

SUPPLEMENTARY TABLES

Supplementary Table 1. X-ray data collection and processing.

The $CC_{1/2}$ criterion was used to determine the resolution range. Values for the outer shell are given in parentheses.

Sample	SpoT _{Ab} -ppGpp complex	Mn ²⁺ -free SpoT _{Ab} ^{NTD}
Diffraction source	Soleil PX1	Soleil PX2
Wavelength (Å)	0.9786	0.9801
Temperature (K)	100.0	100.0
Detector	Eiger-X 16M	Eiger-X 16M
Crystal-detector distance (mm)	402.12	254.68
Rotation range per image (°)	0.01	0.10
Exposure time per image (s)	0.01	0.004
Space group	P2 ₁ 2 ₁ 2 ₁	P4 ₁ 22
<i>a</i> , <i>b</i> , <i>c</i> (Å)	128.8, 133.8, 211.3	90.9, 90.9, 262.4
α , β , γ (°)	90.0, 90.0, 90.0	90.0 90.0 90.0
Mosaicity (°)	0.20	0.20
Resolution range (Å)	48.88 – 2.51	85.90 – 2.79
Total N°. of reflections	1158971 (58614)	628934 (33155)
N°. of unique reflections	83804 (4191)	25329 (1230)
Completeness (ellipsoidal %)	95.5 (72.6)	95.6 (86.4)
Redundancy	13.8 (14.0)	24.8 (27.0)
$\langle I/\sigma(I) \rangle$	9.5 (1.5)	10.1 (2.0)
$CC_{1/2}$	0.995 (0.712)	0.990 (0.487)
R_{pim}	0.051 (0.459)	0.108 (0.689)
Overall <i>B</i> factor / Wilson plot (Å ²)	60.6	44.3
R-factor (%)	21.7	24.6
R _{free} -factor (%)	25.0	28.6
Ramachandran profile (%)		
Core	97.0	96.4
Allowed	3.0	3.6
Outliers	0.0	0.0
R.m.s. deviations		
Bond lengths (Å)	0.012	0.014
Bond angles (°)	1.56	1.55
Number of atoms	22600	5158
Macromolecules	21520	4893
Solvent	872	242
Other	208	23
B-factors (Å ²)		
All atoms	69.9	49.4
Macromolecules	69.8	49.6
Solvent atoms	54.5	39.0
Other atoms	147.3	103.3
PDB ID	7QPR	7QPS

Supplementary Table 2. SAXS parameters.

Theoretically and experimentally determined SAXS parameters of the different species. The quality of the SAXS-based models was assessed based on the metrics recently proposed by Rambo and Tainer.

Sample	R_g (Å)	D_{max} (Å)	V_P (Å ³)	V_C	Conformation
SpoT _{Ab}	37.0	102.9	1.6	625	τ-state
SpoT _{Ab} ^{L356D}	36.3	102.7	1.5	613	τ-state
SpoT _{Ab} ^{L356D}	40.6	135.3	1.7	742	relaxed state
SpoT _{Ab} ^{E379K/W382K}	35.8	103.9	1.4	607	relaxed state
SpoT _{Ab} ^{I637D/R614D}	35.6	103.1	1.3	583	τ-state
RelA _{Ab}	42.0	140.0	2.5	903	relaxed state
Rel _{Bs}	36.6	101.3	1.3	520	τ-state
Rel _{Bs}	41.0	139.4	1.8	696	relaxed state