Structure *16*

Supplemental Data

Structure of the PduU Shell Protein

from the Pdu Microcompartment of *Salmonella*

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Table S1. Data Collection and Refinement Statistics

Data collection	
Cell dimensions	
a, *b*, *c* (Å)	74.1, 74.1, 218.0
α, β, γ (°)	90, 90, 120
Space group	R3 (indexed as H3)
Molecules/asymmetric unit	4
Resolution (Å) (last shell)	72.7-1.80 (1.85-1.80)
No. reflections total	205624
No. reflections unique	40948
R_{sym} (last shell)	15.9% (50.5%)
$I/\sigma I$ (last shell)	11.85 (2.33)
Completeness (last shell)	99.2% (93.5%)
Redundancy	5.0
Refinement	
Resolution (Å)	1.80
No. reflections R_{work}	38881
No. reflections R_{free}	2063
R_{work} / R_{free}	20.3 / 24.2%
No. atoms non-H_2O	3527
No. solvent O atoms	167
Average *B* factor all atoms (Å^2)	30.1
Est. coordinate error (Å)(Read, 1986)	0.116
R.M.S. deviations from ideality	
Bond lengths (Å)	.012
Bond angles (°)	1.43
Ramachandran plot:	
Most favored	94.0%
Allowed	5.0%
Generously allowed	1.0%
Disallowed	0%

$R_{\text{sym}} = \sum_{hkl} \sum_{i} \left| I_i(hkl) - \overline{I(hkl)} \right| / \sum_{hkl} \sum_{i} I_i(hkl)$

$R_{\text{work}} = \sum \left| F_{obs} - F_{calc} \right| / \sum F_{obs}$

$R_{\text{free}} = \sum \left| F_{obs} - F_{calc} \right| / \sum F_{obs}$, calculated using a random set containing 5% of reflections that were not included throughout refinement

Supplemental References

Read, R.J. (1986). Improved Fourier coefficients for maps using phases from partial structures with errors. Acta Cryst. A *42*, 140–149.