

Supplementary Table S3: Data collection and refinement statistics for BOS

Data Collection	
PDB code	6ZBS
Space group	<i>P4₃2₁2</i>
Cell dimensions:	
a,b,c (Å)	66.20 66.20 226.38
α,β,γ (°)	90, 90, 90
No. of copies in a.u.	1
Resolution (Å)	45.84-2.35
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Upper resolution shell (Å)	2.434-2.35
Unique reflections	21,933 (2,130)
Completeness (%)	99.83 (99.77)
Multiplicity	19.3 (21.1)
Average $I/\sigma(I)$	49.73 (5.75)
R-pim	0.165 (0.2717)
CC1/2	0.75 (0.824)
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Refinement	
Resolution range (Å)	45.84-2.35
No. of reflections ($I/\sigma(I) > 0$)	21,906
No. of reflections in test set	1,112
R-working / R-free	0.2059 / 0.2590
No. of protein atoms	3324
No. of water molecules	111
Overall average B factor (Å ²)	43.73
Root mean square deviations:	
- bond length (Å)	0.006
- bond angle (°)	0.85
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Ramachandran Plot	
Most favored (%)	95.45
Additionally allowed (%)	3.83
Disallowed (%)	0.72

* Values in parentheses refer to the data of the corresponding upper resolution shell.