SUPPLEMENTARY INFORMATION

Combinatorial Virtual Library Screening Study of Transforming Growth Factor Beta-2 – Chondroitin Sulfate System

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10          20          30          40          50
MHYCVLSAFL  ILHLVTVALS  LSTCSTLDMD  QFMRKRIEAI  RGQILSKLKL
        60          70          80          90         100
TSPPEDYPEP  EEVPPEVISI  YNSTRDLLQE  KASRRAAACE  RERSDEEYYA
       110         120         130         140         150
KEVYKIDMPP  FFPSENAIPP  TFYRPYFRIV  RFDVSAMEKN  ASNLVKAEFR
       160         170         180         190         200
VFRLQNPKAR  VPEQRIELYQ  ILKSKDLTSP  TQRYIDSKVV  KTRAEGEWLS
       210         220         230         240         250
FDVTDAVHEW  LHHKDRNLGF  KISLHCPCCT  FVPSNNYIIP  NKSEELEARF
       260         270         280         290         300
AGIDGTSTYT  SGDQKTIKST  RKKNSGKTPH  LLLMLLPSYR  LESQQTNRRK
       310         320         330         340         350
KRALDAAYCF  RNVQDNCCLR  PLYIDFKRDL  GWKWIHEPKG  YNANFCAGAC
       360         370         380         390         400
PYLWSSDTQH  SRVLSLYNTI  NPEASASPCC  VSQDLEPLTI  LYYIGKTPKI
       410
EQLSNMIVKS  CKCS
