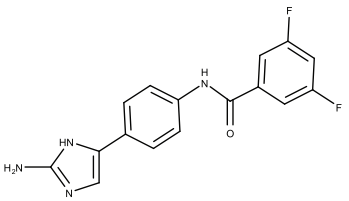
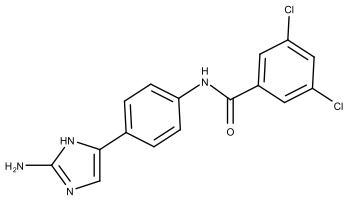
Supplementary Table 1. Data collection and refinement statistics (molecular replacement)

	QseBN (5UIC)
Data collection	
Space group	$P4_12_12$
Cell dimensions	
a, *b*, *c* (Å)	47.737, 47.737, 191.789
α, β, γ (°)	90, 90, 90
Resolution (Å)	38.25–2.50 (2.58–2.50)[a]
R_{sym}	0.116 (0.862)
$CC_{1/2}$	0.120 (0.990)
$I / \sigma I$	60.760 (9.250)
Completeness (%)	99.6 (99.7)
Redundancy	18.1 (19.6)
Refinement	
Resolution (Å)	38.25–2.50
No. reflections	8353
R_{work} / R_{free}	0.2254/0.3012
No. atoms	
Protein	1,876
Water	40
B-factors (Å^2)	
Protein	65.49
Water	48.78
R.m.s. deviations	
Bond lengths (Å)	0.002
Bond angles (°)	0.560

[a]Values in parenthesis correspond to the highest-resolution shell.



AGL-503



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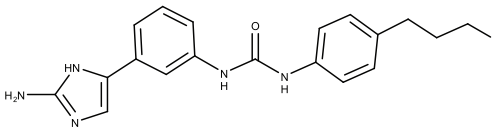

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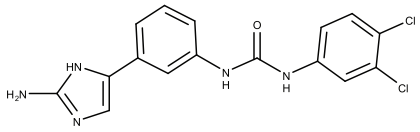

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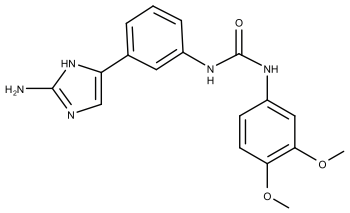

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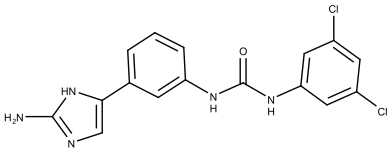

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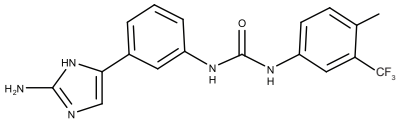

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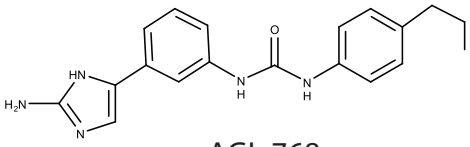

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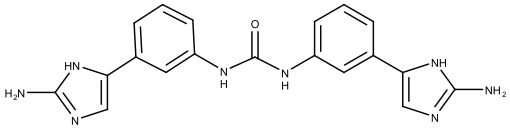

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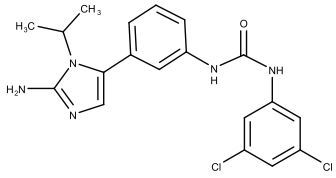

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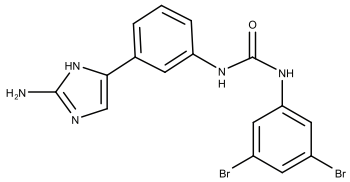

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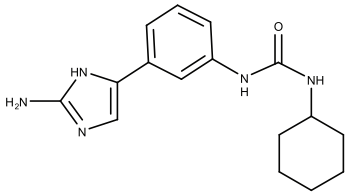

