Appendix A. RMSDs of the mutants against their wild types

Protein ID	Mutation	Type[a]	RMSD (Å)	1st and 2nd largest deviations (Å)		Corresponding residues[b]		Resolution (Å)
T4 Lysozyme (wild type: 3lzm. ***Resolution- 1.7*** **)**								
220l	C54t, C97a, M102a	C-c, C-h, H-a	0.16	0.53	0.39	Asn 55	Ala 98	1.8
221l	A49s, C54t, C97a	H-c, C-c, C-h	0.112	0.32	0.25	Asn 40	Lys 43	1.7
222l	C54t, C97a, M102a	C-c, C-h, H-h	0.17	0.39	0.37	Arg 52	Gly 113	1.9
223l	L133g	H-g	0.212	0.89	0.43	Gly 113	Glu 22	1.9
224l	C54t, A93s, C97a	C-c, H-c, C-h	0.22	0.27	0.27	Val 57	Gly 77	1.8
227l	C54t, C97a, F104a	C-c, C-h, H-h	0.20	0.43	0.39	Asn 40	Thr 109	2.0
229l	C54t, R95a, C97a	C-c, C-h, C-h	0.18	0.33	0.31	Asn 40	Thr 109	1.8
230l	M6l, C54t, C97a	H-h, C-c, C-h	0.19	0.62	0.39	Arg 76	Thr 115	1.9
231l	C54t, C97a, M106k	C-c, C-h, H-c	0.21	0.56	0.48	Arg 76	Arg52	2.5
232l	C54t, C97a, M120k	C-c, C-h, H-c	0.18	0.42	0.36	Arg 76	Gly 113	1.7
233l	C54t, C97a, M120l	C-c, C-h, H-h	0.16	0.54	0.33	Gly 77	Asn 40	1.9
234l	C54t, C97a, M106l	C-c, C-h, H-h	0.18	0.52	0.49	Gly 77	Leu 106	1.9
235l	C54t, C97a, V111a	C-c, C-h, H-h	0.16	0.45	0.38	Gly 113	Arg 76	1.9
236l	C54t, V87a, C97a	C-c, H-h, C-h	0.12	0.49	0.44	Lys 83	Asn 40	1.9
237l	C54t, C97a, V149a	C-c, C-h, H-h	0.15	0.44	0.32	Arg 76	Asn 40	1.7
238l	C54t, C97a, V103a	C-c, C-h, H-h	0.17	0.56	0.38	Arg 76	Gly 113	1.8
239l	I17a, C54t, C97a	H-h, C-c, C-h	0.19	0.62	0.36	Pro 37	Gly 113	1.8
240l	I27a, C54t, C97a	H-h, C-c, C-h	0.17	0.40	0.36	Lys 16	Ala 49	1.7
241l	I29a, C54t, C97a	H-h, C-c, C-h	0.23	0.89	0.64	Leu 13	Ala 29	1.7
242l	I50a, C54t, C97a	H-h, C-c, C-h	0.16	0.40	0.35	Ala 50	Ser 38	1.8
243l	C54t, I58a, C97a	C-c, H-h, C-h	0.15	0.36	0.35	Asn 40	Ala 63	1.7
244l	C54t, C97a, I100a	C-c, C-h, H-h	0.20	0.59	0.44	Val 75	Ser 38	1.7
245l	M6a, C54t, C97a	H-h, C-c, C-h	0.17	0.55	0.36	Asn 40	Arg 76	1.8
246l	C54t, F67a, C97a	C-c, H-h, C-h	0.23	0.51	0.50	Asp 61	Asn 40	1.8
247l	C54t, L84a, C97a	C-c, H-h, C-h	0.37	2.25	0.43	Ala 112	Asn 40	1.7
248l	T27a, I29a, C54t, C97a	C-h, H-h, C-c, C-h	0.21	0.59	0.48	Lys 16	Ser 36	1.9
249l	I27a, C54t, I58a, C97a	H-h, C-c, H-h, C-h	0.19	0.49	0.34	Leu 46	Ala 93	1.9
