

Appendix B. B-factors of the largest deviated residues

Protein	Mutation	Position of largest deviation	Corresponding B-factor	Largest B-factor	Corresponding residue
T4 Lysozyme (wild type: 3lzm)					
220l	C54t, C97a, M102a	Asn 55	67.28	67.28	Asn 55
221l	A49s, C54t, C97a	Asn 40	35.36	66.55	Lys 162
222l	C54t, C97a, M102a	Arg 52	36.14	62.54	Lys 162
223l	L133g	Gly 113	37.99	87.24	Asn 55
224l	C54t, A93s, C97a	Val 57	22.70	56.23	Lys 162
227l	C54t, C97a, F104a	Asn 40	29.96	54.42	Lys 162
229l	C54t, R95a, C97a	Asn 40	25.11	57.56	Lys 162
230l	M6l, C54t, C97a	Arg 76	22.45	41.61	Asn 55
231l	C54t, C97a, M106k	Arg 76	22.21	57.70	Lys 162
232l	C54t, C97a, M120k	Arg 76	16.93	37.76	Lys 162
233l	C54t, C97a, M120l	Gly 77	8.58	45.38	Lys 162
234l	C54t, C97a, M106l	Gly 77	14.36	43.82	Asn 55
235l	C54t, C97a, V111a	Gly 113	29.95	68.89	Lys 162
236l	C54t, V87a, C97a	Lys 83	31.06	65.42	Lys 162
237l	C54t, C97a, V149a	Arg 76	22.14	51.25	Lys 162
238l	C54t, C97a, V103a	Arg 76	16.39	55.04	Lys 162
239l	I17a, C54t, C97a	Pro 37	65.77	100.00	Asn 55
240l	I27a, C54t, C97a	Lys 16	22.44	50.72	Lys 162
241l	I29a, C54t, C97a	Leu 13	22.92	76.84	Lys 162
242l	I50a, C54t, C97a	Ala 50	18.01	52.12	Lys 162
243l	C54t, I58a, C97a	Asn 40	31.98	67.62	Lys 162
244l	C54t, C97a, I100a	Val 75	20.73	52.29	Lys 162
245l	M6a, C54t, C97a	Asn 40	31.93	51.24	Lys 162
246l	C54t, F67a, C97a	Asp 61	10.17	55.98	Lys 162
247l	C54t, L84a, C97a	Ala 112	58.13	78.14	Thr 109
248l	T27a, I29a, C54t, C97a	Lys 16	21.12	52.40	Lys 35
249l	I27a, C54t, I58a, C97a	Leu 46	14.90	53.21	Lys 162
250l	I29a, C54t, I58a, C97a	Leu 13	19.90	61.32	Lys 162
251l	C54t, C97a, L121a, L133a	Gly 113	48.75	73.15	Lys 124
253l	D20a, C54t, C97a	Thr 21	38.16	51.70	Lys 162
254l	D20s, C54t, C97a	Gly 77	10.95	46.49	Lys 162
255l	D20n, C54t, C97a	Gly 77	14.81	48.93	Lys 162
256l	M6i	Asn 40	32.64	86.82	Asn 163
2178	C54t, C97a, V111i	Gly 113	19.64	47.87	Glu 108
102l	Ins N40-a, C54t, C97a	Asn 40	48.90	100.00	Ser 36
104l	Ins S44-aa, C54t, C97a	Ala 41	64.31	79.89	Thr 115
107l	S44g, C54t, C97a	Asn 40	47.10	50.87	Ser 36
108l	S44i, C54t, C97a	Asn 40	25.45	42.98	Lys 162
109l	S44k, C54t, C97a	Gly 113	25.45	40.40	Asn 55
110l	S44l, C54t, C97a	Thr 15	11.87	42.54	Lys 162
111l	S44n, C54t, C97a	Gly 113	36.60	44.94	Lys 162
112l	S44p, C54t, C97a	Asn 40	45.44	45.44	Asn 40
113l	S44r, C54t, C97a	Gly 113	27.49	46.14	Lys 162
114l	S44t, C54t, C97a	Gly 77	15.90	43.19	Lys 162
115l	S44v, C54t, C97a	Gly 113	14.35	46.04	Lys 162
118l	C54t, C97a, A130s	Gly 56	17.78	34.82	Lys 162
119l	C54t, C97a, A134s	Val 57	16.64	48.61	Lys 162

