2.632376
H	-7.209454	1.861744	-1.308626
C	-5.290062	1.410862	-2.189175
H	-4.503443	1.95352	-2.733192
H	-5.703862	0.673579	-2.886849
C	-4.617133	0.678738	-1.013479
H	-3.721252	0.16	-1.379287
C	-5.534188	-0.361038	-0.378595
C	-5.771616	-2.66684	0.34914
H	-5.972075	-2.435152	1.4018
H	-5.195151	-3.591215	0.284201
H	-6.735332	-2.803205	-0.149211
C	6.054885	2.510525	-1.707296
H	5.202995	2.578648	-2.389027
H	6.037781	3.359191	-1.016097
H	6.98565	2.571696	-2.276836
H	3.560963	-3.948374	-1.343421
H	-1.477089	-2.111058	-4.866946
H	-6.593559	4.097116	-0.410721

03 even C$^{\beta}$-aza analogue: (*M*)-helix

C	-5.444467	-2.77787	0.964642
C	-4.514577	-1.607397	1.165228
O	-3.321742	-1.777104	1.427439
N	-5.069411	-0.377326	1.020781
C	-4.241076	0.804291	0.797868
C	-4.051379	1.082962	-0.714077
C	-5.346542	1.582684	-1.364011
C	-5.890436	2.816882	-0.641521
C	-6.107831	2.533981	0.846959
C	-4.816944	2.034659	1.500875
C	-3.563446	-0.177635	-1.414765
O	-4.330671	-1.065879	-1.75765
N	-2.211223	-0.224129	-1.618847
N	-1.656423	-1.371362	-2.171754
C	-1.239941	-2.365141	-1.175353
C	-0.870225	-3.668954	-1.894306
C	0.093419	-3.468549	-3.068652
C	-0.430948	-2.384533	-4.010947
C	-0.709619	-1.093656	-3.246641
C	-0.099096	-1.844209	-0.294402
O	1.077491	-1.841765	-0.694253
N	-0.466137	-1.357444	0.903697
C	0.498601	-0.810197	1.852793
C	0.036675	0.559267	2.407461
C	-1.18386	0.417599	3.318309
C	-0.885691	-0.553613	4.464037
C	-0.449602	-1.919488	3.924564
C	0.766675	-1.782595	3.004786
C	-0.192586	1.461043	1.210056
O	-1.288572	1.578657	0.671286
N	0.942743	2.049694	0.738463
N	0.962842	2.529788	-0.569221
C	1.600002	1.557384	-1.455998
C	1.515858	2.049946	-2.906838
C	2.040402	3.479297	-3.05788
C	1.303199	4.407688	-2.091026
C	1.430744	3.915788	-0.652111
C	3.051907	1.24449	-1.069035
O	3.873677	2.139124	-0.860682
N	3.363718	-0.072154	-1.004826
C	4.710867	-0.502984	-0.662579
C	4.87645	-0.725625	0.867905
C	4.104023	-1.961873	1.334552
C	4.533517	-3.210873	0.562949
C	4.329775	-3.009706	-0.940127
C	5.091785	-1.775213	-1.427835
C	4.434698	0.526449	1.609038
O	3.285129	0.662382	2.033652
N	5.368035	1.494032	1.760125
C	4.968835	2.83307	2.157822
H	-6.00109	-0.367242	0.622564
H	-1.626758	0.425778	-1.082636
H	-1.456189	-1.405489	1.152919
H	1.836176	1.797002	1.175685
H	2.598485	-0.749941	-0.980993
H	6.210125	1.406839	1.206453
H	-3.263696	0.578111	1.220945
H	-4.055335	2.824501	1.452465
H	-4.976695	1.798124	2.559097

H	-6.903826	1.78291	0.96416
H	-6.461845	3.434681	1.361172
H	-5.174943	3.644788	-0.74828
H	-6.82633	3.143945	-1.109189
H	-5.160327	1.804397	-2.4212
H	-6.091563	0.775691	-1.353788
H	-3.281284	1.861489	-0.785009
H	0.239002	-0.670067	-2.872248
H	-1.180988	-0.350355	-3.896371
H	-1.366643	-2.716669	-4.478251
H	0.291876	-2.186115	-4.810763
H	1.079747	-3.180331	-2.692259
H	0.206411	-4.415868	-3.608806
H	-0.453126	-4.374478	-1.166676
H	-1.808863	-4.095203	-2.268976
H	-2.116358	-2.540682	-0.54186
H	1.421576	-0.650637	1.293585
H	1.057109	-2.754317	2.58627
H	1.627499	-1.398299	3.570068
H	-0.218062	-2.600197	4.751747
H	-1.284613	-2.368492	3.368155
H	-1.773215	-0.663329	5.097362
H	-0.088297	-0.14019	5.099114
H	-1.475627	1.402364	3.702682
H	-2.036371	0.039693	2.741146
H	0.887531	0.94102	2.988729
H	2.470196	4.013831	-0.306607
H	0.784536	4.498741	0.011052
H	0.238856	4.443077	-2.358136
H	1.696413	5.428085	-2.158325
H	3.115565	3.505938	-2.847942
H	1.896243	3.814897	-4.091163
H	2.059917	1.352818	-3.555473
H	0.458048	2.01558	-3.199434
H	1.018617	0.631418	-1.357991
H	5.367408	0.317088	-0.972128
H	4.922292	-1.604269	-2.496784
H	6.169806	-1.94075	-1.29182
H	3.256164	-2.897575	-1.142699
H	4.667204	-3.891956	-1.495965
H	5.592514	-3.429892	0.766676
H	3.956957	-4.075321	0.910679
H	4.241662	-2.096215	2.413973
H	3.034437	-1.793624	1.170671
H	5.950632	-0.883329	1.049364
H	4.39772	3.316379	1.356644
H	5.862622	3.417425	2.382161
H	4.349114	2.767902	3.053471
H	-5.093653	-3.624758	1.555505
H	-6.479118	-2.542112	1.227787
H	-5.404154	-3.042045	-0.098229

04 even C$^{\beta}$-aza analogue: (*P*)-helix

C	5.238078	2.5741	-2.148309
C	5.392766	1.307763	-1.333434
O	6.291991	1.15902	-0.509094
N	4.497886	0.32231	-1.604307
C	4.631317	-1.017363	-1.057688
C	4.394669	-1.129164	0.47555
C	4.577524	-2.592486	0.913325
C	3.750156	-3.596818	0.102048
C	3.964106	-3.420248	-1.40249
C	3.725251	-1.972037	-1.83069
C	3.03858	-0.577382	0.893339
O	2.056232	-1.289406	1.099026
N	3.020883	0.773875	1.027267
N	1.845854	1.47456	1.305549
C	1.473046	2.356392	0.181382
C	2.444683	3.517326	-0.011471
C	2.5358	4.329264	1.285256
C	2.908655	3.423643	2.464532
C	1.945403	2.237208	2.558552
C	1.30182	1.491868	-1.068889
O	1.928289	1.694375	-2.111454
N	0.418662	0.489347	-0.913008
C	0.107877	-0.457495	-1.971329
C	-0.158367	-1.875947	-1.415869
C	-0.458087	-2.831631	-2.58472
C	-1.545012	-2.327496	-3.54111
C	-1.247503	-0.912066	-4.038859
C	-1.025012	0.044525	-2.866743
C	-1.267384	-1.903965	-0.362378
O	-2.444173	-2.124533	-0.63426
N	-0.817808	-1.659024	0.897834
N	-1.695015	-1.682241	1.992284
C	-1.635519	-0.398766	2.720696
C	-0.310466	-0.170196	3.441772
C	-0.010133	-1.347848	4.3742
C	-0.056723	-2.674133	3.608195
C	-1.395159	-2.818287	2.879284
C	-1.97467	0.72259	1.729912
O	-1.289668	1.741381	1.633598
N	-3.063416	0.471576	0.984394
C	-3.531821	1.352355	-0.07803
C	-4.401894	0.558696	-1.078152
C	-4.904568	1.497554	-2.187164
C	-5.570907	2.775656	-1.665797
C	-4.668417	3.506845	-0.670381

C	-4.26172	2.578615	0.475198
C	-5.542448	-0.168834	-0.36681
O	-6.621136	0.35292	-0.106019
N	-5.256497	-1.446737	-0.002568
C	-6.242341	-2.245662	0.699026
H	3.658047	0.567181	-2.124606
H	3.881701	1.281912	0.83134
H	-0.036229	0.424077	-0.005459
H	0.188275	-1.537028	1.058895
H	-3.4657	-0.458081	1.071264
H	-4.375821	-1.869012	-0.287791
H	5.678376	-1.31705	-1.206421
H	3.908395	-1.849029	-2.9049
H	2.677401	-1.693915	-1.64354
H	4.994025	-3.700532	-1.666598
H	4.025138	-4.615044	0.401223
H	2.689777	-3.463171	0.338864
H	5.643782	-2.833579	0.802485
H	4.340788	-2.685051	1.978957
H	5.168035	-0.515341	0.951284
H	0.925508	2.579842	2.773966
H	2.240667	1.53632	3.346357
H	3.939516	3.060963	2.34003
H	2.889443	3.983274	3.406348
H	3.266784	5.137591	1.177309
H	1.562784	4.800159	1.484534
H	3.436195	3.133588	-0.286872
H	2.116132	4.135342	-0.853385
H	0.481823	2.74595	0.452647
H	1.011472	-0.525414	-2.592415
H	-0.764566	1.049025	-3.219442
H	-1.94034	0.130134	-2.267773
H	-0.344188	-0.92052	-4.666541
H	-1.620531	-3.016924	-4.39012
H	-2.509224	-2.338156	-3.023999
H	0.480294	-2.960868	-3.144047
H	-0.730637	-3.815866	-2.187961
H	0.760732	-2.203186	-0.913108
H	-2.216507	-2.865803	3.6061
H	-1.435773	-3.725733	2.269793
H	0.07892	-3.522792	4.288568
H	0.769189	-2.708927	2.884662
H	0.970257	-1.214505	4.844565
H	-0.752349	-1.372828	5.186425
H	-0.365835	0.772045	3.997558
H	0.487864	-0.050452	2.699102
H	-2.448426	-0.449245	3.460919
H	-2.641429	1.705936	-0.622722
H	-3.59655	3.088673	1.180253
H	-5.152779	2.245416	1.022386
H	-3.762248	3.864883	-1.182847
H	-5.807877	3.428366	-2.514504
H	-6.51253	2.511227	-1.175536
H	-4.033987	1.771395	-2.802208
H	-5.593904	0.948337	-2.838504
H	-3.766896	-0.213905	-1.528092
H	-6.596357	-1.712887	1.585917
H	-5.778515	-3.186438	0.999576
H	-7.108785	-2.453349	0.062468
H	4.21235	2.719177	-2.498085
H	5.562047	3.428484	-1.550862
H	5.900592	2.499656	-3.017391
H	3.301384	-4.090464	-1.962268
H	-2.067469	-0.551241	-4.67002
H	-5.177842	4.392196	-0.273993