250l	I29a, C54t, I58a, C97a	H-h, C-c, H-h, C-h	0.24	0.88	0.66	Leu 13	Ala 29	1.8
251l	C54t, C97a, L121a, L133a	C-c, C-h, H-h, H-h	0.38	1.10	1.20	Gly 113	Arg 54	2.6
253l	D20a C54t, C97a	C-h, C-c, C-h	0.17	0.42	0.32	Thr 21	Lys 16	2.0
254l	D20s, C54t, C97a	C-c, C-c, C-h	0.15	0.43	0.38	Gly 77	Asn 40	1.9
255l	D20n, C54t, C97a	C-c, C-c, C-h	0.13	0.36	0.33	Gly 77	Asn 40	1.8
256l	M6i	H-h	0.16	0.33	0.27	Asn 40	Gly 113	1.8
2l78	C54t, C97a, V111i	C-c, C-h, H-h	0.37	2.26	0.36	Gly 113	Glu 22	2.0
102l	Ins N40-a, C54t, C97a	Ins h, C-c, C-h	0.23	2.34		Asn 40		1.7
104l	Ins S44-aa, C54t, C97a	Ins h,h, C-c, C-h	1.24	6.48	1.31	Ala 41	Arg 76	2.8
107l	S44g, C54t, C97a	C-g, C-c, C-h	0.13	0.35	0.34	Asn 40	Gly 113	1.8
108l	S44i, C54t, C97a	C-h, C-c, C-h	0.11	0.24	0.23	Asn 40	Thr 15	1.8
109l	S44k, C54t, C97a	C-c, C-c, C-h	0.15	0.49	0.28	Gly 113	Gly 56	1.8
110l	S44l, C54t, C97a	C-h, C-c, C-h	0.15	0.57	0.26	Thr 15	Asn 53	1.7
111l	S44n, C54t, C97a	C-c, C-c, C-h	0.17	0.54	0.45	Gly 113	Ser 38	1.8
112l	S44p, C54t, C97a	C-h, C-c, C-h	0.15	0.67	0.20	Asn 40	Leu 79	1.8
113l	S44r, C54t, C97a	C-c, C-c, C-h	0.14	0.50	0.30	Gly 113	Thr 54	1.8
114l	S44t, C54t, C97a	C-c, C-c, C-h	0.11	0.28	0.25	Gly 77	Thr 54	1.8
115l	S44v, C54t, C97a	C-h, C-c, C-h	0.12	0.25	0.25	Gly 113	Val 44	1.8
118l	C54t, C97a, A130s	C-c, C-h, H-c	0.12	0.26	0.26	Gly 56	Gly 77	1.8
119l	C54t, C97a, A134s	C-c, C-h, H-c	0.12	0.31	0.21	Val 57	Gly 77	1.6
120l	A41s, C54t, C97a	H-c, C-c, C-c	0.14	0.37	0.29	Thr 54	Arg 76	1.8
122l	C54t, A73s, C97a	C-c, H-c, C-c	0.11	0.23	0.21	Asn 40	Ala 93	1.8
123l	C54t, A82s, C97a	C-c, H-c, C-c	0.13	0.29	0.25	Asn 40	Ala 93	1.8

125l	C54t, C97a, A98s	C-c, C-h, H-c	0.15	0.31	0.28	Asn 40	Gly 77	1.8
126l	C54t, C97a, V149t	C-c, C-h, H-c	0.14	0.30	0.22	Lys 43	Trp 58	1.8
127l	C54t, V75t, C97a	C-c, H-c, C-h	0.21	0.49	0.41	Thr 75	Glu 108	1.8
128l	C54t, V87t, C97a	C-c, H-c, C-h	0.16	0.34	0.33	Lys 83	Asn 53	1.7
129l	C54t, A93t, C97a	C-c, H-c, C-h	0.14	0.28	0.25	Asn 40	Gly 113	1.7
130l	C54t, C97a, T151s	C-c, C-h, C-c	0.14	0.35	0.25	Asn 40	Glu 108	1.7
131l	T26s, C54t, C97a	C-c, C-c, C-h	0.15	0.35	0.32	Asn 40	Thr 21	1.7
137l	S44f, C54t, C97a	C-h, C-c, C-h	0.53	1.22	1.20	Arg 137	Thr 21	1.8
