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Research article

Molecular dynamics simulations of metalloproteins: A folding study of rubredoxin from *Pyrococcus furiosus*

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Supplementary

Table S1. Secondary structure persistency per-residue of the APO simulation.

#Residue	Strand	Helix	Turn	#Residue	Strand	Helix	Turn
1	0.00	0.00	0.00	28	0.00	0.00	0.00
2	0.97	0.00	0.00	29	0.00	0.58	0.25
3	1.00	0.00	0.00	30	0.00	0.58	0.41
4	1.00	0.00	0.00	31	0.00	0.58	0.38
5	1.00	0.00	0.00	32	0.00	0.00	0.00
6	0.00	0.00	0.49	33	0.00	0.00	0.00
7	0.00	0.00	0.49	34	0.00	0.00	0.93
8	0.02	0.00	0.32	35	0.00	0.00	0.93
9	0.00	0.00	0.09	36	0.00	0.00	0.00

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#Residue	Strand	Helix	Turn	#Residue	Strand	Helix	Turn
10	0.09	0.00	0.00	37	**0.91**	0.00	0.00
11	1.00	0.00	0.00	38	**0.42**	0.00	0.00
12	1.00	0.00	0.00	39	0.00	0.01	0.98
13	0.95	0.00	0.00	40	0.00	0.01	0.99
14	0.00	0.02	0.97	41	0.00	0.01	0.98
15	0.00	0.02	0.98	42	0.00	0.00	0.42
16	0.00	0.02	0.97	43	**0.42**	0.00	0.00
17	0.10	0.00	0.00	44	**0.91**	0.00	0.00
18	**0.98**	0.00	0.00	45	0.00	0.67	0.32
19	0.00	0.23	0.76	46	0.00	0.67	0.33
20	0.00	0.23	0.76	47	0.00	0.67	0.01
21	0.00	0.23	0.76	48	0.99	0.00	0.00
22	0.00	0.00	0.99	49	1.00	0.00	0.00
23	**0.98**	0.00	0.00	50	0.99	0.00	0.00
24	0.00	0.00	0.94	51	0.05	0.00	0.00
25	0.00	0.00	0.94	52	**0.78**	0.00	0.00
26	0.00	0.00	0.94	53	0.00	0.00	0.00
27	0.00	0.00	0.00				

The residues involved in a native helix and β-strand are colored in blue and green, respectively. Residues with significant (>0.3) persistency of non-native secondary structures are in bold.

Table S2. Secondary structure persistency per-residue of the F-cMD simulation.

#Residue	Strand	Helix	Turn	#Residue	β-sheet	Helix	Turn
1	0.00	0.00	0.00	28	**0.41**	0.00	0.00
2	0.41	0.00	0.00	29	0.01	0.00	0.00
3	0.01	0.00	0.00	30	0.00	0.00	0.00
4	0.00	0.00	0.00	31	0.00	0.00	0.00
5	0.00	0.00	0.00	32	0.00	0.00	0.00
6	0.00	0.00	0.00	33	0.00	0.00	0.00
7	0.00	0.00	0.00	34	0.00	0.15	0.85
8	0.01	0.00	0.00	35	0.00	0.15	0.85
9	0.00	0.00	0.00	36	0.00	0.15	0.79
10	0.00	0.00	0.00	37	0.00	0.00	0.00
11	0.00	0.08	0.40	38	0.00	0.00	0.00
12	0.00	0.12	0.46	39	0.00	0.00	0.00
13	0.00	**0.52**	0.37	40	0.01	0.00	0.00
14	0.00	**0.52**	0.43	41	0.01	0.00	0.00
15	0.00	**0.49**	0.35	42	0.00	0.00	0.00
16	0.00	0.27	0.24	43	0.00	0.00	0.00
17	0.00	0.11	0.26	44	0.00	0.00	0.00
18	0.00	0.00	0.29	45	0.01	0.00	0.00

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#Residue	Strand	Helix	Turn	#Residue	β-sheet	Helix	Turn
19	0.00	0.00	0.29	46	0.00	0.00	0.00
20	0.01	0.07	0.04	47	0.00	0.37	0.57
21	0.01	0.07	0.30	48	0.00	**0.41**	0.57
22	0.01	0.07	0.28	49	0.00	**0.50**	0.48
23	**0.37**	0.00	0.00	50	0.00	**0.45**	0.31
24	0.00	0.00	0.00	51	**0.37**	0.19	0.15
25	0.00	0.14	0.72	52	0.00	0.07	0.10
26	0.00	0.14	0.73	53	0.00	0.00	0.00
27	0.00	0.14	0.26				

The residues involved in native helix and β-strand structures are colored in blue and green, respectively. Residues with significant (>0.3) persistency of non-native strand and helix are in bold and underlined bold, respectively.

Table S3. Secondary structure persistency per-residue of the F-aMD simulation.

