Supporting Information

The role of the oligosaccharide chain polarity in protein-glycosaminoglycan interactions

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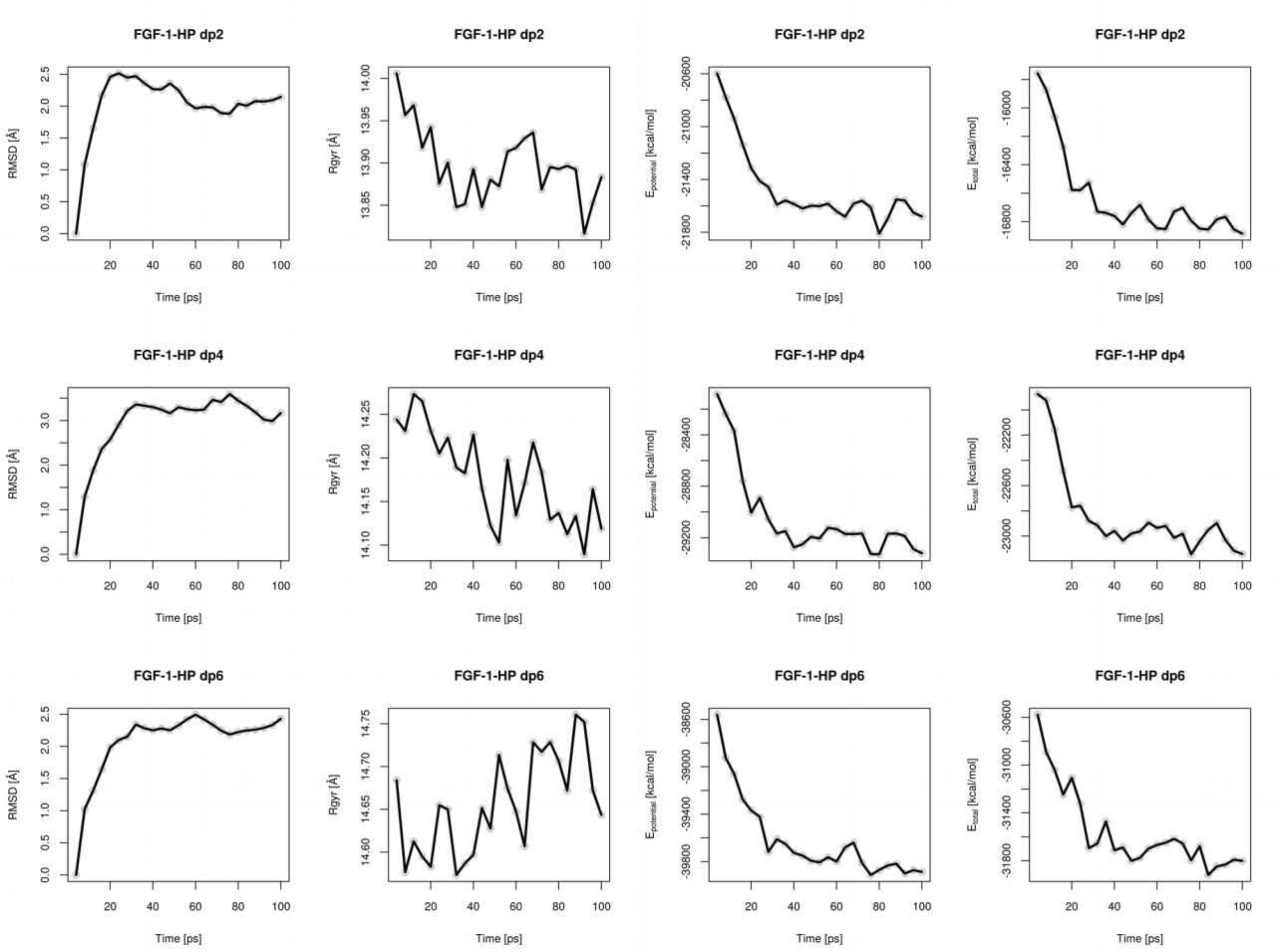

Figure S1: Equilibration of dynamic and thermodynamic parameters in FGF-1-HP systems.

