Data Report

Jay Doe

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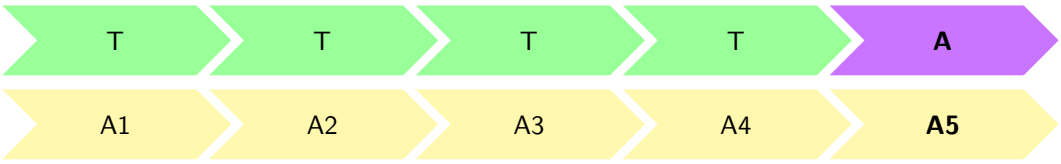
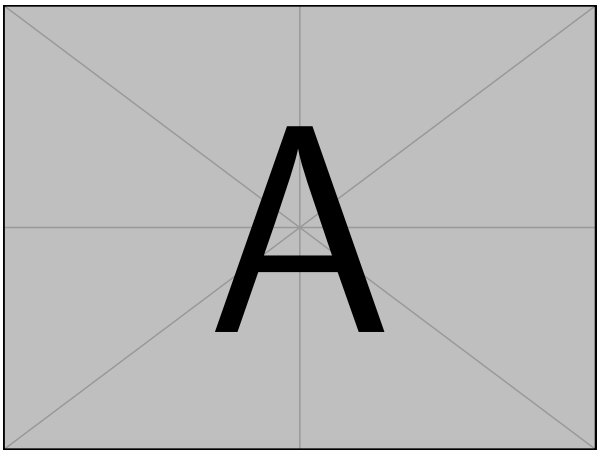
Analyses