05 odd C^{β}-aza analogue: (*M*)-helix

C	5.570372	-0.954071	2.834831
C	4.66724	-1.064579	1.632708
O	3.473656	-1.309074	1.732713
N	5.295901	-0.860207	0.429961
N	4.510961	-0.615409	-0.698716
C	4.279992	0.829574	-0.942994
C	5.540329	1.558859	-1.418382
C	6.114694	0.874036	-2.661479
C	6.352977	-0.615165	-2.397284
C	5.070413	-1.274719	-1.883947
C	3.716471	1.449627	0.337
O	4.45636	1.736548	1.27807
N	2.381009	1.621366	0.348988
C	1.677792	2.095321	1.526979
C	1.12325	0.942697	2.409975
C	0.473202	1.547643	3.666077
C	-0.564598	2.638927	3.367015
C	-0.01599	3.710001	2.420605
C	0.581796	3.090292	1.155082
C	0.145893	0.04716	1.648616
O	-1.07605	0.144528	1.785024
N	0.733571	-0.840747	0.812335
N	-0.044314	-1.696052	0.018157
C	0.179932	-1.426574	-1.41842
C	1.576386	-1.817007	-1.887867
C	1.826999	-3.298383	-1.591542
C	1.604572	-3.584886	-0.103419
C	0.214004	-3.11241	0.328259
C	-0.132108	0.049566	-1.666241
O	0.741058	0.871232	-1.963994
N	-1.427673	0.372386	-1.504993

C	-1.930893	1.737827	-1.56338
C	-2.832176	2.051343	-0.345848
C	-3.331843	3.503639	-0.430501
C	-3.962246	3.870758	-1.77837
C	-3.038153	3.513672	-2.944626
C	-2.629086	2.039834	-2.891133
C	-3.97432	1.045531	-0.25
O	-5.018426	1.145338	-0.884817
N	-3.692866	-0.009359	0.567148
N	-4.646505	-1.01821	0.755699
C	-4.096787	-2.340218	0.415997
C	-3.014717	-2.813691	1.385662
C	-3.557777	-2.795694	2.817998
C	-4.124533	-1.415976	3.168529
C	-5.167261	-0.992342	2.13122
C	-3.631102	-2.355225	-1.042141
O	-2.688555	-3.053043	-1.415404
N	-4.338069	-1.575705	-1.883486
C	-3.998164	-1.507724	-3.290751
H	6.186781	-0.36927	0.491878
H	1.840692	1.351382	-0.475534
H	1.753308	-0.945873	0.835186
H	-2.041558	-0.368073	-1.175408
H	-2.794947	-0.048045	1.062502
H	-5.011529	-0.921558	-1.488428
H	4.295735	-1.228349	-2.661381
H	5.227222	-2.325784	-1.625326
H	7.156619	-0.73966	-1.657292
H	6.687163	-1.125222	-3.307821
H	5.404413	0.982309	-3.493575
H	7.043717	1.364722	-2.971372
H	5.29439	2.606631	-1.62511
H	6.277957	1.573293	-0.605017
H	3.513894	0.864306	-1.731005
H	2.431591	2.609197	2.13566
H	-0.198946	2.573111	0.578789
H	1.00561	3.863229	0.503402
H	0.76957	4.286663	2.930269
H	-0.807958	4.420492	2.155692
H	-1.450388	2.177073	2.920421
H	-0.879371	3.103036	4.309407
H	0.014793	0.750615	4.261547
H	1.280874	1.978599	4.274221
H	1.981501	0.322688	2.698638
H	0.060282	-3.241245	1.40489
H	-0.569496	-3.672247	-0.197865
H	1.698354	-4.657527	0.103701
H	2.375573	-3.073856	0.48829
H	2.846337	-3.575492	-1.885149
H	1.140816	-3.914095	-2.191035
H	1.675697	-1.598024	-2.957795
H	2.320519	-1.207892	-1.360556
H	-0.575332	-2.034753	-1.93655
H	-1.045982	2.383302	-1.494483
H	-3.515565	1.399917	-2.990863
H	-1.940519	1.791992	-3.707575
H	-2.131447	4.13582	-2.903559
H	-3.529383	3.734003	-3.898941
H	-4.910576	3.337121	-1.88848
H	-4.18285	4.944757	-1.78933
H	-4.040236	3.692275	0.384434
H	-2.461892	4.153462	-0.252041
H	-2.219199	1.937019	0.556444
H	-5.545483	0.017357	2.314885
H	-6.023601	-1.679	2.153462
H	-3.308181	-0.680602	3.196593
H	-4.582485	-1.422945	4.164633
H	-4.353972	-3.549161	2.916795
H	-2.767673	-3.074572	3.52393
H	-2.691087	-3.818065	1.094976
H	-2.138397	-2.158297	1.295899
H	-4.952796	-3.030701	0.474177
H	-2.969908	-1.153099	-3.432767
H	-4.685787	-0.815915	-3.77928
H	-4.082934	-2.496188	-3.751338
H	5.187818	-1.59636	3.628691
H	6.607029	-1.217774	2.608774
H	5.535421	0.088759	3.168924

06 odd C$^{\beta}$-aza analogue: (*P*)-helix

C	6.186783	2.207929	-1.776425
C	6.130002	0.953127	-0.92502
O	7.035993	0.627975	-0.17488
N	4.960269	0.261227	-1.036088
N	4.7983	-0.960018	-0.380137
C	4.359633	-0.838685	1.020093
C	4.430936	-2.222929	1.669306
C	3.675629	-3.291515	0.871436
C	4.123365	-3.289046	-0.590685
C	4.016814	-1.89215	-1.19267
C	2.966408	-0.199998	1.187731
O	1.984495	-0.838972	1.582778
N	2.901741	1.114885	0.880983
C	1.658675	1.877373	0.815001
C	1.395682	2.374633	-0.626688
C	2.378451	3.471664	-1.036803
C	2.348375	4.633328	-0.040321
C	2.64125	4.148556	1.382211

C	1.660196	3.049459	1.79858
C	1.453835	1.167989	-1.554434
O	2.429177	0.917488	-2.257729
N	0.357957	0.374766	-1.469277
N	0.323785	-0.882239	-2.066399
C	0.194966	-1.931883	-1.052927
C	0.236823	-3.307431	-1.731081
C	-0.747469	-3.426172	-2.896995
C	-0.523064	-2.280097	-3.883892
C	-0.625637	-0.929229	-3.184058
C	-1.053936	-1.776482	-0.177333
O	-2.192	-1.842974	-0.658182
N	-0.813723	-1.577215	1.134135
C	-1.873451	-1.427819	2.121912
C	-2.057891	0.048737	2.572275
C	-0.842077	0.54218	3.362992
C	-0.580732	-0.350076	4.578368
C	-0.382185	-1.805841	4.149207
C	-1.586178	-2.307044	3.346468
C	-2.348126	0.922028	1.362708
O	-1.455005	1.346996	0.635053
N	-3.666633	1.165966	1.145512
N	-4.113362	1.684117	-0.068027
C	-4.446293	0.574982	-0.973046
C	-5.011121	1.110037	-2.294118
C	-6.149956	2.102988	-2.068355
C	-5.656586	3.240363	-1.173996
C	-5.152156	2.698135	0.159055
C	-5.406794	-0.423642	-0.314872
O	-6.398985	-0.060214	0.317383
N	-5.082512	-1.724575	-0.477221
C	-5.897846	-2.759628	0.128836
H	4.182855	0.599243	-1.610986
H	3.751808	1.536005	0.524932
H	-0.425844	0.669631	-0.877623
H	0.151174	-1.385513	1.409045
H	-4.362249	0.68888	1.721567
H	-4.126295	-1.943212	-0.745484
H	4.446981	-1.870356	-2.198423
H	2.963363	-1.570834	-1.288332
H	5.169613	-3.612459	-0.658655
H	3.853664	-4.275668	1.31974
H	2.598225	-3.098349	0.932242
H	5.492098	-2.49177	1.72494
H	4.043229	-2.161351	2.69103
H	5.094011	-0.178213	1.498302
H	0.863702	1.18138	1.07967
H	0.640141	3.457016	1.828823
H	1.891667	2.672278	2.801833
H	3.671775	3.765631	1.432613
H	2.590139	4.983337	2.089768
H	3.072022	5.400365	-0.338408
H	1.356076	5.106243	-0.063023
H	3.394027	3.054306	-1.091551
H	2.144997	3.815477	-2.050453
H	0.373206	2.777388	-0.624655
H	-0.337317	-0.121	-3.862724
H	-1.658004	-0.747592	-2.843586
H	0.476598	-2.367533	-4.328732
H	-0.605699	-4.3913	-3.396209
H	-1.775063	-3.394587	-2.520285
H	1.258848	-3.441825	-2.109439
H	0.061188	-4.084526	-0.977647
H	1.067476	-1.831449	-0.399802
H	-2.793153	-1.765165	1.631423
H	-2.477769	-2.301381	3.988492
H	-1.432836	-3.33854	3.010642
H	-0.233482	-2.446391	5.025651
H	0.533406	-1.882022	3.545923
H	0.302397	0.009264	5.117869
H	-1.429503	-0.284929	5.275143
H	-0.997806	1.584581	3.666004
H	0.040297	0.526084	2.714235
H	-2.935168	0.057135	3.23622
H	-4.683838	3.493136	0.74797
H	-5.99194	2.279336	0.732739
H	-4.840509	3.775552	-1.677103
H	-6.497395	2.494997	-3.030557
H	-6.996828	1.59792	-1.58897
H	-4.192061	1.610409	-2.82638
H	-5.332082	0.26095	-2.908152
H	-3.501192	0.056807	-1.173856
H	-5.838506	-2.730162	1.223573
H	-5.553763	-3.731774	-0.226783
H	-6.943046	-2.616919	-0.154139
H	5.35415	2.286826	-2.480995
H	6.192944	3.085638	-1.122422
H	7.130379	2.201466	-2.327216
H	3.520823	-3.98875	-1.181778
H	-1.253562	-2.32087	-4.699356
H	-6.456487	3.963324	-0.981178

07 even C^{α}-aza analogue: (*M*)-helix

C	5.215216	-2.724082	1.775891
C	4.473012	-2.052445	0.644217
O	3.288012	-2.287205	0.422894
N	5.198757	-1.168795	-0.094945
C	4.558741	-0.201867	-0.983308

