Electronic supplementary information (ESI)

Probing the role of electrostatics of polypeptide main-chain in protein folding by perturbing N-terminal residue stereochemistry: A DFT study with oligoalanine models

Bhupesh Goyal,* Kinshuk Raj Srivastava, Anil Kumar, G. Naresh Patwari, and Susheel Durani*

Department of Chemistry, Indian Institute of Technology Bombay,

Mumbai–400076, India

*Corresponding author

E-mail address: bhupesh@iitbombay.org

Present Address

[1]Department of Chemistry, School of Basic and Applied Sciences, Sri Guru Granth Sahib World University, Fatehgarh Sahib–140406, Punjab, India

[2]Department of Chemistry, University of Toronto, Toronto, ON, M5S 3H6

[3]Department of Physics and Astronomy, Michigan State University, East Lansing, USA

Table of Contents

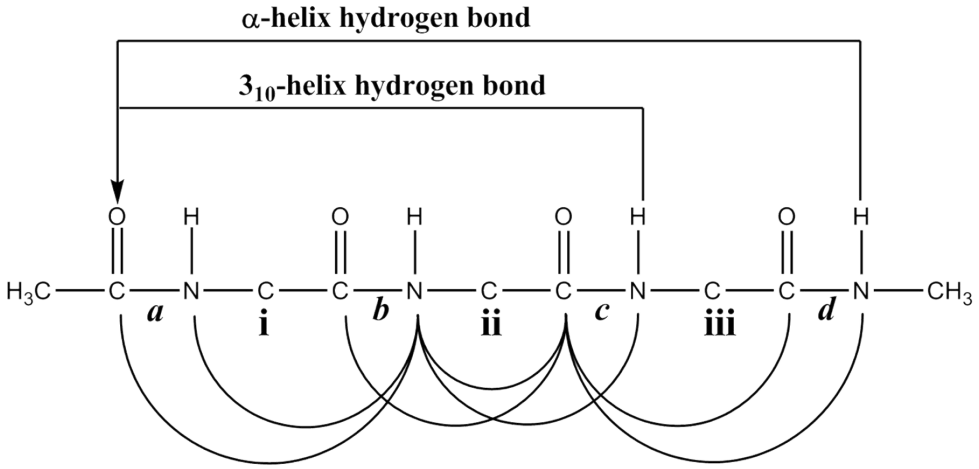


Fig. S1. Interactions of peptides **a**, **b**, **c**, and **d** of residues **i**, **ii**, and **iii** shown as curved lines define sequence-local electrostatics (C_{local}). Interactions of peptides **a** and **d**, and of **a** and **c** characterizing α-helix and 3_{10}-helix hydrogen bonds (C_{Hb}) are noted to be excluded from C_{local}. Interactions characterizing C_{local} are noted to encompass the chain segments that define C_{local}.

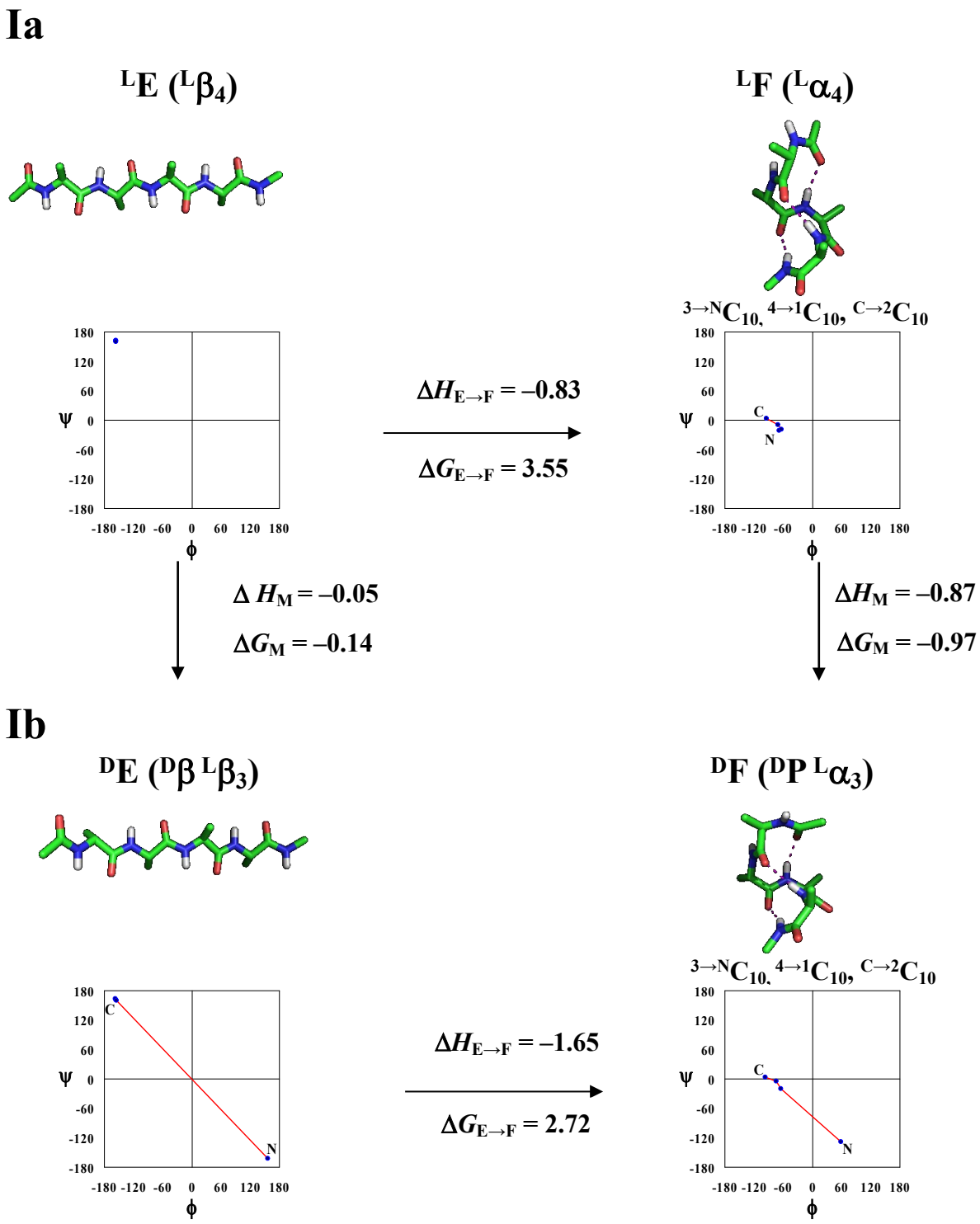


Fig. S2. Enthalpy change ($\Delta H_{E\rightarrow F}$, ΔH_M) and free energy change ($\Delta G_{E\rightarrow F}$, ΔG_M) (kcal/mol) in folding (subscript E→F) of end-protected tetraalanine (**Ia**, **Ib**) from $^{L/D}$**E** to $^{L/D}$**F** structures and their mutation of the folds (subscript M) from ^{L}**E**/^{L}**F** to ^{D}**E**/^{D}**F** structures in vacuum, showing the accompanying changes in φ, ψ's and hydrogen bonds.

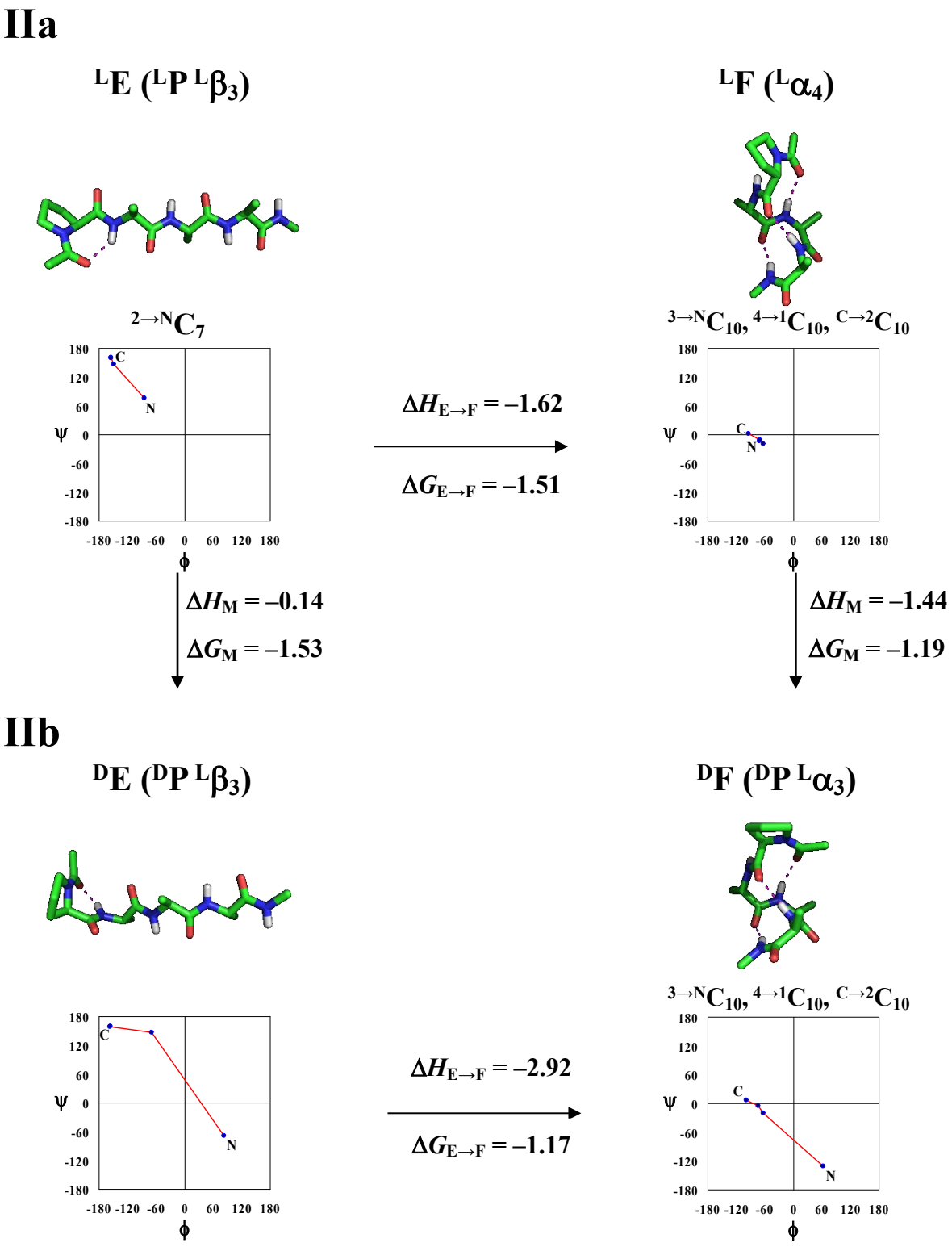


Fig. S3. Enthalpy change ($\Delta H_{E\rightarrow F}$, ΔH_M) and free energy change ($\Delta G_{E\rightarrow F}$, ΔG_M) (kcal/mol) in folding (subscript E→F) of end-protected proline (**IIa**, **IIb**) peptides from $^{L/D}$**E** to $^{L/D}$**F** structures and their mutation of the folds (subscript M) from ^{L}**E**/^{L}**F** to ^{D}**E**/^{D}**F** structures in vacuum, showing the accompanying changes in φ, ψ's and hydrogen bonds.

