

Table S1. A list of the structures of benchmark proteins selected for this study with the respective numbers of residues in the sequence (#res), the numbers of residues after truncation (#res.t), and the ranges of residues after truncation (range_t). The entries are grouped according to secondary-structure class. PDB codes in boldface font correspond to NMR structures, those in regular font correspond to X-ray structures.

α proteins				β proteins				$\alpha+\beta$ proteins			
PDB ID^a	# res.	#res.t	range_t	PDB ID^a	# res.	#res.t	range_t	PDB ID^a	# res.	#res.t	range_t
1A6S	87	87	1-87	1AH9	71	63	5-67	1A80	277	276	2-277
1ACP	77	71	3-73	1BK2	57	55	2-56	1ADG	374	373	2-374
1ALA	316	316	1-316	1CSP	67	67	1-67	1AKY	218	216	2-217
1AUM	70	70	1-70	1ED7	45	45	1-45	1CFJ	532	530	1-530
1BAL	51	33	16-48	1HRF	67	45	7-51	1CLB	75	72	2-73
1ENH	54	48	4-51	1IYV	79	71	3-73	1CTF	68	68	1-68
1EO0	77	73	2-73	1MJC	69	69	1-69	1E0G	48	46	2-47
1FEX	59	54	5-58	1NOA	113	113	1-113	1EM7	56	56	1-56
1GAB	53	44	9-52	1RUW	69	69	1-69	1G6E	87	86	2-87

1HNS	47	39	6-44	1TEN	89	89	1-89	1GHH	81	80	1-79
1HYP	75	73	1-73	1TPN	50	43	5-47	1HYW	58	52	3-52
1IYR	83	72	4-75	1WIU	93	93	1-93	1IG5	75	75	1-75
1J7O	76	71	5-75	1WKT	88	85	4-88	1IQO	88	87	2-88
1K40	126	124	3-126	1XCD	305	305	1-305	1K8B	52	51	1-51
1L2Y	20	18	2-19	2K9G	73	62	9-70	1LEB	72	66	4-69
1LQ7	67	65	3-67	2KYW	87	78	2-79	1OGQ	313	310	3-312
1P68	102	98	4-101	2LGN	66	65	2-66	1OIX	168	168	1-168
1POU	71	66	5-70	2LVC	90	87	4-90	1OPD	85	81	1-81
1PRV	56	36	5-40	3PUC	98	97	1-97	1PGA	56	56	1-56
1RIJ	23	17	5-21	4F98	62	60	3-62	1PHT	83	83	1-83
1ROP	56	56	1-56	4M9O	97	95	1-95	1PTF	87	86	1-86

1YRF	35	34	1-34					1QRE	210	208	3-210
2BF9	36	34	1-34					1STU	68	66	1-66
2CRB	97	69	11-79					1THX	108	104	3-106
2E7N	117	108	10-117					1TIG	88	87	1-87
2HEP	42	23	8-30					1UBQ	76	71	1-71
2HI3	73	47	9-55					1VIG	71	67	4-70
2YGS	92	91	1-91					2ACY	98	93	5-97
3ICB	75	74	1-75					2BBY	69	62	5-66
3WFW	138	134	1-134					2FMR	65	64	2-65
								2L09	62	48	3-50
								2LZM	164	162	1-162
								2M6Q	91	82	2-83

								2MQ8	112	97	1-97
								2N2U	77	63	3-65
								2PTL	78	59	19-77
								2RGF	97	97	1-97
								3CI2	64	63	2-64
								3E8Y	30	29	1-29
								3KYW	54	53	1-53
								3KYY	54	53	1-53
								3NCM	92	92	1-92
								4N6T	79	79	1-79
								4OZU	390	389	2-390
								4QRL	110	110	1-110

								4R7E	69	69	1-69
								4RTE	124	123	2-124
								5D14	70	68	1-68
								6DNB	411	409	1-410

Table S2. The Pearson (r_p) and Spearman (r_s) correlation coefficients of the RMSF profiles over the truncated structures calculated from B-factors (X-ray structures) or NMR ensembles (NMR structures) and those predicted with UNRES-flex, UNRES-DSSP-flex, CABS-flex, and NOLB, respectively.

#	PDB ID	UNRES-flex		UNRES-DSSP-flex		CABS-flex		NOLB	
		r_s	r_p	r_s	r_p	r_s	r_p	r_s	r_p
1	1A6S	0.52	0.34	0.59	0.56	0.75	0.81	0.17	-0.08
2	1A80	0.42	0.40	0.49	0.44	0.59	0.50	0.67	0.66
3	1ACP	0.22	0.20	0.46	0.35	0.42	0.38	0.22	0.22
4	1ADG	0.31	0.30	0.36	0.31	0.45	0.41	0.45	0.40
5	1AH9	0.71	0.65	0.74	0.72	0.79	0.68	0.21	0.21
6	1AKY	0.40	0.38	0.44	0.58	0.52	0.73	0.71	0.73
7	1ALA	0.47	0.43	0.58	0.54	0.52	0.49	0.55	0.48
8	1AUM	0.40	0.24	0.52	0.43	0.28	0.11	0.44	0.46

9	1BAL	0.27	0.26	0.32	0.27	0.05	-0.08	0.08	-0.05
10	1BK2	0.36	0.22	0.14	0.05	0.37	0.22	0.47	0.54
11	1CFJ	0.53	0.53	0.56	0.59	0.37	0.40	0.68	0.67
12	1CLB	0.33	0.30	0.56	0.58	0.81	0.88	0.09	-0.08
13	1CSP	0.41	0.49	0.50	0.51	0.50	0.45	0.28	0.28
14	1CTF	0.29	0.27	0.38	0.36	0.10	0.05	0.41	0.40
15	1E0G	0.42	0.62	0.58	0.66	0.61	0.73	0.28	0.14
16	1ED7	0.49	0.45	0.59	0.53	0.33	0.22	0.00	-0.02
17	1EM7	0.31	0.28	0.46	0.42	0.52	0.53	0.69	0.61
18	1ENH	0.52	0.62	0.39	0.51	0.48	0.51	0.35	0.34
19	1EO0	0.29	0.36	0.33	0.41	0.31	0.37	0.30	0.34
20	1FEX	0.50	0.39	0.64	0.46	0.54	0.40	-0.13	-0.21
21	1G6E	0.59	0.43	0.69	0.53	0.46	0.41	0.48	0.33
22	1GAB	0.20	0.16	0.22	0.18	0.39	0.38	0.57	0.46
23	1GHH	0.28	0.35	0.40	0.52	0.21	0.36	0.07	0.09
24	1HNS	0.53	0.49	0.67	0.66	0.81	0.81	0.16	0.16
25	1HRF	-0.18	-0.12	-0.18	-0.12	0.25	0.43	0.45	0.45
26	1HYP	0.72	0.62	0.62	0.54	0.69	0.54	0.60	0.57
27	1HYW	0.60	0.57	0.58	0.56	0.64	0.60	-0.03	-0.02
28	1IG5	0.77	0.62	0.78	0.75	0.75	0.61	0.76	0.74
29	1IQO	0.41	0.32	0.56	0.44	0.62	0.50	0.18	0.06

30	1IYR	0.21	0.53	0.52	0.61	0.69	0.74	0.44	0.07
31	1IYV	0.47	0.42	0.47	0.42	0.63	0.67	0.12	0.33
32	1J7O	0.17	0.11	0.09	0.05	-0.37	-0.29	0.23	0.04
33	1K40	0.78	0.78	0.82	0.85	0.68	0.64	0.55	0.55
34	1K8B	0.34	0.31	0.46	0.43	0.16	0.14	0.17	-0.01
35	1L2Y	0.56	0.57	0.72	0.62	0.70	0.54	-0.23	-0.14
36	1LEB	0.22	0.23	0.35	0.32	0.86	0.82	-0.05	-0.12
37	1LQ7	0.66	0.66	0.67	0.60	0.69	0.81	0.67	0.49
38	1MJC	0.76	0.80	0.63	0.69	0.58	0.67	0.60	0.65
39	1NOA	0.45	0.43	0.36	0.38	0.42	0.40	0.65	0.66
40	1OGQ	0.08	0.06	0.20	0.17	0.62	0.59	0.45	0.50
41	1OIX	0.25	0.25	0.49	0.49	0.21	0.32	0.51	0.54
42	1OPD	0.55	0.52	0.57	0.62	0.35	0.40	0.43	0.40
43	1P68	0.61	0.51	0.58	0.56	0.69	0.56	0.47	0.34
44	1PGA	0.21	0.18	0.16	0.13	0.31	0.14	0.30	0.20
45	1PHT	0.79	0.77	0.83	0.70	0.72	0.67	0.82	0.78
46	1POU	0.32	0.24	0.54	0.47	0.49	0.65	-0.22	-0.15
47	1PRV	0.63	0.53	0.69	0.54	0.49	0.60	0.52	0.60
48	1PTF	0.29	0.29	0.41	0.42	0.51	0.39	0.52	0.60
49	1QRE	0.77	0.71	0.74	0.71	0.71	0.76	0.80	0.83
50	1RIJ	0.46	0.48	0.74	0.78	0.71	0.68	-0.28	-0.19

51	1ROP	0.53	0.52	0.50	0.59	0.43	0.54	0.49	0.55
52	1RUW	0.39	0.49	0.35	0.47	0.36	0.62	0.29	0.48
53	1STU	0.46	0.48	0.40	0.48	0.55	0.88	0.38	0.17
54	1TEN	0.48	0.48	0.44	0.46	0.56	0.61	0.29	0.35
55	1THX	0.37	0.32	0.36	0.38	0.58	0.46	0.48	0.45
56	1TIG	0.40	0.42	0.47	0.48	0.64	0.49	0.72	0.61
57	1TPN	0.57	0.70	0.76	0.87	0.49	0.58	0.14	0.02
58	1UBQ	0.49	0.49	0.47	0.40	0.52	0.50	0.65	0.67
59	1VIG	0.79	0.66	0.27	0.33	0.85	0.86	0.53	0.48
60	1WIU	0.70	0.48	0.77	0.66	0.67	0.47	0.59	0.45
61	1WKT	0.66	0.47	0.80	0.59	0.72	0.55	0.48	0.37
62	1XCD	0.71	0.64	0.74	0.70	0.58	0.49	0.31	0.41
63	1YRF	0.58	0.69	0.35	0.60	0.58	0.62	0.32	0.45
64	2ACY	0.33	0.27	0.27	0.29	0.26	0.33	0.44	0.47
65	2BBY	0.55	0.62	0.75	0.82	0.51	0.76	0.38	0.48
66	2BF9	0.29	0.21	-0.06	0.02	0.27	0.06	0.34	0.33
67	2CRB	0.56	0.44	0.52	0.47	0.50	0.66	0.49	0.39
68	2E7N	0.61	0.57	0.69	0.67	0.72	0.83	0.09	0.06
69	2FMR	0.63	0.58	0.83	0.78	0.77	0.60	0.42	0.33
70	2HEP	0.71	0.61	0.51	0.43	0.58	0.73	0.14	0.38
71	2HI3	0.63	0.45	0.34	0.19	0.64	0.75	-0.14	-0.14

72	2K9G	0.78	0.80	0.61	0.61	0.71	0.52	0.39	0.31
73	2KYW	0.75	0.63	0.78	0.69	0.72	0.67	0.19	-0.02
74	2L09	0.43	0.36	0.29	0.20	0.44	0.68	0.00	-0.18
75	2LGN	0.72	0.53	0.56	0.57	0.77	0.61	0.37	0.36
76	2LVC	0.79	0.73	0.85	0.77	0.71	0.49	0.36	0.16
77	2LZM	0.37	0.46	0.23	0.33	0.46	0.49	0.49	0.55
78	2M6Q	0.45	0.45	0.43	0.50	0.58	0.55	0.25	0.03
79	2MQ8	0.59	0.49	0.73	0.62	0.76	0.58	0.28	0.22
80	2N2U	0.14	0.17	0.43	0.41	0.55	0.48	0.39	0.37
81	2PTL	0.56	0.43	0.52	0.41	0.72	0.72	0.53	0.68
82	2RGF	0.55	0.37	0.51	0.32	0.40	0.19	0.29	0.18
83	2YGS	0.16	0.15	0.07	0.05	0.11	0.01	0.33	0.27
84	3CI2	0.32	0.23	0.52	0.40	0.65	0.62	-0.16	-0.24
85	3E8Y	0.54	0.30	0.48	0.43	0.18	0.12	0.55	0.52
86	3ICB	0.15	0.13	0.31	0.30	0.33	0.19	0.68	0.56
87	3KYW	0.51	0.51	0.49	0.45	0.49	0.44	0.47	0.56
88	3KYY	0.49	0.41	0.44	0.41	0.52	0.36	0.53	0.63
89	3NCM	0.71	0.44	0.57	0.39	0.68	0.34	0.39	0.24
90	3PUC	0.57	0.47	0.67	0.53	0.60	0.46	0.57	0.47
91	3WFW	0.55	0.62	0.55	0.64	0.38	0.50	0.43	0.54
92	4F98	0.75	0.66	0.73	0.68	0.71	0.64	0.58	0.62

93	4M9O	0.64	0.60	0.55	0.51	0.52	0.43	0.64	0.55
94	4N6T	0.41	0.34	0.53	0.52	0.84	0.73	0.76	0.79
95	4OZU	0.49	0.48	0.31	0.36	0.44	0.48	0.61	0.63
96	4QRL	0.69	0.61	0.47	0.46	0.81	0.81	0.79	0.78
97	4R7E	0.46	0.47	0.44	0.46	0.59	0.55	0.37	0.34
98	4RTE	0.49	0.52	0.38	0.30	0.74	0.81	0.71	0.74
99	5D14	0.56	0.56	0.46	0.44	0.35	0.40	0.52	0.53
100	6DNB	0.46	0.34	0.58	0.41	0.51	0.37	0.58	0.36
Average:		0.48	0.44	0.44	0.48	0.53	0.51	0.38	0.35

Table S3. The Pearson (r_p) and Spearman (r_s) correlation coefficients of the RMSF profiles over the full structures calculated from B-factors (X-ray structures) or NMR ensembles (NMR structures) and those predicted with UNRES-flex, UNRES-DSSP-flex, CABS-flex, and NOLB, respectively.

#	PDB ID	UNRES-flex		UNRES-DSSP-flex		CABS-flex		NOLB	
		r_s	r_p	r_s	r_p	r_s	r_p	r_s	r_p
1	1A6S	0.52	0.34	0.59	0.56	0.75	0.81	0.17	-0.08
2	1A80	0.42	0.39	0.49	0.42	0.59	0.51	0.67	0.64
3	1ACP	0.38	0.59	0.55	0.67	0.36	0.30	0.25	0.18
4	1ADG	0.32	0.33	0.37	0.34	0.45	0.41	0.46	0.41
5	1AH9	0.77	0.84	0.79	0.82	0.83	0.79	0.19	0.31
6	1AKY	0.42	0.42	0.45	0.62	0.53	0.76	0.71	0.72
7	1ALA	0.47	0.43	0.58	0.54	0.52	0.49	0.55	0.48

8	1AUM	0.40	0.24	0.52	0.43	0.28	0.11	0.44	0.46
9	1BAL	0.71	0.94	0.77	0.96	0.47	0.68	0.73	0.81
10	1BK2	0.42	0.39	0.21	0.20	0.39	0.21	0.52	0.60
11	1CFJ	0.54	0.56	0.56	0.61	0.38	0.41	0.69	0.69
12	1CLB	0.40	0.46	0.60	0.64	0.82	0.87	0.12	-0.07
13	1CSP	0.41	0.49	0.50	0.51	0.50	0.45	0.28	0.28
14	1CTF	0.29	0.27	0.38	0.36	0.10	0.05	0.41	0.40
15	1EOG	0.49	0.78	0.63	0.77	0.65	0.84	0.33	0.25
16	1ED7	0.49	0.45	0.59	0.53	0.33	0.22	0.00	-0.02
17	1EM7	0.31	0.28	0.46	0.42	0.52	0.53	0.69	0.61
18	1ENH	0.66	0.91	0.57	0.89	0.62	0.83	0.54	0.76
19	1EO0	0.40	0.59	0.43	0.66	0.36	0.31	0.38	0.39
20	1FEX	0.62	0.88	0.73	0.88	0.64	0.79	0.07	0.57
21	1G6E	0.60	0.49	0.70	0.57	0.47	0.44	0.49	0.40
22	1GAB	0.52	0.88	0.54	0.92	0.64	0.95	0.71	0.84
23	1GHH	0.30	0.52	0.42	0.67	0.24	0.57	0.10	0.16
24	1HNS	0.72	0.82	0.81	0.93	0.86	0.84	0.41	0.62
25	1HRF	0.55	0.87	0.55	0.87	0.69	0.79	0.39	0.05
26	1HYP	0.74	0.72	0.65	0.68	0.71	0.63	0.61	0.54
27	1HYW	0.71	0.76	0.70	0.82	0.73	0.81	0.19	0.46
28	1IG5	0.77	0.62	0.78	0.75	0.75	0.61	0.76	0.74

29	1IQO	0.43	0.41	0.57	0.50	0.63	0.53	0.21	0.29
30	1IYR	0.47	0.79	0.68	0.91	0.79	0.91	0.53	0.22
31	1IYV	0.55	0.80	0.55	0.80	0.65	0.86	0.24	0.07
32	1J7O	0.33	0.79	0.25	0.83	-0.15	0.52	0.37	0.67
33	1K4O	0.79	0.82	0.82	0.85	0.68	0.59	0.57	0.55
34	1K8B	0.37	0.41	0.49	0.65	0.20	0.37	0.19	0.08
35	1L2Y	0.68	0.84	0.77	0.60	0.76	0.58	-0.12	-0.01
36	1LEB	0.51	0.85	0.62	0.88	0.89	0.86	0.07	0.48
37	1LQ7	0.69	0.77	0.70	0.78	0.72	0.72	0.69	0.92
38	1MJC	0.76	0.80	0.63	0.69	0.58	0.67	0.60	0.65
39	1NOA	0.45	0.43	0.36	0.38	0.42	0.40	0.65	0.66
40	1OGQ	0.08	0.06	0.19	0.16	0.63	0.62	0.46	0.56
41	1OIX	0.25	0.25	0.49	0.49	0.21	0.32	0.51	0.54
42	1OPD	0.60	0.60	0.62	0.70	0.35	0.32	0.45	0.33
43	1P68	0.65	0.67	0.63	0.72	0.72	0.64	0.48	0.42
44	1PGA	0.21	0.18	0.16	0.13	0.31	0.14	0.30	0.20
45	1PHT	0.79	0.77	0.83	0.70	0.72	0.67	0.82	0.78
46	1POU	0.43	0.58	0.62	0.67	0.51	0.66	-0.07	0.02
47	1PRV	0.87	0.77	0.88	0.74	0.67	0.40	-0.24	-0.23
48	1PTF	0.31	0.34	0.43	0.47	0.53	0.45	0.50	0.54
49	1QRE	0.78	0.74	0.74	0.74	0.72	0.77	0.81	0.84

50	1RIJ	0.78	0.90	0.85	0.86	0.58	0.43	-0.02	0.03
51	1ROP	0.53	0.52	0.50	0.59	0.43	0.54	0.49	0.55
52	1RUW	0.39	0.49	0.35	0.47	0.36	0.62	0.29	0.48
53	1STU	0.48	0.49	0.44	0.49	0.58	0.88	0.40	0.18
54	1TEN	0.48	0.48	0.44	0.46	0.56	0.61	0.29	0.35
55	1THX	0.43	0.49	0.42	0.59	0.62	0.60	0.52	0.54
56	1TIG	0.42	0.53	0.48	0.59	0.65	0.60	0.73	0.66
57	1TPN	0.72	0.91	0.85	0.92	0.65	0.70	0.36	0.62
58	1UBQ	0.58	0.77	0.53	0.64	0.59	0.75	0.71	0.85
59	1VIG	0.82	0.88	0.38	0.82	0.87	0.88	0.58	0.78
60	1WIU	0.70	0.48	0.77	0.66	0.67	0.47	0.59	0.45
61	1WKT	0.69	0.63	0.82	0.75	0.73	0.54	0.50	0.52
62	1XCD	0.71	0.64	0.74	0.70	0.58	0.49	0.31	0.41
63	1YRF	0.61	0.78	0.40	0.73	0.62	0.77	0.35	0.41
64	2ACY	0.42	0.67	0.38	0.78	0.35	0.63	0.52	0.60
65	2BBY	0.67	0.72	0.82	0.77	0.56	0.54	0.45	0.60
66	2BF9	0.40	0.67	0.11	0.65	0.38	0.39	0.42	0.57
67	2CRB	0.84	0.91	0.82	0.95	0.81	0.94	0.76	0.67
68	2E7N	0.69	0.81	0.75	0.88	0.78	0.93	0.17	0.72
69	2FMR	0.64	0.61	0.84	0.80	0.78	0.63	0.44	0.40
70	2HEP	0.94	0.96	0.91	0.97	0.48	0.76	0.05	0.31

71	2HI3	0.89	0.93	0.81	0.92	0.84	0.90	0.14	0.06
72	2K9G	0.86	0.77	0.76	0.74	0.80	0.51	0.53	0.73
73	2KYW	0.82	0.85	0.84	0.96	0.79	0.70	0.30	0.01
74	2L09	0.73	0.95	0.67	0.86	0.66	0.91	0.25	0.02
75	2LGN	0.73	0.66	0.58	0.59	0.78	0.63	0.40	0.50
76	2LVC	0.81	0.84	0.86	0.88	0.71	0.40	0.42	0.69
77	2LZM	0.39	0.53	0.26	0.44	0.48	0.52	0.50	0.58
78	2M6Q	0.58	0.86	0.57	0.80	0.66	0.68	0.34	0.10
79	2MQ8	0.73	0.98	0.83	0.99	0.84	0.96	0.37	0.20
80	2N2U	0.51	0.96	0.65	0.98	0.67	0.90	0.41	0.03
81	2PTL	0.80	0.95	0.78	0.94	0.85	0.85	0.74	0.81
82	2RGF	0.55	0.37	0.51	0.32	0.40	0.19	0.29	0.18
83	2YGS	0.18	0.21	0.10	0.18	0.14	0.12	0.35	0.30
84	3CI2	0.35	0.45	0.54	0.56	0.67	0.71	-0.11	0.05
85	3E8Y	0.58	0.59	0.53	0.70	0.26	0.38	0.59	0.70
86	3ICB	0.18	0.18	0.34	0.38	0.35	0.25	0.69	0.61
87	3KYW	0.51	0.51	0.49	0.45	0.49	0.44	0.47	0.56
88	3KYY	0.49	0.41	0.44	0.41	0.52	0.36	0.53	0.63
89	3NCM	0.71	0.44	0.57	0.39	0.68	0.34	0.39	0.24
90	3PUC	0.58	0.46	0.68	0.52	0.61	0.46	0.58	0.50
91	3WFW	0.59	0.61	0.59	0.70	0.35	0.39	0.44	0.45

92	4F98	0.77	0.67	0.76	0.73	0.73	0.76	0.61	0.63
93	4M9O	0.66	0.67	0.58	0.59	0.55	0.47	0.66	0.60
94	4N6T	0.41	0.34	0.53	0.52	0.84	0.73	0.76	0.79
95	4OZU	0.50	0.49	0.32	0.38	0.45	0.51	0.61	0.62
96	4QRL	0.69	0.61	0.47	0.46	0.81	0.81	0.79	0.78
97	4R7E	0.46	0.47	0.44	0.46	0.59	0.55	0.37	0.34
98	4RTE	0.51	0.56	0.39	0.38	0.74	0.82	0.71	0.73
99	5D14	0.60	0.78	0.51	0.70	0.38	0.45	0.56	0.59
100	6DNB	0.47	0.41	0.59	0.47	0.52	0.42	0.59	0.41
Average:		0.56	0.62	0.58	0.65	0.58	0.59	0.43	0.45

Table S4. The average Pearson's (r_p) and Spearman's correlation coefficients (r_s) between fluctuation profiles calculated for truncated structures with UNRES-flex, UNRES-DSSP-flex, CABS-flex, and NOLB.

A: NMR structures

	Secondary-structure type							
	α		β		$\alpha + \beta$		all	
	r_p	r_s	r_p	r_s	r_p	r_s	r_p	r_s
UNRES-flex	0.410	0.449	0.522	0.586	0.427	0.474	0.441	0.489
	0.153	0.172	0.236	0.264	0.138	0.163	0.176	0.200
UNRES-DSSP-flex	0.466	0.516	0.574	0.613	0.488	0.525	0.498	0.541
	0.181	0.174	0.248	0.275	0.154	0.151	0.194	0.197
CABS-flex	0.524	0.498	0.536	0.618	0.608	0.614	0.558	0.568
	0.300	0.279	0.129	0.173	0.191	0.163	0.235	0.226
NOLB	0.128	0.185	0.238	0.300	0.166	0.247	0.167	0.234
	0.249	0.277	0.172	0.171	0.237	0.202	0.233	0.234

B: X-ray structures

	Secondary-structure type							
	α		B		$\alpha + \beta$		all	
	r_p	r_s	r_p	r_s	r_p	r_s	r_p	r_s
UNRES-flex	0.465	0.501	0.527	0.553	0.396	0.417	0.447	0.474
	0.195	0.169	0.149	0.145	0.159	0.168	0.178	0.173
UNRES-DSSP-flex	0.473	0.467	0.496	0.512	0.426	0.431	0.457	0.460
	0.198	0.202	0.181	0.182	0.148	0.157	0.176	0.182
CABS-flex	0.392	0.439	0.497	0.519	0.499	0.524	0.460	0.492
	0.209	0.165	0.131	0.104	0.189	0.190	0.194	0.171
NOLB	0.512	0.512	0.502	0.468	0.573	0.578	0.537	0.532
	0.130	0.129	0.120	0.150	0.158	0.150	0.145	0.149

C: All structures

	Secondary-structure type							
	α		B		$\alpha + \beta$		all	
	r_p	r_s	r_p	r_s	r_p	r_s	r_p	r_s
UNRES-flex	0.436	0.474	0.525	0.570	0.410	0.444	0.444	0.482
	0.176	0.173	0.200	0.216	0.150	0.169	0.177	0.187
UNRES-DSSP-flex	0.469	0.493	0.537	0.565	0.455	0.474	0.477	0.500
	0.189	0.190	0.222	0.241	0.154	0.161	0.186	0.194
CABS-flex	0.461	0.470	0.517	0.571	0.550	0.566	0.509	0.530
	0.269	0.234	0.131	0.153	0.198	0.183	0.221	0.204
NOLB	0.310	0.340	0.364	0.380	0.384	0.425	0.352	0.383
	0.278	0.273	0.199	0.182	0.284	0.242	0.268	0.246

Table S5. The average Pearson's (r_p) and Spearman's correlation coefficients (r_s) between fluctuation profiles calculated for full structures with UNRES-flex, UNRES-DSSP-flex, CABS-flex, and NOLB.

A: NMR structures

Secondary-structure type								
	α		β		$\alpha + \beta$		all	
	r_p	r_s	r_p	r_s	r_p	r_s	r_p	r_s
UNRES-flex	0.759	0.625	0.735	0.698	0.681	0.580	0.724	0.624
	0.171	0.184	0.152	0.116	0.212	0.148	0.188	0.164
UNRES-DSSP-flex	0.803	0.680	0.774	0.723	0.715	0.623	0.763	0.668
	0.130	0.163	0.131	0.122	0.192	0.131	0.161	0.148
CABS-flex	0.672	0.590	0.600	0.695	0.706	0.666	0.669	0.642
	0.217	0.245	0.183	0.129	0.213	0.164	0.212	0.200
NOLB	0.361	0.282	0.358	0.356	0.292	0.318	0.334	0.312
	0.340	0.293	0.272	0.159	0.242	0.192	0.293	0.234

B: X-ray structures

Secondary-structure type								
	α		β		$\alpha + \beta$		all	
	r_p	r_s	r_p	r_s	r_p	r_s	r_p	r_s
UNRES-flex	0.560	0.529	0.552	0.563	0.453	0.434	0.512	0.494
	0.210	0.166	0.126	0.142	0.182	0.170	0.190	0.172
UNRES-DSSP-flex	0.594	0.503	0.524	0.525	0.492	0.449	0.535	0.484
	0.175	0.178	0.154	0.173	0.167	0.154	0.174	0.170
CABS-flex	0.464	0.464	0.513	0.528	0.541	0.537	0.508	0.509
	0.196	0.160	0.149	0.106	0.197	0.186	0.191	0.167
NOLB	0.562	0.537	0.518	0.478	0.589	0.590	0.565	0.548
	0.131	0.116	0.126	0.156	0.165	0.147	0.149	0.145

C: All structures

Secondary-structure type								
	α		β		$\alpha + \beta$		all	
	r_p	r_s	r_p	r_s	r_p	r_s	r_p	r_s

UNRES-flex	0.665	0.580	0.648	0.634	0.559	0.502	0.618	0.559
	0.215	0.182	0.167	0.146	0.227	0.176	0.217	0.180
UNRES-DSSP-flex	0.704	0.596	0.655	0.628	0.595	0.530	0.649	0.576
	0.185	0.192	0.190	0.178	0.211	0.168	0.203	0.184
3CABS-flex	0.574	0.530	0.559	0.615	0.617	0.597	0.588	0.575
	0.232	0.218	0.173	0.145	0.220	0.188	0.217	0.196
NOLB	0.456	0.403	0.434	0.415	0.451	0.464	0.449	0.430
	0.281	0.260	0.230	0.169	0.252	0.217	0.259	0.228

Table S6. ANOVA results, shown as significance levels (expressed as p-values), of the Pearson's (r_p) and Spearman's (r_s) correlation coefficients between the fluctuation profiles calculated with UNRES-flex, UNRES-DSSP-flex, CABS-flex, and NOLB and the corresponding experimental profiles. The analysis has been carried out for truncated structures. The values in the 'Method' and 'Secondary structure' columns indicate the significance of the dependence of a correlation coefficient on fluctuation-profile-prediction method and on secondary-structure type (α , β , or $\alpha+\beta$, respectively). The values in the 'Interaction column' indicate the significance of the simultaneous dependence of a correlation coefficient on the prediction method and secondary-structure type. The p-values lower than 0.05 (indicating statistical significance) are in red font and higher values (corresponding to weak or no statistical significance) are in green font.

Significance level	r_p/r_s	Method	Secondary structure	Interaction
	NMR structures			
r_p		<0.001	0.082	0.82
r_s		<0.001	0.016	0.94
X-ray structures				
r_p		0.040	0.42	0.14
r_s		0.17	0.60	0.069
All structures				
r_p		<0.001	0.074	0.37
r_s		<0.001	0.024	0.19

Table S7. Significance of differences, expressed as p-values, of the Pearson's (r_p) and Spearman's (r_s) correlation coefficients of fluctuation profiles, corresponding to truncated structures, calculated with UNRES-flex, UNRES-DSSP-flex, CABS-flex, and NOLB assessed by the two sample t-test depending on structure-determination method and secondary-structure class. The p-values with the "-" sign indicate that the respective correlation coefficients are greater for the method in the left column (Method 1), while the "+" sign means that the correlation coefficients are greater for the method in the right column (Method

2). The p-values lower than 0.05 (indicating statistical significance) are in red font and higher values (corresponding to weak or no statistical significance) are in green font.

A: NMR structures, Pearson coefficient (r_p)

Significance level	Method 1	Method 2	Secondary-structure type			
			α	β	$\alpha + \beta$	all
UNRES-flex	UNRES-DSSP-flex	UNRES-DSSP-flex	+ 0.31	+ 0.64	+ 0.22	+ 0.42
		CABS-flex	+ 0.15	+ 0.88	+ 0.0024	+ 0.35
		NOLB	- <0.001	- 0.0060	- <0.001	- <0.001
UNRES-DSSP-flex	UNRES-DSSP-flex	CABS-flex	+ 0.47	- 0.67	+ 0.046	+ 0.36
		NOLB	- <0.001	- 0.0022	- <0.001	- <0.001
CABS-flex	CABS-flex	NOLB	- <0.001	- <0.001	- <0.001	- <0.001

B: NMR structures, Spearman coefficient (r_s)

Significance level	Method 1	Method 2	Secondary-structure type			
			α	β	$\alpha + \beta$	all
UNRES-flex	UNRES-DSSP-flex	UNRES-DSSP-flex	+ 0.31	+ 0.64	+ 0.22	+ 0.42
		CABS-flex	+ 0.15	+ 0.88	+ 0.0024	+ 0.35
		NOLB	- <0.001	- 0.0060	- <0.001	- <0.001
UNRES-DSSP-flex	UNRES-DSSP-flex	CABS-flex	+ 0.47	- 0.67	+ 0.046	+ 0.36
		NOLB	- <0.001	- 0.0022	- <0.001	- <0.001
CABS-flex	CABS-flex	NOLB	- <0.001	- <0.001	- <0.001	- <0.001

C: X-ray structures, Pearson coefficient (r_p)

Significance level	Method 1	Method 2	Secondary-structure type			
			α	β	$\alpha + \beta$	all

	UNRES-flex	UNRES-DSSP-flex	+ 0.91	- 0.70	+ 0.52	+ 0.65
		CABS-flex	- 0.30	- 0.66	+ 0.061	+ 0.24
		NOLB	+ 0.41	- 0.70	+ <0.001	+ 0.0073
	UNRES-DSSP-flex	CABS-flex	- 0.25	- 0.99	+ 0.17	+ 0.35
		NOLB	+ 0.50	- 0.94	+ 0.0035	+ 0.31
	CABS-flex	NOLB	+ 0.052	+ 0.94	+ 0.18	+ 0.30

D: X-ray structures, Spearman coefficient (r_s)

Significance level	Method 1	Method 2	Secondary-structure type			
			α	B	$\alpha + \beta$	all
UNRES-flex	UNRES-DSSP-flex	UNRES-DSSP-flex	- 0.60	- 0.61	+ 0.78	- 0.70
		CABS-flex	- 0.28	- 0.58	+ 0.061	+ 0.22
		NOLB	+ 0.84	- 0.24	+ 0.0021	+ 0.25
UNRES-DSSP-flex	UNRES-DSSP-flex	CABS-flex	- 0.66	+ 0.92	+ 0.092	+ 0.39
		NOLB	+ 0.45	- 0.58	+ 0.0033	+ 0.26
CABS-flex	CABS-flex	NOLB	+ 0.16	- 0.41	+ 0.30	+ 0.29

E: All structures, Pearson coefficient (r_p)

Significance level	Method 1	Method 2	Secondary-structure type			
			α	β	$\alpha + \beta$	all
UNRES-flex	UNRES-DSSP-flex	UNRES-DSSP-flex	+ 0.44	+ 0.86	+ 0.19	+ 0.41
		CABS-flex	+0.63	- 0.90	+ <0.001	+ 0.38
		NOLB	- 0.023	- 0.015	- 0.61	- 0.31
UNRES-DSSP-flex	UNRES-DSSP-flex	CABS-flex	- 0.89	- 0.74	+ 0.019	+ 0.43
		NOLB	- 0.0053	- 0.013	- 0.17	- 0.10
CABS-flex	CABS-flex	NOLB	- 0.020	- 0.0063	- 0.0034	- 0.0090

F: All structures, Spearman coefficient (r_s)

can ce	Method 1	Method 2	Secondary-structure type			
			α	β	$\alpha + \beta$	all

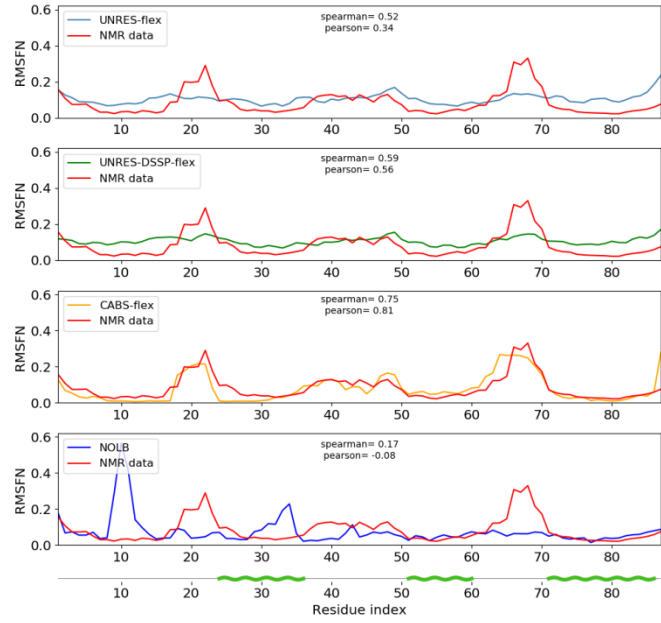
	UNRES-flex	UNRES-DSSP-flex	+ 0.66	- 0.94	+ 0.40	+ 0.59
		CABS-flex	- 0.94	- 1.0	+ 0.0027	+ 0.49
		NOLB	- 0.014	- 0.0045	- 0.69	- 0.34
	UNRES-DSSP-flex	CABS-flex	- 0.65	+ 0.93	+ 0.021	+ 0.40
		NOLB	- 0.0067	- 0.0091	- 0.28	- 0.14
		CABS-flex	NOLB	- 0.031	- <0.001	- 0.0043

Table S8. PDB codes of NMR structures with low similarity of the fluctuation profiles estimated from NMR ensembles and those calculated with a given method.

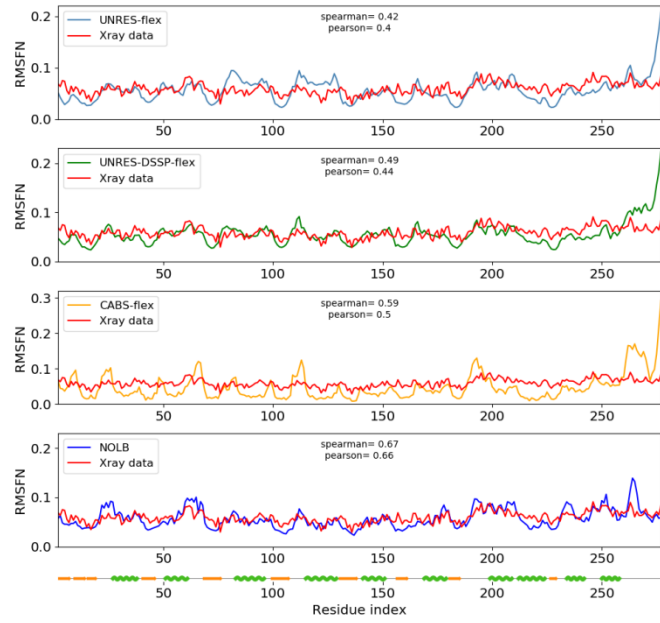
method	structure with $r_p \leq 0.2$
UNRES-flex	1ACP, 1BAL, 1GAB, 1HRF, 1J7O, 1LEB, 1POU, 2N2U, 3CI2
UNRES-DSSP-flex	1BAL, 1GAB, 1HRF, 1J7O, 2HI3, 2L09
CABS-flex	1BAL, 1ED7, 1J7O, 1K8B, 2RGF
NOLB	1A6S, 1ACP, 1AH9, 1BAL, 1CLB, 1E0G, 1ED7, 1FEX, 1GHH, 1HNS, 1HYW, 1IQO, 1IYR, 1J7O, 1K8B, 1L2Y, 1LEB, 1POU, 1RIJ, 1STU, 1TPN, 2E7N, 2HI3, 2KYW, 2L09, 2LVC, 2M6Q, 2MQ8, 2RGF, 3CI2, 3NCM

Figure S1. Normalized fluctuation profiles (RMSFN, dimensionless) calculated from NMR ensembles or X-ray B-factors (red line) and the corresponding profile predicted by UNRES-flex (light-blue line), UNRES-DSSP-flex (green line), CABS-flex (yellow line), and NOLB (blue line). Except for NOLB, the fluctuation profiles are averaged over three simulations. The Pearson (r_p) and Spearman (r_s) coefficients for the correlation between the experimental and predicted profiles are shown in each panel. The solid orange and wavy green lines below the abscissa of each panel indicate the β -sheet and α -helical structure, respectively. The analyses were carried out for truncated structures.