1. Overview

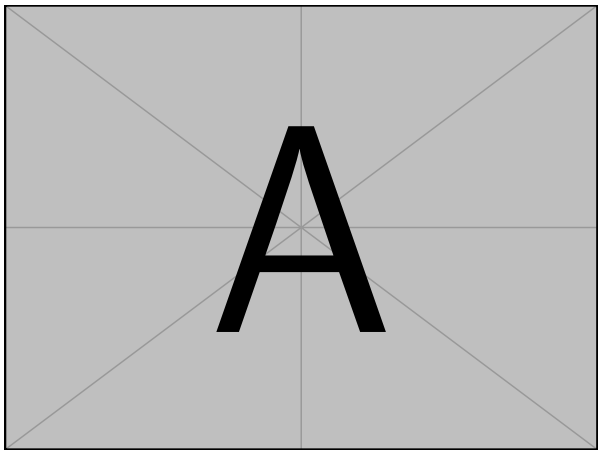
1.1. Example Nucleic Acid



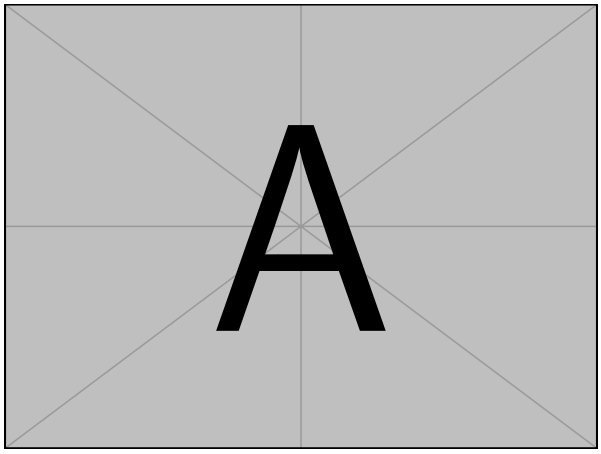
2. X-X Distances



(a) R1

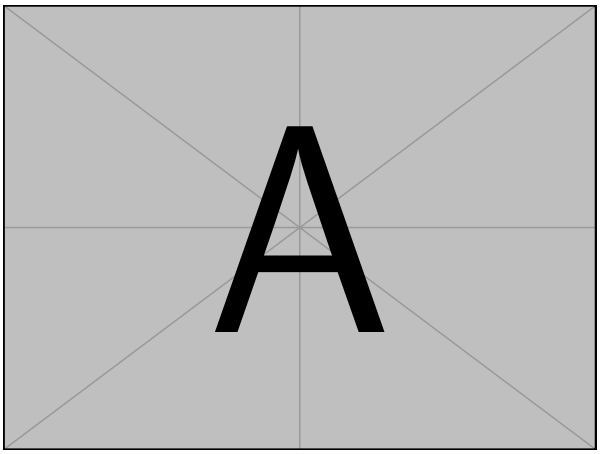


(b) R2

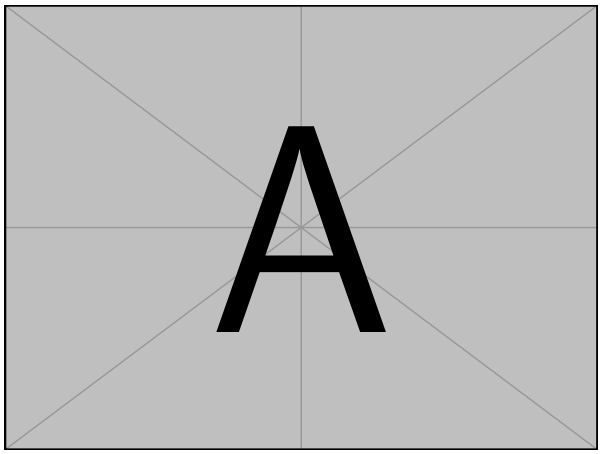


(c) R3

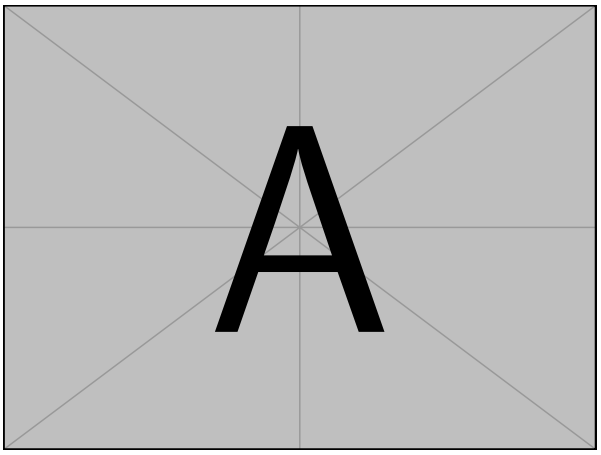
Figure 1: X-X distances for the R systems.