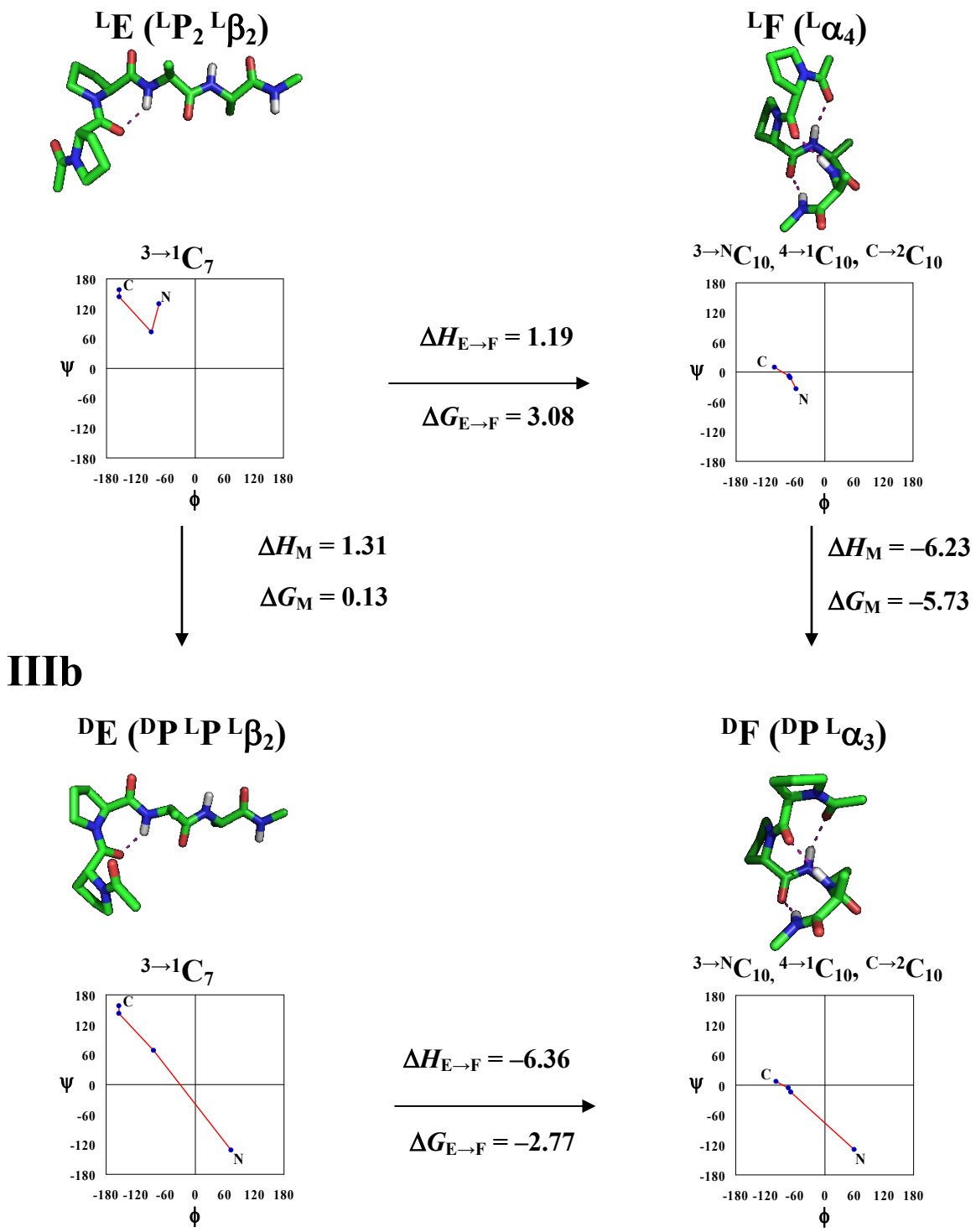


Fig. S4. Enthalpy change ($\Delta H_{E\rightarrow F}$, ΔH_M) and free energy change ($\Delta G_{E\rightarrow F}$, ΔG_M) (kcal/mol) in folding (subscript E→F) of end-protected diproline (**IIIa**, **IIIb**) peptides from $^{L/D}$**E** to $^{L/D}$**F** structures and their mutation of the folds (subscript M) from ^{L}**E**/^{L}**F** to ^{D}**E**/^{D}**F** structures in vacuum, showing the accompanying changes in φ, ψ's and hydrogen bonds.

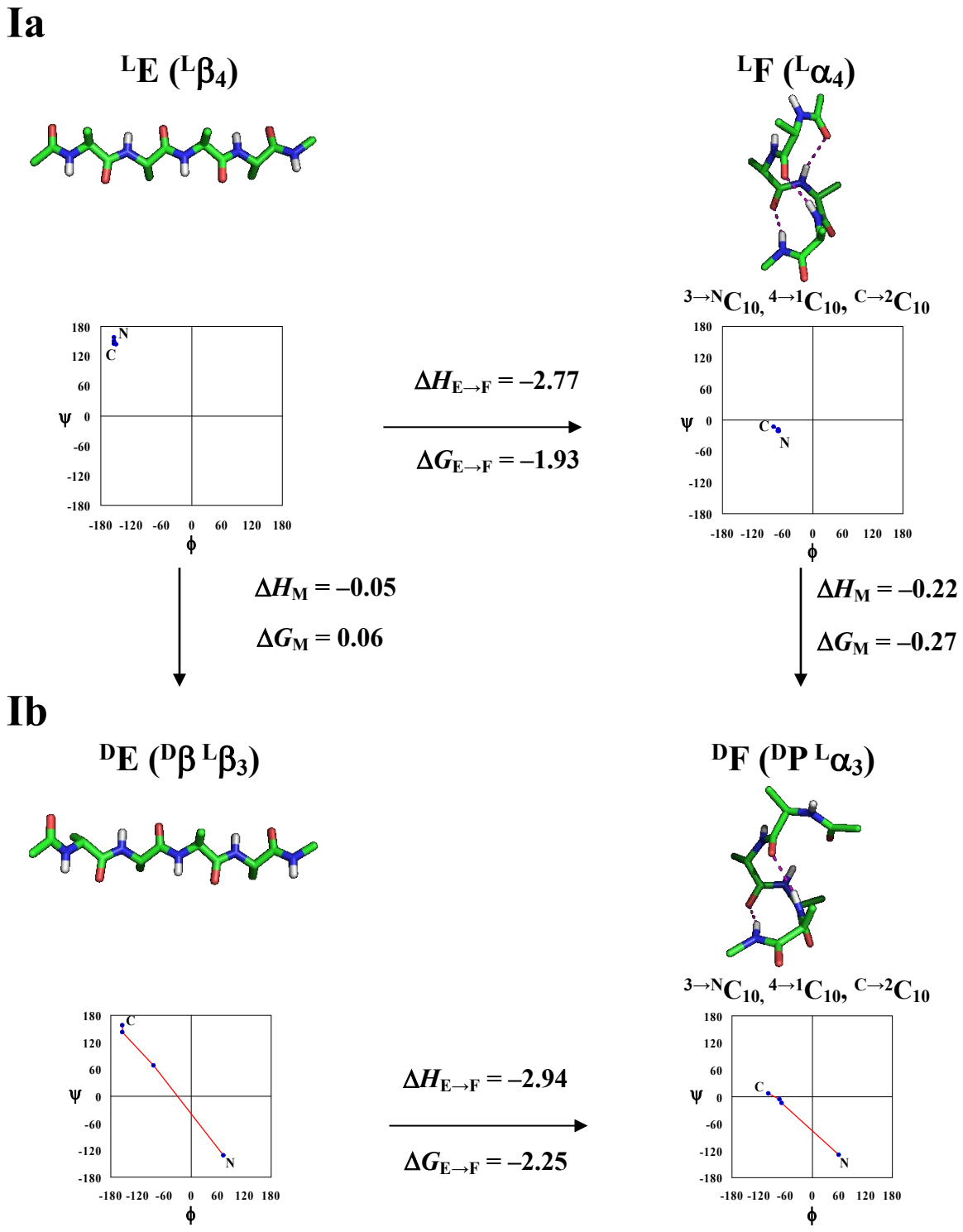


Fig. S5. Enthalpy change ($\Delta H_{E\rightarrow F}$, ΔH_M) and free energy change ($\Delta G_{E\rightarrow F}$, ΔG_M) (kcal/mol) in folding (subscript E→F) of end-protected tetraalanine (**Ia**, **Ib**) from $^{L/D}$**E** to $^{L/D}$**F** structures and their mutation of the folds (subscript M) from ^{L}**E**/^{L}**F** to ^{D}**E**/^{D}**F** structures in solvent, showing the accompanying changes in φ, ψ's and hydrogen bonds.

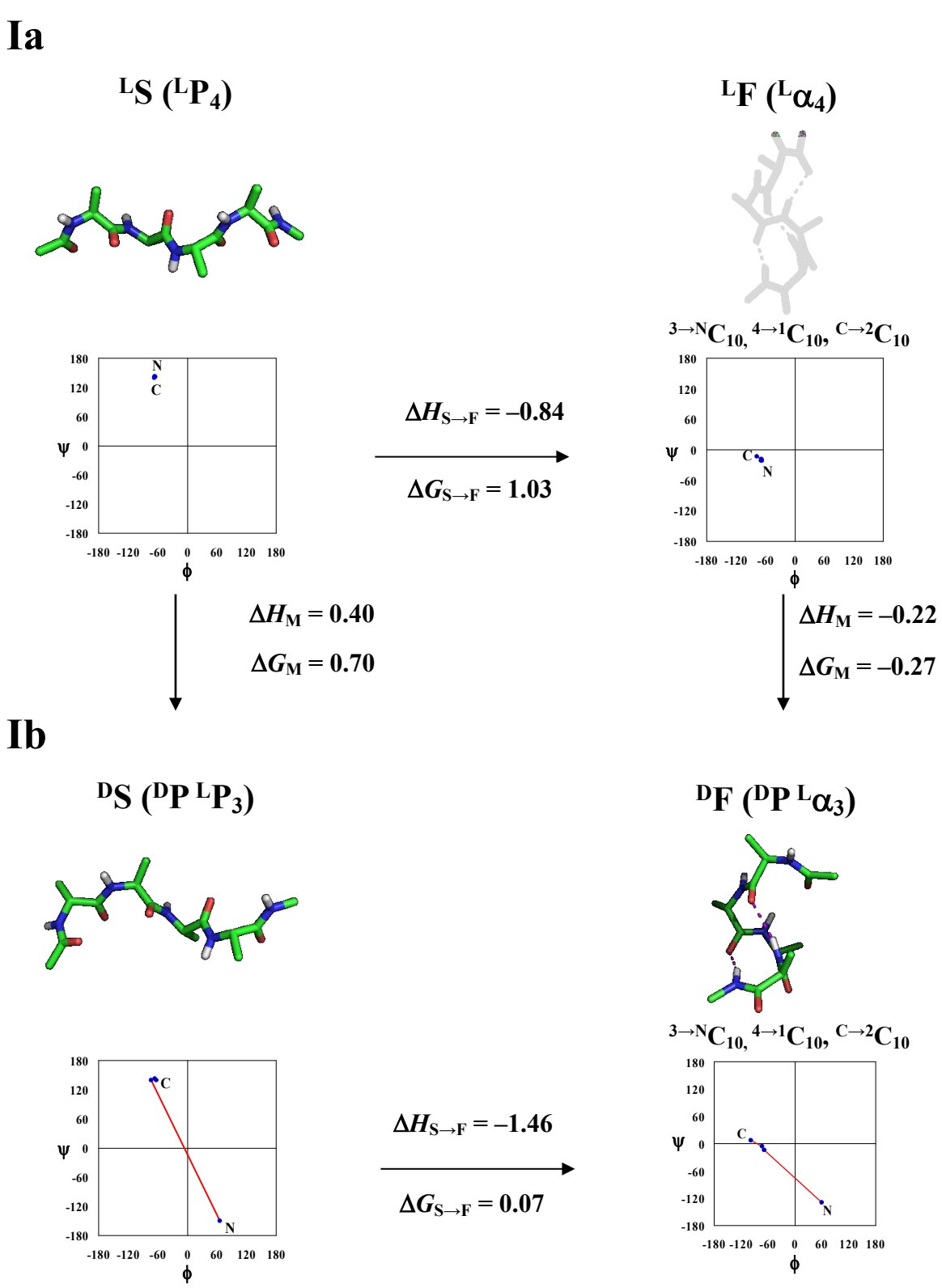


Fig. S6. Enthalpy change ($\Delta H_{S\rightarrow F}$, ΔH_M) and free energy change ($\Delta G_{S\rightarrow F}$, ΔG_M) (kcal/mol) in folding (subscript S→F) of end-protected tetraalanine (**Ia**, **Ib**) from $^{L/D}$**S** to $^{L/D}$**F** structures and their mutation of the folds (subscript M) from ^{L}**S**/^{L}**F** to ^{D}**S**/^{D}**F** structures in solvent, showing the accompanying changes in φ, ψ's and hydrogen bonds.

