Folding of a LysM domain: entropy-enthalpy compensation in the transition state of an 'ideal' two-state folder
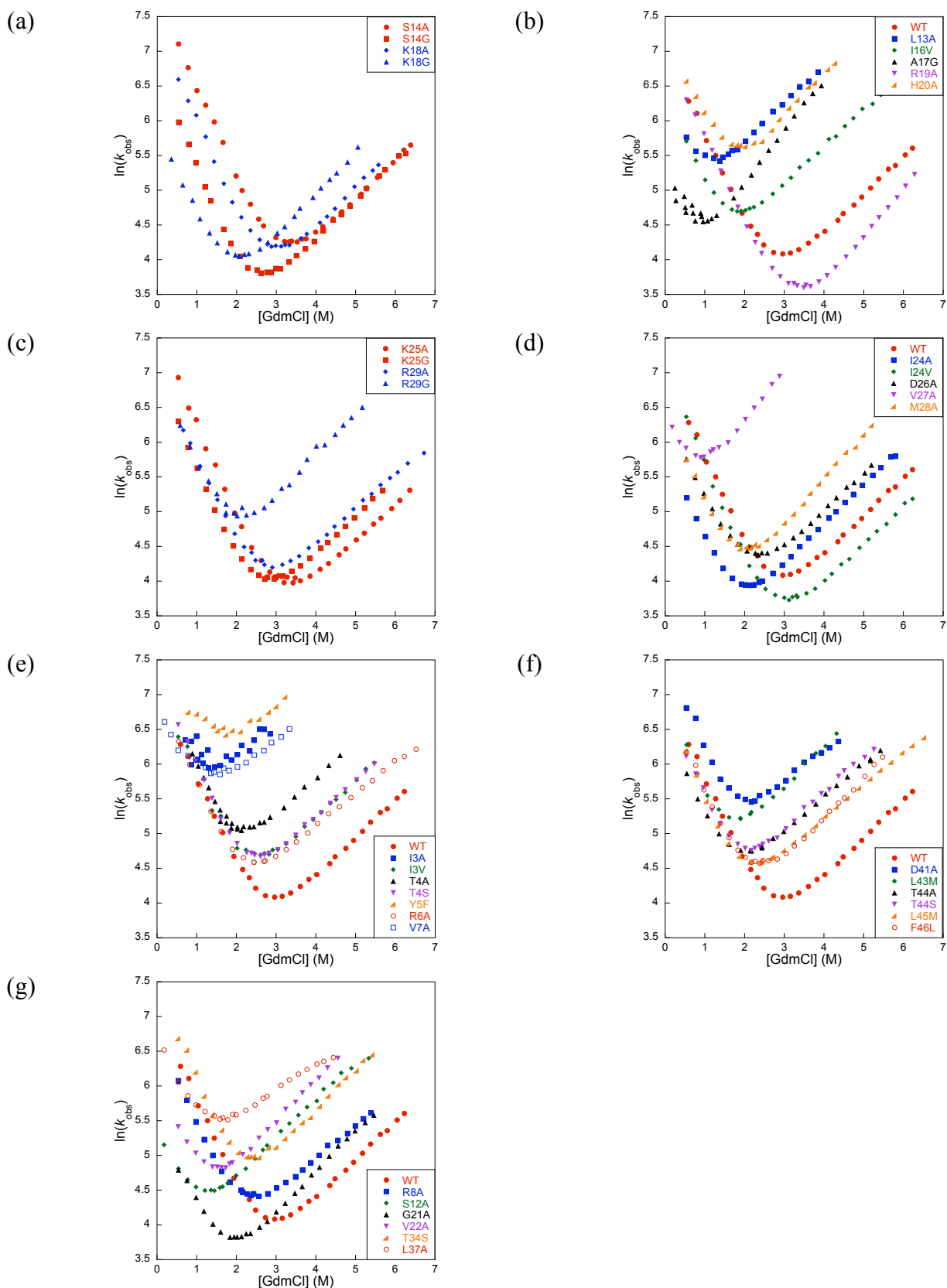
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