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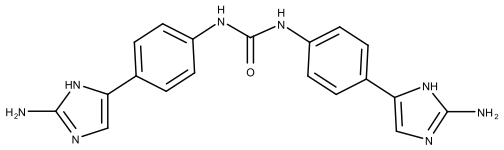

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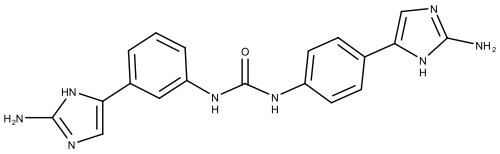

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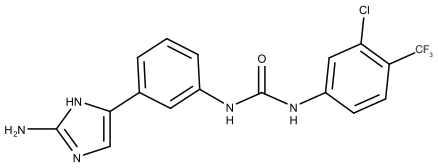
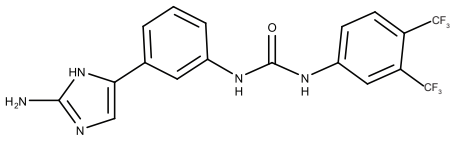
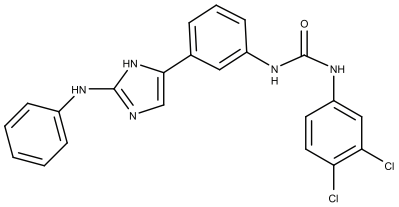


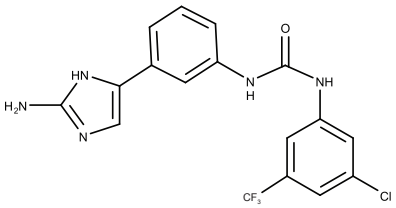
AGL-793



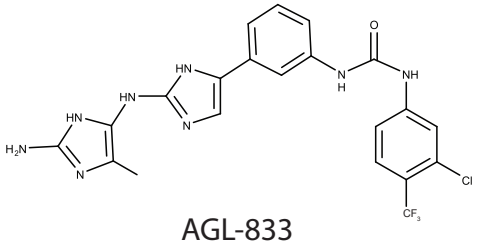
AGL-802



AGL-810



AGL-811



AGL-833

Fig. S1 2-AI compounds. Structures of compounds used in thermal shift assay. Structures of AGL-621, 702, 736, 753, 754, 773, 774, 782, 806, and 808 are not shown due to pending patent.