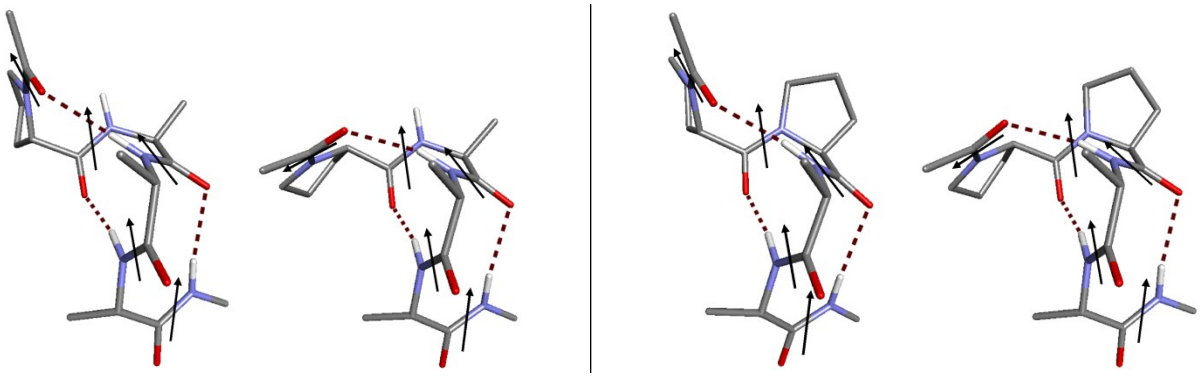
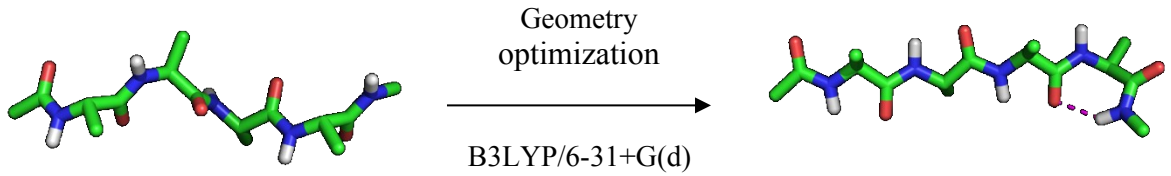
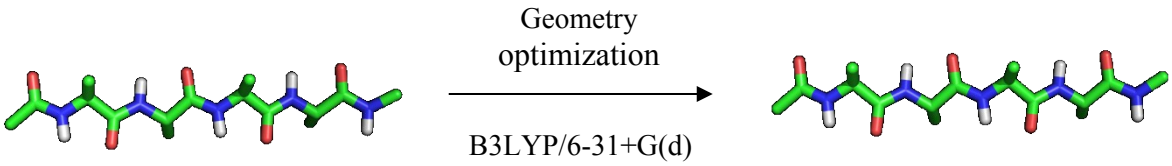


Fig. S7. The end-protected proline (**IIa**, **IIb**) and diproline (**IIIa**, **IIIb**) peptides as 3_{10}-helix (^{L}**F**) and ^{D}PPII-capped-3_{10}-helix (^{D}**F**) folds are identical in the donor-acceptor specificity of backbone hydrogen bonds, however, distinct in geometry of dipoles of backbone peptide units due to a ~90^{o} tilt in the dipole of a backbone peptide unit caused by the L- to D-stereochemical mutation of the N-terminal residue. The model peptides are shown in stick representation with hydrogen bonds between backbone CO and NH groups shown as dashed line in brown colour.



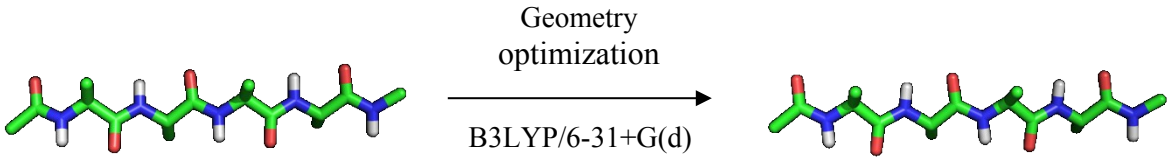
	φ	ψ
Ala_1	–78.0	149.0
Ala_2	–78.0	149.0
Ala_3	–78.0	149.0
Ala_4	–78.0	149.0

	φ	ψ
Ala_1	–156.2	162.4
Ala_2	–156.3	162.7
Ala_3	–154.7	158.6
Ala_4	–83.7	77.2



	φ	ψ
Ala_1	–156.2	162.4
Ala_2	–156.3	162.7
Ala_3	–154.7	158.6
Ala_4	–154.2	159.6

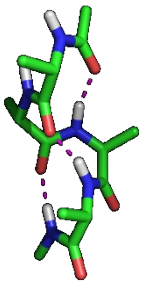
	φ	ψ
Ala_1	–155.7	161.6
Ala_2	–156.6	162.7
Ala_3	–155.7	161.8
Ala_4	–156.5	161.1



	φ	ψ
Ala_1	–155.0	160.0
Ala_2	–155.0	160.0
Ala_3	–155.0	160.0
Ala_4	–155.0	160.0

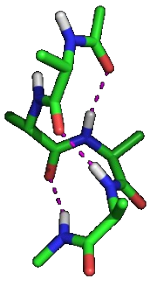
	φ	ψ
Ala_1	–155.7	161.7
Ala_2	–156.3	162.5
Ala_3	–155.9	161.9
Ala_4	–156.4	159.8

Fig. S8. Minimum energy conformers of end-protected tetraalanine (**Ia**) achieved from different starting structures in correspondence of polyproline-II and extended β-conformation. All minima are extended β-structures with exception of one structure having a terminal residue locked in a hydrogen-bonded γ-turn structure.



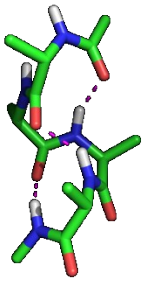
Geometry optimization

B3LYP/6-31+G(d)



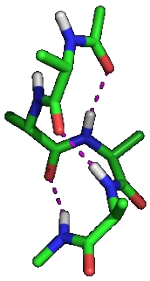
	φ	ψ
Ala_1	–50.0	–30.0
Ala_2	–50.0	–30.0
Ala_3	–50.0	–30.0
Ala_4	–50.0	–30.0

	φ	ψ
Ala_1	–68.1	–21.1
Ala_2	–63.5	–18.5
Ala_3	–70.8	–9.6
Ala_4	–94.7	3.3



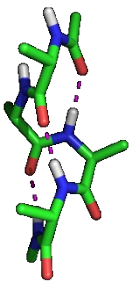
Geometry optimization

B3LYP/6-31+G(d)



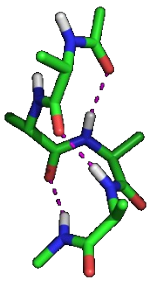
	φ	ψ
Ala_1	–55.0	–35.0
Ala_2	–55.0	–35.0
Ala_3	–55.0	–35.0
Ala_4	–55.0	–35.0

	φ	ψ
Ala_1	–68.1	–21.1
Ala_2	–63.5	–18.5
Ala_3	–70.8	–9.6
Ala_4	–94.7	3.2



Geometry optimization

B3LYP/6-31+G(d)



	φ	ψ
Ala_1	–45.0	–25.0
Ala_2	–45.0	–25.0
Ala_3	–45.0	–25.0
Ala_4	–45.0	–25.0

	φ	ψ
Ala_1	–68.1	–21.2
Ala_2	–63.4	–18.5
Ala_3	–70.8	–9.7
Ala_4	–94.6	3.2

Fig. S9. Optimized geometry in end-protected tetraalanine (**Ia**) achieved in independent runs of optimization starting with 3_{10}-helical folds varied by ± 5° in φ, ψ's. The optimized structures converge to similar conformation irrespective of the starting conformation.

Table S1. Specific dihedral angles for **E** and **F** folds of end-protected tetraalanine (**Ia**, **Ib**), proline (**IIa**, **IIb**) and diproline (**IIIa**, **IIIb**) peptides in correspondence of the optimized structures obtained in vacuum.

		Ia		**Ib**		**IIa**		**IIb**		**IIIa**		**IIIb**	
Residue		^{L}**E**	^{L}**F**	^{D}**E**	^{D}**F**	^{L}**E**	^{L}**F**	^{D}**E**	^{D}**F**	^{L}**E**	^{L}**F**	^{D}**E**	^{D}**F**
1	φ1	–155.7	–68.1	155.9	58.6	–85.3	–72.4	82.8	61.9	–72.9	–58.2	73.1	60.3
	ψ1	161.7	–21.1	–162.0	–128.7	76.4	–12.4	–68.2	–130.2	129.6	–33.6	–131.8	–129.6
	ω1	174.7	177.7	–179.9	–178.7	–178.5	172.7	170.1	–179.3	–173.8	–179.5	–171.7	–176.5
2	φ2	–156.3	–63.5	–156.9	–64.4	–149.7	–63.1	–69.3	–64.1	–88.4	–69.0	–83.4	–68.6
	ψ2	162.5	–18.5	160.8	–20.1	146.7	–18.5	147.5	–19.6	72.5	–11.6	68.1	–14.0
	ω2	174.7	178.1	–179.9	178.9	–178.5	178.3	170.1	178.4	–173.8	175.1	–171.7	176.1
3	φ3	–155.9	–70.8	–157.4	–74.7	–155.0	–70.2	–157.8	–74.3	–153.2	–71.6	–153.3	–72.9
	ψ3	161.9	–9.6	163.5	–4.4	161.6	–10.2	159.3	–5.1	143.4	–7.8	142.9	–6.2
	ω3	174.6	173.9	174.8	171.0	173.4	174.2	176.1	171.5	–178.7	173.6	–177.0	171.5
4	φ4	–156.4	–94.7	–155.2	–96.9	–155.0	–94.5	–156.1	–99.2	–154.4	–101.6	–153.8	–98.6
	ψ4	159.8	3.3	160.1	4.0	159.6	2.5	160.0	6.8	158.2	9.1	157.3	6.5
	ω4	175.2	177.0	174.8	177.3	174.8	176.9	174.5	177.2	174.3	176.8	174.3	176.9

Table S2. Specific dihedral angles for **E, S** and **F** folds of end-protected tetraalanine (**Ia**, **Ib**) in correspondence of the optimized structures obtained in presence of solvent.

		Ia			**Ib**		
Residue		^{L}**E**	^{L}**S**	^{L}**F**	^{D}**E**	^{D}**S**	^{D}**F**
1	φ1	–154.0	–66.1	–68.7	151.9	65.5	66.4
	ψ1	150.5	141.1	–21.1	–152.5	–149.7	–142.8
	ω1	175.1	176.9	–179.9	–173.6	–173.0	–171.9
2	φ2	–153.1	–66.9	–66.6	–158.1	–73.7	–71.5
	ψ2	157.2	139.5	–20.9	143.5	139.1	–20.9
	ω2	175.1	176.9	–179.9	–173.6	–173.0	–171.9
3	φ3	–149.2	–65.8	–68.1	–154.5	–66.4	–69.8
	ψ3	143.4	142.3	–18.4	152.1	142.8	–19.7
	ω3	176.9	174.9	179.9	177.3	173.5	179.7
4	φ4	–154.0	–65.3	–77.7	–153.0	–62.6	–81.8
	ψ4	145.1	141.4	–13.6	146.8	139.4	–11.5
	ω4	178.6	177.2	175.6	176.6	175.4	177.1

Table S3. Thermodynamic parameters for **E, S** and **F** folds of end-protected tetraalanine (**Ia**, **Ib**), proline (**IIa**, **IIb**) and diproline (**IIIa**, **IIIb**) peptides in correspondence of the optimized structures obtained in vacuum and in presence of solvent.

