

Supporting Information

Acyl carrier protein structural classification and normal mode analysis

David C. Cantu, Michael J. Forrester, Katherine Charov, and Peter J. Reilly

Dept. of Chemical and Biological Engineering, Iowa State University

Table S1: Amino acid identities between randomly chosen sequences in two families based on pairwise alignments. Values are shown as a percentage; those above the diagonal are based on the shorter sequence compared, while those below the diagonal are based on the longer sequence compared.

Figure S1: Color map representation of Table S1.

Figure S2: Detailed phylogenetic tree of the 16 ACP families.

Figure S3: Individual residue fluctuations of the five slowest vibrational normal modes for Protein Data Bank (PDB) ACP1 structures 1T8K, 1X3O, 2EHS, 2EHT, 2QNW, ACP5 structure 2AF8, and ACP17 structure 1HQB. Fluctuation scale normalized to largest residue fluctuation within each structure. Residues corresponding with α -helices are highlighted.

Figure S4: Slowest mode visualizations of individual tertiary structures. S4A and S4B: 1T8K head-on and side view; S4C and S4D: 1X3O head-on and side view; S4E: 2EHS head-on; S4F and S4G: 2EHT head-on and side view; S4H and S4I: 2QNW head-on and side view; S4J and S4K: 2AF8 head-on and side view; S4L and S4M: 1HQB head-on and side view. Red through gray/blue: high through low degrees of fluctuation.

Figure S5: Overlap charts between the 20 slowest vibrational normal modes of two structures, 0 being no overlap and 1 complete overlap. Shown for two conformers (2EHS and 2EHT) of a single structure in ACP1, two bacterial structures (1T8K and 1X3O) in ACP1, a bacterial (1T8K) and a eukaryotic (2QNW) structure in ACP1, an ACP1 (1T8K) and ACP5 (2AF8), an ACP1 (1T8K) and ACP17 (1HQB), and an ACP5 (2AF8) and ACP17 (1HQB).

Figure S6: Comparative residue fluctuations of the three most overlapped vibrational normal modes between compared cases (see Figure S5). Fluctuation scale normalized to largest residue fluctuation between the two compared structures. See table for corresponding modes in each comparison and color key:

Comparison	1 st most overlapped modes	2 nd most overlapped modes	3 rd most overlapped modes
Two conformers	6 (red) and 6 (red lined)	2 (green) and 1 (green lined)	7 (blue) and 5 (blue lined)
Two Bacterial	1 (red) and 4 (red lined)	2 (green) and 3 (green lined)	2 (green) and 1 (green dotted)
Bacterial and Eukaryotic	1 (red) and 1 (red lined)	1 (red) and 3 (red dotted)	6 (green) and 5 (green lined)
ACP1 and ACP5	1 (red) and 1 (red lined)	2 (green) and 4 (green lined)	2 (green) and 3 (green dotted)
ACP1 and ACP17	4 (red) and 2 (green lined)	1 (green) and 1 (green lined)	2 (blue) and 3 (blue lined)
ACP5 and ACP17	1 (red) and 1 (green lined)	2 (green) and 5 (green lined)	2 (green) and 9 (green dotted)

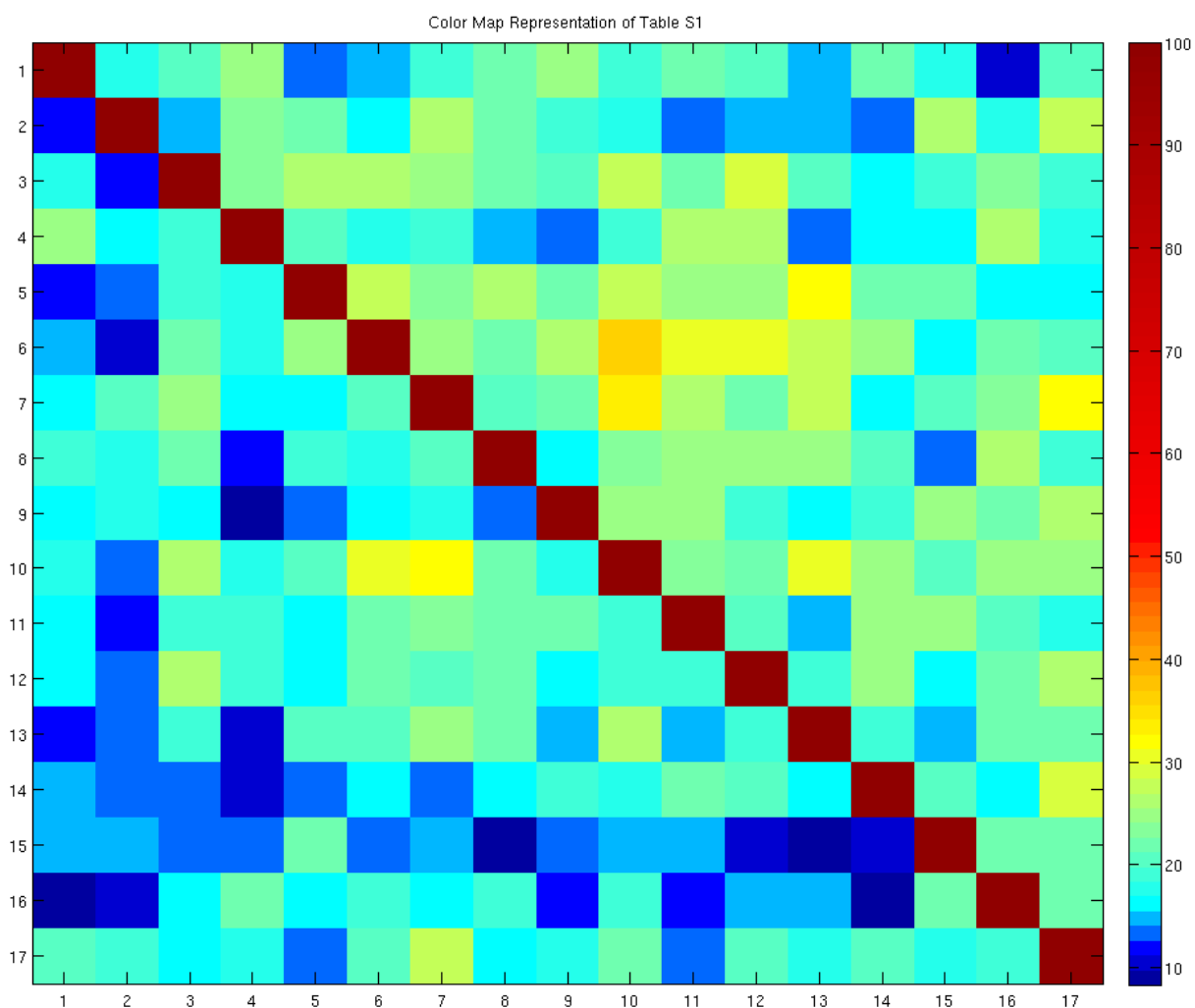
Figure S7: Tertiary structure models for ACP15 and 16 predicted by threading.

