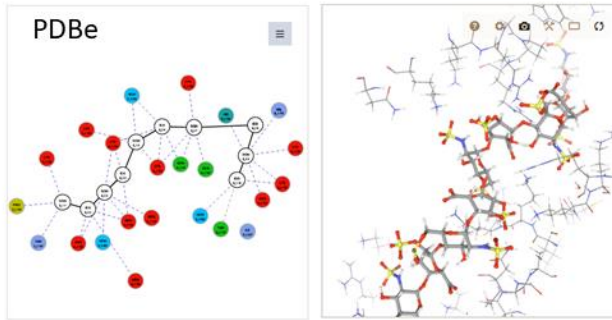


Supplementary Figures

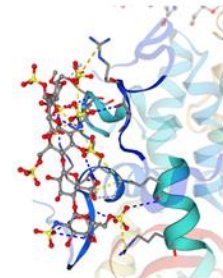
2GD4



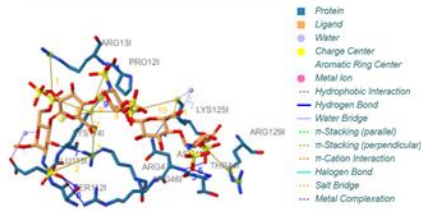
SWISS-MODEL

Ligands

ZDO: 14 residues within 4Å
 IDS: 9 PLIP interactions
 SUS: 9 interactions with SGN.2 chain C
 Hydrogen bonds:
 C:N 56, C:T 55,
 C:T 55, C:N 56,
 C:K 136, C:P 23,
 C:N 56, C:K 125,
 C:R 57, C:R 58,
 C:S 123,
 C:E 124,
 C:K 125
 Water bridges:
 C:K 136,
 C:E 124
 Salt bridges:
 C:K 136, C:R 58,
 C:K 125,
 C:R 140,
 C:K 125,
 C:K 125,
 C:K 136, C:R 24

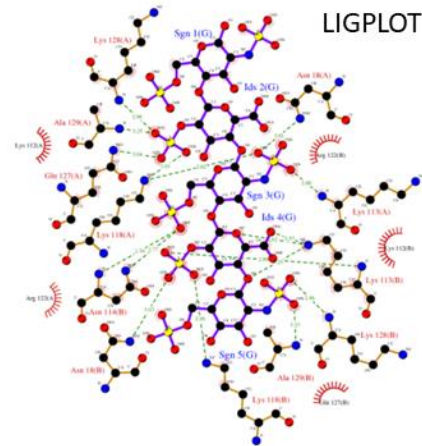


Composite ligand consists of ZDO:F.1, IDS:F.2, SUS:F.3, BDP:F.4, SGN:F.5.
 Interacting chains: 1



PLIP

LIGPLOT of interactions involving ligand SGN-IDS-SGN-IDS-SGN



LIGPLOT

Download visualization in PyMol (Lack) format | es | en | img

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein-donor?	Sidechain	Donor Atom	Acceptor Atom
1	121	PRO	2.30	2.67	101.82	✓	✓	10600 [O3]	2233 [O2]
2	441	THR	3.02	4.00	170.82	✓	✓	2390 [N4]	10954 [O3]
3	441	THR	2.99	3.00	122.04	✓	✓	10954 [O3]	2390 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	131	ARG	5.37	✓	Sulfate	10696, 10686
2	471	ARG	4.95	✓	Sulfonamide	10678, 10678, 10679, 10680, 10681

Water Bridges

Index	Residue	AA	Dist. A-W	Dist. D-W	Donor Angle	Water Angle	Protein-donor?	Donor Atom	Acceptor Atom	Water Atom
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Figure S1. Detailed of the analysis of GAG binding in crystal structure of a ternary FG1-FGFR2-Heparin complex (PDB 2GD4) available from different sources ; PDBe ; Swiss-Model ; PLIP, LIGPOLY.

1f0o

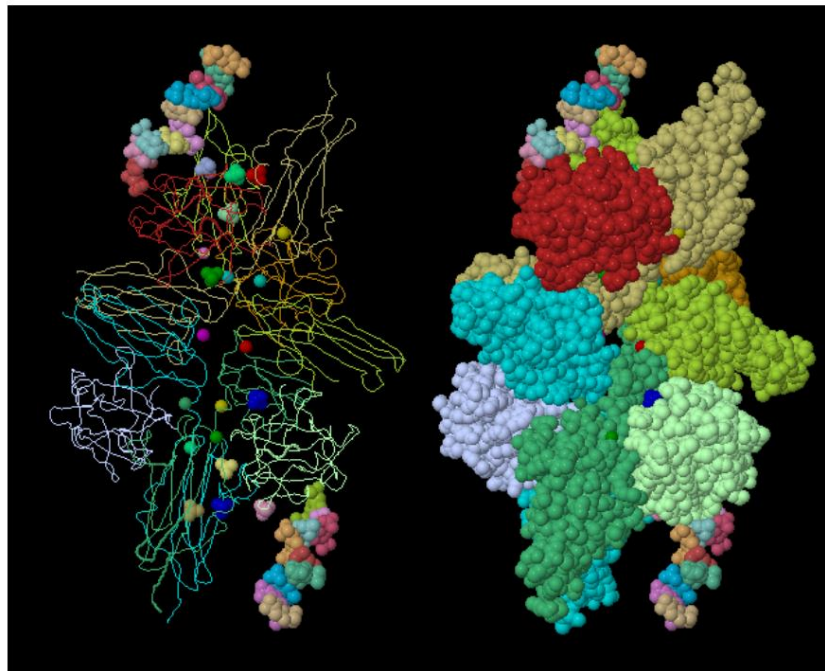


Figure S2. Quaternary organisation in the crystal Structure of the Antithrombin-S195A Factor Xa-Pentasaccharide Complex (PDB 1EO0) computed and displayed by PISA.