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Overview

Tables for cluster selection

ubq site	cluster id	N frames	ensemble %	aa %	σ^2 internal RMSD	coefficient	mean abs diff to exp w/ coeff	mean abs diff to exp w/o coeff
k6	0	131969	12	3	0.01	0.00	5.43	4.97
	1	96726	9	1	0.10	0.00	5.43	5.15
	2	43256	4	4	0.21	0.00	5.43	5.10
	3	39818	4	1	0.10	0.00	5.43	5.06
	4	27491	2	74	0.12	0.00	5.43	4.92
	5	17686	2	0	0.14	0.43	3.38	5.07
	6	15884	1	32	0.03	0.00	5.43	5.00
	7	13093	1	17	0.11	0.00	5.43	5.07
	8	12241	1	3	0.02	0.00	5.43	4.98
	9	7014	1	1	0.03	0.57	3.66	5.16
	10	6479	1	18	0.21	0.00	5.43	5.14
	11	5848	1	0	0.05	0.00	5.43	5.32
	12	2955	0	3	0.03	0.00	5.43	5.09
sum and combination	final linear combination	Σ 420460	Σ 38		Σ 1.0	final combination: 4.72		

		N frames	ensemble %	aa %	σ^2 internal RMSD	coefficient	mean abs diff to exp w/ coeff	mean abs diff to exp w/o coeff
ubq site	cluster id							
	0	186366	17	3	0.19	0.42	3.80	3.21
	1	99803	9	1	0.06	0.00	5.41	3.31
	2	48921	4	16	0.07	0.00	5.41	3.27
	3	44759	4	2	0.05	0.00	5.41	3.25
	4	28701	3	5	0.01	0.00	5.41	3.35
	5	22909	2	13	0.26	0.00	5.41	3.33
	6	16151	1	7	0.06	0.00	5.41	3.60
	7	14024	1	2	0.01	0.00	5.41	3.19
k29	8	12681	1	5	0.19	0.00	5.41	4.21
	9	11039	1	15	0.08	0.00	5.41	3.79
	10	7428	1	3	0.25	0.00	5.41	4.82
	11	7142	1	7	0.04	0.00	5.41	3.24
	12	6436	1	0	0.00	0.58	3.33	3.15
	13	5148	0	7	0.06	0.00	5.41	4.28
	14	4662	0	2	0.14	0.00	5.41	4.16
	15	4606	0	36	0.10	0.00	5.41	4.77
	16	4112	0	1	0.00	0.00	5.41	3.14
	17	3379	0	1	0.01	0.00	5.41	3.25
sum and combination	final linear	Σ 528267	Σ 48		Σ 1.0		final combination: 3.03	

ubq site	cluster id	N frames	ensemble %	aa %	σ^2 internal RMSD	coefficient	mean abs diff	abs diff to exp w/o coeff
k33	0	119908	10	2	0.02	0.00	7.89	4.48
	1	95897	8	1	0.02	0.00	7.89	4.45
	2	31411	3	1	0.02	0.00	7.89	4.45
	3	30973	3	47	0.14	0.00	7.89	4.16
	4	29716	3	2	0.08	0.00	7.89	4.36
	5	29250	2	2	0.03	0.00	7.89	4.57
	6	22921	2	1	0.01	0.06	7.67	4.60
	7	21385	2	18	0.22	0.00	7.89	4.47
	8	21253	2	4	0.05	0.09	7.45	3.91
	9	20462	2	9	0.06	0.00	7.89	4.12
	10	9469	1	1	0.00	0.00	7.89	4.47
	11	9425	1	34	0.17	0.00	7.89	4.15
	12	9010	1	100	0.16	0.00	7.89	4.34
	13	7593	1	81	0.20	0.00	7.89	4.38
	14	6179	1	11	0.17	0.00	7.89	4.21
	15	6174	1	3	0.08	0.00	7.89	4.55
	16	5877	0	3	0.29	0.09	7.51	4.41
	17	5140	0	6	0.13	0.00	7.89	4.53
	18	4838	0	100	0.38	0.00	7.89	4.75
	19	4735	0	1	0.01	0.00	7.89	4.90
	20	4326	0	1	0.25	0.77	4.58	4.08
	21	3231	0	4	0.04	0.00	7.89	4.05
	22	3050	0	100	0.05	0.00	7.89	4.36
	23	2584	0	100	0.00	0.00	7.89	4.06
sum final linear Σ							final combination:	
and combination							4.07	
Σ 43								
Σ 504807								
Σ 1.0								