Table S1. Percentage of identical residues at aligned positions between two sequences present in different ACP families^a

	1	2	3	4	5	6	7	8	9	10	11	12	13	15	16	17
1	100	18.2	20.6	25.0	13.8	15.0	18.6	21.7	24.1	19.2	21.7	21.0	14.5	17.5	10.0	20.0
2	12.5	100	14.6	23.6	21.8	16.4	25.5	21.8	18.5	18.2	12.7	14.6	14.6	25.5	18.2	27.3
3	17.5	11.8	100	23.5	26.5	26.5	25.0	22.1	20.4	27.9	21.7	29.0	21.0	19.1	23.5	19.1
4	24.4	15.9	19.5	100	20.7	18.3	18.6	14.5	13.0	19.2	26.7	25.8	12.9	15.9	25.6	17.3
5	11.6	12.6	19.0	17.9	100	27.4	22.9	26.1	22.2	27.4	25.0	24.2	32.3	22.1	15.5	16.1
6	14.3	10.7	21.4	17.9	24.2	100	24.3	21.7	25.9	35.6	30.0	30.7	27.4	15.5	21.4	21.0
7	16.3	20.0	24.3	15.9	16.8	20.2	100	20.3	22.2	32.9	26.7	22.6	27.4	20.0	22.9	31.4
8	18.8	17.4	21.7	12.2	19.0	17.9	20.0	100	16.7	23.2	25.0	24.2	24.2	13.0	26.1	18.8
9	16.3	18.2	16.2	8.5	12.6	16.7	17.1	13.0	100	24.1	24.1	18.5	16.7	24.1	22.2	25.9
10	17.5	13.7	26.0	17.1	21.1	31.0	31.5	21.9	17.8	100	23.3	22.6	30.7	20.6	24.7	24.7
11	16.3	11.7	19.1	19.5	15.8	21.4	22.9	21.7	21.7	19.2	100	20.0	15.0	25.0	20.0	18.3
12	16.3	12.9	26.5	19.5	15.8	22.6	20.0	21.7	16.1	19.2	19.4	100	19.4	16.1	22.6	25.8
13	11.3	12.9	19.1	9.8	21.1	20.2	24.3	21.7	14.5	26.0	14.5	19.4	100	14.5	22.6	22.6
15	14.1	14.1	13.1	13.1	21.2	13.1	14.1	9.1	13.1	15.2	15.2	10.1	9.1	100	21.7	22.2
16	8.3	10.3	16.5	21.7	15.5	18.6	16.5	18.6	12.4	18.6	12.4	14.4	14.4	21.2	100	22.2
17	19.8	18.5	16.1	17.1	13.7	20.2	27.2	16.1	17.3	22.2	13.6	19.8	17.3	18.2	18.6	100

^a Percentages above the 100% diagonal are based on the number of residues of the shorter chain being compared, while those below the 100% diagonal are based on the number of residues of the longer chain being compared.

Figure S1. Identical residues at aligned positions between two sequences present in different ACP families^a



^a Percentages above the 100% diagonal are based on the number of residues of the shorter chain being compared, while those below the 100% diagonal are based on the number of residues of the longer chain being compared.

Figure S2: Detailed phylogenetic tree of ACP families.

