Supplementary Table S1. Number of structures determined using iodide derivative data using SAD/SIRAS/MIRAS phasing methods

SAD phasing method

PDB id	Res. (Å)	No. of sites	Redundancy	SG	X-ray source	Detector	Programs	Reference
1BN2	2.80	5	-	$P2_12_12_1$	RIGAKU/MSC RU-H2R	SIEMENS DETECTOR		Chen *et al*. 1991
-	1.62	12	3.2	$P2_1$	NSLS BEAMLINE X9B	ADSC MAR165	SHELXS	Dauter *et al*. 2000
1GWG	2.01	9	9.1	F432	ELLIOT GX-13	MAR 180CM PLATE		
1GWA	1.85	23	12.5	$P2_12_12_1$	RIGAKU RU300	JUPITER CCD	SHARP,	Evans & Bricogne, 2002
1GW9	1.55	29	18.8	I222	RIGAKU RU300	MAR-345 (IP)	SHELXD	
1GWD	1.77	4	12.1	$P4_32_12$	ELLIOT GX-13	MAR 180CM PLATE		
1OXS	1.65	12/31	5.5	$P2_12_12_1$	ESRF BEAMLINE ID14-2	ADSC QUANTUM 4	SnB, SHARP	Verdon *et al*. 2001, 2003
1OJ5	2.21	5	16.8	$P6_2$	SIEMENS M18X	MARRESEARCH	SHELXD/E	Razeto *et al*. 2004
1T6H	2.01	1 Iod-Phe	19.4	$P3_221$	RIGAKU RU300	RIGAKU RAXIS IV	SOLVE	Xie *et al*. 2004
1SD5	1.68	9/16	11.0	$P4_32_12$	HAMBURG BW7A	MAR CCD	SOLVE/SHELXD	Morth *et al*. 2004
1UTX	1.90	15	14.8	$P4_1$	SIEMENS M18X	MAR345	SHELXD/E	Rumpel *et al*. 2004
1YRI	1.00	3	25.8	$P3_121$	APS BEAMLINE 22-ID	MAR CCD	SOLVE	Chiu *et al*. 2005
1WY4	1.55	2	26.4	$C222_1$	RIGAKU	RIGAKU RAXIS IV	SOLVE	Chiu *et al*. 2005
1ZCR	1.80	6	-	$P2_12_12$	ENRAF-NONIUS FR 591	MACSCIENCE 2030H	CNS	Hörnberg *et al*. 2005
1V1G	2.70	7	3.7	$I4_1$	ESRF BEAMLINE BM16		SHARP	Sánchez-Barrena *et al*. 2005
-	3.0	6	-	$C222_1$	ENRAF-NONIUS FR591	MAR345	SHARP	Kostrewa *et al*. 2005
2D8P	2.30	3	-	$P4_12_12$	RIGAKU RU300	RIGAKU RAXIS IV++	SHARP	
2D8O	2.38	3	-	$P4_12_12$	RIGAKU RU300 Cr	R-AXIS VII		Miyatake *et al*. 2006
2D91	2.10	2	-	$P4_32_12$	RIGAKU RU300	RIGAKU RAXIS IV++		
2ANX	1.04	8	4.4	C2	ALS BEAMLINE 8.2.2	ADSC QUANTUUM 315	SHELXC/D/E	Mooers & Matthews, 2006
2C3V	1.39	3 Iod-Tyr	7.8	$P2_1$	RIGAKU MM-002	RIGAKU R-AXIS IV++	SHARP	Boraston *et al*. 2006

2OYY	2.50	13	-	H3	ENRAF-NONIUS FR591	MAR 345dtb	SHARP	Jeoung *et al*. 2007
2Q2L	2.37	10	6.3	C2	RIGAKU MICROMAX-007	MAR 345dtb	PHENIX	Yogavel *et al*. 2007
3E3T	1.60	1 + 3 I3C	11.2	$P2_12_12_1$	MACSCIENCE	BRUKER SMART 6000	SHELXD	Beck *et al*. 2008
3E3S	1.73	5 I3C	26.8	$P4_12_12$	MACSCIENCE	MAR scanner 345 mm		
3E3D	1.55	4 I3C	26.1	$P4_32_12$	MACSCIENCE	MAR scanner 345 mm		
3D11	2.31	19	3.3	$P2_13$	APS BEAMLINE 24-ID-C		PHENIX	Xu *et al*. 2008
-	1.75	3	7.5	$P2_12_12_1$	RIGAKU RUH3R	RIGAKU RAXIS IV	SHELXD/E	Van Itallie *et al*. 2008

Ab initio phasing method

PDB id	Res. (Å)	No. of sites	SG	X-ray source	Detector	Programs used	Reference
1TUK	1.12	2	C2	ESRF BM14	MAR CCD	SnB	Hoh *et al*. 2005
1HC0	1.82	11	$P4_32_12$	ENRAF-NONIUS FR591	MAR 345DTB	SHELXL-97	Ondrácek *et al*. 2005
2ANV	1.04	6	C2	ALS BEAMLINE 8.2.2	ADSC QUANTUUM 315	SIR V. 2002	Mooers & Matthews, 2006

