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**Software developments in automated structure solutions and
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Data sets used for testing

For testing of the new algorithms presented in Chapters 2 and 3 a total of 134 data sets were used. A majority of 78 data sets was provided by the Joint Center for Structural Genomics (JCSG, <http://www.jcsg.org/>): 1vjn, 1vjr, 1vjz, 1vk4, 1vkm, 1vlm, 1vqr, 1z82, 1zy9, 1zyb, 2a2m, 2a2o, 2a3n, 2a6b, 2aml, 2avn, 2b8m, 2etd, 2etj, 2ets, 2etv, 2evr, 2f4p, 2fea, 2ffj, 2fg0, 2fg9, 2fna, 2fqp, 2fur, 2fzt, 2g0t, 2g42, 2gc9, 2nlv, 2nuj, 2nvw, 2o08, 2o1q, 2o2x, 2o2z, 2o3l, 2o62, 2o7t, 2o8q, 2obp, 2oc5, 2od5, 2od6, 2oh3, 2okc, 2okf, 2ooj, 2opk, 2osd, 2otm, 2ozg, 2ozj, 2p10, 2p4o, 2p7h, 2p7i, 2p97, 2pg3, 2pg4, 2pgc, 2pim, 2pn1, 2pnk, 2ppv, 2pr7, 2pr, 2prv, 2prx, 2pv4, 2pw4, 2b78, 2b79; 23 data sets from Mueller-Dieckmann et al. (2007): 2g4h, 2g4i, 2g4j, 2g4k, 2g4p, 2g4q, 2g4l, 2g4n, 2g4o, 2g4r, 2g4s, 2g4t, 2g4u, 2g4v, 2g4w, 2g4x, 2g4y, 2g4z, 2ill, 2g51, 2g52, 2g54, 2g55; and 33 from various other individual data set contributors: 1e42 (Owen, Vallis, et al. 2000), 1e6i (Owen, Ornaghi, et al. 2000), 1hf8 (Ford et al. 2001), 2ahy (Shi et al. 2006), 2hba, 2o0h (Sun et al. 2007), 2rkk (Xiao et al. 2008), 3bpj, 2fdn (Dauter et al. 1997), 1of3 (Boraston et al. 2003), 1i4u (Gordon et al. 2001), 1dw9 (Walsh et al. 2000), 2v0o (Henne et al. 2007), 1fse (Ducros et al. 2001), 1xib (Carrell et al. 1989), 1fj2 (Devedjiev et al. 2000), 1h29 (Matias et al. 2002), 1c8u (Li et al. 2000), 1lvy (Schiltz et al. 1997), 1lz8 (Dauter et al. 1999), 1e3m (Lamers et al. 2000), 1ga1 (Dauter et al. 2001), 1djl (White et al. 2000), 1dtx (Skarzyński 1992), 1dpx (Weiss 2001), 1mso (Smith et al. 2003), 1ocy (Thomassen et al. 2003), 1rju (Calderone 2004), 1rgg & 2sar (Sevcik et al. 1996, 1991), 1m32 (Chen et al. 2002). Finally, two data sets that were used have not been deposited in the PDB: a subtilisin savinase (sav3, Betzel et al. 1988; Dauter et al. 2002) and glucose isomerase (gilu, Dauter et al. 2002) data set.

Table A.1: The raw data summarized in Chapter 3. The PDB code is given by the first column. For data sets SAD data is taken from peak wavelength MAD data ($\ast$) or the inflection wavelength ($\dagger$) or were phased on a partial heavy atom substructure or substructure from another data set ($\ast$). data sets not deposited in the PDB are shown in italics. The maximum resolution is denoted by R , followed by the fraction of the substructure that was detected and the map correlation after experimental phasing as S and M_{Ph} , respectively. M_{σ_A} and M_{SAD-DM} denote the map correlation with the map generated from the deposited model phases with the map after density modification and phase combination with the σ_A and the *SAD-DM* algorithm, respectively. The difference between the two is given by ΔM . Similarly the fraction built with BUCCANEER and ARP/wARP are denoted by B and A , respectively.