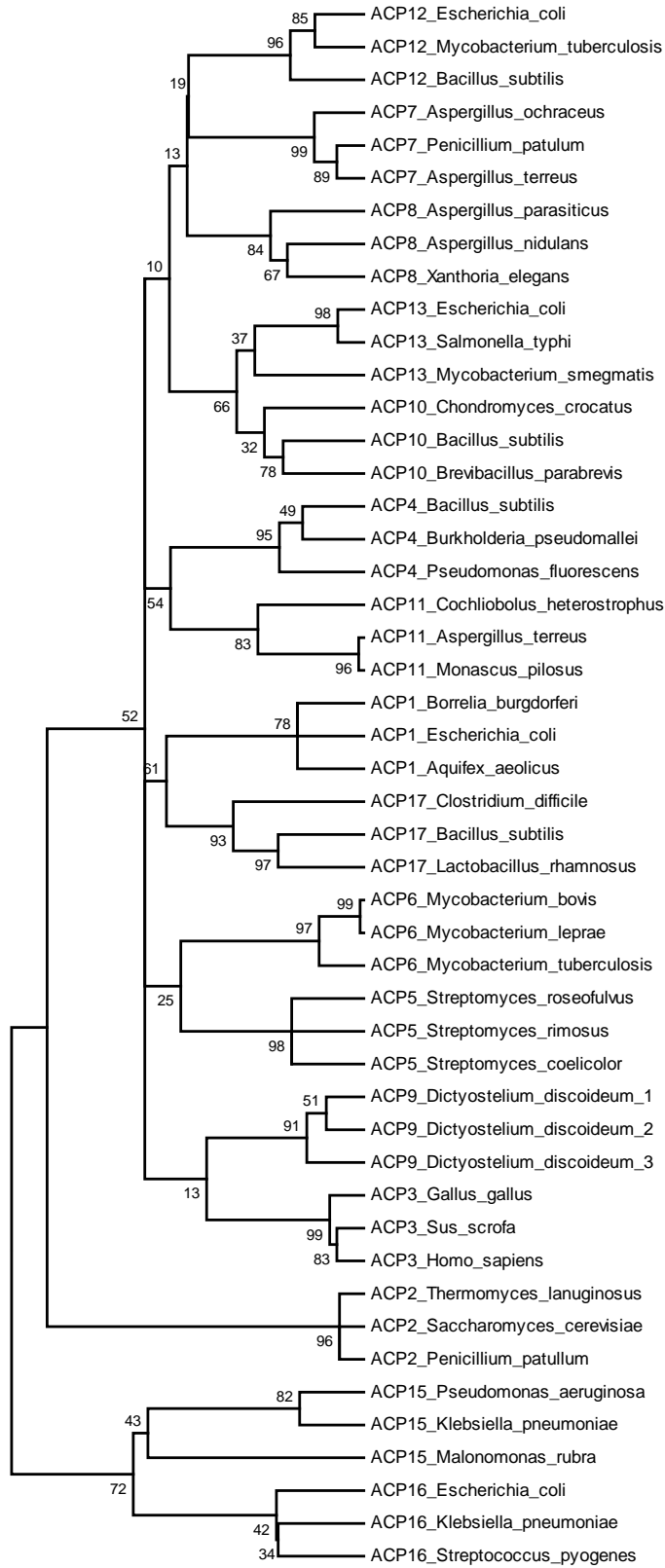
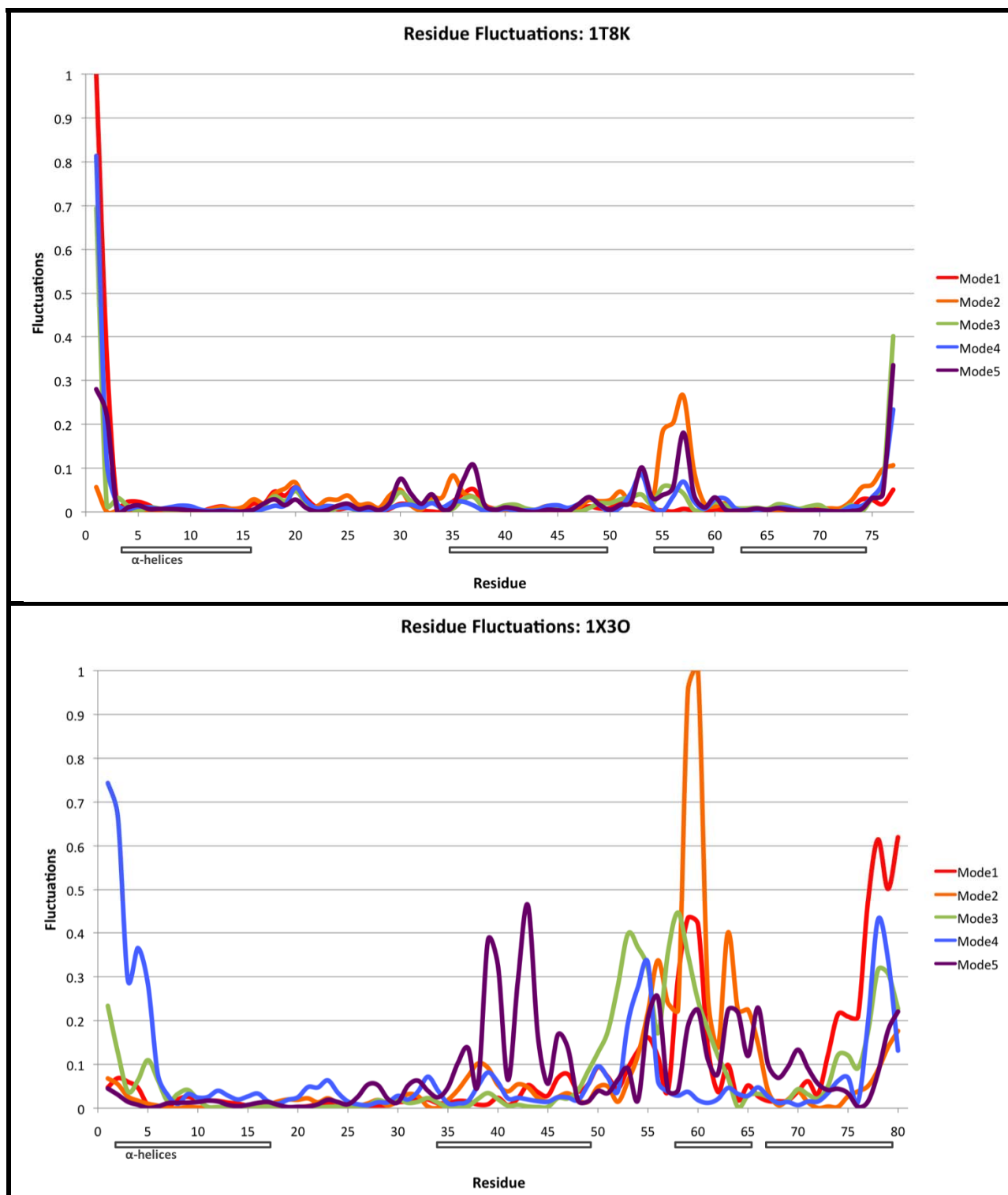