C	4.434663	1.171161	-0.284884	H	-6.197119	-0.583622	-2.037169
C	5.79068	1.868634	-0.153182	H	3.553053	-0.58146	-1.163681
C	6.485885	1.992004	-1.510576	H	4.65943	0.507772	-2.994295
C	6.651062	0.620722	-2.171086	H	5.410006	-1.075129	-2.755519
C	5.296794	-0.077263	-2.317362	H	7.327217	0.000885	-1.563116
C	3.785606	0.972205	1.081847	H	7.127128	0.720768	-3.15285
O	4.446299	0.952399	2.114596	H	5.8882	2.637585	-2.170163
N	2.437366	0.781727	1.050253	H	7.460741	2.477729	-1.38942
C	1.651824	0.872977	2.25335	H	5.650731	2.853651	0.305169
N	0.831661	-0.318725	2.585591	H	6.422767	1.30608	0.546643
C	0.22864	-0.144333	3.915445	H	3.767302	1.779217	-0.911581
C	-0.683031	1.083976	3.997124	H	2.375179	0.962377	3.069993
C	0.068398	2.340871	3.556291	H	0.003279	1.949298	1.418897
C	0.753523	2.113543	2.206574	H	1.362779	2.982119	1.928122
C	-0.038729	-0.876804	1.645551	H	0.834892	2.593375	4.303667
O	-1.235672	-1.074113	1.910379	H	-0.612609	3.19857	3.50004
N	0.498561	-1.228808	0.452292	H	-1.547913	0.917495	3.343917
C	-0.372384	-1.752844	-0.596737	H	-1.056985	1.195736	5.02205
C	0.085882	-1.257298	-1.989503	H	-0.320065	-1.054579	4.161845
C	1.359558	-1.956485	-2.459103	H	1.059897	-0.043398	4.625394
C	1.166293	-3.475313	-2.467326	H	-1.355683	-1.322254	-0.40924
C	0.774025	-3.974632	-1.07361	H	-0.757179	-3.597043	0.435027
C	-0.497681	-3.279406	-0.582382	H	-1.344053	-3.542336	-1.233489
C	0.213848	0.249308	-1.874787	H	0.621711	-5.060339	-1.08671
O	1.291069	0.812702	-1.660984	H	1.597438	-3.771331	-0.377206
N	-0.968067	0.917249	-1.935487	H	2.090351	-3.963549	-2.797974
C	-1.138906	2.224981	-1.339285	H	0.383152	-3.745682	-3.191564
N	-1.916583	2.074833	-0.08784	H	1.647327	-1.585105	-3.450193
C	-2.100612	3.379328	0.579444	H	2.179692	-1.718514	-1.774996
C	-2.722676	4.442927	-0.329795	H	-0.739686	-1.496458	-2.673618
C	-1.876902	4.609026	-1.595692	H	-0.139415	2.54629	-1.018726
C	-1.689995	3.268157	-2.31418	H	-2.641905	2.917554	-2.722359
C	-3.175705	1.409362	-0.267655	H	-0.975279	3.367486	-3.139201
O	-3.937328	1.641185	-1.203519	H	-0.890657	5.008953	-1.315168
N	-3.45633	0.521053	0.711601	H	-2.332815	5.340135	-2.271828
C	-4.747726	-0.154652	0.728791	H	-3.743352	4.147792	-0.599052
C	-4.763873	-1.454773	-0.122829	H	-2.783921	5.390971	0.21826
C	-3.912553	-2.550028	0.523971	H	-2.697023	3.211376	1.483328
C	-4.383587	-2.846688	1.949422	H	-1.105599	3.717387	0.90147
C	-4.352409	-1.580461	2.808973	H	-5.453679	0.556692	0.286829
C	-5.180071	-0.46509	2.166049	H	-5.123978	0.457163	2.756042
C	-4.316377	-1.15837	-1.546075	H	-6.236291	-0.768102	2.138986
O	-3.136064	-1.226283	-1.892293	H	-3.310583	-1.259353	2.929204
N	-5.289276	-0.809753	-2.419889	H	-4.741847	-1.788951	3.812341
C	-4.931063	-0.230348	-3.702531	H	-5.406676	-3.252547	1.92703
H	6.112343	-0.929114	0.270819	H	-3.743027	-3.616863	2.393071
H	1.964264	0.884031	0.15017	H	-3.945099	-3.453878	-0.096053
H	1.506219	-1.384582	0.407693	H	-2.869526	-2.220667	0.557214
H	-1.807206	0.355546	-2.095813	H	-5.812996	-1.787863	-0.151583
H	-2.674628	0.15798	1.263459	H	-4.413931	0.725598	-3.560131

H	-5.839605	-0.078202	-4.287417
H	-4.270914	-0.916472	-4.236652
H	4.760133	-3.695089	1.973775
H	6.280808	-2.847083	1.564192
H	5.105824	-2.094982	2.666203

08 even C^{α}-aza analogue: (*P*)-helix

C	-5.877078	2.53188	1.606271
C	-5.827276	1.16684	0.950411
O	-6.737383	0.753017	0.239335
N	-4.727318	0.415676	1.221623
C	-4.674931	-0.995679	0.877867
C	-4.362558	-1.294474	-0.617531
C	-4.395683	-2.815424	-0.839998
C	-3.500634	-3.604323	0.124775
C	-3.763117	-3.229562	1.584991
C	-3.696703	-1.715944	1.801168
C	-3.038441	-0.680437	-1.052054
O	-2.001018	-1.340394	-1.159213
N	-3.079562	0.650494	-1.317872
C	-1.87413	1.486312	-1.364283
N	-1.760803	2.271812	-0.133128
C	-2.734501	3.357169	-0.005637
C	-2.631716	4.301828	-1.197367
C	-2.839065	3.536494	-2.504288
C	-1.832248	2.389953	-2.591147
C	-1.515842	1.547173	1.036479
O	-2.170787	1.726971	2.068267
N	-0.517086	0.626043	0.943611
C	-0.164409	-0.200545	2.085692
C	0.107596	-1.669416	1.681838
C	0.384368	-2.495923	2.951491
C	1.464959	-1.900657	3.863101
C	1.181652	-0.433111	4.191764
C	0.971353	0.393051	2.921036
C	1.229763	-1.814424	0.658822
O	2.41486	-1.913102	0.992229
N	0.827147	-1.849179	-0.635641
C	1.776704	-1.912088	-1.747439
N	1.751188	-0.66559	-2.528646
C	0.554598	-0.500957	-3.370377
C	0.405638	-1.678441	-4.32398
C	0.293995	-2.973019	-3.520146
C	1.537492	-3.125011	-2.646878
C	2.029807	0.467752	-1.730172
O	1.203109	1.363126	-1.539667
N	3.2589	0.46611	-1.176601
C	3.707314	1.45087	-0.201764
C	4.470155	0.755689	0.948922
C	4.98465	1.802205	1.950973
C	5.762119	2.952168	1.302932
C	4.950533	3.60391	0.182005
C	4.525015	2.565423	-0.858385
C	5.58692	-0.133721	0.408438
O	6.711695	0.273426	0.137326
N	5.22141	-1.426794	0.19551
C	6.198595	-2.396249	-0.262694
H	-3.957944	0.827349	1.750307
H	-3.966751	1.108407	-1.140109
H	0.160597	0.751882	0.191226
H	-0.166507	-1.714608	-0.836219
H	3.921597	-0.23483	-1.486908
H	4.311838	-1.740398	0.529258
H	-5.685673	-1.394404	1.041103
H	-3.932	-1.463247	2.841933
H	-2.682092	-1.344063	1.599706
H	-4.761027	-3.580904	1.884472
H	-3.675016	-4.677051	-0.019591
H	-2.451452	-3.410722	-0.11953
H	-5.437281	-3.140295	-0.71137
H	-4.118079	-3.039394	-1.875704
H	-5.163603	-0.82399	-1.201528
H	-1.036399	0.800511	-1.415635
H	-0.812044	2.787021	-2.652499
H	-2.007335	1.769906	-3.477202
H	-3.86658	3.144429	-2.542036
H	-2.728736	4.201421	-3.367272
H	-3.377058	5.097161	-1.087017
H	-1.639999	4.771507	-1.196813
H	-3.760366	2.957913	0.061944
H	-2.538571	3.873127	0.936079
H	-1.058966	-0.216984	2.719563
H	0.710456	1.42858	3.167792
H	1.893639	0.415889	2.324359
H	0.274374	-0.361233	4.809578
H	1.514758	-2.488319	4.787302
H	2.436953	-1.983026	3.36855
H	-0.562173	-2.553659	3.509151
H	0.649309	-3.521639	2.670595
H	-0.804982	-2.046127	1.202897
H	2.756604	-2.012131	-1.279914
H	2.41929	-3.235198	-3.290953
H	1.477729	-4.012028	-2.007931
H	0.193426	-3.841293	-4.180017
H	-0.608638	-2.935387	-2.893693
H	-0.486438	-1.522894	-4.940496
H	1.272717	-1.725122	-4.995607
H	0.662919	0.44364	-3.909186

H	-0.355676	-0.432364	-2.759386
H	2.796834	1.89281	0.224145
H	3.91421	3.021831	-1.645873
H	5.414734	2.12818	-1.331791
H	4.051713	4.079597	0.602855
H	6.009191	3.695603	2.070109
H	6.702311	2.566621	0.897548
H	4.1077	2.212963	2.473528
H	5.60117	1.304676	2.70828
H	3.754308	0.096248	1.453018
H	6.664486	-2.052971	-1.190237
H	5.692613	-3.346984	-0.439496
H	6.991911	-2.539814	0.478531
H	-4.939807	2.801856	2.100123
H	-6.137441	3.284532	0.857594
H	-6.680618	2.514938	2.349047
H	-3.042333	-3.733595	2.240071
H	2.001565	-0.012395	4.784793
H	5.532335	4.39823	-0.29867

