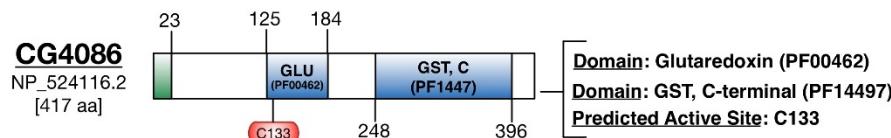


A.**B.**

CG4086/1-417

1	10	TT	TTT	40
CG4086/1-417	M . C T R L A S A T V L A G V R P P . . F A A S G G C A L R L I T K R N P D A A F A R R Q F A V A V			
PTGES2/1-377	M D P A A R V V R A L W P G G C A L A W R L G G R P Q P L L E T Q S R A C F A G A A G G P S P V A A A			

CG4086/1-417

50	TT	70	80	90	100	α_1
CG4086/1-417	E N G G G R K K P N G T F K L A V L G A . . . T V G A A T G S V Y T M Y Q R W T D G S S H K E H E E T K P T R L D G I P					
PTGES2/1-377	R K C S P R L L G A A A L A L G G A L G L Y H T A . . . R W H L R A Q D L H A E R S A					

CG4086/1-417

110	α_2	120	β_1	130	α_3	140	150	160	α_1
CG4086/1-417	A G V R I T K R Y V N P K D T S G L D T V L F Q F Q T C P F C C K V R A F L D E M G T S V A V V E V D A V L R Q D I R W								
PTGES2/1-377	A Q L S L S S R L Q L T L Y Q Y K T C P F C S K V R A F L D E H A L P Y Q V V E V N P V R R A E I K F								

★

CG4086/1-417

170	β_3	180	β_4	190	α_4	200	210	α_5	220	β_5	η_1
CG4086/1-417	S S V K K V P M V L I R Q Q D G K Y V O M V D S S A I I S L I A T H L Q D K R T D I G E L A Q F Y P H T S F F D D D G K										
PTGES2/1-377	S S Y R K V P . I L V A O E G E S S Q Q L N D S S V I I S A L K T Y I V V S G . Q P L E E I I T Y Y P A M K A V N E Q G K										

CG4086/1-417

230	β_6	TT	240	α_6	250	α_7	260	α_8	270	α_9
CG4086/1-417	K K N D I L N K Y F L M Y R E H T P K G V . . S K E T D E T D R K W R S W A D S H L V H L I S P N C Y Q T M G E S L E T									
PTGES2/1-377	E V T E F G N K Y W L M L N E K E A Q Q V Y G G K E A R T E E M K W R Q W A D W L V H L I S P N V Y R T P T E A L A S									

CG4086/1-417

290	α_{10}	300	α_{11}
CG4086/1-417	F E W F S Q A G E W D V H F P K W E R D L M V Y C G A T A M W A I A K M L K R R H A L S D D V R S H M Y D A L D Q W T T		
PTGES2/1-377	F D Y I V R E G K . . . F G A V E G A V A K Y M G A A A M Y I L I S K E R L K S R E R L O D N V R E D L Y E A A D K W V A		