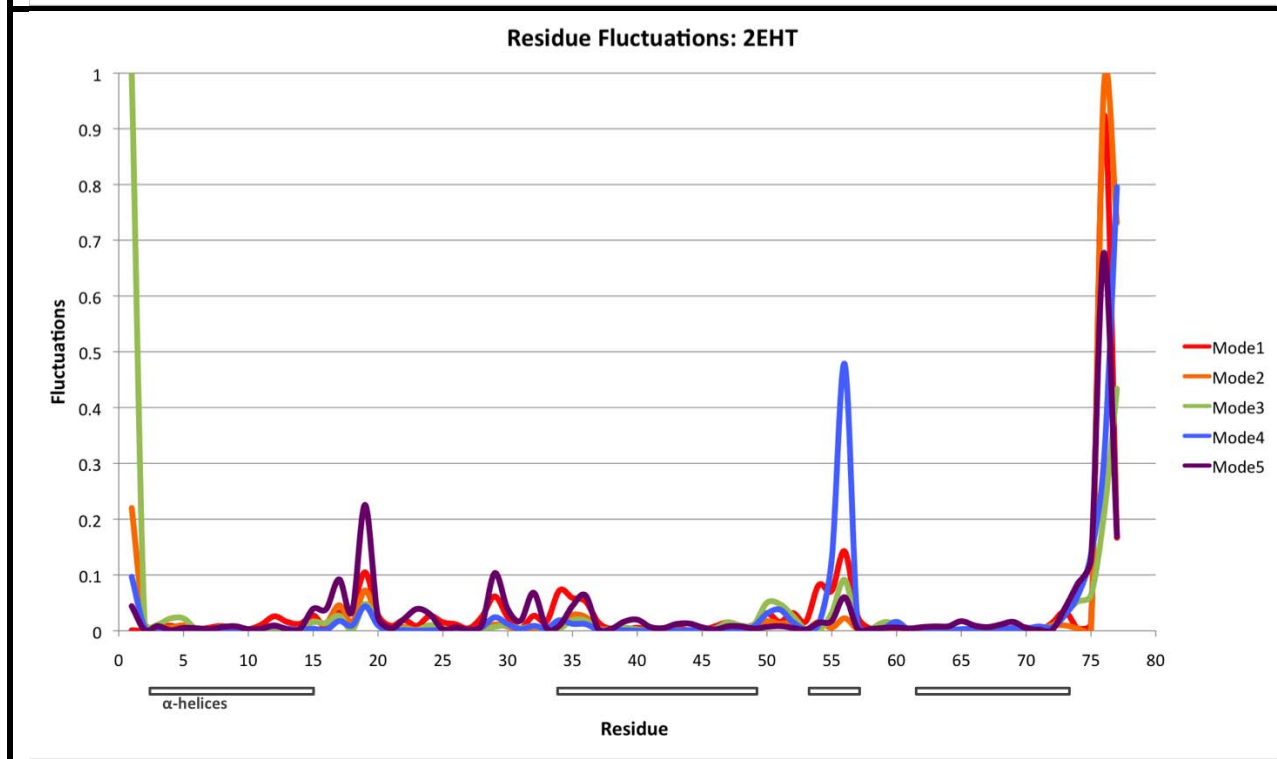
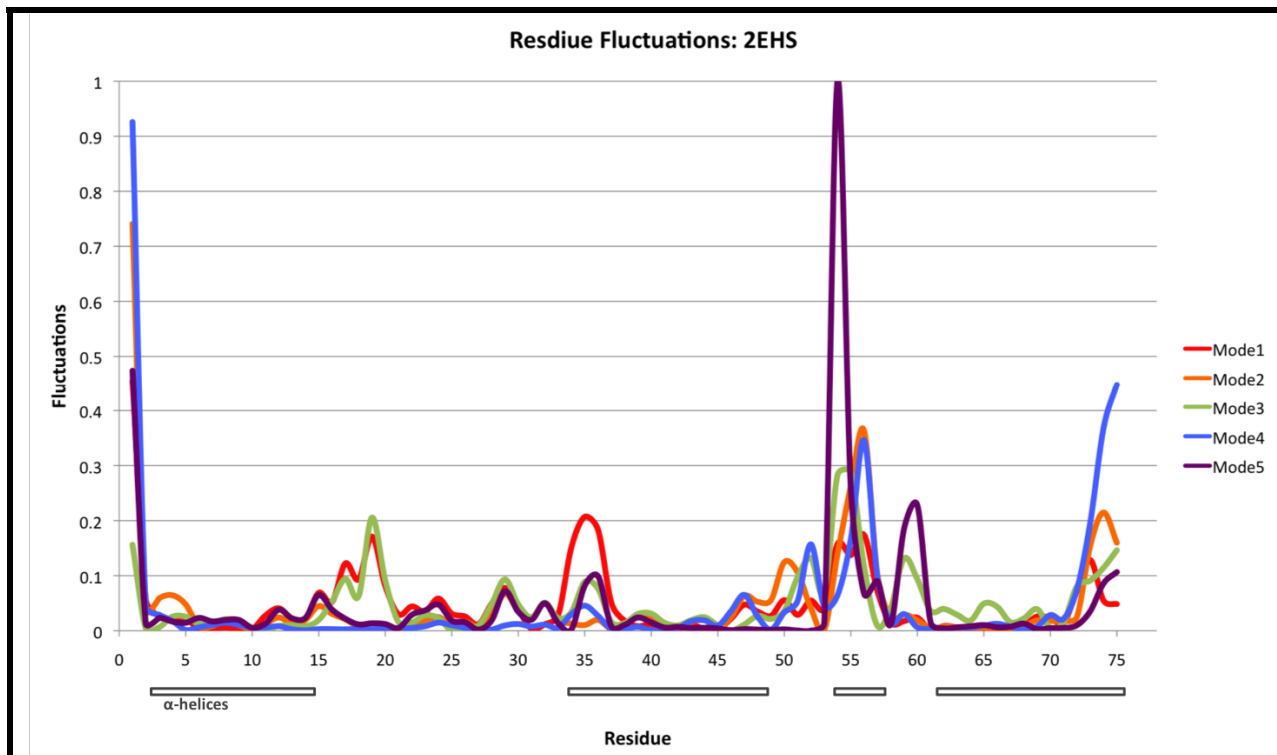