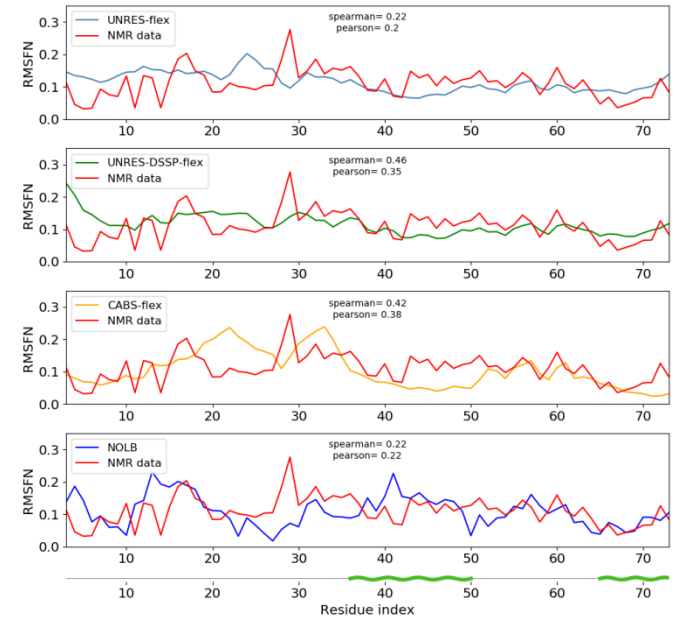
1A6S truncated RMSFN profiles



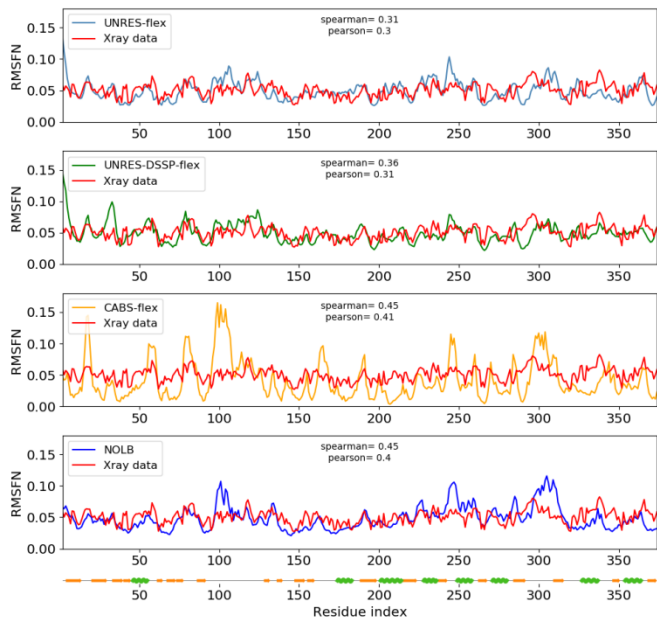
1A80 truncated RMSFN profiles



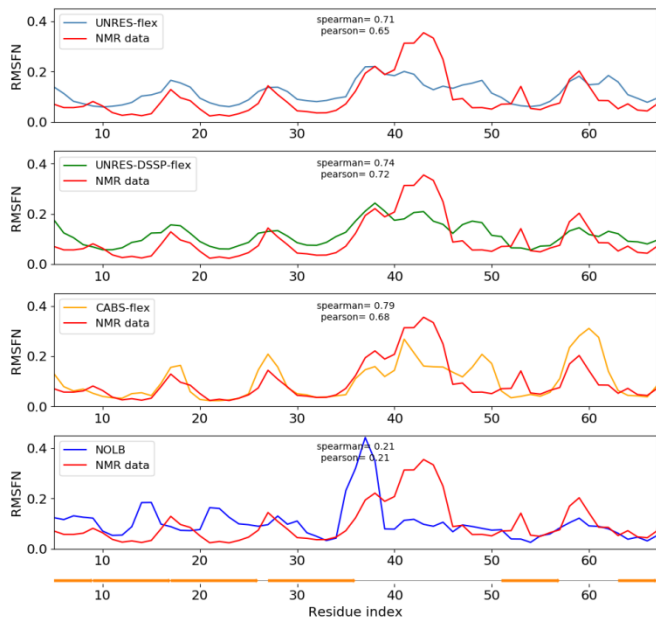
1ACP truncated RMSFN profiles



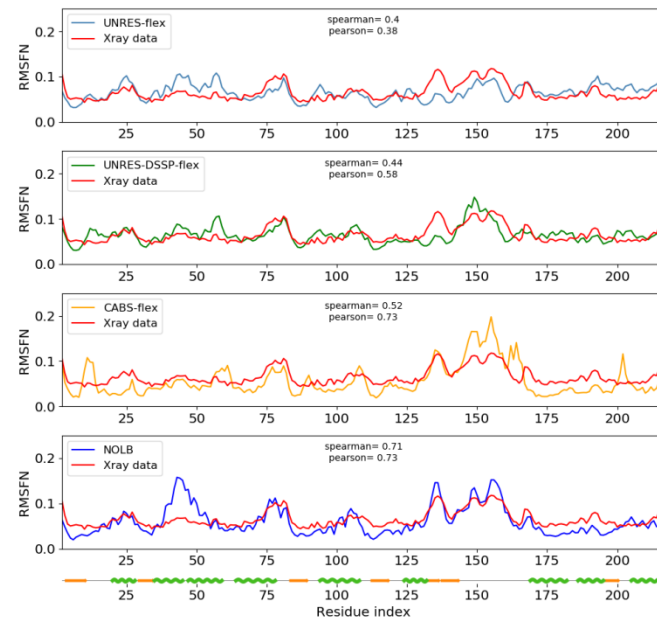
1ADG truncated RMSFN profiles



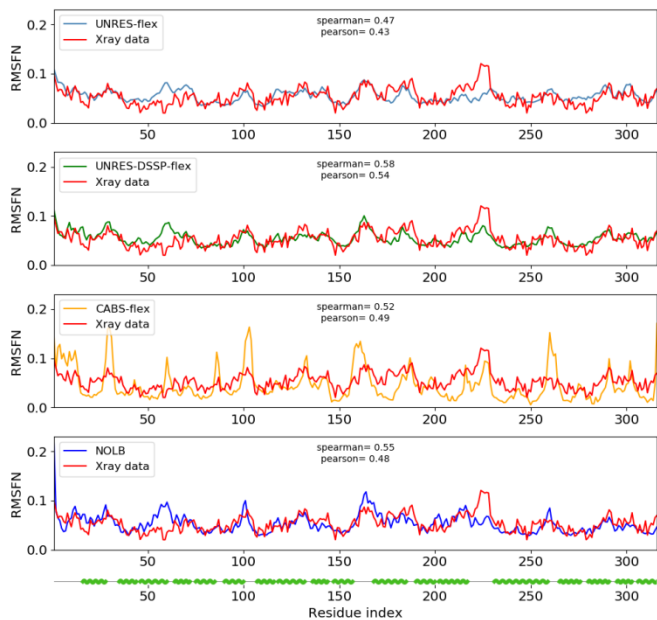
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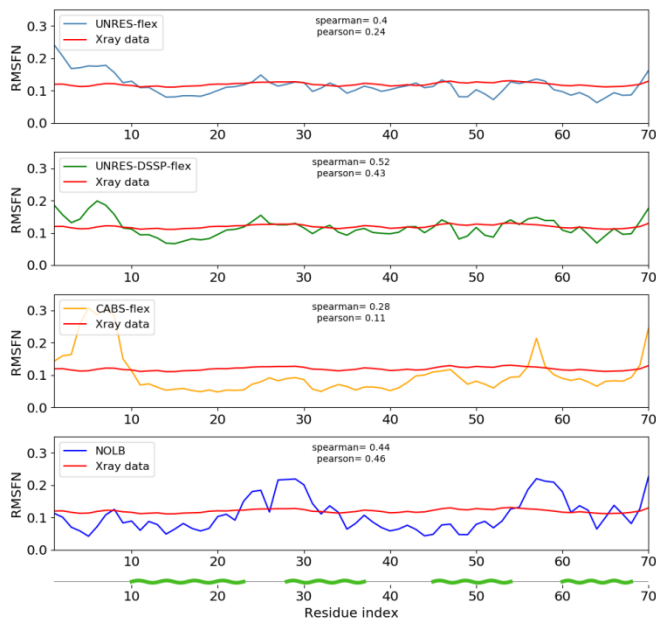
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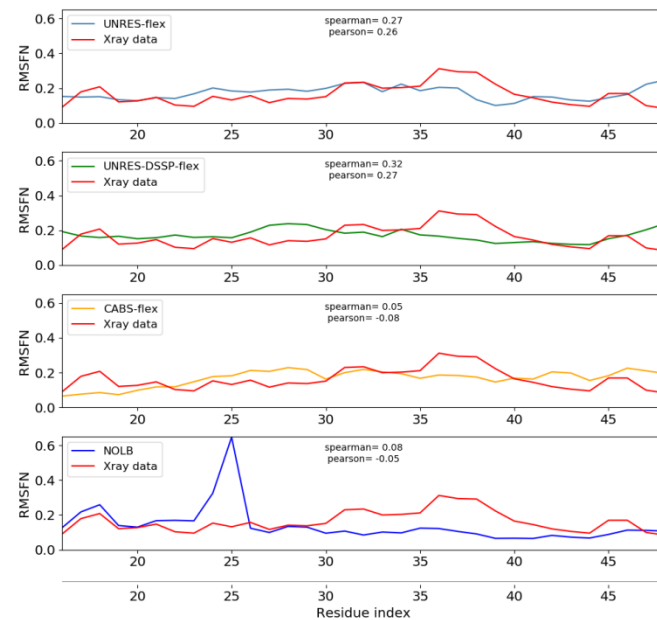
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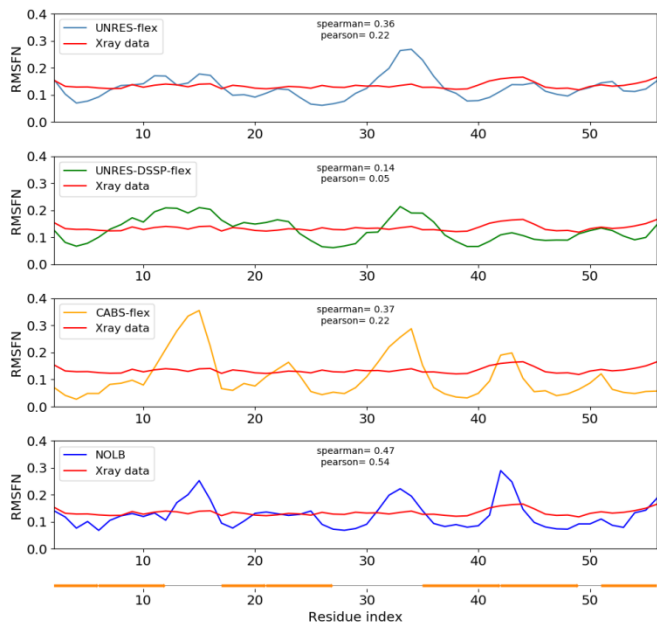
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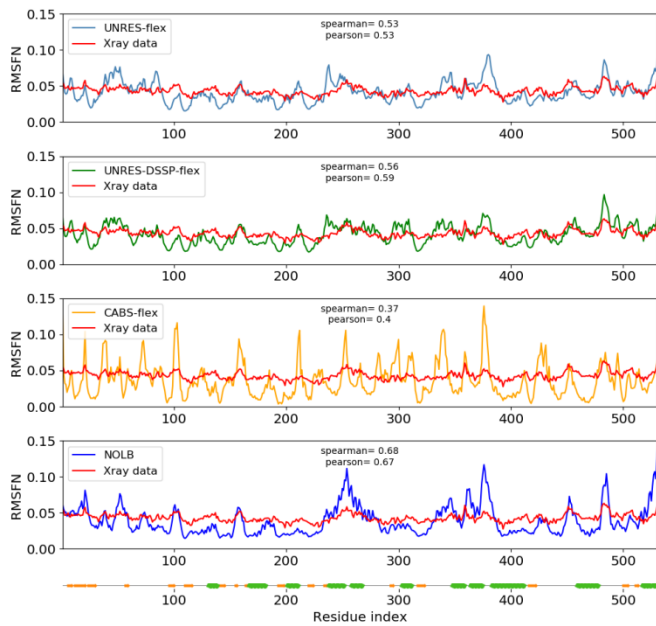
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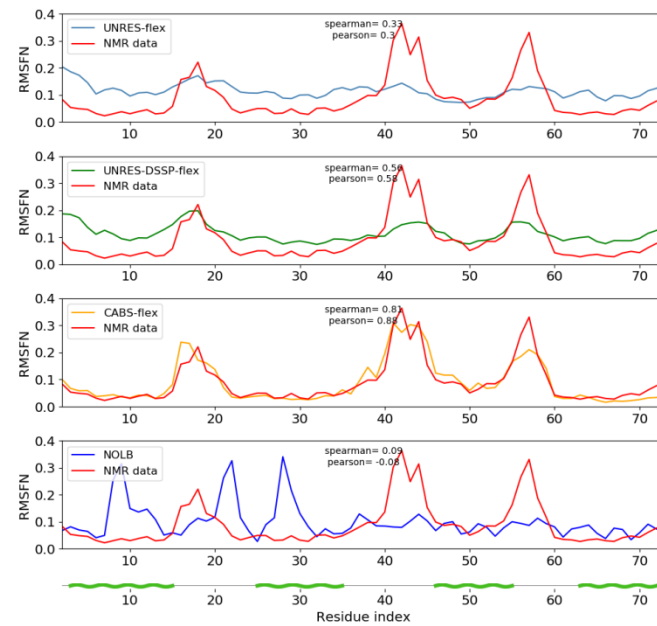
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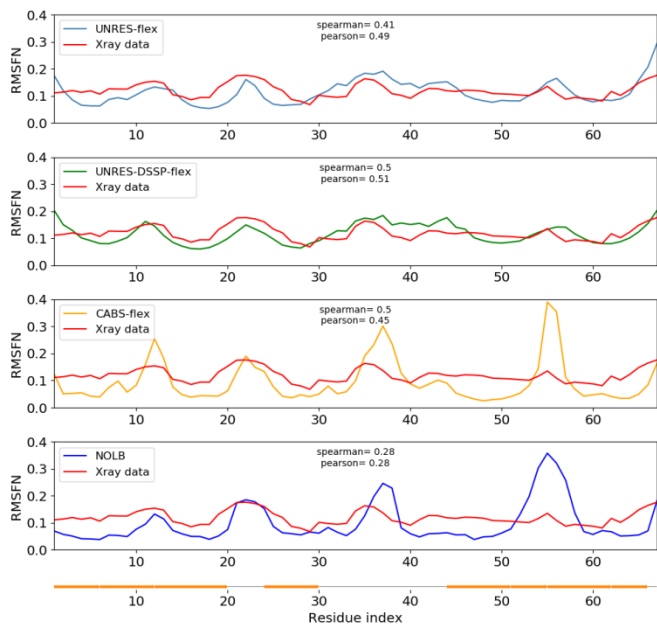
1CFJ truncated RMSFN profiles



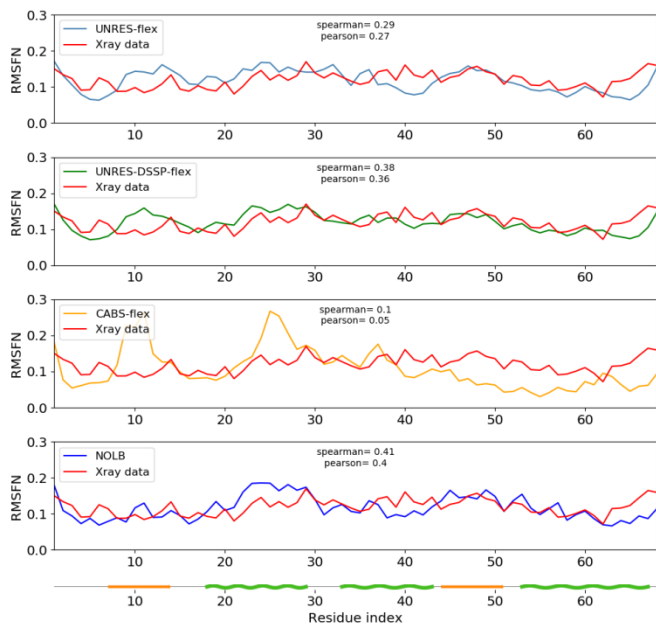
1CLB truncated RMSFN profiles



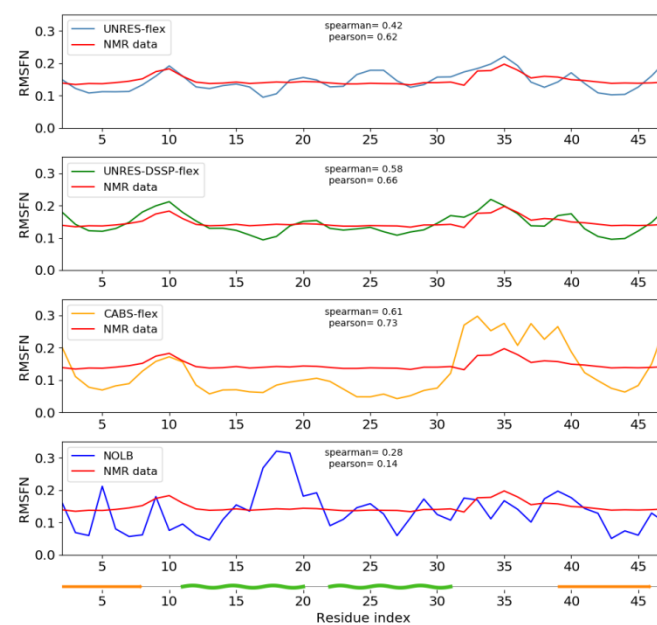
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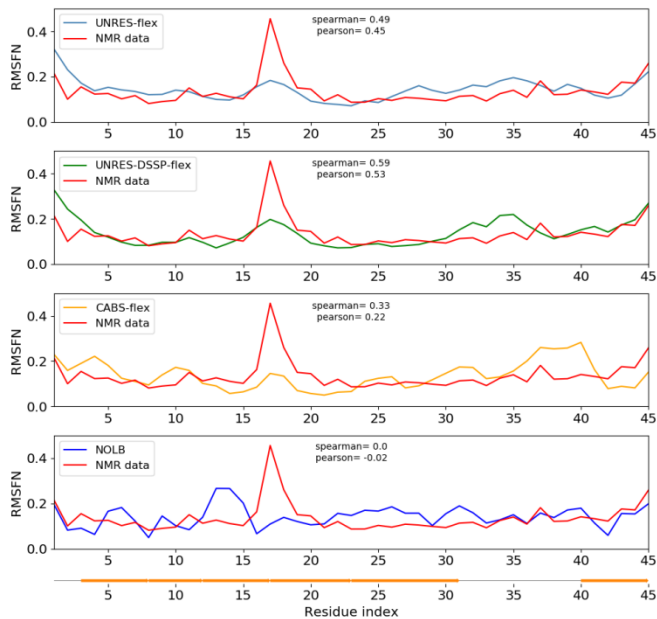
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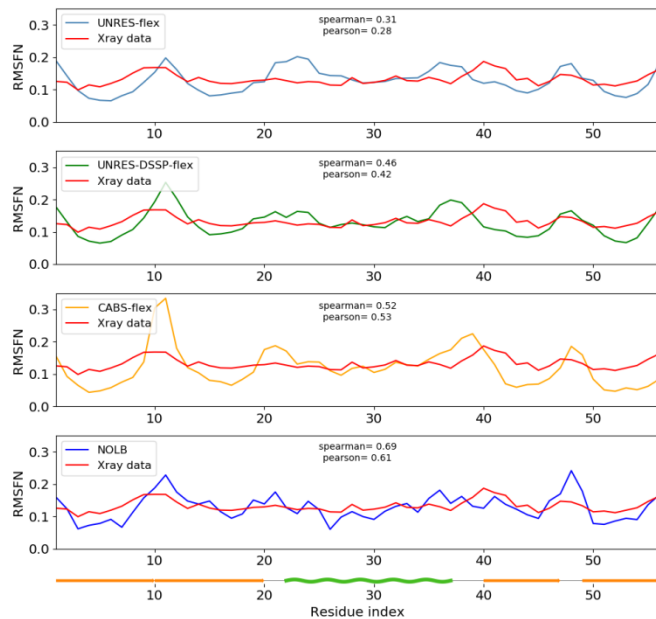
1EOG truncated RMSFN profiles