CG4086/1-417

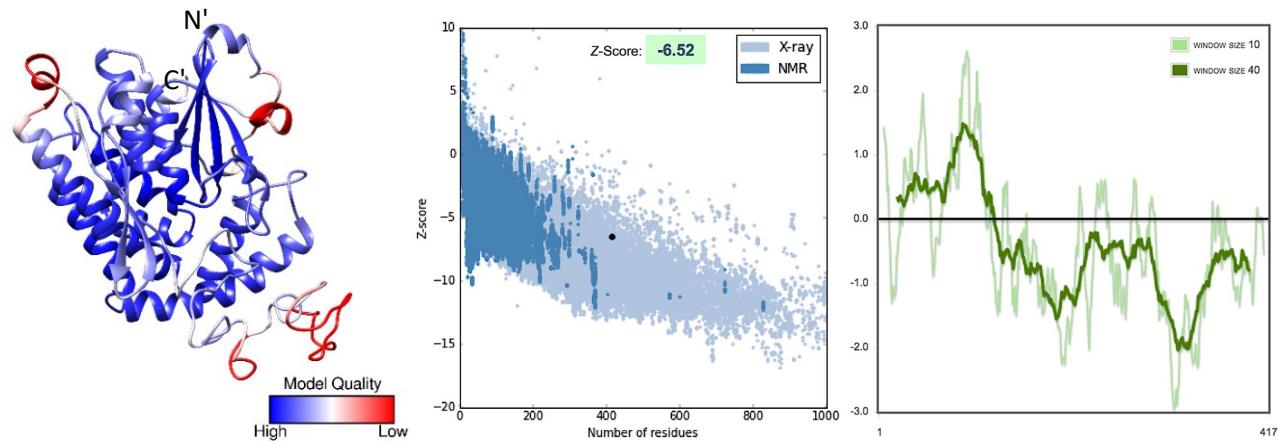
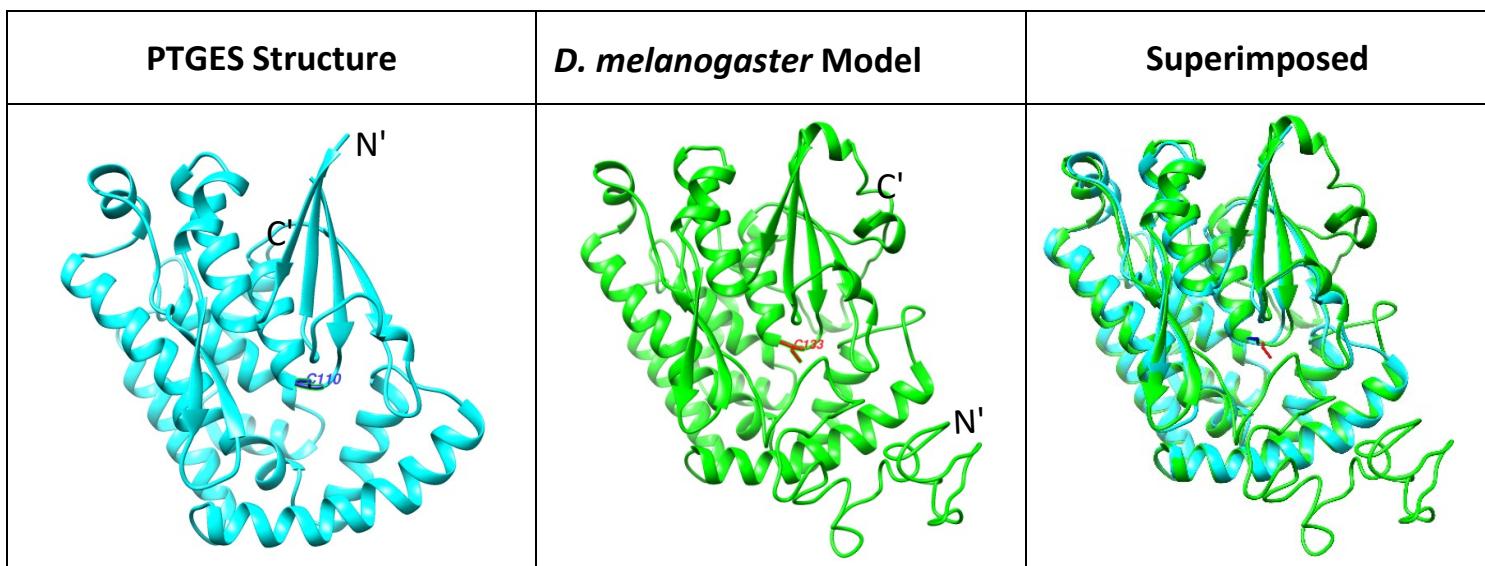
350	TT	360	α_{12}	370	α_{13}	380	α_{14}
CG4086/1-417	E L K K R N T K F M G G K Q P S L A D L S V F G V L I S S M E G C Q T E K D C I O N T S I G K W F Y D V K A L V E K N R G						
PTGES2/1-377	A V G K . D R P F M G G Q K P N L A D L A V Y G V L R V M E G I L D A F D D L M Q H T H I Q P W Y L R V E R A I T E . . .						