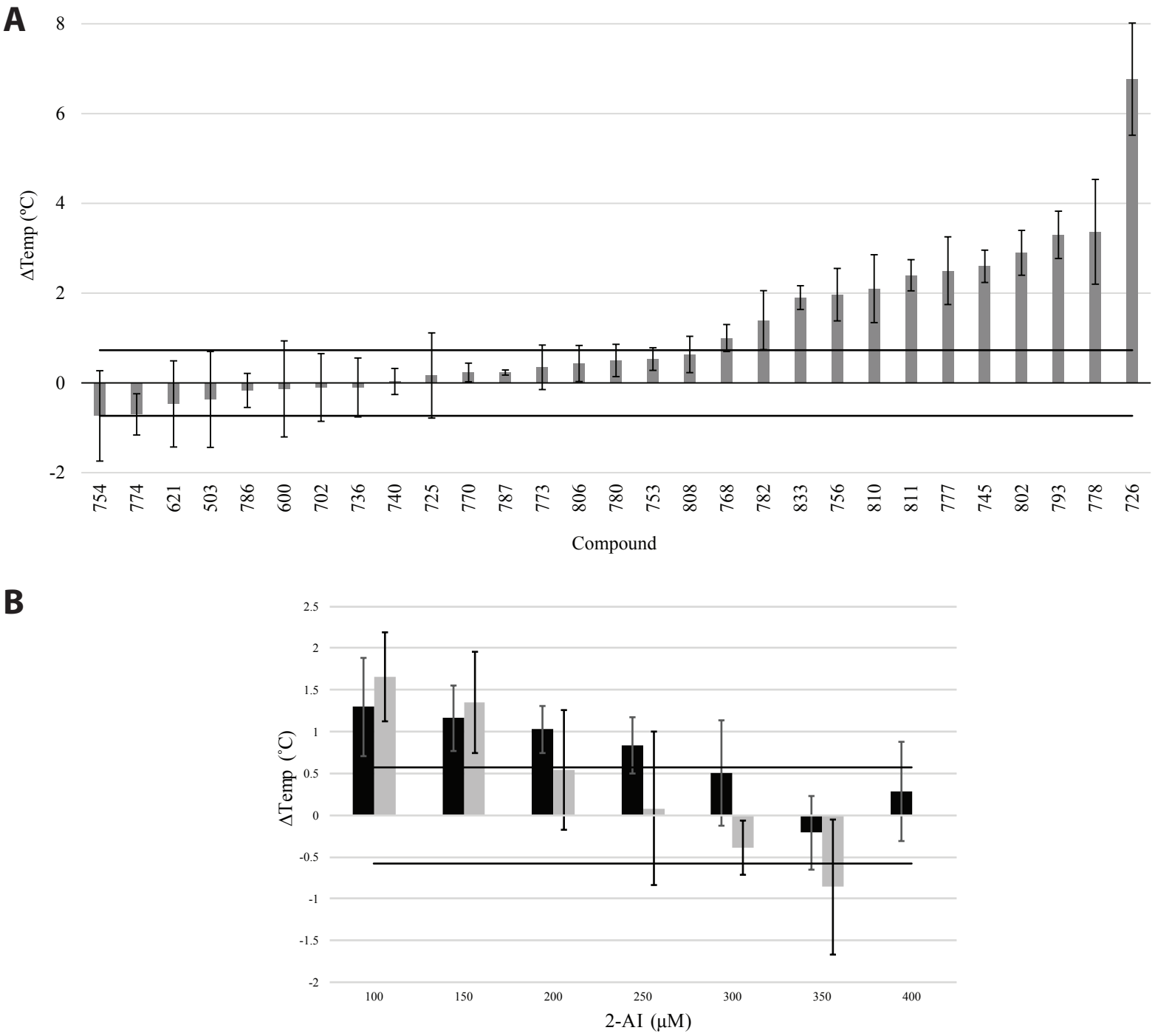


Fig. S2 Thermal shift of QseB and QseBN upon addition of 2-AI compounds. A) The average change in QseB melting temperature is plotted for each 2-AI compound tested. The thick horizontal black lines represents the standard deviation of the average melting temperature of QseB in the absence of any compound. The compound identifcation number is listed on the x-axis. B) The average change in QseBN melting temperature is plotted for AGL-600 (black) and AGL-726 (grey). The thick horizontal black line represents the standard deviation of the average melting temperature of QseBN in the absence of any compound. AGL-726 precepitated at 400 μM so no value could be determined.

