



STRUCTURAL
BIOLOGY

Volume 74 (2018)

Supporting information for article:

Structure of ISG15 from the bat species *Myotis davidii* and the impact of interdomain ISG15 interactions on viral protein engagement

Caroline Langley, Octavia Goodwin, John V. Dzimianski, Courtney M. Daczkowski and Scott D. Pegan

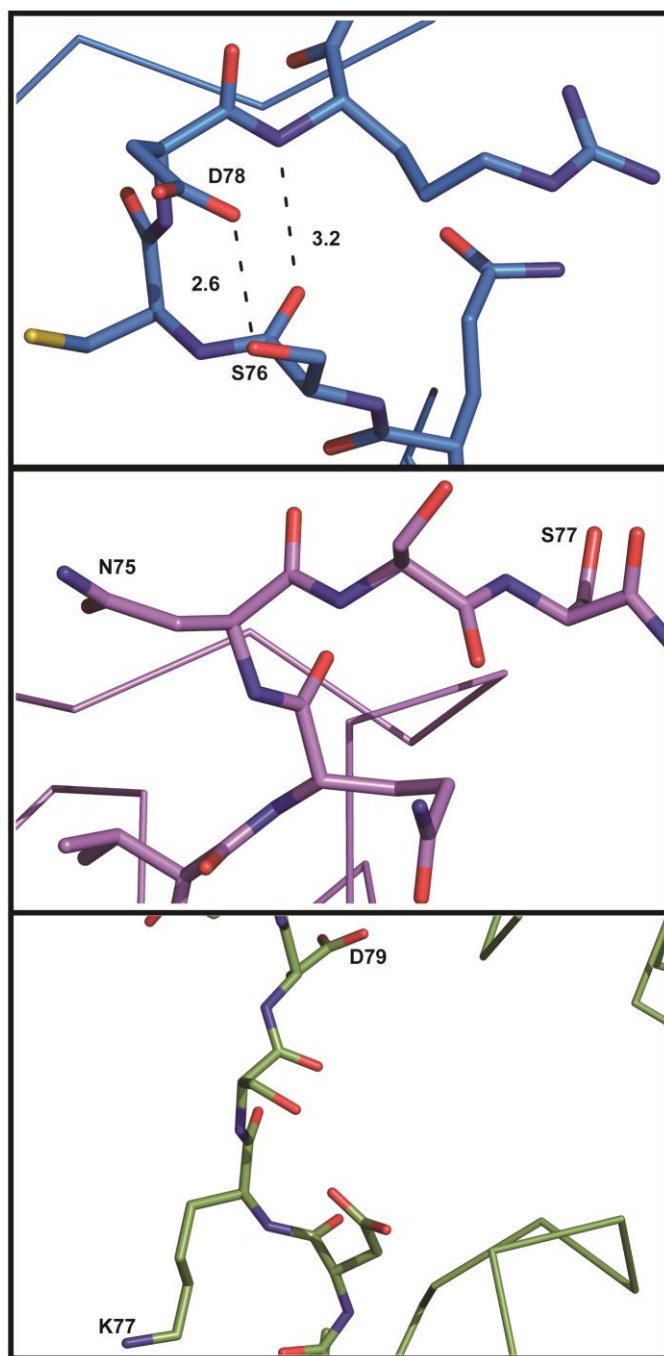


Figure S1 Hinge region of bISG15 (blue), mISG15 (purple), and hISG15 (green) highlighting residues forming reverse turn in bISG15 and lack thereof in mISG15 and hISG15.