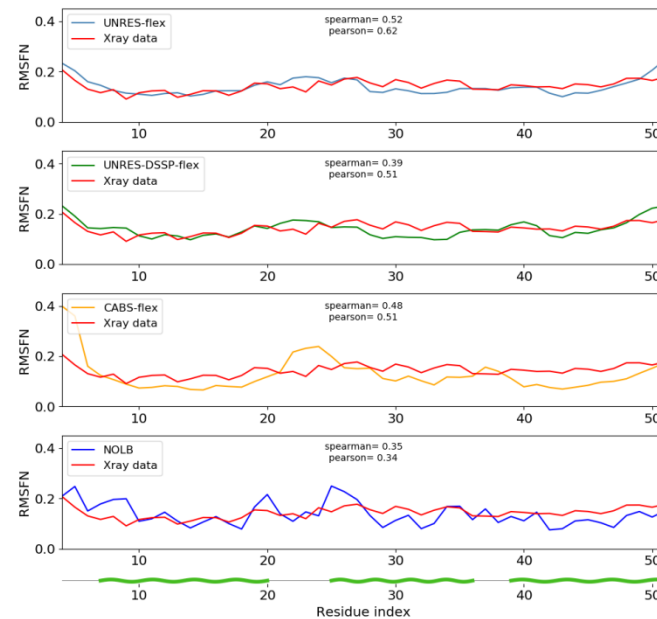
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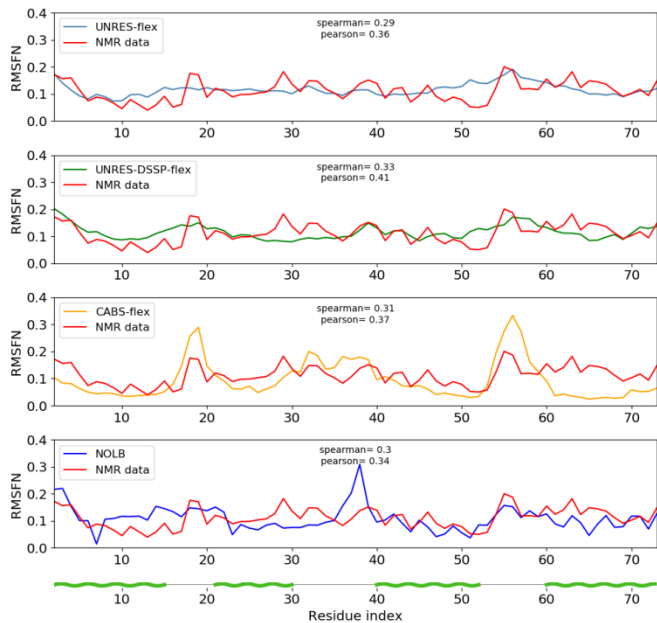
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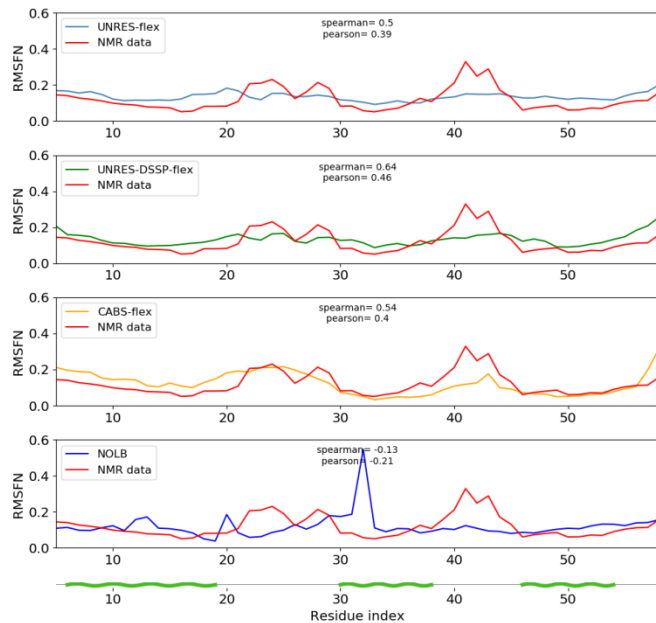
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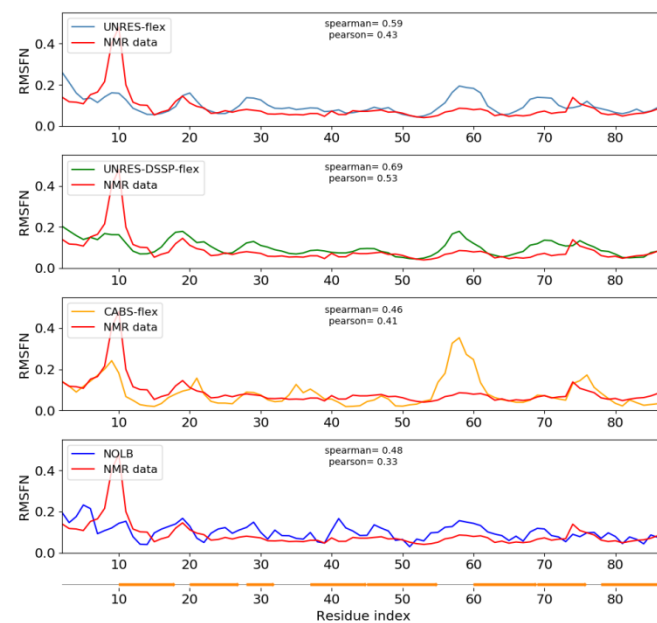
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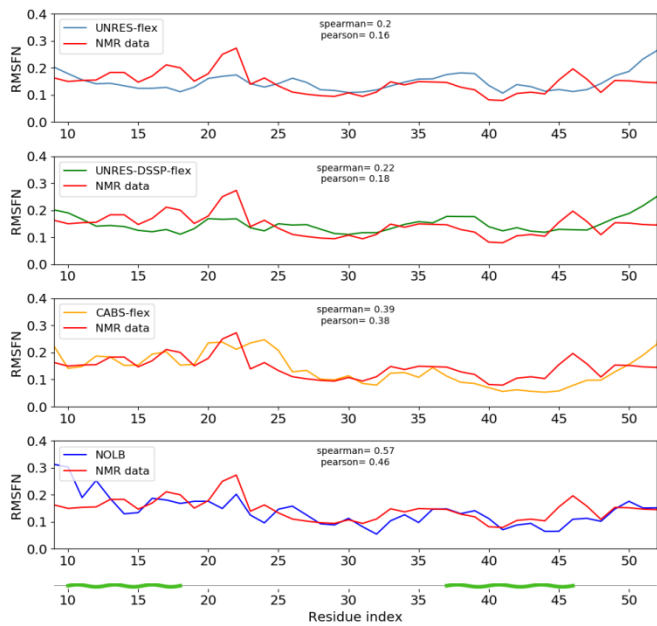
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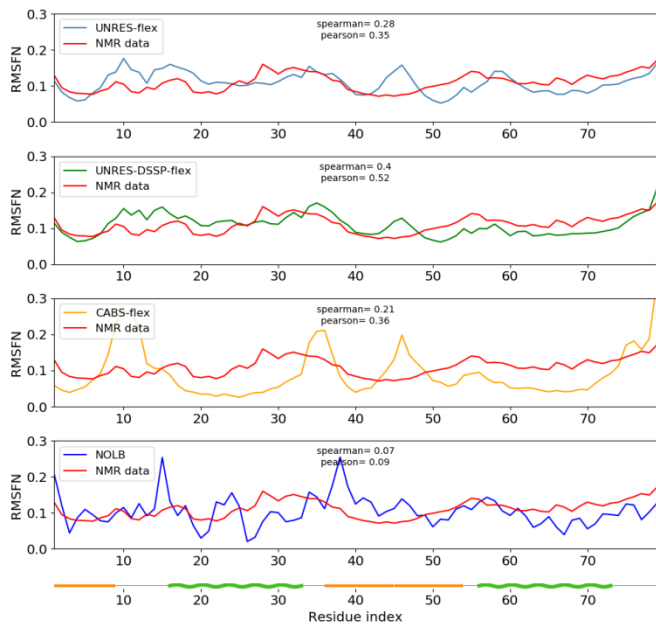
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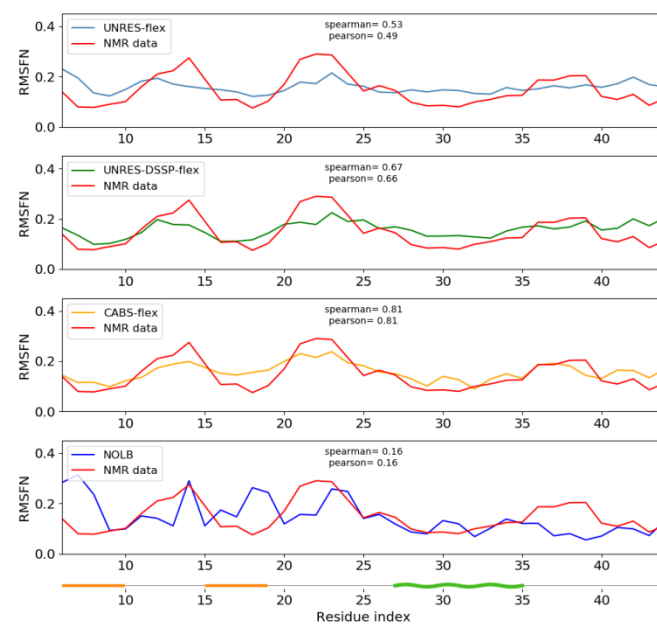
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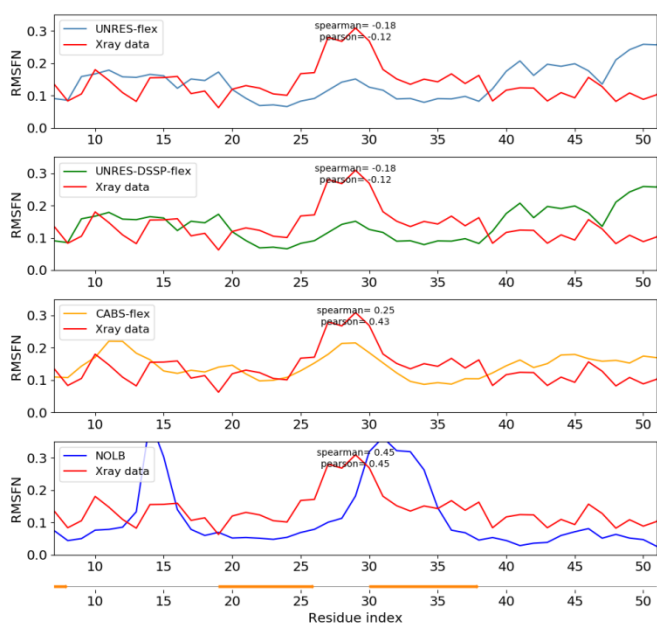
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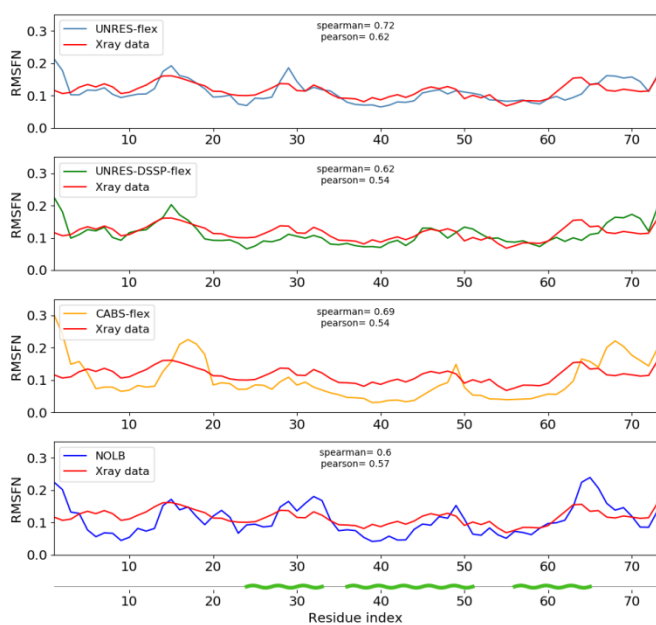
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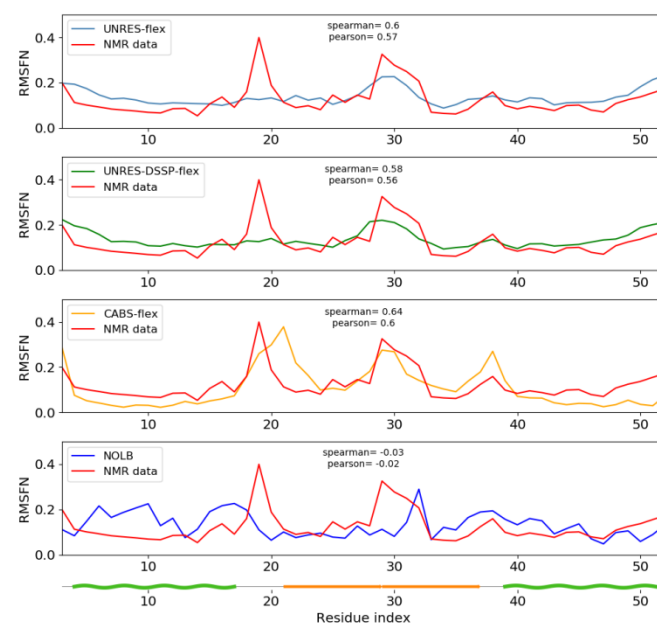
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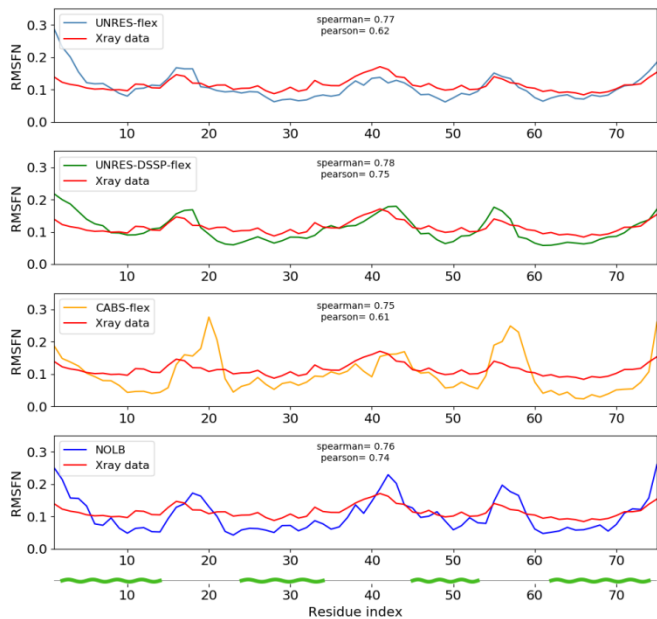
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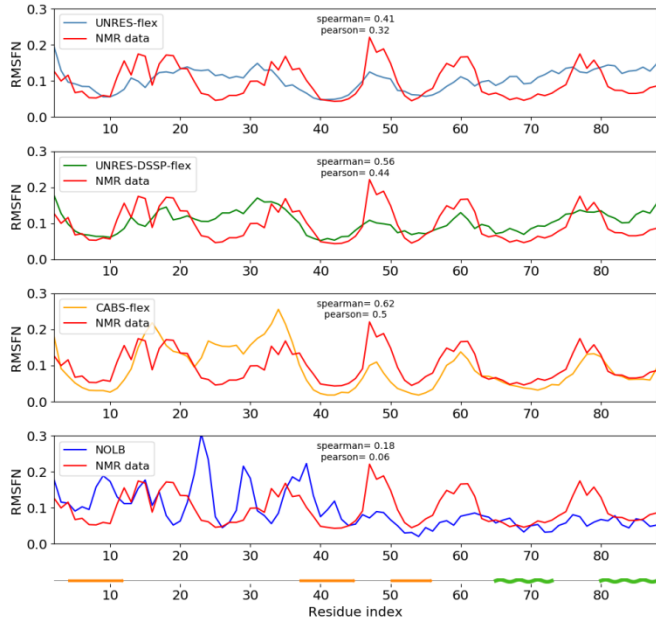
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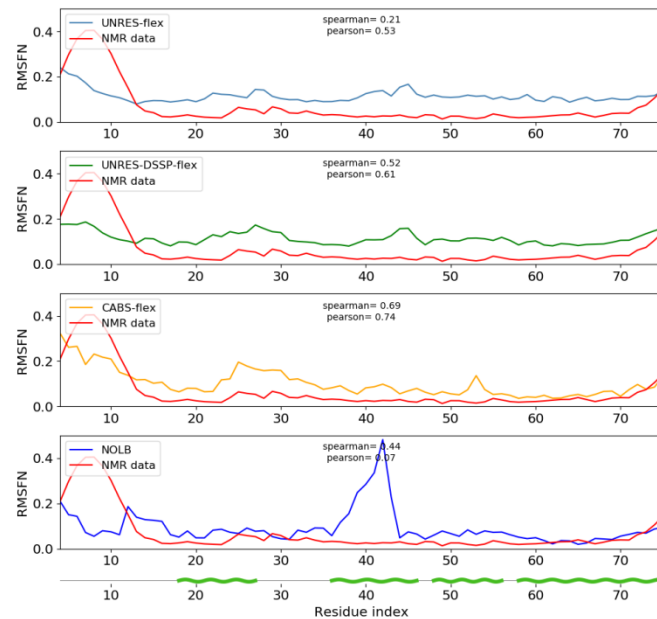
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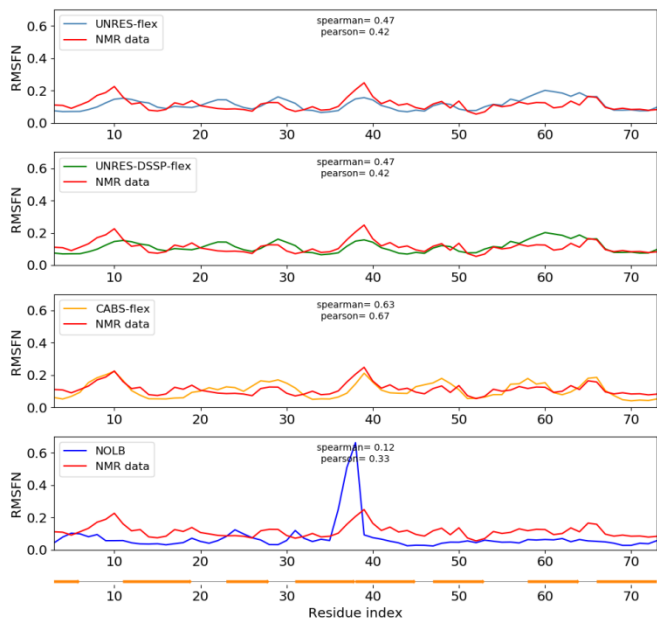
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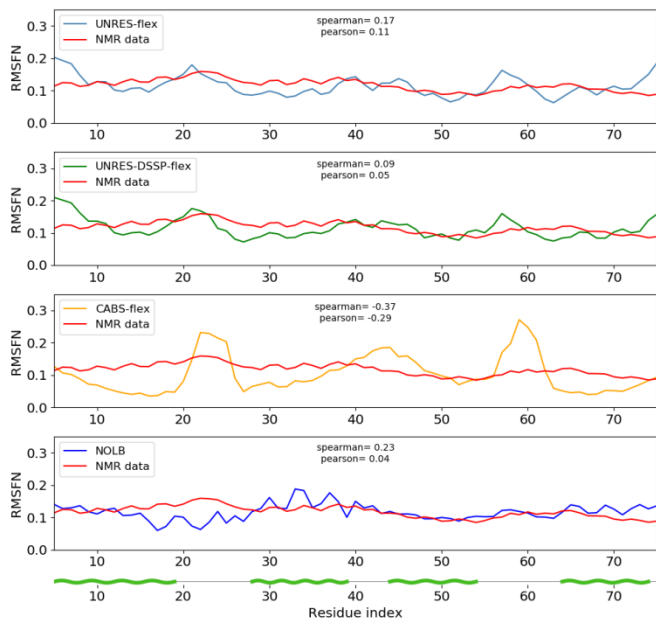
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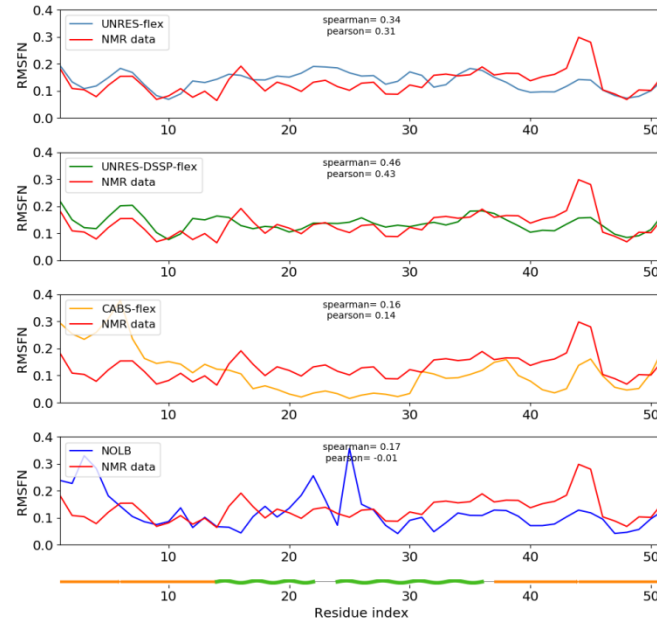
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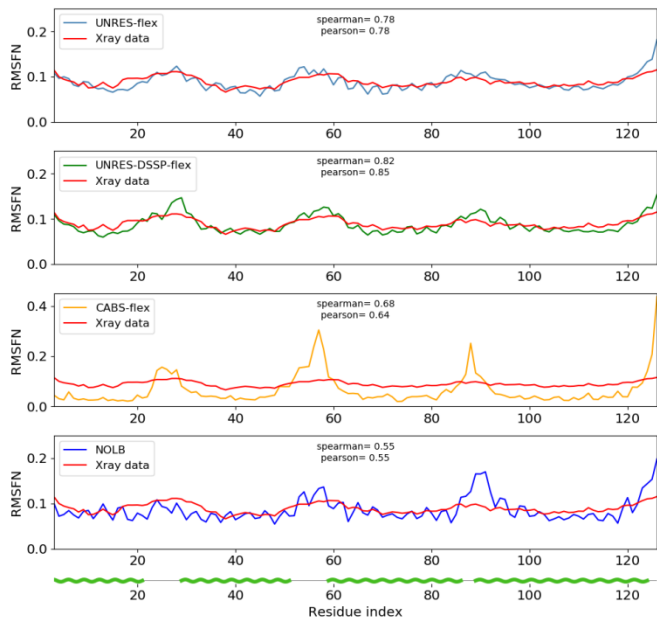
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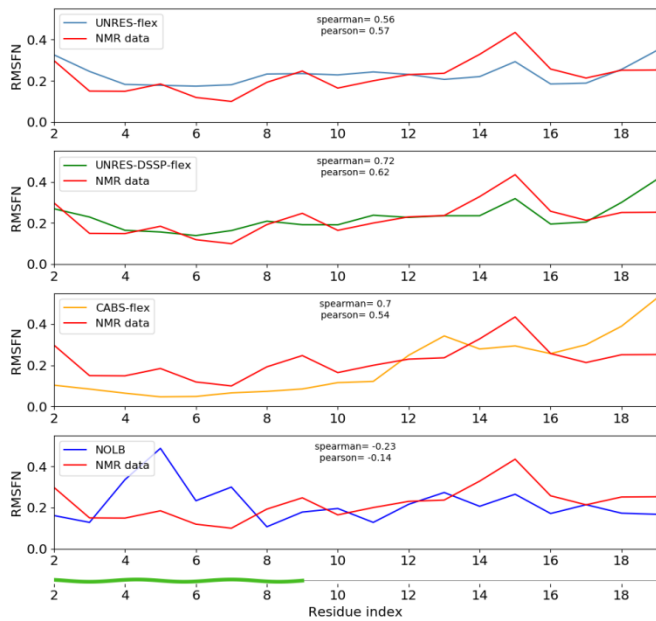
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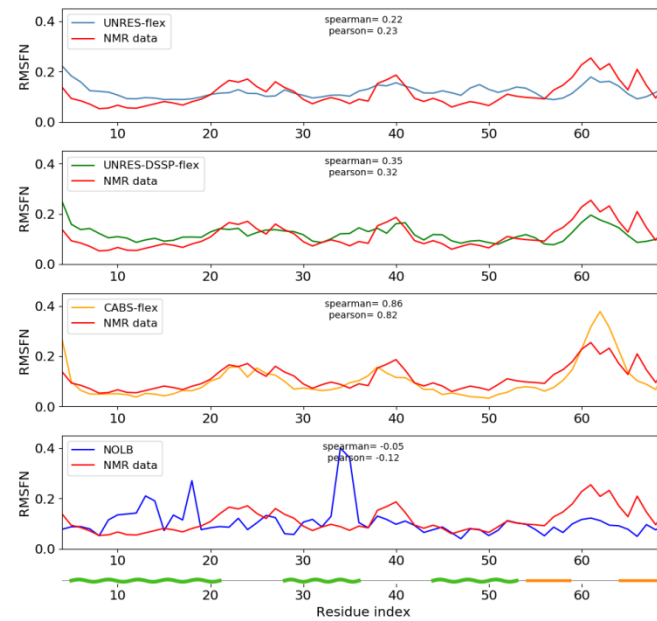
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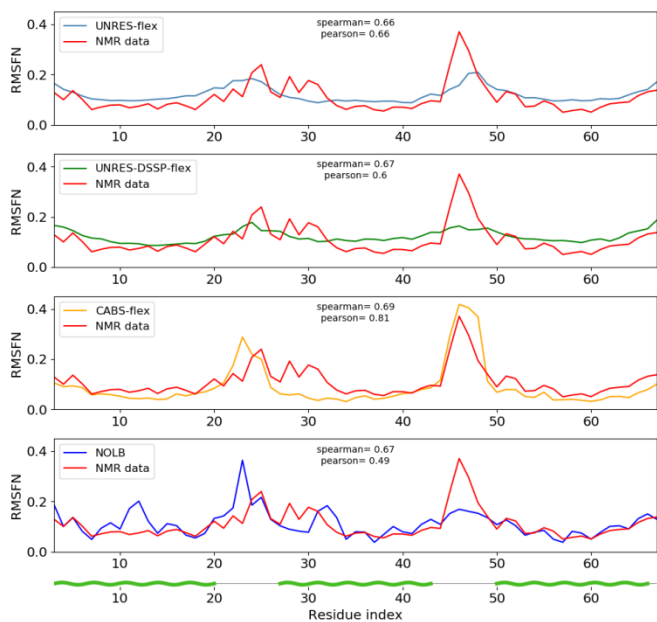
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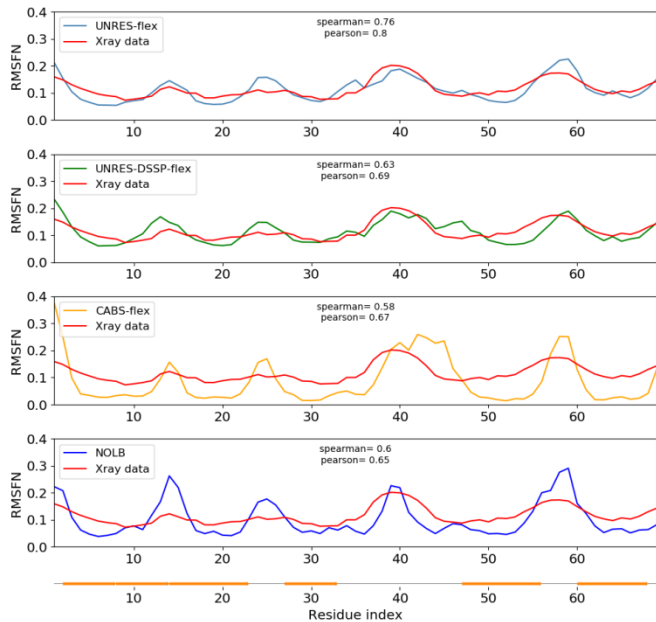
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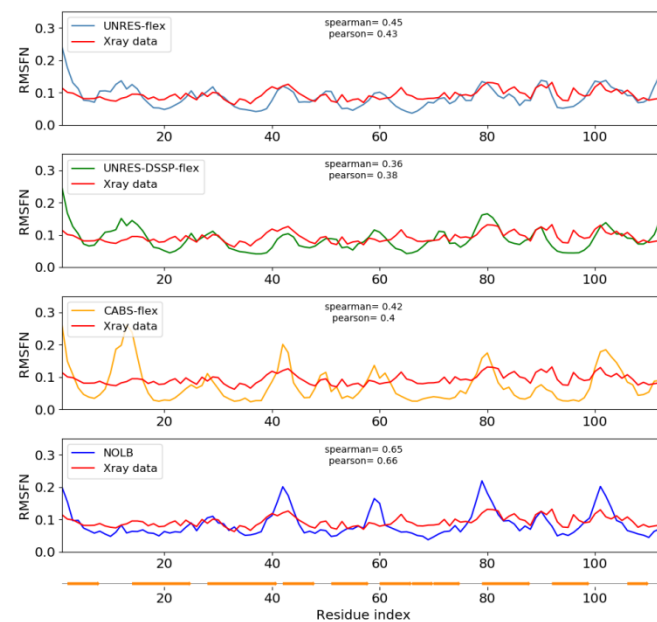
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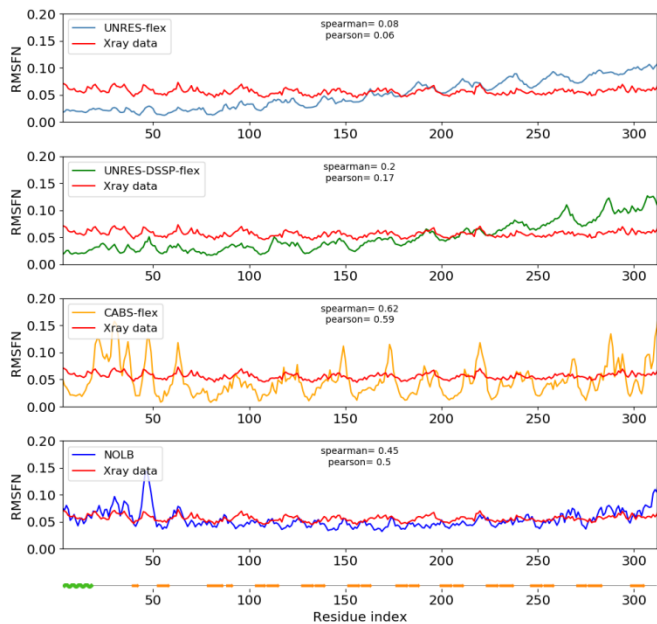
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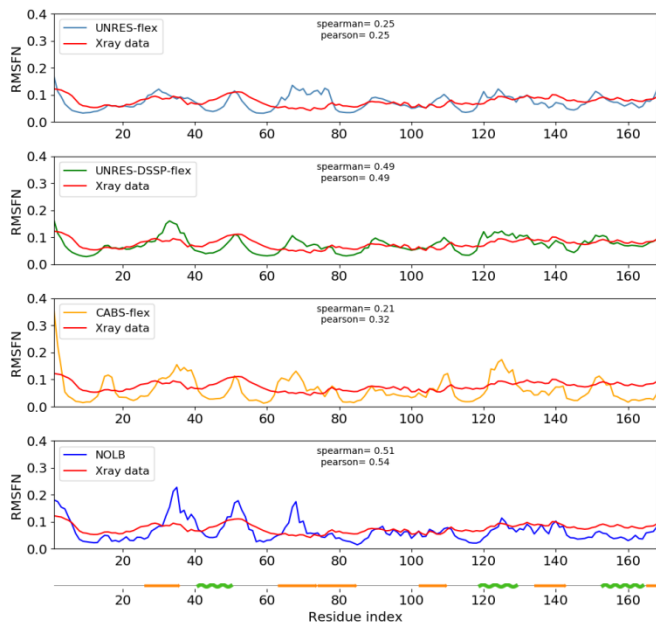
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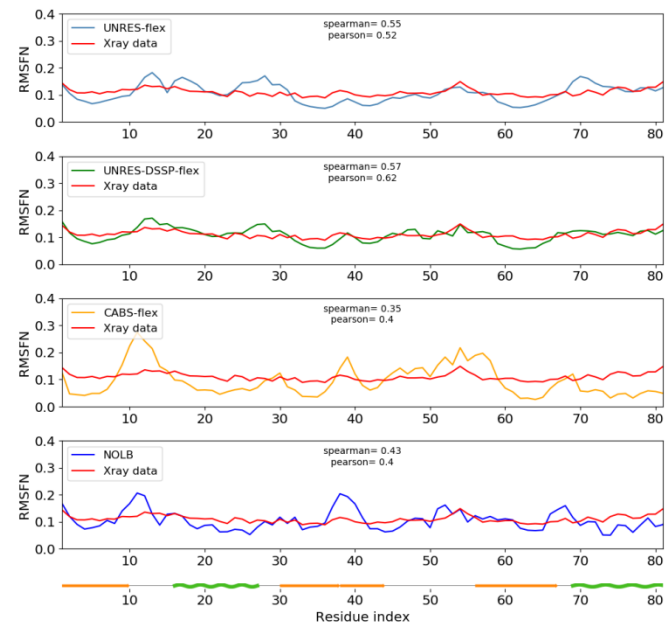
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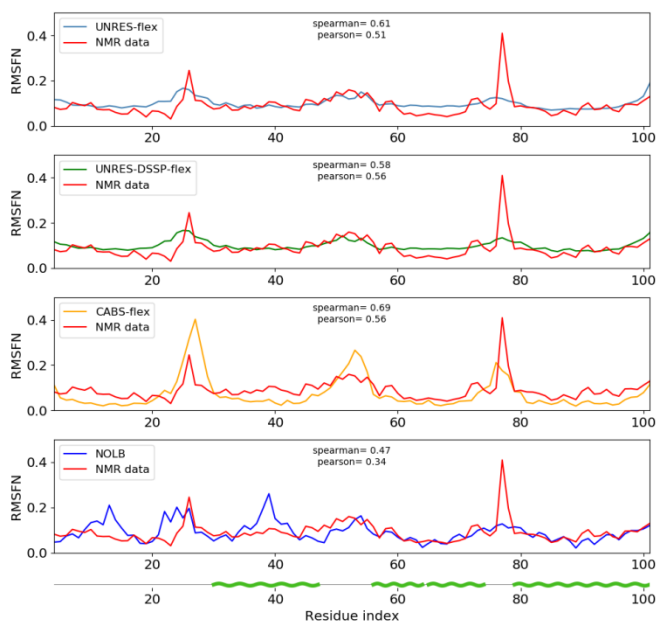
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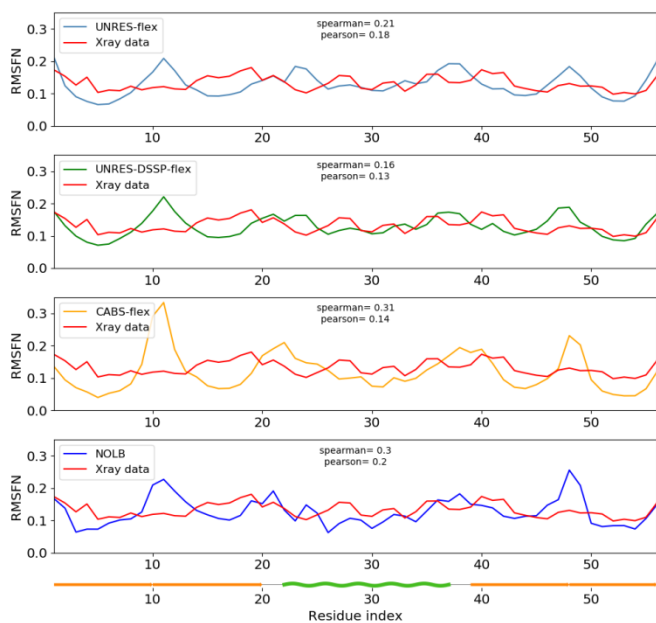
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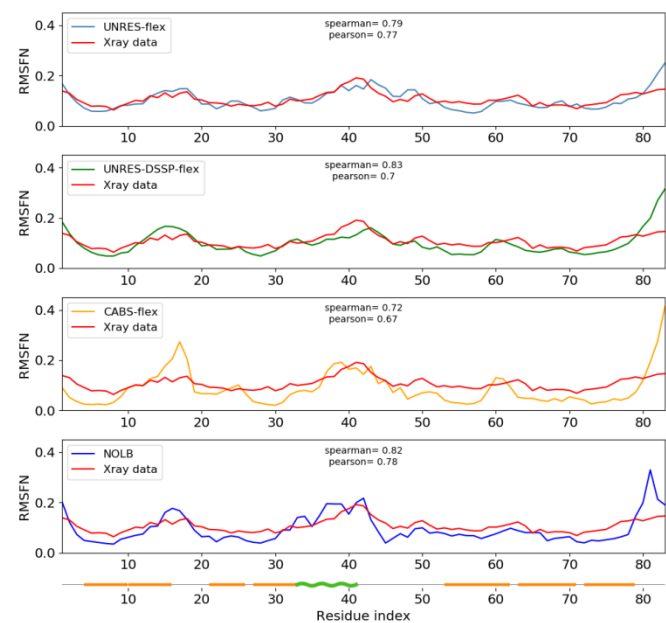
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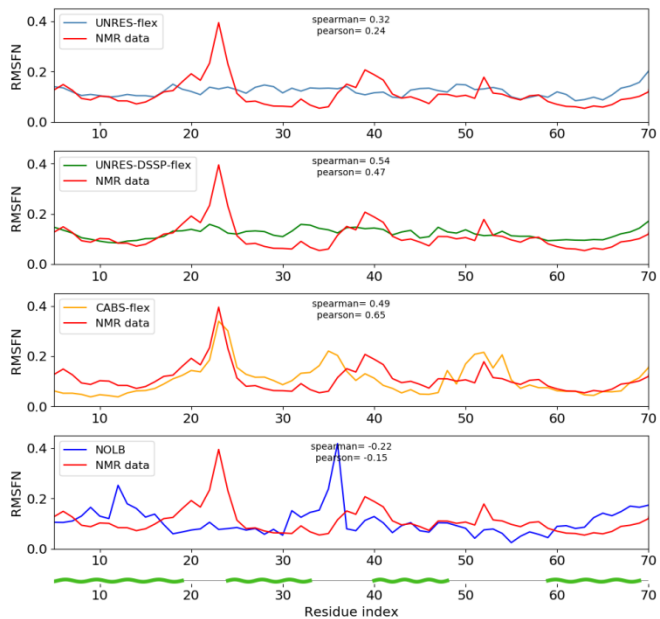
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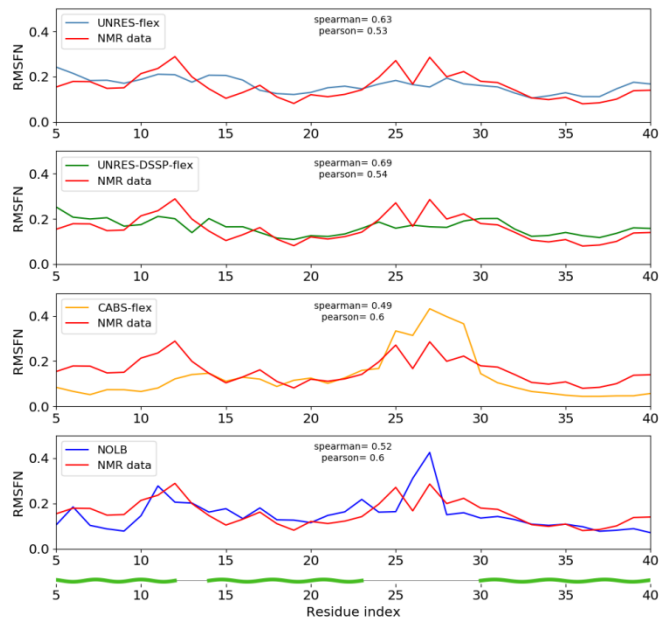
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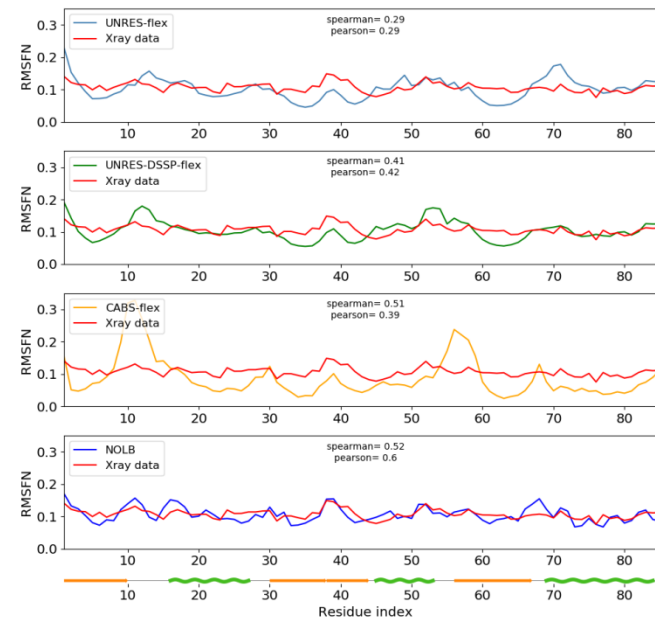
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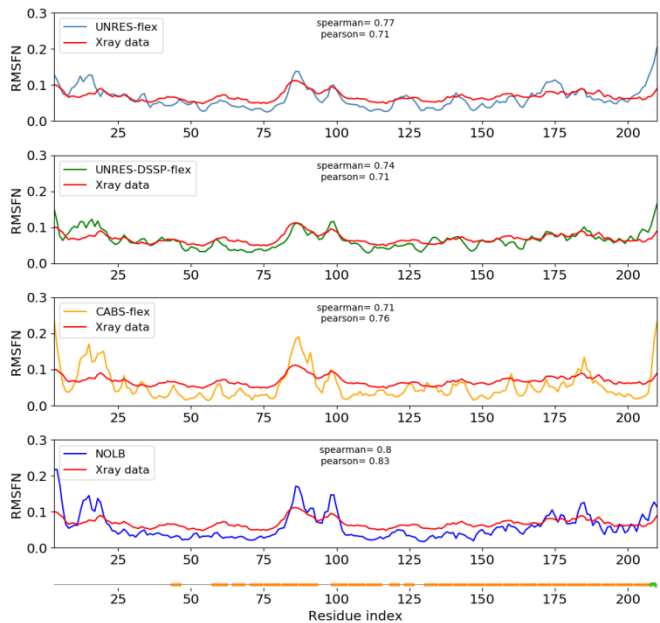
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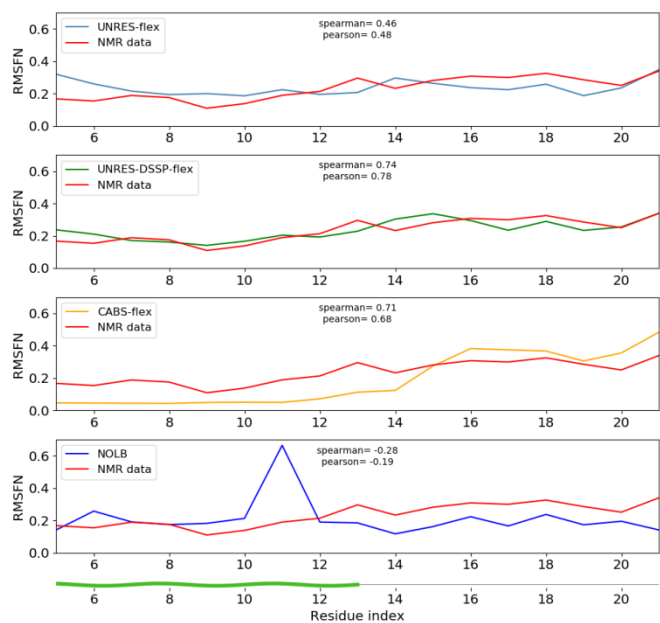
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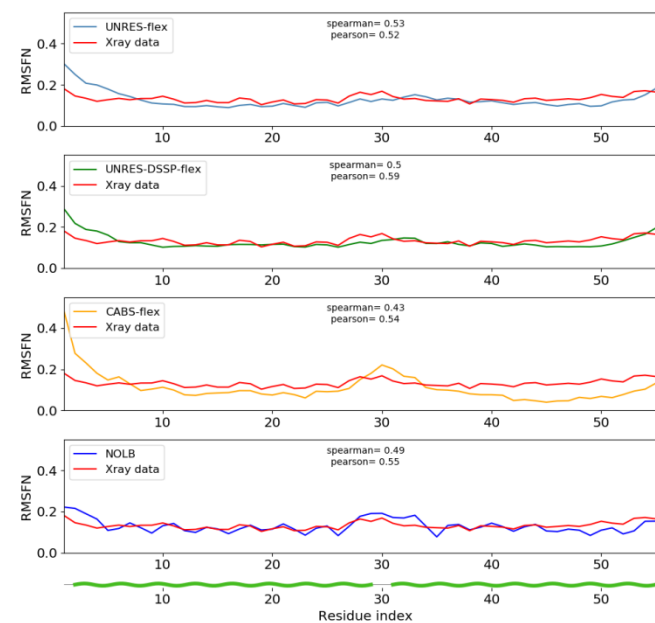
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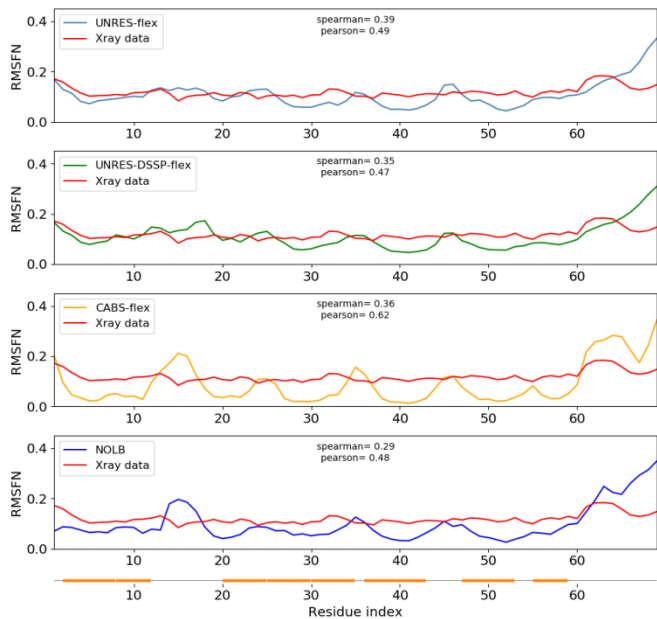
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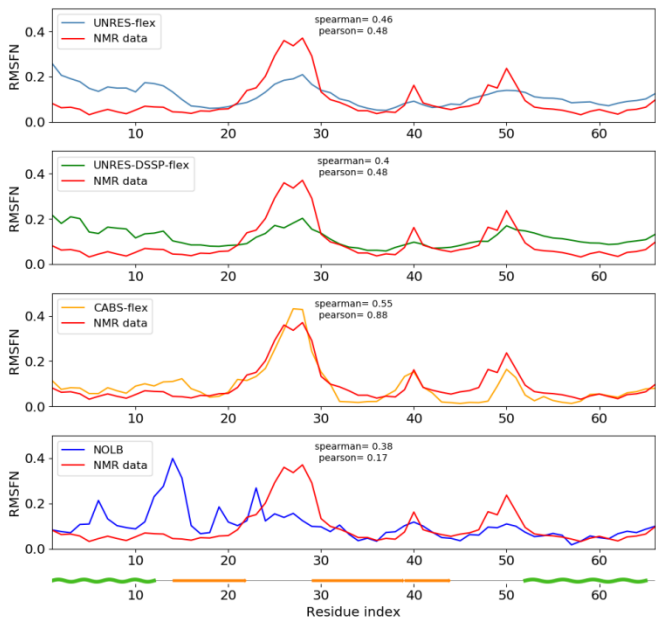
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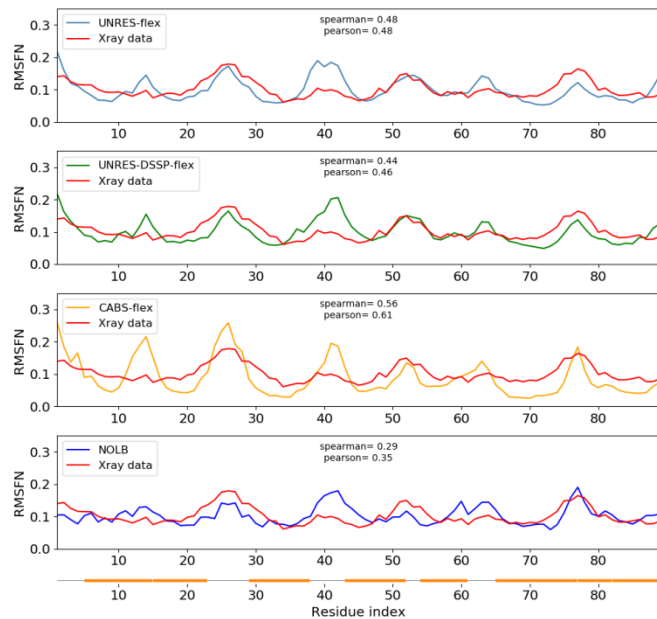
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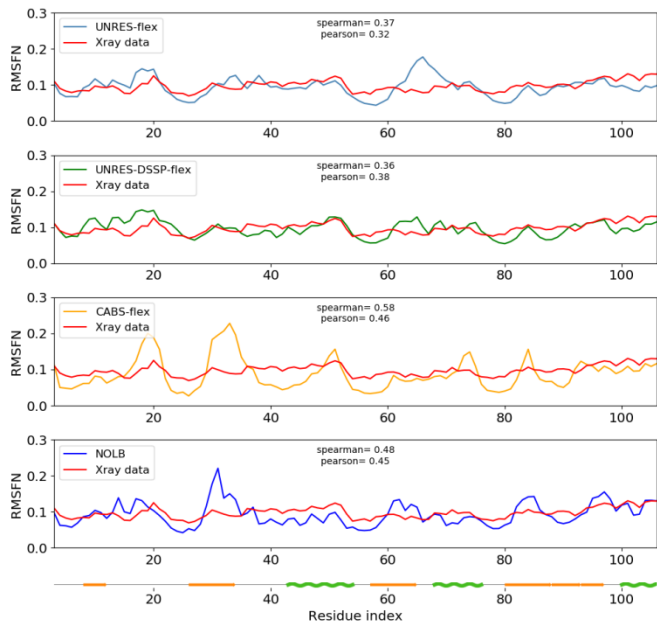
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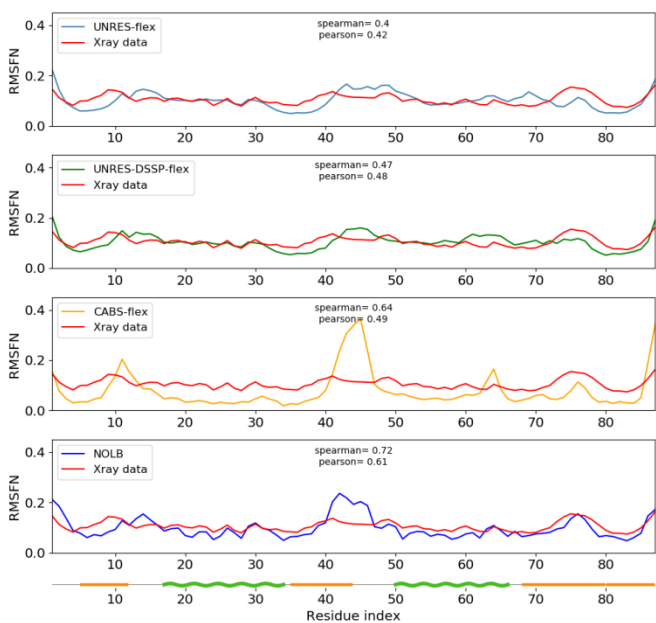
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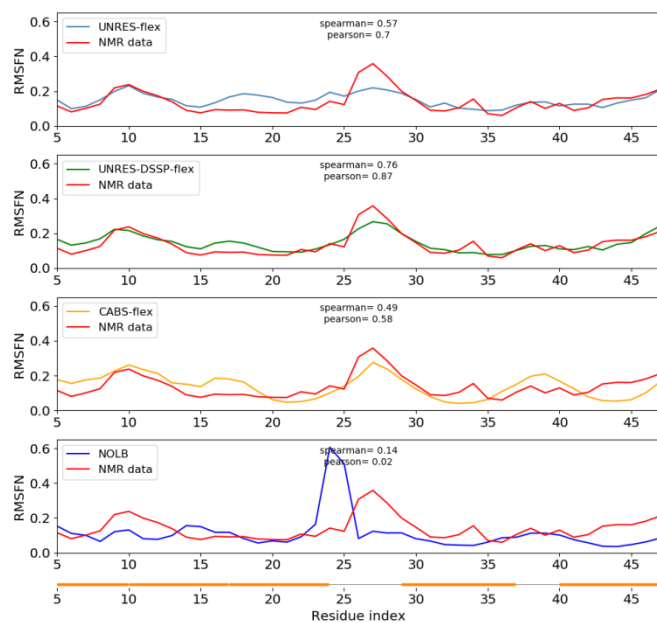
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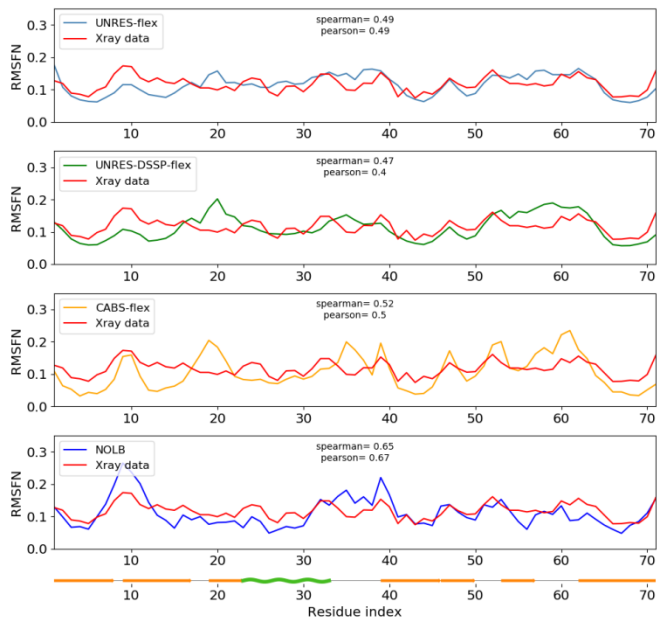
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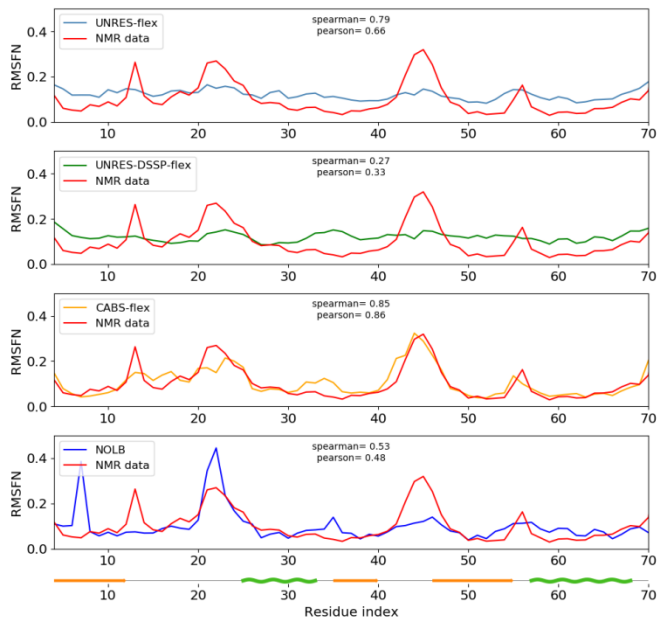