09 add C$^{\alpha}$-aza analogue: (*M*)-helix

C	5.587731	-3.157448	0.609912
C	4.577311	-2.16782	0.069881
O	3.377005	-2.437041	0.074787
N	5.082512	-1.003015	-0.405551
C	4.265156	0.136397	-0.846283
N	4.37463	1.251441	0.085105
C	5.657431	1.953626	0.089082
C	5.998443	2.443513	-1.313765
C	5.985902	1.286022	-2.311905
C	4.631523	0.579065	-2.260831
C	3.763103	1.123261	1.336187
O	4.285699	1.546292	2.360668
N	2.550472	0.483008	1.319953
C	1.844183	0.283897	2.572591
C	1.066133	-1.053486	2.577791
C	0.385952	-1.241811	3.947576
C	-0.444505	-0.036689	4.40954
C	0.361328	1.262709	4.350197
C	0.969351	1.475819	2.962395
C	0.056129	-1.160024	1.438273
O	-1.107799	-0.757789	1.562038
N	0.510051	-1.732483	0.29965
C	-0.318562	-1.836205	-0.910263
N	0.236518	-1.016301	-1.990832
C	1.463074	-1.541882	-2.600413
C	1.214843	-2.945073	-3.140884
C	0.754269	-3.859217	-2.00538
C	-0.508723	-3.278619	-1.369937
C	0.288551	0.348606	-1.652392
O	1.354435	0.967483	-1.563723
N	-0.921149	0.897923	-1.408066
C	-1.075832	2.240934	-0.874473
C	-2.003912	2.236159	0.357571
C	-2.170962	3.669197	0.901044
C	-2.585986	4.67946	-0.171972
C	-1.614543	4.651882	-1.354176
C	-1.50438	3.244988	-1.947576
C	-3.358541	1.604988	0.071258
O	-4.154764	2.073156	-0.741273
N	-3.641728	0.499435	0.818706
C	-4.874079	-0.250103	0.615477
N	-4.698411	-1.363773	-0.340437
C	-3.841395	-2.441532	0.180703
C	-4.442874	-3.018226	1.455944
C	-4.580974	-1.917192	2.506706
C	-5.427288	-0.777605	1.938866
C	-4.294081	-0.909974	-1.619346
O	-3.157705	-1.08424	-2.061347
N	-5.265318	-0.293134	-2.328239
C	-4.930954	0.549039	-3.461808
H	6.083417	-0.871399	-0.341683
H	2.007023	0.553617	0.46023
H	1.492879	-2.009655	0.258052
H	-1.744169	0.3625	-1.689181
H	-2.858231	0.048378	1.289069
H	-6.147398	-0.141935	-1.859856
H	3.241338	-0.220075	-0.854986
H	3.837426	1.260286	-2.588127
H	4.611162	-0.300073	-2.914415
H	6.796254	0.580836	-2.069369
H	6.185405	1.644336	-3.327412
H	5.256766	3.193272	-1.616964
H	6.977951	2.934395	-1.295202
H	5.575454	2.781054	0.794408
H	6.461899	1.300645	0.473097
H	2.625745	0.18638	3.335232
H	0.176062	1.603275	2.213322
H	1.593241	2.376319	2.943067
H	1.176547	1.226783	5.087787
H	-0.272338	2.114649	4.622391
H	-1.331063	0.056141	3.774731
H	-0.791651	-0.216235	5.434433
H	-0.238185	-2.142809	3.925718
H	1.182222	-1.424021	4.682807
H	1.808935	-1.847608	2.430047
H	-1.288323	-1.427312	-0.641293
H	-0.835187	-3.872393	-0.508535

H	-1.325759	-3.266329	-2.102467
H	0.558708	-4.872692	-2.372543
H	1.554258	-3.934149	-1.255041
H	2.139574	-3.321824	-3.592615
H	0.448122	-2.905708	-3.925436
H	1.758477	-0.850848	-3.394446
H	2.287857	-1.588385	-1.875704
H	-0.080224	2.534481	-0.516754
H	-2.470713	2.937828	-2.365007
H	-0.762843	3.217684	-2.754567
H	-0.619439	4.978202	-1.016433
H	-1.934661	5.361104	-2.125913
H	-3.595353	4.442549	-0.524427
H	-2.616151	5.682914	0.269353
H	-2.890001	3.664085	1.729436
H	-1.2021	3.972122	1.324757
H	-1.518846	1.622591	1.123199
H	-5.577361	0.46308	0.181967
H	-5.493968	0.06033	2.640081
H	-6.444673	-1.142757	1.751442
H	-3.581019	-1.550975	2.781563
H	-5.040334	-2.302667	3.423385
H	-5.42717	-3.452372	1.236454
H	-3.796742	-3.824375	1.820978
H	-3.756208	-3.201675	-0.600387
H	-2.828738	-2.074499	0.397743
H	-4.489291	1.493673	-3.124168
H	-5.839962	0.750028	-4.031552
H	-4.219615	0.019668	-4.097459
H	5.349329	-4.148916	0.219717
H	6.620882	-2.904463	0.36006
H	5.485818	-3.191568	1.698665

10 add C^{α}-aza analogue: (*P*)-helix

C	5.736755	2.633453	-2.066389
C	5.88046	1.330241	-1.306925
O	6.942886	0.968964	-0.829224
N	4.718624	0.612987	-1.175388
C	4.705871	-0.707259	-0.601436
N	4.167314	-0.79422	0.783171
C	4.377634	-2.141862	1.323605
C	3.641096	-3.196261	0.495138
C	4.079384	-3.116138	-0.968105
C	3.945025	-1.685831	-1.501683
C	2.975988	-0.199174	1.174932
O	2.170786	-0.781872	1.919833
N	2.764598	1.076677	0.767678
C	1.487719	1.749766	0.951023
C	1.087451	2.505299	-0.341406
C	1.982893	3.719452	-0.592985
C	1.979735	4.657055	0.617503
C	2.4	3.919223	1.891862
C	1.501249	2.70724	2.146364
C	1.128705	1.495885	-1.473945
O	2.116476	1.372905	-2.202142
N	0.039627	0.691607	-1.575827
C	0.14212	-0.608125	-2.20379
N	0.287729	-1.627389	-1.137568
C	0.472979	-2.971321	-1.723557
C	-0.640823	-3.351238	-2.704774
C	-0.759643	-2.297419	-3.809821
C	-0.957718	-0.892072	-3.227793
C	-0.783359	-1.618009	-0.193259
O	-1.959707	-1.438997	-0.513361
N	-0.404717	-1.846096	1.079138
C	-1.421941	-1.956671	2.116403
C	-1.844902	-0.580375	2.700563
C	-0.712751	0.027467	3.538114
C	-0.291793	-0.915089	4.666411
C	0.152075	-2.267563	4.104852
C	-0.95292	-2.883419	3.243241
C	-2.296978	0.393781	1.618225
O	-1.504058	1.121622	1.022258
N	-3.632683	0.443146	1.38295
C	-4.221866	1.355472	0.433403
N	-4.395105	0.837413	-0.940276
C	-4.749995	1.941805	-1.841614
C	-6.073692	2.592277	-1.432087
C	-6.028798	3.042283	0.03106
C	-5.549213	1.914315	0.953027
C	-5.095419	-0.347124	-1.198391
O	-5.877144	-0.452789	-2.134266
N	-4.82587	-1.394884	-0.338025
C	-5.385568	-2.684418	-0.720557
H	3.896266	0.901157	-1.708635
H	3.518177	1.541005	0.280814
H	-0.718509	0.836403	-0.906432
H	0.574373	-1.668926	1.324414
H	-4.243471	-0.221424	1.841271
H	-3.838084	-1.432116	-0.092191
H	5.755031	-1.010371	-0.512444
H	4.338712	-1.611122	-2.522109
H	2.888593	-1.378172	-1.518463
H	5.131147	-3.426574	-1.050839
H	3.833898	-4.195258	0.903822
H	2.562557	-3.00467	0.573437
H	5.45901	-2.328874	1.303004
H	4.04845	-2.149784	2.362752

H	0.746496	0.970533	1.125645
H	0.467795	3.036565	2.325294
H	1.827515	2.151572	3.0336
H	3.443367	3.585332	1.793801
H	2.37127	4.597323	2.751982
H	2.644577	5.508215	0.431591
H	0.969043	5.067871	0.754717
H	3.008664	3.383945	-0.801495
H	1.651219	4.243423	-1.49672
H	0.051314	2.835848	-0.187086
H	1.103184	-0.611848	-2.731389
H	-0.881017	-0.137263	-4.018702
H	-1.941214	-0.798668	-2.759873
H	0.160831	-2.310447	-4.41259
H	-0.419612	-4.335192	-3.135557
H	-1.592449	-3.433769	-2.166136
H	1.437259	-2.954405	-2.250231
H	0.559687	-3.69176	-0.90296
H	-2.293476	-2.409509	1.630374
H	-1.823058	-3.105574	3.87657
H	-0.625549	-3.831627	2.801572
H	0.405202	-2.95671	4.918658
H	1.063364	-2.123987	3.510675
H	0.523615	-0.458895	5.238281
H	-1.130781	-1.061196	5.36367
H	-1.031533	0.998215	3.936536
H	0.150385	0.210777	2.88997
H	-2.703272	-0.782665	3.359482
H	-3.497759	2.171766	0.337239
H	-5.4137	2.284655	1.97582
H	-6.287994	1.099827	0.982218
H	-5.335487	3.890185	0.131427
H	-6.288135	3.44573	-2.085697
H	-6.872221	1.856296	-1.578427
H	-3.929579	2.670009	-1.795334
H	-4.803801	1.54783	-2.856765
H	-6.46993	-2.600313	-0.806188
H	-5.143385	-3.410541	0.058956
H	-4.995155	-3.037477	-1.682573
H	4.762606	2.73992	-2.551538
H	5.882238	3.461114	-1.364984
H	6.531455	2.691787	-2.813609
H	3.499049	-3.810909	-1.585764
H	-1.584075	-2.544052	-4.486795
H	-7.012206	3.399563	0.35492

Cartesian Coordinates of two helices of *c*-ACPC pentamer **2** and its aza-analogues optimized at the M06-2X/6-31+G(d) level of theory**:**