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TGF-β2

Figure S1. The sequence of TGF-β2 extracted from Uniprot ID: P61812. The region of TGF-β2 is shown in gray. The mapping of potential GAG binding was done by considering the presence of Cardin and Weintraub consensus sequence motif ([–XBBXBX–] and [–XBBBXXBX–]; B = basic residue and X = hydropathic residue.). The sequence region belonging to TGF-β2 did not show any consensus sequence pattern. See Methods for details.
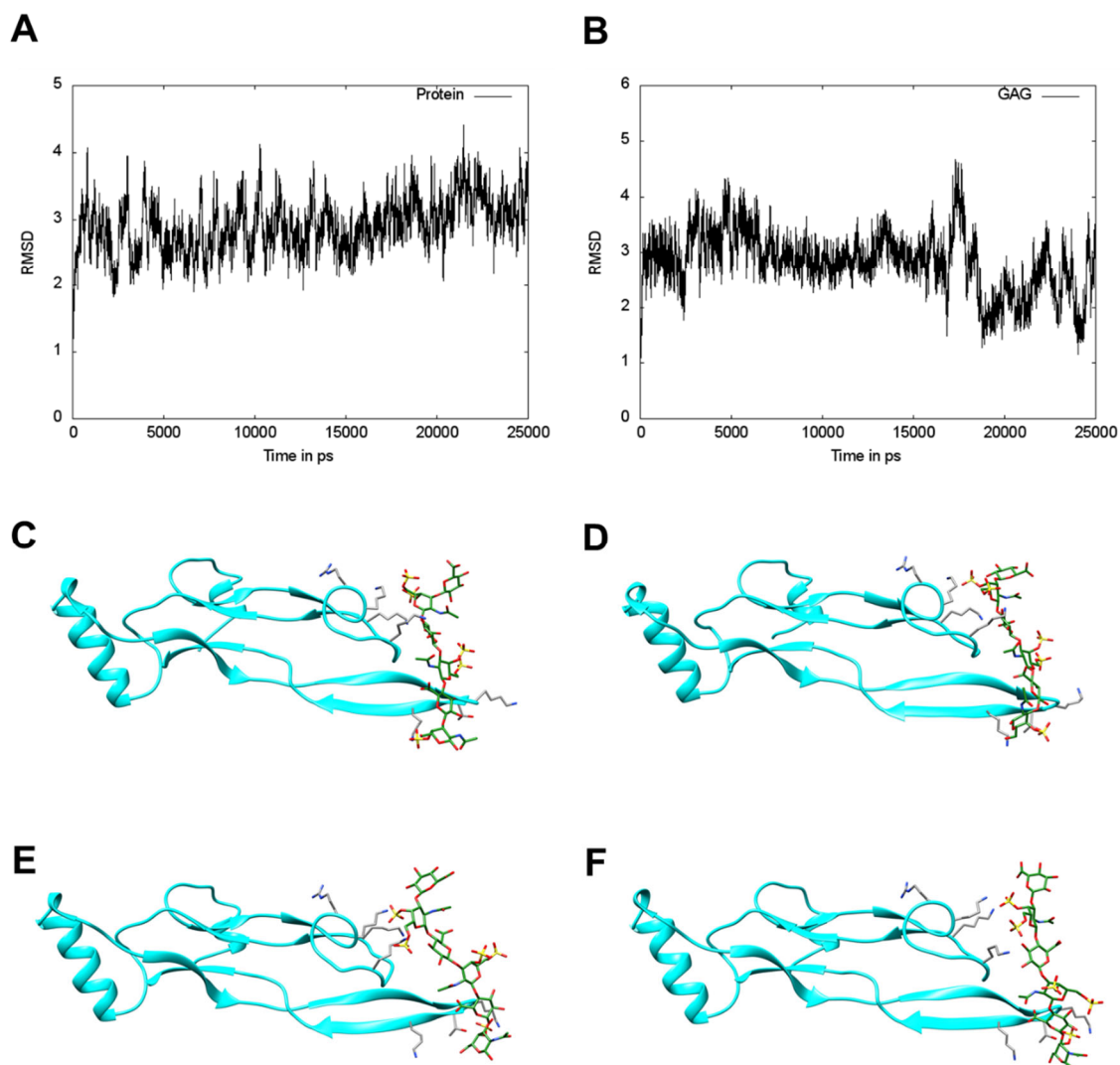
Figure S2. Conformational sampling of CS06 bound in BS1 of TGF-β2 from MD simulation to give an overall picture on the movement of protein (A) and ligand (B) was in presence of solvent (see **Movie SM1**). (C) through (F) show representative frames of the MD simulation showing the bound hexasaccharide (in green sticks) and the interacting residues (shown as sticks). See Methods for details.
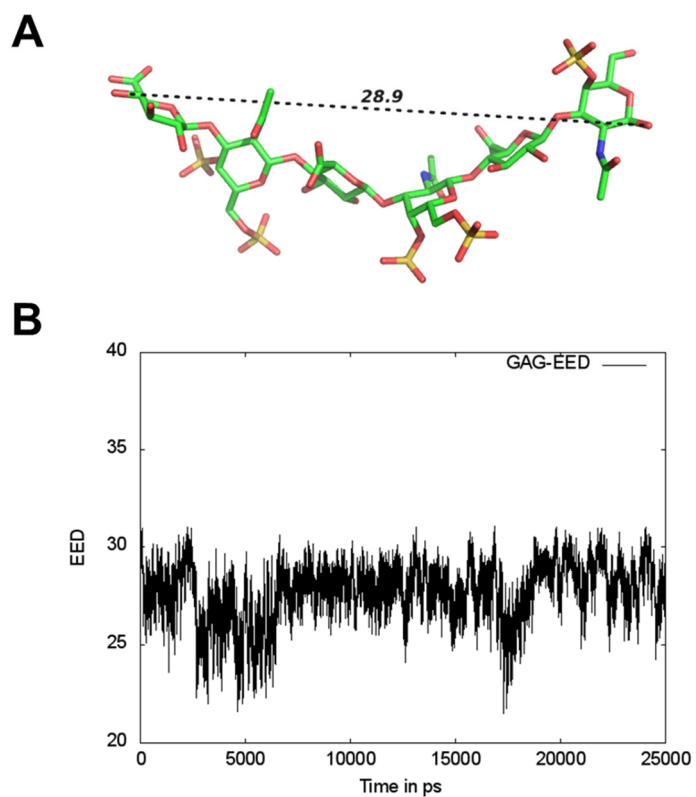
A

B

Figure S3. Conformational space exploration of TGF-β2-CS06 complex in BS1. A) A representative structure showing the end-to-end distance (EED) of the CS06. B) Time-based fluctuation of the EED during the MD simulation for the bound CS06.