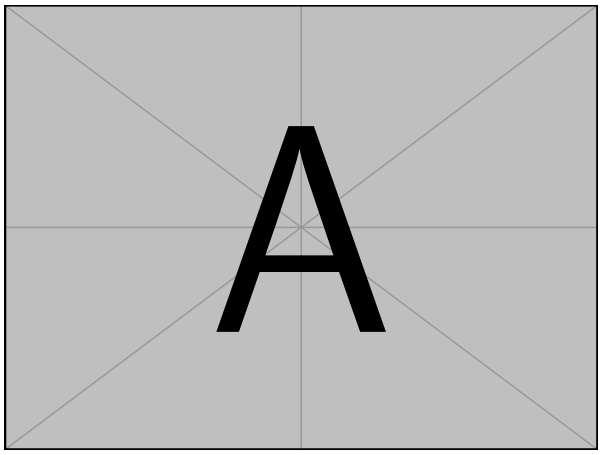
(a) S1



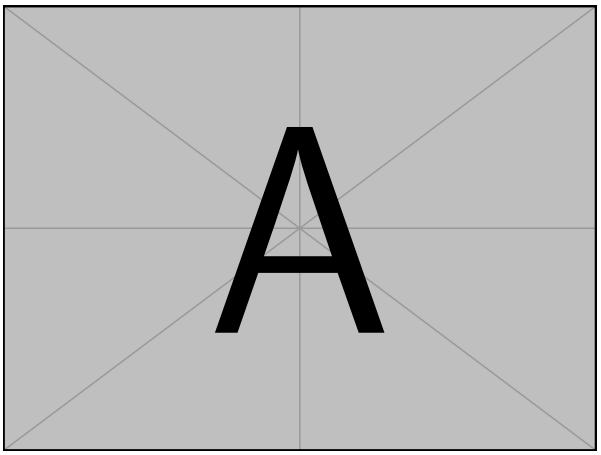
(b) S2



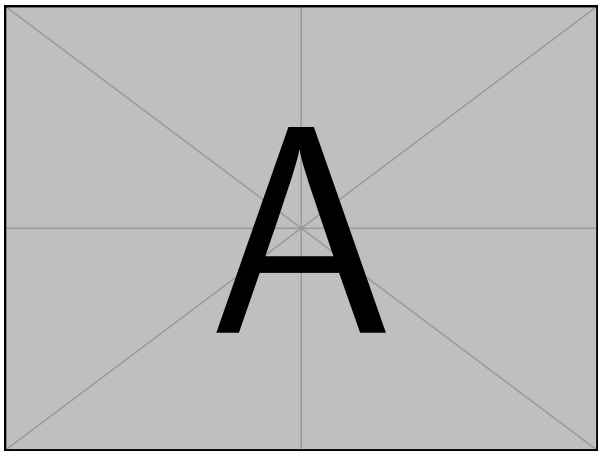
(c) S3



(d) S4



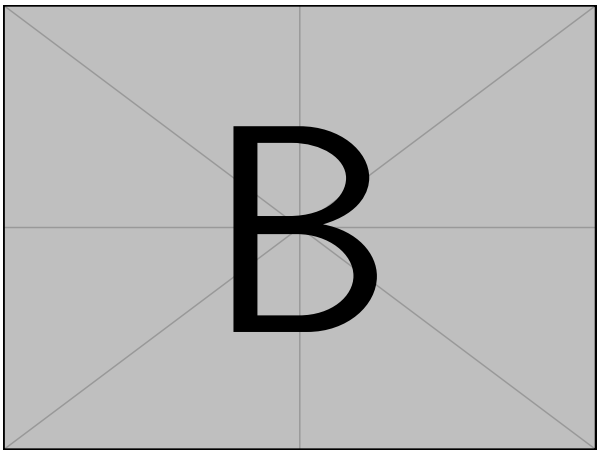
(e) S5



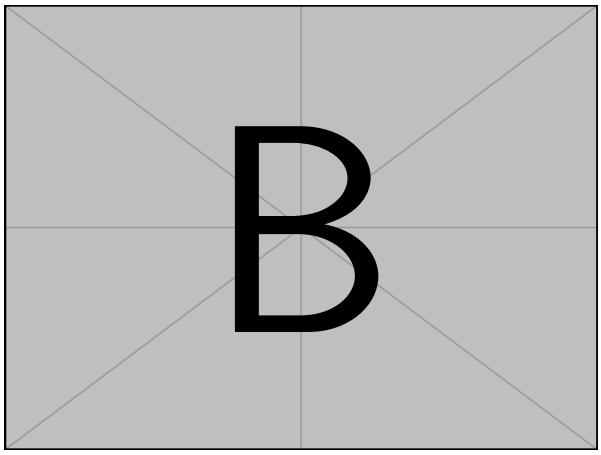
(f) S6

Figure 2: X-X distances for the S systems.