01 *c*-ACPC pentamer: (*M*)-helix

C	5.196066	-2.589739	0.492742
C	4.552448	-1.677599	-0.527726
O	3.486277	-1.963208	-1.075701
N	5.228618	-0.528029	-0.778582
C	4.581969	0.624825	-1.399624
C	4.18009	1.702744	-0.335924
C	5.341069	2.726526	-0.315619
C	6.376935	2.225066	-1.342351
C	5.550157	1.37734	-2.315675
C	3.954594	1.01452	1.002188
O	4.884987	0.80677	1.782823
N	2.697035	0.562891	1.202116
C	2.336283	-0.257455	2.334201
C	1.647495	-1.594781	1.969519
C	1.150176	-2.065287	3.346687
C	0.756056	-0.777004	4.119133
C	1.373902	0.400341	3.333886
C	0.473944	-1.400361	1.020157
O	-0.618003	-0.992294	1.442387
N	0.686347	-1.724986	-0.266996
C	-0.350797	-1.653533	-1.288063
C	-0.266878	-0.371372	-2.152453
C	0.950039	-0.630412	-3.046173
C	0.982222	-2.167553	-3.260891
C	-0.125223	-2.740287	-2.344091
C	-0.207036	0.873319	-1.29245
O	0.861347	1.3332	-0.870328
N	-1.408865	1.399349	-0.992067
C	-1.601218	2.43872	-0.007601
C	-2.263755	1.962748	1.309532
C	-2.62023	3.301586	1.972806
C	-3.001512	4.26118	0.814073
C	-2.499592	3.588528	-0.481871
C	-3.517243	1.138075	1.045976
O	-4.605142	1.661732	0.79269
N	-3.362903	-0.204901	1.125559
C	-4.500284	-1.101943	1.055951
C	-4.859089	-1.574147	-0.388166
C	-3.9609	-2.803664	-0.655534
C	-3.346786	-3.197486	0.709439
C	-4.174109	-2.427708	1.749161
C	-4.704685	-0.452835	-1.397756
O	-3.632628	-0.227	-1.96295
N	-5.814471	0.287365	-1.622667
C	-5.731393	1.574969	-2.288418
H	4.741436	-3.57881	0.430797
H	6.276754	-2.667548	0.343372
H	5.024533	-2.167264	1.490563
H	5.970471	-0.315091	-0.118382
H	3.705883	0.235977	-1.91823
H	3.247406	2.165306	-0.673794
H	4.96587	3.71268	-0.606607
H	5.76794	2.809271	0.686501
H	6.912166	3.040462	-1.837245
H	7.133297	1.601473	-0.847602
H	4.968241	2.03327	-2.975444
H	6.139503	0.698034	-2.938428
H	1.986328	0.789728	0.501304
H	3.274022	-0.503899	2.844405
H	2.367291	-2.2848	1.516282
H	0.319582	-2.77157	3.265453
H	1.974274	-2.577915	3.855101
H	-0.330848	-0.676632	4.164949
H	1.129318	-0.815227	5.147126
H	0.601712	0.943779	2.778551
H	1.901473	1.119598	3.966989
H	1.64374	-1.936059	-0.557724
H	-1.315696	-1.719339	-0.780538
H	-1.188041	-0.349974	-2.74745
H	0.891219	-0.069825	-3.983397
H	1.849196	-0.303959	-2.5163
H	0.807953	-2.441113	-4.305365
H	1.962829	-2.562208	-2.979156
H	-1.058509	-2.869171	-2.90424
H	0.133927	-3.703547	-1.894058
H	-2.235087	0.922373	-1.357611
H	-0.605278	2.816433	0.244733
H	-1.558169	1.363959	1.894194
H	-3.425047	3.196586	2.704701
H	-1.734578	3.673132	2.500602
H	-4.083855	4.402386	0.775907
H	-2.543103	5.244273	0.959528
H	-3.339832	3.169608	-1.04648
H	-1.957232	4.26745	-1.146586
H	-2.421941	-0.580525	1.257659
H	-5.347699	-0.576719	1.507118
H	-5.911544	-1.88415	-0.362582
H	-4.559014	-3.619393	-1.07288
H	-3.194367	-2.555303	-1.394919
H	-3.367831	-4.277526	0.880461

H	-2.298177	-2.883387	0.770284
H	-5.113011	-2.956159	1.955083
H	-3.654361	-2.275549	2.70037
H	-6.561676	0.178065	-0.948877
H	-5.451751	2.355788	-1.571264
H	-6.696926	1.813092	-2.73963
H	-4.974136	1.510592	-3.070534

02 *c*-ACPC pentamer: (*P*)-helix

C	5.976334	1.208087	-2.260147
C	5.914905	0.21481	-1.120805
O	6.60288	0.339845	-0.106829
N	5.085202	-0.840065	-1.31395
C	4.921493	-1.88743	-0.327899
C	4.494081	-1.470435	1.107535
C	4.063533	-2.815872	1.707258
C	3.435291	-3.622146	0.542376
C	3.831168	-2.878172	-0.750539
C	3.341327	-0.486234	1.071863
O	2.161184	-0.855823	1.11756
N	3.681092	0.815546	0.995423
C	2.689308	1.879033	1.021101
C	2.100376	2.254521	-0.369087
C	3.130797	3.229833	-0.984547
C	4.059508	3.67024	0.173215
C	3.349555	3.191292	1.448439
C	1.799063	1.055479	-1.2572
O	2.685048	0.5224	-1.932691
N	0.521334	0.6325	-1.250278
C	0.089414	-0.541691	-1.970291
C	-0.232677	-1.786107	-1.098955
C	-0.869291	-2.716625	-2.13954
C	-1.661432	-1.787227	-3.100831
C	-1.189316	-0.348874	-2.794217
C	-1.227536	-1.448317	-0.000507
O	-2.447287	-1.573124	-0.171218
N	-0.708446	-1.008946	1.161664
C	-1.552433	-0.676619	2.294961
C	-2.005839	0.810331	2.298485
C	-0.749631	1.563181	2.763348
C	0.029064	0.572638	3.66768
C	-0.748205	-0.7597	3.595156
C	-2.540339	1.281536	0.956342
O	-1.788337	1.671031	0.06029
N	-3.882859	1.248554	0.812387
C	-4.546233	1.430881	-0.464851
C	-5.071544	0.127515	-1.120085
C	-5.946609	0.685565	-2.247976
C	-6.567128	1.997474	-1.693644
C	-5.786079	2.330154	-0.403005
C	-5.905409	-0.668478	-0.121532
O	-7.116286	-0.504245	0.006339
N	-5.206767	-1.528756	0.658815
C	-5.896336	-2.381419	1.606847
H	5.066106	1.19881	-2.864403
H	6.153901	2.207614	-1.857953
H	6.828135	0.945573	-2.896482
H	4.30064	-0.677443	-1.939091
H	5.885171	-2.401317	-0.215192
H	5.339145	-1.018443	1.632057
H	4.953419	-3.326881	2.089939
H	3.370146	-2.684544	2.541599
H	3.802528	-4.652667	0.538927
H	2.347578	-3.662876	0.644573
H	4.17318	-3.543479	-1.5487
H	2.978357	-2.30285	-1.136631
H	4.670397	1.041635	0.923898
H	1.897239	1.554917	1.699332
H	1.15895	2.781166	-0.16351
H	3.689257	2.720856	-1.772951
H	2.62049	4.083193	-1.440278
H	5.03942	3.183843	0.0837
H	4.243208	4.747863	0.181826
H	2.562814	3.899657	1.734064
H	4.015406	3.062669	2.307856
H	-0.172181	1.11638	-0.676714
H	0.918127	-0.823952	-2.627635
H	0.683128	-2.181161	-0.645517
H	-0.069025	-3.235157	-2.679036
H	-1.508103	-3.472785	-1.677598
H	-1.466065	-2.054677	-4.143808
H	-2.736398	-1.887722	-2.931706
H	-0.999255	0.248117	-3.690801
H	-1.928176	0.186507	-2.184731
H	0.3041	-0.883172	1.224635
H	-2.412194	-1.35335	2.277171
H	-2.798155	0.897113	3.054051
H	-0.169562	1.833108	1.874657
H	-1.005899	2.494593	3.276077
H	1.051598	0.431732	3.301994
H	0.105192	0.932054	4.697474
H	-0.099776	-1.640719	3.613593
H	-1.448612	-0.84152	4.433528
H	-4.421897	0.811053	1.55151
H	-3.797059	1.863377	-1.134484
H	-4.233724	-0.485688	-1.469379
H	-5.310565	0.898298	-3.114748
H	-6.711308	-0.03017	-2.558303

H	-6.483612	2.805075	-2.42745
H	-7.626688	1.855945	-1.471745
H	-5.512586	3.385642	-0.315527
H	-6.382473	2.062251	0.476982
H	-4.220669	-1.679728	0.452072
H	-6.500057	-1.779223	2.291682
H	-5.15459	-2.945788	2.175149
H	-6.568603	-3.079582	1.096299

03 even C$^{\beta}$-aza analogue: (*M*)-helix

C	5.189632	-2.527537	-0.238921
C	4.438617	-1.437897	-0.971741
O	3.37221	-1.657239	-1.550199
N	5.014386	-0.211962	-0.920497
C	4.267412	1.018532	-1.17701
C	3.962829	1.77621	0.157153
C	5.130928	2.772555	0.351213
C	6.040393	2.613023	-0.886049
C	5.115653	2.024752	-1.957832
C	3.829946	0.749827	1.272941
O	4.785937	0.377785	1.939982
N	2.579526	0.221924	1.359395
N	2.315883	-0.872696	2.167032
C	1.739985	-2.021171	1.465264
C	1.369914	-2.934068	2.639459
C	0.97678	-1.966601	3.784252
C	1.490717	-0.583576	3.347334
C	0.494214	-1.661638	0.649857
O	-0.546057	-1.309967	1.227697
N	0.605784	-1.773064	-0.681606
C	-0.485091	-1.498147	-1.60701
C	-0.370146	-0.104237	-2.275267
C	0.772818	-0.284351	-3.283863
C	0.735927	-1.784096	-3.685772
C	-0.378153	-2.421267	-2.824171
C	-0.170989	0.987104	-1.244109
O	0.935135	1.27909	-0.794392
N	-1.33229	1.556563	-0.841377
N	-1.3751	2.411339	0.2492
C	-1.897864	1.791029	1.477284
C	-2.052467	3.015619	2.38067
C	-2.448663	4.164624	1.418564
C	-2.143741	3.637596	0.005642
C	-3.247185	1.096386	1.253206
O	-4.291387	1.739566	1.119812
N	-3.205909	-0.253114	1.204104
C	-4.413861	-1.052566	1.119549
C	-4.904381	-1.327245	-0.337716
C	-4.124136	-2.576602	-0.807747
C	-3.440911	-3.160007	0.451836
C	-4.139934	-2.469329	1.632153
C	-4.736261	-0.115203	-1.23318
O	-3.684974	0.10822	-1.836915
N	-5.807474	0.706322	-1.316494
C	-5.678586	2.044766	-1.864073
H	4.831391	-3.50207	-0.571925
H	6.269328	-2.454938	-0.397501
H	4.998644	-2.410672	0.835658
H	5.786374	-0.129854	-0.265574
H	3.343979	0.728054	-1.678886
H	3.012156	2.299686	0.017974
H	4.738941	3.792763	0.406899
H	5.665043	2.566951	1.28229
H	6.505006	3.554205	-1.193734
H	6.857333	1.911071	-0.673264
H	4.45525	2.806396	-2.353894
H	5.640143	1.557533	-2.796521
H	1.83534	0.608075	0.768506
H	2.496133	-2.456689	0.80433
H	0.564858	-3.627465	2.382821
H	2.252709	-3.517213	2.914609
H	-0.107	-1.940907	3.913763
H	1.425464	-2.283637	4.729073
H	0.655148	0.082428	3.089301
H	2.116374	-0.089265	4.095972
H	1.545258	-1.905937	-1.063556
H	-1.421761	-1.592034	-1.052405
H	-1.322618	0.057076	-2.794098
H	0.659313	0.386697	-4.139869
H	1.722916	-0.048949	-2.796852
H	0.53885	-1.922784	-4.752324
H	1.704572	-2.247576	-3.472774
H	-1.336398	-2.399992	-3.355982
H	-0.171815	-3.457134	-2.538145
H	-2.214145	1.178525	-1.20332
H	-1.161979	1.066729	1.840098
H	-2.795931	2.856105	3.16469
H	-1.087475	3.222389	2.851205
H	-3.511118	4.396781	1.51234
H	-1.878711	5.070492	1.640236
H	-3.074595	3.414535	-0.536478
H	-1.540082	4.318516	-0.600911
H	-2.29202	-0.711969	1.217965
H	-5.185927	-0.525716	1.688805
H	-5.972952	-1.565697	-0.263574
H	-4.812604	-3.298495	-1.257115
H	-3.398662	-2.298871	-1.577375
H	-3.519783	-4.249567	0.503138