120l	A41s, C54t, C97a	Thr 54	18.46	36.26	Ser 36
122l	C54t, A73s, C97a	Asn 40	22.10	37.29	Lys 162
123l	C54t, A82s, C97a	Asn 40	23.52	44.73	Lys 162
125l	C54t, C97a, A98s	Asn 40	23.83	38.86	Lys 162
126l	C54t, C97a, V149t	Asn 40	25.10	49.27	Lys 162
127l	C54t, V75t, C97a	Thr 75	15.17	35.47	Ser 36
128l	C54t, V87t, C97a	Lys 83	31.90	39.05	Ser 36
129l	C54t, A93t, C97a	Asn 40	29.10	51.70	Ser 36
130l	C54t, C97a, T151s	Asn 40	28.68	56.14	Lys 162
131l	T26s, C54t, C97a	Asn 40	23.85	51.76	Lys 162
137l	S44f, C54t, C97a	Arg 137	21.29	40.23	Thr 109
138l	C54t, A93c, C97a	Cys 93	10.57	73.79	Asn 55
139l	C54t, N68c, A93c, C97a	Asn 40	33.69	60.78	Lys 162
140l	C54t, C97a, L121a, A129m, F153l	Gly 113	37.17	64.96	Lys 162
141l	C54t, C97a, L121a, A129m, V149i	Gly 113	22.32	84.29	Asn 55

Myoglobin (wild type 105m)

101m	F46v, D122n	Gly 121	19.49	47.07	Gly 153
102m	H64a, D122n	Gly 121	15.19	40.00	Gly 153
106m	V68f, D122n	Gly 121	14.17	43.92	Gly 153
109m	D122n	Gly 121	15.02	40.60	Gly 153
1ch1	L89g, D122n	Gly 121	20.13	66.99	Gly 153
1ch2	L89f, D122n	Gly 121	17.19	54.60	Gln 152
1ch3	L89w, D122n	Gly 121	22.61	68.13	Gln 152
1ch5	H97v, D122n	Gly 121	24.10	55.71	Gln 152
1ch7	H97f, D122n	Gly 121	13.46	56.69	Gln 152
1ch9	H97q, D122n	Gly 121	17.69	67.63	Gln 152
1cik	I99a, D122n	Gly 121	18.17	95.10	Gly 153
1cio	I99v, D122n	Gly 121	14.73	69.22	Gly 153
1co8	L104a, D122n	Gly 121	19.72	83.40	Gly 153
1co9	L104v, D122n	Gly 121	18.04	70.97	Gly 153
1cp0	L104n, D122n	Gly 121	21.79	94.44	Gly 153
1cp5	L104f, D122n	Gly 121	19.96	86.15	Gly 153
1cpw	L104w, D122n	Gly 121	17.91	96.68	Gly 153
1fcs	H64v, T67r	Gly 121	15.85	76.73	Gly 153
1hrm	H93y	Ala 94	17.79	58.39	Gly 153
1jdo	L29f, D122n	Gly 121	18.39	83.90	Gln 152
1ltw	L29w, D122n	Gly 121	18.30	50.30	Gly 153
1mcy	F29l, Q64h, D122n	Gly 121	21.40	52.20	Gly 153
1mdn	V68n	His 119	21.42	79.17	Gly 153
1mgn	H64y, D122n	Gly 121	16.20	45.40	Gly 153
1mlf	V68a, D122n	Gly 121	16.00	55.90	Gly 153
1mlj	V68f, D122n	Gly 121	15.60	49.60	Gly 153
1mlm	V68i, D122n	Gly 121	17.00	48.80	Gly 153
1mls	V68l, D122n	Gly 121	15.10	46.10	Gly 153
1mlu	H64g, V68a, D122n	Gly 121	16.80	56.00	Gly 153
1mnh	H64v, T67r	Gly 121	4.67	56.50	Gly 1
1mni	H64v, V68h	Gly 121	31.28	82.25	Gly 153
1mno	V68n	His 119	21.19	74.52	Gly 153
1moa	L29f, D122n	Gly 121	16.80	43.40	Gly 153
1mob	H64g, D122n	Gly 121	19.10	54.20	Gly 153
1moc	H64t, D122n	Gly 121	18.40	49.30	Gly 153
1mti	F46l, D122n	Gly 121	13.00	42.70	Gly 153
1mtj	F46v, D122n	Gly 121	18.60	49.40	Gly 153
1myh	K45r	Gly 121	31.16	65.06	Gly 153
1myi	K45s	Gly 121	38.88	79.92	Gly 153