Peptide		Medium	Basis Set	E / Hartrees	U / Hartrees	H / Hartrees	G / Hartrees
Ia	^{L}**E**	vacuum	6-31+G(d)	–1237.456419	–1237.426463	–1237.425518	–1237.524427
	^{L}**F**	vacuum	6-31+G(d)	–1237.456889	–1237.427780	–1237.426836	–1237.518764
Ib	^{D}**E**	vacuum	6-31+G(d)	–1237.456533	–1237.426540	–1237.425595	–1237.524646
	^{D}**F**	vacuum	6-31+G(d)	–1237.458335	–1237.429174	–1237.428230	–1237.520312
Ia	^{L}**E**	solvent	6-31+G(d)	–1237.509116	–1237.479926	–1237.478982	–1237.572094
	^{L}**S**	solvent	6-31+G(d)	–1237.512512	–1237.482991	–1237.482047	–1237.576812
	^{L}**F**	solvent	6-31+G(d)	–1237.513192	–1237.484335	–1237.483390	–1237.575167
Ib	^{D}**E**	solvent	6-31+G(d)	–1237.509217	–1237.479999	–1237.479055	–1237.572006
	^{D}**S**	solvent	6-31+G(d)	–1237.511133	–1237.482358	–1237.481413	–1237.575698
	^{D}**F**	solvent	6-31+G(d)	–1237.513680	–1237.484677	–1237.483733	–1237.575590
IIa	^{L}**E**	vacuum	6-31+G(d)	–1314.831978	–1314.803124	–1314.802180	–1314.895857
	^{L}**F**	vacuum	6-31+G(d)	–1314.835552	–1314.805698	–1314.804754	–1314.898257
IIb	^{D}**E**	vacuum	6-31+G(d)	–1314.832912	–1314.803346	–1314.802402	–1314.898297
	^{D}**F**	vacuum	6-31+G(d)	–1314.837772	–1314.807992	–1314.807048	–1314.900155
IIIa	^{L}**E**	vacuum	6-31+G(d)	–1392.207330	–1392.176832	–1392.175888	–1392.274977
	^{L}**F**	vacuum	6-31+G(d)	–1392.205737	–1392.174935	–1392.173990	–1392.270064
IIIb	^{D}**E**	vacuum	6-31+G(d)	–1392.206168	–1392.174740	–1392.173796	–1392.274775
	^{D}**F**	vacuum	6-31+G(d)	–1392.215440	–1392.184871	–1392.183926	–1392.279195

Cartesian coordinates of the optimized geometries of end-protected tetraalanine (**Ia**, **Ib**), proline (**IIa**, **IIb**) and diproline (**IIIa**, **IIIb**) peptides in fully-extended (^{L}**E** and ^{D}**E**), fully-folded structures (^{L}**F** and ^{D}**F**) and ^{D}PPII-capped-3_{10}-helix folds in vacuum.

Ia (^{L}E: $^{L}\beta_4$)

1	6	0	-8.839097	0.778152	-0.034685
2	6	0	-7.669262	-0.112475	0.352778
3	8	0	-7.794182	-1.030303	1.164982
4	7	0	-6.483878	0.166432	-0.256868
5	1	0	-6.377112	0.967384	-0.870372
6	6	0	-5.258777	-0.553230	0.045803
7	6	0	-5.167893	-1.888468	-0.721182
8	6	0	-4.088037	0.374409	-0.317835
9	8	0	-4.236679	1.329341	-1.087080
10	7	0	-2.896745	0.053641	0.236846
11	1	0	-2.790975	-0.760180	0.836241
12	6	0	-1.660235	0.749739	-0.083373
13	6	0	-1.515362	2.063979	0.710082
14	6	0	-0.509655	-0.221201	0.233156
15	8	0	-0.678208	-1.194480	0.974010
16	7	0	0.681333	0.083719	-0.328696
17	1	0	0.802439	0.913417	-0.903040
18	6	0	1.903270	-0.655733	-0.048442
19	6	0	2.006535	-1.941736	-0.892585
20	6	0	3.073022	0.298934	-0.342099
21	8	0	2.921316	1.297098	-1.053633
22	7	0	4.260297	-0.046366	0.202916
23	1	0	4.368129	-0.888942	0.761220
24	6	0	5.491797	0.684468	-0.055449
25	6	0	5.612856	1.938966	0.832971
26	6	0	6.649288	-0.294792	0.208517
27	8	0	6.489184	-1.288041	0.918942
28	7	0	7.832630	0.034016	-0.368998
29	1	0	7.871893	0.866207	-0.942681
30	6	0	9.061844	-0.721859	-0.164163
31	1	0	9.765165	-0.171027	0.471731
32	1	0	9.538051	-0.935249	-1.126416
33	1	0	8.802572	-1.661341	0.325614
34	1	0	6.528107	2.497977	0.606137
35	1	0	5.630306	1.658341	1.891528
36	1	0	4.756326	2.594094	0.651720
37	1	0	5.487265	0.992924	-1.107780
38	1	0	2.913570	-2.504633	-0.645264
39	1	0	2.025893	-1.698925	-1.960678
40	1	0	1.140345	-2.576977	-0.687978
41	1	0	1.900659	-0.928290	1.013524
42	1	0	-0.598568	2.595379	0.430537

43	1	0	-1.487424	1.861126	1.786327
44	1	0	-2.369301	2.711366	0.492420
45	1	0	-1.667359	0.982748	-1.154837
46	1	0	-4.262180	-2.442445	-0.448662
47	1	0	-5.156631	-1.709663	-1.802193
48	1	0	-6.036967	-2.503216	-0.470956
49	1	0	-5.246472	-0.765578	1.121695
50	1	0	-9.222123	1.268570	0.866291
51	1	0	-9.642886	0.151030	-0.433790
52	1	0	-8.581378	1.541984	-0.775461

Ia (^{L}F: $^{L}\alpha_4$)

1	6	0	5.389262	1.201086	-0.808989
2	6	0	4.040430	0.509135	-0.823485
3	8	0	2.991229	1.123656	-1.017460
4	7	0	4.040387	-0.843416	-0.594325
5	1	0	4.934023	-1.317581	-0.546929
6	6	0	2.857633	-1.669432	-0.861278
7	6	0	3.232913	-3.155448	-0.812911
8	6	0	1.676755	-1.385457	0.082717
9	8	0	0.538299	-1.709937	-0.255693
10	7	0	1.950615	-0.788453	1.269363
11	1	0	2.903900	-0.504526	1.455430
12	6	0	0.901289	-0.428469	2.219258
13	6	0	1.521576	0.033404	3.542468
14	6	0	-0.089664	0.628717	1.687028
15	8	0	-1.183528	0.746237	2.247189
16	7	0	0.287504	1.381443	0.626660
17	1	0	1.184674	1.217359	0.175365
18	6	0	-0.606015	2.377274	0.033927
19	6	0	0.186572	3.341174	-0.855793
20	6	0	-1.803314	1.780016	-0.741791
21	8	0	-2.704148	2.534580	-1.104449
22	7	0	-1.800640	0.439494	-0.968968
23	1	0	-1.007004	-0.120877	-0.671579
24	6	0	-2.930525	-0.259135	-1.573775
25	6	0	-2.445603	-1.330140	-2.558474
26	6	0	-3.905649	-0.874924	-0.541888
27	8	0	-4.870980	-1.534572	-0.933802
28	7	0	-3.653853	-0.649138	0.768695
29	1	0	-2.869765	-0.069555	1.047266
30	6	0	-4.555130	-1.134527	1.801704
31	1	0	-4.124687	-0.890958	2.775706
32	1	0	-4.685684	-2.218645	1.719732
33	1	0	-5.543752	-0.668441	1.714365
34	1	0	-3.305914	-1.867232	-2.964876
35	1	0	-1.787478	-2.052560	-2.061170
36	1	0	-1.890566	-0.863094	-3.379444
37	1	0	-3.512903	0.497091	-2.109431

38	1	0	-0.500768	4.066427	-1.297895
39	1	0	0.701918	2.808424	-1.662869
40	1	0	0.937188	3.877746	-0.265223
41	1	0	-1.069957	2.936355	0.853063
42	1	0	0.726125	0.295040	4.244655
43	1	0	2.155087	0.918199	3.400350
44	1	0	2.126294	-0.766742	3.984177
45	1	0	0.284689	-1.315179	2.397748
46	1	0	2.345433	-3.761988	-1.010205
47	1	0	3.629823	-3.435572	0.170374
48	1	0	3.983404	-3.389200	-1.577083
49	1	0	2.473688	-1.422674	-1.857624
50	1	0	6.200444	0.570459	-0.431525
51	1	0	5.320315	2.106649	-0.199756
52	1	0	5.633217	1.512226	-1.831187

Ib (^{D}E: $^{D}\beta\,^{L}\beta_3$)

1	6	0	-8.409812	-0.815951	-1.615721
2	6	0	-7.405021	-0.963314	-0.484131
3	8	0	-7.515485	-1.843432	0.370731
4	7	0	-6.385846	-0.059898	-0.474430
5	6	0	-5.310454	-0.102732	0.501335
6	6	0	-5.712084	0.559849	1.834846
7	6	0	-4.101627	0.608409	-0.129038
8	8	0	-4.233792	1.378944	-1.085364
9	7	0	-2.907291	0.356237	0.454021
10	6	0	-1.659498	0.940930	-0.012985
11	6	0	-1.458785	2.375863	0.514103
12	6	0	-0.530366	0.011954	0.464058
13	8	0	-0.701783	-0.775218	1.399734
14	7	0	0.646120	0.141780	-0.188249
15	6	0	1.852916	-0.572072	0.202048
16	6	0	1.863376	-2.021552	-0.323635
17	6	0	3.039453	0.233628	-0.354398
18	8	0	2.881922	1.071905	-1.247747
19	7	0	4.246192	-0.058345	0.179327
20	6	0	5.486782	0.526113	-0.306565
21	6	0	5.741511	1.920281	0.300703
22	6	0	6.612885	-0.455762	0.063869
23	8	0	6.460292	-1.287161	0.959631
24	7	0	7.763417	-0.314020	-0.641942
25	6	0	8.966814	-1.092264	-0.377188
26	1	0	-6.263581	0.611186	-1.225555
27	1	0	-2.809649	-0.341139	1.186812
28	1	0	0.771783	0.824763	-0.930452
29	1	0	4.357961	-0.782467	0.883900
30	1	0	7.800025	0.395091	-1.362353
31	1	0	9.734835	-0.482196	0.113270
32	1	0	9.368929	-1.493082	-1.312965

33	1	0	8.696795	-1.918314	0.281991
34	1	0	6.658682	2.365989	-0.101378
35	1	0	5.836381	1.852503	1.389742
36	1	0	4.903731	2.579215	0.056287
37	1	0	5.410402	0.621640	-1.396355
38	1	0	2.759980	-2.555857	0.009948
39	1	0	1.836598	-2.033399	-1.418772
40	1	0	0.985884	-2.549649	0.059282
41	1	0	1.898807	-0.593349	1.297493
42	1	0	-0.533807	2.813814	0.122259
43	1	0	-1.411366	2.379420	1.608594
44	1	0	-2.297959	2.999104	0.192457
45	1	0	-1.685142	0.967016	-1.108801
46	1	0	-4.905998	0.482318	2.573305
47	1	0	-6.596143	0.054094	2.233009
48	1	0	-5.945823	1.619435	1.681907
49	1	0	-5.067235	-1.154960	0.693268
50	1	0	-9.404677	-0.659423	-1.186158
51	1	0	-8.440998	-1.751815	-2.183195
52	1	0	-8.182323	0.009192	-2.298323

