

Table S7. The information of the template for molecular docking.

Protein	UniProt Accession	Template	Seq Identity (%)	QMEANDisCo Global ¹	Resolution (Å)
AcnA	Q6G9K9	2b3y.1.A	51.87	0.79 ± 0.05	1.85
Icd	Q8NW61	1hqs.1.A	78.62	0.83 ± 0.05	1.55

¹ QMEANDisCo Global represent an overall model quality measurement with higher numbers indicating higher quality.