1myj	V68t	Gly 121	27.44	76.92	Gly 153
1obm	L29f, H64q, V68f, D122n	Gly 121	14.30	39.90	Gly 153
1ofj	L29h, H64l, D122n	Gly 121	15.80	50.32	Gly 153
1ofk	F43h, H64l, D122n	Gly 121	17.20	50.90	Gly 153
1tes	D123n	Gly 121	18.00	43.90	Gly 154
1xch	L104n	Lys 45	24.85	52.18	Gly 153
1yca	V68t	Gly 121	24.98	39.38	Gly 153
2mgb	H64g, D122n	Gly 121	18.50	54.50	Gly 153
2mgc	H64l, D122n	Gly 121	15.10	36.60	Gly 153
2mgf	H64q, D122n	Gly 121	17.90	52.30	Gly 153
2mgi	H64t, D122n	Gly 121	17.90	48.70	Gly 153
2mgj	H64v, D122n	Gly 121	19.10	49.30	Gly 153
2mm1	K45r, C110a	Gly 121	14.71	40.99	Gly 153
2spm	L29f, D122n	Gly 121	16.60	44.90	Gly 153
2spo	L29v, D122n	Gly 121	17.00	46.90	Gly 153

Transthyretin (wild type: 1bmz A)

1tsh	A60t	Ser 85	30.84	69.03	Pro 102
1ttc	V30m	Met 30	15.88	40.00	Gly 1
1ttb	A109t	Cys 10	30.43	53.79	Gly 1
2trh	R10c	His 56	22.18	58.17	Gly 101
2try	S77y	Gly 101	19.16	49.59	Pro 102
1bzd	S6g	Ser 100	36.54	68.21	Pro 102
1bze	M119t	Ser 100	38.87	64.43	Glu 7
1bz8	delV122	Pro 102	58.23	66.58	Pro 102
1ttr	V122i	Ser 85	23.98	85.88	Ser 8

HIV aspartic proteinase (wild type: 1dif A)

1a30	Q7k, L33i, L63i	Pro 39	36.09	47.71	Gly 68
1axa	A28s	Ser 37	53.17	61.13	Pro 1
1az5	S4h	Pro 40	21.87	84.97	Gly 52
1gnm	V82d	Gly 51	20.36	30.76	Arg 41
1gnn	V82n	Ser 37	29.00	38.61	Arg 41

Barnase (wild type: 1a2p A)

1brh	L14a	Glu 60	35.95	35.95	Glu 60
1bne	A43c, S80c	Asn 41	15.11	28.85	Ser 67
1bnf	T70c, S92c	Gly 68	27.82	32.00	Ser 67
1bng	S85c, H102c	Gly 68	28.08	32.00	Ser 67
1bri	I76a	Ser 67	24.36	33.46	Ser 67
1brj	I88a	Lys 66	38.10	42.37	Glu 60
1brk	I96a	Ser 67	30.19	30.19	Ser 67
1b20	R69s	Lys 66	31.39	35.08	Gln 2
1b3s	H102a	Arg 59	30.35	59.40	Gln 62
1b2u	K27a	Gln 104	22.69	59.76	Ala 32

Lactoferrin (wild type 1bka)

1hse	H253m	Arg 313	76.79	86.29	Pro 142
1dsn	D60s	Ile 314	79.73	80.00	Thr 139
1vfd	R121e	Arg 313	52.43	80.00	Pro 142
1vfe	R121s	Arg 313	38.76	57.38	Thr 139

Dihydrofolate reductase (wild type 4dfr A)

1dhi	D27S	Ser 135	37.01	83.19	Pro 130
1dhj	D27S, F137S	Val 136	36.63	81.73	Pro 130
1dra	D27e	Ser 135	44.43	72.25	Pro 130
1drb	D27c	Gly 67	63.43	70.58	Pro 130
2drc	W22f	Val 136	40.90	70.08	Pro 130

α -1-antitrypsin (wild type: 2psi)

1atu	F51l, T59a, T68a, A70g, M374i, S381a	Ala 355	22.34	33.08	Leu 353
1kct	T59a, T68a, A70g	Ala 350	20.00	20.00	His 20
1psi	F51l	Ala 348	34.53	73.90	Lys 394

BP-RNase A (wild type: 1rph)

1a5q	P93a	Lys 37	71.92	98.33	Tyr 92
3rsk	K7a, R10a, K66a	Ser 89	63.13	100.00	Lys 1
3rsd	D121n	Asn 67	14.09	44.51	Ser 21

Adenylate kinase (wild type: 1ake A)

1dvr	D89v, R165i	Glu 113	13.15		
3aky	I213f	Glu 113	21.20	104.91	Glu 3

Calmodulin (wild type: 4cln)

1ahr	del-Thr 79, del-Asp 80	Asp 131	35.73	74.73	Ala 1
1deg	del-Glu 84	Gly 113	20.00	20.00	Thr 5