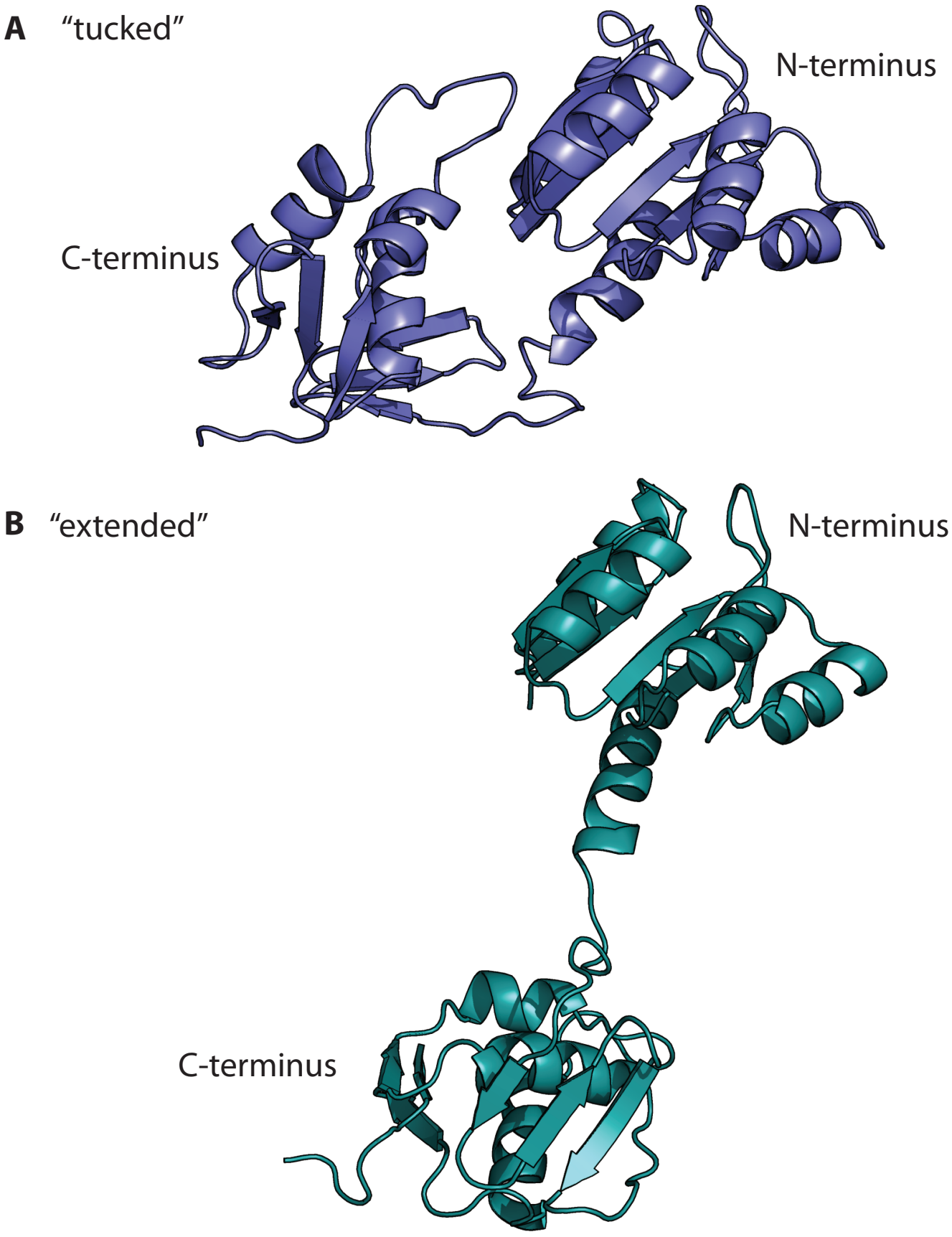


Fig. S3 "Tucked" and "extended" conformations. The QseB C-terminal domain moves significantely relative to the N-terminal domain. The two extremes of the C-terminal domain movement spans the "tucked" conformation (A) to the "extended" conformation (B).