Table S1

	Source Atom	Target Atom	Distance (Å)
bISG15	Phe 40 CB	Pro 143 CD	3.51
		Pro 143 CG	3.99
	Phe 40 CG	Pro 143 CD	3.33
		Pro 143 CG	3.85
	Phe 40 CD1	Pro 143 CD	3.43
		Pro 143 CG	3.46
	Phe 40 CD2	Pro 143 CD	3.85
		Thr 142 CB	4.39
		Thr 142 CG2	4.07
		Thr 142 CA	4.38
	Phe 40 CE1	Pro 143 CD	4.05
		Pro 143 CG	4.1
	Phe 40 CE2	Pro 143 CD	4.41
	Phe 40 CZ	Pro 143 CD	4.5
		Leu 81 CD1	4.48
	Arg 41 CD	Cys 77 CA	3.89
		Cys 77 CB	4.46
	Arg 41 CZ	Cys 77 CA	3.87
	Gln 75 CD	Arg 79 CB	4.12
		Arg 79 CG	4.47
Gln 75 O	Cys 77 N	3.46	
Ser 76 OG	Asp 78 OD2	2.60	
	Phe 41 CA	Leu 98 CD1	4.49
	Phe 41 CB	Leu 98 CB	4.07
		Leu 98 CG	4.3
		Leu 98 CD1	3.25
	Phe 41 CG	Gly 136 CA	3.83
		Gly 136 C	4.27
		Leu 98 CB	3.99
		Leu 98 CD1	3.97
	Phe 41 CD1	Thr 99 CG2	4.36
		Leu 98 C	4.27
		Gly 136 CA	4.12
		Leu 98 CB	3.72
		Leu 98 CD1	4.48
	Phe 41 CD2	Gly 136 CA	3.45
Gly 136 C		3.4	

mISG15	Phe 41 CE1	Thr 99 CG2	4.08
		Leu 98 C	4.19
		Gly 136 CA	4.11
		Leu 98 CB	4.38
	Phe 41 CE2	Glu 137 CD	3.94
		Gly 136 CA	3.43
		Gly 136 C	3.17
		Glu 137 CG	4.16
		Glu 137 CA	4.01
	Phe 41 CZ	Glu 137 CD	4.3
		Gly 136 CA	3.77
		Gly 136 C	3.88
		Leu 134 CD1	4.45
		Glu 137 CG	4.27
	Gln 42 CG	Thr 99 CG2	3.75
	Gln 42 CD	Thr 98 CG2	3.96
hISG15	His 39 CG	Pro 136 CG	4.14
	His 39 ND1	H ₂ O	3.50
	His 39 CD2	Thr 101 CB	4.38
		Thr 101 CG2	4.02
	His 39 CE1	Pro 136 CB	4.23
		Pro 136 CG	4.09
		Pro 136 CD	4.46
	Ala 40 CB	Glu 139 CD	4.12
	Phe 41 N	Glu 139 OE1	3.43
	Phe 41 CA	Glu 139 CD	4.44
	Phe 41 CB	Glu 139 CD	3.86
		Gly 138 C	3.93
		Glu 139 CA	4.36
	Phe 41 CG	Glu 139 CD	4.43
		Gly 138 CA	3.94
		Gly 138 C	3.65
	Phe 41 CD1	Gly 138 CA	4.02
		Gly 138 C	4.15
	Phe 41 CD2	Pro 136 CG	3.98
		Glu 139 CD	4.01
		Gly 138 CA	3.83
		Gly 138 C	3.64
		Glu 139 CA	4.37
Phe 41 CE1	Leu 100 CB	3.99	
	Gly 138 CA	4.01	

	Phe 41 CE2	Pro 136 CB	3.87
		Pro 136 CG	3.75
		Leu 100 C	4.29
		Gly 138 CA	3.81
		Gly 138 C	4.14
	Phe 41 CZ	Thr 101 CA	4.26
		Thr 101 CG2	3.97
		Leu 100 CA	4.5
		Leu 100 C	3.75
		Leu 100 CB	3.95
	Gln 42 CD	Gly 138 CA	3.9
		Thr 101 CG2	4.16
	Asp 76 OD2	Ser 78 OG	2.62
	Glu 139 OE2	H ₂ O	3.43