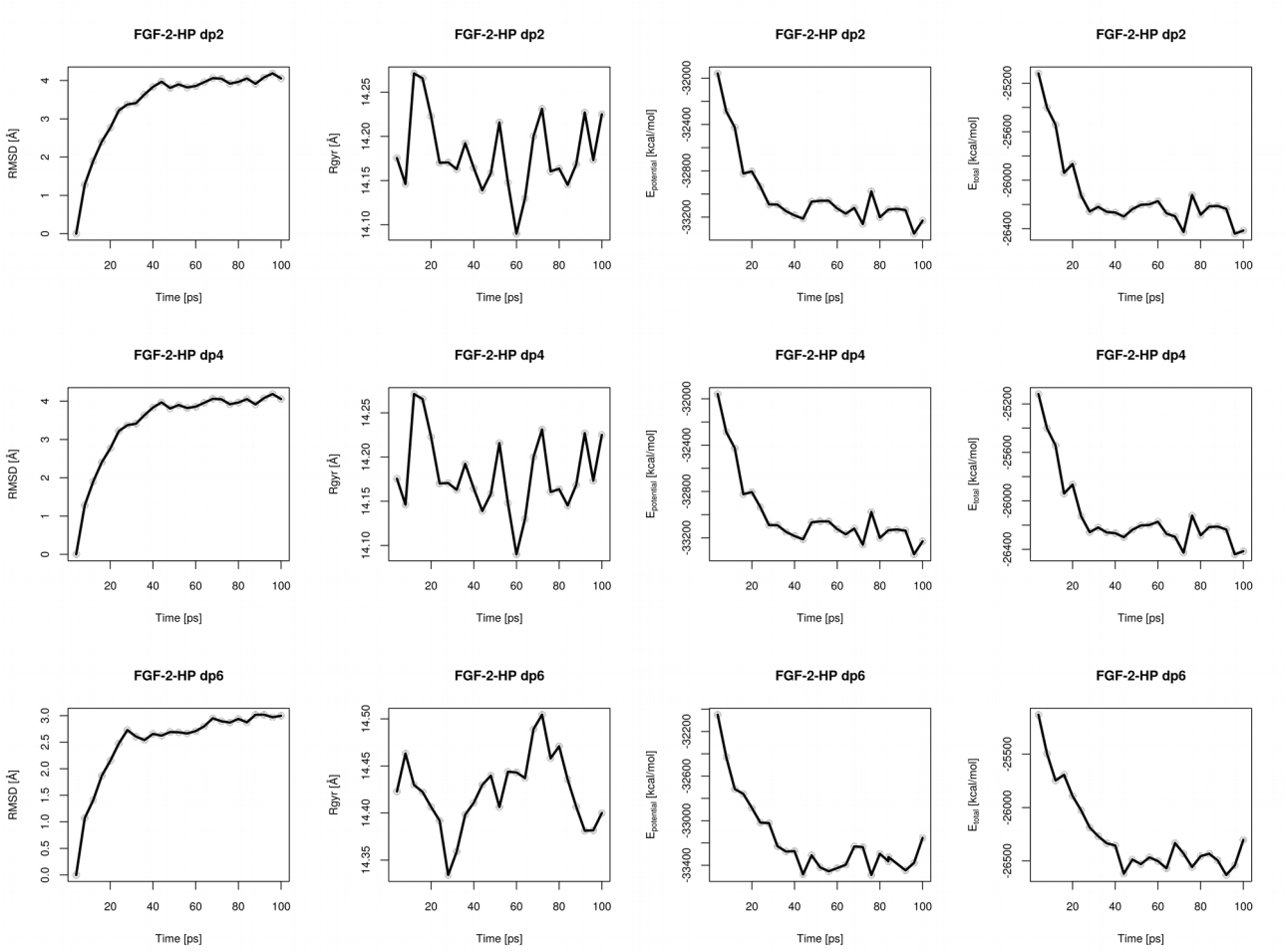

Figure S2: Equilibration of dynamic and thermodynamic parameters in FGF-2-HP systems.