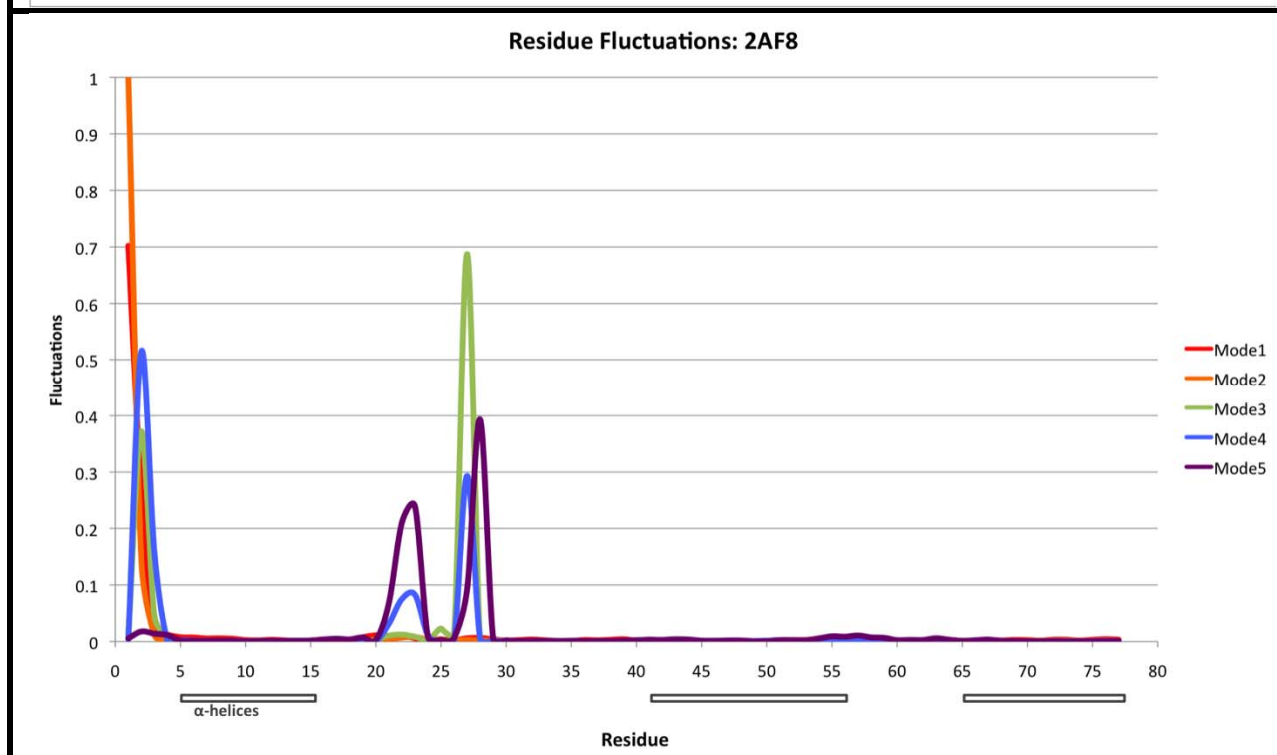
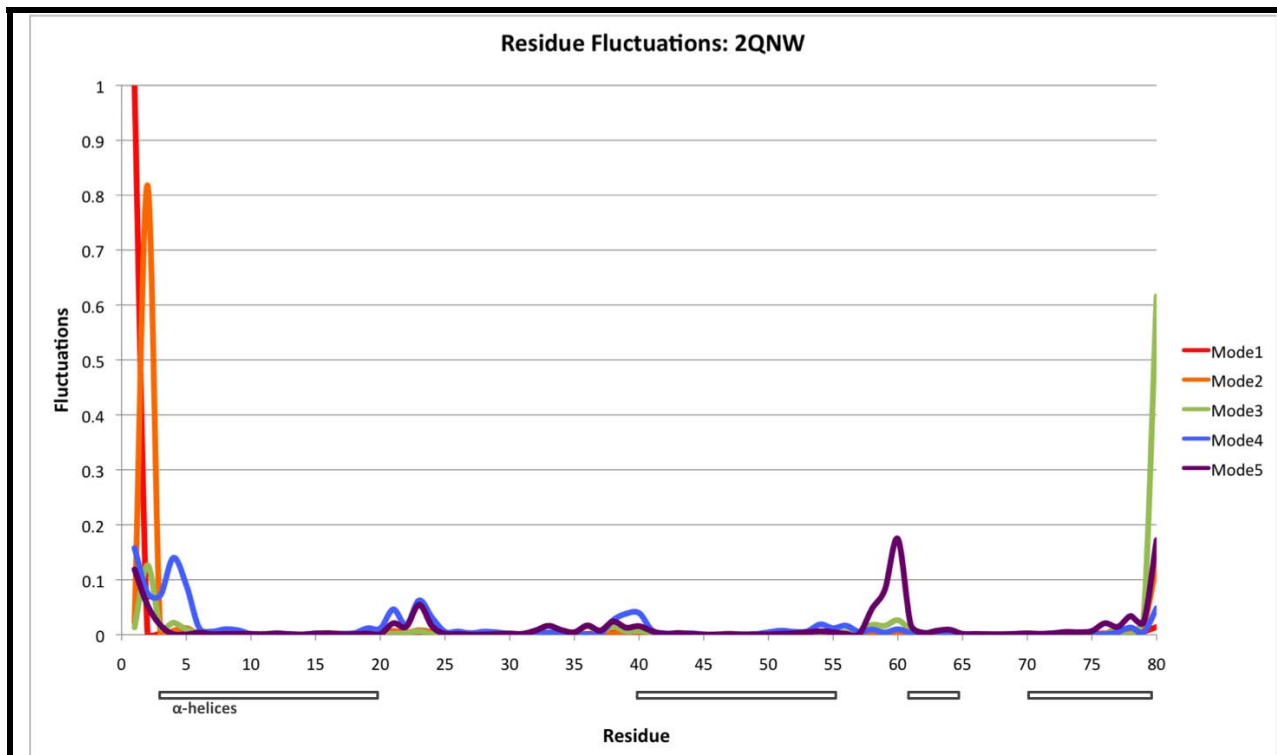