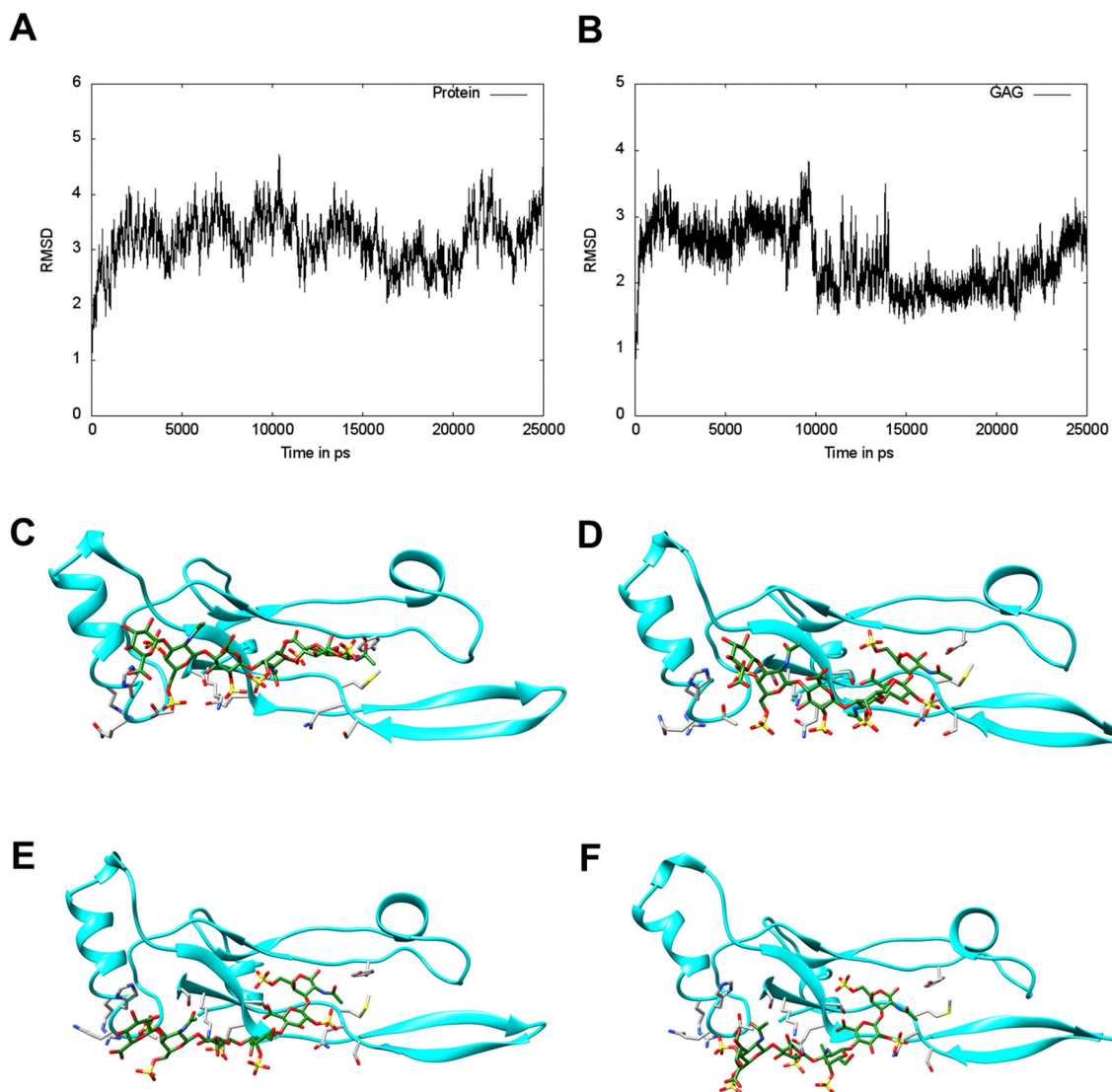
Figure S4. Conformational sampling of CS06 bound in BS2 of TGF-β2 from MD simulation to give an overall picture on the movement of protein (A) and ligand (B) was in presence of solvent (see **Movie SM2**). (C) through (F) show representative frames of the MD simulation showing the bound hexasaccharide (in green sticks) and the interacting residues (shown as sticks). See Methods for details.
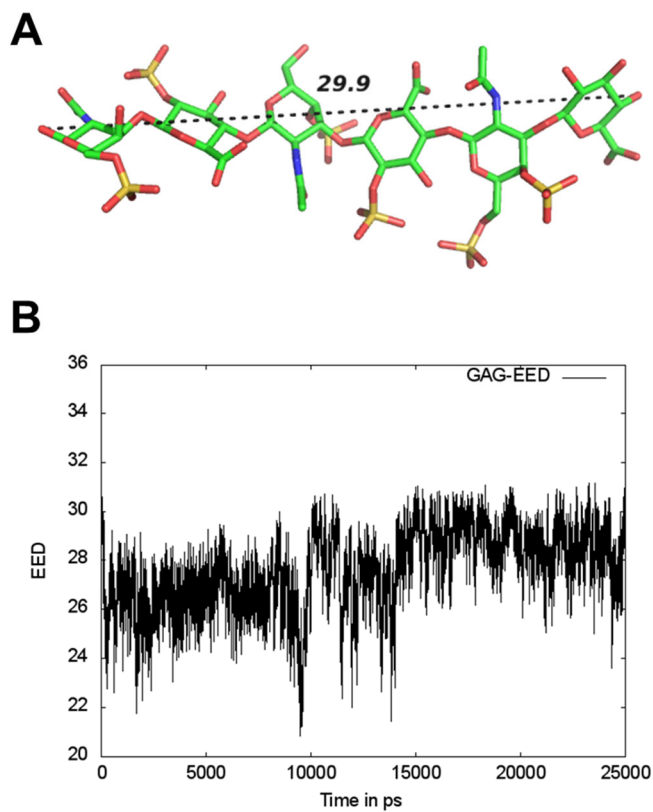
A

B

Figure S5. Conformational space exploration of TGF-β2-CS06 complex in BS2. A) A representative structure showing the end-to-end distance (EED) of the CS06. B) Time based fluctuation of the EED during the MD simulation for the bound CS06.