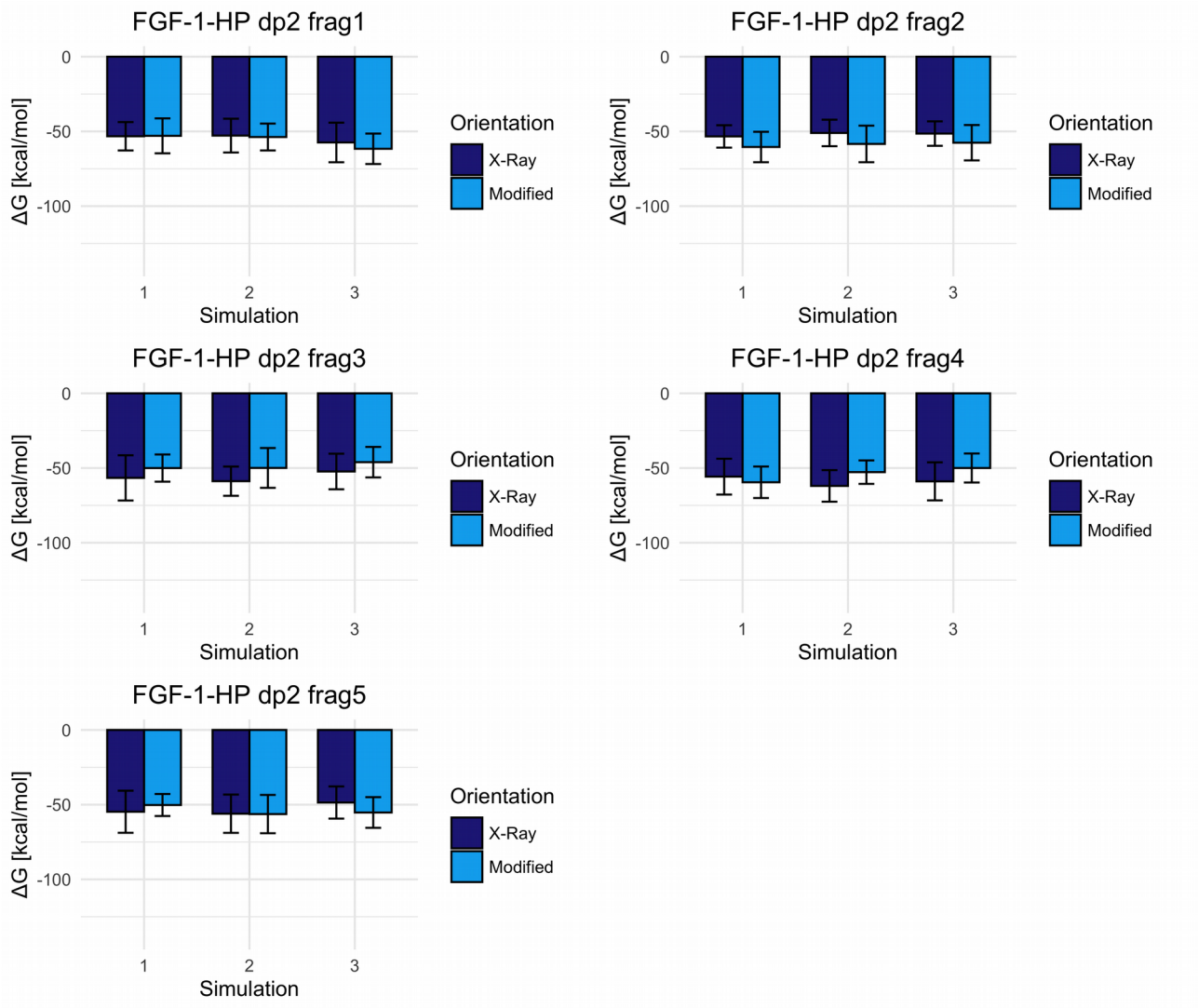

Figure S3: Binding free energies for different HP fragments of FGF-1-HP dp2 complexes. The X-Ray and Modified represent the ΔG values for FGF-1-HP complexes with HP in parallel and antiparallel orientation, respectively. Each simulation was repeated three times.