138l	C54t, A93c, C97a	C-c, H-c, C-h	0.19	0.50	0.45	Cys 93	Asn 40	1.7
139l	C54t, N68c, A93c, C97a	C-c, C-c, H-c, C-h	0.19	0.39	0.36	Asn 40	Gly 77	1.7
140l	C54t, C97a, L121a, A129m, F153l	C-c, C-h, H-h, H-h, H-h	0.22	1.01	0.38	Gly 113	Arg 54	2.1
141l	C54t, C97a, L121a, A129m, V149i	C-c, C-h, H-h, H-h, H-h	0.17	0.47	0.33	Gly 113	Asn 40	2.0

Myoglobin (wild type 105m. ***Resolution- 2.0*****)**

101m	F46v, D122n	H-h, C-c	0.82	3.97	1.43	Gly 121	His 64	2.0
102m	H64a, D122n	C-h, C-c	0.84	3.86	1.59	Gly 121	Asp 60	1.8
106m	V68f, D122n	H-h, C-c	0.79	3.81	1.23	Gly 121	Glu 59	1.9
109m	D122n	C-p	0.80	3.96,	1.18	Gly 121	His 48	1.8
1ch1	L89g, D122n	H-g, C-c	0.80	3.77	1.06	Gly 121	His 48	1.9
1ch2	L89f, D122n	H-h, C-c	0.80	3.83	1.09	Gly 121	His 48	1.8
1ch3	L89w, D122n	H-c, C-c	0.78	3.84	0.84	Gly 121	His 48	2.0
1ch5	H97v, D122n	C-h, C-c	0.95	3.84	1.17	Gly 121	Val 97	2.1
1ch7	H97f, D122n	C-h, C-c	0.80	3.91	0.97	Gly 121	His 48	1.9
1ch9	H97q, D122n	C-c, C-c	0.80	3.71	1,18	Gly 121	His 48	1.8
1cik	I99a, D122n	H-h, C-c	0.92	3.96	1.02	Gly 121	Lys 16	1.7
1cio	I99v, D122n	H-h, C-c	0.79	3.77	1.05	Gly 121	His 48	1.6
1co8	L104a, D122n	H-h, C-c	0.79	3.77	1.09	Gly 121	His 48	1.8
1co9	L104v, D122n	H-h, C-c	0.78	3.75	1.07	Gly 121	His 48	1.6
1cp0	L104n, D122n	H-c, C-c	0.79	3.91	1.00	Gly 121	His 48	2.0
1cp5	L104f, D122n	H-h, C-c	0.77	3.77	1.10	Gly 121	His 48	2.1
1cpw	L104w, D122n	H-c, C-c	0.77	3.83	0.98	Gly 121	His 48	2.2
1fcs	H64v, T67r	C-h, C-c	0.83	3.99	0.88	Gly 121	His 48	1.6
1hrm	H93y	C-c	0.68	1.43,	1.11	Ala 94	Lys 42	1.7
1jdo	L29f, D122n	H-h, C-c	0.80	3.88	1.21	Gly 121	His 48	1.9
1ltw	L29w, D122n	H-c, C-c	0.80	3.99	1.06	Gly 121	His 48	1.7
1mcy	F29l, Q64h, D122n	H-h, C-c, C-c	0.81	3.90	1.27	Gly 121	His 48	1.7
1mdn	V68n	H-c	3.89	7.17	2.81	His 119	His 48	1.9
1mgn	H64y, D122n	C-c, C-c	0.84	3.85	1.37	Gly 121	His 48	1.9
1mlf	V68a, D122n	H-h, C-c	0.93	3.95	1.13	Gly 121	His 48	2.0
1mlj	V68f, D122n	H-h, C-c	0.93	3.77	1.31	Gly 121	His 48	2.0
1mlm	V68i, D122n	H-h, C-c	0.90	3.84	1.20	Gly 121	His 48	1.8
1mls	V68l, D122n	H-h, C-c	0.80	3.93	1.04	Gly 121	his 48	1.7
1mlu	H64g, V68a, D122n	C-g, H-h, C-c	0.98	3.88	1.33	Gly 121	Asp 60	1.9
1mnh	H64v, T67r	C-h, C-c	1.06	4.43	1.83	Gly 121	His 48	2.3