Ib (^{D}F: ^{D}P $^{L}\alpha_3$)

1	6	0	-2.821496	-3.174004	0.841418
2	6	0	-2.960405	-1.715181	0.461787
3	8	0	-2.786149	-0.804308	1.280085
4	7	0	-3.292324	-1.442536	-0.829831
5	1	0	-3.272305	-2.188916	-1.512327
6	6	0	-3.372912	-0.069667	-1.314895
7	6	0	-3.766076	-0.060236	-2.795566
8	6	0	-2.017059	0.639344	-1.119919
9	8	0	-0.970485	0.148285	-1.542205
10	7	0	-2.062662	1.839348	-0.483809
11	1	0	-2.924643	2.114421	-0.029751
12	6	0	-0.866245	2.644444	-0.249522
13	6	0	-1.258546	4.031542	0.272551
14	6	0	0.167664	1.989353	0.689238
15	8	0	1.332506	2.398526	0.661697
16	7	0	-0.253045	1.000299	1.513070
17	1	0	-1.198379	0.631335	1.431994
18	6	0	0.669721	0.312466	2.416048
19	6	0	-0.096374	-0.352515	3.564377
20	6	0	1.614122	-0.694960	1.718966
21	8	0	2.496800	-1.235454	2.383023
22	7	0	1.435467	-0.904761	0.386062
23	1	0	0.665345	-0.450435	-0.096085
24	6	0	2.373861	-1.677943	-0.421420
25	6	0	1.632209	-2.604216	-1.392771
26	6	0	3.400424	-0.806379	-1.184336
27	8	0	4.203454	-1.343246	-1.950736

28	7	0	3.375574	0.528562	-0.963641
29	1	0	2.720222	0.928415	-0.301094
30	6	0	4.342531	1.413216	-1.595146
31	1	0	4.087095	2.442739	-1.334593
32	1	0	4.318402	1.293568	-2.683193
33	1	0	5.361076	1.193627	-1.254005
34	1	0	2.356202	-3.136651	-2.014191
35	1	0	0.964505	-2.032599	-2.048528
36	1	0	1.033498	-3.332333	-0.833926
37	1	0	2.962290	-2.276771	0.280653
38	1	0	0.610369	-0.886746	4.203770
39	1	0	-0.842029	-1.061535	3.188656
40	1	0	-0.615051	0.404330	4.162905
41	1	0	1.346680	1.069966	2.824761
42	1	0	-0.357191	4.627227	0.436753
43	1	0	-1.798967	3.960842	1.225002
44	1	0	-1.892135	4.550847	-0.455095
45	1	0	-0.341487	2.750177	-1.204110
46	1	0	-3.874240	0.968067	-3.154557
47	1	0	-4.722866	-0.574048	-2.940499
48	1	0	-2.996085	-0.550146	-3.401332
49	1	0	-4.139864	0.447201	-0.725122
50	1	0	-3.111862	-3.861563	0.041253
51	1	0	-3.437843	-3.369627	1.724051
52	1	0	-1.779329	-3.369794	1.115879

IIa (^{L}E: ^{L}P $^{L}\beta_3$)

1	6	0	6.340787	2.515227	1.135160
2	6	0	5.396616	1.727305	0.243768
3	8	0	4.378706	2.241464	-0.234524
4	7	0	5.720505	0.424887	0.000513
5	6	0	4.950863	-0.379240	-0.975676
6	6	0	5.963843	-1.438719	-1.431144
7	6	0	6.853886	-1.648493	-0.194109
8	6	0	6.971026	-0.241324	0.412728
9	6	0	3.694522	-1.010036	-0.321670
10	8	0	3.648576	-2.207367	-0.025411
11	7	0	2.666926	-0.150889	-0.122974
12	1	0	2.800078	0.843256	-0.313471
13	6	0	1.426173	-0.573192	0.509399
14	6	0	1.480619	-0.430244	2.044063
15	6	0	0.281493	0.274807	-0.061766
16	8	0	0.440183	1.458591	-0.359302
17	7	0	-0.912815	-0.362075	-0.169522
18	1	0	-1.027463	-1.330078	0.114713
19	6	0	-2.134361	0.324694	-0.556572
20	6	0	-2.256884	0.467279	-2.087500
21	6	0	-3.307557	-0.482656	0.020881
22	8	0	-3.174784	-1.664109	0.354340

23	7	0	-4.485340	0.178065	0.107382
24	1	0	-4.580849	1.141411	-0.201046
25	6	0	-5.720171	-0.467180	0.524603
26	6	0	-5.841556	-0.540026	2.060244
27	6	0	-6.876532	0.344880	-0.083750
28	8	0	-6.719810	1.518456	-0.421667
29	7	0	-8.060675	-0.313544	-0.177942
30	1	0	-8.088265	-1.289435	0.086405
31	6	0	-9.285689	0.304420	-0.667835
32	1	0	-10.083204	0.225933	0.079254
33	1	0	-9.617556	-0.169087	-1.598881
34	1	0	-9.075608	1.357294	-0.860092
35	1	0	-6.758077	-1.060942	2.360641
36	1	0	-5.856191	0.466579	2.491708
37	1	0	-4.985522	-1.088048	2.463550
38	1	0	-5.718163	-1.486891	0.121204
39	1	0	-3.163029	1.018841	-2.362794
40	1	0	-2.288870	-0.518978	-2.563594
41	1	0	-1.389887	1.016182	-2.465217
42	1	0	-2.114685	1.326855	-0.111794
43	1	0	0.548176	-0.778759	2.503795
44	1	0	1.638980	0.616714	2.324086
45	1	0	2.305223	-1.033789	2.435864
46	1	0	1.282049	-1.628489	0.256959
47	1	0	7.066073	-0.259725	1.503936
48	1	0	7.838938	0.296502	0.005521
49	1	0	7.834876	-2.069693	-0.436150
50	1	0	6.351199	-2.323855	0.504719
51	1	0	6.551494	-1.040286	-2.267559
52	1	0	5.471084	-2.358326	-1.752331
53	1	0	4.629596	0.281508	-1.787460
54	1	0	6.443936	2.046191	2.120853
55	1	0	5.936201	3.521089	1.256480
56	1	0	7.343812	2.581643	0.696080

IIa (^{L}F: $^{L}\alpha_4$)

1	6	0	4.941060	1.847096	-0.708836
2	6	0	3.664230	1.030638	-0.767533
3	8	0	2.567148	1.549911	-1.004463
4	7	0	3.764013	-0.311191	-0.517776
5	6	0	2.620366	-1.202403	-0.794297
6	6	0	3.249398	-2.616767	-0.794506
7	6	0	4.513333	-2.465701	0.068932
8	6	0	5.015123	-1.060774	-0.287231
9	6	0	1.441468	-1.071371	0.180640
10	8	0	0.359712	-1.585271	-0.106723
11	7	0	1.641535	-0.369740	1.325508
12	1	0	2.529504	0.100156	1.444442

13	6	0	0.548867	-0.054653	2.241378
14	6	0	1.099152	0.564119	3.530798
15	6	0	-0.539404	0.851340	1.625687
16	8	0	-1.649200	0.892973	2.165172
17	7	0	-0.228058	1.558360	0.513685
18	1	0	0.696602	1.479905	0.094708
19	6	0	-1.212243	2.411461	-0.154199
20	6	0	-0.513086	3.369302	-1.124750
21	6	0	-2.342346	1.638454	-0.874009
22	8	0	-3.313586	2.268603	-1.288364
23	7	0	-2.203136	0.291842	-1.001134
24	1	0	-1.360552	-0.160822	-0.659521
25	6	0	-3.253657	-0.561263	-1.548229
26	6	0	-2.657695	-1.649328	-2.449785
27	6	0	-4.168568	-1.192996	-0.471781
28	8	0	-5.067448	-1.964690	-0.814113
29	7	0	-3.940359	-0.857903	0.819501
30	1	0	-3.215754	-0.188714	1.055733
31	6	0	-4.794674	-1.354319	1.886609
32	1	0	-4.389522	-1.008337	2.840267
33	1	0	-4.825093	-2.448850	1.877012
34	1	0	-5.821751	-0.987430	1.773589
35	1	0	-3.457041	-2.301164	-2.810285
36	1	0	-1.930902	-2.260533	-1.901300
37	1	0	-2.150414	-1.192617	-3.306702
38	1	0	-3.906245	0.089846	-2.138104
39	1	0	-1.266327	3.982971	-1.624567
40	1	0	0.056303	2.822815	-1.884994
41	1	0	0.178895	4.024687	-0.584858
42	1	0	-1.732537	2.989232	0.616877
43	1	0	0.271469	0.796000	4.205764
44	1	0	1.642556	1.495646	3.326701
45	1	0	1.775112	-0.135542	4.035014
46	1	0	0.026997	-0.986780	2.478316
47	1	0	5.606051	-0.600371	0.510195
48	1	0	5.628306	-1.079777	-1.199788
49	1	0	5.263651	-3.235670	-0.133513
50	1	0	4.259868	-2.515298	1.134740
51	1	0	3.521770	-2.890552	-1.820049
52	1	0	2.550228	-3.371027	-0.425391
53	1	0	2.191660	-0.954839	-1.770374
54	1	0	5.374307	1.836301	0.298953
55	1	0	4.703688	2.876457	-0.980868
56	1	0	5.700256	1.455520	-1.395875

IIb (^{D}E: ^{D}P $^{L}\beta_3$)

1	6	0	-5.134138	-0.972972	2.852398
2	6	0	-5.022399	-0.104184	1.614334

3	8	0	-5.001704	1.134355	1.696116
4	7	0	-4.928484	-0.740409	0.416541
5	6	0	-4.903814	0.002071	-0.864653
6	6	0	-5.388388	-1.042473	-1.876703
7	6	0	-4.850052	-2.367465	-1.309267
8	6	0	-4.993579	-2.200748	0.212640
9	6	0	-3.476177	0.517668	-1.189053
10	8	0	-2.817251	0.079177	-2.132828
11	7	0	-3.029812	1.492906	-0.356998
12	1	0	-3.585250	1.670431	0.481811
13	6	0	-1.645670	1.929802	-0.388649
14	6	0	-1.486899	3.209126	0.445740
15	6	0	-0.707401	0.825159	0.152266
16	8	0	-1.039608	0.077972	1.072230
17	7	0	0.520824	0.790018	-0.423773
18	1	0	0.755465	1.391501	-1.206746
19	6	0	1.567721	-0.121112	0.004590
20	6	0	1.379416	-1.537548	-0.578030
21	6	0	2.906535	0.482490	-0.445910
22	8	0	2.968691	1.296776	-1.371714
23	7	0	4.000561	0.034524	0.214142
24	1	0	3.930325	-0.658526	0.953702
25	6	0	5.354412	0.410045	-0.160665
26	6	0	5.751377	1.784870	0.414629
27	6	0	6.286060	-0.697437	0.361245
28	8	0	5.938112	-1.441732	1.278536
29	7	0	7.505093	-0.758267	-0.234809
30	1	0	7.690339	-0.135474	-1.009995
31	6	0	8.546194	-1.697304	0.160738
32	1	0	9.464732	-1.164259	0.430047
33	1	0	8.764308	-2.403426	-0.648656
34	1	0	8.185311	-2.251865	1.027874
35	1	0	6.759351	2.072569	0.093764
36	1	0	5.727666	1.762587	1.509458
37	1	0	5.046878	2.541357	0.058113
38	1	0	5.399405	0.458297	-1.255560
39	1	0	2.151579	-2.222381	-0.208596
40	1	0	1.425650	-1.511501	-1.672108
41	1	0	0.400776	-1.919852	-0.275958
42	1	0	1.533150	-0.182388	1.098655
43	1	0	-0.453460	3.568805	0.408246
44	1	0	-1.746897	3.021625	1.493719
45	1	0	-2.142836	3.995835	0.057850
46	1	0	-1.384570	2.132556	-1.433356
47	1	0	-5.959719	-2.586604	0.566436
48	1	0	-4.198954	-2.708987	0.768901
49	1	0	-3.795921	-2.478025	-1.581429
50	1	0	-5.392919	-3.244629	-1.675430
51	1	0	-5.015058	-0.834263	-2.881139
52	1	0	-6.485212	-1.046109	-1.897409