H	-2.373097	-2.91239	0.463473
H	-5.098246	-2.958207	1.846262
H	-3.5472	-2.464976	2.552185
H	-6.529176	0.5702	-0.620509
H	-5.239627	2.720637	-1.121206
H	-6.664708	2.408846	-2.158831
H	-5.033814	2.002597	-2.742644

04 even C$^{\beta}$-aza analogue: (*P*)-helix

C	5.868229	0.941278	-2.535823
C	5.800498	0.226757	-1.20371
O	6.396281	0.636715	-0.206353
N	5.079056	-0.921219	-1.198485
C	4.986487	-1.789603	-0.043808
C	4.484181	-1.184369	1.295861
C	4.21028	-2.454048	2.116018
C	3.690892	-3.508754	1.105746
C	4.01669	-2.948524	-0.295135
C	3.212121	-0.375844	1.11446
O	2.093348	-0.875525	1.240281
N	3.415157	0.927172	0.817444
N	2.340903	1.823998	0.700574
C	1.965297	2.09496	-0.715871
C	3.078238	2.993923	-1.271504
C	3.614936	3.74158	-0.024106
C	2.791757	3.15269	1.148395
C	1.712322	0.795238	-1.473734
O	2.620776	0.199342	-2.055049
N	0.439343	0.368691	-1.418324
C	0.024302	-0.930339	-1.892496
C	-0.261077	-1.987637	-0.789926
C	-0.880345	-3.115444	-1.623883
C	-1.712376	-2.404984	-2.727761
C	-1.273422	-0.923945	-2.707539
C	-1.267493	-1.4722	0.236453
O	-2.461736	-1.765869	0.172759
N	-0.742781	-0.653524	1.174519
N	-1.531182	-0.169335	2.236031
C	-1.822734	1.278747	2.061557
C	-0.52783	2.021346	2.411682
C	0.193976	1.075055	3.399905
C	-0.720071	-0.173786	3.468125
C	-2.37708	1.543182	0.664326
O	-1.664495	1.949788	-0.257293
N	-3.687217	1.276991	0.530379
C	-4.370805	1.208355	-0.747873
C	-4.982236	-0.180411	-1.066526
C	-5.850816	0.142798	-2.286192
C	-6.397307	1.575882	-2.045952
C	-5.562979	2.1647	-0.887064
C	-5.834936	-0.669888	0.102857
O	-7.047971	-0.489782	0.153974
N	-5.143299	-1.256951	1.113519
C	-5.850171	-1.819517	2.248325
H	4.933731	0.844475	-3.095492
H	6.10442	1.993554	-2.368331
H	6.677013	0.496554	-3.125546
H	4.340918	-0.99074	-1.891531
H	5.99253	-2.17649	0.167961
H	5.257989	-0.549501	1.734055
H	5.152259	-2.785942	2.565337
H	3.499883	-2.270282	2.925262
H	4.17226	-4.477161	1.270529
H	2.613731	-3.653199	1.219418
H	4.439703	-3.693336	-0.975469
H	3.109506	-2.542829	-0.763959
H	4.366021	1.232806	0.60313
H	1.020982	2.650631	-0.647147
H	3.848191	2.365791	-1.725986
H	2.70129	3.668684	-2.044236
H	4.685924	3.555045	0.112005
H	3.483867	4.824161	-0.095082
H	1.891571	3.750187	1.329909
H	3.33848	3.05663	2.088923
H	-0.249184	0.948713	-0.932123
H	0.848421	-1.316303	-2.501552
H	0.665257	-2.266599	-0.275668
H	-0.072316	-3.704069	-2.072177
H	-1.490813	-3.785033	-1.015004
H	-1.526085	-2.858575	-3.705891
H	-2.781875	-2.497025	-2.522668
H	-1.124695	-0.496303	-3.702931
H	-2.014818	-0.302744	-2.187301
H	0.267915	-0.468214	1.170896
H	-2.60245	1.504116	2.800361
H	0.069561	2.148744	1.505807
H	-0.733087	3.010943	2.829586
H	1.183741	0.817088	3.009899
H	0.325373	1.520258	4.38989
H	-0.182465	-1.121319	3.542146
H	-1.418045	-0.101132	4.308947
H	-4.145538	0.822613	1.315495
H	-3.618249	1.433932	-1.510085
H	-4.190684	-0.910025	-1.265069
H	-5.221791	0.116227	-3.183539
H	-6.653559	-0.586739	-2.412658
H	-6.307395	2.183213	-2.951855
H	-7.453648	1.539635	-1.771987

H	-5.233505	3.193258	-1.060426
H	-6.142197	2.150449	0.043355
H	-4.163363	-1.50087	0.957262
H	-6.513002	-1.068902	2.686383
H	-5.117313	-2.139352	2.991024
H	-6.465093	-2.676333	1.951089

05 odd C^{β}-aza analogue: (*M*)-helix

C	5.971778	-0.826713	2.264719
C	4.90026	-1.080498	1.234223
O	3.740733	-1.320227	1.542178
N	5.339596	-1.015776	-0.062013
N	4.392244	-0.904832	-1.093146
C	4.199194	0.512264	-1.50953
C	5.445899	0.871857	-2.339167
C	5.915704	-0.487517	-2.919709
C	4.929584	-1.518589	-2.31633
C	3.94151	1.388431	-0.287028
O	4.862377	1.727886	0.456367
N	2.64686	1.693767	-0.091209
C	2.16776	2.31288	1.121459
C	1.591673	1.324729	2.173035
C	0.945857	2.296933	3.168529
C	0.386369	3.462822	2.307099
C	1.020333	3.305113	0.9067
C	0.534421	0.413956	1.558545
O	-0.666296	0.699211	1.601839
N	1.010831	-0.689403	0.949923
N	0.129187	-1.652033	0.426355
C	-0.031663	-1.532909	-1.049066
C	1.269158	-2.08036	-1.648858
C	1.732408	-3.142792	-0.624581
C	0.746043	-2.984624	0.561079
C	-0.397748	-0.106812	-1.438236
O	0.463491	0.759165	-1.628894
N	-1.715162	0.132028	-1.530778
C	-2.25839	1.466032	-1.671391
C	-2.893319	2.077482	-0.392119
C	-3.564729	3.326284	-0.972757
C	-4.105762	2.894327	-2.361424
C	-3.373931	1.579486	-2.714972
C	-3.93928	1.15022	0.230697
O	-5.141352	1.285653	0.029574
N	-3.399674	0.149878	0.976458
N	-4.220945	-0.745837	1.690282
C	-4.185119	-2.082365	1.045614
C	-2.842149	-2.713072	1.425434
C	-2.475999	-2.036266	2.767803
C	-3.615467	-1.013187	3.006757
C	-4.456919	-1.923704	-0.448261
O	-3.621586	-2.208666	-1.309284
N	-5.684365	-1.434909	-0.712162
C	-6.102236	-1.029545	-2.040855
H	5.698384	-1.328026	3.193527
H	6.957641	-1.164368	1.934233
H	6.009227	0.254913	2.435604
H	6.208154	-0.495062	-0.185003
H	3.30877	0.505739	-2.150046
H	5.204483	1.602201	-3.115194
H	6.202218	1.324692	-1.689782
H	5.889596	-0.505093	-4.012072
H	6.945603	-0.709418	-2.620961
H	4.081483	-1.68399	-2.990505
H	5.374306	-2.484961	-2.07218
H	1.944187	1.30625	-0.726985
H	3.025633	2.811448	1.584264
H	2.392613	0.713843	2.604044
H	0.167586	1.814734	3.764065
H	1.718959	2.661867	3.853224
H	-0.703137	3.405355	2.246463
H	0.642097	4.42955	2.751529
H	0.303353	2.868863	0.199015
H	1.377302	4.247297	0.481177
H	2.020155	-0.870298	0.924074
H	-0.874813	-2.193534	-1.292504
H	1.112882	-2.484	-2.653241
H	2.003729	-1.272727	-1.711135
H	1.693012	-4.157404	-1.030713
H	2.760079	-2.937606	-0.310242
H	-0.06544	-3.717952	0.494297
H	1.212476	-3.068835	1.5451
H	-2.357754	-0.648904	-1.387851
H	-1.416816	2.108147	-1.94866
H	-2.117344	2.293356	0.350838
H	-4.356378	3.703144	-0.321998
H	-2.808873	4.112287	-1.082856
H	-5.184807	2.730625	-2.310669
H	-3.92179	3.668718	-3.112163
H	-4.044786	0.718704	-2.610448
H	-2.97392	1.559991	-3.732899
H	-2.383069	0.12216	1.124149
H	-5.014241	-2.648353	1.490154
H	-2.916199	-3.801905	1.494175
H	-2.095209	-2.470886	0.666593
H	-2.40785	-2.74885	3.594614
H	-1.508917	-1.532122	2.674809
H	-4.400908	-1.443153	3.637647
H	-3.287458	-0.071414	3.451572

H	-6.121856	-0.949496	0.066698
H	-6.14899	0.063035	-2.09811
H	-7.087074	-1.446829	-2.268682
H	-5.376675	-1.409265	-2.761641