1mni	H64v, V68h	C-h, H-c	0.76	2.79	1.03	Gly 121	Phe 46	2.0
1mno	V68n	H-p	3.90	7.09	2.75	His 119	His 48	1.9
1moa	L29f, D122n	H-h, C-c	0.83	3.95	1.38	Gly 121	His 48	1.9
1mob	H64g, D122n	C-g, C-c	0.98	3.90	1.21	Gly 121	His 48	2.2
1moc	H64t, D122n	C-c, C-c	0.84	3.93	1.53	Gly 121	His 48	2.0
1mti	F46l, D122n	H-h, C-c	0.80	3.94	1.37	Gly 121	Asp 60	1.9
1mtj	F46v, D122n	H-h, C-c	0.85	3.92	1.59	Gly 121	Asp 60	1.7
1myh	K45r	C-c	0.88	3.09	0.86	Gly 121	Thr 95	1.9
1myi	K45s	C-c	0.72	2.65	1.03	Gly 121	Ser 45	2.0
1myj	V68t	H-c	0.86	2.75	1.91	Gly 121	Lys 45	1.9
1obm	L29f, H64q, V68f, D122n	H-h, P-p, H-h, C-p	0.83	3.86	1.54	Gly 121	Asp 60	1.8
1ofj	L29h, H64l, D122n	H-c, C-h, C-c	0.82	3.91	1.43	Gly 121	His 48	1.8
1ofk	F43h, H64l, D122n	H-c, C-h, C-c	0.81	3.83	1.40	Gly 121	His 48	1.8
1tes	D123n	C-c	0.79	3.93	1.19	Gly 121	His 48	1.7

1xch	L104n	H-c	0.62	0.97	0.82	Lys 45	Gln 91	1.7
1yca	V68t	H-c	0.76	2.84	0.92	Gly 121	Lys 45	2.2
2mgb	H64g, D122n	H-g, C-c	0.97	3.97	1.34	Gly 121	Asp 60	2.0
2mgc	H64l, D122n	C-h, C-c	0.84	3.97	1.31	Gly 121	His 48	1.9
2mgf	H64q, D122n	C-c, C-c	0.90	3.87	1.35	Gly 121	His 48	1.8
2mgi	H64t, D122n	C-c, C-c	0.85	3.91	1.58	Gly 121	Asp 60	2.0
2mgj	H64v, D122n	C-h, C-c	0.86	3.98	1.47	Gly 121	His 48	2.0
2mm1	K45r, C110a	C-c, C-c	0.84	2.79	1.47	Gly 121	Lys 16	2.8
2spm	L29f, D122n	H-h, C-c	0.80	4.04	0.89	Gly 121	Lys 16	1.7
2spo	L29v, D122n	H-h, C-c	0.84	3.74	1.16	Gly 121	His 48	1.7
Transthyretin (wild type: 1bmz A *Resolution- 2.0*)								
1tsh	A60t	H-c	0.24	0.80	0.52	Ser 85	Glu 63	1.7
1ttc	V30m	H-h	0.33	0.71	0.68	Met 30	Ser 100	1.7
1ttb	A109t	H-c	0.23	0.58	0.56	Cys 10	Ser 100	1.7
2trh	R10c	C-c	0.23	0.70	0.49	His 56	Ser 100	1.9
2try	S77y	C-c	0.26	0.70	0.58	Gly 101	Ser 100	2.0
1bzd	S6g	C-g	0.20	0.71	0.57	Ser 100	Glu 62	1.9
1bze	M119t	H-c	0.21	0.62	0.55	Ser 100	Gly 101	1.8
1bz8	delV122	del-h	0.91	5.29	4.66	Pro 102	Asp 99	2.0
1ttr	V122i	H-h	0.18	0.58	0.41	Ser 85	Ser 100	1.9
HIV aspartic proteinase (wild type: 1dif A *Resolution- 1.7*)								
1a30	Q7k, L33i, L63i	C-c,H-h,H-h	0.44	1.07	0.80	Pro 39	Gly 51	2.0
1axa	A28s	H-c	0.41	1.46	0.86	Ser 37	Gly 51	2.0
1az5	S4h	C-c	1.25	4.73	2.03	Pro 40	Phe 53	2.0
