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Supporting information for article:

Comparison of four different crystal forms of *Mycobacterium tuberculosis* ESX-1 secreted protein regulator, EspR

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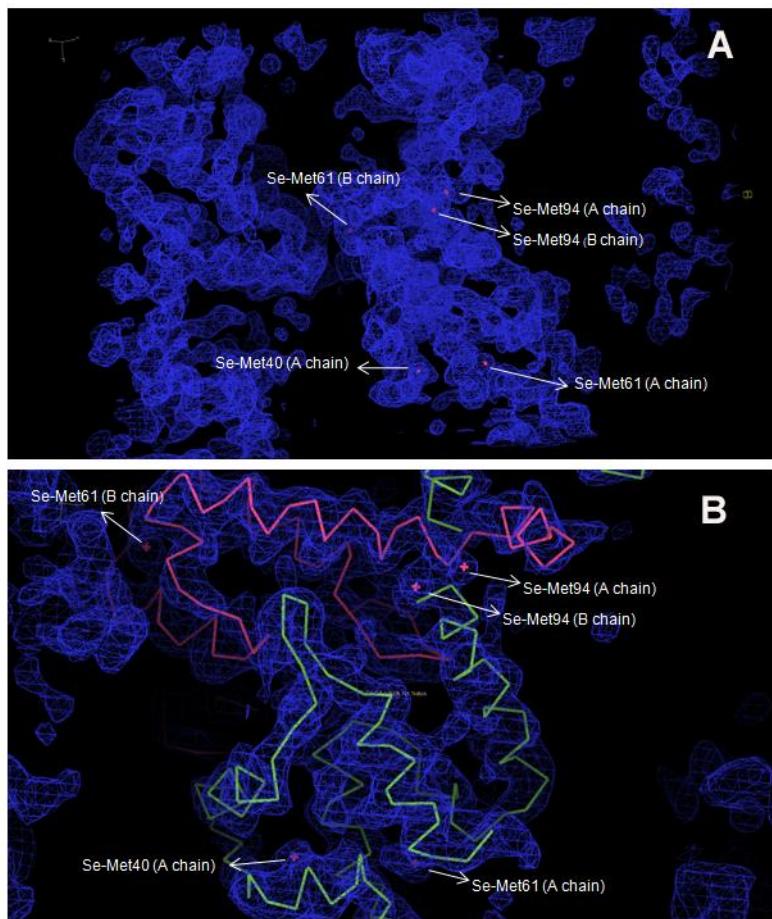


Figure S1 **A**, Experimental electron density map of EspR obtained from SAD phasing using 6 selenium sites obtained from SHELXD program together with density modification. **B**, C α backbone of EspR fitted in the experimental electron density map obtained from Se-SAD phasing together with 6 selenium sites.

Table S1 Residues involved in crystallographic contacts in different EspR crystal forms

Crystal form P3 ₂ 21 (4NDW)	Residues in Chain A	Residues in Chain B
	Arg120	Glu123, Arg120
	Glu123	Arg120
	Leu124	Glu123
	Ala127	Arg126, Glu123
Crystal form P2 ₁ (3QF3)	Arg54	Asn11, Asp15
Crystal form P2 ₁ 2 ₁ 2 ₁ , (3QWG)	Val17	Arg70
	Tyr18	Arg70
	Pro19	Arg70, Asn67
	Pro20	Lys72, Ile71, Arg70,
	Arg22	Asn67, Glu37,
	His25	Arg70
	Glu29	Glu37
	Ala32	Ala36
	Lys35	Glu80
	Ala36	Ala32, Ala36
	Glu37	Arg22, Glu29
	Tyr45	Glu80
	Gln48	Glu80
	ARg54	Glu80
	Ser58	Glu83
	Asn67	Pro19, Erg22
	Phe68	Arg70
	Arg70	Pro19, Tyr18, Arg70, Val17, Tyr18, His25, Phe68, Phe69
	Ile71	Pro20
	Lys72	Pro20
	Glu80	Lys35
	Lys84	Thr55, Asn56
	Lys87	Asn53, Thr55, Gly52
	Glu88	Arg54
	Trp91	Arg54, Glu88, Gln48
	Leu92	Leu92
	Met95	Tyr81, Lys84, Leu85, Glu88
	Arg96	Tyr81, Lys72, Arg70