06 odd C$^{\beta}$-aza analogue: (*P*)-helix

C	5.888548	1.998234	-1.724066
C	5.837544	0.757004	-0.857885
O	6.504872	0.64456	0.165842
N	5.015776	-0.217179	-1.331488
N	4.925593	-1.446593	-0.670546
C	4.439476	-1.435992	0.725207
C	4.222161	-2.928837	0.968876
C	3.769679	-3.493009	-0.400125
C	4.070053	-2.377801	-1.41549
C	3.143314	-0.6466	0.867449
O	2.036177	-1.178944	0.719374
N	3.287678	0.665705	1.129307
C	2.160657	1.579757	1.276399
C	1.672006	2.18959	-0.061577
C	2.711054	3.277846	-0.385645
C	3.387104	3.635698	0.964717
C	2.617837	2.828962	2.029903
C	1.480603	1.151928	-1.156699
O	2.393616	0.77871	-1.887716
N	0.215292	0.675896	-1.219864
N	-0.133193	-0.339593	-2.091199
C	-0.335566	-1.669806	-1.49239
C	-0.892949	-2.434022	-2.691725
C	-1.770856	-1.396923	-3.435547
C	-1.308925	-0.025057	-2.910001
C	-1.334029	-1.672818	-0.323442
O	-2.543297	-1.866036	-0.506558
N	-0.799793	-1.447241	0.892093
C	-1.574964	-1.501155	2.12078
C	-1.961604	-0.09226	2.678238
C	-0.804524	0.325364	3.614797
C	0.138601	-0.895763	3.703633
C	-0.72828	-2.081011	3.258018
C	-2.223536	0.87068	1.532528
O	-1.348078	1.591922	1.063601
N	-3.486519	0.804568	1.051001
N	-3.880023	1.439659	-0.118396
C	-4.580889	0.553627	-1.0733
C	-5.11039	1.565388	-2.086329
C	-5.409594	2.842145	-1.258859
C	-4.765633	2.595457	0.11428
C	-5.721405	-0.213465	-0.39041
O	-6.844803	0.261371	-0.254515
N	-5.364572	-1.417136	0.120835
C	-6.351122	-2.267146	0.760876
H	5.084511	2.03159	-2.463486
H	5.855975	2.887686	-1.090314
H	6.849057	1.997875	-2.249262
H	4.168355	0.095633	-1.815496
H	5.219298	-0.999452	1.353847
H	5.173557	-3.371475	1.273729
H	3.486782	-3.106472	1.756562
H	4.312683	-4.409629	-0.642864
H	2.701903	-3.723276	-0.393333
H	4.608538	-2.720736	-2.303372
H	3.141031	-1.880241	-1.741882
H	4.236064	1.022271	1.215665
H	1.349777	1.035326	1.767476
H	0.70171	2.645612	0.165404
H	3.434793	2.885545	-1.103471
H	2.232666	4.144983	-0.84928
H	4.444641	3.342519	0.954829
H	3.364821	4.708107	1.174914
H	1.727673	3.378135	2.356094
H	3.212028	2.589853	2.917782
H	-0.47837	1.020069	-0.54841
H	0.633084	-2.038638	-1.140784
H	-0.053851	-2.746798	-3.318905
H	-1.459223	-3.317636	-2.391667
H	-1.641537	-1.476483	-4.51762
H	-2.827522	-1.558932	-3.208708
H	-1.011962	0.671347	-3.699493
H	-2.086236	0.464956	-2.301267
H	0.206582	-1.265538	0.937788
H	-2.469572	-2.089409	1.898627
H	-2.883623	-0.222001	3.258357
H	-0.299707	1.21269	3.223024
H	-1.200817	0.583884	4.601387
H	0.984353	-0.782663	3.014892
H	0.554773	-1.032739	4.705385
H	-0.152803	-2.954176	2.936167
H	-1.394641	-2.389918	4.073062
H	-4.155926	0.187201	1.508398
H	-3.861308	-0.156955	-1.487844
H	-4.331919	1.759861	-2.829947
H	-5.997624	1.189224	-2.599111
H	-4.98835	3.726454	-1.743261
H	-6.48531	2.989679	-1.148711
H	-4.162316	3.430063	0.480905
H	-5.531246	2.351297	0.865254
H	-4.430768	-1.772258	-0.081556
H	-6.882127	-1.707696	1.535322

H	-5.842166	-3.12102	1.210867
H	-7.091507	-2.627061	0.038606

07 even C^{α}-aza analogue: (*M*)-helix

C	6.03162	-2.224747	0.677008
C	5.044087	-1.427818	-0.138173
O	3.896358	-1.823426	-0.327659
N	5.493691	-0.24559	-0.640582
C	4.564791	0.763078	-1.135287
C	3.997655	1.642411	0.008026
C	5.131293	2.643687	0.310942
C	6.000866	2.710998	-0.973862
C	5.298172	1.793199	-1.994234
C	3.579761	0.82073	1.218564
O	4.390223	0.441119	2.057603
N	2.251228	0.537725	1.274633
C	1.648545	-0.116413	2.392429
N	1.046606	-1.462287	2.148431
C	0.304579	-1.697021	3.392614
C	-0.364045	-0.351279	3.754763
C	0.490863	0.693206	3.010778
C	0.298963	-1.702602	0.98629
O	-0.899677	-2.02155	1.032637
N	0.978365	-1.63214	-0.180547
C	0.322571	-1.966209	-1.436054
C	-0.022429	-0.712491	-2.323501
C	1.055637	-0.658652	-3.434542
C	2.063026	-1.772641	-3.104851
C	1.234588	-2.805745	-2.340024
C	-0.059466	0.532773	-1.460753
O	0.957005	1.195963	-1.232931
N	-1.264118	0.81567	-0.909809
C	-1.482715	2.015147	-0.148484
N	-2.225302	1.833537	1.129364
C	-2.479747	3.225545	1.52665
C	-2.817973	4.004525	0.230547
C	-2.2748	3.104359	-0.897064
C	-3.41439	1.053128	1.086148
O	-4.538188	1.547099	1.173327
N	-3.202609	-0.280641	1.008336
C	-4.314571	-1.211355	0.926934
C	-4.732517	-1.47464	-0.549957
C	-3.659666	-2.457084	-1.017613
C	-3.527864	-3.435229	0.160816
C	-3.900005	-2.612152	1.421745
C	-4.821862	-0.191461	-1.346223
O	-3.858944	0.266277	-1.966797
N	-6.013947	0.447285	-1.313635
C	-6.109056	1.834384	-1.735767
H	5.836114	-3.288633	0.536457
H	7.070585	-1.998806	0.423363
H	5.859499	-1.970883	1.728493
H	6.371887	0.091842	-0.263498
H	3.765579	0.24522	-1.667231
H	3.123239	2.158811	-0.40283
H	4.724099	3.621235	0.583726
H	5.709992	2.283916	1.166866
H	6.104477	3.73052	-1.354576
H	7.01785	2.354388	-0.770137
H	4.54995	2.359284	-2.560159
H	5.980316	1.325267	-2.710525
H	1.662892	0.871968	0.511018
H	2.445162	-0.275505	3.124034
H	-0.399731	-2.516521	3.261186
H	1.040527	-1.979732	4.154036
H	-1.397185	-0.326434	3.393872
H	-0.380133	-0.191283	4.836518
H	-0.094583	1.159765	2.208878
H	0.877337	1.489125	3.654434
H	1.995972	-1.553264	-0.15081
H	-0.591401	-2.497498	-1.166228
H	-1.016937	-0.868194	-2.75839
H	0.584207	-0.84784	-4.404742
H	1.527316	0.326767	-3.478858
H	2.540377	-2.186538	-3.998418
H	2.8548	-1.401277	-2.447786
H	0.606278	-3.376025	-3.036421
H	1.837022	-3.511726	-1.760753
H	-2.095495	0.367949	-1.305201
H	-0.494262	2.396738	0.126797
H	-3.272776	3.260571	2.272159
H	-1.552685	3.602851	1.974677
H	-3.899436	4.134796	0.140744
H	-2.35475	4.995441	0.232443
H	-3.085997	2.619717	-1.451849
H	-1.634352	3.627898	-1.612877
H	-2.252566	-0.654111	1.015885
H	-5.13676	-0.782234	1.506238
H	-5.714363	-1.969659	-0.536696
H	-3.907054	-2.942023	-1.966814
H	-2.723922	-1.902509	-1.157509
H	-4.225068	-4.270912	0.033578
H	-2.518336	-3.845818	0.23406
H	-4.740868	-3.069322	1.952492
H	-3.06471	-2.535604	2.122342
H	-6.664883	0.141331	-0.601825
H	-5.617041	2.490508	-1.007207
H	-7.16209	2.106634	-1.825514

H	-5.625158	1.943249	-2.707401

08 even C^{α}-aza analogue: (*P*)-helix

C	3.934666	2.865396	-2.026386
C	4.443879	1.790833	-1.09661
O	5.136314	2.035332	-0.109145
N	4.097865	0.513932	-1.411496
C	4.681973	-0.651614	-0.765598
C	4.464195	-0.800108	0.770424
C	4.782822	-2.28225	1.005292
C	4.366895	-3.031837	-0.28552
C	4.094013	-1.942533	-1.342902
C	3.029275	-0.455681	1.111041
O	2.132313	-1.314917	1.111304
N	2.803002	0.848057	1.348928
C	1.482019	1.474864	1.345824
N	1.188726	2.073447	0.04562
C	1.145643	3.538863	0.089954
C	1.855599	3.851583	1.405529
C	1.43017	2.676287	2.294248
C	0.813473	1.405776	-1.094038
O	0.693252	1.99212	-2.171707
N	0.575842	0.06058	-0.964252
C	0.411595	-0.777675	-2.139697
C	0.130334	-2.253729	-1.758291
C	-0.354285	-2.846757	-3.089456
C	-1.120676	-1.705267	-3.803926
C	-0.765371	-0.404508	-3.050313
C	-0.9567	-2.313181	-0.696616
O	-2.153131	-2.219515	-0.990137
N	-0.528917	-2.450202	0.578765
C	-1.397022	-2.230372	1.73567
N	-1.183244	-0.91613	2.317743
C	-0.408399	-0.953747	3.561111
C	0.06554	-2.408197	3.631063
C	-1.041554	-3.169562	2.892092
C	-1.717727	0.275899	1.87203
O	-1.424997	1.333307	2.433476
N	-2.571748	0.207506	0.811176
C	-2.994963	1.422159	0.125785
C	-3.965997	1.117323	-1.037636
C	-4.511214	2.514253	-1.366322
C	-4.612833	3.248255	-0.006715
C	-3.774097	2.420852	0.994332
C	-5.086283	0.183715	-0.588631
O	-6.085452	0.587726	-0.004243
N	-4.90469	-1.130558	-0.872484
C	-5.837291	-2.119848	-0.370476
H	2.898876	2.68683	-2.335554
H	4.015097	3.828773	-1.520662
H	4.566735	2.891675	-2.921058
H	3.48633	0.366054	-2.206131
H	5.770412	-0.624573	-0.914889
H	5.137829	-0.129752	1.309373
H	5.858781	-2.387465	1.177356
H	4.267796	-2.664936	1.88984
H	5.157861	-3.712956	-0.612143
H	3.469778	-3.633274	-0.116204
H	4.512374	-2.177192	-2.326712
H	3.013142	-1.797577	-1.463833
H	3.601342	1.468927	1.218645
H	0.752243	0.710544	1.61832
H	1.629555	3.964068	-0.790536
H	0.101568	3.880062	0.104913
H	2.943205	3.856536	1.252648
H	1.565772	4.821406	1.816215
H	0.393459	2.794414	2.622599
H	2.065784	2.520075	3.169646
H	0.895334	-0.403165	-0.119403
H	1.335259	-0.772009	-2.745515
H	1.03194	-2.747855	-1.376024
H	0.52068	-3.150725	-3.674474
H	-0.972677	-3.734475	-2.933516
H	-0.833776	-1.649598	-4.858313
H	-2.197948	-1.884756	-3.768659
H	-0.510612	0.429738	-3.703729
H	-1.59233	-0.082954	-2.409937
H	0.470886	-2.367795	0.757052
H	-2.425276	-2.362938	1.389337
H	0.420815	-0.240431	3.528233
H	-1.048819	-0.6821	4.409759
H	1.020106	-2.511472	3.102715
H	0.204696	-2.75175	4.658771
H	-0.74687	-4.158653	2.534126
H	-1.920538	-3.277378	3.537152
H	-2.605509	-0.648968	0.267817
H	-2.110634	1.922047	-0.304562
H	-3.441155	0.666431	-1.887484
H	-3.798985	3.019957	-2.027943
H	-5.472016	2.45926	-1.884197
H	-4.241647	4.27447	-0.092659
H	-5.652759	3.295552	0.322704
H	-3.101637	3.023613	1.605671
H	-4.42627	1.855227	1.667738
H	-4.025244	-1.449146	-1.262558
H	-5.921236	-2.058916	0.719989
H	-5.479654	-3.110454	-0.656066
H	-6.832374	-1.956407	-0.793829