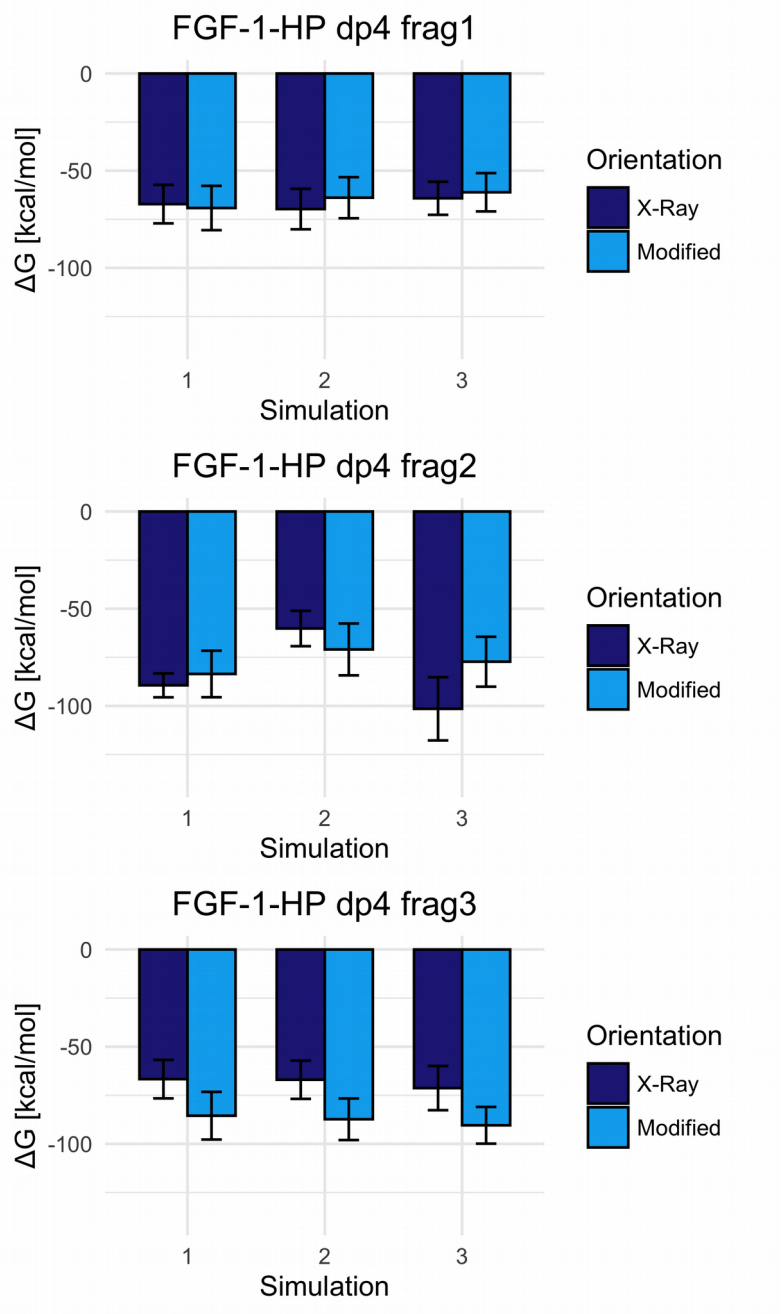

Figure S4: Binding free energies for different HP fragments of FGF-1-HP dp4 complexes. The X-Ray and Modified represent the ΔG values for FGF-1-HP complexes with HP in parallel and antiparallel orientation, respectively. Each simulation was repeated three times.

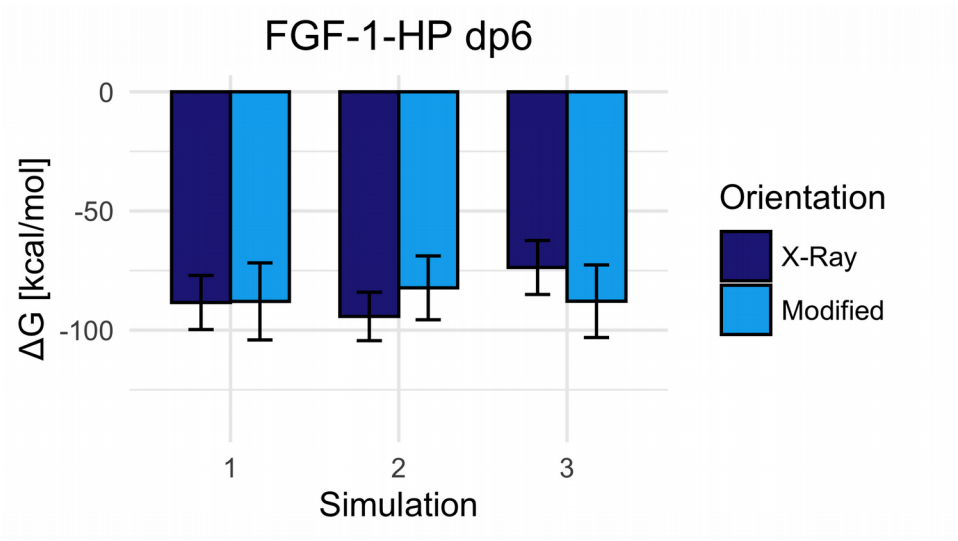

Figure S5: Binding free energies for FGF-1-HP dp6 complexes. The X-Ray and Modified represent the ΔG values for FGF-1-HP complexes with HP in parallel and antiparallel orientation, respectively. Each simulation was repeated three times.