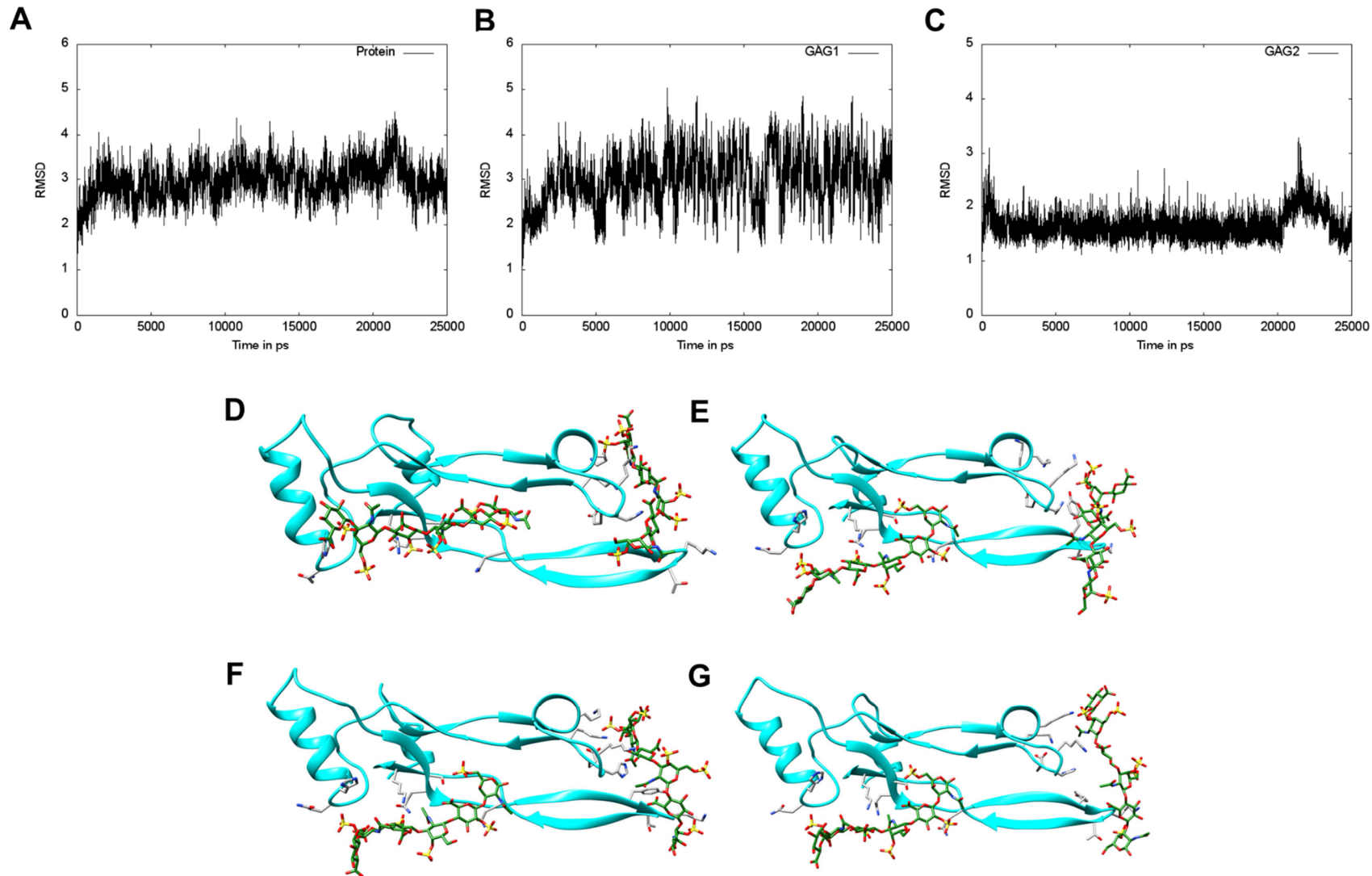
Figure S6. Conformational sampling of two CS06 sequences simultaneously bound in BS1 and BS2 of TGF-β2 from MD simulation to give an overall picture on the movement of protein (A) and ligand (B) was in presence of solvent (see **Movie SM3**). (C) through (F) show representative frames of the MD simulation showing the bound hexasaccharides (in green sticks) and the interacting residues (shown as sticks). See Methods for details.
