

Supplementary Materials

Table S1. Intermolecular symmetry generated contacts within H-bond distance in SpeG structures.

Monomer	Open state	Intermediate state	Closed state
1	G95-N170, -x+3/2, y-1/2, -z+2 [a-b+2c] R100-R154, -x+3/2, y-1/2, -z+2 [a-b+2c] K129-R171, -x+3/2, y-1/2, -z+2 [a-b+2c] E136-N152, -x+3/2, y-1/2, -z+2 [a-b+2c] Y168-K129, -x+3/2, y-1/2, -z+2 [a-b+2c] R171-Q94, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-G95, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-F98, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-A99, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-R100, -x+3/2, y-1/2, -z+2 [a-b+2c]	R100-R154, -x+1/2, y+1/2, -z [-b+c] R100-E126, -x+1/2, y+1/2, -z [-b+c] R100-R154, -x+1/2, y+1/2, -z [-b+c] R104-E126, -x+1/2, y+1/2, -z [-b+c] K129-L169, -x+1/2, y+1/2, -z [-b+c] E173-G95, -x+1/2, y+1/2, -z [-b+c] E173-G97, -x+1/2, y+1/2, -z [-b+c] E173-F98, -x+1/2, y+1/2, -z [-b+c] E173-A99, -x+1/2, y+1/2, -z [-b+c] E173-R100, -x+1/2, y+1/2, -z [-b+c]	R100-R154, -x+1/2, y+1/2, -z [-a-b] E136-N152, -x+1/2, y+1/2, -z [-a-b] E173-G95, -x+1/2, y+1/2, -z [-a-b] E173-G97, -x+1/2, y+1/2, -z [-a-b] E173-F98, -x+1/2, y+1/2, -z [-a-b] E173-A99, -x+1/2, y+1/2, -z [-a-b] E173-R100, -x+1/2, y+1/2, -z [-a-b]
2	N170-G95, -x+3/2, y-1/2, -z+2 [a-b+2c] R171-K129, -x+3/2, y-1/2, -z+2 [a-b+2c]	L169-K129, -x+1/2, y+1/2, -z [c]	
3	Q94-R171, -x+3/2, y-1/2, -z+2 [a-b+2c] G95-E173-x+3/2, y-1/2, -z+2 [a-b+2c], F98-E173, -x+3/2, y-1/2, -z+2 [a-b+2c] A99-E173, -x+3/2, y-1/2, -z+2 [a-b+2c] R100-E173-x+3/2, y-1/2, -z+2 [a-b+2c], K129-Y168-x+3/2, y-1/2, -z+2 [a-b+2c], N152-E136, -x+3/2, y-1/2, -z+2 [a-b+2c] R154-R100, -x+3/2, y-1/2, -z+2 [a-b+2c]	G95-E173, -x+1/2, y+1/2, -z [c] G97-E173, -x+1/2, y+1/2, -z [c] F98-E173, -x+1/2, y+1/2, -z [c] A99-E173, -x+1/2, y+1/2, -z [c] R100-E173, -x+1/2, y+1/2, -z [c] E126-R100, -x+1/2, y+1/2, -z [c] E126-N104, -x+1/2, y+1/2, -z [c] R154-R100, -x+1/2, y+1/2, -z [c]	G95-E173, -x+1/2, y+1/2, -z [-a] G97-E173, -x+1/2, y+1/2, -z [-a] F98-E173, -x+1/2, y+1/2, -z [-a] A99-E173, -x+1/2, y+1/2, -z [-a] R100-E173, -x+1/2, y+1/2, -z [-a] N152-E136, -x+1/2, y+1/2, -z [-a] R154-R100, -x+1/2, y+1/2, -z [-a]
4	R100-R154, -x+1/2, y+1/2, -z+1 [c] K129-N170, -x+1/2, y+1/2, -z+1 [c] R171-N127, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-G95, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-G97, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-F98, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-A99, -x+3/2, y-1/2, -z+2 [a-b+2c] E173-R100, -x+3/2, y-1/2, -z+2 [a-b+2c]	R100-R154, -x+1/2, y+1/2, -z [-a] E136-N152, -x+1/2, y+1/2, -z [-a] E173-G95, -x+1/2, y+1/2, -z [-a] E173-G97, -x+1/2, y+1/2, -z [-a] E173-F98, -x+1/2, y+1/2, -z [-a] E173-A99, -x+1/2, y+1/2, -z [-a] E173-R100, -x+1/2, y+1/2, -z [-a]	R100-R154, -x+1/2, y+1/2, -z [-a-c] D108-K129, -x+1/2, y+1/2, -z [-a-c] R171-N127, -x+1/2, y+1/2, -z [-a-c] E173-F98, -x+1/2, y+1/2, -z [-a-c] E173-A99, -x+1/2, y+1/2, -z [-a-c] E173-R100, -x+1/2, y+1/2, -z [-a-c]
5	R154-E136, -x+1/2, y+1/2, -z+1 [+c] N170-K129, -x+1/2, y-1/2, -z+1 [-b+c]		
6	G95-E173, -x+1/2, y-1/2, -z+1 [-b+c] G97-E173, -x+1/2, y-1/2, -z+1 [-b+c] F98-E173, -x+1/2, y-1/2, -z+1 [-b+c] A99-E173, -x+1/2, y-1/2, -z+1 [-b+c] R100-E173, -x+1/2, y-1/2, -z+1 [-b+c] N127-R171, -x+1/2, y-1/2, -z+1 [-b+c] E136-R154, -x+1/2, y-1/2, -z+1 [-b+c] R154-R100, -x+1/2, y-1/2, -z+1 [-b+c]	G95-E173, -x+1/2, y+1/2, -z [-a-b] G97-E173, -x+1/2, y+1/2, -z [-a-b] F98-E173, -x+1/2, y+1/2, -z [-a-b] A99-E173, -x+1/2, y+1/2, -z [-a-b] R100-E173, -x+1/2, y+1/2, -z [-a-b] E126-R104, -x+1/2, y+1/2, -z [-a-b] K129-D108, -x+1/2, y+1/2, -z [-a-b] N152-E136, -x+1/2, y+1/2, -z [-a-b] R154-R100, -x+1/2, y+1/2, -z [-a-b]	F98-E173, -x+1/2, y+1/2, -z [-a-b-c] A99-E173, -x+1/2, y+1/2, -z [-a-b-c] R100-E173, -x+1/2, y+1/2, -z [-a-b-c] K129-D108, -x+1/2, y+1/2, -z [-a-b-c] R154-R100, -x+1/2, y+1/2, -z [-a-b-c]