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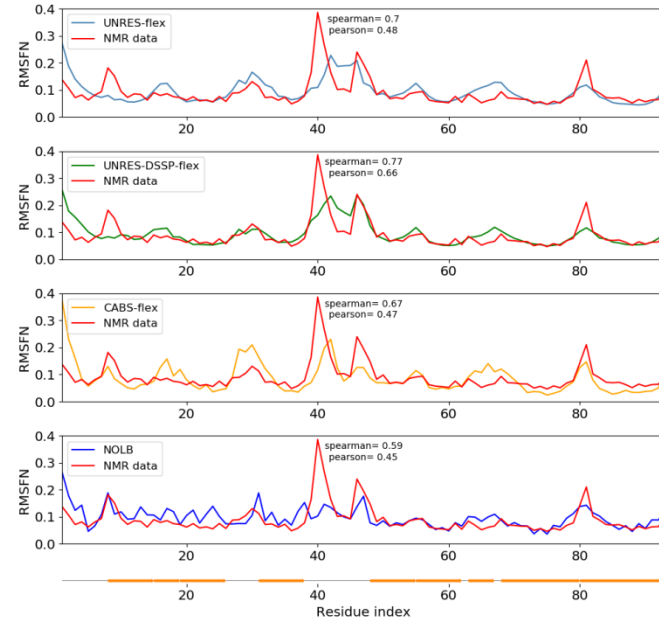
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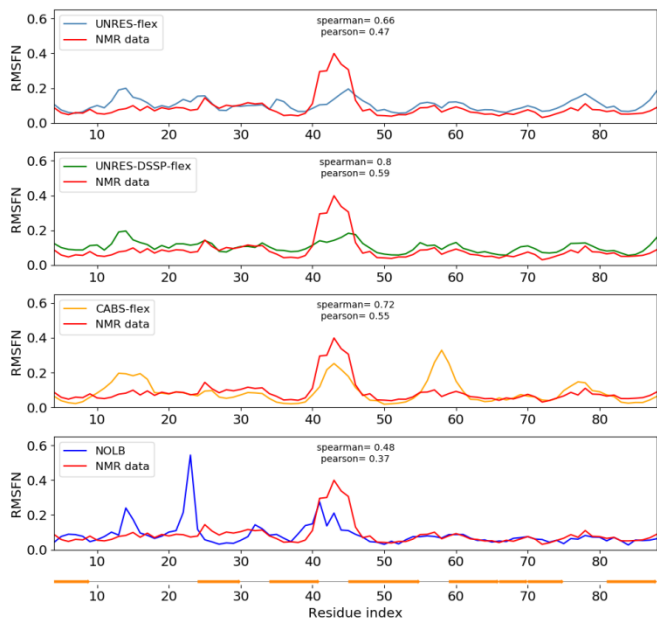
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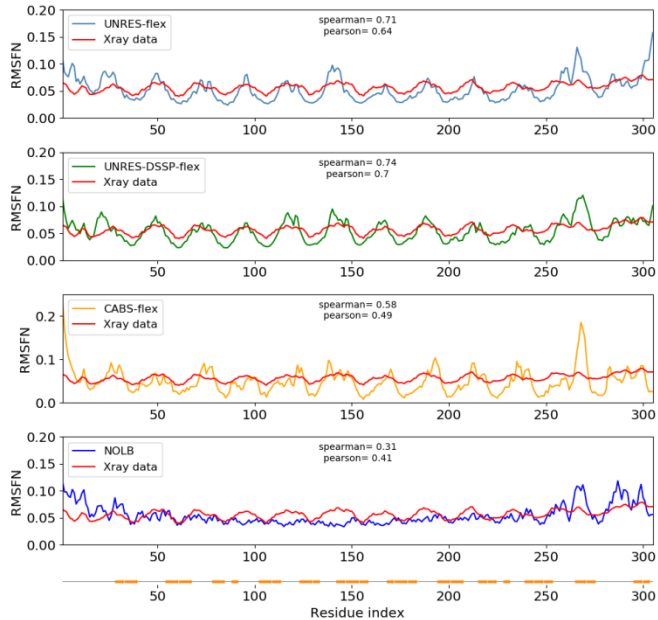
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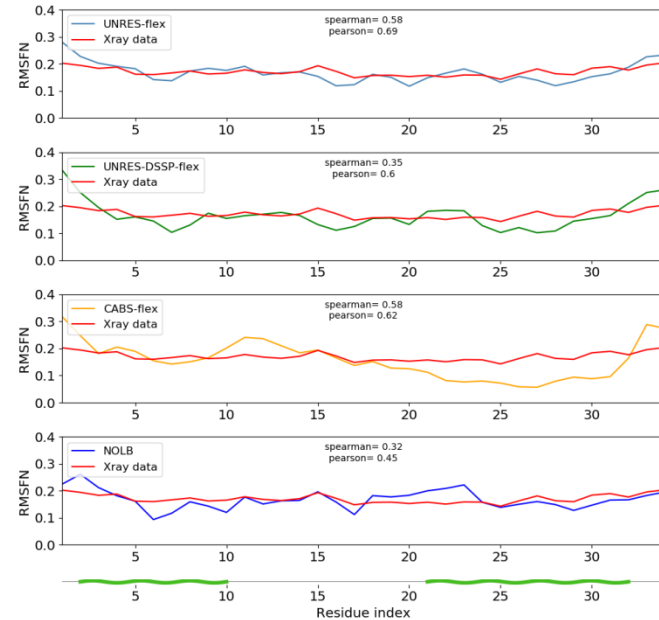
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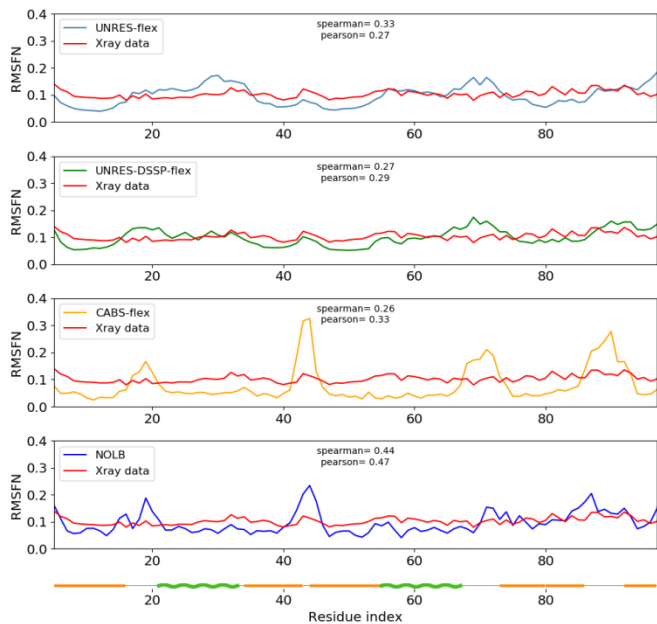
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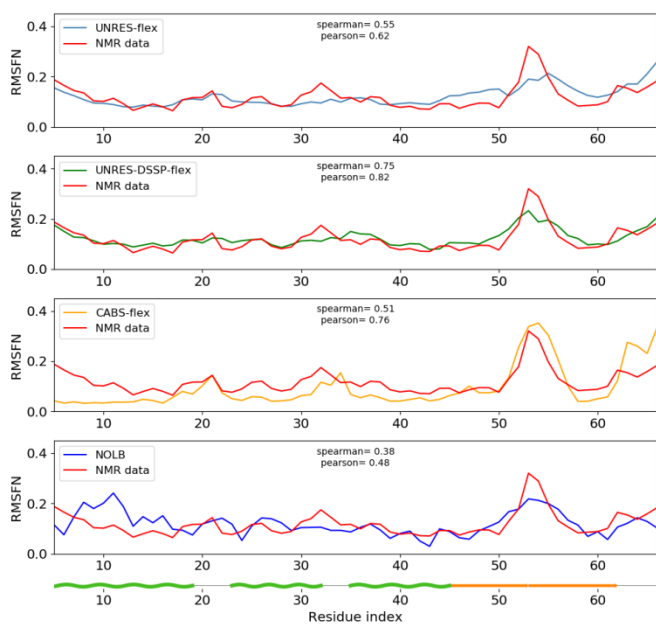
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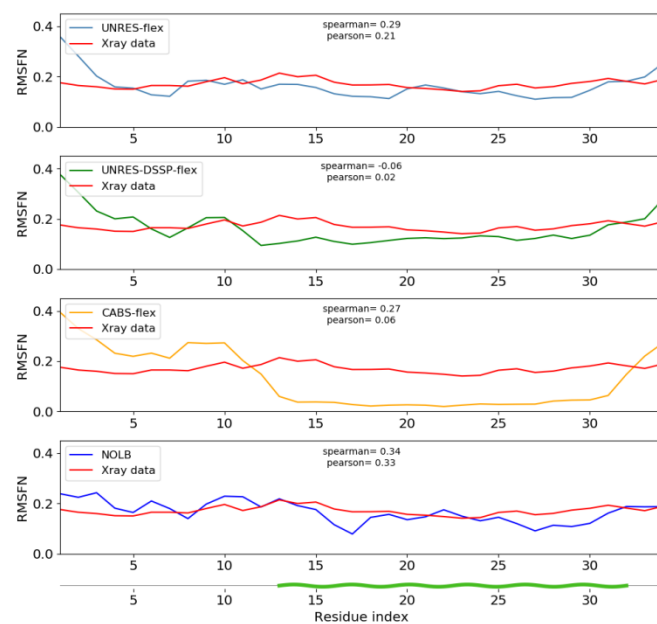
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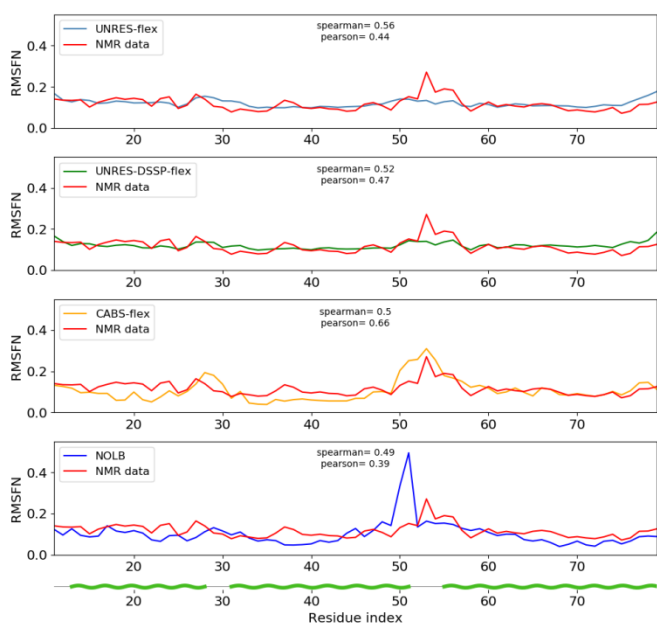
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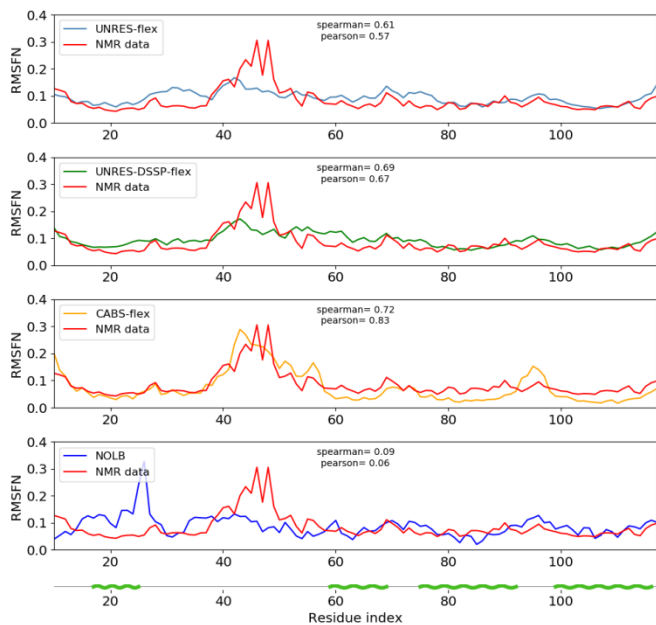
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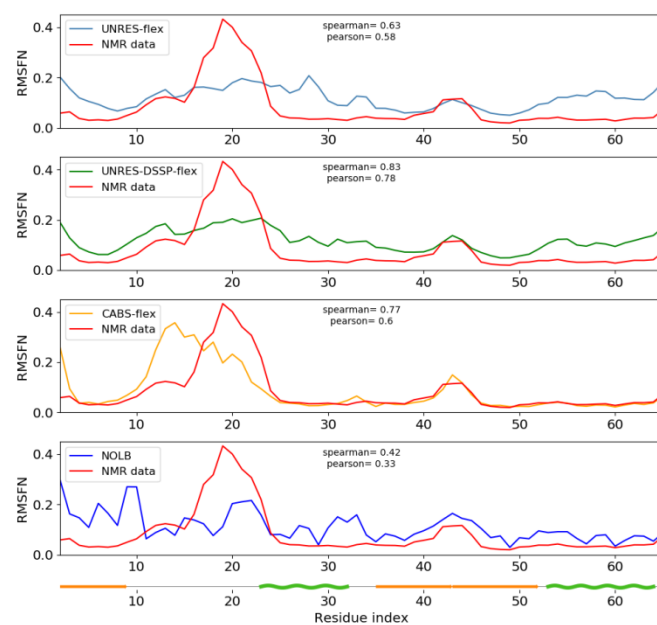
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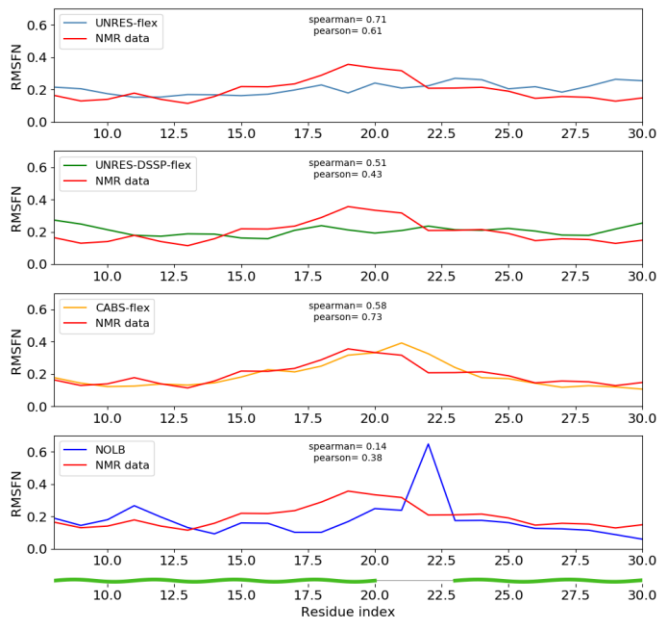
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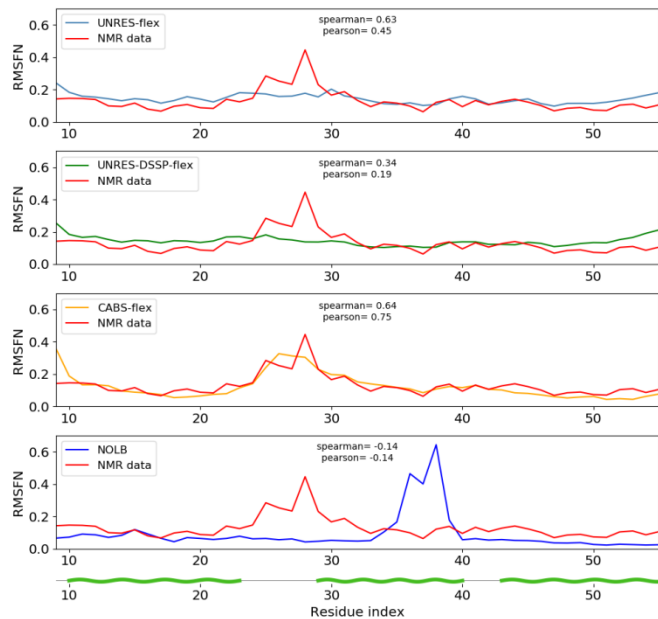
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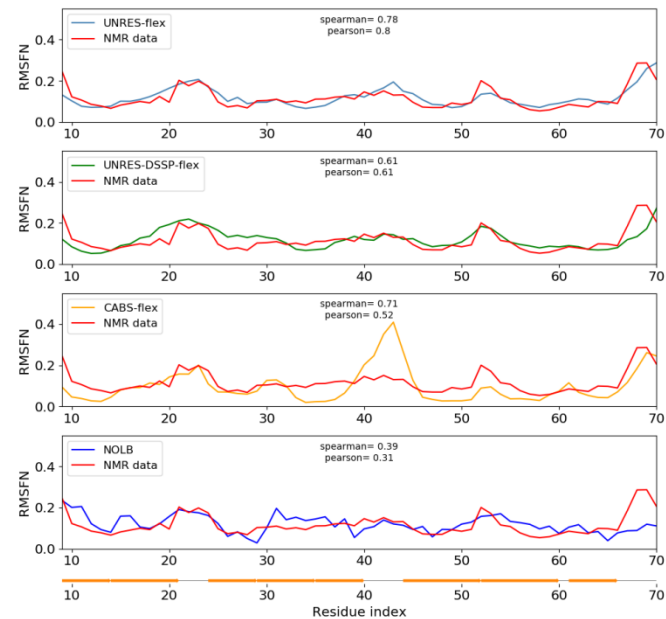
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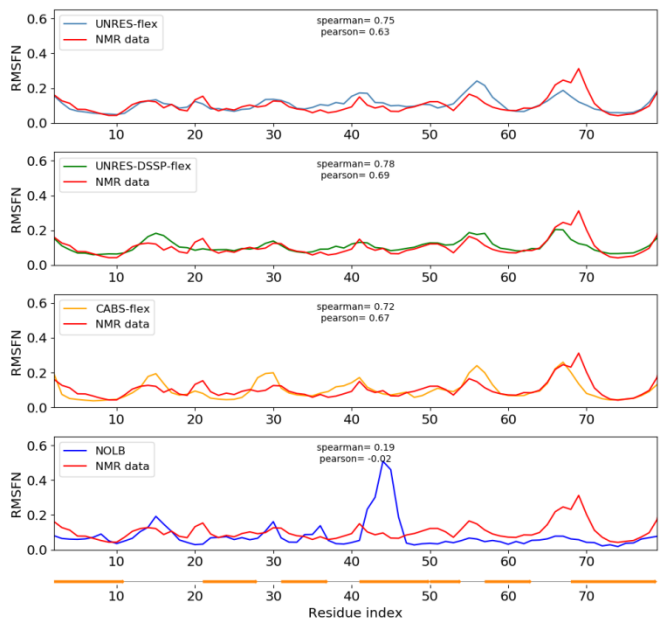
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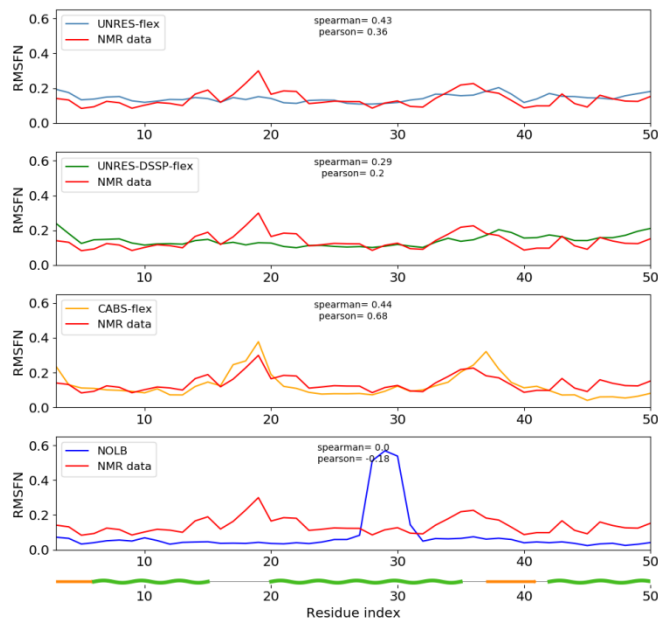
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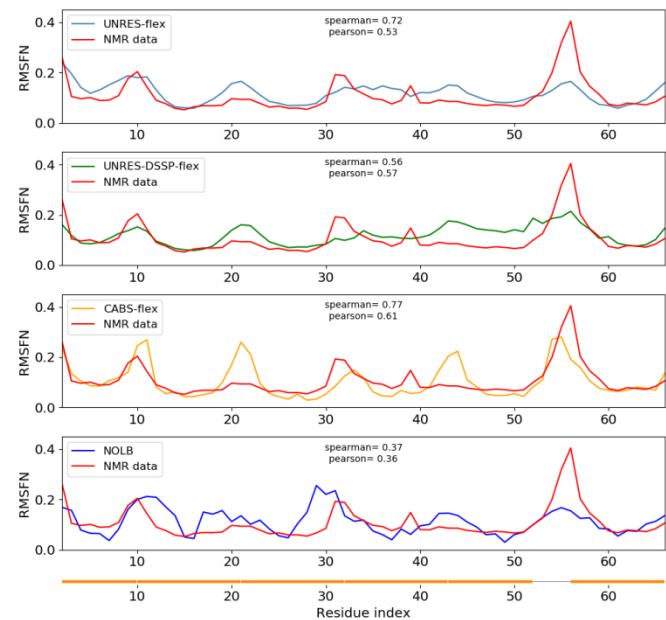
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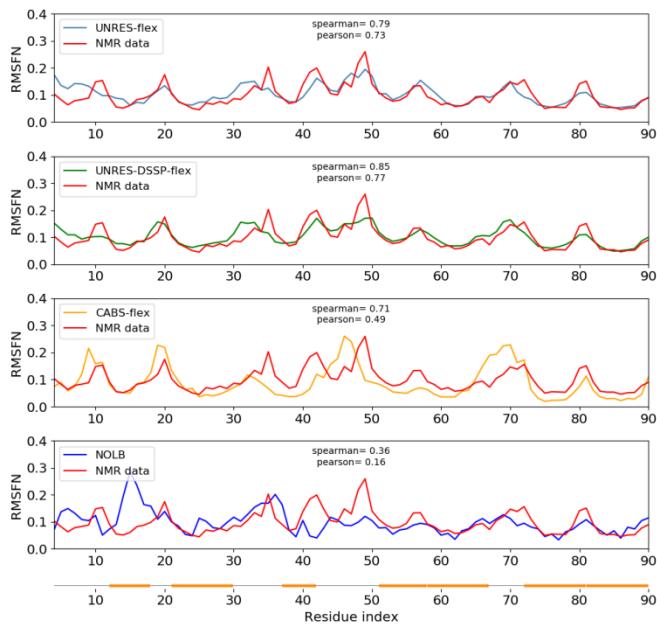
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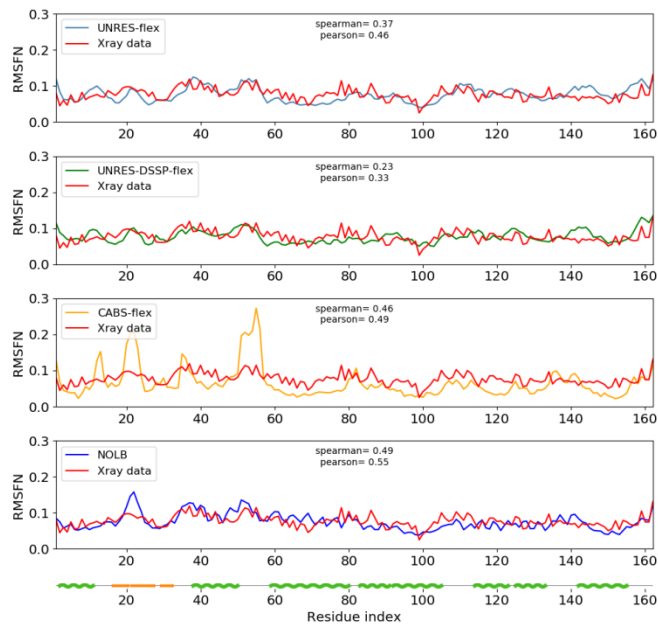
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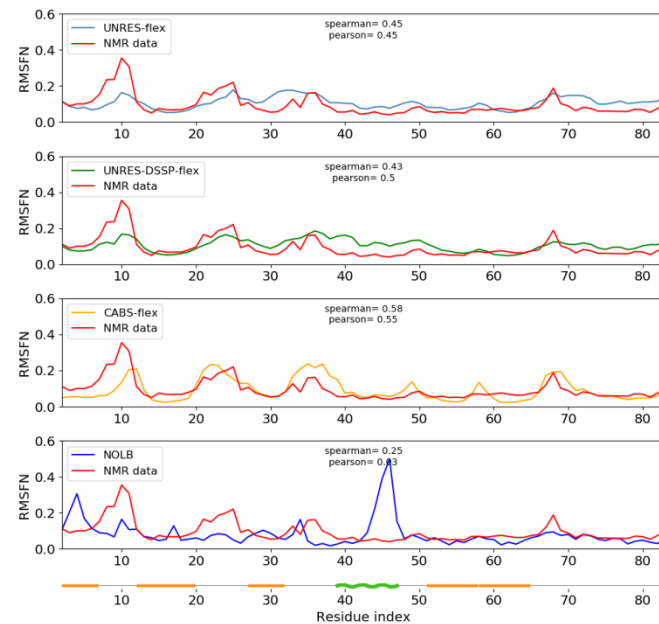
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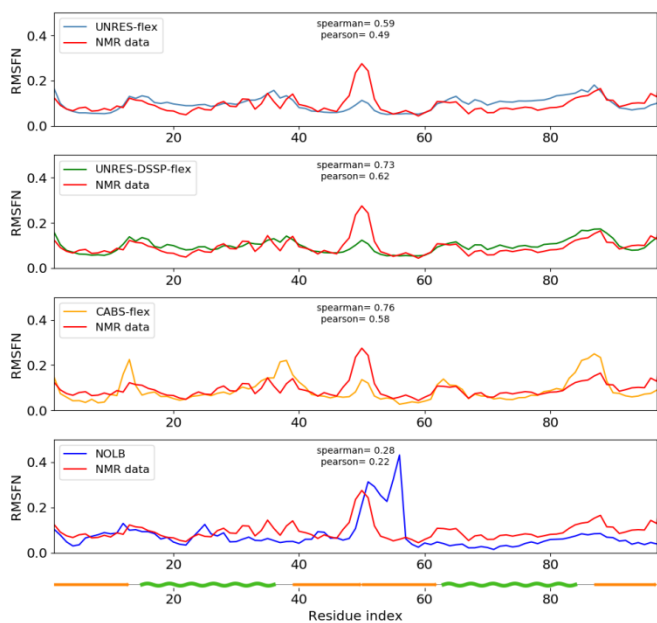
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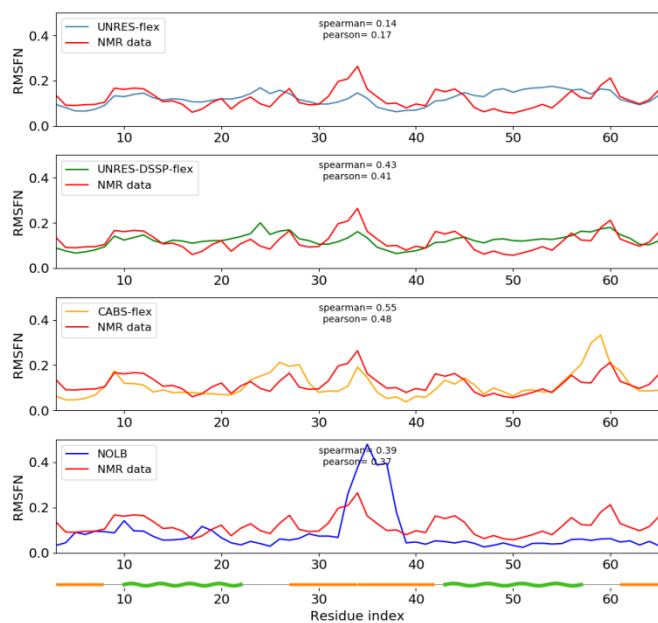
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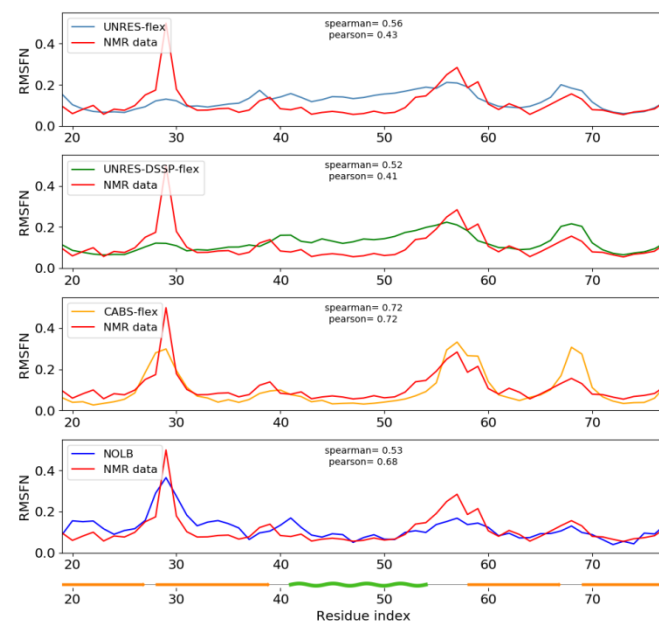
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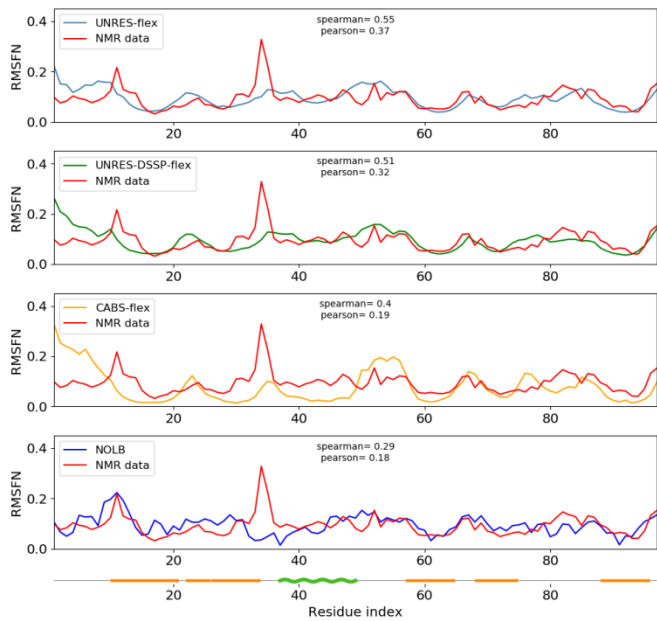
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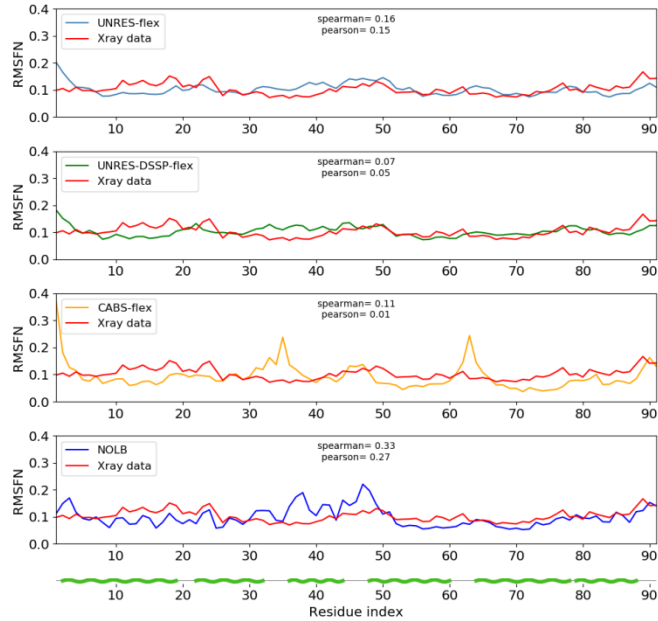
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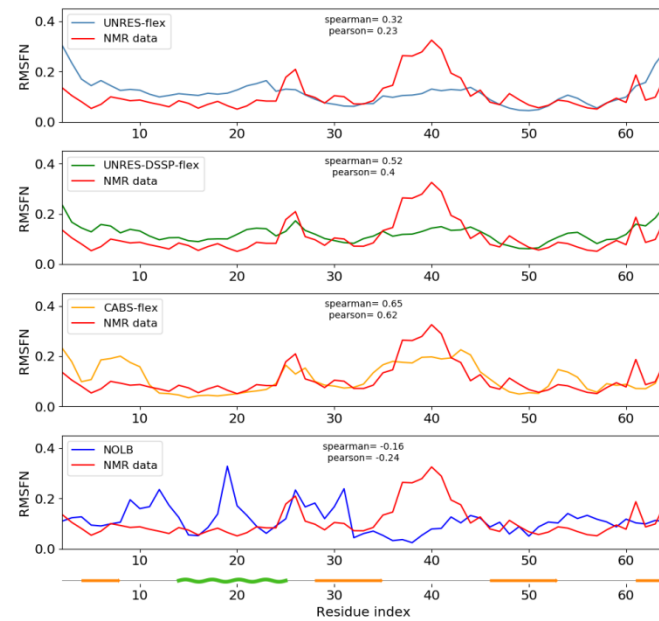
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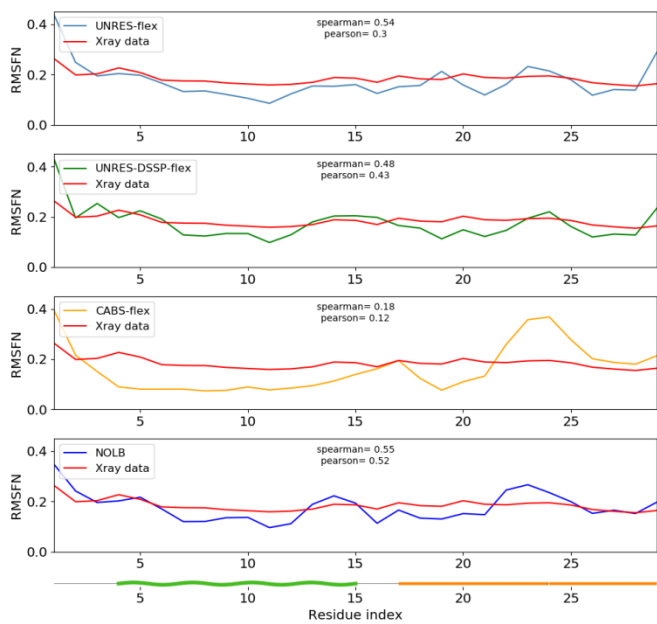
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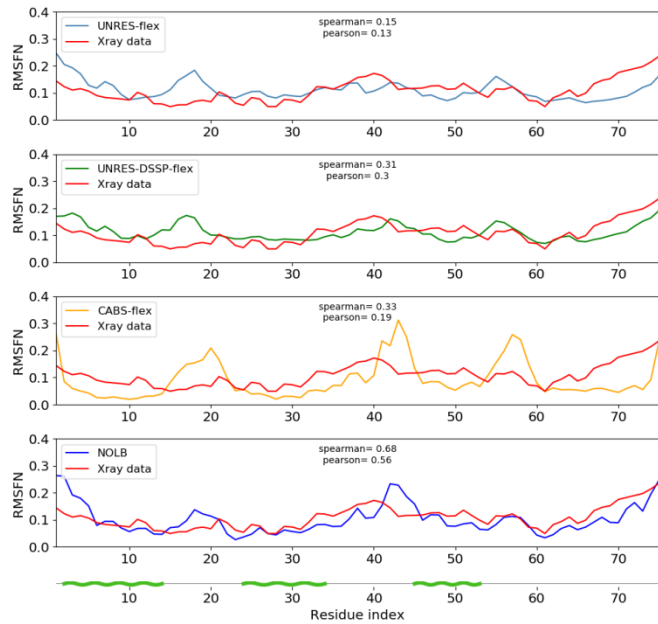
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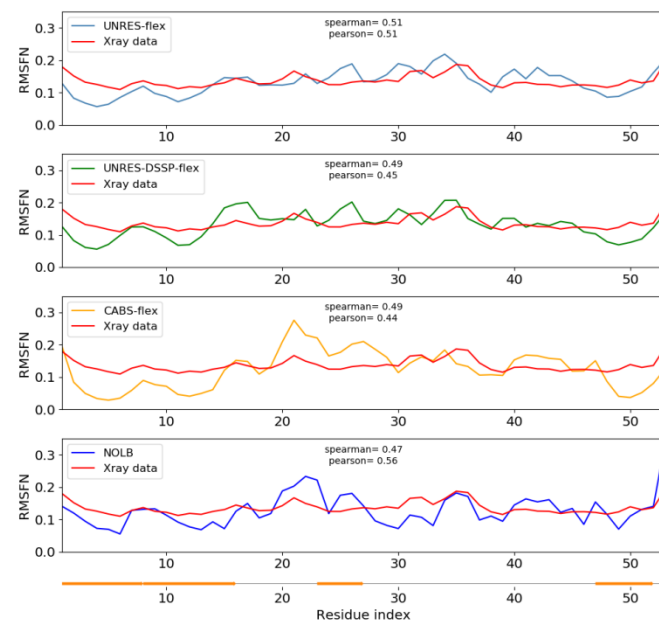
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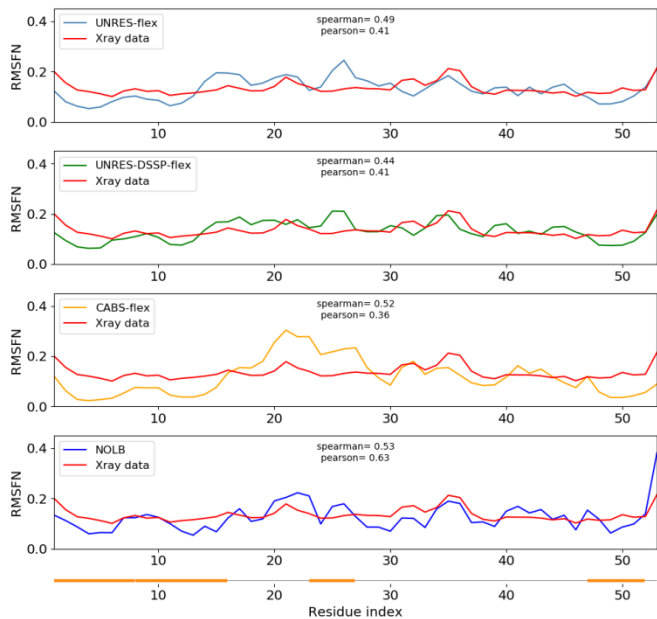
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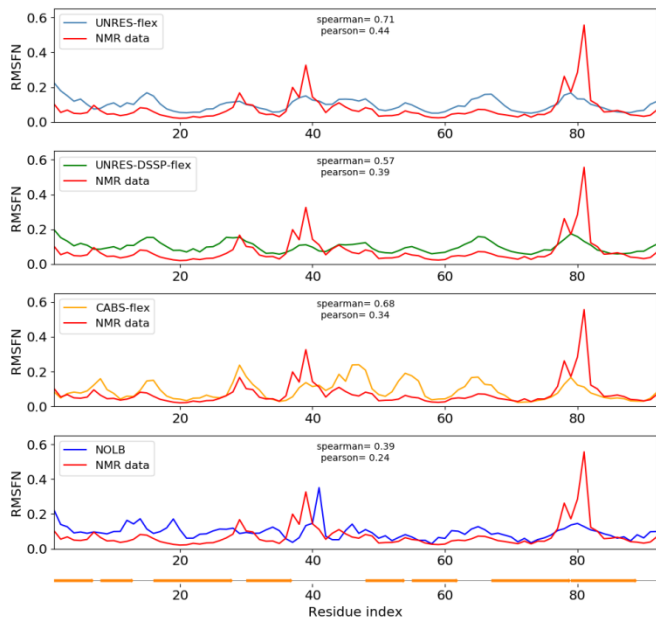
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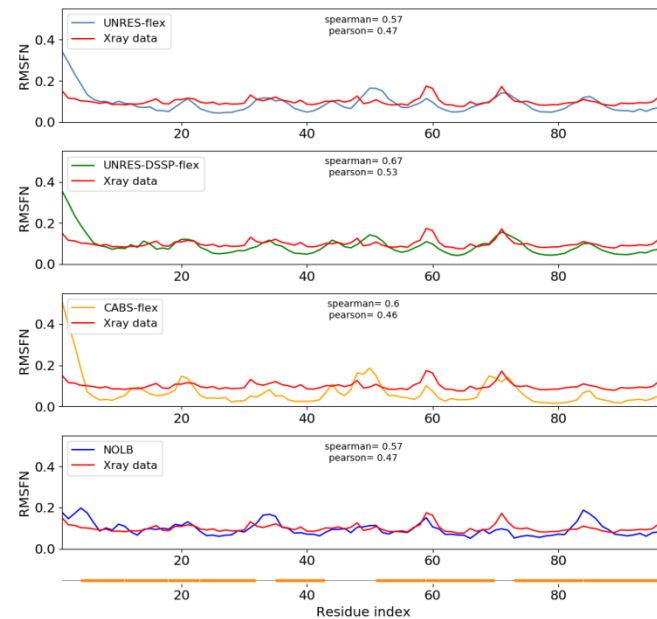
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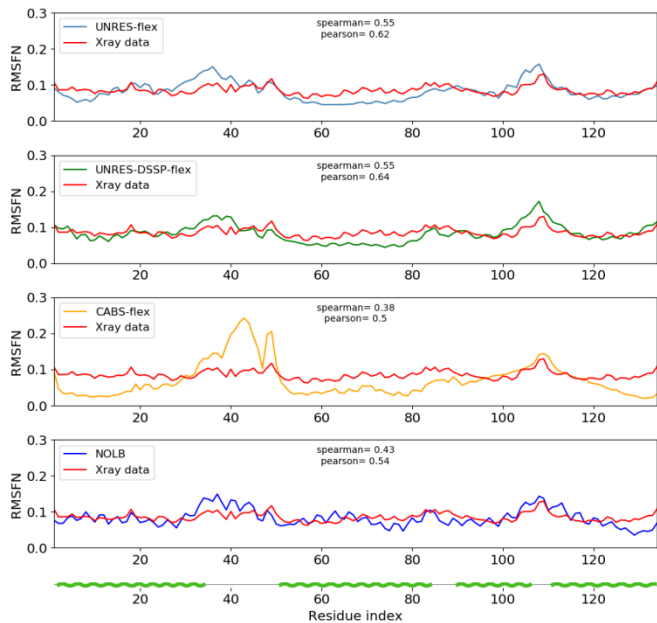
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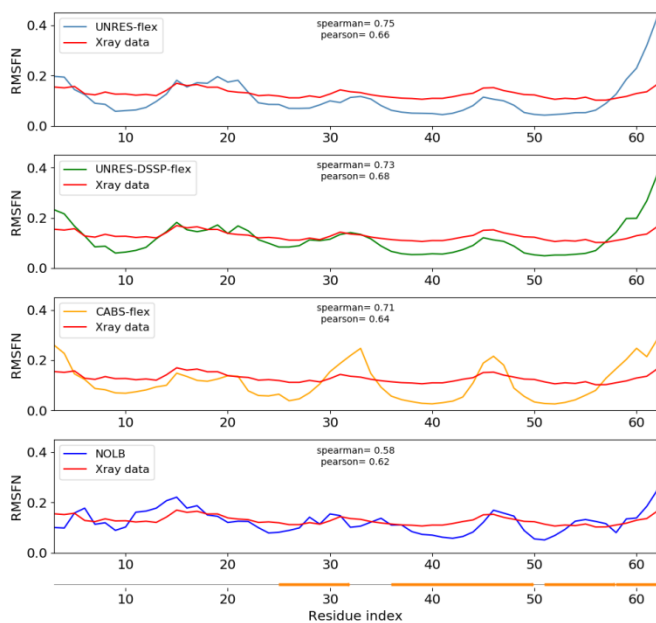
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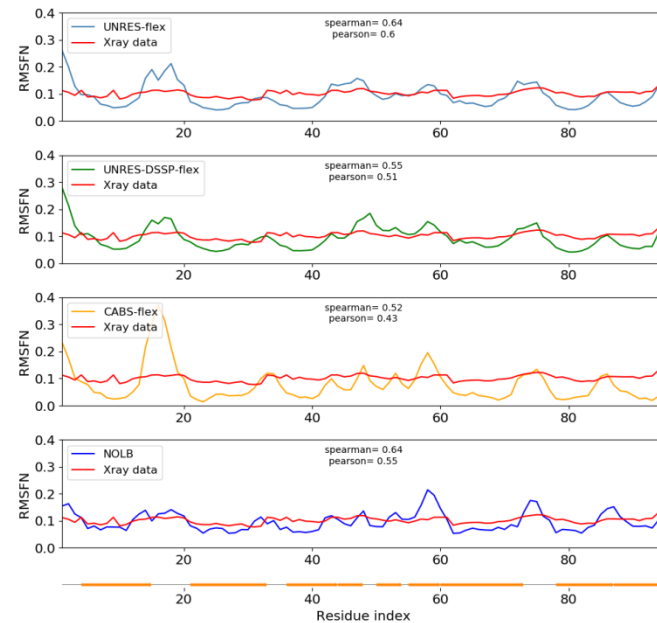
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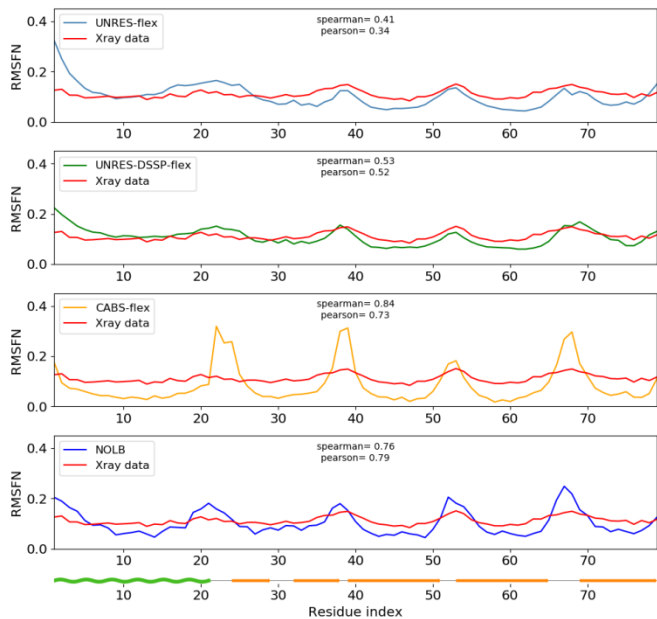
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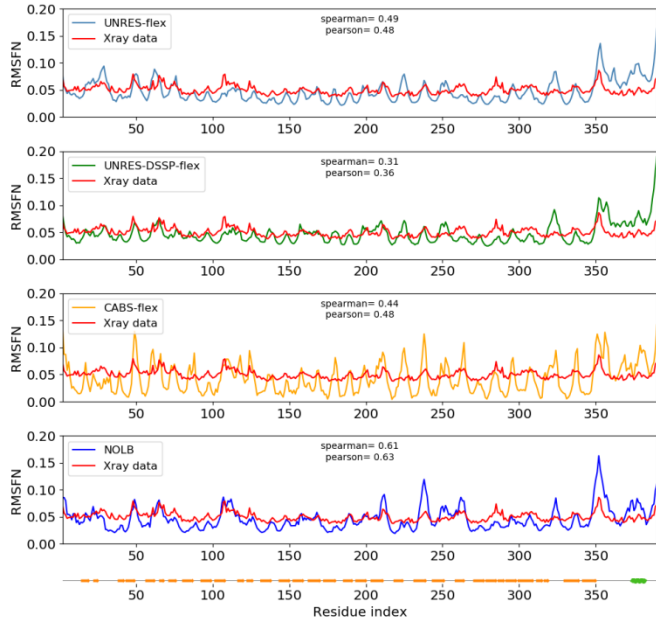
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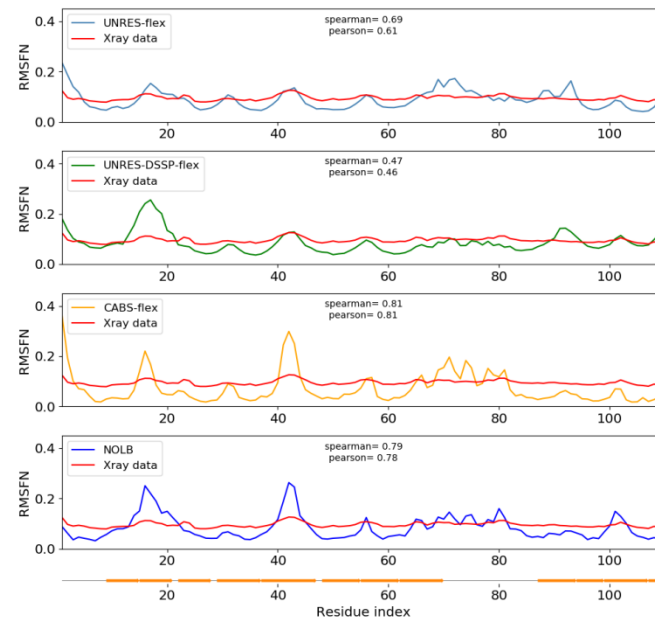
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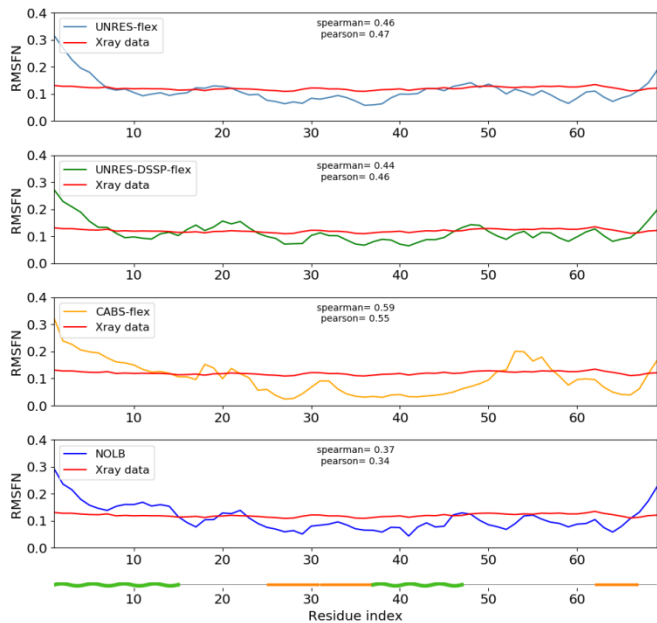
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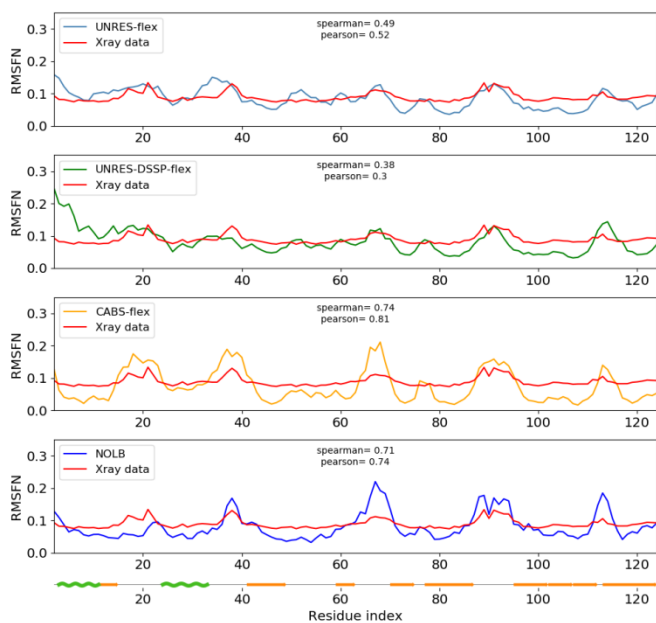
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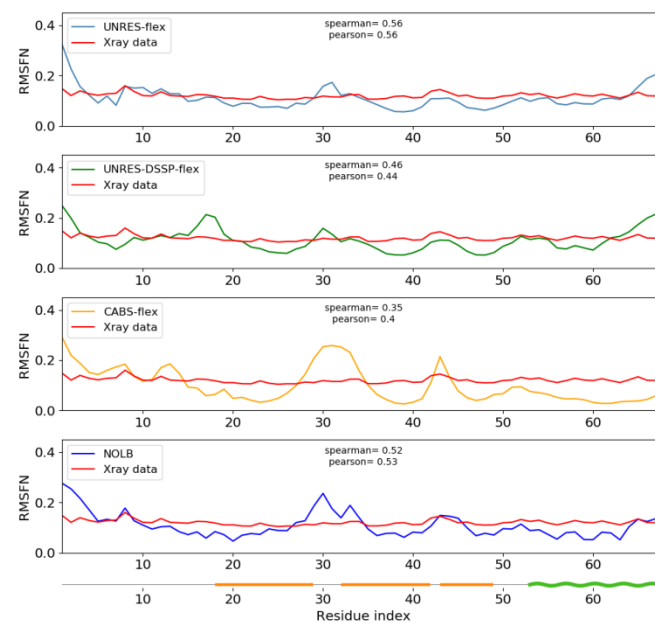
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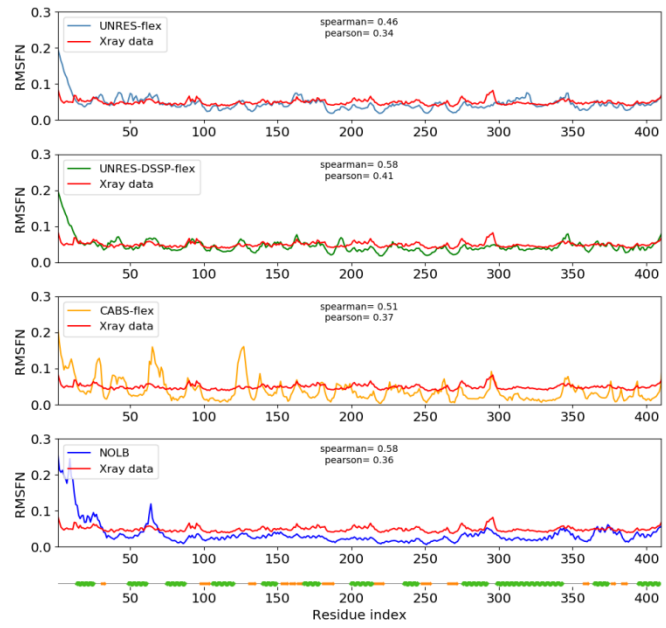
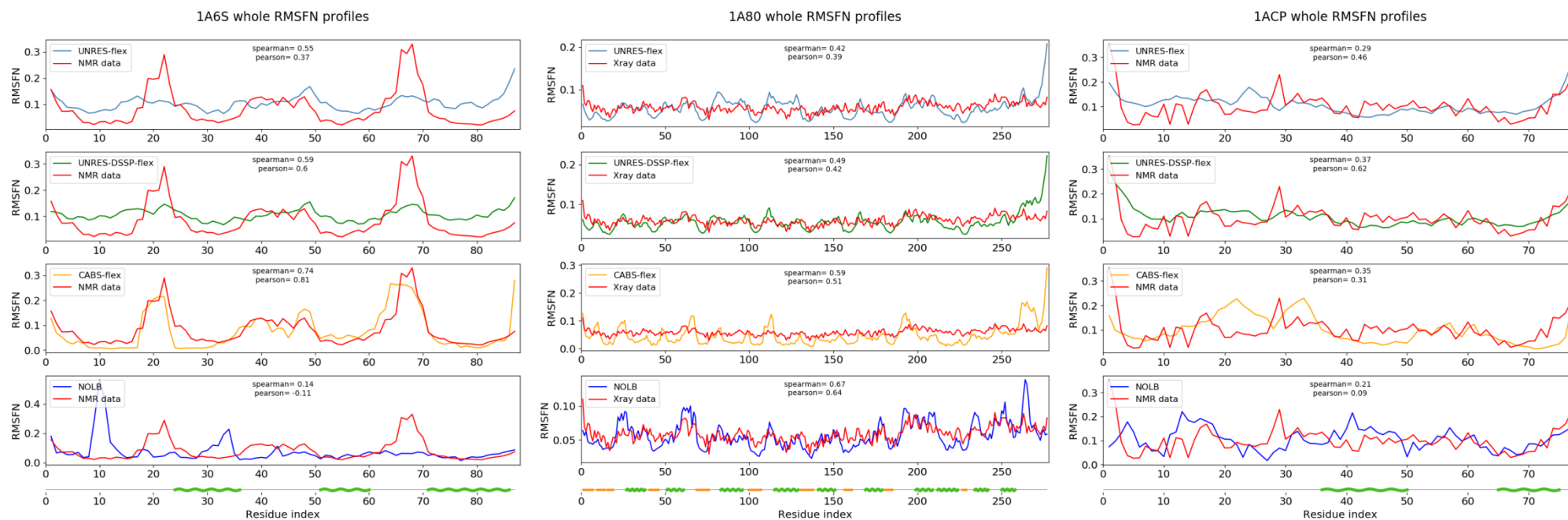
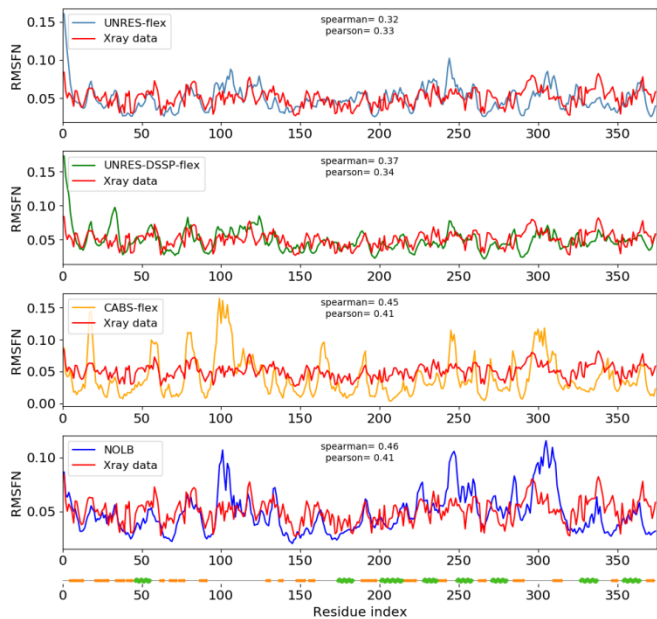