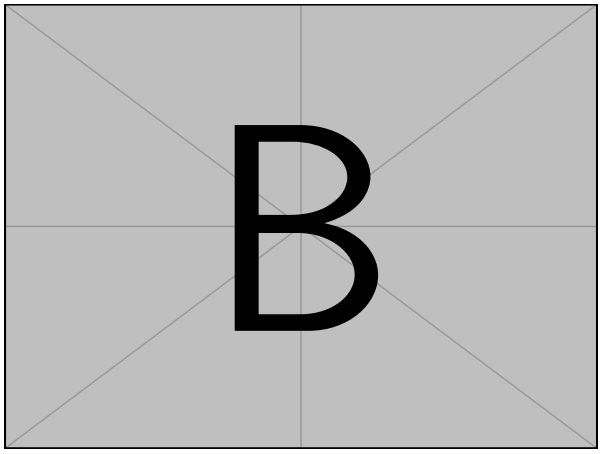
3. Backbone RMSD



(a) R1

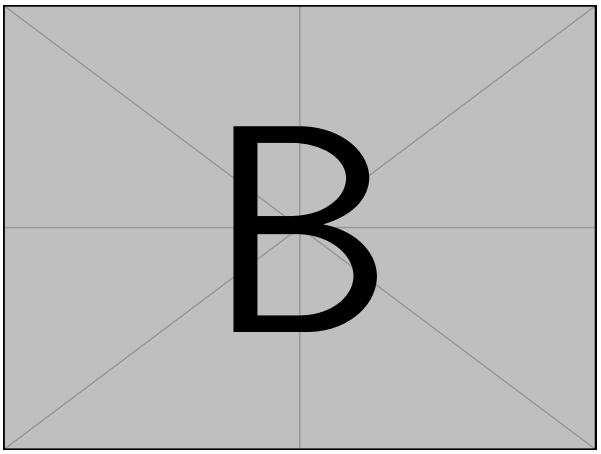


(b) R2

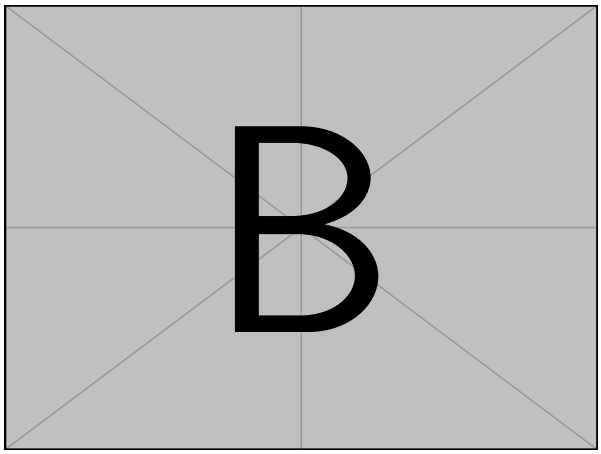


(c) R3

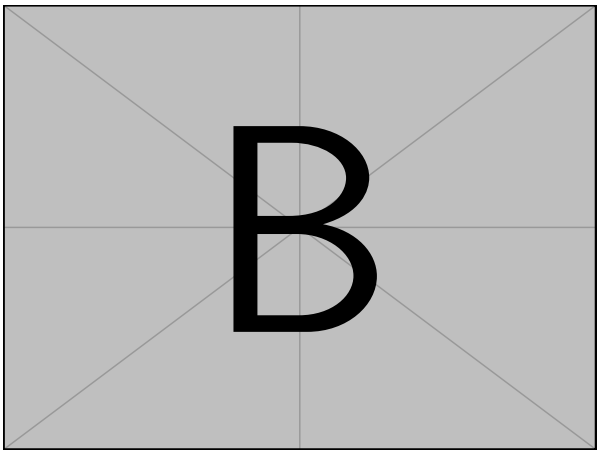
Figure 3: Root mean square deviation (RMSD) for the backbone of the R systems.