Figure S3: Individual residue fluctuations







Residue Fluctuations: 1HQB

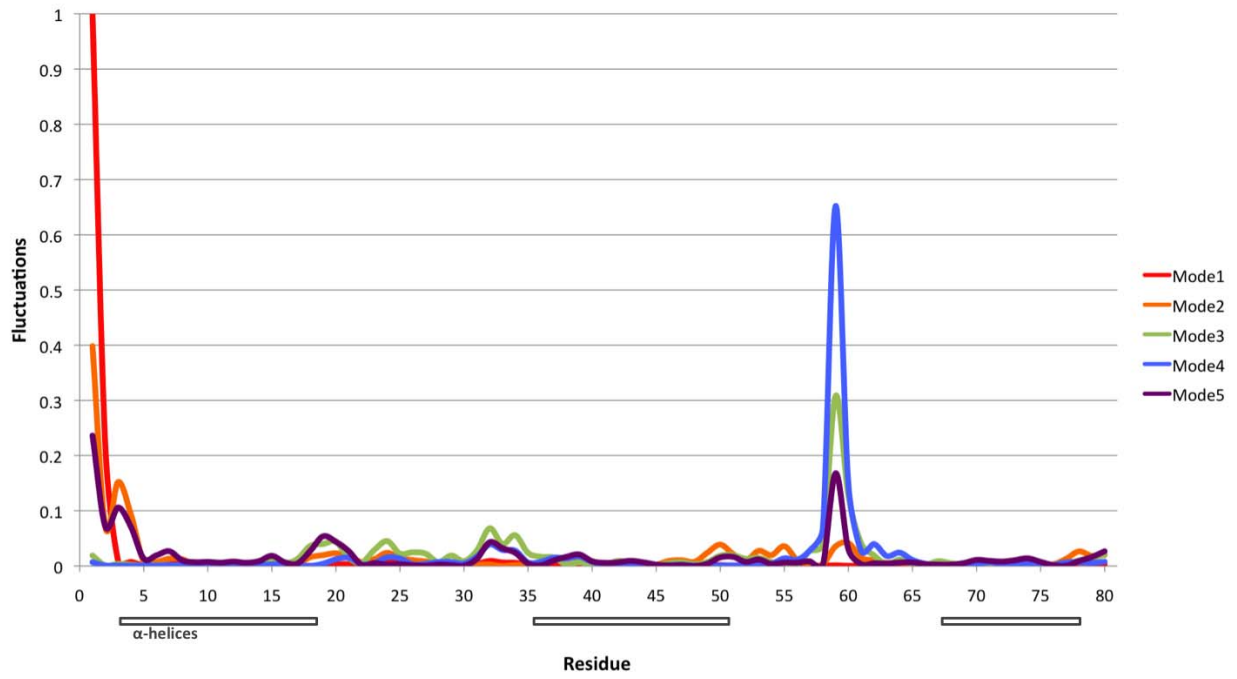
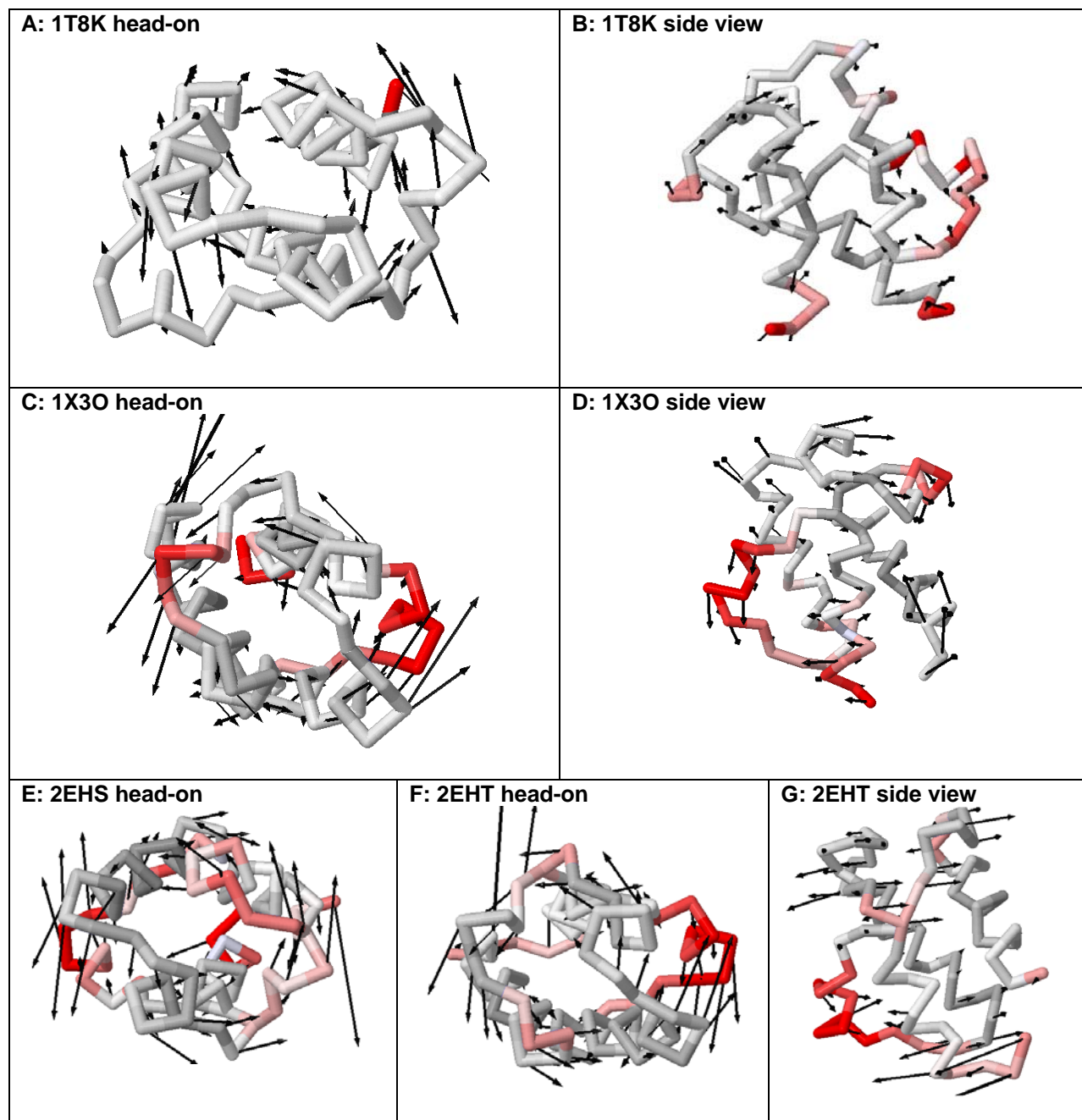


