Supplementary Information

Supplementary Materials and methods

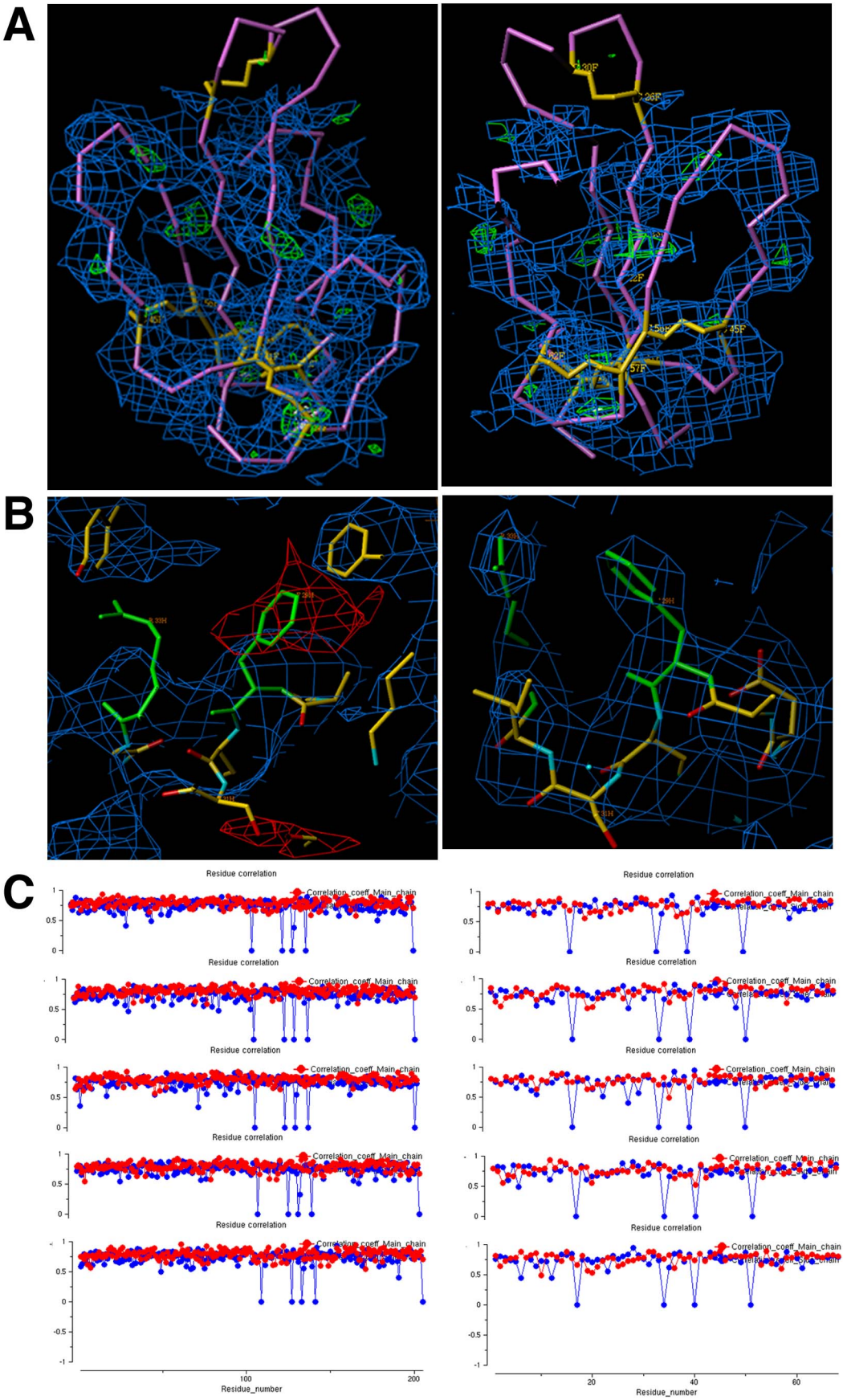
Supplementary Table

Refinement step (R-factor / R-free (%))		
1-Rigid-body 1 (AChBP)		43.1 (41.1) / 43.2 (48.2)
2-Rigid-body 2 (AChBP + 1 Cbtx)		43.0 (41.0) / 43.1 (48.2)
3-Rigid-body 3 (AChBP + 5 Cbtx)		42.6 (40.6) / 42.1 (48.5)
4-Restrained refinement		33.1(35.2) / 37.8 (47.1)
Coordinate shifts [1](ΔTg (Å))		
1-Rigid-body 1 (AChBP subunit A / B / C / D / E)	x	0.05 / -0.11 / -0.06 / -0.07 / 0.0
	y	0.02 / 0.05 / 0.05 / -0.26 / 0.09
	z	0.0 / 0.38 / 0.16 / -0.19 / -0.32
2-Rigid-body 2 (Cbtx molecule H)	x	0.1
	y	1.08
	z	0.59
3-Rigid-body 3 (Cbtx molecule F / G / I / J)	x	-0.94 / 0.29 / 0.31 / -0.29
	y	-0.63 / -0.46 / 0.74 / -0.2
	z	0.27 / -0.55 / -0.11 / 1.27
Non-crystallographic restraints (Å)		
AChBP (subunit A / B / C / D / E), main chains (side chains)		0.02 (0.3) / 0.02 (0.3) / 0.03 (0.31) / 0.02 (0.29) / 0.02 (0.36)
Cbtx (molecule F / G / H / I / J), main chains (side chains)		0.03 (0.38) / 0.02 (0.25) / 0.03 (0.29) / 0.02 (0.31) / 0.02 (0.24)
Ramachandran outliers [2] (%)		
AChBP (subunit A / B / C / D / E)		4.6 / 5.1 / 4.1 / 7.0 / 4.6
Cbtx (molecule F / G / H / I / J)		9.7 / 9.7 / 6.5 / 9.8 / 9.7

[1] Shift of center of mass along the x,y,z axis

[2] Kleywegt GJ, Jones TA (1996) Phi/psi-chology: Ramachandran revisited. *Structure* **4**: 1395-1400

Supplementary Figure Quality of the structure. (**A**) View of the unaveraged electron density maps, contoured at 1 σ (blue) and 3 σ (green), calculated after the first rigid-body refinement step in which a single Cbtx molecule (magenta with yellow disulfide bridges) has been positioned. (**B**) View of the tip of Cbtx loop II, with residues Phe29 and Arg33 in green, in the original model (left) and after rebuilding (right), with the electron density maps contoured at 1 σ (blue) and -3 σ (red). (**C**) Plots showing real-space fit *versus* residue number for the five AChBP subunits (left, subunits A to E from top to bottom) and the five bound Cbtx molecules (right, molecules F to J from top to bottom).


A
B
C
Residue correlation
Correlation_coeff_Main_chain
Residue_number