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Supporting information for article:

Crystal and solution structures of a novel antimicrobial peptide from *Chrysomya megacephala*

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Table S1 Molecualr replacement using *AMPLE* with *QUARK* ab initio structure prediction.

Ensemble_name	c1_t48_r1_unmod
MR_program	Phaser
Solution_Type	Marginal
<i>Phaser_LLG</i>	127.0
<i>Phaser_TFZ</i>	8.4
<i>Refmac_Rwork</i>	0.5206
<i>Refmac_Rfree</i>	0.5146
<i>ARP_final_Rwork</i>	0.2306
<i>ARP_final_Rfree</i>	0.545
<i>SHELXE_CC</i>	40.79
<i>SHELXE_ACL</i>	53
<i>SXRBUCC_final_Rwork</i>	0.3279
<i>SXRBUCC_final_Rfree</i>	0.3116
<i>SXRARP_final_Rwork</i>	0.3151
<i>SXRARP_final_Rfree</i>	0.365

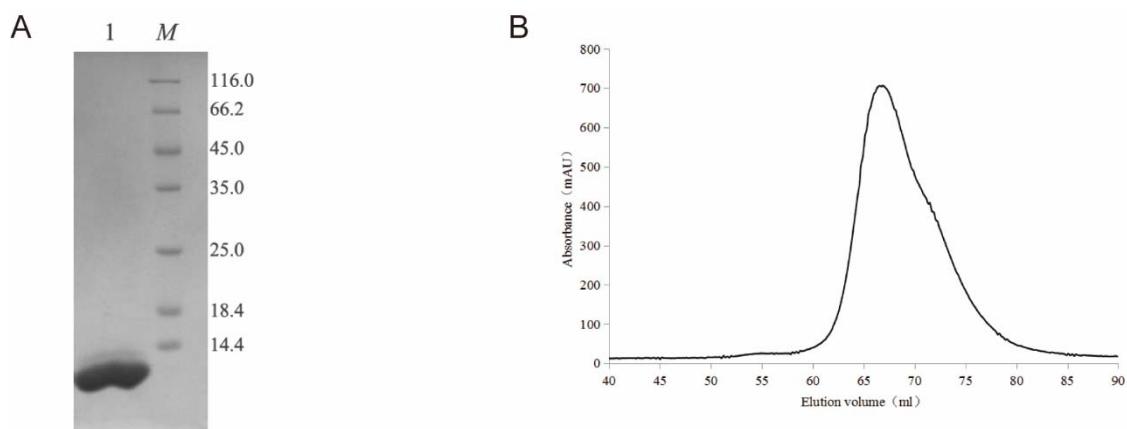


Figure S1 Purification of recombinant PSK. (a) Analysis of purified PSK on a 15% SDS-PAGE gel. Lane 1, purified PSK with theoretical molecular weight of 10.4 kDa; lane *M*, protein markers (labelled in kDa). (b) The elution profile of PSK from a Superdex 75 16/600 column.

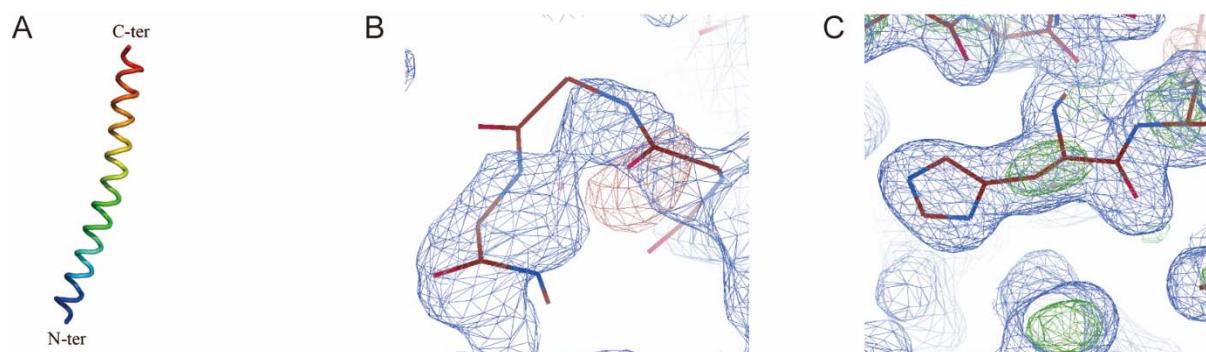


Figure S2 Molecular replacement in solving the PSK structure using *AMPLE* with *QUARK ab initio* structure prediction. (a) The representative model in the ensemble producing the solution with highest Z-score in molecular replacement using *Phaser*. (b) Local electron density of the PSK model with side chain truncation to C_β after molecular replacement using *Phaser* and refinement using *REFMAC*. (c) Representative local electron density of the rebuilt PSK model after density modification, main-chain tracing and model rebuilding using *SHELXE* and *Buccaneer*. A same model region is shown in panels (b) and (c), where the $2F_o - F_c$ density at 1.0σ contour is shown as blue mesh while the $F_o - F_c$ density at 3.0 and -3.0σ contours is colored in green and red, respectively.