1gnm	V82d	H-c	0.41	1.06	0.98	Gly 51	Ser 37	2.3
1gnn	V82n	H-c	0.39	0.87	0.81	Ser 37	Gly 51	2.3
Barnase (wild type: 1a2p A *Resolution- 1.5*)								
1brh	L14a	H-h	0.10	0.46	0.34	Glu 60	Gly 40	2.0
1bne	A43c, S80c	H-c, C-c	3.79	5.07	4.88	Asn 41	Ala 32	2.1
1bnf	T70c, S92c	C-c, C-c	1.06	6.22	0.75	Gly 68	Gly 40	2.0
1bng	S85c, H102c	C-c, C-c	0.22	6.27	0.75	Gly 68	Gly 40	2.1
1bri	I76a	H-h	0.23	0.62	0.49	Ser 67	Gly 48	1.9
1brj	I88a	H-h	0.18	0.42	0.27	Lys 66	Gly 40	2.0
1brk	I96a	H-h	0.29	0.75	0.49	Ser 67	Gly 40	2.0
1b20	R69s	C-c	0.30	1.06	0.96	Lys 66	Arg 59	1.7
1b3s	H102a	C-h	0.50	1.84	0.96	Arg 59	Gln 104	2.3
1btu	K27a	C-h	0.50	1.27	0.72	Gln 104	Ser 67	1.6
Lactoferrin (wild type: 1bka *Resolution- 2.4*)								
1hse	H253m	C-h	0.49	1.87	1.67	Arg 313	Pro 284	2.2
1dsn	D60s	C-c	1.29	2.07	1.76	Ile 314	Gln 186	2.0
1vfd	R121e	C-c	0.67	3.01	1.67	Arg 313	Pro 284	2.3
1vfe	R121s	C-c	0.60	2.25	1.85	Arg 313	Gly 101	2.3
Dihydrofolate reductase (wild type: 4dfr A *Resolution- 1.7*)								
1dhi	D27S	C-c	0.23	0.88	0.58	Ser 135	Pro 66	1.9
1dhj	D27S, F137S	C-c, H-c	0.28	1.00	0.69	Val 136	Ser 27	1.8
1dra	D27e	C-c	0.25	0.85	0.54	Ser 135	Glu 27	1.9
1drb	D27c	C-c	0.29	0.97	0.85	Gly 67	Ser 135	1.9
2drc	W22f	C-h	0.18	0.50	0.43	Val 136	Gly 67	1.9
α-1-antitrypsin (wild type: 2psi *Resolution- 2.0*)								
1atu	F51l, T59a, T68a, A70g, M374i, S381a	H-h, C-h, C-h, C-g, H-h, C-h	2.19	9.37	7.57	Ala 355	Glu 354	2.7
1kct	T59a, T68a, A70g	C-h, C-h, H-g	2.60	13.37	12.11	Ala 350	Pro 357	3.4
1psi	F51l	H-h	0.30	3.60	0.69	Ala 348	Ala 350	2.9

BP-RNase A (wild type: 1rph *Resolution- 2.2*)								
1a5q	P93a	C-h	0.28	0.71	0.45	Lys 37	Ser 21	2.3
3rsk	K7a, R10a, K66a	C-h, C-h, C-h	0.34	1.48	0.60	Ser 89	Ser 22	2.0
3rsd	D121n	C-c	0.39	1.04	0.98	Asn 67	Gly 88, Ser 21	1.6
Adenylate kinase (wild type: 1ake A *Resolution- 1.9*)								
1dvr	D89v, R165i	C-h, C-h	12.74	27.78	22.35	Glu 113, Arg 128	Thr 158	2.3
3aky	I213f	H-h	12.19	27.56,	22.00	Glu 113, Thr 158	Arg 128	2.2
Calmodulin (wild type: 4cln *Resolution- 2.2*)								
1ahr	del-Thr 79, del-Asp 80	del H, del C	11.66	26.35	25.45	Asp 131	Gly 113	1.8
1deg	del-Glu 84	del C	10.93	22.00	19.43	Gly 113	Glu 127	2.9