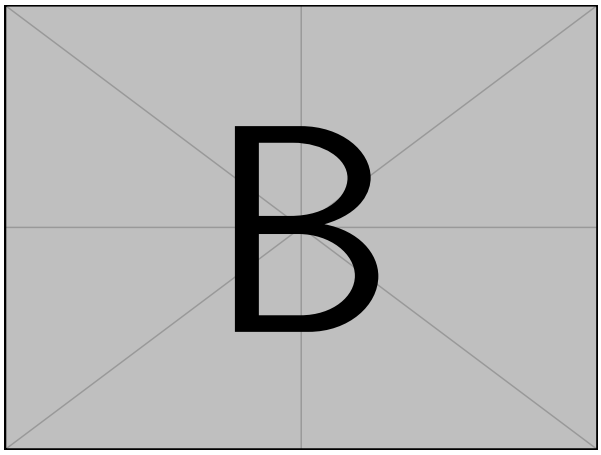
(a) S1



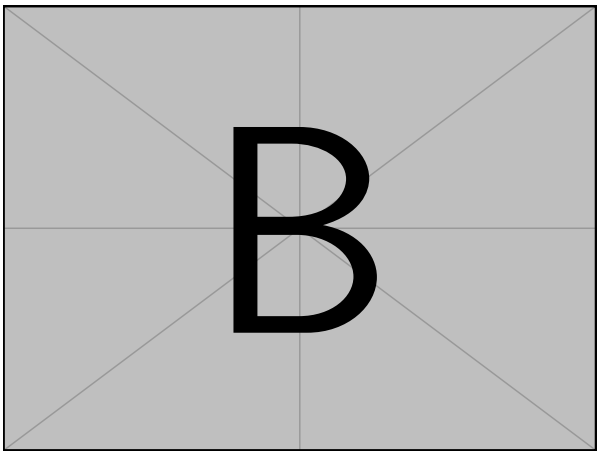
(b) S2



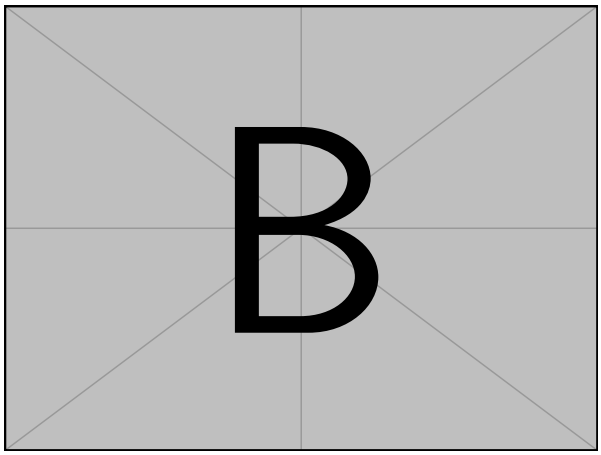
(c) S3



(d) S4



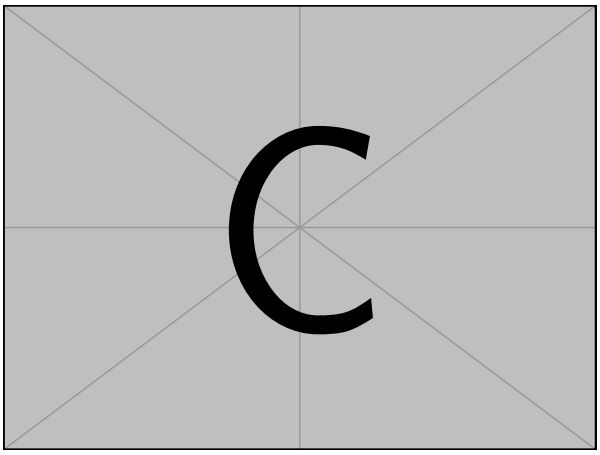
(e) S5



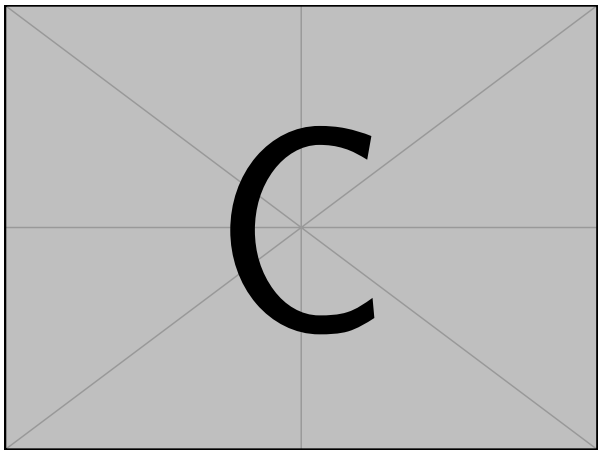
(f) S6

Figure 4: Root mean square deviation (RMSD) for the backbone of the S systems.