53	1	0	-5.574773	0.863216	-0.778036
54	1	0	-5.958804	-1.691543	2.779977
55	1	0	-5.294766	-0.321904	3.712959
56	1	0	-4.208174	-1.540758	3.004563

IIb (^{D}F: ^{D}P $^{L}\alpha_3$)

1	6	0	-2.987180	-1.541646	2.523105
2	6	0	-2.862076	-0.474376	1.455007
3	8	0	-2.389081	0.646679	1.702632
4	7	0	-3.278169	-0.786431	0.200688
5	6	0	-3.192194	0.219882	-0.863402
6	6	0	-3.808770	-0.497212	-2.088343
7	6	0	-3.577524	-1.991983	-1.805388
8	6	0	-3.741046	-2.099430	-0.282664
9	6	0	-1.730253	0.630401	-1.102514
10	8	0	-0.843918	-0.205212	-1.289364
11	7	0	-1.490762	1.968185	-1.123692
12	1	0	-2.223374	2.594003	-0.813098
13	6	0	-0.158779	2.520354	-1.355101
14	6	0	-0.244363	4.039004	-1.547038
15	6	0	0.872920	2.172188	-0.262170
16	8	0	2.074254	2.274261	-0.530548
17	7	0	0.413299	1.777533	0.948938
18	1	0	-0.581534	1.614696	1.093979
19	6	0	1.329426	1.398127	2.024412
20	6	0	0.631768	1.491122	3.385258
21	6	0	1.997414	0.015750	1.834389
22	8	0	2.875791	-0.331199	2.622070
23	7	0	1.594189	-0.734406	0.772754
24	1	0	0.835572	-0.404044	0.182910
25	6	0	2.265663	-1.968017	0.378670
26	6	0	1.250646	-3.072482	0.060494
27	6	0	3.253908	-1.784928	-0.798650
28	8	0	3.801536	-2.771866	-1.295516
29	7	0	3.490493	-0.522265	-1.224013
30	1	0	3.032776	0.264735	-0.777317
31	6	0	4.449383	-0.252259	-2.283926
32	1	0	4.439932	0.820321	-2.490151
33	1	0	4.184563	-0.802283	-3.193241
34	1	0	5.459700	-0.557168	-1.987567
35	1	0	1.777431	-3.968269	-0.276804
36	1	0	0.562849	-2.754531	-0.732232
37	1	0	0.666613	-3.313352	0.955958
38	1	0	2.879465	-2.268724	1.233771
39	1	0	1.325870	1.170748	4.165948
40	1	0	-0.260084	0.856188	3.419132
41	1	0	0.324874	2.523677	3.584782
42	1	0	2.167868	2.101859	1.997874
43	1	0	0.756056	4.440758	-1.726014

44	1	0	-0.655254	4.531255	-0.656459
45	1	0	-0.877394	4.281864	-2.407799
46	1	0	0.240447	2.061493	-2.265035
47	1	0	-4.791051	-2.262150	0.000075
48	1	0	-3.139818	-2.904985	0.147115
49	1	0	-2.559242	-2.272634	-2.089389
50	1	0	-4.279455	-2.637336	-2.342317
51	1	0	-3.359568	-0.168815	-3.029970
52	1	0	-4.881171	-0.272715	-2.131484
53	1	0	-3.775027	1.102339	-0.575031
54	1	0	-3.959777	-2.044576	2.495449
55	1	0	-2.846002	-1.073445	3.498512
56	1	0	-2.210925	-2.305486	2.388639

IIIa (^{L}E: $^{L}P_2$ $^{L}\beta_2$)

1	6	0	-6.000396	-2.395395	-1.658415
2	6	0	-5.300273	-1.323512	-0.841502
3	8	0	-5.515348	-0.119969	-1.023497
4	7	0	-4.414989	-1.747203	0.103335
5	6	0	-3.693606	-0.766398	0.923631
6	6	0	-3.063083	-1.641142	2.031687
7	6	0	-2.840533	-3.004027	1.351403
8	6	0	-4.038080	-3.139741	0.396674
9	6	0	-2.612983	-0.056672	0.085486
10	8	0	-1.783164	-0.733020	-0.540851
11	7	0	-2.568426	1.298253	0.101560
12	6	0	-1.629769	2.010666	-0.799642
13	6	0	-2.339431	3.342324	-1.073270
14	6	0	-3.140031	3.601930	0.213107
15	6	0	-3.614494	2.203908	0.637462
16	6	0	-0.244110	2.199164	-0.133580
17	8	0	0.150948	3.300621	0.256305
18	7	0	0.494580	1.066088	-0.031426
19	1	0	0.087850	0.173814	-0.316291
20	6	0	1.808524	1.068263	0.595198
21	6	0	1.725219	0.911516	2.127345
22	6	0	2.629007	-0.078672	-0.006684
23	8	0	2.119323	-1.168994	-0.269699
24	7	0	3.950007	0.180070	-0.181647
25	1	0	4.353554	1.080129	0.059155
26	6	0	4.893020	-0.831997	-0.627403
27	6	0	4.901469	-0.974382	-2.163314
28	6	0	6.279313	-0.419282	-0.105734
29	8	0	6.534218	0.753830	0.167705
30	7	0	7.186628	-1.426864	-0.010406
31	1	0	6.880921	-2.367406	-0.222315
32	6	0	8.570354	-1.224774	0.396536
33	1	0	9.258861	-1.565556	-0.384975

34	1	0	8.786755	-1.763953	1.325893
35	1	0	8.717069	-0.156782	0.562896
36	1	0	5.588640	-1.766121	-2.484172
37	1	0	5.209940	-0.034208	-2.633069
38	1	0	3.894922	-1.230161	-2.505805
39	1	0	4.588660	-1.788755	-0.186128
40	1	0	2.723004	0.953996	2.580209
41	1	0	1.263469	-0.046898	2.388052
42	1	0	1.123082	1.725294	2.542579
43	1	0	2.273078	2.032861	0.366089
44	1	0	-3.691933	2.108736	1.725626
45	1	0	-4.578037	1.944977	0.185335
46	1	0	-3.983523	4.282998	0.062057
47	1	0	-2.481449	4.033548	0.973737
48	1	0	-3.014777	3.219669	-1.928219
49	1	0	-1.627356	4.140100	-1.293486
50	1	0	-1.500940	1.404251	-1.701853
51	1	0	-3.773448	-3.675689	-0.520398
52	1	0	-4.877047	-3.667782	0.872930
53	1	0	-2.792522	-3.830166	2.068284
54	1	0	-1.911063	-2.982067	0.777507
55	1	0	-3.776539	-1.732196	2.860143
56	1	0	-2.138961	-1.210581	2.428630
57	1	0	-4.407398	-0.047930	1.328079
58	1	0	-5.290862	-2.887470	-2.335434
59	1	0	-6.780859	-1.918176	-2.253237
60	1	0	-6.446206	-3.171301	-1.025344

IIIa (^{L}F: $^{L}\alpha_4$)

1	6	0	-4.366802	-0.148091	2.535752
2	6	0	-3.201446	-0.470563	1.618933
3	8	0	-2.035273	-0.196409	1.929027
4	7	0	-3.486619	-1.051341	0.419110
5	6	0	-2.401984	-1.584299	-0.422867
6	6	0	-3.145631	-2.276418	-1.600309
7	6	0	-4.583649	-1.725985	-1.551795
8	6	0	-4.819108	-1.450055	-0.061834
9	6	0	-1.287569	-0.618105	-0.866451
10	8	0	-0.155107	-1.104805	-0.977395
11	7	0	-1.497812	0.701255	-1.131473
12	6	0	-0.338324	1.510951	-1.560026
13	6	0	-0.971211	2.823503	-2.069751
14	6	0	-2.288069	2.922950	-1.286149
15	6	0	-2.760541	1.465376	-1.202400
16	6	0	0.718721	1.751670	-0.466235
17	8	0	1.810136	2.221910	-0.804198
18	7	0	0.412000	1.434080	0.814275
19	1	0	-0.462838	0.958738	1.026596
20	6	0	1.405886	1.538854	1.882659

21	6	0	0.722986	1.548833	3.254392
22	6	0	2.514462	0.460675	1.829463
23	8	0	3.482283	0.572471	2.580793
24	7	0	2.368087	-0.543869	0.925067
25	1	0	1.515973	-0.607271	0.374236
26	6	0	3.402124	-1.543734	0.680649
27	6	0	2.811178	-2.958586	0.665112
28	6	0	4.219374	-1.277042	-0.606115
29	8	0	5.023944	-2.120017	-1.009771
30	7	0	4.023874	-0.091406	-1.230765
31	1	0	3.368990	0.583749	-0.851893
32	6	0	4.795195	0.278539	-2.406415
33	1	0	4.364198	1.188979	-2.829487
34	1	0	4.762201	-0.524101	-3.149759
35	1	0	5.846890	0.460488	-2.152771
36	1	0	3.597499	-3.682375	0.438110
37	1	0	2.028216	-3.046988	-0.097591
38	1	0	2.373583	-3.192190	1.641715
39	1	0	4.114665	-1.451347	1.506966
40	1	0	1.487450	1.605170	4.033141
41	1	0	0.126167	0.643472	3.409027
42	1	0	0.060595	2.417066	3.343814
43	1	0	1.943844	2.480855	1.736150
44	1	0	-3.389481	1.276118	-0.333597
45	1	0	-3.323335	1.186682	-2.104499
46	1	0	-3.029448	3.567804	-1.768324
47	1	0	-2.104899	3.313420	-0.278171
48	1	0	-1.172849	2.738172	-3.144212
49	1	0	-0.303265	3.675539	-1.922873
50	1	0	0.201558	0.987738	-2.353351
51	1	0	-5.551434	-0.656455	0.113514
52	1	0	-5.166040	-2.354696	0.459414
53	1	0	-5.317020	-2.426774	-1.961858
54	1	0	-4.661961	-0.792922	-2.120709
55	1	0	-3.146287	-3.358760	-1.434221
56	1	0	-2.652232	-2.099409	-2.559989
57	1	0	-1.839620	-2.323567	0.154953
58	1	0	-5.016497	0.619430	2.096547
59	1	0	-3.966850	0.227858	3.478498
60	1	0	-4.985892	-1.031506	2.729796

IIIb (^{D}E: ^{D}P ^{L}P $^{L}\beta_2$)

1	6	0	-2.409430	-3.420698	2.101598
2	6	0	-2.948167	-2.101305	1.577120
3	8	0	-2.889997	-1.060440	2.239890
4	7	0	-3.497799	-2.111912	0.329494
5	6	0	-4.014385	-0.866965	-0.247523
6	6	0	-4.805734	-1.361566	-1.480948
7	6	0	-4.067303	-2.642974	-1.908967