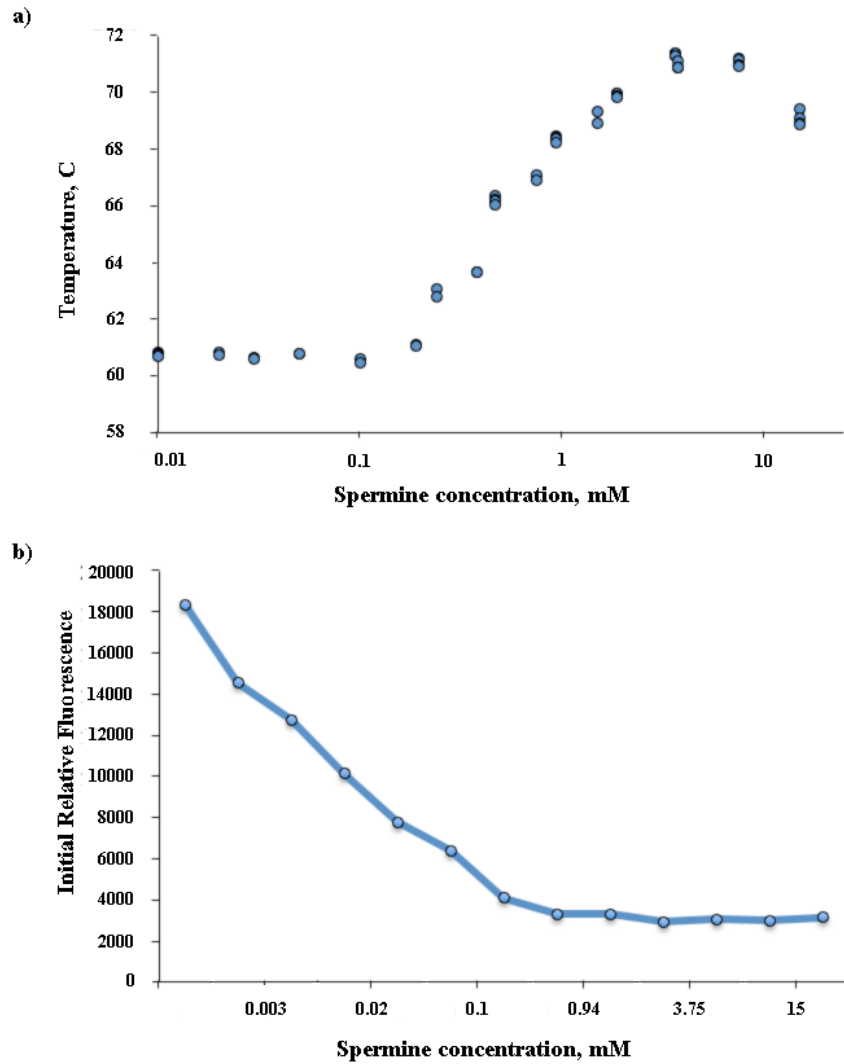


Figure S1. Fluorescence thermal shift analysis. Plots of ΔT_m (a) and initial relative fluorescence (b) vs spermine concentration. (a) Above 0.1 mM of spermine the significant increase in the temperature (T_m maximum is 71.3 °C at 3.7 mM of spermine) indicates polyamine binding. The transition progressively goes down when the spermine concentration increases (> 10 mM). (b) Plot shows the initial relative fluorescence vs spermine concentration at low temperature.

Table S2. Volume fractions of possible SpeG oligomeric states in absence and presence of polyamine calculated in the program OLIGOMER.

SpeG concentration mg/mL	χ^2	R _g Å	Dodecamer apo-close/spermine-close %	Dodecamer apo-open/apo-intermediate %	Decamer %	Octamer %	Hexamer I/II %	Tetramer %	Dimer %	Monomer %
SpeG oligomeric states in ligand-free form										
0.45	0.18	35.0	0/0	0/0	20.7	0	0/0	31.4	42.7	5.2
0.9	0.19	36.8	0/0	24.3/0	0	0	0/0	43.1	29.1	3.5
1.8	0.22	38.5	0/0	36.1/0	0	0	0/0	47.0	16.9	0
3.6	0.25	39.7	0/0	45.2/0	0	4.7	0/0	45.2	5.0	0
7.2	0.54	40.3	0/0	33.6/0	0	50.3	0/0	14.8	1.3	0
SpeG oligomeric states in presence of spermine										
0.4	0.22	42.6	33.1/0	66.9/0	0	0	0/0	0	0	0
0.8	0.35	42.5	35.2/0	64.8/0	0	0	0/0	0	0	0
1.6	0.51	42.5	31.7/11.4	56.9/0	0	0	0/0	0	0	0
3.3	0.83	42.4	28.7/23.2	48.1/0	0	0	0/0	0	0	0
7.2	0.96	42.1	45.6/25.3	29.1/0	0	0	0/0	0	0	0

Dodecamer apo-close is calculated from the close structure from the C2 space group (Figure 3b); Dodecamer spermine-close is calculated from the close structure with spermine in I222 space group (Figure 3d); Dodecamer apo-open is calculated from the open structure in the C2 space group (Figure 3a); and Dodecamer apo-intermediate is