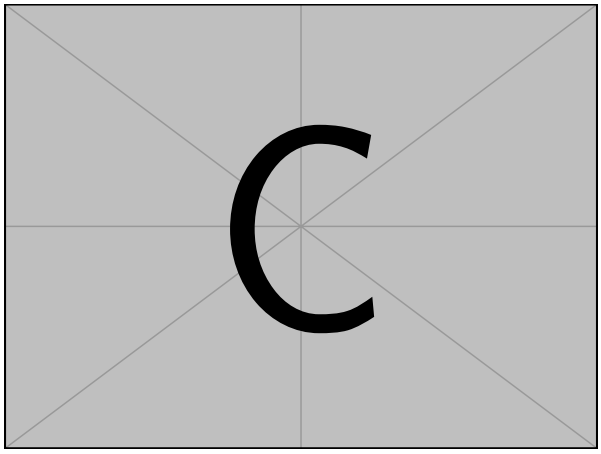
4. Root Mean Square Fluctuations



(a) R1

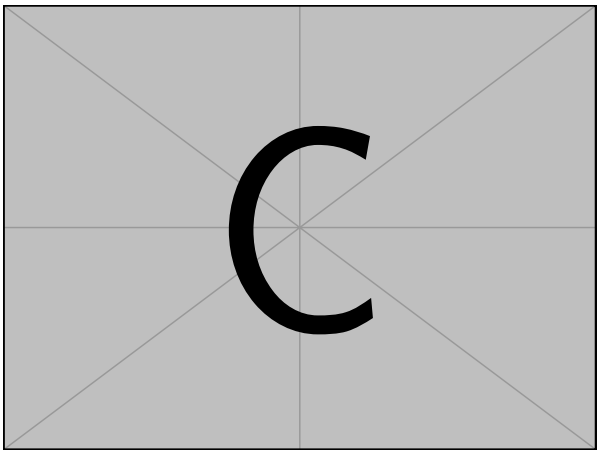


(b) R2

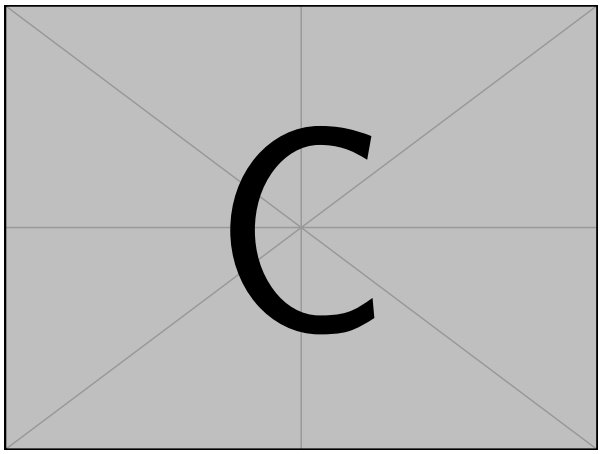


(c) R3

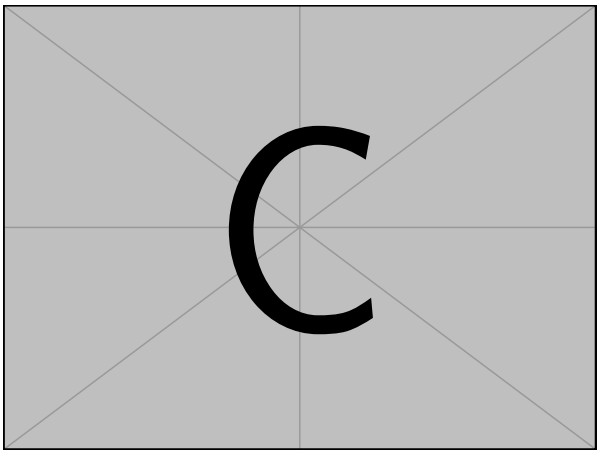
Figure 5: Root mean square fluctuation (RMSF) for the backbone of the R systems.