CG4086/1-417

410	β_7	α_{15}	
CG4086/1-417	Q L Q R E R I E N M A A T A		
PTGES2/1-377 A S P A H		

C.

<i>CG4086/1-417</i>	1 - - - - - MSCIRLASATVLAGVRPPAASGGALRLLTKRN	PDAAFARRQFAVAVENGGRKKPNTF	61
<i>1Z9H/88-377</i>	88 ERSAVQLSLSSR - - - - -	- - - - -	99
<i>CG4086/1-417</i>	62 KLAVALGATVGAATGSVYTMQRWTDGSSHKEHEETK	PTRLDGIPAGVRITKRYVNPKDTSGLDIVLFQFQTC	134
<i>1Z9H/88-377</i>	100 - - - - -	LQLTLYQYKTC	111
<i>CG4086/1-417</i>	135 F CCKVRAFLDYMGISYAVVEVDABL RQDI RWSSVKVPMVL I RQGDGKYVQMVDSAAISLIA THLQDKRTDI	- - - - -	207
<i>1Z9H/88-377</i>	112 FCSKVRAFLDFHALPYQVVEVNPNVLRAEIKFSSYRKVPILVAQE - GESSQQLNDSSVIIISALKTYLVSGQ - PL	- - - - -	182
<i>CG4086/1-417</i>	208 GELAQFYPHHTSFFDDGKKKNDILNKYFLMYREHTPKG - V - SKETDETDRKWRWSWADSHLVHLISPNCYQTMG	- - - - -	278
<i>1Z9H/88-377</i>	183 EEIITYYPAMKAVNDQGKEVTEFGNKYWLMLNEKEAQQVYSGKEARTFEEMKWRQWADDWLVHLISPNVYRTPT	- - - - -	255
<i>CG4086/1-417</i>	279 ESLETTFEWFSQAGEWDVHF PKWERDLMVYCGATAMWAIAKMLKRRHALSDDVRSHMYDAL DQWTTELKKRNTK	- - - - -	351
<i>1Z9H/88-377</i>	256 EALASF DYIVREGK - - - FGAVEGAVAKYMGAAAMYLIISKRLKSRRHLQDNVBEDLYEAADKWWAAVG - KDRP	- - - - -	323
<i>CG4086/1-417</i>	352 FMGGKQPSLADLSVFGVLSSMEGCQTFKDCLQNTSIGKWFYDVKA LVEKN - - - RQLQERIENMAIA	- - - - -	417
<i>1Z9H/88-377</i>	324 FMGGQQKPNLADLAVYGVLRVMEGLDAFDLDMQHTHIQPWYL RVERAITEASPAH - - - - -	- - - - -	377

D.**E.**

F.	Length (AA)	Domain Architecture (Pfam, range)	Functional Residues (aligned matches in <i>D. melanogaster</i>)	Sequence ID%	Structural Overlap (RMSD)
Prostaglandin-E-synthase 2 (PTGES2, NP_079348.1, PDB: 1Z9H)	377	GST-N3 domain (PF13417) 104-175 GST-C3 (PF14497) 201-368	C110		
Suppressor of ref(2)P sterility (CG4086, NP_524116.2)	417	Glutaredoxin domain (PF00462) 125-184 GST-C domain (PF14497) 248-396	C133	33% ID 49% SIM	0.814 Å

S2 Fig. Sequence and structural details of the modeled fly PTGES2 candidate. A. Domain architecture of PTGES2 and CG4086 and known/predicted functional residues B. Pairwise alignment of CG4086 and 1Z9H generated from structural superposition showing shared secondary structure elements and known/predicted functional residues (marked with a red asterisk) C. Pairwise alignment of CG4086 and 1Z9H generated from structural superposition with conserved residues highlighted using the physicochemical color scheme (CLUSTALX) D. Validation of the CG4086 model: ProQ2 quality score mapped to a 3D model of CG4086 (left); ProSA global quality score ranking (middle) and per-residue quality graph (right) E. Truncated PTGES2 (1Z9H, cyan-blue) superimposed on the predicted structure of CG4086 (green-red) with potential matches for conserved functional residues highlighted F. Summary of features shared by PTGES2 and potential *D. melanogaster* ortholog CG4086.