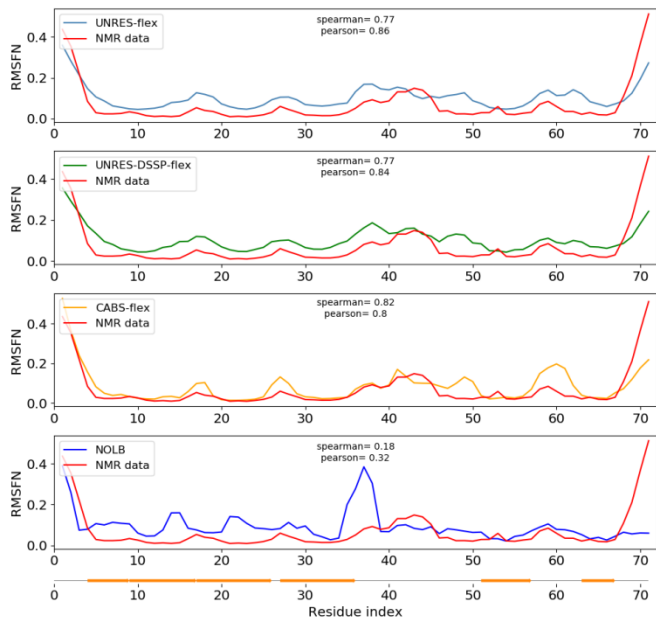
Figure S2. Normalized fluctuation profiles (RMSFN, dimensionless) calculated from NMR ensembles or X-ray B-factors (red line) and the corresponding profile predicted by UNRES-flex (light-blue line), UNRES-DSSP-flex (green line), CABS-flex (yellow line), and NOLB (blue line). Except for NOLB, the fluctuation profiles are averaged over three simulations. The Pearson (r_p) and Spearman (r_s) coefficients for the correlation between the experimental and predicted profiles are shown in each panel. The solid orange and wave green lines below the abscissa of each panel indicate the β -sheet and α -helical structure, respectively. The analyses were carried out for full structures.