PDB ID	R (Å)	S	M_{Ph}	M_{σ_A}	M_{SAD-DM}	ΔM	B_{SAD-DM}	B_{σ_A}	A_{SAD-DM}	A_{σ_A}
1vjn	3	0.38	0.08	0.03	0.03	0	0.02	0.02	0	0
1vjr	2.4	1	0.41	0.8	0.6	0.2	0.87	0.54	0.89	0.93
1vjz	2.5	1	0.41	0.72	0.55	0.17	0.81	0.37	0.3	0.08
1vk4	2	1	0.58	0.85	0.78	0.07	0.92	0.93	0.85	0.83
1vkm	2.6	0.98	0.51	0.76	0.61	0.15	0.96	0.64	0.77	0.62
1vlm	2.8	1	0.34	0	0	0	0.01	0	0	0
1vqr	2.77	0.86	0.4	0.6	0.41	0.19	0.58	0.11	0.15	0.05
1z82	2.05	0.85	0.4	0.47	0.43	0.04	0.09	0.06	0.06	0.06
1zyb	2.1	1	0.34	0.53	0.4	0.14	0.39	0.16	0.38	0.11
2a3n	1.23	1	0.58	0.84	0.8	0.05	0.98	0.98	0.97	0.96
2a6b	2.1	1	0.3	0.58	0.4	0.18	0.86	0.08	0.85	0.6
2aml	1.5	0.75	0.52	0.71	0.62	0.1	0.96	0.62	0.94	0.93
2avn	2.35	0.9	0.42	0.83	0.73	0.1	0.98	0.96	0.87	0.92
2etd	2.3	1	0.28	0.17	0.16	0.01	0.05	0.02	0.03	0.02

Table A.1 Continued from previous page

PDB ID	R (Å)	S	M_{Ph}	M_{σ_A}	M_{SAD-DM}	ΔM	B_{SAD-DM}	B_{σ_A}	A_{SAD-DM}	A_{σ_A}
2etj	1.74	1	0.36	0.5	0.4	0.1	0.06	0.09	0.44	0.22
2ets	2.25	1	0.39	0.81	0.68	0.13	0.97	0.93	0.93	0.93
2evr	1.6	1	0.48	0.91	0.91	0	0.91	0.92	0.96	0.96
2f4p	1.9	1	0.3	0.39	0.35	0.04	0.02	0.03	0.06	0.06
2fea	2	1	0.49	0.84	0.72	0.12	0.81	0.94	0.92	0.92
2fg0	1.79	1	0.41	0.86	0.74	0.12	0.97	0.94	0.94	0.93
2fg9	2.2	1	0.5	0.83	0.65	0.18	0.9	0.74	0.77	0.69
2fna	2	0.89	0.33	0.34	0.31	0.03	0.05	0.02	0.04	0.02
2fqp	1.8	1	0.47	0.6	0.56	0.03	0.17	0.03	0.45	0.37
2fur	1.9	1	0.41	0.51	0.48	0.03	0.1	0.04	0.24	0.19
2gc9	1.7	1	0.44	0.64	0.6	0.04	0.78	0.59	0.89	0.89
2nlv	1.33	0.53	0.43	0.68	0.64	0.04	0.56	0.68	0.94	0.89
2nuj	2	1	0.45	0.89	0.88	0.02	0.98	0.96	0.88	0.87
2nwv	1.85	1	0.3	0.66	0.42	0.24	0.52	0.02	0.88	0.11
2o08	2.5	1	0.4	0.72	0.49	0.23	0.79	0.23	0.67	0.1
2o1q	2	0.89	0.46	0.51	0.5	0	0.03	0.07	0.39	0.31
2o2x	1.5	1	0.55	0.71	0.67	0.04	0.87	0.89	0.92	0.92
2o2z	2.6	1	0.46	0.81	0.78	0.03	0.97	0.96	0.88	0.91
2o3l	2.05	0.92	0.48	0.84	0.74	0.1	0.87	0.95	0.87	0.85
2o62	1.75	1	0.41	0.76	0.57	0.2	0.88	0.31	0.92	0.91
2o7t	2.1	1	0.35	0.3	0.3	0	0.06	0.05	0.02	0.02
2o8q	2.5	1	0.44	0.81	0.75	0.06	0.9	0.75	0.74	0.77