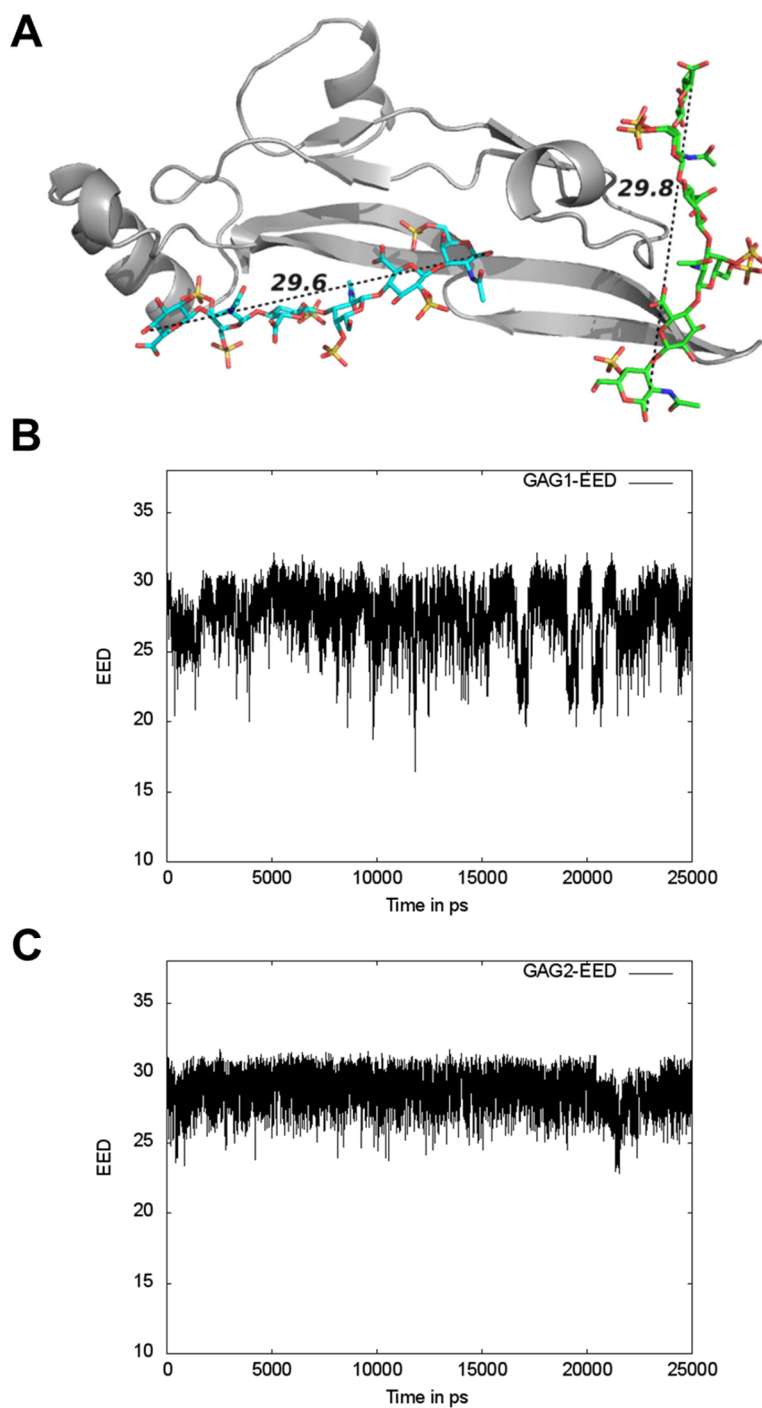
Figure S7. Conformational sampling of two CS06 sequences simultaneously bound in BS1 and BS2 of TGF-β2. A) A representative structure showing the end-to-end distance (EED) of the CS06. B) Time based fluctuation of the EED during the MD simulation for the bound CS06.