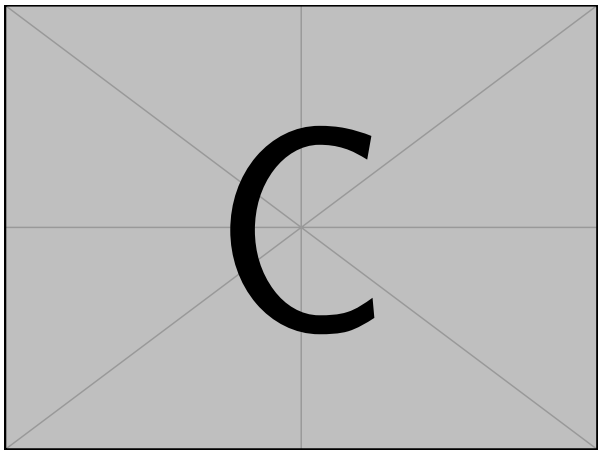
(a) S1



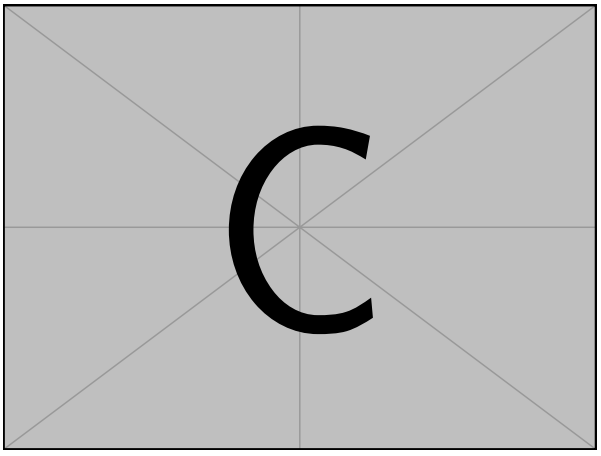
(b) S2



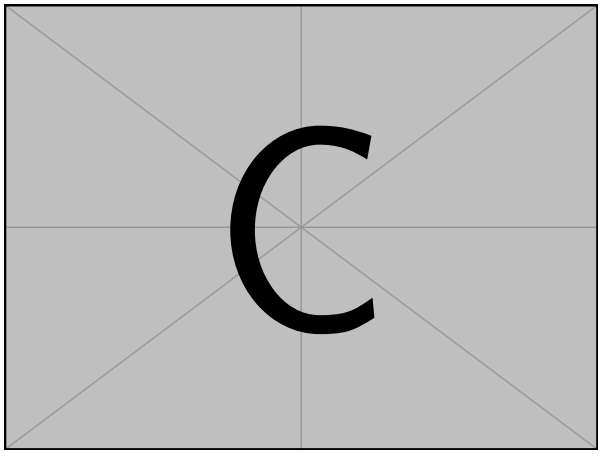
(c) S3



(d) S4



(e) S5



(f) S6

Figure 6: Root mean square fluctuation (RMSF) for the backbone of the S systems.

5. Hydrogen Bond Analysis

Table 1: Selected values for hydrogen bond interactions across total simulation time. All values are an average of the total simulation time for each replicate (%). Acceptor–donor interactions affected at a 20 % threshold are highlighted yellow, at a 50 % threshold are highlighted orange, and at an 80 % threshold are highlighted purple.

Acceptor	Donor	WT A	A123B	A123C	A123D	A123E	A123F
C112@O	S122@N	1.00	60.00	61.00	-	62.00	63.00
R543@O	R532@NH2	1.00	-	-	82.00	83.00	85.00
G302@O	R938@N1	80.00	45.00	47.00	48.00	49.00	50.00