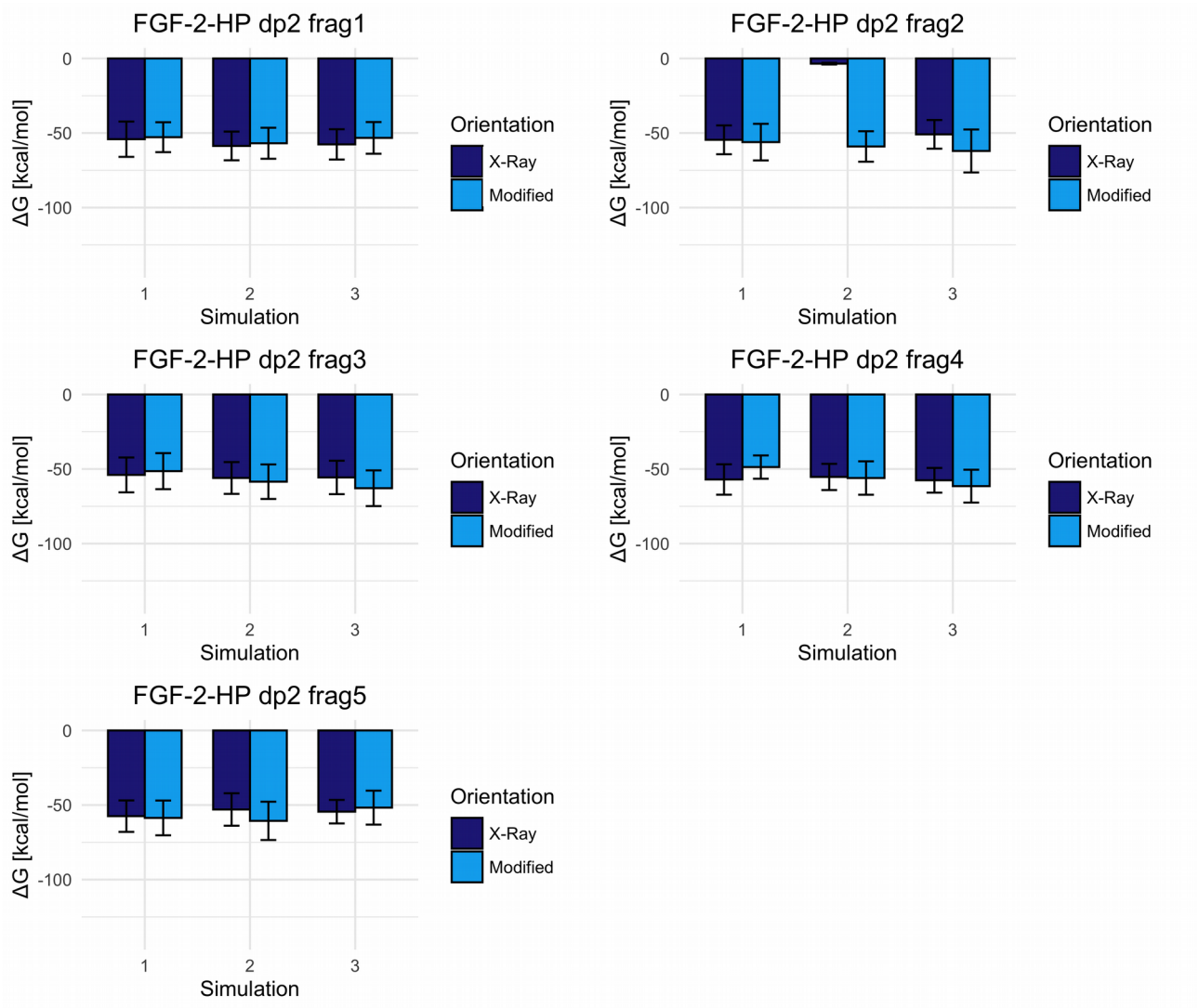

Figure S6: Binding free energies for different HP fragments of FGF-2-HP dp2 complexes. The X-Ray and Modified represent the ΔG values for FGF-2-HP complexes with HP in parallel and antiparallel orientation, respectively. Each simulation was repeated three times.