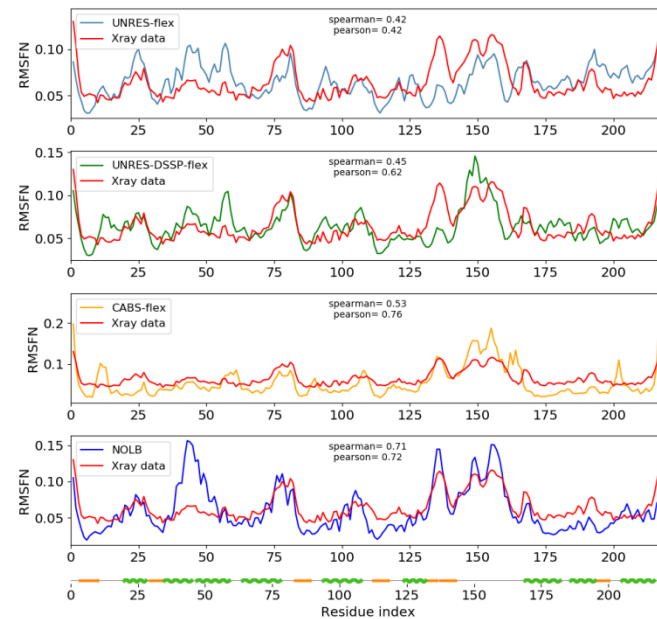
1ADG whole RMSFN profiles



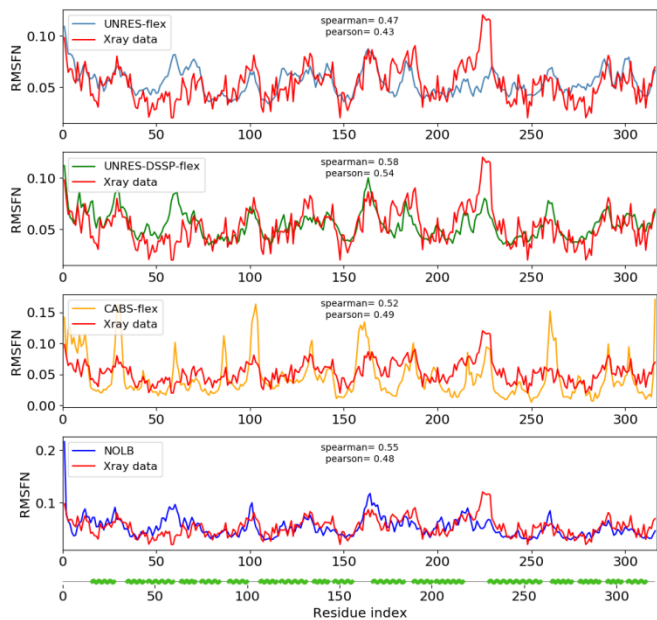
1AH9 whole RMSFN profiles



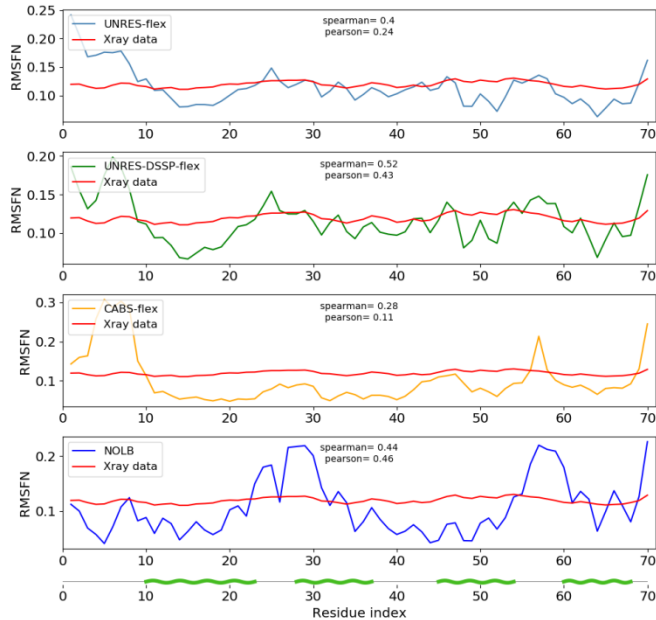
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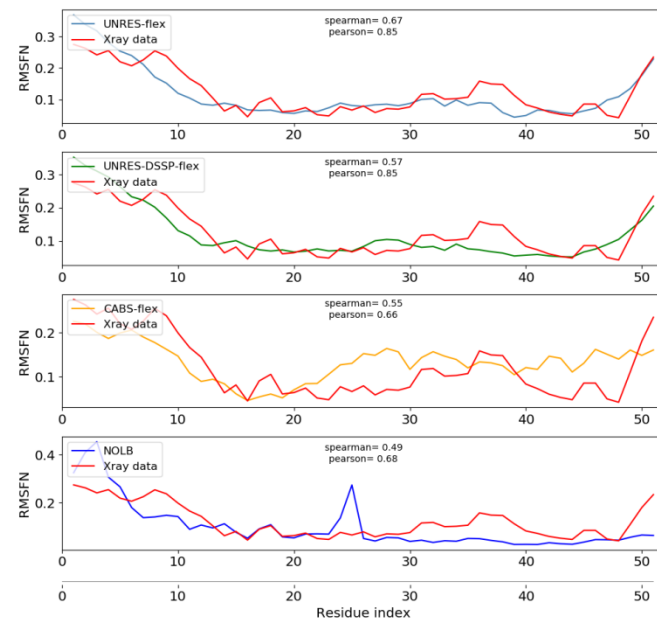
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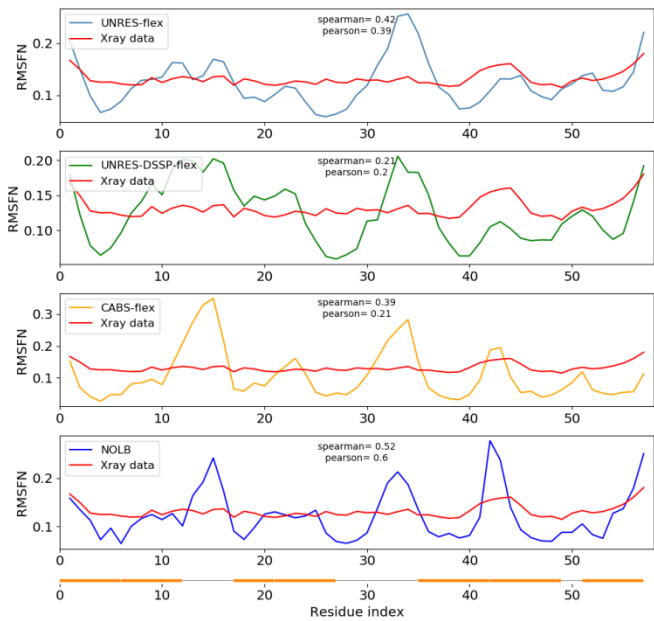
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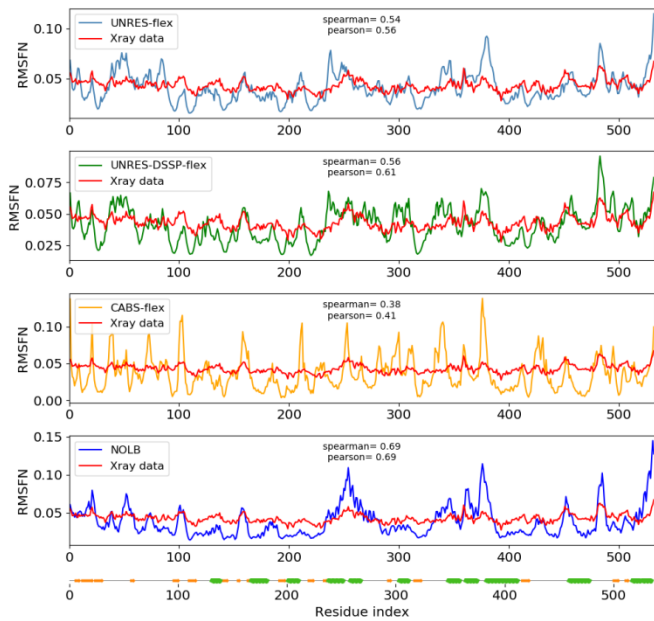
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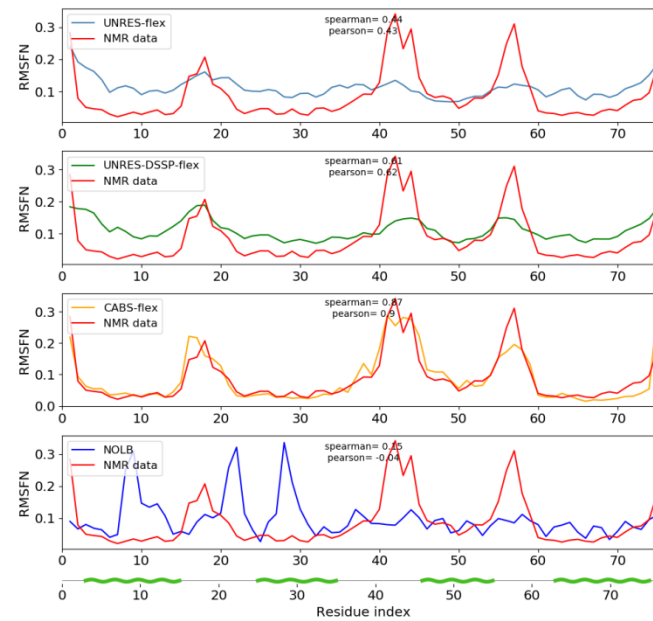
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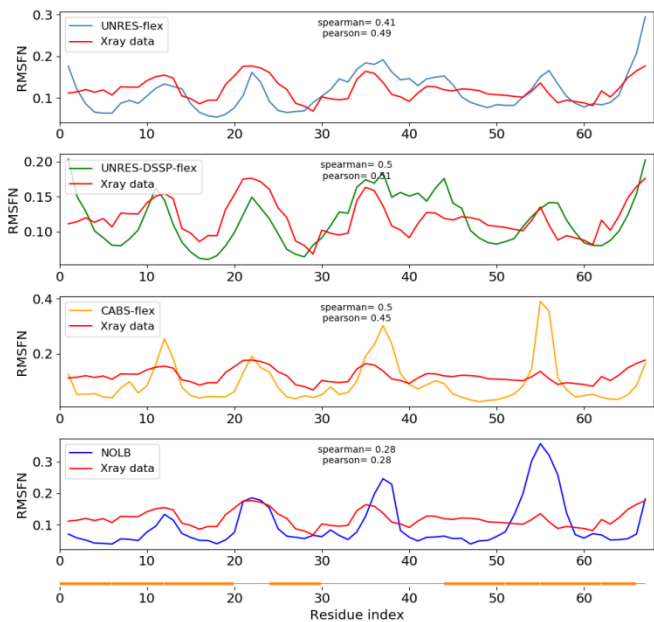
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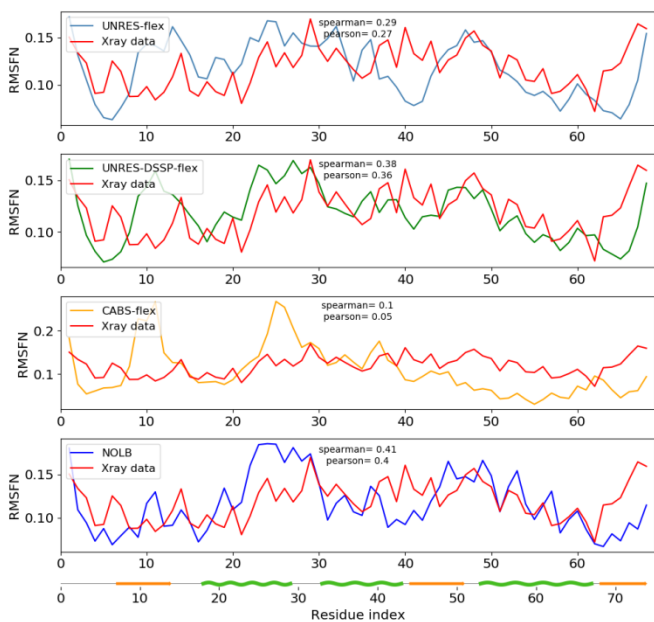
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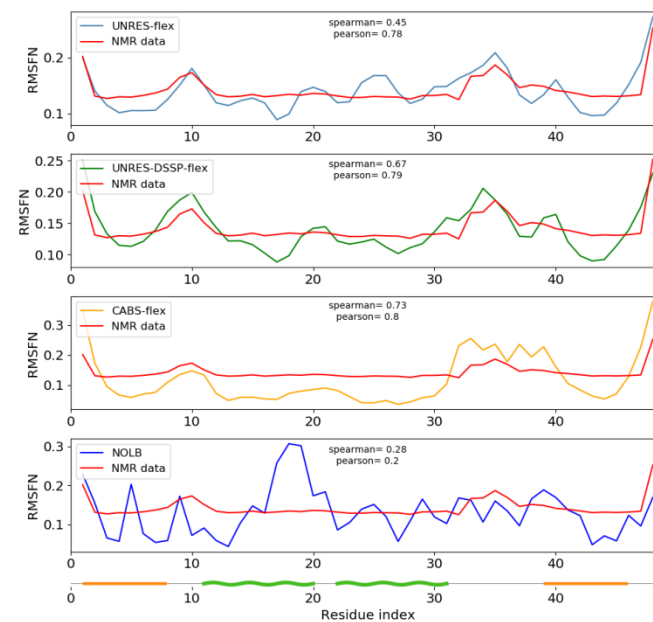
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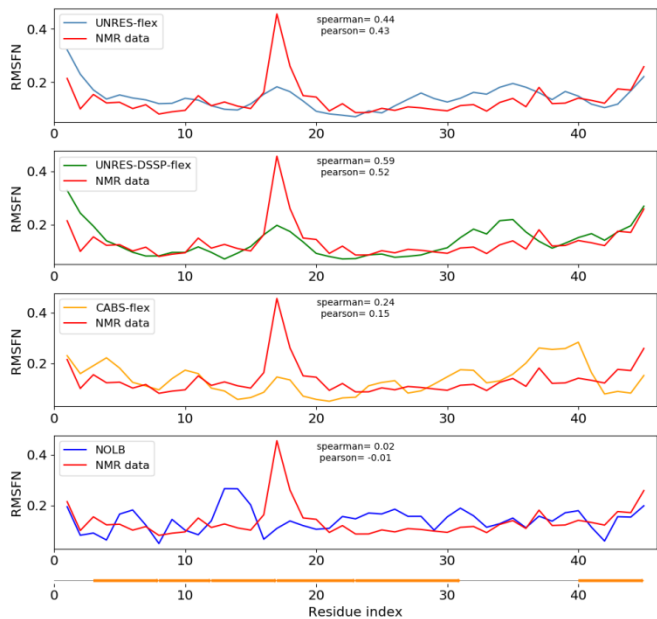
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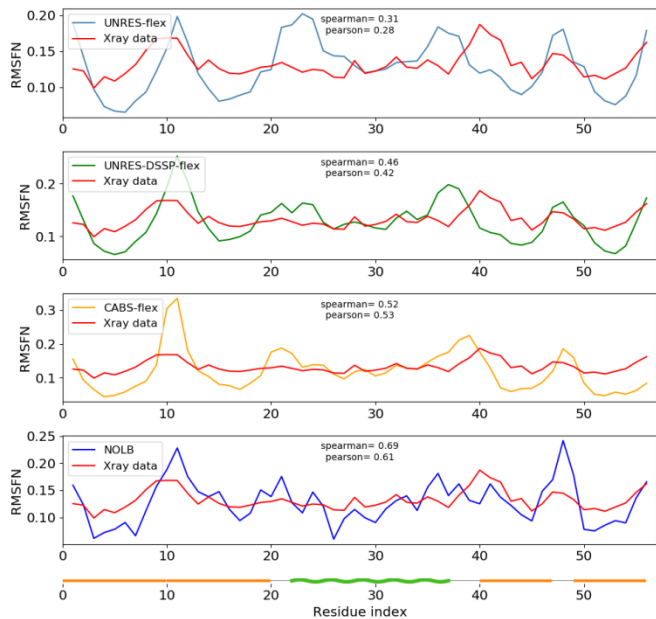
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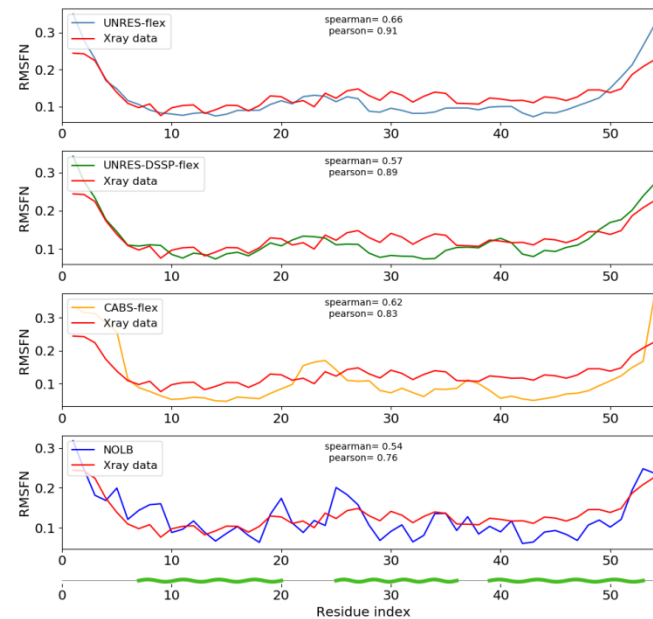
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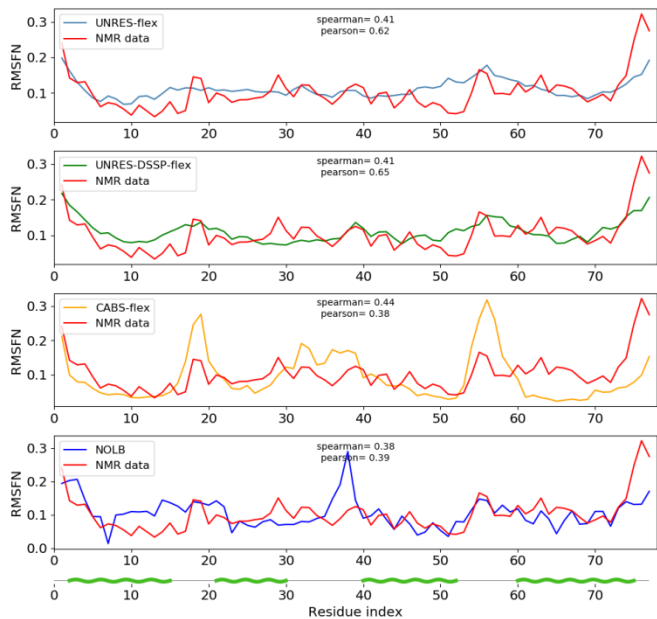
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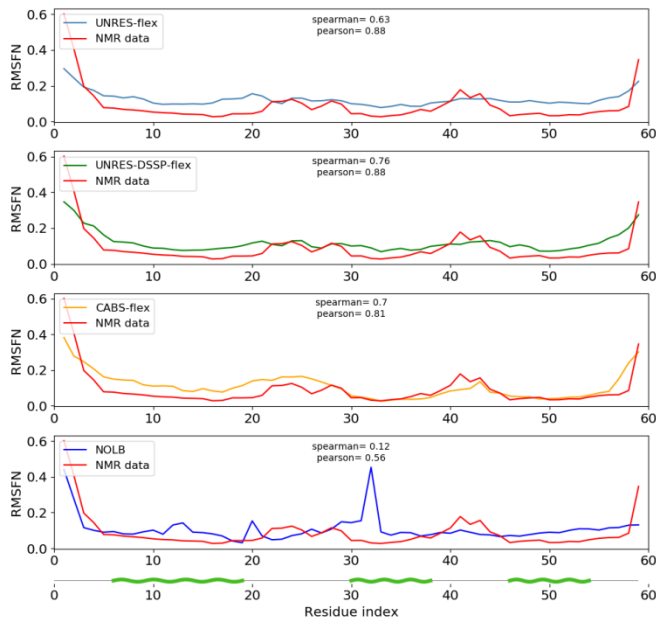
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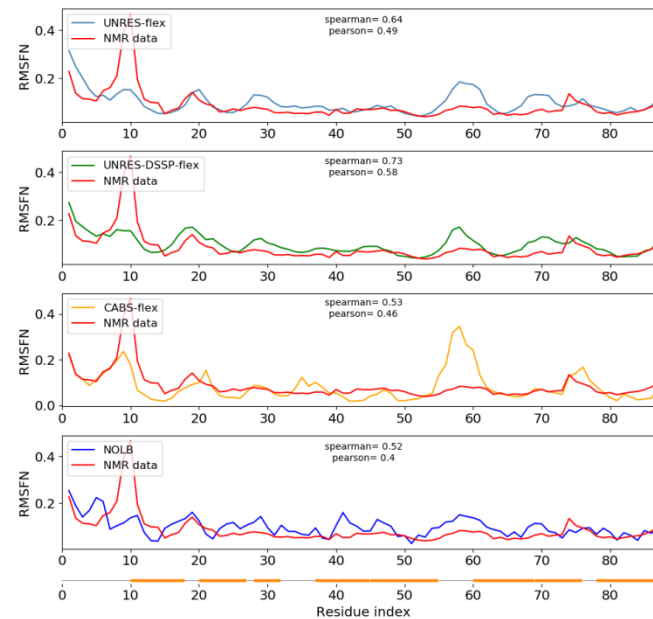
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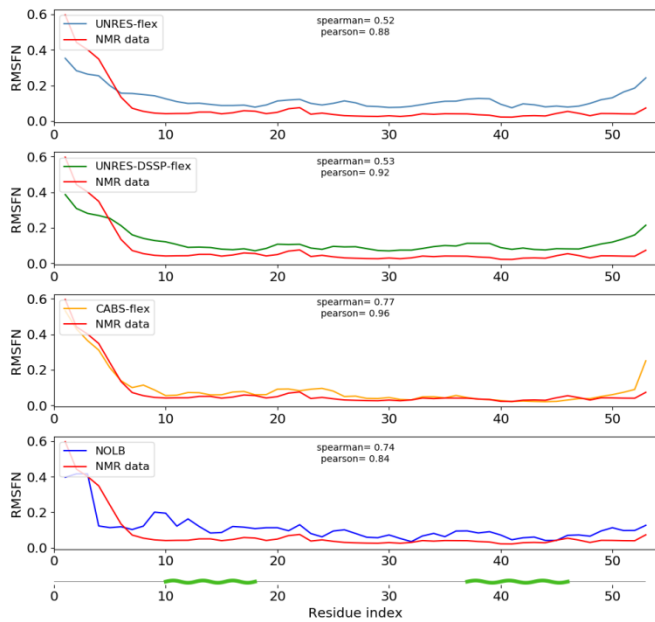
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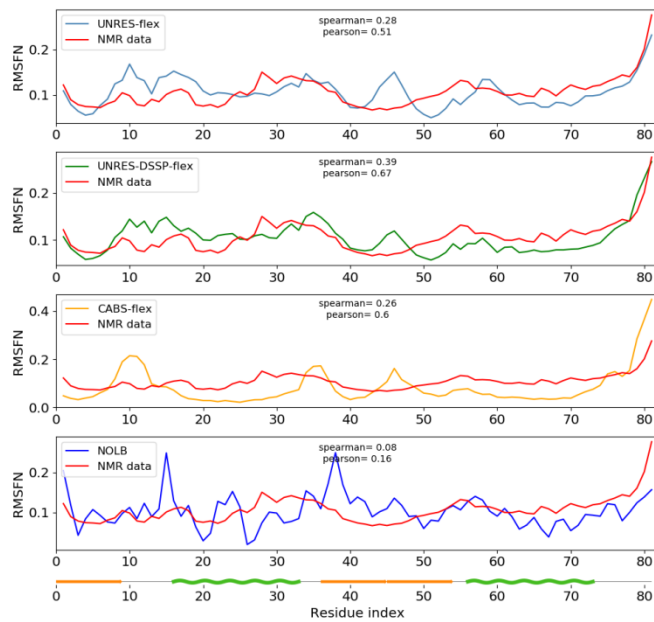
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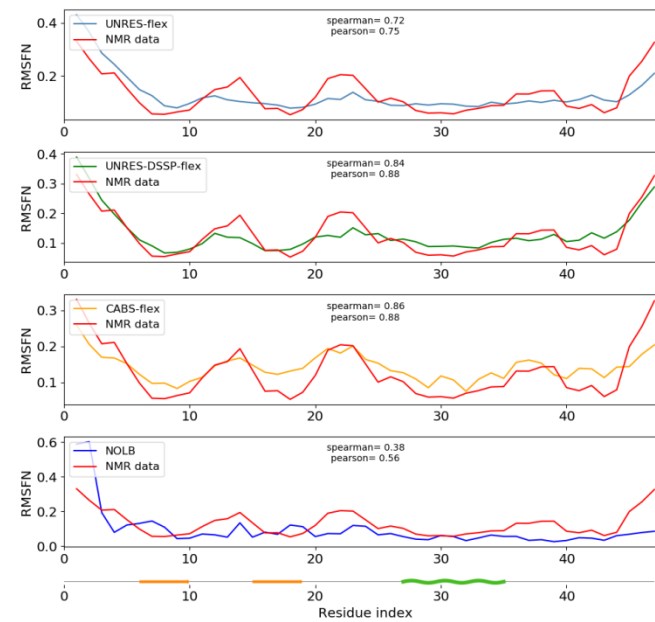
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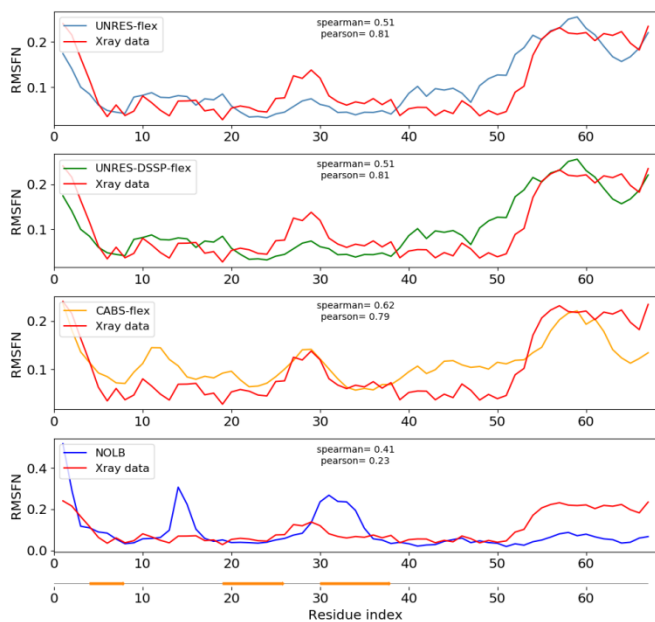
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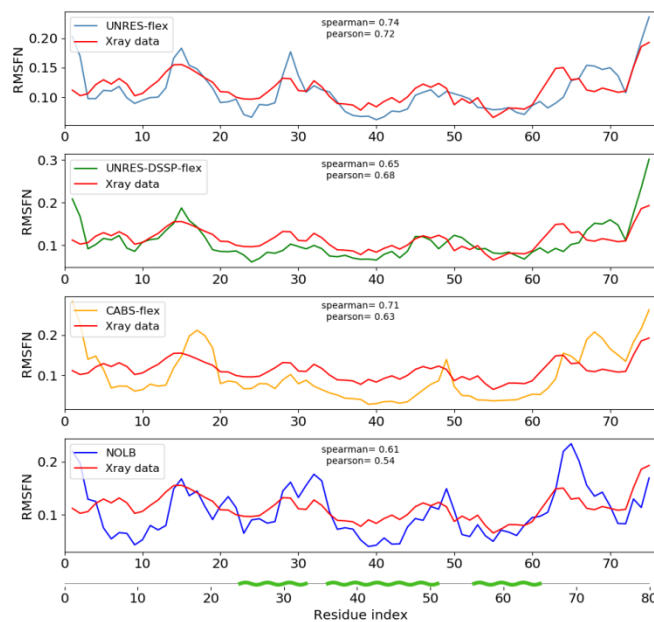
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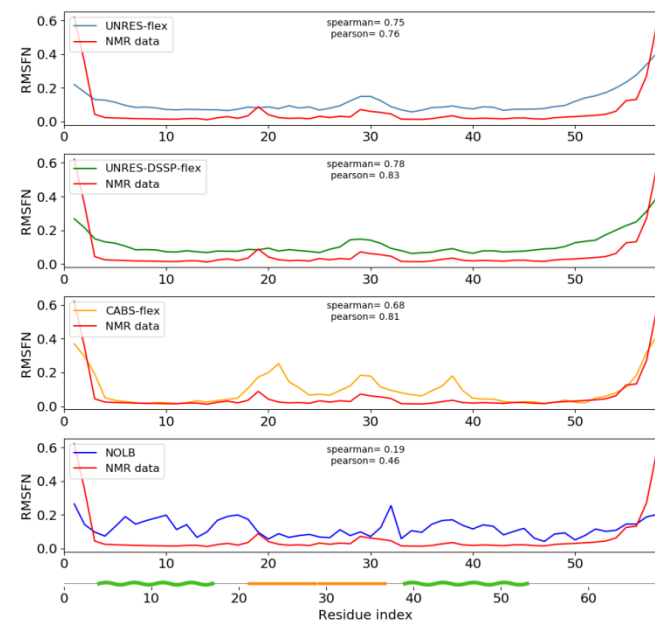
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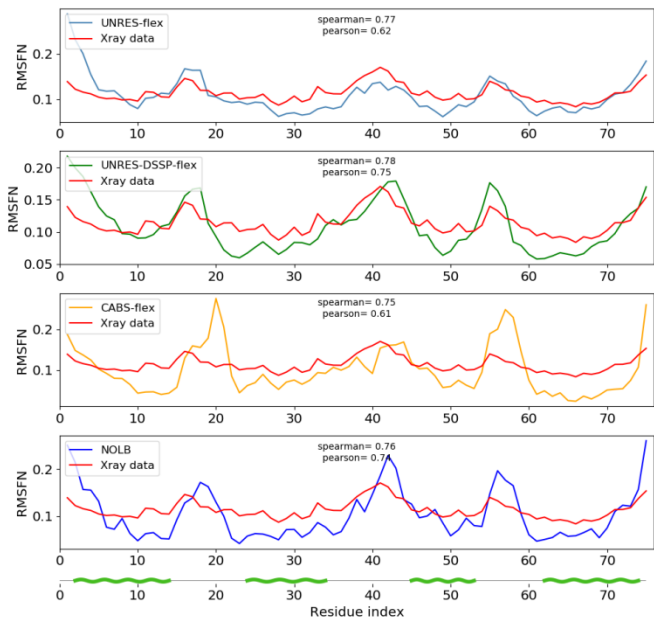
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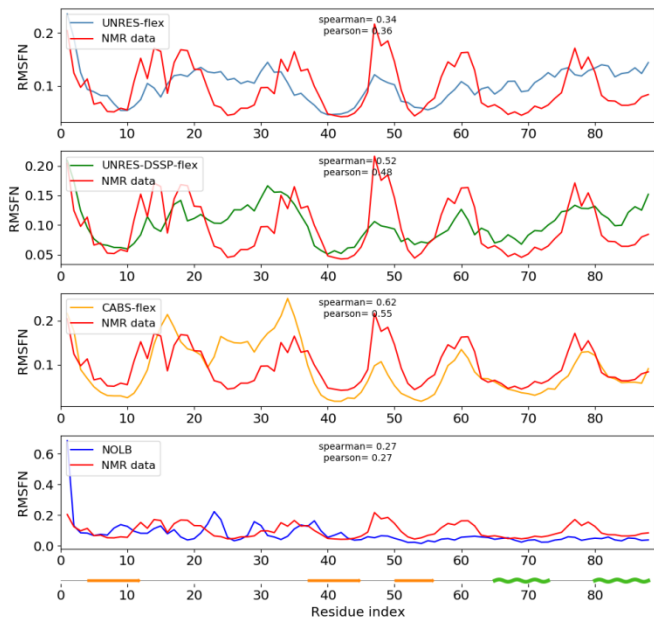
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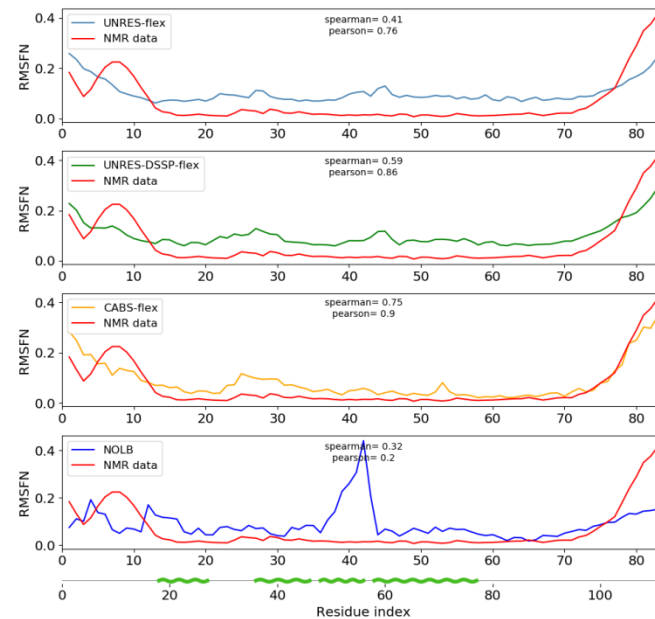
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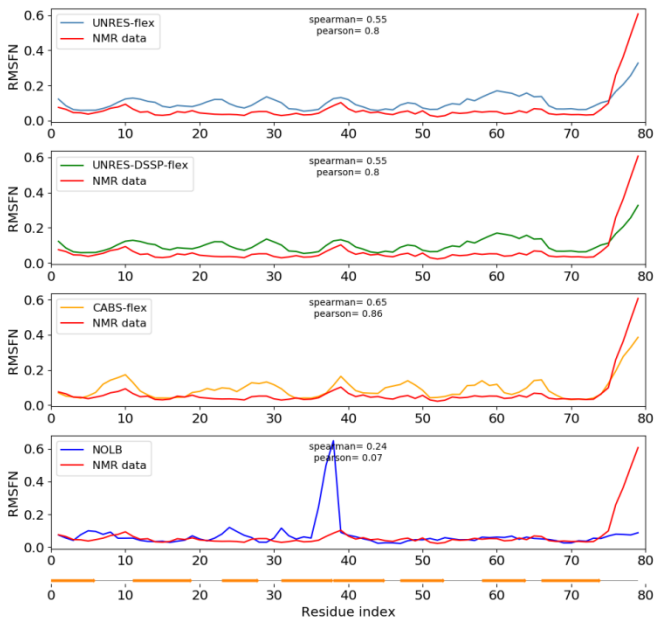
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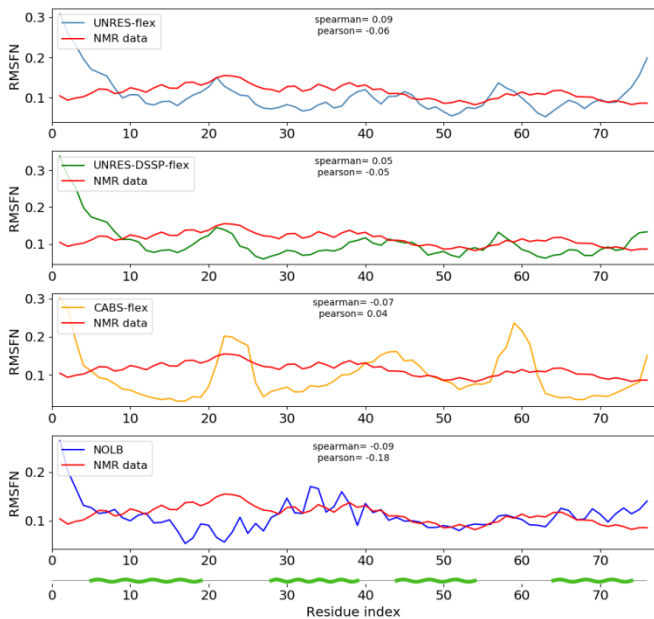
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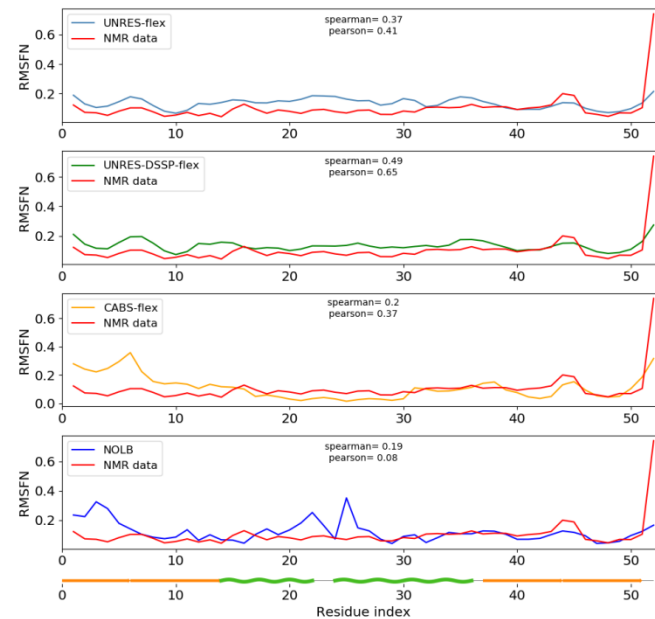
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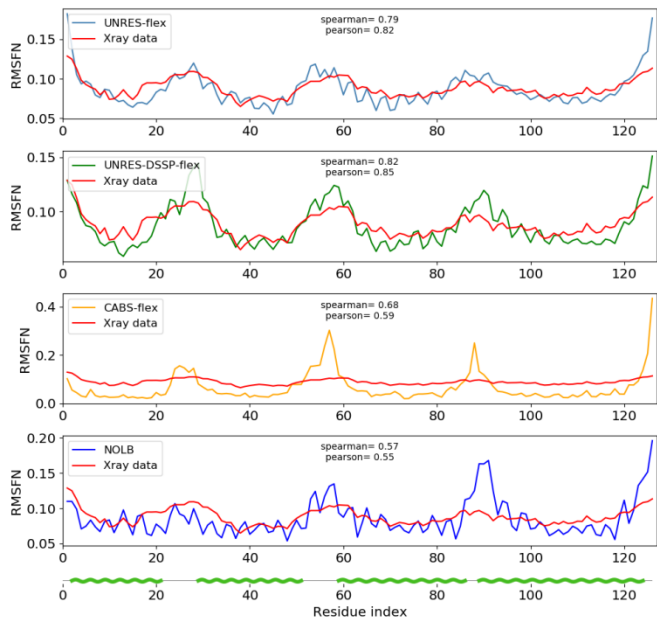
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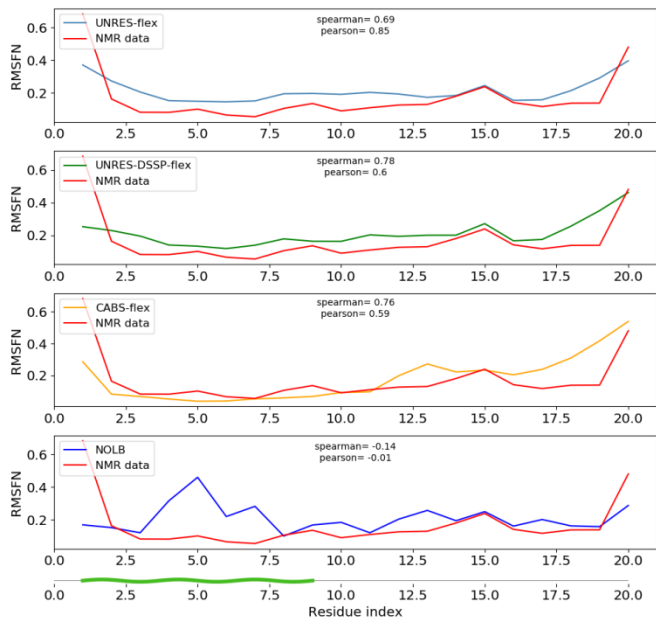
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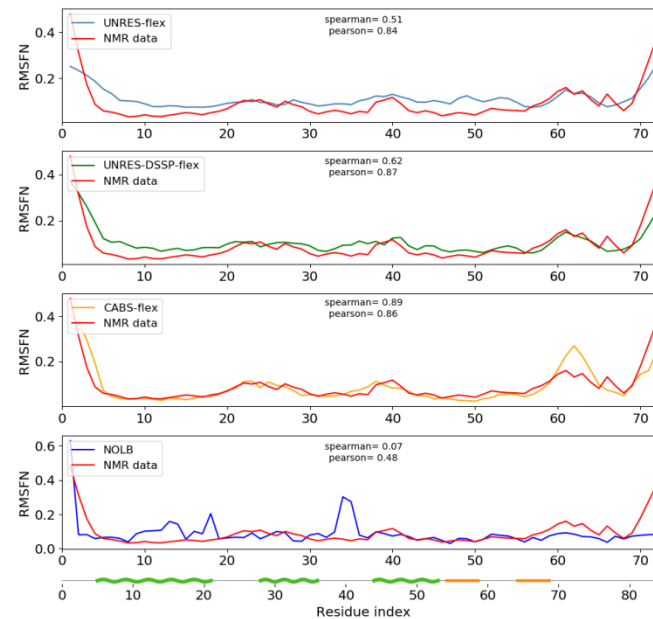
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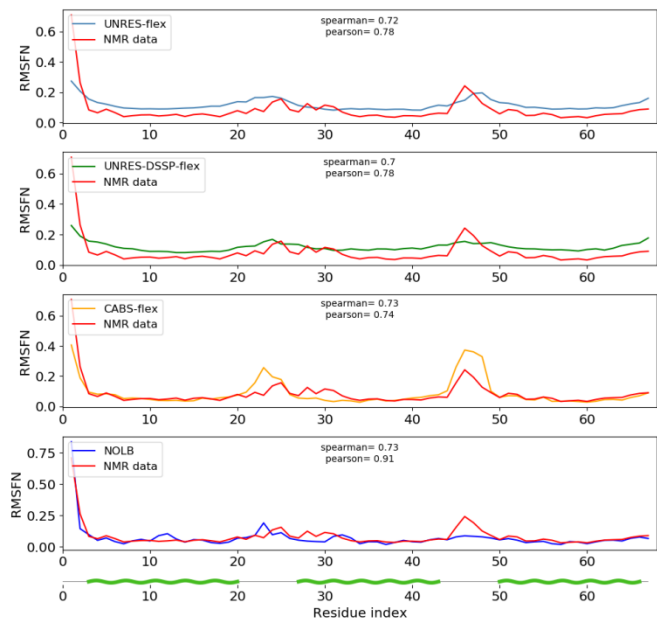
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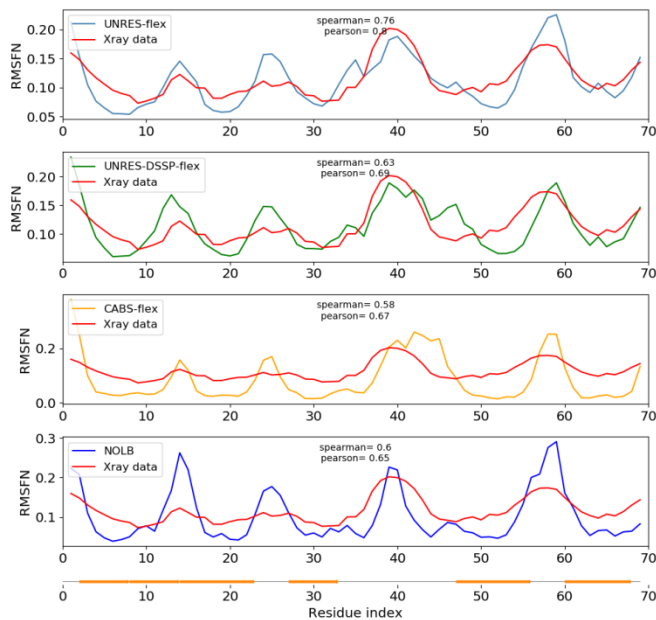
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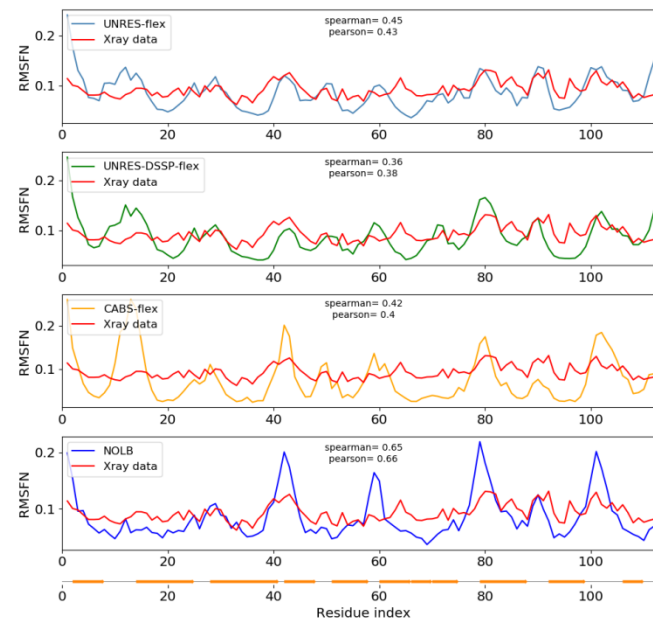
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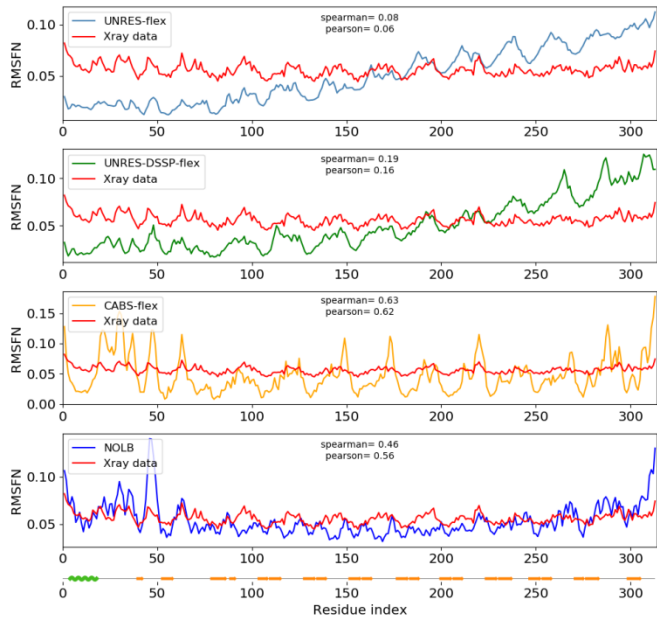
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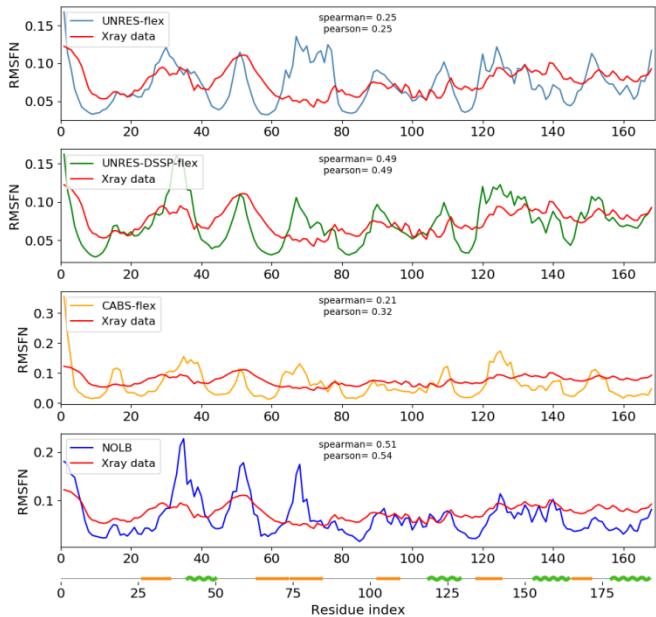
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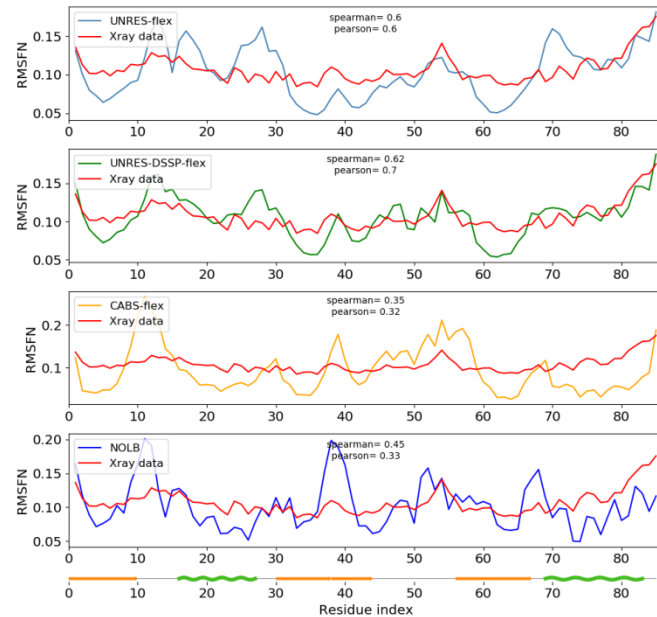
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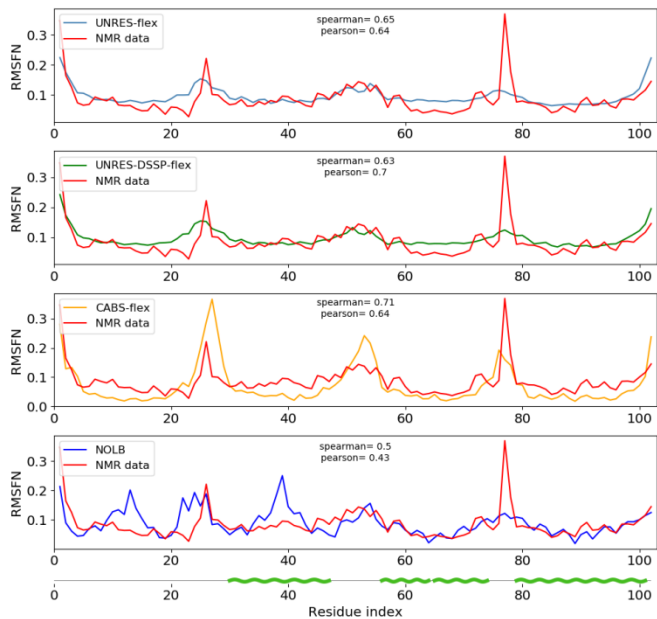
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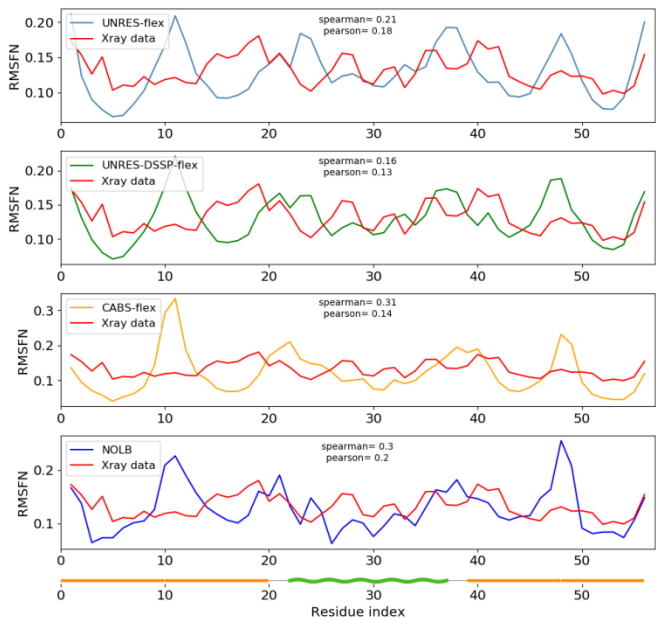
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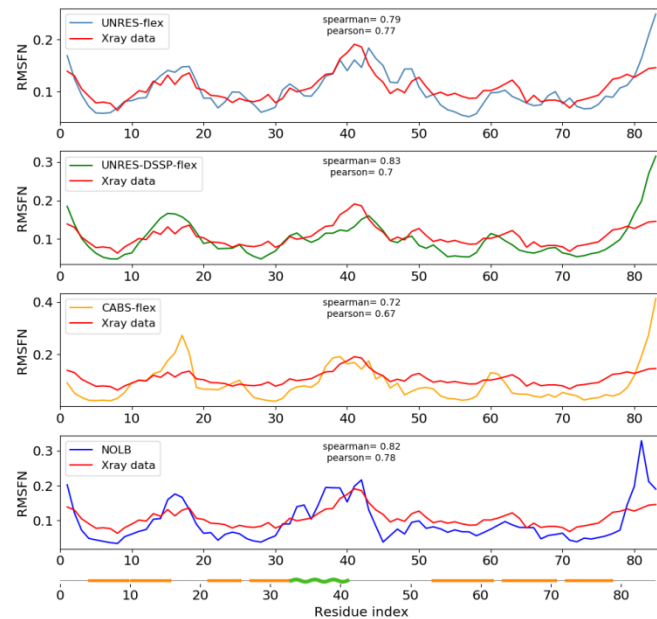
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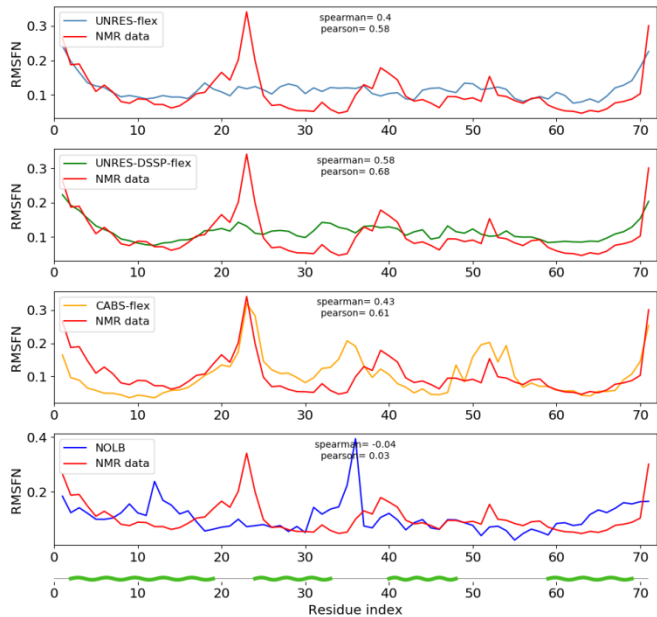
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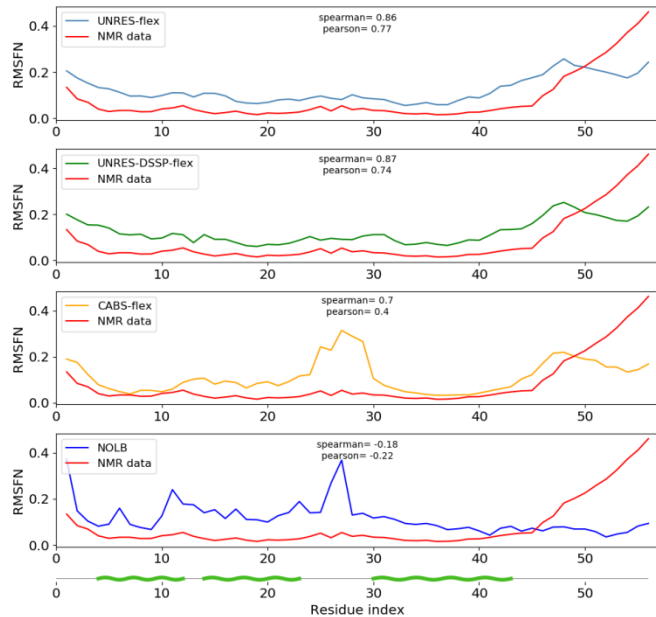
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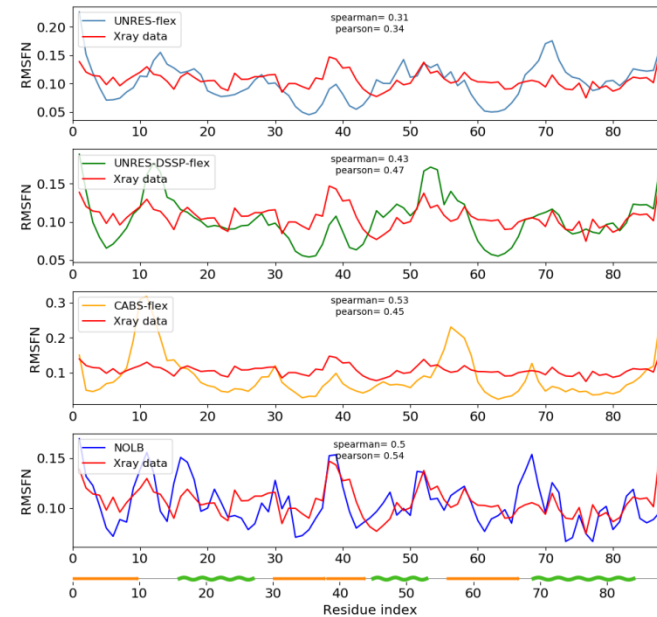