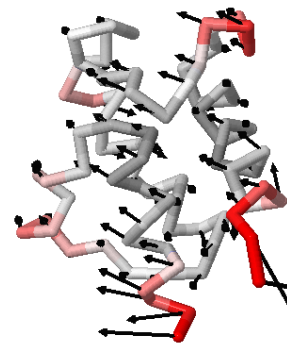
Figure S4: Slowest mode visualizations



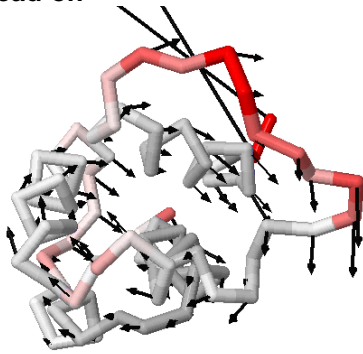
H: 2QNW head-on



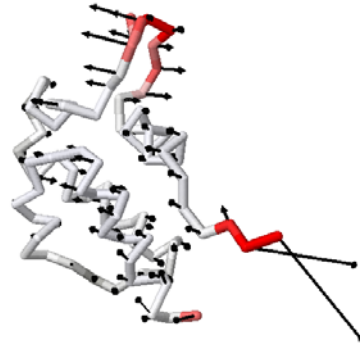
I: 2QNW side view



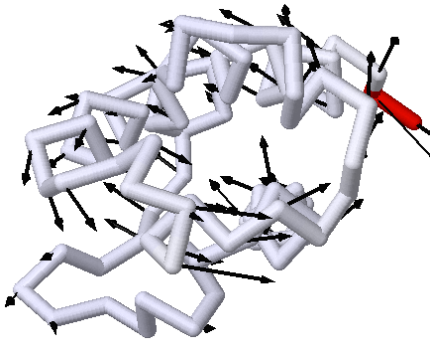
J: 2AF8 head-on



K: 2AF8 side view



L: 1HQB head-on



M: 1HQB side view

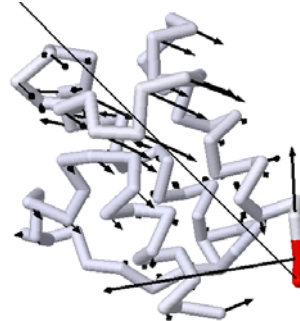


Figure S5: Normal mode overlap charts

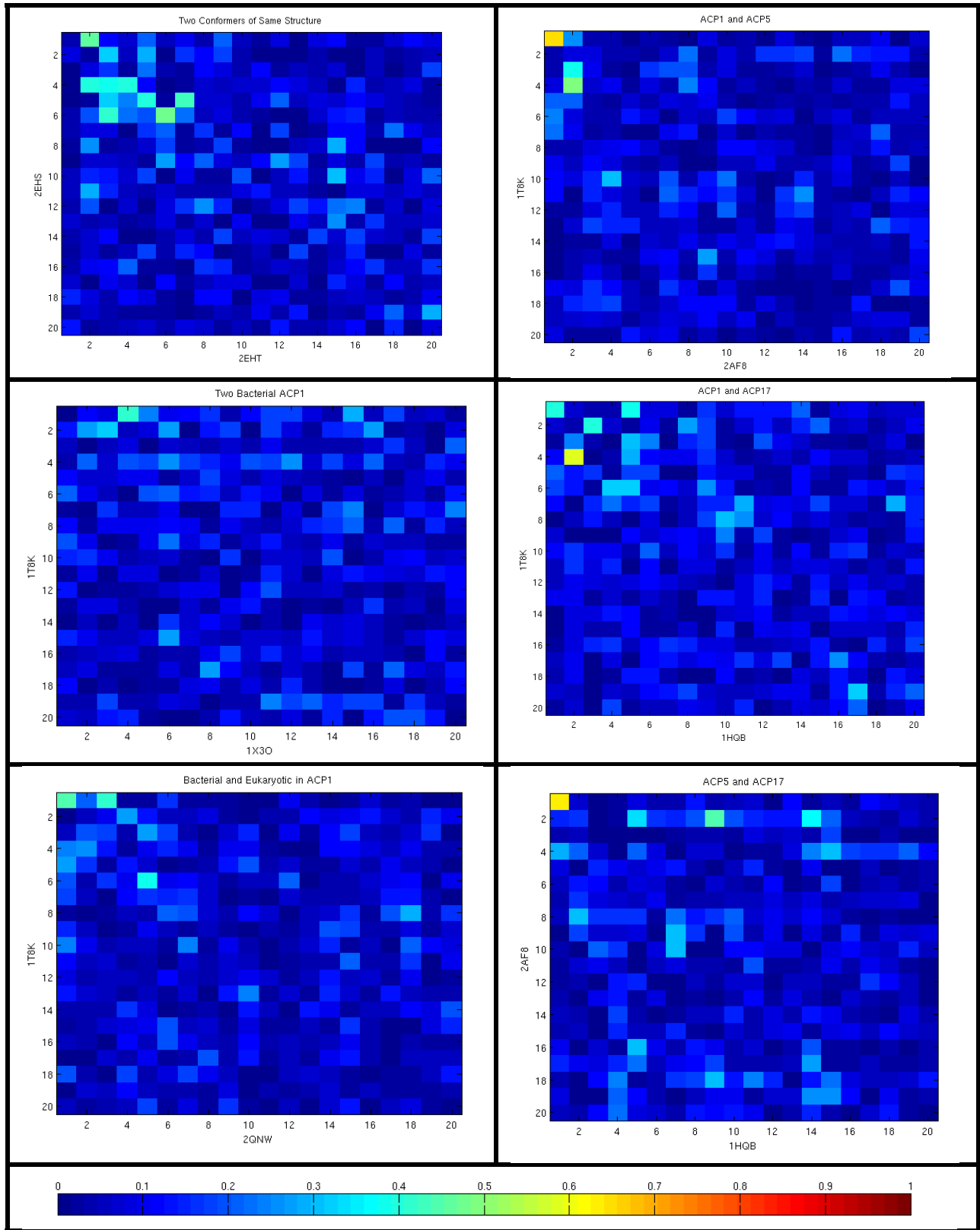
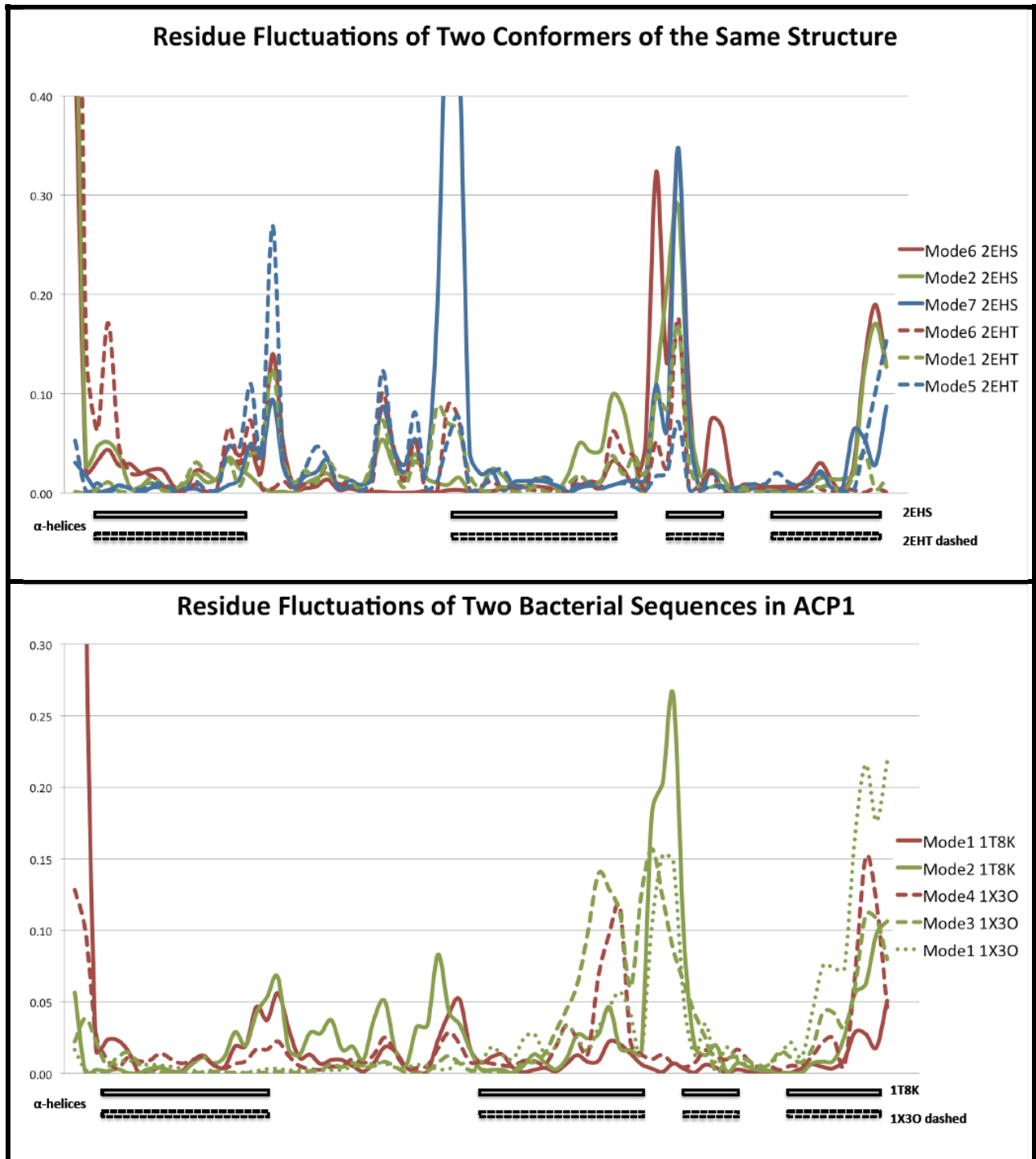
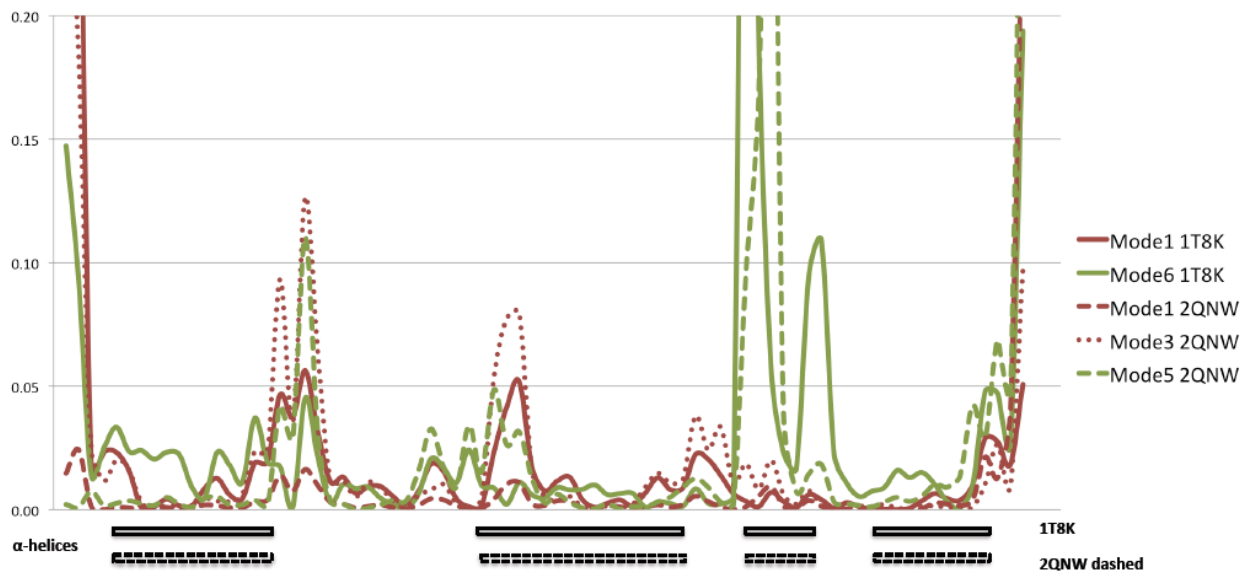