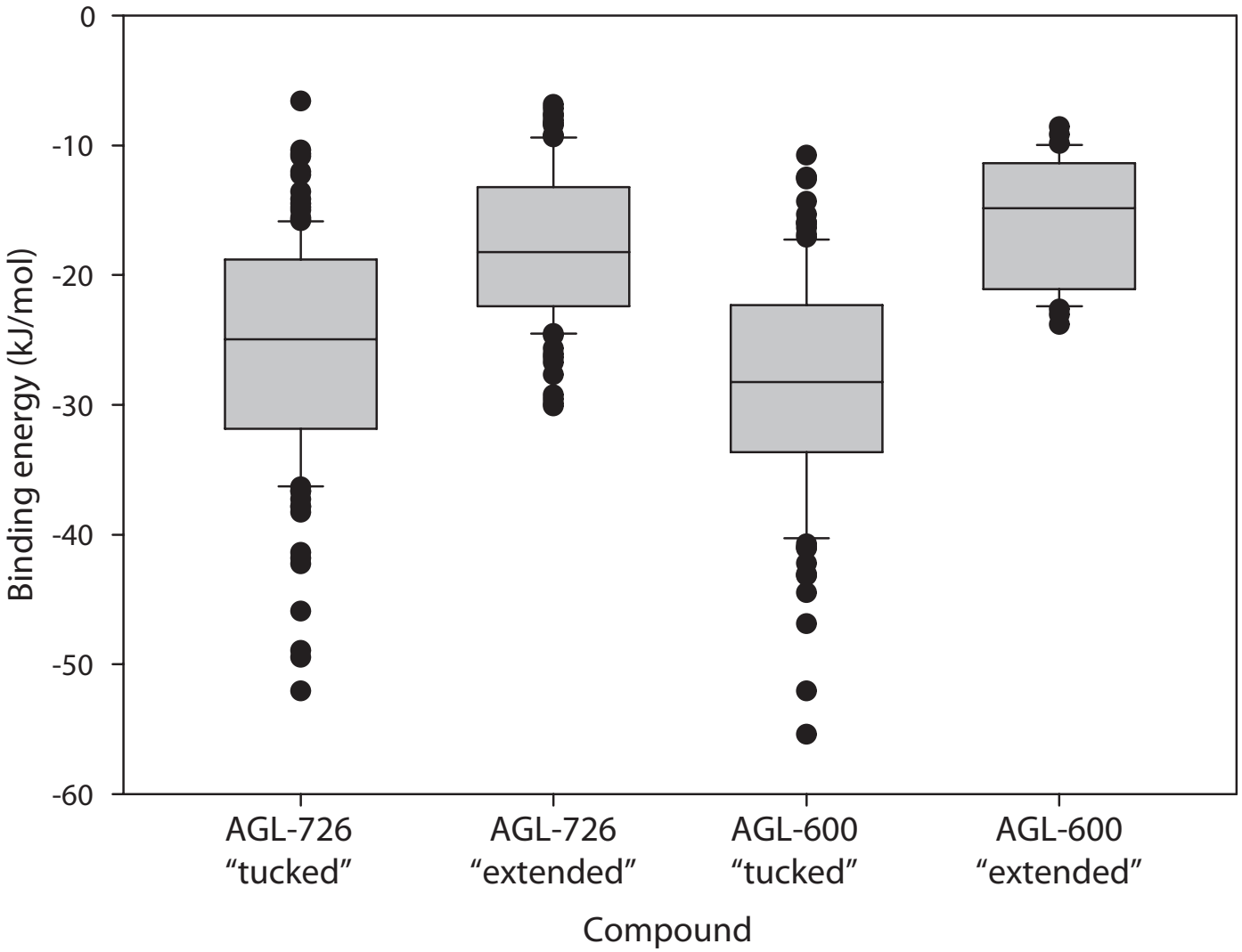


Fig. S4 Molecular docking results. The results from the highest populated cluster represented as box plots. The middle bar within each box represents the median scored complex, the box represents 50% of the data, and the 'tails' represent 25% of the data. Black circles signify solutions that are statistical outliers and were not included in the overall analysis.