09 odd C^{α}-aza analogue: (*M*)-helix

C	4.657361	-3.037552	0.690959
C	3.870353	-1.985948	-0.058922
O	2.827358	-2.265677	-0.648532
N	4.378192	-0.729352	-0.019589
C	3.623447	0.448899	-0.445698
N	3.281622	1.293927	0.695376
C	4.129006	2.487913	0.79262
C	5.177506	2.274764	-0.305287
C	4.438961	1.397936	-1.322897
C	2.600588	0.830619	1.805922
O	2.770766	1.296403	2.927742
N	1.741641	-0.209033	1.552323
C	1.076224	-0.882889	2.648649
C	0.338621	-2.164147	2.19193
C	-0.549191	-2.509175	3.409234
C	-0.680438	-1.207399	4.249828
C	0.01877	-0.105466	3.440147
C	-0.516624	-1.894996	0.957557
O	-1.61137	-1.328775	1.046649
N	-0.003506	-2.311851	-0.217807
C	-0.655441	-2.079429	-1.505455
N	0.173024	-1.262067	-2.385698
C	0.922551	-2.058525	-3.365671
C	0.565508	-3.503018	-2.996561
C	-0.801534	-3.367936	-2.316086
C	0.552835	0.027027	-2.129112
O	1.486283	0.566377	-2.724227
N	-0.138227	0.657931	-1.110672
C	0.19102	2.043787	-0.812227
C	-0.547364	2.584334	0.433167
C	-0.153389	4.070734	0.39222
C	-0.020498	4.435043	-1.113479
C	-0.082146	3.101229	-1.888884
C	-2.057229	2.435841	0.285509
O	-2.717483	3.240467	-0.373431
N	-2.629717	1.364246	0.896572
C	-4.04728	1.055351	0.730261
N	-4.27222	-0.18479	-0.003203
C	-4.68066	-1.299802	0.859171
C	-4.512997	-0.730797	2.26987
C	-4.742154	0.770571	2.067469
C	-3.816139	-0.448568	-1.266836
O	-3.891137	-1.569178	-1.769924
N	-3.206254	0.59723	-1.928501
C	-2.87238	0.422677	-3.333306
H	4.53514	-3.998924	0.190525
H	5.720149	-2.79546	0.771915
H	4.242452	-3.11933	1.70182
H	5.196358	-0.570927	0.556692
H	2.754672	0.074309	-0.984299
H	3.525969	3.384405	0.595277
H	4.548969	2.575115	1.797112
H	5.535884	3.216009	-0.728256
H	6.048409	1.743532	0.100064
H	3.734181	1.992258	-1.915579
H	5.089124	0.85007	-2.008376
H	1.344456	-0.293156	0.619144
H	1.857005	-1.189675	3.358774
H	1.058807	-2.956173	1.958765
H	-1.524378	-2.87477	3.078579
H	-0.079542	-3.305355	3.994139
H	-1.724943	-0.960948	4.45896
H	-0.182589	-1.333818	5.217164
H	-0.684964	0.368553	2.748668
H	0.474932	0.675221	4.052875
H	0.965535	-2.628299	-0.244559
H	-1.627055	-1.630803	-1.298014
H	0.59599	-1.797493	-4.37975
H	1.990966	-1.84572	-3.280345
H	0.547547	-4.163053	-3.867035
H	1.305751	-3.894034	-2.289251
H	-1.597149	-3.21645	-3.054322
H	-1.07618	-4.211878	-1.67985
H	-1.122054	0.402063	-1.01715
H	1.262868	2.069861	-0.573443
H	-0.204346	2.077599	1.342502
H	-0.885391	4.697968	0.906039
H	0.806475	4.186637	0.907323
H	-0.829158	5.100023	-1.424013
H	0.925202	4.955247	-1.298537
H	-1.084713	2.947368	-2.302907
H	0.641809	3.027315	-2.702863
H	-2.041542	0.599117	1.225813
H	-4.485786	1.914041	0.216297
H	-5.721188	-1.574475	0.645886
H	-4.044024	-2.165581	0.665602
H	-5.207885	-1.174502	2.987354
H	-3.489362	-0.91609	2.613772
H	-5.81282	0.979334	1.959619
H	-4.341134	1.401676	2.863733
H	-3.378283	1.548889	-1.614598
H	-2.293866	1.290204	-3.658256
H	-3.763473	0.316304	-3.962551
H	-2.257762	-0.473281	-3.45283

10 odd C^{α}-aza analogue: (*P*)-helix

C	5.69536	1.198023	-2.427694
C	5.564194	0.037101	-1.467904
O	6.42664	-0.256387	-0.64948
N	4.40934	-0.683875	-1.592053
C	4.17139	-1.883939	-0.85448
N	3.743543	-1.774462	0.57541
C	3.228986	-3.106953	0.888009
C	2.422383	-3.53595	-0.352393
C	3.03879	-2.71109	-1.499202
C	3.069771	-0.698008	1.11904
O	2.03854	-0.827673	1.79857
N	3.638176	0.518601	0.92589
C	3.009723	1.733185	1.418603
C	2.084442	2.445445	0.35686
C	2.88267	3.681221	-0.132376
C	4.311806	3.474584	0.38438
C	4.083109	2.78402	1.72965
C	1.732958	1.516237	-0.793573
O	2.471597	1.394659	-1.77248
N	0.572056	0.827554	-0.653917
C	0.041897	0.026163	-1.720449
N	-0.297753	-1.392368	-1.392449
C	-0.919605	-1.831412	-2.653288
C	-1.810995	-0.652073	-3.121557
C	-1.253446	0.562918	-2.35271
C	-1.131107	-1.622798	-0.275404
O	-2.238223	-2.162005	-0.386664
N	-0.610411	-1.263565	0.91682
C	-1.362996	-1.397029	2.153392
C	-1.789035	-0.002164	2.693019
C	-0.527054	0.483118	3.406612
C	-0.027164	-0.763201	4.151215
C	-0.488321	-1.9683	3.292636
C	-2.266682	0.918768	1.587632
O	-1.528233	1.763139	1.07732
N	-3.547031	0.736794	1.178708
C	-4.142224	1.509908	0.122393
N	-4.631486	0.748267	-1.058594
C	-5.273291	1.815412	-1.840645
C	-6.003257	2.723945	-0.814548
C	-5.357419	2.355267	0.537666
C	-5.508897	-0.34368	-0.811707
O	-6.656525	-0.380524	-1.230625
N	-4.9519	-1.356086	-0.079226
C	-5.713588	-2.589662	0.046551
H	4.744133	1.727648	-2.537801
H	6.472137	1.873033	-2.066181
H	5.992309	0.814118	-3.409565
H	3.612036	-0.206613	-2.00817
H	5.111108	-2.445814	-0.829125
H	4.091946	-3.767565	1.036624
H	2.647225	-3.07468	1.807673
H	2.486214	-4.61396	-0.523009
H	1.367348	-3.271928	-0.228665
H	3.425049	-3.318374	-2.322488
H	2.287243	-2.023294	-1.90868
H	4.602461	0.541999	0.612166
H	2.426581	1.454554	2.298404
H	1.157568	2.748078	0.857376
H	2.83782	3.786935	-1.218655
H	2.457472	4.586567	0.314794
H	4.864688	2.809697	-0.291995
H	4.876656	4.407674	0.467101
H	3.677893	3.506039	2.448852
H	4.97808	2.334584	2.171368
H	-0.07254	1.126827	0.081029
H	0.827939	-0.031041	-2.478714
H	-0.106329	-2.015038	-3.364401
H	-1.469229	-2.757174	-2.496274
H	-1.754213	-0.520013	-4.205689
H	-2.855514	-0.827593	-2.850745
H	-1.053687	1.436941	-2.979311
H	-1.941983	0.863997	-1.552904
H	0.383388	-1.032054	0.987391
H	-2.225706	-2.028428	1.929937
H	-2.598821	-0.153341	3.421368
H	0.205293	0.788564	2.650218
H	-0.712559	1.340907	4.059914
H	1.058323	-0.746374	4.27196
H	-0.477158	-0.814294	5.149077
H	0.357726	-2.515401	2.869451
H	-1.076416	-2.673977	3.887381
H	-4.100775	-0.004945	1.593375
H	-3.348894	2.16657	-0.245832
H	-4.475665	2.364182	-2.353739
H	-5.9413	1.380597	-2.581408
H	-5.867069	3.7815	-1.057336
H	-7.074228	2.510371	-0.810571
H	-5.057663	3.21843	1.138023
H	-6.03187	1.736932	1.142614
H	-3.943248	-1.479091	-0.189346
H	-6.670823	-2.386548	0.530717
H	-5.134663	-3.284375	0.65783
H	-5.914751	-3.044838	-0.929673