Table A.1 Continued from previous page

PDB ID	R (Å)	S	M_{Ph}	M_{σ_A}	M_{SAD-DM}	ΔM	B_{SAD-DM}	B_{σ_A}	A_{SAD-DM}	A_{σ_A}
2obp	1.7	1	0.52	0.89	0.89	0	0.98	0.98	0.94	0.93
2oc5	1.68	1	0.56	0.92	0.92	0	1	1	0.97	0.94
2od5	1.98	1	0.33	0.86	0.68	0.18	0.97	0.88	0.85	0.81
2od6	1.9	0.95	0.46	0.72	0.61	0.12	0.9	0.39	0.91	0.83
2oh3	2	0.8	0.47	0.82	0.76	0.06	0.95	0.93	0.89	0.9
2okc	2.2	1	0.47	0.69	0.57	0.12	0.71	0.3	0.28	0.15
2okf	1.6	1	0.44	0.82	0.75	0.06	0.92	0.87	0.78	0.78
2ooj	1.84	0.92	0.42	0.72	0.56	0.16	0.7	0.25	0.93	0.71
2opk	2.1	1	0.4	0.82	0.6	0.22	0.96	0.26	0.93	0.65
2osd	2.3	0.57	0.19	0.14	0.14	0	0.04	0.03	0.01	0
2otm	1.9	0.83	0.41	0.85	0.67	0.18	0.97	0.81	0.95	0.94
2ozg	2.05	1	0.4	0.57	0.5	0.08	0.31	0.19	0.32	0.13
2ozj	1.6	0.67	0.44	0.7	0.67	0.03	0.32	0.26	0.78	0.77
2p4o	1.95	1	0.34	0.39	0.36	0.04	0.05	0.05	0.03	0.05
2p7h	1.85	1	0.37	0.81	0.57	0.24	0.95	0.26	0.79	0.81
2p7i	1.84	1	0.45	0.84	0.67	0.16	0.95	0.85	0.89	0.89
2p97	1.6	1	0.41	0.82	0.81	0.01	0.98	0.94	0.93	0.93
2pg3	2.4	0.75	0.44	0.75	0.62	0.13	0.83	0.49	0.69	0.25
2pg4	2.2	0.33	0.31	0.33	0.29	0.04	0.13	0.11	0.05	0.04
2pim	2.2	0.8	0.4	0.62	0.52	0.1	0.81	0.26	0.72	0.38
2pn1	2	1	0.39	0.41	0.39	0.02	0.02	0.01	0.06	0.04
2pr7	1.55	1	0.39	0.7	0.6	0.1	0.96	0.88	0.95	0.89