#Residue	Strand	Helix	Turn	#Residue	β-sheet	Helix	Turn
1	0.00	0.00	0.00	28	0.17	**0.32**	0.16
2	0.09	0.00	0.06	29	0.12	0.30	0.33
3	0.12	0.00	0.07	30	0.05	0.25	0.39
4	0.14	0.00	0.01	31	0.02	0.13	0.43
5	0.00	0.00	0.01	32	0.11	0.05	0.08
6	0.08	0.00	0.25	33	0.01	0.09	0.12
7	0.00	0.00	0.27	34	0.00	0.10	0.31
8	**0.32**	0.00	0.05	35	0.01	0.09	0.32
9	0.05	0.04	0.11	36	0.00	0.01	0.10
10	0.01	0.13	0.12	37	0.01	0.00	0.00
11	0.04	0.16	0.11	38	0.00	0.00	0.00
12	0.07	0.17	0.11	39	0.01	0.00	0.00
13	0.09	0.19	0.12	40	0.01	0.00	0.00
14	0.01	0.15	0.33	41	0.03	0.00	0.34
15	0.00	0.12	0.35	42	0.00	0.00	0.36
16	0.02	0.08	0.33	43	**0.31**	0.00	0.01
17	0.04	0.05	0.15	44	0.04	0.01	0.03
18	0.16	0.05	0.03	45	0.00	0.57	0.08
19	0.07	0.10	0.33	46	0.00	0.62	0.07
20	0.01	0.13	0.38	47	0.01	0.79	0.11
21	0.02	0.12	0.42	48	0.00	**0.80**	0.10
22	0.08	0.07	0.27	49	0.00	**0.65**	0.22
23	0.06	0.05	0.15	50	0.00	**0.53**	0.26
24	0.07	0.03	0.05	51	0.01	**0.39**	0.24
25	0.06	0.17	0.18	52	0.01	0.08	0.13
26	0.05	0.23	0.22	53	0.00	0.00	0.00
27	0.08	**0.31**	0.17				

The residues involved in a native helix or β-strand structure in the crystal are colored in blue and green, respectively. Residues with significant (>0.3) persistency of non-native strand or helix structure are in bold and underlined bold, respectively.

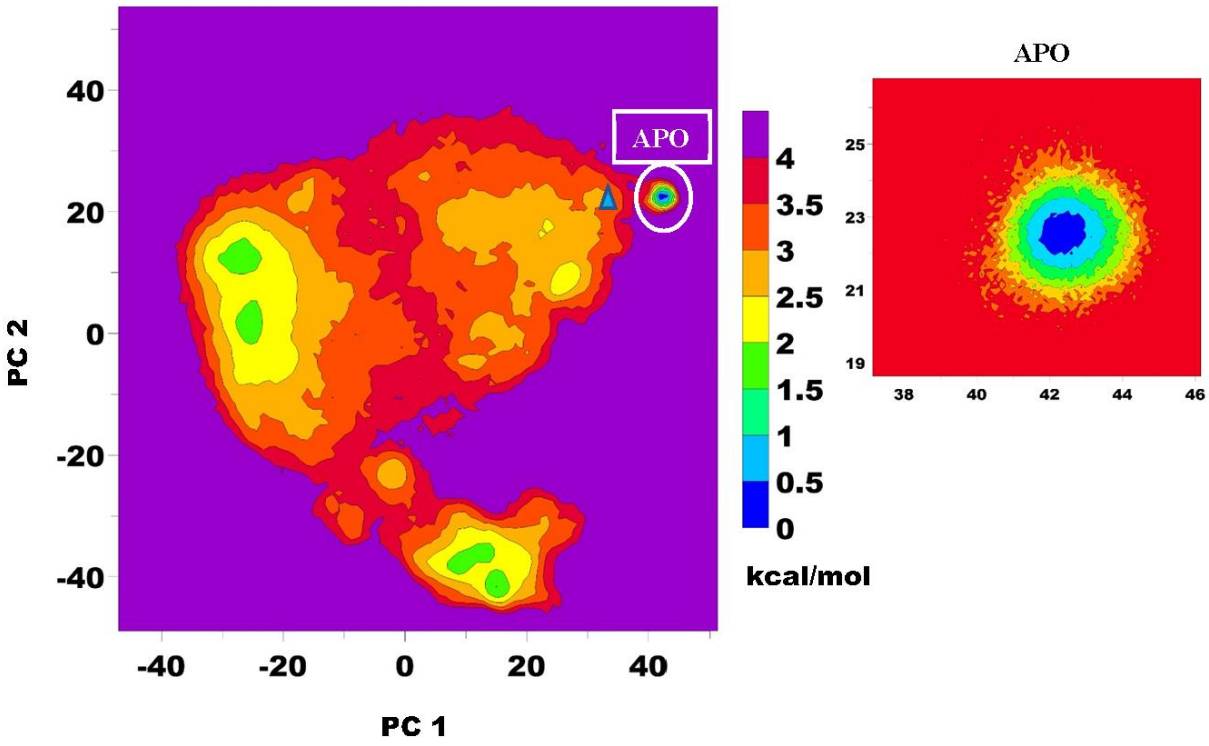

Figure S1. Principal Component Analysis of the F-aMD and APO trajectories. Projection of the two conformational ensembles on the first two eigenvectors. The APO region is zoomed on the right. The F-aMD conformation closest to the crystal structure at 2.2 μs is projected with a cyan triangle.