8	6	0	-3.600334	-3.263332	-0.581273
9	6	0	-2.855028	0.058719	-0.663050
10	8	0	-1.934065	-0.390705	-1.362717
11	7	0	-2.900171	1.357328	-0.285276
12	6	0	-1.916273	2.337569	-0.800783
13	6	0	-2.657457	3.670788	-0.647887
14	6	0	-3.487039	3.469670	0.631800
15	6	0	-3.935278	1.999936	0.557259
16	6	0	-0.585790	2.321248	0.003779
17	8	0	-0.238041	3.285287	0.690606
18	7	0	0.156949	1.197538	-0.132752
19	1	0	-0.219791	0.409249	-0.662520
20	6	0	1.394977	1.013549	0.612246
21	6	0	1.143462	0.441684	2.022237
22	6	0	2.302789	0.070952	-0.185907
23	8	0	1.855764	-0.905842	-0.788825
24	7	0	3.628394	0.364932	-0.140555
25	1	0	3.978320	1.163676	0.379282
26	6	0	4.639291	-0.491395	-0.737806
27	6	0	4.822431	-0.204629	-2.242324
28	6	0	5.948196	-0.251188	0.030018
29	8	0	6.160053	0.803551	0.629463
30	7	0	6.862865	-1.251797	-0.031928
31	1	0	6.609110	-2.120857	-0.480787
32	6	0	8.167536	-1.142202	0.609933
33	1	0	8.761064	-2.020648	0.346880
34	1	0	8.066795	-1.085853	1.699407
35	1	0	8.683744	-0.240906	0.266619
36	1	0	5.560897	-0.882043	-2.687148
37	1	0	5.157659	0.826625	-2.397079
38	1	0	3.866728	-0.348855	-2.754008
39	1	0	4.310130	-1.530337	-0.615358
40	1	0	2.085602	0.335700	2.573565
41	1	0	0.658356	-0.537380	1.957750
42	1	0	0.490134	1.120066	2.578384
43	1	0	1.860616	1.999506	0.709033
44	1	0	-3.979620	1.516638	1.537534
45	1	0	-4.917816	1.914018	0.074874
46	1	0	-4.341471	4.150393	0.701863
47	1	0	-2.849559	3.629684	1.506528
48	1	0	-3.311189	3.823027	-1.515997
49	1	0	-1.965100	4.510928	-0.572006
50	1	0	-1.692767	2.082635	-1.842016
51	1	0	-4.331571	-3.988665	-0.195718
52	1	0	-2.635744	-3.770754	-0.683348
53	1	0	-3.199143	-2.383304	-2.519628
54	1	0	-4.705610	-3.326262	-2.478637
55	1	0	-4.850434	-0.613709	-2.278612
56	1	0	-5.834086	-1.589682	-1.174441
57	1	0	-4.658404	-0.379211	0.484614

58	1	0	-3.138167	-4.233459	2.001685
59	1	0	-2.150617	-3.291952	3.153849
60	1	0	-1.508221	-3.712881	1.548094

IIIb (^{D}F: ^{D}P $^{L}\alpha_3$)

1	6	0	-2.398697	-2.475296	2.405249
2	6	0	-2.539715	-1.314109	1.442012
3	8	0	-2.310747	-0.143683	1.792251
4	7	0	-2.915941	-1.592822	0.169196
5	6	0	-3.053110	-0.496685	-0.801342
6	6	0	-3.493739	-1.218853	-2.098009
7	6	0	-2.944140	-2.647915	-1.943094
8	6	0	-3.076829	-2.925380	-0.438895
9	6	0	-1.706613	0.226743	-0.968394
10	8	0	-0.680147	-0.422872	-1.210112
11	7	0	-1.683675	1.579372	-0.860873
12	6	0	-0.425551	2.305350	-1.091793
13	6	0	-0.876947	3.778844	-1.165938
14	6	0	-2.102775	3.827822	-0.238951
15	6	0	-2.796710	2.475265	-0.473364
16	6	0	0.656723	2.077004	-0.021398
17	8	0	1.814150	2.431630	-0.269003
18	7	0	0.294479	1.497268	1.148670
19	1	0	-0.646232	1.124772	1.265454
20	6	0	1.285927	1.174766	2.173862
21	6	0	0.612059	0.983850	3.536570
22	6	0	2.189692	-0.031724	1.825644
23	8	0	3.143583	-0.288226	2.558404
24	7	0	1.893311	-0.731970	0.696569
25	1	0	1.064163	-0.495220	0.157217
26	6	0	2.767560	-1.771099	0.162789
27	6	0	1.961030	-3.001856	-0.269307
28	6	0	3.673710	-1.284941	-0.994449
29	8	0	4.380408	-2.096134	-1.597481
30	7	0	3.661450	0.036636	-1.285287
31	1	0	3.087038	0.676698	-0.747678
32	6	0	4.530477	0.589472	-2.312330
33	1	0	4.296590	1.650478	-2.425010
34	1	0	4.372503	0.075719	-3.266295
35	1	0	5.586370	0.476818	-2.039328
36	1	0	2.630723	-3.740747	-0.715708
37	1	0	1.200108	-2.729321	-1.010472
38	1	0	1.461102	-3.446207	0.598764
39	1	0	3.449974	-2.045084	0.973622
40	1	0	1.369156	0.710190	4.275450
41	1	0	-0.148444	0.196543	3.497935
42	1	0	0.125822	1.912976	3.853476
43	1	0	1.981694	2.018185	2.228847
44	1	0	-3.293228	2.101752	0.425981

45	1	0	-3.532624	2.540887	-1.285833
46	1	0	-2.767258	4.670646	-0.451861
47	1	0	-1.785645	3.907369	0.807080
48	1	0	-1.165728	4.016697	-2.196764
49	1	0	-0.076359	4.463358	-0.875157
50	1	0	0.028999	1.967525	-2.026737
51	1	0	-4.063794	-3.341133	-0.189847
52	1	0	-2.310913	-3.614266	-0.072855
53	1	0	-1.889831	-2.674249	-2.231646
54	1	0	-3.490859	-3.378594	-2.547171
55	1	0	-3.122945	-0.719196	-2.997664
56	1	0	-4.589223	-1.229088	-2.146317
57	1	0	-3.820154	0.196839	-0.451859
58	1	0	-3.230353	-3.183763	2.328598
59	1	0	-2.349566	-2.079099	3.420792
60	1	0	-1.470530	-3.024143	2.201407

Cartesian coordinates of the optimized geometries of end-protected tetraalanine (**Ia**, **Ib**) in fully-extended (^{L}**E** and ^{D}**E**), semi-extended (^{L}**S** and ^{D}**S**), and fully-folded structures (^{L}**F** and ^{D}**F**) in presence of solvent.

Ia (^{L}S: $^{L}P_4$)

1	6	0	-7.693995	-0.299482	1.180429
2	6	0	-6.513967	-0.279630	0.240244
3	8	0	-6.186345	-1.291574	-0.417206
4	7	0	-5.833206	0.880646	0.133583
5	1	0	-6.097954	1.657388	0.729071
6	6	0	-4.650542	1.034804	-0.704518
7	6	0	-4.241326	2.511720	-0.744576
8	6	0	-3.487877	0.179191	-0.171500
9	8	0	-3.247805	0.083969	1.046356
10	7	0	-2.730362	-0.422665	-1.107200
11	1	0	-2.973803	-0.302177	-2.085015
12	6	0	-1.549307	-1.218267	-0.787987
13	6	0	-1.045554	-1.917741	-2.055598
14	6	0	-0.429126	-0.338322	-0.204939
15	8	0	-0.152460	0.776096	-0.686152
16	7	0	0.256050	-0.872005	0.822796
17	1	0	0.001152	-1.797174	1.152753
18	6	0	1.416303	-0.227899	1.426873
19	6	0	1.834344	-1.004074	2.680496
20	6	0	2.586548	-0.159034	0.429459
21	8	0	2.850444	-1.100065	-0.341454
22	7	0	3.324372	0.964548	0.479547
23	1	0	3.055365	1.697014	1.128308
24	6	0	4.507694	1.182385	-0.346922
25	6	0	4.997839	2.623132	-0.161293
26	6	0	5.630213	0.193899	0.017258
27	8	0	5.886539	-0.099375	1.203167
28	7	0	6.343069	-0.283849	-1.013901
29	1	0	6.075374	-0.018204	-1.954661
30	6	0	7.502864	-1.150417	-0.837107
31	1	0	7.908562	-1.383133	-1.822430
32	1	0	7.220518	-2.083022	-0.338552
33	1	0	8.274234	-0.652081	-0.241190
34	1	0	5.854094	2.817448	-0.813510
35	1	0	5.300195	2.803081	0.876341
36	1	0	4.200819	3.326890	-0.423609
37	1	0	4.228312	1.026486	-1.394276
38	1	0	2.685468	-0.515049	3.162962
39	1	0	2.119088	-2.031595	2.427996
40	1	0	1.003311	-1.031906	3.393101
41	1	0	1.135897	0.791820	1.708573
42	1	0	-0.168431	-2.529646	-1.825553

43	1	0	-0.767860	-1.184787	-2.821007
44	1	0	-1.825345	-2.572458	-2.458493
45	1	0	-1.832283	-1.970799	-0.044596
46	1	0	-3.370522	2.646952	-1.392320
47	1	0	-3.990087	2.875592	0.258025
48	1	0	-5.063901	3.114482	-1.143624
49	1	0	-4.897584	0.699291	-1.716490
50	1	0	-7.870892	0.664877	1.664555
51	1	0	-7.521696	-1.059685	1.950315
52	1	0	-8.589140	-0.590333	0.619950

Ib (^{D}S: ^{D}P ^{L}P$_3$)

1	6	0	-5.907625	3.082081	0.293061
2	6	0	-5.153746	1.919184	-0.310659
3	8	0	-4.114674	2.071302	-0.986999
4	7	0	-5.676365	0.694295	-0.083683
5	1	0	-6.484613	0.619753	0.524482
6	6	0	-5.066397	-0.538282	-0.561191
7	6	0	-6.006468	-1.718300	-0.280909
8	6	0	-3.703849	-0.787655	0.111469
9	8	0	-3.469616	-0.444404	1.284560
10	7	0	-2.809051	-1.459371	-0.638338
11	1	0	-3.047107	-1.686789	-1.598484
12	6	0	-1.523492	-1.919064	-0.126681
13	6	0	-0.923162	-2.945754	-1.093886
14	6	0	-0.545606	-0.744580	0.050316
15	8	0	-0.431542	0.147866	-0.810166
16	7	0	0.207956	-0.776892	1.164846
17	1	0	0.084724	-1.545928	1.815494
18	6	0	1.280889	0.174758	1.428355
19	6	0	1.798345	-0.022426	2.857897
20	6	0	2.431231	-0.008233	0.421585
21	8	0	2.794002	-1.135430	0.037515
22	7	0	3.035492	1.123134	0.015505
23	1	0	2.705613	2.010214	0.381363
24	6	0	4.205662	1.135133	-0.857997
25	6	0	4.567811	2.584142	-1.201012
26	6	0	5.402165	0.438537	-0.186842
27	8	0	5.678762	0.631249	1.014924
28	7	0	6.146722	-0.344070	-0.981718
29	1	0	5.859827	-0.473799	-1.944925
30	6	0	7.354865	-1.016703	-0.516984
31	1	0	7.768774	-1.588959	-1.348153
32	1	0	7.124933	-1.697790	0.308543
33	1	0	8.099419	-0.290307	-0.175844
34	1	0	5.434369	2.609923	-1.868257
35	1	0	4.809554	3.150398	-0.294484
36	1	0	3.729435	3.072149	-1.709207
37	1	0	3.954217	0.595043	-1.776731

38	1	0	2.583942	0.705167	3.080059
39	1	0	2.207818	-1.030113	2.991118
40	1	0	0.982094	0.124214	3.572955
41	1	0	0.876520	1.186648	1.325030
42	1	0	0.037389	-3.306785	-0.714641
43	1	0	-0.761821	-2.502420	-2.082893
44	1	0	-1.597761	-3.802189	-1.196196
45	1	0	-1.693496	-2.390553	0.846367
46	1	0	-5.570115	-2.647429	-0.658697
47	1	0	-6.966397	-1.561075	-0.783747
48	1	0	-6.185933	-1.828802	0.794647
49	1	0	-4.908128	-0.452387	-1.641160
50	1	0	-6.939706	3.104010	-0.074886
51	1	0	-5.410676	4.017582	0.029538
52	1	0	-5.945347	2.988854	1.384625