calculated from the intermediate state in the C2 spacegroup (Figure 3c). Zeroes above indicate that the calculated scattering was included in the OLIGOMER fitting but gave a result of 0.0%. The decrease in open dodecamer from 3.3 to 7.2 mg/mL and increase of octamer is likely an anomaly due to the influence of the structure factor, which could not be removed for these data.

Table S3. Volume fractions of a minimal set of possible SpeG oligomeric states in absence and presence of polyamine calculated in the program OLIGOMER.

SpeG concentration mg/mL	χ^2	R_g Å	Dodecamer apo-open/ spermine-close %	Tetramer %	Dimer %	Monomer %
SpeG oligomeric states in ligand-free form						
0.45	0.18	35.0	16.6/-	32.6	42.1	8.7
0.9	0.19	36.8	24.3/-	43.1	29.1	3.5
1.8	0.22	38.5	36.1/-	47.0	16.9	0
3.6	0.25	39.7	47.3/-	48.2	4.5	0
7.2	0.74	40.6	57.4/-	42.6	0	0
SpeG oligomeric states in presence of spermine						
0.4	0.22	42.6	66.9/33.1	-	-	-
0.8	0.35	42.5	64.8/35.2	-	-	-
1.6	0.51	42.5	61.3/38.6	-	-	-
3.3	0.85	42.4	57.4/42.6	-	-	-
7.2	1.01	42.1	38.7/61.3	-	-	-

Dodecamer spermine-close is calculated from the close structure with spermine in I222 space group (Figure 3d); Dodecamer apo-open is calculated from the open structure in the C2 space group (Figure 3a). A minimal set of states were produced by first eliminating those which were zero in the previous calculation (Table S2) for the medium concentrations where the data had both good signal to noise and minimal structure factor. Additionally the apo-close form was removed due to its similarity to the spermine-close form. There is minimal impact on the χ^2 value and no change in the calculated scattering curves as compared to the fitting of the full set (Table S2).