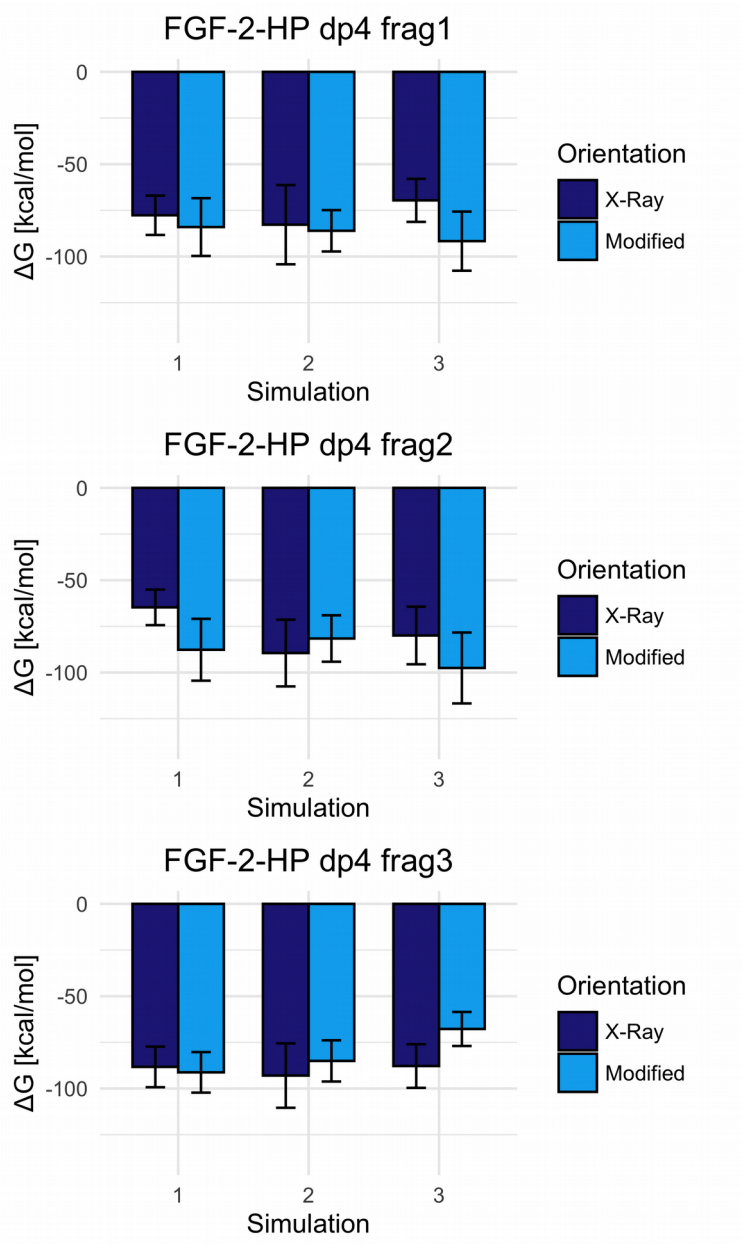

Figure S7: Binding free energies for different HP fragments of FGF-2-HP dp4 complexes. The X-Ray and Modified represent the ΔG values for FGF-2-HP complexes with HP in parallel and antiparallel orientation, respectively. Each simulation was repeated three times.