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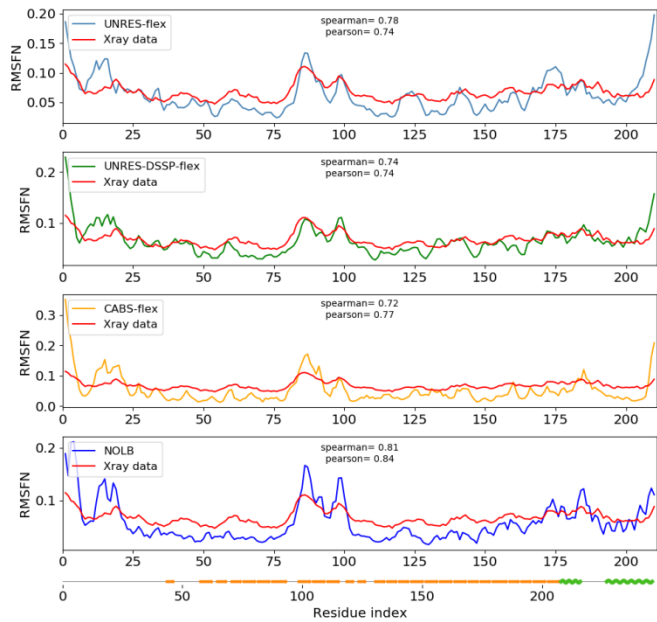
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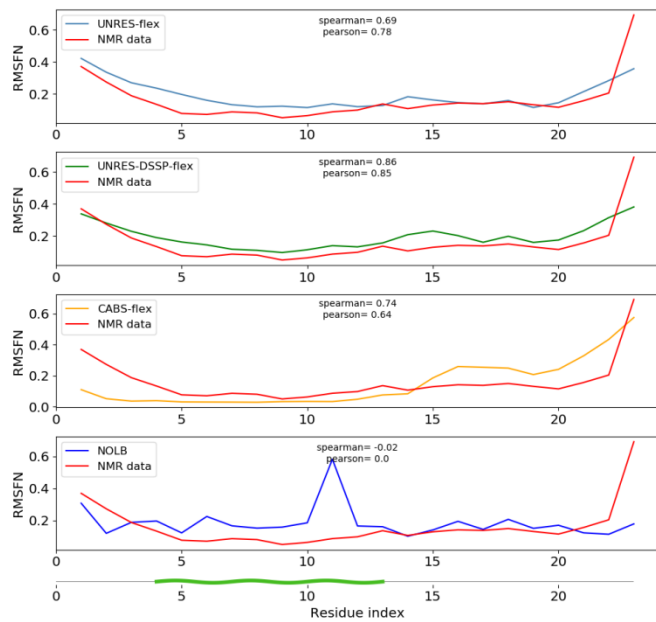
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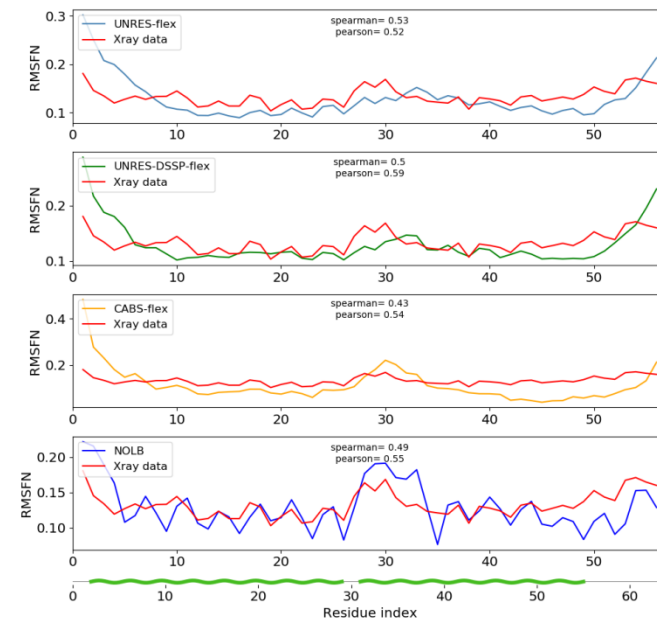
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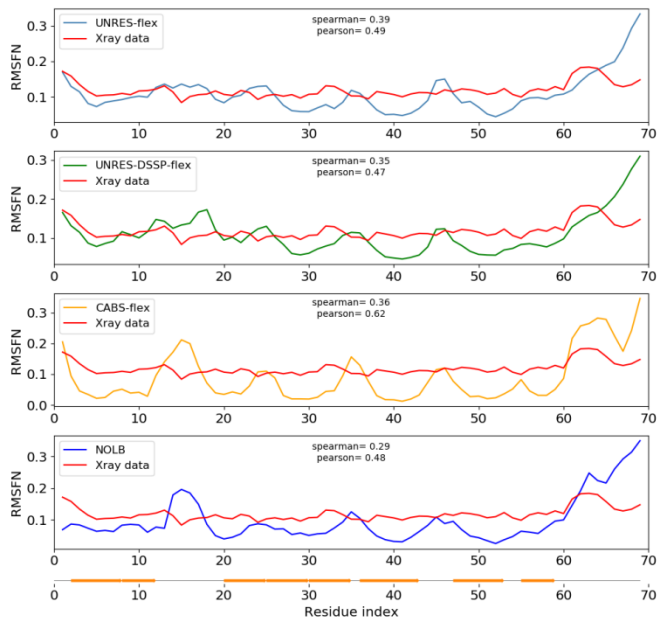
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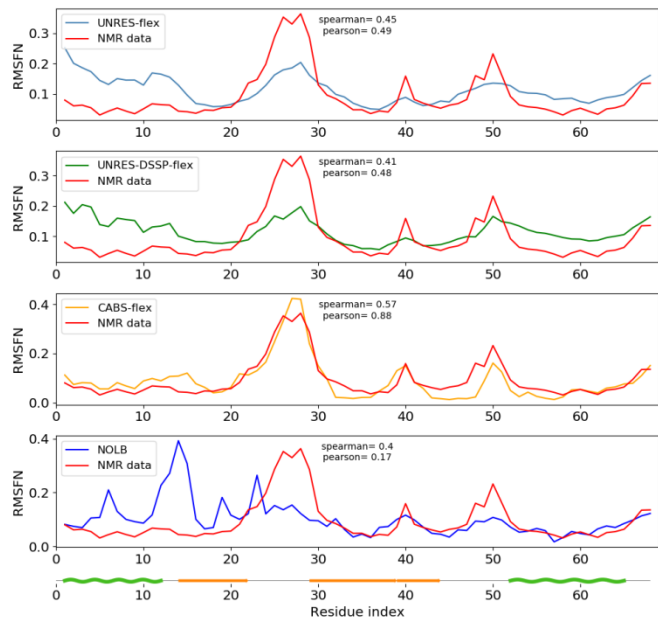
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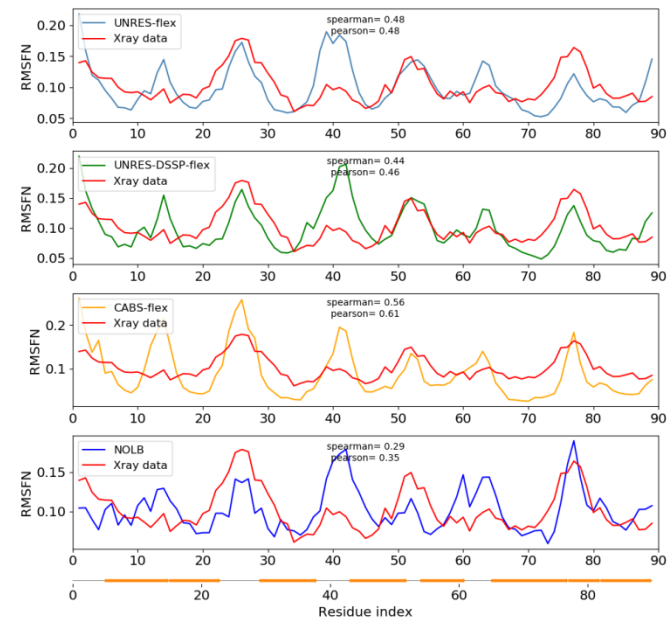
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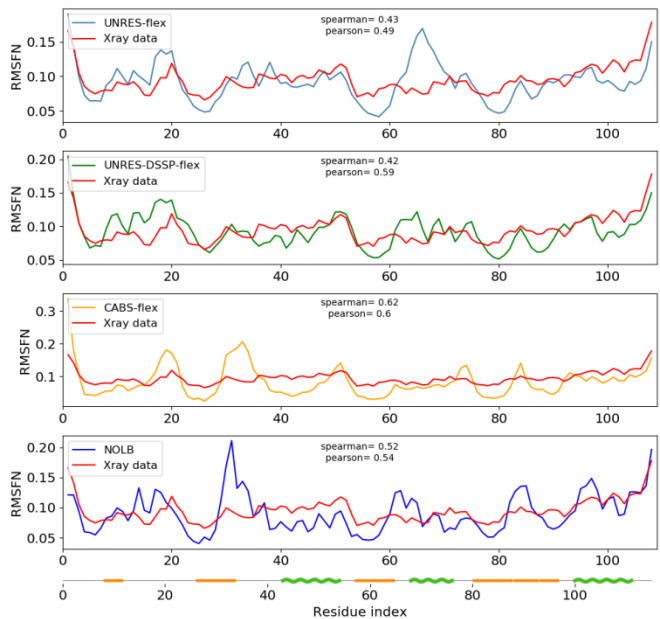
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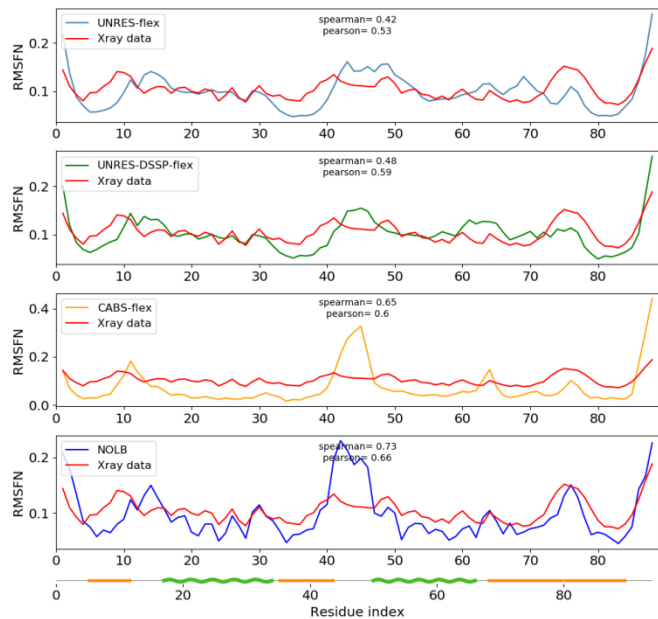
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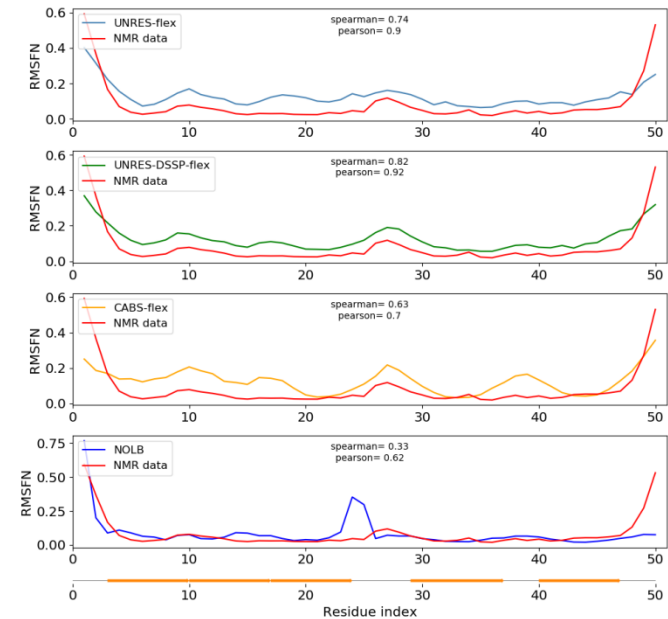
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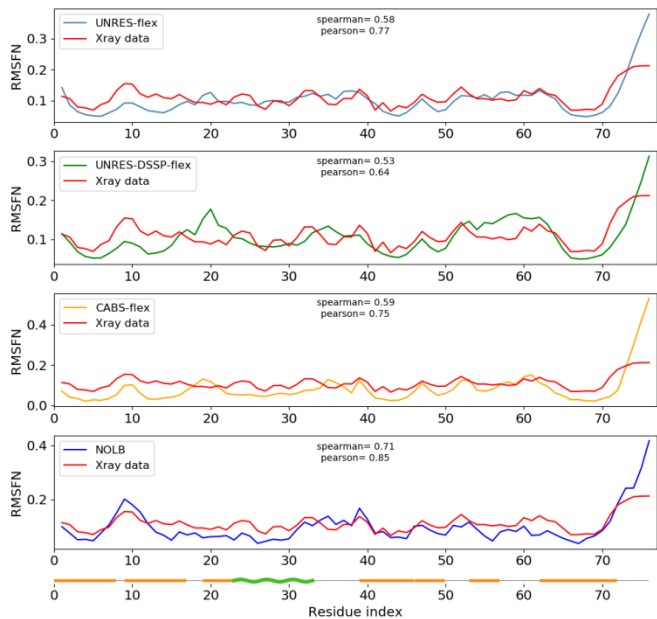
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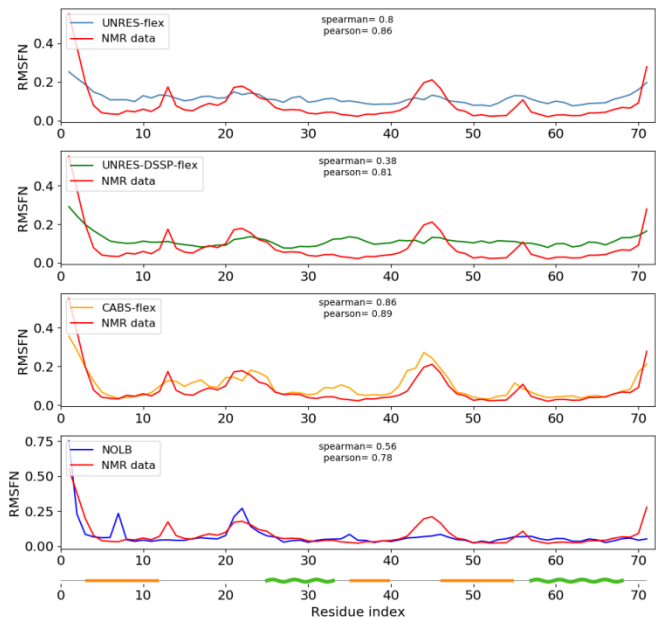
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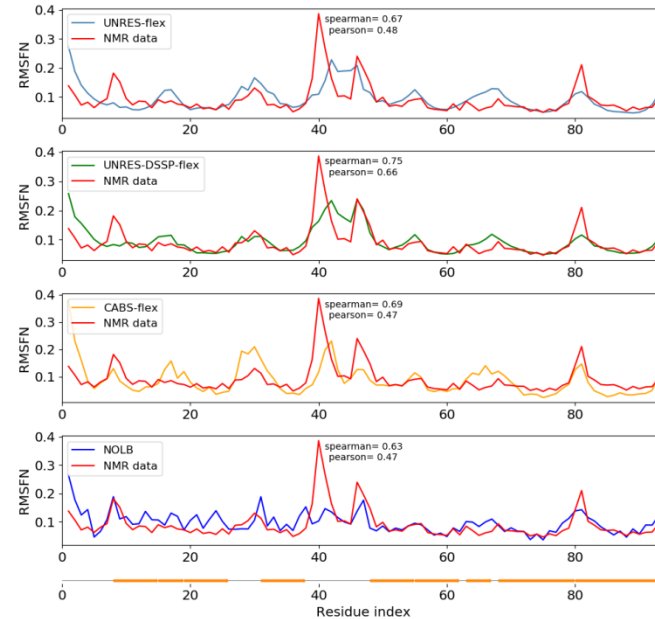
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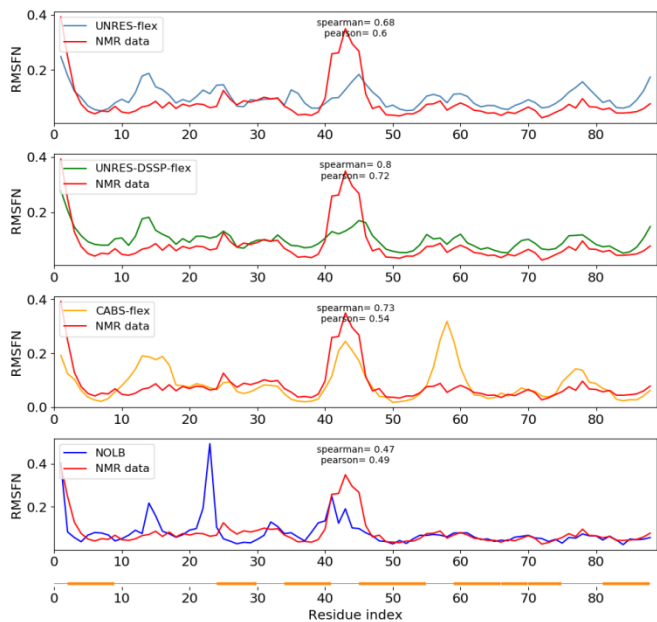
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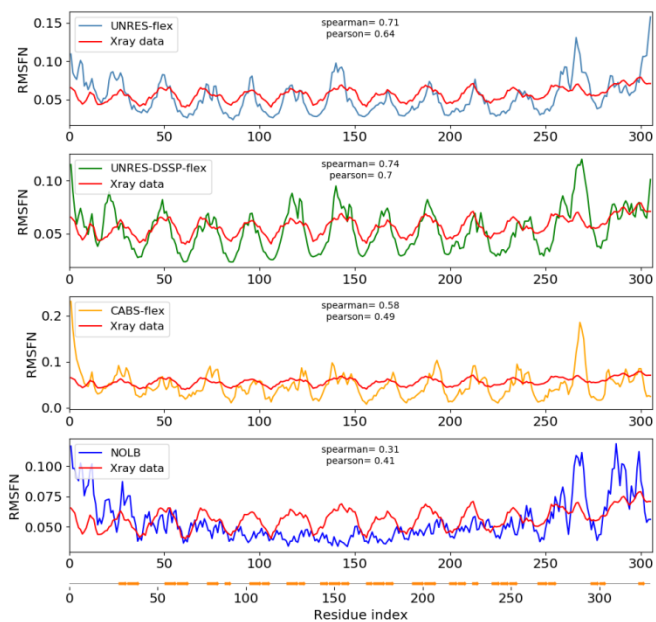
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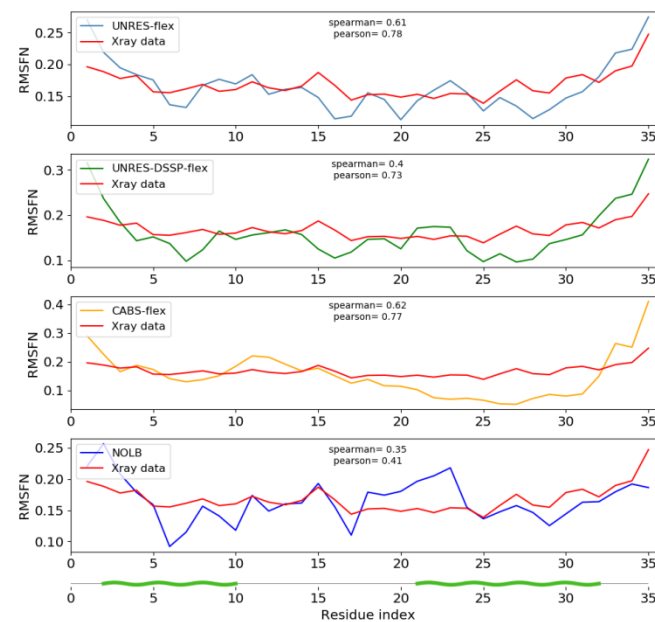
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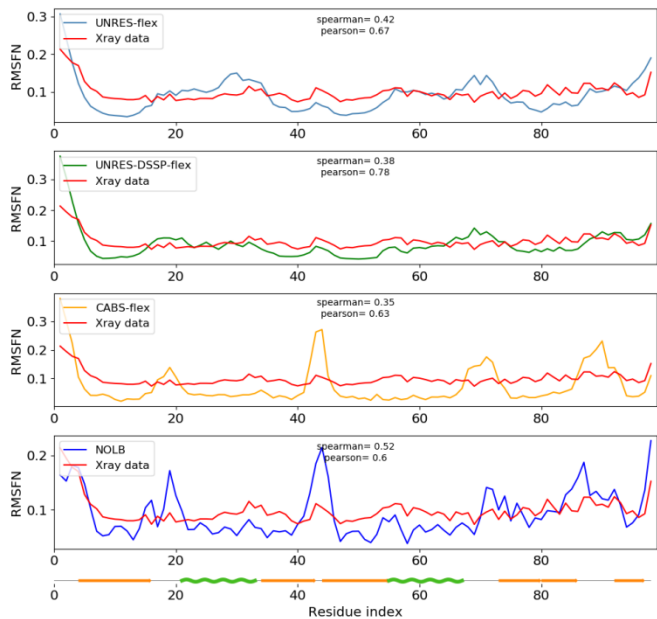
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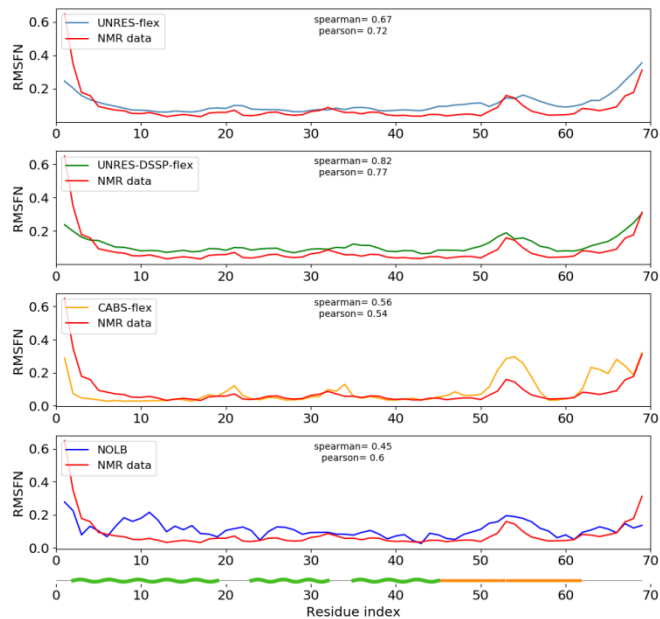
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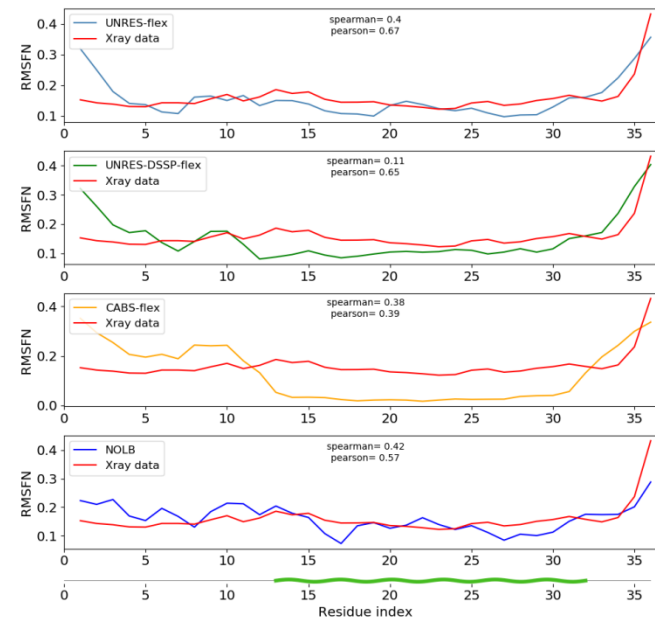
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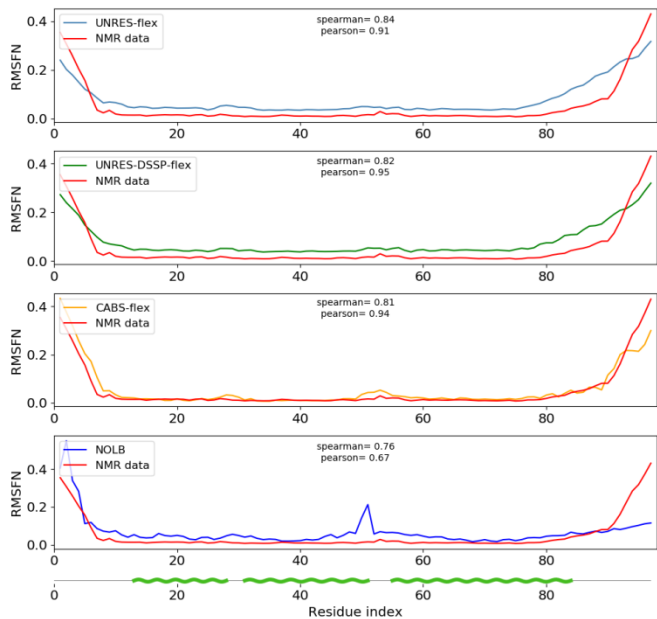
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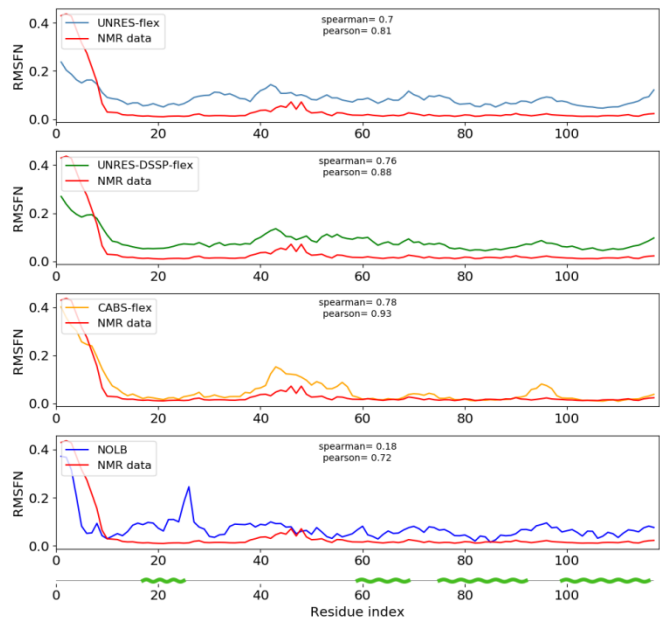
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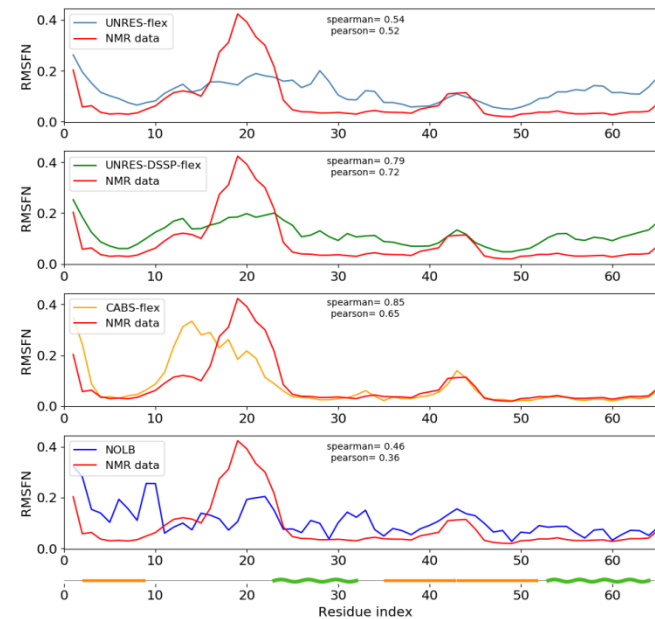
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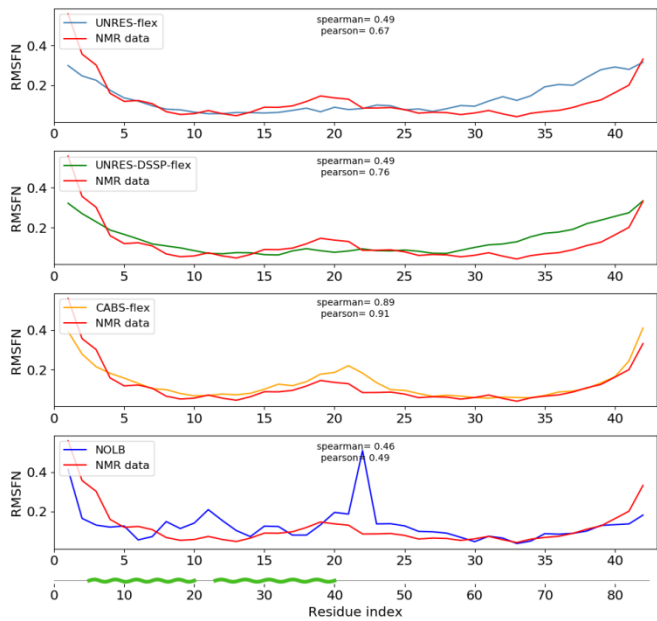
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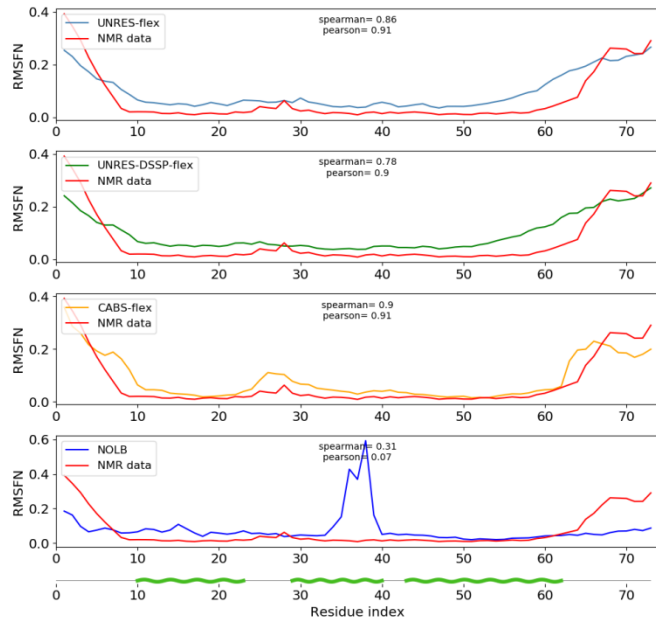
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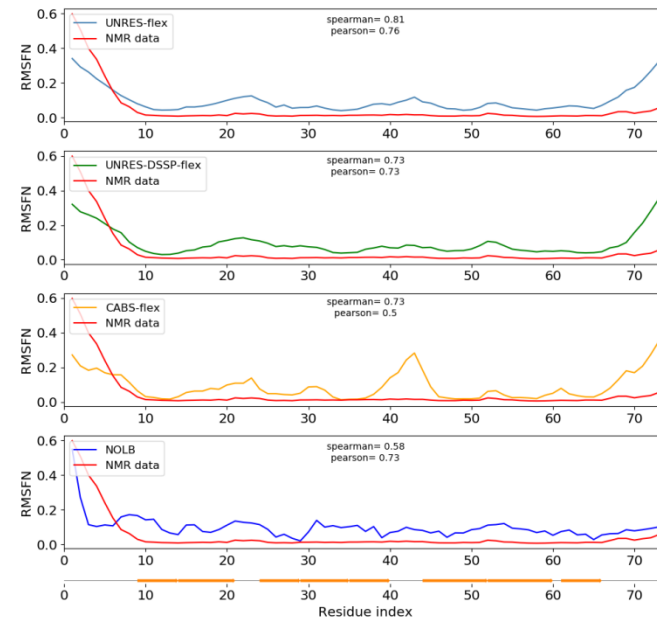
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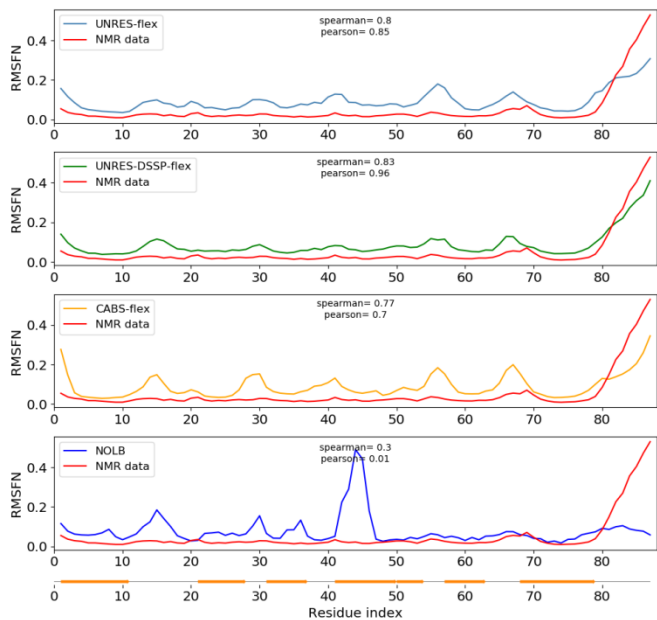
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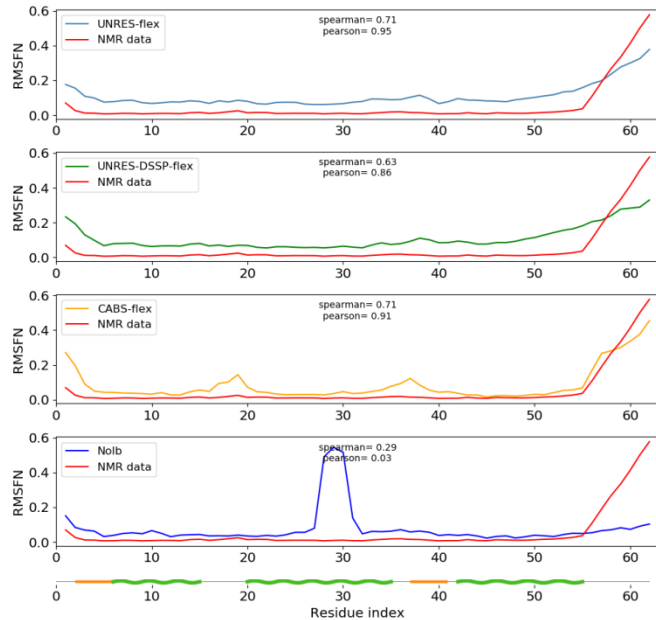
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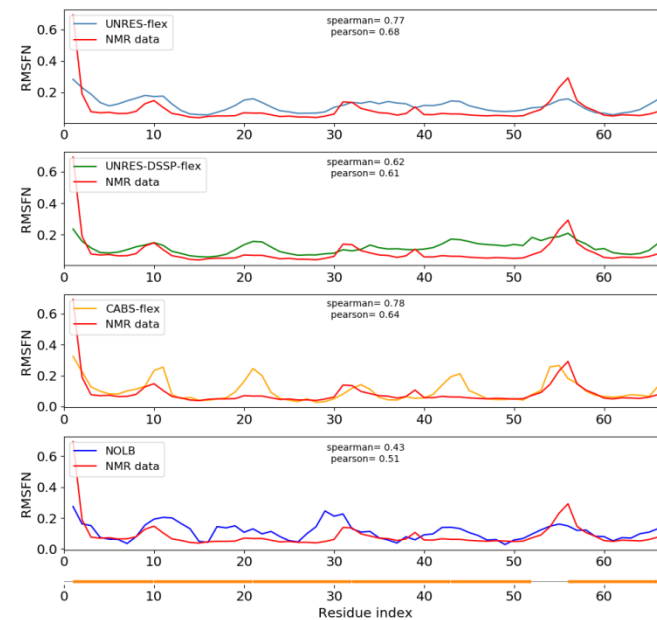
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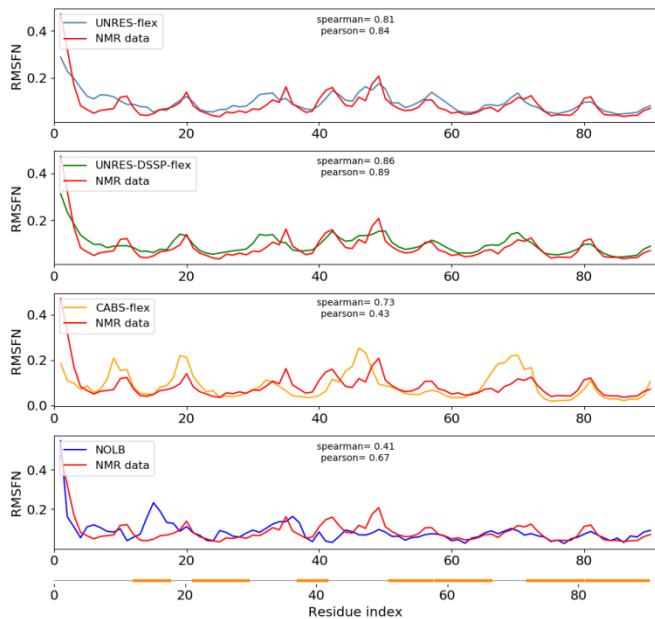
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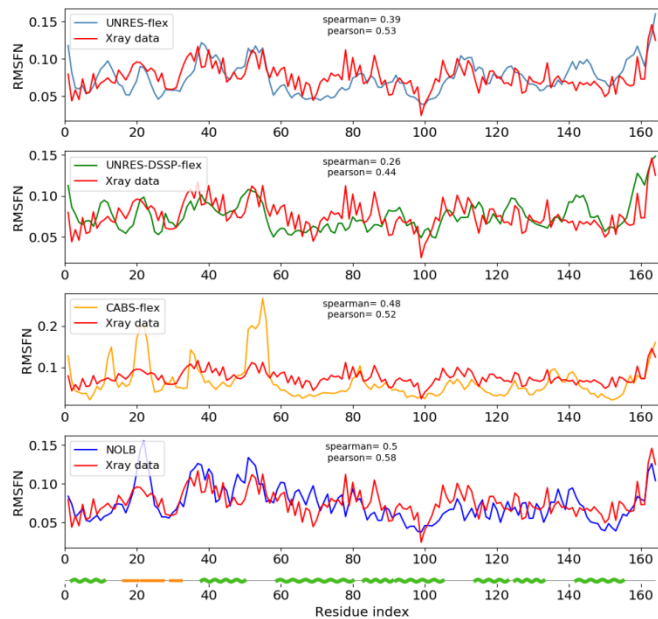
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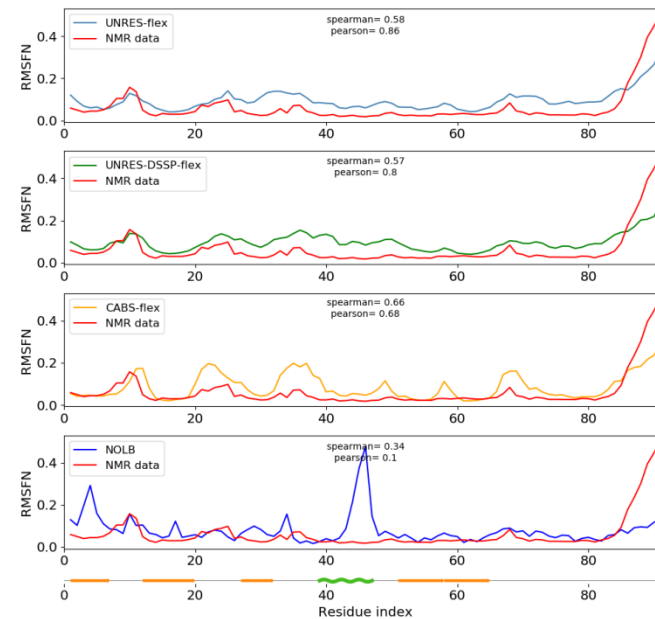
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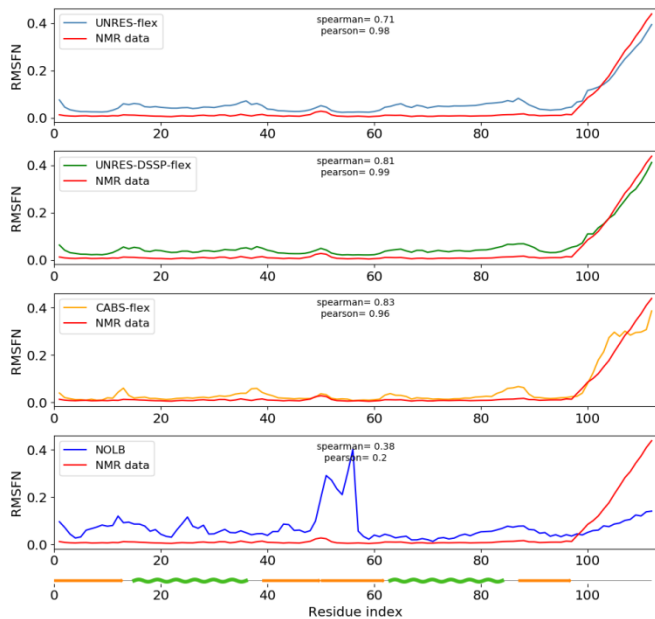
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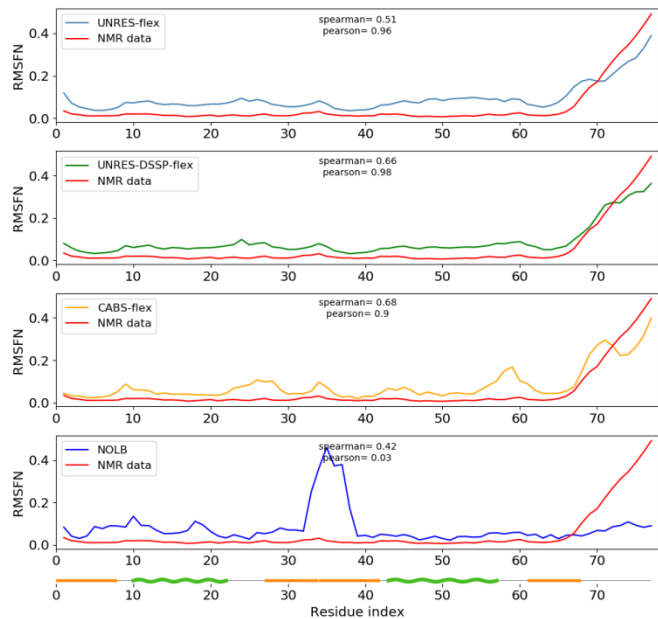
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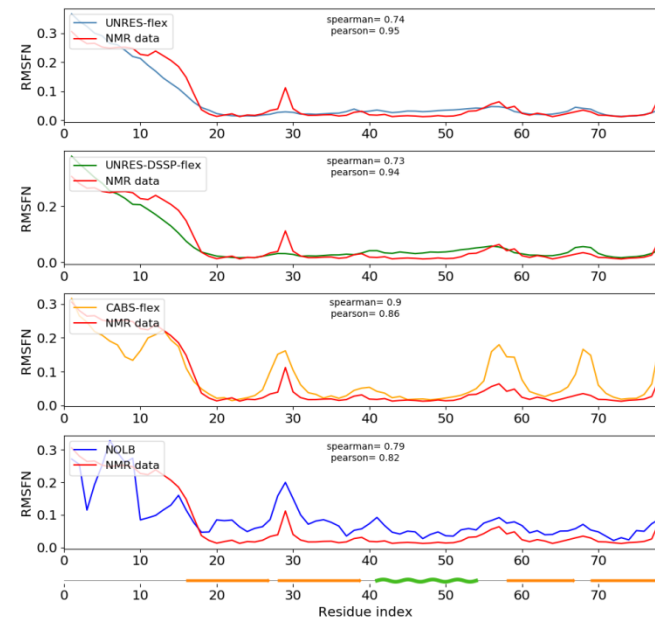
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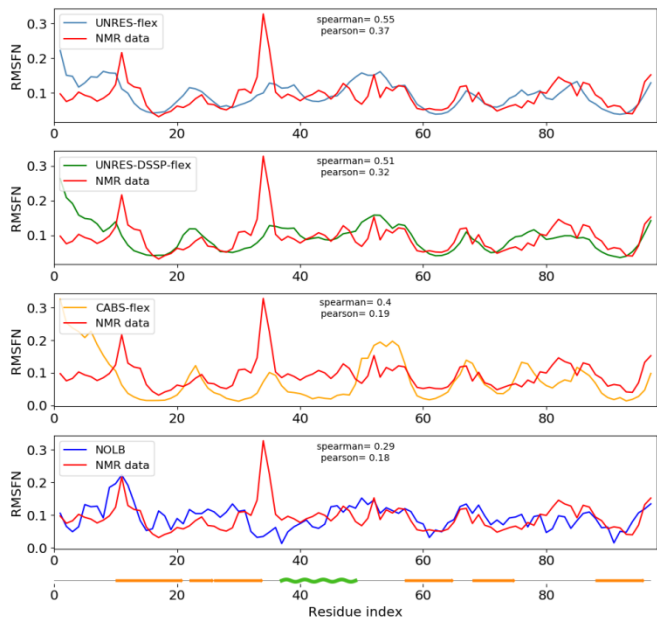
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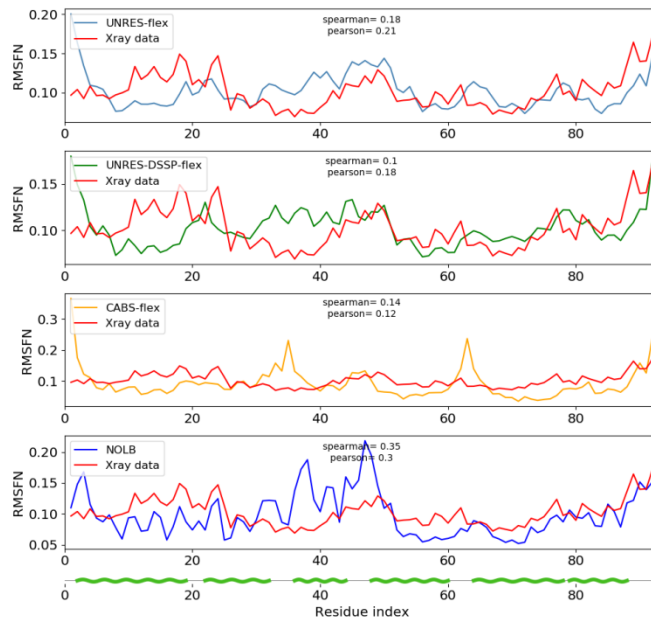
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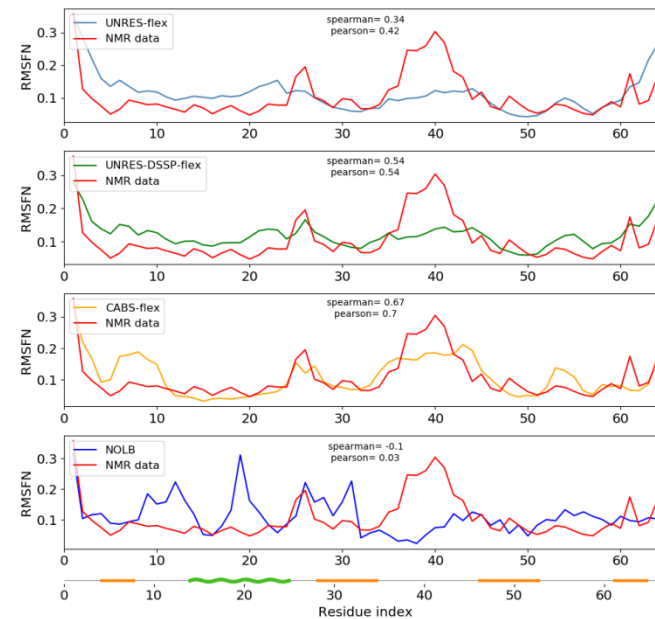
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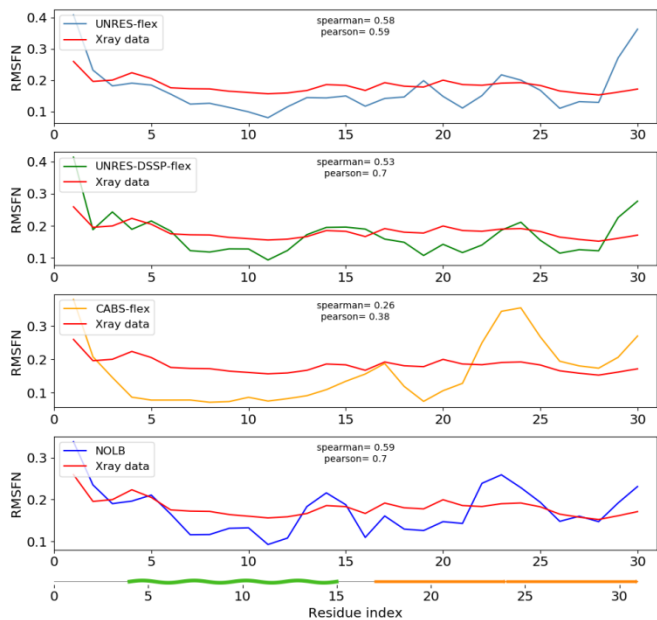
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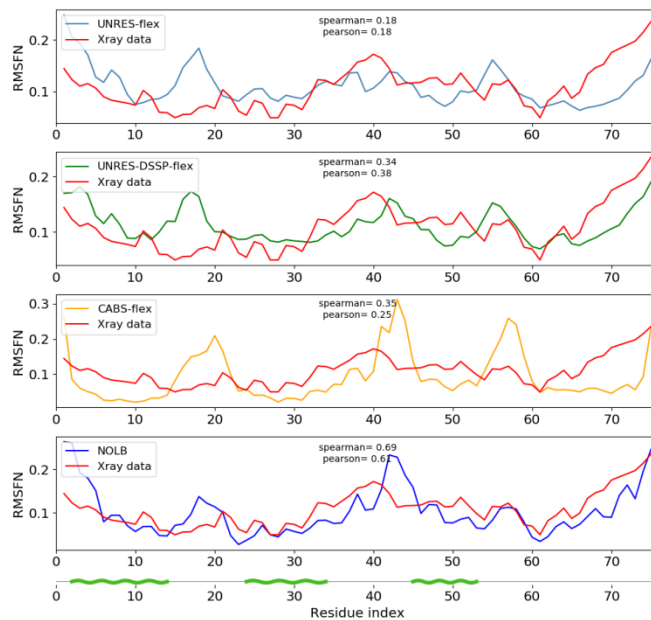
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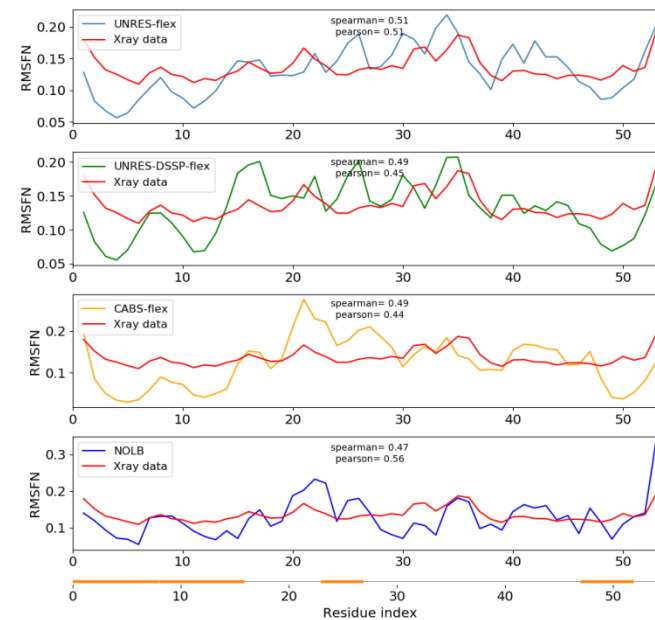
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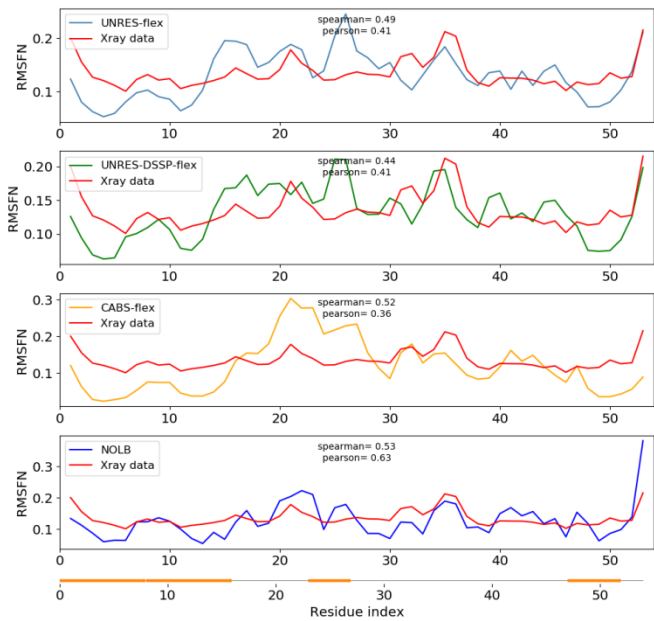
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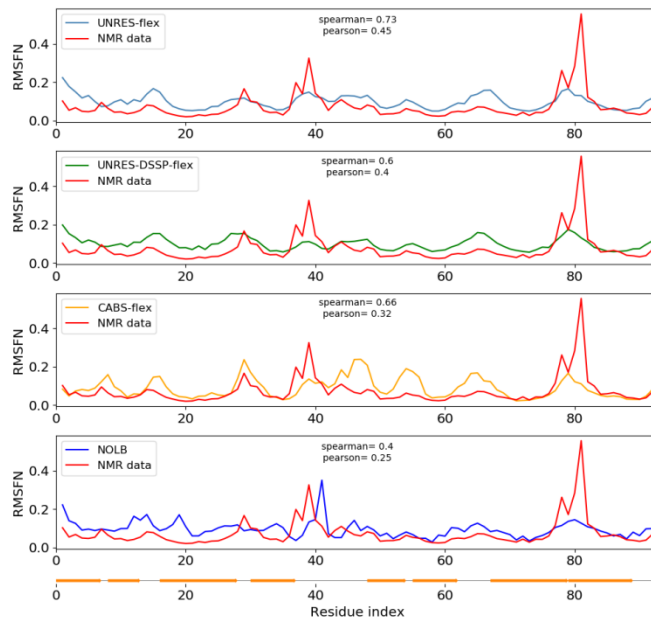
3KYW whole RMSFN profiles