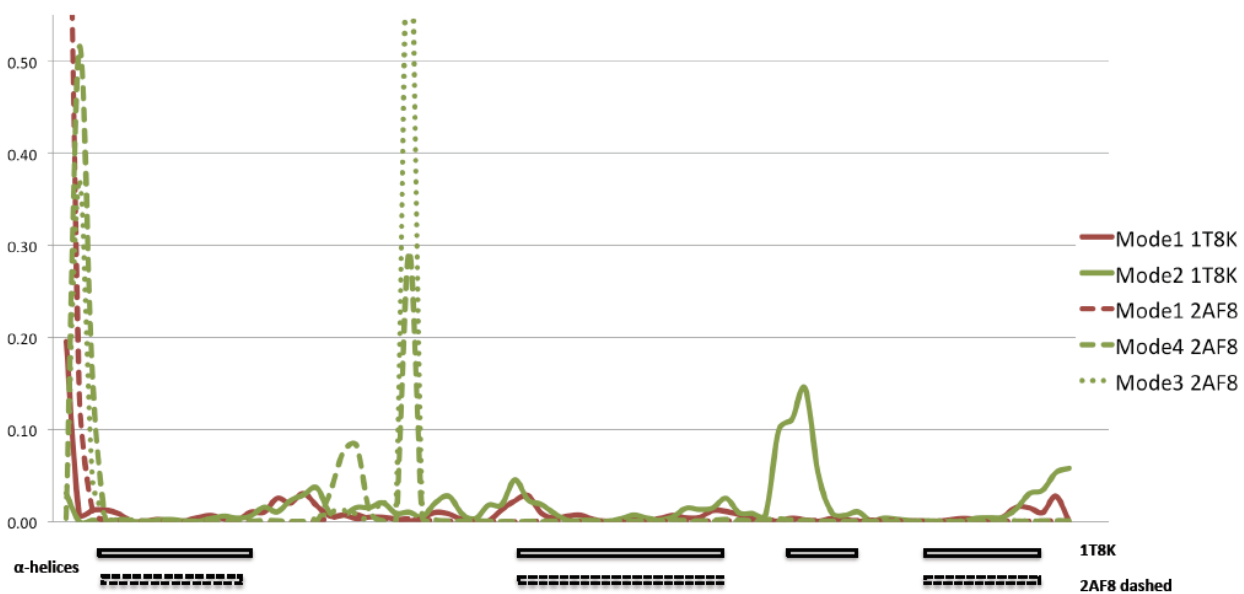
Figure S6: Residue fluctuation comparisons



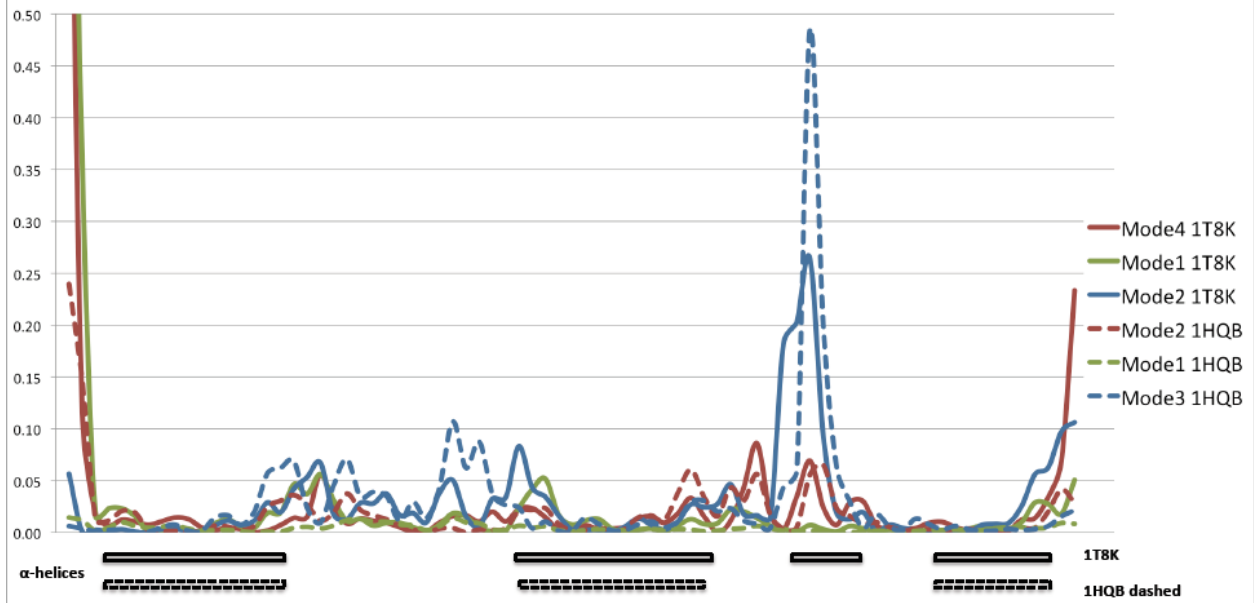
Residue Fluctuations of a Bacterial and Eukaryotic Structure in ACP1



Residue Fluctuations of ACP1 and ACP5



Residue Fluctuations of ACP1 and ACP17



Residue Fluctuations of ACP5 and ACP17

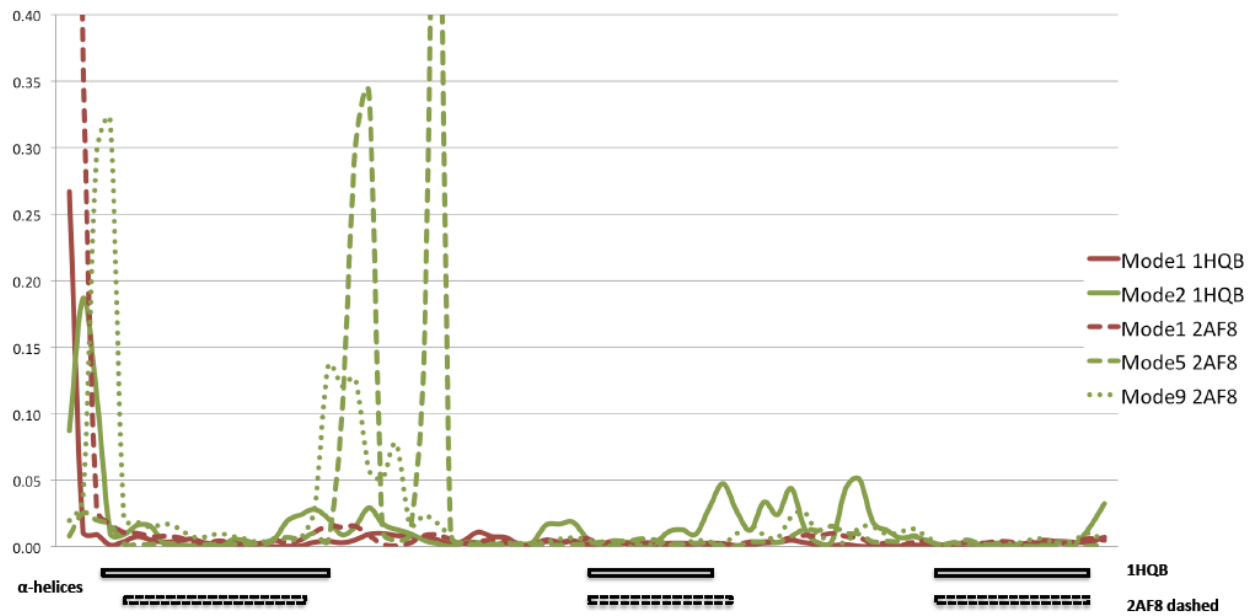


Figure S7: Tertiary structure models for ACP15 and 16 predicted by threading