Table A.1 Continued from previous page

PDB ID	R (Å)	S	M_{Ph}	M_{σ_A}	M_{SAD-DM}	ΔM	B_{SAD-DM}	B_{σ_A}	A_{SAD-DM}	A_{σ_A}
2prv	1.3	1	0.31	0.4	0.38	0.01	0.04	0.02	0.75	0.63
2pv4	1.95	1	0.49	0.84	0.71	0.13	0.98	0.9	0.91	0.86
2pw4	1.45	1	0.48	0.83	0.79	0.04	0.93	0.95	0.96	0.95
1e42	2.2	0.5	0.06	0.02	0.02	0	0.02	0	0.01	0.01
1e6i	1.87	0.83	0.36	0.62	0.43	0.19	0.87	0.08	0.93	0.86
1hf8	2	0.5	0.31	0.65	0.39	0.26	0.79	0.09	0.65	0.09
2b78	1.94	1	0.27	0.41	0.31	0.1	0	0.01	0.09	0.05
2b79	2.35	1	0.32	0.58	0.45	0.13	0.26	0.09	0.06	0.04
2hba	2.28	0.75	0.36	0.48	0.39	0.09	0.39	0.07	0.07	0.22
2o0h	3.29	0.64	0.28	0	0	0.02	0.03	0.02	0.01	0
2rkk	2.99	1	0.44	0.64	0.55	0.09	0.82	0.46	0.19	0.09
3bpj	2.28	0.78	0.39	0.63	0.55	0.08	0.79	0.81	0.71	0.58
2ill	2.2	1	0.29	0.65	0.43	0.21	0.29	0.11	0.56	0.15
2g4h	2	1	0.52	0.88	0.89	0	0.98	0.98	0.94	0.93
1of3	2	0.75	0.37	0.89	0.84	0.06	0.94	0.87	0.95	0.95
1i4u	2.6	0.5	0.31	0.25	0.24	0.01	0.01	0.01	0.02	0.01
1dw9*	2.4	0.97	0.58	0.86	0.79	0.08	0.92	0.92	0.95	0.97
2v0o	3.1	1	0.09	0.07	0.07	0	0.01	0.02	0	0
1fse†	2.73	0.83	0.34	0.48	0.35	0.13	0.27	0.11	0.02	0.02
1fse*	2.73	1	0.41	0.71	0.5	0.21	0.93	0.58	0.67	0.34
<i>gilu</i>	1.5	1	0.43	0.91	0.9	0.01	0.97	0.97	0.95	0.95
1fj2	1.8	1	0.49	0.73	0.66	0.07	0.98	0.97	0.92	0.92

Table A.1 Continued from previous page

PDB ID	R (Å)	S	M_{Ph}	M_{σ_A}	M_{SAD-DM}	ΔM	B_{SAD-DM}	B_{σ_A}	A_{SAD-DM}	A_{σ_A}
2g4k	1.82	0.95	0.39	0.53	0.45	0.08	0.14	0.14	0.6	0.2
1h29*	2.81	0.91	0.41	0.5	0.42	0.09	0.1	0.06	0.04	0.03
2g4m	1.8	1	0.56	0.91	0.91	0	0.92	0.86	0.9	0.88
1c8u [†]	2.5	1	0.44	0.78	0.62	0.16	0.91	0.52	0.91	0.83
1c8u*	2.5	1	0.52	0.83	0.72	0.11	0.96	0.89	0.95	0.93
1lvy	1.87	1	0	0.01	0	0.02	0	0.01	0	0
1lz8	1.53	0.94	0.58	0.77	0.68	0.1	0.71	0.61	0.98	0.95
2g4q	1.84	0.8	0.5	0.7	0.58	0.12	0.73	0.43	0.98	0.95
1e3m*	3	0.98	0.51	0.79	0.72	0.07	0.9	0.78	0.69	0.66
2g4s	2.2	0.75	0.24	0.59	0.36	0.23	0.49	0.15	0.67	0.12
2g4u on Ca*	1.84	1	0.46	0.66	0.5	0.16	0.42	0.01	0.93	0.65
2g4u on Na*	2.15	1	0.49	0.71	0.55	0.16	0.85	0.25	0.96	0.54
2g4v	2.14	0.93	0.47	0.63	0.53	0.1	0.48	0.33	0.9	0.32
1ga1*	1.8	1	0.3	0.61	0.61	0	0.9	0.94	0.92	0.91
1rgg & 2sar*	2.53	0.57	0.33	0.42	0.34	0.07	0.1	0.05	0.03	0.01
<i>sav3</i>	1.75	1	0.48	0.71	0.61	0.1	0.7	0.7	0.93	0.94
1djl	2.48	0.94	0.45	0.82	0.62	0.21	0.98	0.61	0.95	0.93
2g4z	1.98	0.54	0.46	0.8	0.62	0.18	0.93	0.65	0.96	0.94
2g51	1.84	0.29	0.1	0.06	0.09	0	0.03	0.01	0	0
2g55	1.82	0.83	0.52	0.75	0.6	0.15	0.79	0.52	0.97	0.96
1dpx	1.64	0.75	0.55	0.71	0.61	0.1	0.81	0.22	0.95	0.94
1ocy	2.74	1	0.37	0.5	0.45	0.06	0.19	0.15	0.3	0.28

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