

Monobody 7c12/Abl1 SH2 domain complex	
<b>Data collection</b>	
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Cell dimensions	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	39.34, 49.40, 107.35
α, β, γ (°)	90, 90, 90
Resolution (Å)	2.10 (2.18-2.10)
<i>R</i> <sub>sym</sub>	13.3 (55.6)
<i>I</i> / σ <i>I</i>	11.8 (2.4)
Completeness (%)	99.2 (99.3)
Redundancy	5.2 (5.1)
<b>Refinement</b>	
Resolution (Å)	2.10
No. reflections	11957
<i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	0.19/0.25
No. atoms	1726
Protein	1581
Ligand/ion	29
Water	127
<i>B</i> -factors	
Protein	23.27
Ligand/ion	54.82
Water	35.85
R.m.s. deviations	
Bond lengths (Å)	0.013
Bond angles (°)	1.378

**Table S1. Data collection and refinement statistics (molecular replacement) for Monobody 7c12/Abl SH2 domain complex structure, related to Figure 6**

Sample No.	Origin	Age	Gender	WBC (x 10 <sup>3</sup> )	Phase of Disease	BCR/ABL BM %	BCR/ABL PB %	Ph+ Metaphases %	Best response to Imatinib/Nilotinib
51	PB	64	m	273.6	AP	65.907	66.907	100	IM-resistant + NI-resistant
60	BM	87	f	230	AP	83.53	80.674	64	IM-resistant
61	BM	32	m	142.1	CP	63.388	53.965	100	CCyR, MMR
88	BM	46	f	184.5	CP	45.037	43.177	100	CCyR, MMR
111	BM	33	m	190	CP	38.866	26.735	100	IM-resistant
112	BM	74	m	47.1	CP	22.897	23.01	83	CHR
113	PB	74	m	47.1	CP	22.897	23.01	83	CHR

**Table S2. Clinical characteristics of primary CML samples used in this study, related to Figure 7**

Abbreviations used: PB, peripheral blood; BM, bone marrow; WBC, white blood cells; AP, accelerated phase; CP, chronic phase; IM, Imatinib; NI, Nilotinib; CCyR, Complete Cytogenetic Response; MMR, Major Molecular Response; CHR, Complete Hematologic Response.