

**Structural studies on MRG701 chromodomain reveal a novel dimerization  
interface of MRG proteins in green plants**

Yanchao Liu, Hong Wu, Yu Yu and Ying Huang

## Supplementary Tables

**Table S1.  $K_d$  value (mM) of wild type proteins and mutants measured by ITC assay.**

protein	peptide	$K_d$	$\Delta H$	$\Delta S$
MRG701 <sup>CD</sup>	H3K36me3	$0.51 \pm 0.03$	$-4.8 \pm 0.19$	-14.9
MRG701 <sup>CD</sup>	H3K4me3	$0.33 \pm 0.01$	$-3.6 \pm 0.08$	3.5
MRG701 <sup>CD</sup>	H3K9me3	n.d.	n.d.	n.d.
MRG701 <sup>CD</sup>	H3K27me3	n.d.	n.d.	n.d.
MRG701 <sup>CD</sup> W56A	H3K36me3	$0.26 \pm 0.01$	$-8.2 \pm 0.12$	-11.7
MRG701 <sup>CD</sup> W56A	H3K4me3	$0.25 \pm 0.03$	$-7.1 \pm 0.33$	-7.7
MRG701 <sup>CD</sup> Y62A	H3K36me3	n.d.	n.d.	n.d.
MRG701 <sup>CD</sup> Y62A	H3K4me3	n.d.	n.d.	n.d.
MRG1 <sup>CD</sup>	H3K36me3	$0.46 \pm 0.04$	$-3.1 \pm 0.15$	4.5
MRG1 <sup>CD</sup>	H3K4me3	$0.65 \pm 0.05$	$-3.7 \pm 0.16$	1.9
MRG1 <sup>CD</sup>	H3K9me3	n.d.	n.d.	n.d.
MRG1 <sup>CD</sup>	H3K27me3	n.d.	n.d.	n.d.
MRG1 <sup>CD</sup> W58A	H3K36me3	$0.66 \pm 0.04$	$-3.7 \pm 0.15$	2.0
MRG1 <sup>CD</sup> W58A	H3K4me3	$0.91 \pm 0.03$	$-1.5 \pm 0.35$	-3.8
MRG2 <sup>CD</sup>	H3K36me3	$0.29 \pm 0.01$	$-4.0 \pm 0.05$	2.35
MRG2 <sup>CD</sup>	H3K4me3	$0.52 \pm 0.02$	$-10.4 \pm 0.25$	-19.7
MRG2 <sup>CD</sup> E75A	H3K36me3	$0.30 \pm 0.01$	$-5.6 \pm 0.11$	-2.8
MRG2 <sup>CD</sup> E75A	H3K4me3	$0.45 \pm 0.03$	$-1.9 \pm 0.06$	8.9

All data were fitted into the one-site model with N value fixed 1.

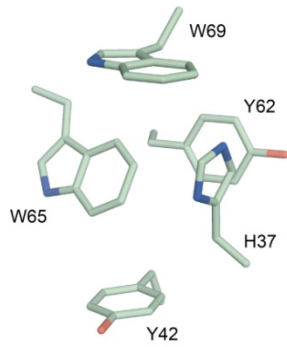
## Supplementary Figure Legends

**Fig. S1 Aromatic cages of MRG proteins.** Residues consisting of aromatic cage are shown as sticks. (A) Aromatic cage of MRG701<sup>CD</sup> is shown in light green. (B) Aromatic cage of MRG15<sup>CD</sup> is shown in violet. (C) Aromatic cage of MRG2<sup>CD</sup> is shown in cyan with tri-methylated lysine on H3K36me3 in yellow. (D) Aromatic cage of Eaf3<sup>CD</sup> is shown in orange with di-methylated lysine on H3K36me2 in yellow. (E) Comparison of the aromatic cages of MRG701, MRG2, MRG15, and Eaf3. Residues are shown as colored sticks as in (A–D).

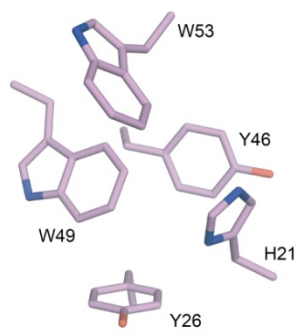
**Fig. S2 Secondary structure analysis via circular dichroism spectroscopy.** Spectra of wild type protein and mutant proteins are superimposed in the UV region of 190 nm-260 nm. (A) MRG701<sup>CD</sup> (black) and MRG701<sup>CD</sup>W56A (green). (B) MRG1<sup>CD</sup> (black) and MRG1<sup>CD</sup>W58A (blue). (C) MRG2<sup>CD</sup> (black) and MRG2<sup>CD</sup>E75A (red).

## Supplementary Figure S1

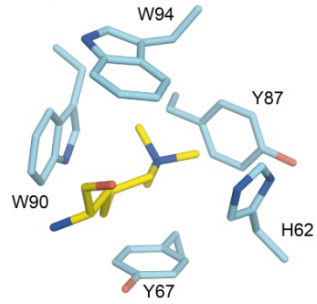
**A** MRG701 (PDB: 4PLI)



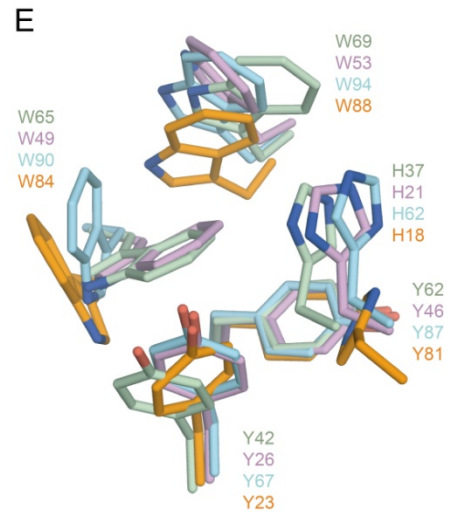
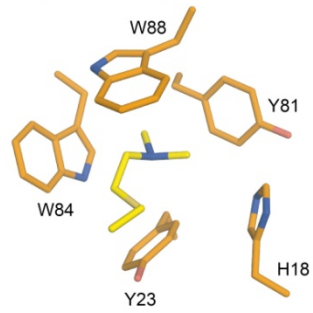
**B** MRG15 (PDB: 2F5K)



**C** MRG2 and H3K36me3 (PDB: 4PLI)



**D** Eaf3 and H3K36me2 (PDB: 2K3Y)



## Supplementary Figure S2