Ia (^{L}E: $^{L}\beta_4$)

1	6	0	8.705516	0.920363	-0.375921
2	6	0	7.531672	0.014586	-0.659722
3	8	0	7.590759	-0.865189	-1.548576
4	7	0	6.426936	0.211831	0.085989
5	1	0	6.430881	0.930971	0.802091
6	6	0	5.202722	-0.570668	-0.050603
7	6	0	5.252930	-1.881521	0.756025
8	6	0	4.035877	0.299041	0.428408
9	8	0	4.195599	1.151565	1.325334
10	7	0	2.852229	0.052561	-0.153341
11	1	0	2.788198	-0.663200	-0.872090
12	6	0	1.604630	0.701036	0.238688
13	6	0	1.415855	2.063309	-0.453640
14	6	0	0.453930	-0.250704	-0.112412
15	8	0	0.580431	-1.112196	-1.005263
16	7	0	-0.681305	-0.062174	0.578314
17	1	0	-0.709393	0.647172	1.305223
18	6	0	-1.908388	-0.821532	0.343418
19	6	0	-1.956562	-2.104662	1.189298
20	6	0	-3.090891	0.094411	0.676963
21	8	0	-3.034833	0.879604	1.644840
22	7	0	-4.170271	-0.038101	-0.108993
23	1	0	-4.130746	-0.664269	-0.908144
24	6	0	-5.405045	0.723939	0.068952
25	6	0	-5.329094	2.098275	-0.618160
26	6	0	-6.548215	-0.105614	-0.520246
27	8	0	-6.373985	-0.793365	-1.548617
28	7	0	-7.728778	-0.021662	0.106251
29	1	0	-7.791943	0.537084	0.949750
30	6	0	-8.927428	-0.699531	-0.376408
31	1	0	-9.177083	-0.372155	-1.390378
32	1	0	-9.752139	-0.451093	0.292649

33	1	0	-8.784324	-1.784649	-0.380775
34	1	0	-6.250161	2.664823	-0.444988
35	1	0	-5.181544	1.982923	-1.697303
36	1	0	-4.490162	2.667947	-0.206554
37	1	0	-5.563870	0.862053	1.141294
38	1	0	-2.859495	-2.681064	0.961472
39	1	0	-1.948698	-1.868496	2.258678
40	1	0	-1.084539	-2.725054	0.959254
41	1	0	-1.935812	-1.087305	-0.715739
42	1	0	0.512510	2.558439	-0.082875
43	1	0	1.333849	1.939736	-1.539004
44	1	0	2.274262	2.706284	-0.236042
45	1	0	1.627165	0.852418	1.321724
46	1	0	4.351231	-2.475959	0.574646
47	1	0	5.330716	-1.675447	1.829196
48	1	0	6.122345	-2.470108	0.446956
49	1	0	5.069684	-0.807513	-1.109474
50	1	0	8.946489	1.486083	-1.282776
51	1	0	9.577125	0.305611	-0.126383
52	1	0	8.514943	1.619861	0.442461

Ib (^{D}E: $^{D}\beta\,^{L}\beta_3$)

1	6	0	-8.105532	-1.584062	-1.459893
2	6	0	-7.154938	-1.306351	-0.320364
3	8	0	-7.198642	-1.974559	0.737530
4	7	0	-6.263034	-0.313989	-0.507736
5	1	0	-6.272119	0.205014	-1.379794
6	6	0	-5.275268	0.087291	0.487193
7	6	0	-5.836590	1.116858	1.485393
8	6	0	-4.064443	0.669428	-0.252069
9	8	0	-4.188786	1.225654	-1.361351
10	7	0	-2.891663	0.552734	0.391141
11	1	0	-2.876218	0.122652	1.311839
12	6	0	-1.640276	1.153900	-0.067784
13	6	0	-1.542479	2.642913	0.305207
14	6	0	-0.499288	0.365536	0.583439
15	8	0	-0.600389	-0.041964	1.758196
16	7	0	0.595275	0.183768	-0.169915
17	1	0	0.603391	0.517865	-1.129398
18	6	0	1.799441	-0.492098	0.306123
19	6	0	1.689200	-2.021921	0.175688
20	6	0	2.985568	0.030072	-0.511994
21	8	0	2.834426	0.413012	-1.689377
22	7	0	4.173266	0.000764	0.111204
23	1	0	4.220149	-0.300502	1.080713
24	6	0	5.434690	0.387254	-0.517949
25	6	0	5.681890	1.902756	-0.423534
26	6	0	6.555866	-0.380984	0.187958
27	8	0	6.489422	-0.629315	1.410855

28	7	0	7.602238	-0.732073	-0.570103
29	1	0	7.581744	-0.505941	-1.557998
30	6	0	8.783700	-1.397921	-0.031500
31	1	0	9.485520	-1.559380	-0.850599
32	1	0	8.518582	-2.364740	0.407339
33	1	0	9.263488	-0.781750	0.735508
34	1	0	6.612982	2.170389	-0.934571
35	1	0	5.748441	2.220463	0.622522
36	1	0	4.858269	2.440126	-0.903879
37	1	0	5.390780	0.093806	-1.570044
38	1	0	2.576808	-2.506090	0.595725
39	1	0	1.588674	-2.316184	-0.874636
40	1	0	0.810937	-2.374117	0.725399
41	1	0	1.938746	-0.230682	1.358443
42	1	0	-0.614067	3.074127	-0.084254
43	1	0	-1.563453	2.772388	1.392464
44	1	0	-2.385261	3.187516	-0.131587
45	1	0	-1.592554	1.046014	-1.154405
46	1	0	-5.096511	1.342283	2.260408
47	1	0	-6.729253	0.708503	1.969419
48	1	0	-6.108008	2.047125	0.974053
49	1	0	-4.968314	-0.808526	1.033000
50	1	0	-7.959019	-0.914063	-2.311555
51	1	0	-9.134180	-1.484045	-1.096880
52	1	0	-7.969605	-2.619330	-1.791685

Ia (^{L}F: $^{L}\alpha_4$)

1	6	0	5.302095	1.330269	-0.849538
2	6	0	4.028582	0.532409	-0.971425
3	8	0	2.967565	1.048126	-1.381379
4	7	0	4.080784	-0.768288	-0.600943
5	1	0	4.969179	-1.152068	-0.296569
6	6	0	2.954496	-1.685710	-0.750734
7	6	0	3.428531	-3.128560	-0.539566
8	6	0	1.775017	-1.376112	0.180310
9	8	0	0.643072	-1.817956	-0.094703
10	7	0	2.014176	-0.644493	1.285298
11	1	0	2.945065	-0.267899	1.430187
12	6	0	0.970652	-0.289882	2.240958
13	6	0	1.600093	0.305232	3.505549
14	6	0	-0.082677	0.667488	1.663983
15	8	0	-1.200107	0.747633	2.212193
16	7	0	0.246222	1.399384	0.582891
17	1	0	1.156904	1.265734	0.148272
18	6	0	-0.682638	2.336780	-0.043917
19	6	0	0.062369	3.233077	-1.039480
20	6	0	-1.877182	1.655322	-0.730910
21	8	0	-2.884520	2.335960	-1.003661
22	7	0	-1.779935	0.343989	-1.027870

23	1	0	-0.949543	-0.169274	-0.739402
24	6	0	-2.885975	-0.422972	-1.594642
25	6	0	-2.353315	-1.671245	-2.308928
26	6	0	-3.954822	-0.821166	-0.560940
27	8	0	-5.047212	-1.275147	-0.968511
28	7	0	-3.666653	-0.696076	0.741140
29	1	0	-2.789340	-0.265128	1.020213
30	6	0	-4.627227	-1.030666	1.787473
31	1	0	-4.169659	-0.808666	2.752486
32	1	0	-4.888272	-2.092913	1.752099
33	1	0	-5.543311	-0.440615	1.680925
34	1	0	-3.183353	-2.229689	-2.749621
35	1	0	-1.821218	-2.327849	-1.611894
36	1	0	-1.668059	-1.380732	-3.111409
37	1	0	-3.399644	0.214932	-2.318968
38	1	0	-0.631442	3.957048	-1.475064
39	1	0	0.505606	2.641994	-1.847994
40	1	0	0.857635	3.782481	-0.525604
41	1	0	-1.124432	2.958642	0.740810
42	1	0	0.817381	0.567558	4.222432
43	1	0	2.178434	1.206591	3.272930
44	1	0	2.263739	-0.429987	3.971829
45	1	0	0.419499	-1.197512	2.505285
46	1	0	2.588283	-3.817885	-0.658326
47	1	0	3.852440	-3.261338	0.462249
48	1	0	4.191085	-3.382827	-1.282766
49	1	0	2.552779	-1.581967	-1.763975
50	1	0	6.149768	0.734209	-0.500874
51	1	0	5.136323	2.160476	-0.154053
52	1	0	5.543616	1.760568	-1.827461

Ib (^{D}F: ^{D}P $^{L}\alpha_3$)

1	6	0	-2.946390	-3.485148	0.800777
2	6	0	-3.011657	-1.987822	0.630361
3	8	0	-2.683748	-1.207747	1.550749
4	7	0	-3.442858	-1.529446	-0.563195
5	1	0	-3.651484	-2.199512	-1.294995
6	6	0	-3.542244	-0.112380	-0.886008
7	6	0	-4.244024	0.059963	-2.238583
8	6	0	-2.150368	0.540532	-0.936886
9	8	0	-1.162909	-0.041130	-1.418756
10	7	0	-2.080427	1.801238	-0.458170
11	1	0	-2.919210	2.226603	-0.075743
12	6	0	-0.887245	2.633342	-0.585342
13	6	0	-1.240687	4.097513	-0.297692
14	6	0	0.275012	2.184720	0.312094
15	8	0	1.433850	2.554792	0.041207
16	7	0	-0.008631	1.419155	1.383078
17	1	0	-0.961099	1.091732	1.511912

18	6	0	1.012807	0.928305	2.303139
19	6	0	0.352553	0.398744	3.581799
20	6	0	1.932101	-0.142846	1.693250
21	8	0	3.026590	-0.381257	2.238140
22	7	0	1.499261	-0.803117	0.599980
23	1	0	0.614490	-0.531784	0.176467
24	6	0	2.307203	-1.795603	-0.103206
25	6	0	1.402835	-2.792783	-0.838201
26	6	0	3.323319	-1.184871	-1.084026
27	8	0	4.194356	-1.926146	-1.591103
28	7	0	3.226960	0.117172	-1.381614
29	1	0	2.529675	0.686935	-0.912755
30	6	0	4.146055	0.772731	-2.305537
31	1	0	3.890098	1.832259	-2.346299
32	1	0	4.060559	0.345459	-3.309628
33	1	0	5.181345	0.669348	-1.965338
34	1	0	2.013773	-3.539278	-1.352452
35	1	0	0.775896	-2.283041	-1.578326
36	1	0	0.754651	-3.310305	-0.124123
37	1	0	2.902292	-2.328491	0.643290
38	1	0	1.118911	0.045240	4.276722
39	1	0	-0.328301	-0.430339	3.358499
40	1	0	-0.212373	1.200191	4.068584
41	1	0	1.674203	1.761856	2.556942
42	1	0	-0.348146	4.721640	-0.393196
43	1	0	-1.642675	4.212880	0.715336
44	1	0	-1.986563	4.450259	-1.017232
45	1	0	-0.509654	2.544658	-1.608913
46	1	0	-4.327772	1.121892	-2.487766
47	1	0	-5.252952	-0.362754	-2.192620
48	1	0	-3.684716	-0.442133	-3.035855
49	1	0	-4.131959	0.380677	-0.106198
50	1	0	-3.290562	-4.028780	-0.083203
51	1	0	-3.558383	-3.773484	1.662252
52	1	0	-1.910922	-3.771219	1.016574