SIRAS phasing method

PDB ID	Res. (Å)	No. of sites	Redundancy	SG	X-ray source	Detector	Programs	Reference
	1.62 1.70	11	3.2 3.8	$P4_32_12$	NSLS BEAMLINE X9B	ADSC MAR165	SHELXS	Dauter *et al*. 2000
	1.62 1.50	9	3.2 3.7	$P2_1$	NSLS BEAMLINE X9B	ADSC MAR165	SHELXS	Dauter *et al*. 2000
	1.60 1.40	8	3.3 3.1	$P2_12_12_1$	NSLS BEAMLINE X9B	ADSC MAR165	SHELXS	Dauter *et al*. 2000
	1.60 1.50	14	3.0 1.9	$P2_1$	NSLS BEAMLINE X9B	ADSC MAR165	SHELXS	Dauter *et al*. 2000
2AXE 1BS9	1.80 1.10	2 Iod-Tyr	6.7 3.4	$P2_12_12_1$	RIGAKU RU-H2R CHESS BEAMLINE F2	IMAGE PLATE CCD area detector	SHELX	Ghosh *et al*. 1999
2AXE 1G66	1.80 0.90	2 Iod-Tyr	6.7 4.4	$P2_12_12_1$	RIGAKU RU-H2R CHESS BEAMLINE A1	IMAGE PLATE CCD PRINCETON 2K	SHELX	Ghosh *et al*. 1999 Ghosh *et al*. 2001
	2.30 2.00	6	15.0 14.2	$P4_32_12$	BRAZILIAN NSLS	MAR345dtb	SnB SHARP	Nagem *et al*. 2001
	1.92 1.83		12.1 8.2	$P4_32_12$	Brazilian NSLS	MAR345dtb	SnB SHARP	Nagem *et al*. 2001

	2.00 2.47	5	7.5 5.5	$P6_322$	RIGAKU MICROMAX-007	MAR345dtb	SHARP SHELXD	Salamitou et al. 2005 Réty *et al.* 2005
2GO2	2.10 1.87	8	5.5 8.5	$P2_12_12_1$	RIGAKU ULTRAX 18	MAR345dtb	SHARP SHELXD	Navarro *et al.* 2005
2D8W	2.00	3		$P2_12_12_1$	RIGAKU FR-E	R-AXIS IV	SHARP	Miyatake *et al.* 2006
2B9X 2B9W	2.22 1.95	13	5.9 5.3	$I2_13$	RIGAKU MICROMAX-007	MARRESEARCH	SHELXD/E	Liavonchanka *et al.* 2006a, b
2IIA	3.00 1.80	4	11.3 4.6	P4	RIGAKU ALS BEAMLINE 4.2.2	RIGAKU RAXIS IV MAR CCD		Vogeley & Luecke, 2006 Vogeley *et al.* 2007
2V8I	1.50 1.90	50	3.6 4.1	$P2_12_12_1$	RIGAKU MM-002	RIGAKU RAXIS IV++	SHELXD SHARP	Abbott *et al.* 2007
	2.20 2.40	12	6.6 5.5	$P2_12_12_1$	BESSY BL1		RATON SHRAP	Jonstrup *et al.* 2007
3E79 3E78	1.90 1.90	2 I3C	4.1 3.5	$P2_1$	RIGAKU RUH3R	RIGAKU RAXIS IV++	SHELXD/E	Sippel *et al.* 2008
3BCA 3BC8	2.25 1.65	42/62	4.7 4.7	I222	BRUKER-NONIUS FR591	MAR345dtb	SHELXC/D/E	Ganichkin *et al.* 2008

MIRAS phasing method

PDB ID	Res. (Å)	No. of HA	Redundancy	SG	X-ray source	Detector	Programs	Reference
	2.30	6 I	15.0					
	2.30	5 Cs	15.2	$P4_32_12$	Brazilian NSLS	MAR345dtb	SnB	Nagem *et al*. 2001
	2.30	3 Gd	15.3				SHARP	
-	2.00		14.2					
	1.92	--I	12.1					
	2.00	--Cs	15.0	$P4_32_12$	Brazilian NSLS	MAR345dtb	SnB	Nagem *et al*. 2001
-	1.83		8.2				SHARP	
	2.3	27 I	4.2		SSRL beamline 9-2			
	3.4	9 I	4.6		NSLS beamline X4A			
	2.7	6 Hg	5.6		APS BIOCARS sector 14D			
	2.9	4 Pb	7.2				PHASES	Hao *et al*. 2002
	2.9	3 Os	5.5					
	3.2	12 Cs	4.0					
1L2Q	1.5		3.6		APS BIOCARS sector 14C			
		--I	-		ENRAF-NONIUS 571			
		--Xe	-	$P3_1$	ESRF BEAMLINE BM14			Mittl *et al*. 2002
1KSO	1.70				ESRF BEAMLINE BM14	MARRESEARCH		

	3.0	5 I	-					Hickenbottom *et al*. 2004
	3.0	2 Hg	-	$P6_322$	Rigaku	Raxis-IV	SOLVE	
	3.0	3 Pt	-				RESOLVE	
1SZI	2.8		-					
	3.5	1 I	3.7					
	3.0	4 Pt	5.9	$P2_12_12_1$	ALS BEAMLINE 8.2.1	ADSC CCD	SOLVE	He & Garcia, 2004
1SG1	2.4		4.8					
	2.30	8 I	3.0					
	2.30	4 Se	5.0		RIGAKU RU300	MARRESEARCH	SOVLE	Bandaru *et al*. 2004
	2.40	4 Se + 5 I	6.0					Doublié *et al*. 2004
1TDH	2.1		12.0					
2H9A	1.90	7/16 I						
	2.30	1 I			ENRAF-NONIUS FR571	MAR345dtb	SHARP	
	2.40	4 Hg		C2			SHELXD	Svetlitchnaia *et al*. 2006
	2.04							
	2.54	4 Fe			ESRF beamline ID 14-2			
	2.80	14 I	3.3			SMART 2K	SOLVE	
	2.62	5 Cs	4.0	$I4_122$	MacScience M06X SRA	DIP2030	RESOLVE	White *et al*. 2008
-	2.62		13.4			DIP2030		

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