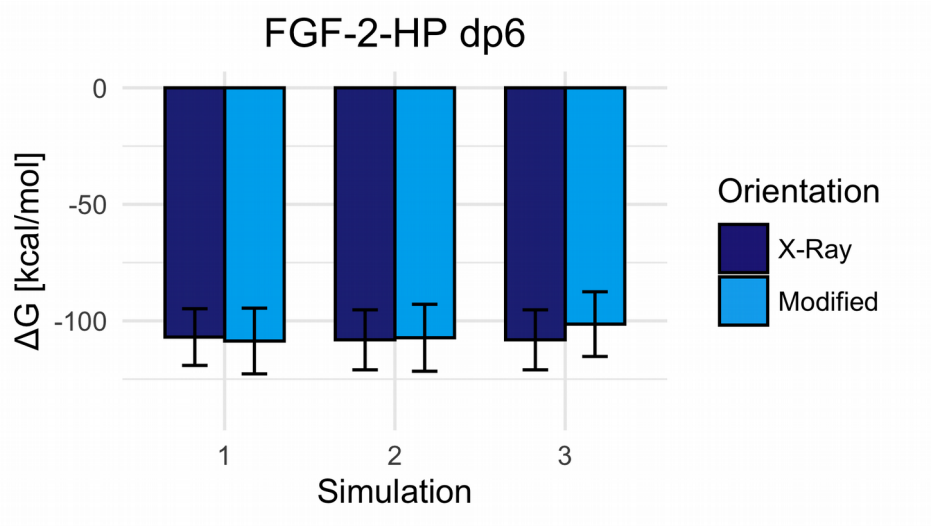

Figure S8: Binding free energies for FGF-1-HP dp6 complexes. The X-Ray and Modified represent the ΔG values for FGF-1-HP complexes with HP in parallel and antiparallel orientation, respectively. Each simulation was repeated three times.

Table S1. H-bonding patterns for X-Ray, Modified and intermediate orientations.

Donor	Acceptor	Occupancy [%]
X-Ray		
K110:NZ	GlcNS(6S)3:N-sulfate	76
K104:NZ	GlcNS(6S)3:N-sulfate	64
A121:N	IdoA(2S)2:O-sulfate	58
K120:N	IdoA(2S)2:O-sulfate	49
K105:N	GlcNS(6S)3:N-sulfate	48
K105:NZ	IdoA(2S)2:COO^-	38
R114:NH	IdoA(2S)4:COO^-	33
N10:ND	GlcNS(6S)3:N-sulfate	25
Modified		
N10:ND	IdoA(2S)2:O-sulfate	81
K110:NZ	IdoA(2S)2:O-sulfate	67
K105:N	IdoA(2S)2:O-sulfate	52
K110:NZ	GlcNS(6S)1:O-sulfate	44
K120:NZ	IdoA(2S)4:COO^-	41
K120:N	GlcNS(6S)3:N-sulfate	36
K104:NZ	GlcNS(6S)1:O5	29
K105:NZ	IdoA(2S)4:O5	29
R114:NE	GlcNS(6S)1:O-sulfate	27
R114:NH	GlcNS(6S)1:O-sulfate	21
Intermediate 1: –59.0°		
K110:NZ	GlcNS(6S)3:N-sulfate	78
K105:N	GlcNS(6S)3:N-sulfate	71
N10:ND	GlcNS(6S)3:N-sulfate	63
Q119:NE	GlcNS(6S)1:O-sulfate	39
K120:NZ	IdoA(2S)4:COO^-	33
K120:NZ	IdoA(2S)4:O5	22
K120:N	IdoA(2S)2:O3	21
Intermediate 2: 137.0°		
R114:NH	IdoA(2S)4:COO^-	79
K110:NZ	GlcNS(6S)3:N-sulfate	53
K105:N	IdoA(2S)2:O-sulfate	40
R114:NE	GlcNS(6S)3:N-sulfate	33
K110:NZ	IdoA(2S)2:O-sulfate	31
N10:ND	IdoA(2S)2:O-sulfate	24

The number of GAG residue (numbers increase from reducing to non-reducing end) is shown after the GAG residue name. The name of the atom/group is indicated after ":".

Only H-bonds with occupancy > 20 % are listed.

Table S2. Similarity between H-bonding patterns for X-Ray, Modified and intermediate orientations.

	X-Ray	Modified	Intermediate 1	Intermediate 2
X-Ray	8/8	0/8	4/8	2/8
Modified	0/10	10/10	1/10	3/10
Intermediate 1	4/7	1/7	7/7	1/7
Intermediate 2	2/6	3/6	1/6	6/6

The number prior to "/" corresponds to the number of common H-bonds, while the number after "/" corresponds to the total number of H-bonds each conformation.

Table S3. Similarity between amino acid residues participating in H-bond formation for X-Ray, Modified and intermediate orientations.

	X-Ray	Modified	Intermediate 1	Intermediate 2
X-Ray	7/7	6/7	4/7	4/7
Modified	6/6	6/6	4/6	4/6
Intermediate 1	4/5	4/5	5/5	3/5
Intermediate 2	4/4	4/4	3/4	4/4

The number prior to "/" corresponds to the number of common amino acid residues participating in H-bond formation, while the number after "/" corresponds to the total number of amino acid residues participating H-bonds for each conformation.