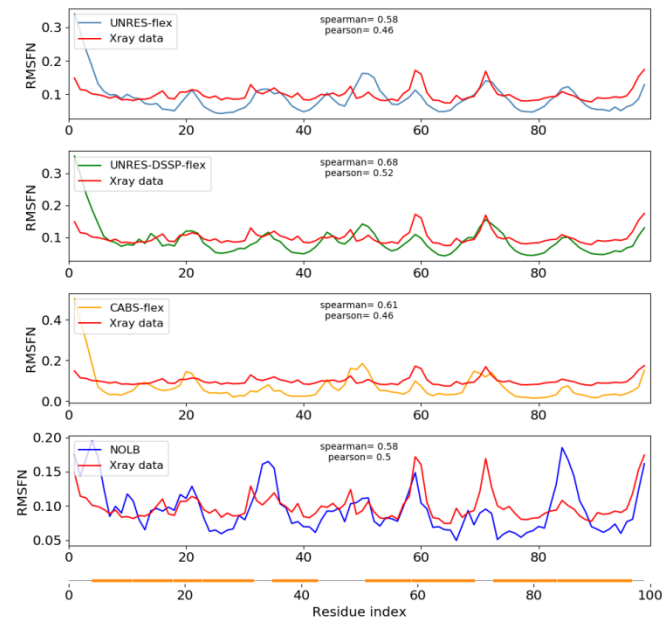
3KYY whole RMSFN profiles



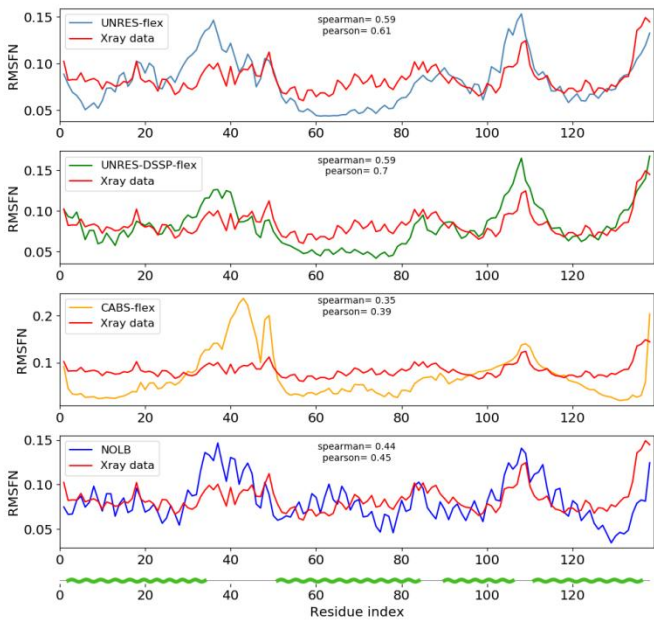
3NCM whole RMSFN profiles



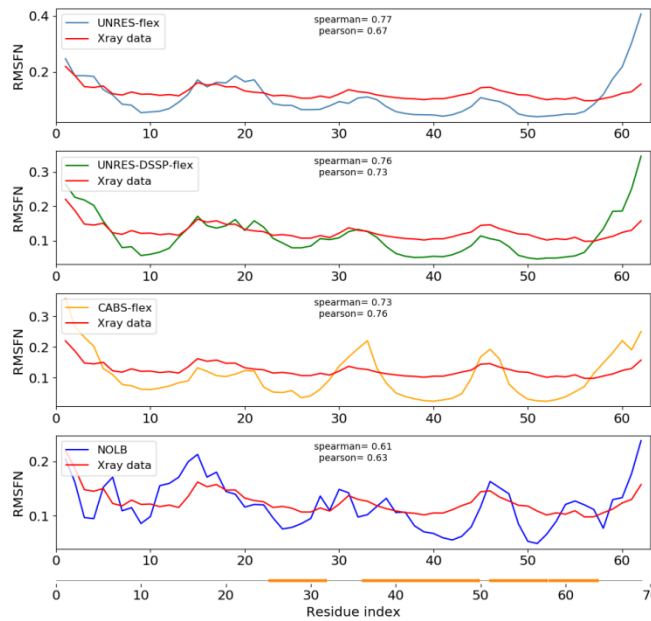
3PUC whole RMSFN profiles



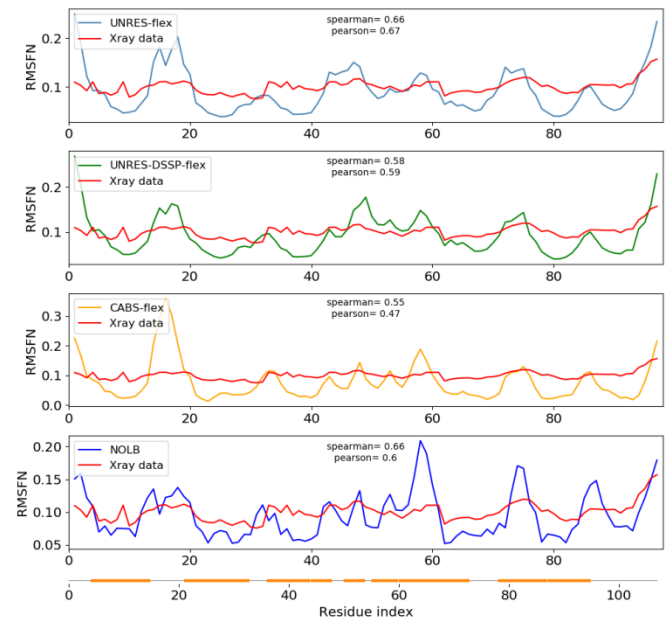
3WFW whole RMSFN profiles



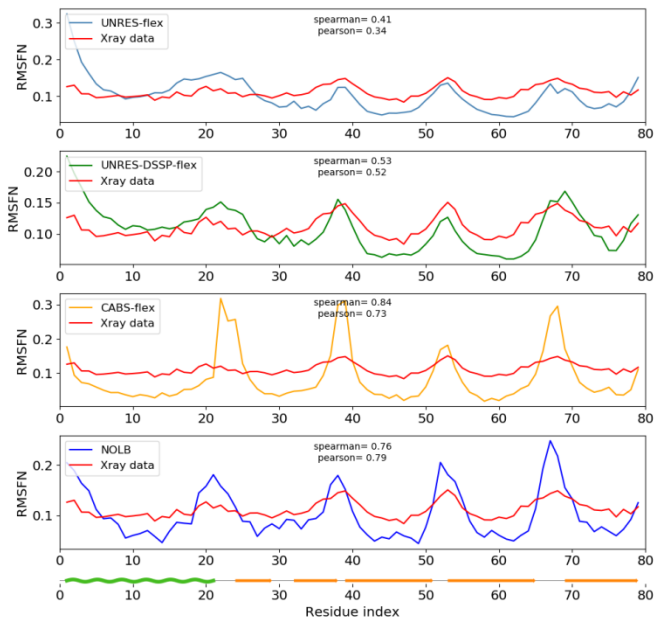
4F98 whole RMSFN profiles



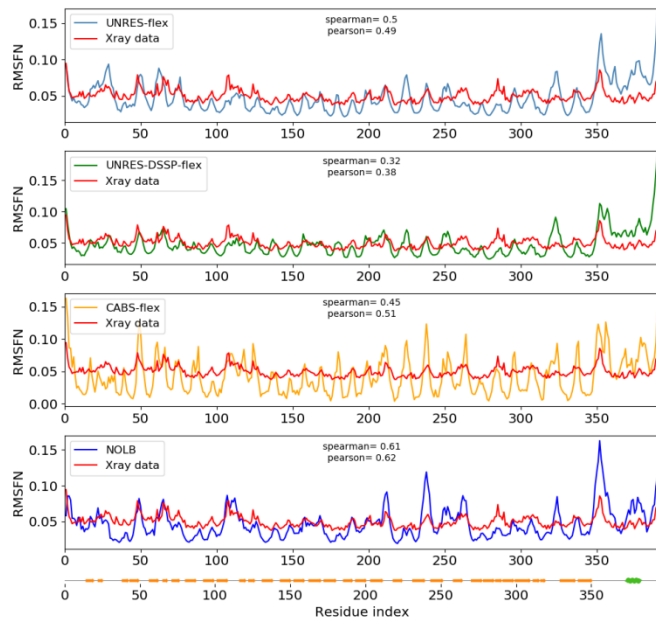
4M9O whole RMSFN profiles



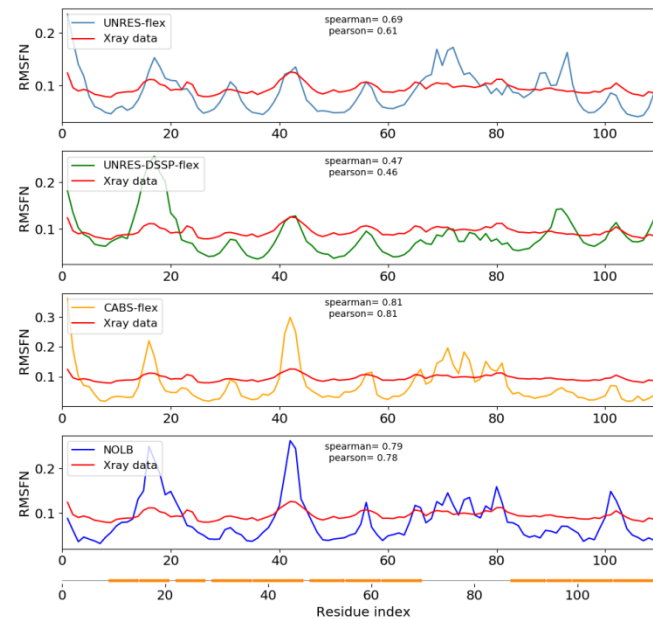
4N6T whole RMSFN profiles



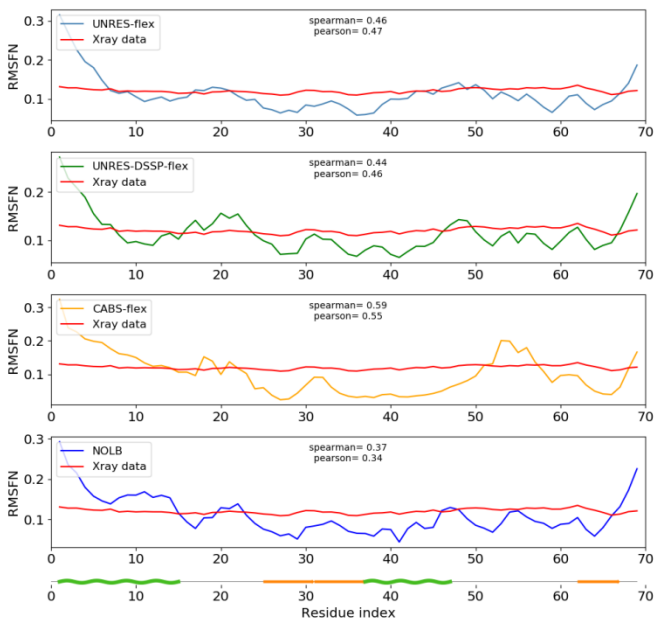
4OZU whole RMSFN profiles



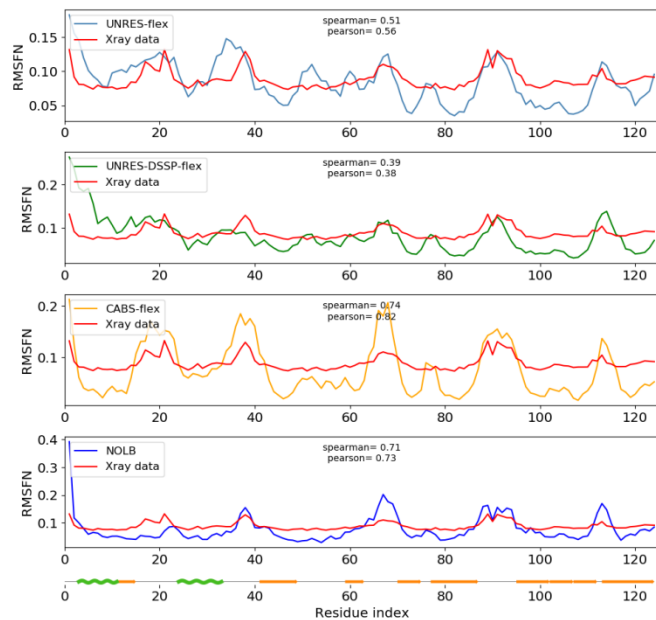
4QRL whole RMSFN profiles



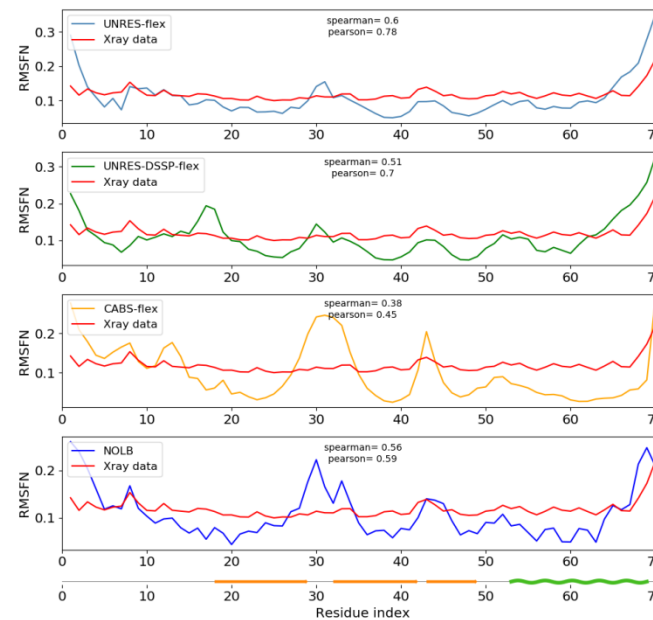
4R7E whole RMSFN profiles



4RTE whole RMSFN profiles



5D14 whole RMSFN profiles



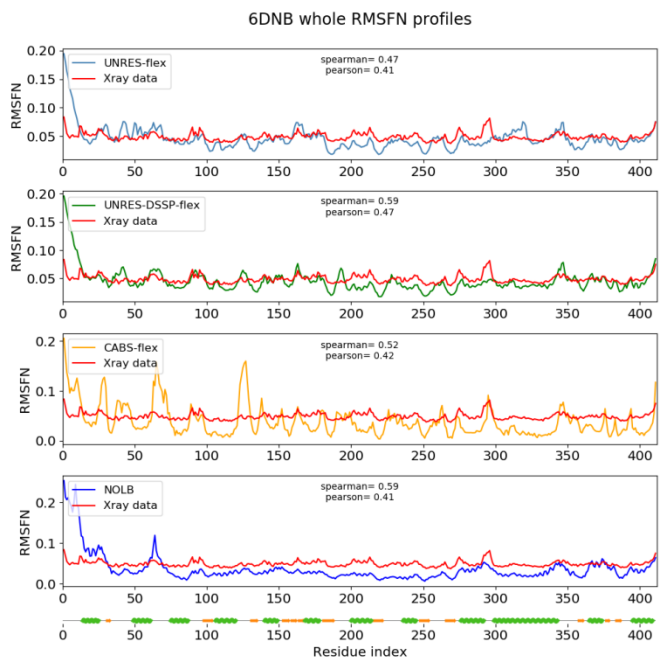
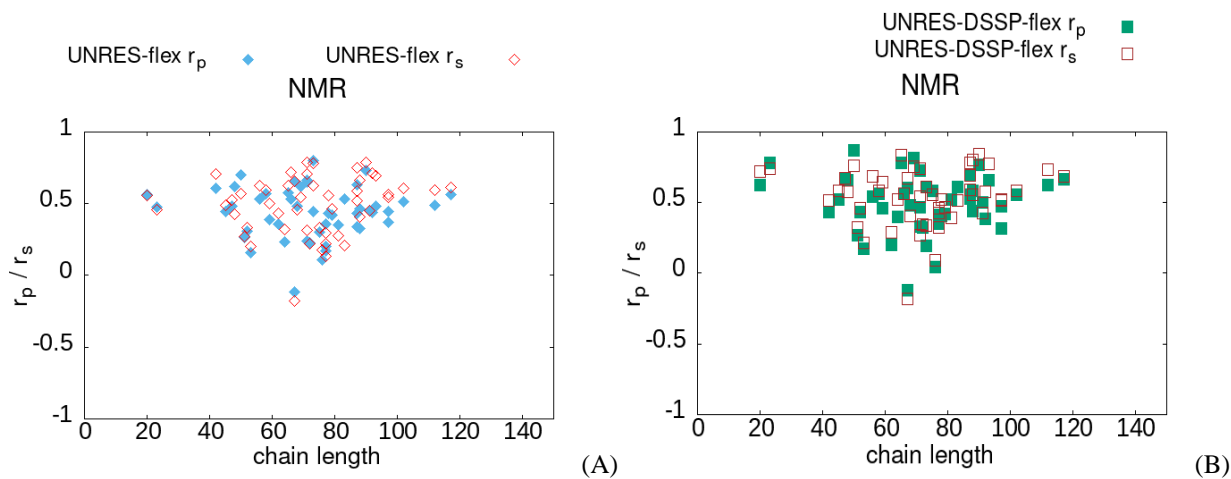
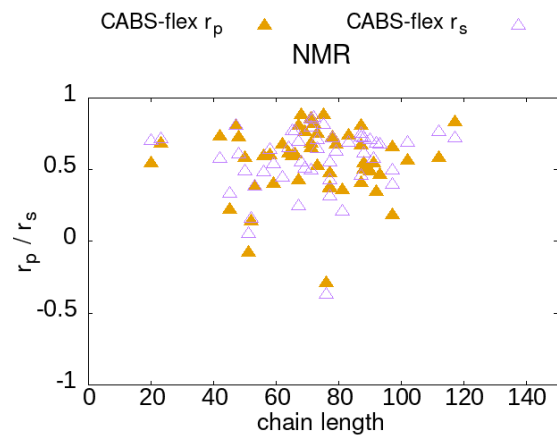
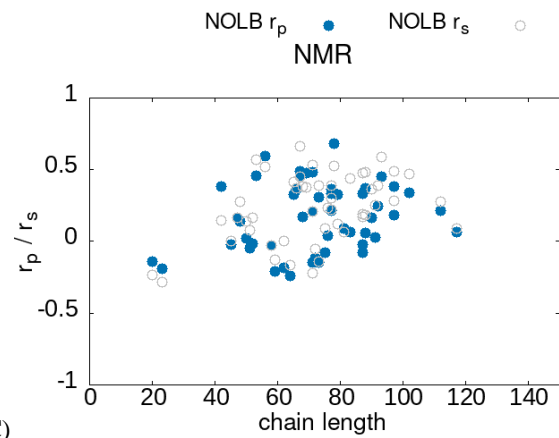


Figure S3. Scatter plots of the Pearson (r_p) and Spearman (r_s) coefficients between the experimental and predicted fluctuation profiles in chain length for the NMR (A-D) and X-ray (E-H) structures and the UNRES-flex (A, E), UNRES-DSSP-flex (B, F), CABS-flex (C,G), and NOLB (D, H) prediction methods.

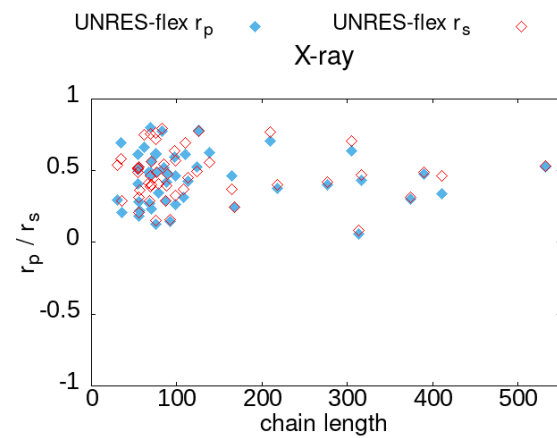




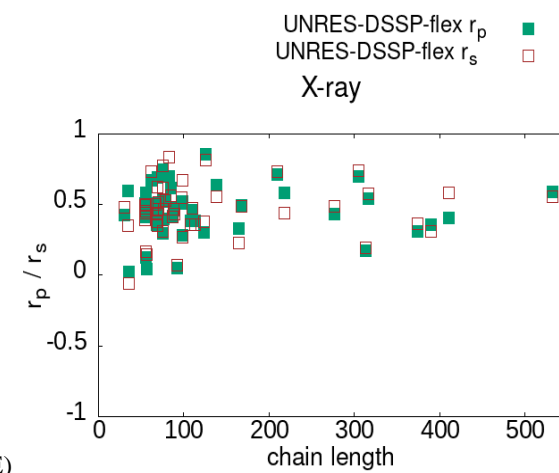
(C)



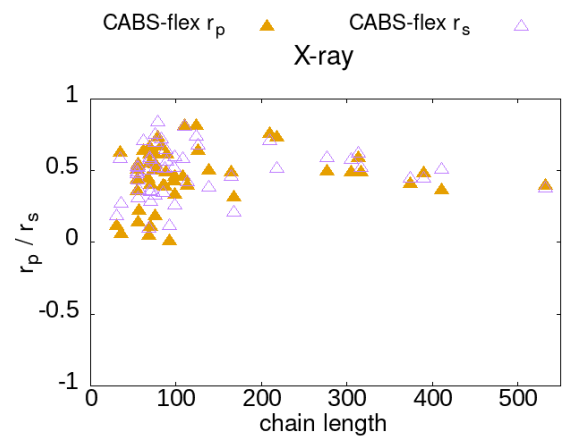
(D)



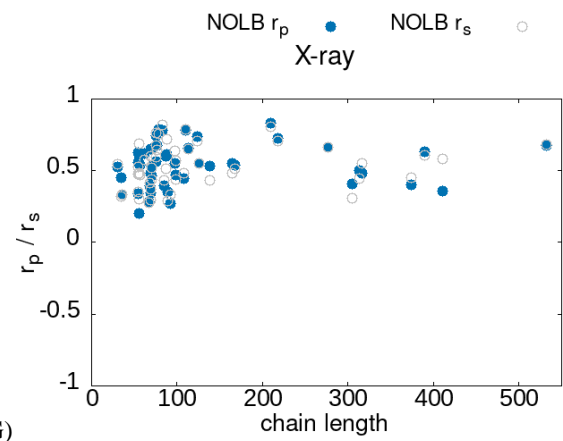
(E)



(F)



(G)



(H)