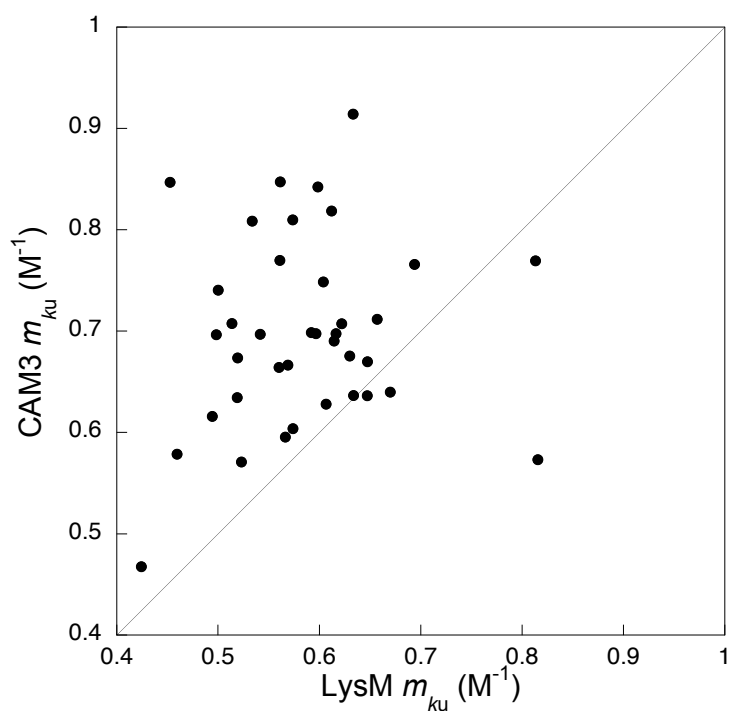
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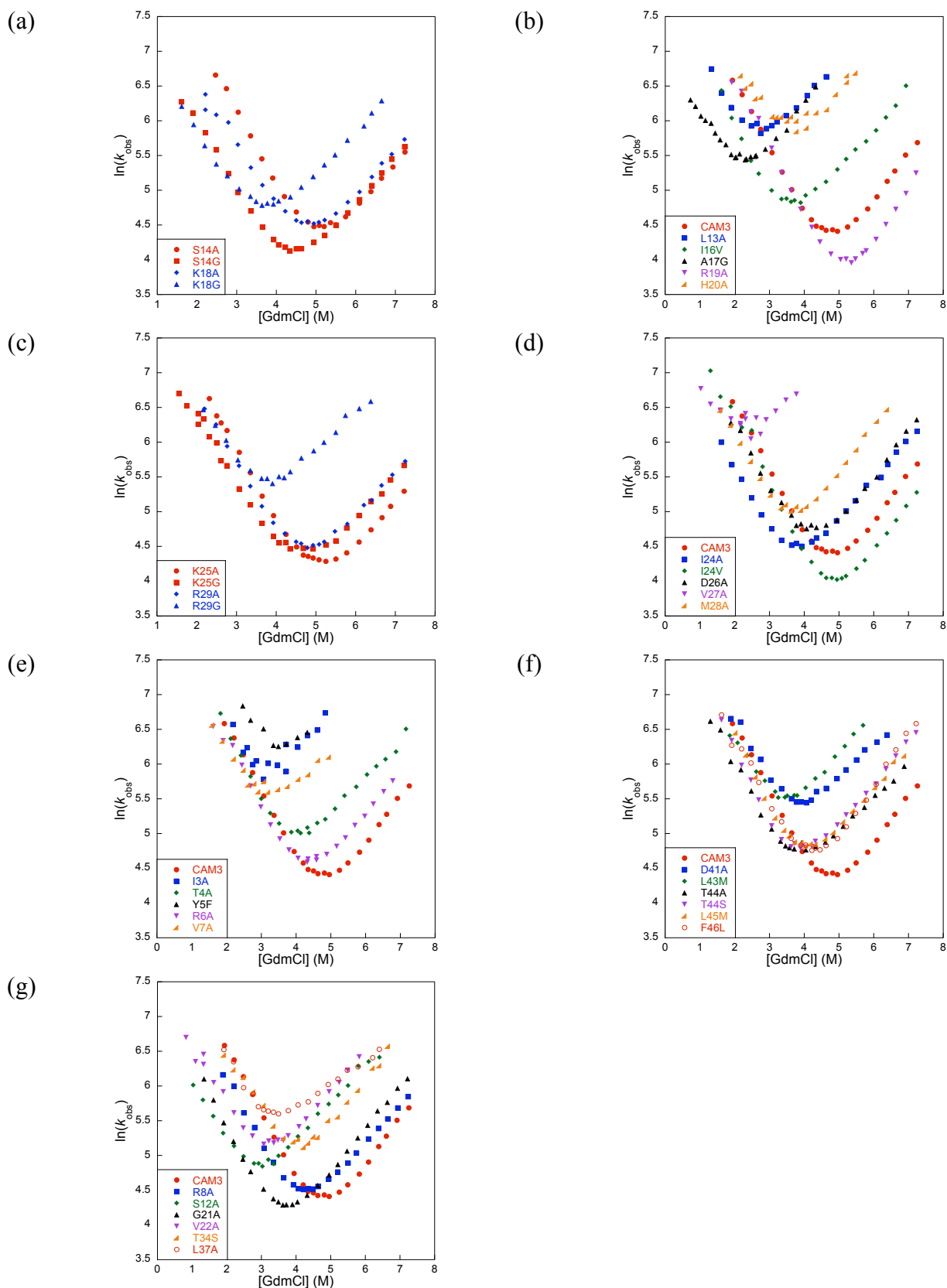[†]Corresponding author; e-mail: jc162@cam.ac.uk; tel: +44 (0) 1223 336426.