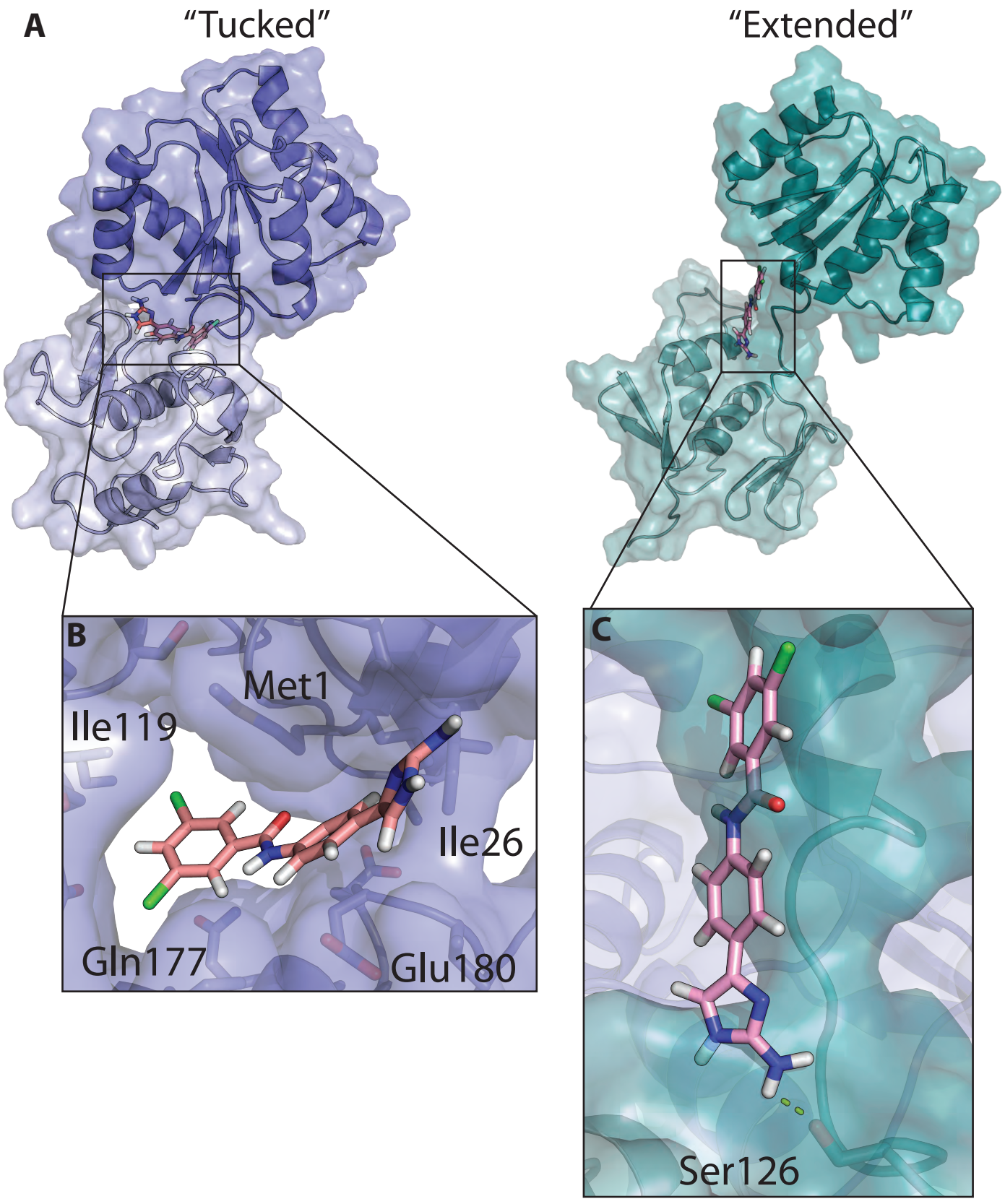


Fig. S5 Molecular docking of AGL-600 to a model of QseB. A) Full-length model of QseB based off of homologous crystal structures. One monomer (blue) takes on the "tucked" conformation with N-terminal domain in dark blue and C-terminal domain in light blue. The second monomer (green) is in the "extended" conformation with N-terminal domain in dark green and C-terminal domain in light green. Surface representation of AGL-600 (pink) docked to the "tucked" (blue) and "extended" (green) conformations. B) Close-up view of binding pocket of the "tucked" conformation. C) Close-up view of "extended" conformation binding site with yellow dashes representing potential H-bonding.