Supplementary Materials

Supplementary Figure 1. Chevron plots for LysM mutants. (a) Helix 1: Ala→Gly scanning mutations. (b) All other mutations in helix 1. (c) Helix 2: Ala→Gly scanning mutations. (d) All other mutations in helix 2. (e) Mutations within β-strand 1. (f) Mutations within β-strand 2. (g) Mutations in the turns and loops between elements of secondary structure.

Supplementary Figure 2. Comparison of unfolding *m*-values, m_{k_u}, for LysM and CAM3. The m_{k_u} values from LysM are plotted against the m_{k_u} values of the same mutant in CAM3. The unfolding *m*-values for CAM3 are consistently higher than those for LysM, suggesting that the transition state of CAM3 is less structured than that of LysM.

Supplementary Figure 3. Chevron plots for mutants of circular protein CAM3. (a) Helix 1: Ala→Gly scanning mutations. (b) All other mutations in helix 1. (c) Helix 2: Ala→Gly scanning mutations. (d) All other mutations in helix 2. (e) Mutations within β-strand 1. (f) Mutations within β-strand 2. (g) Mutations in the turns and loops between elements of secondary structure.

Supplementary Table 1. Contacts lost upon mutation of LysM.

	Mutant	Residues to which contacts have been lost
Strand 1	I3A	D1 T4 Y5 **H20** V22 **L45** V47 K48
	I3V	D1 <u>H20</u> V22 L45 V47 K48
	T4A	<u>S2</u> I3 R6 <u>K42</u> T44
	T4S	R6 K42
	Y5F	V7 L13 I16 L37 L43
	R6A	T4 D41 **K42**
	V7A	**Y5** R6 D11 <u>L13</u> I16 <u>L37</u> L43 D41
Turn 1	R8A	R6 K9 **D11** P39
	S12A	L13 S14 S15
Helix 1	L13A	**Y5** <u>V7</u> S12 I16 <u>I24</u> V27 T34 **L37** <u>L43</u>
	S14A	S12 L13 S15 I24
	S14G	S12 L13 S15 A17 I24
	S14A→G	S12 L13 S15 A17 I24
	S15A	D11 S12 I16 K18
	S15G	D11 S12 S14 I16 K18
	S15A→G	S12 S14 I16 K18
	I16V	<u>Y5</u> V7 D11 S12 L13 S15
	A17G	S14 I16 K18 H20 V22 I24 L45 V47
	K18A	None
	K18G	S15 A17 R19
	K18A→G	S15 A17 R19
	R19A	I16 **H20**
	H20A	**I3 Y5** <u>I16</u> A17 **R19 V22** I24 **L45** V47
Turn 2	G21A	None
	V22A	I3 I16 A17 <u>H20</u> I24 V27 <u>L45</u> <u>V47</u> K48
Helix 2	I24A	Y5 <u>L13</u> S14 I16 A17 H20 V22 M28 <u>V27</u> L45 V47
	I24V	Y5 L13 S14 I16 A17 H20 V22 V27 L45 V47
	K25A	**N23 D26**
	K25G	**N23** I24 **D26** M28
	K25A→G	N23 I24 D26 M28
	D26A	**N23 K25** <u>R29</u> **W30** V47
	V27A	Y5 L13 V22 <u>I24</u> D26 M28 <u>W30</u> N31 T34 L43 T44 <u>L45</u> V47
	M28A	I24 K25 V27 <u>T34</u> L37
	R29A	<u>D26</u> **W30**
	R29G	**D26** M28 **W30**
	R29A→G	D26 M28 <u>W30</u>
Loop	T34S	L13 V27 M28 N31 L37 L43
	L37A	Y5 <u>V7</u> **L13** M28 <u>T34</u> N36 D41 **L43**
Strand 2	D41A	<u>N36</u> <u>Q38</u> <u>K42</u>
	L43M*	**Y5** V7 <u>L13</u> V27 N31 T34 N36 <u>L37</u> T44
	T44A	S2 T4 V27 <u>W30</u> <u>N31</u> L45 **F46**
	T44S	S2 V27 <u>W30</u> N31 L45 <u>F46</u>
	L45M*	<u>I3</u> **Y5** I16 A17 **H20** <u>V22</u> I24 V27 L43 V47
	F46L	<u>S2</u> <u>W30</u> <u>T44</u>

A contact was counted if it involved two side-chain heavy atoms and fell within a distance cut-off of 6 Å. A minimal loss of interactions between two residues (≤ 5 contacts) is indicated by plain text, a moderate loss (≤ 10 contacts) is indicated by <u>underlined</u> text and significant loss of interactions (> 10 contacts) is indicated in **bold**. *The L→M mutations are non-conservative and so the list of residues shows potential contacts lost, not actual contacts lost.