

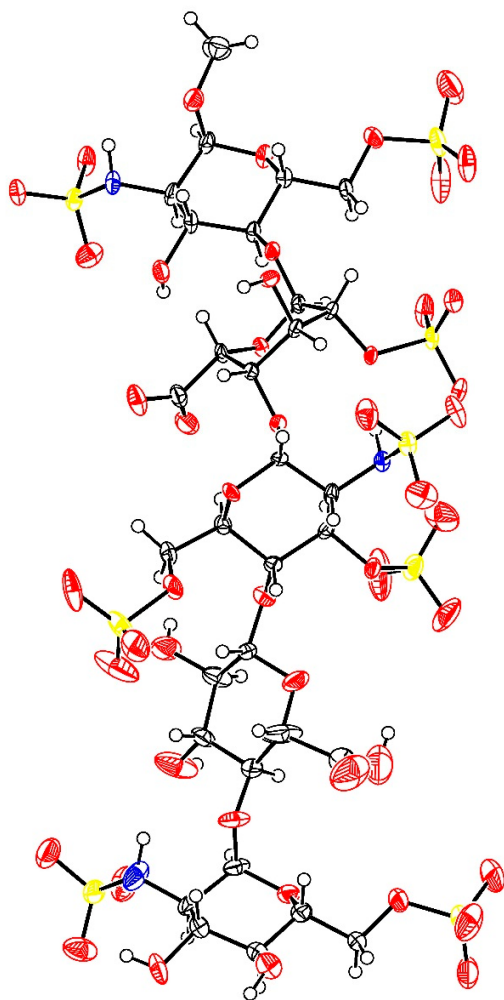


Figure S1: Displacement ellipsoid plot of the pentasaccharide molecule of Fondaparinux drawn at 50% probability level.

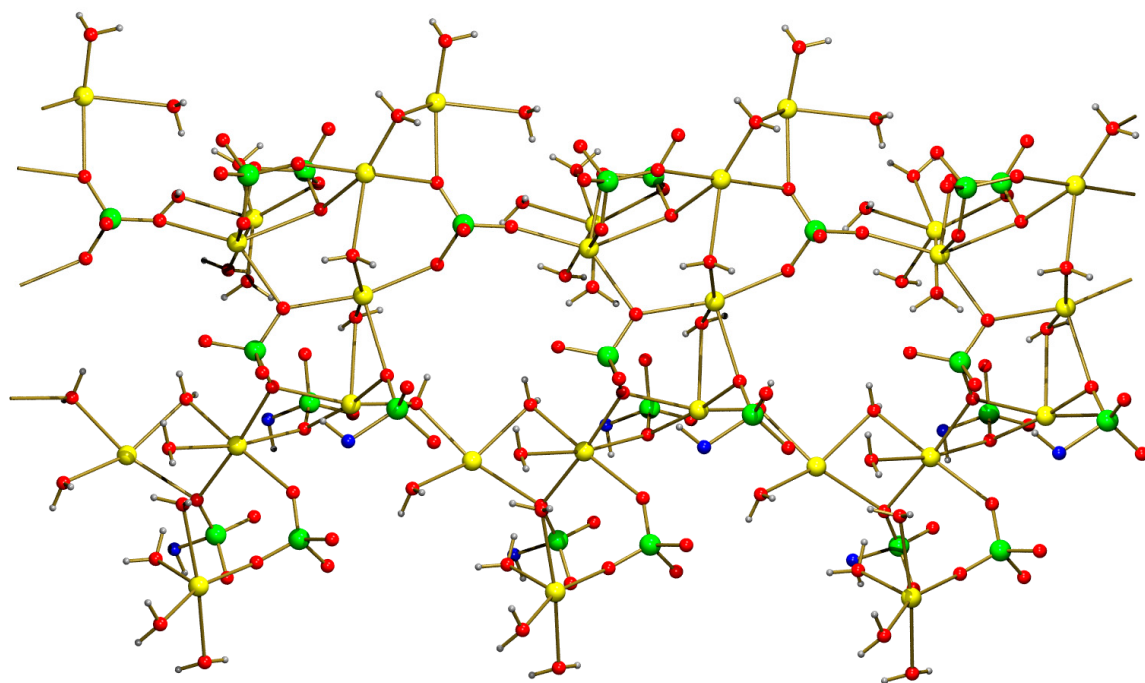


Figure S2: Impression of the crystal packing of Fondaparinux, highlighting the infinite three-dimensional framework formed by Na...O coordination in the substructure of sulfate groups, sodium and coordinated water molecules. The sugar rings have been omitted for clarity.

Table S1: Geometric details of all unique potential hydrogen bonds.

Geometric details of Potential Hydrogen Bonds; distances in Å, angles in °. Standard uncertainties are given in parentheses. Note: no standard uncertainties are given for quantities calculated from coordinates at calculated positions. Geometric criteria used for inclusion in the list:

$$d(D\cdots A) < R(D) + R(A) + 0.50 \text{ Å}$$

$$d(H\cdots A) < R(H) + R(A) - 0.12 \text{ Å}$$

$$D-H\cdots A > 100.0^\circ$$

(D = donor, A = Acceptor, R = Van der Waals radius)

ARU = Asymmetric Residue Unit, the code given is written out in equivalent positions below the H-bond table. For potential bifurcated H-bonds, the Acceptor...Hydrogen...Acceptor angle is included in the Tables, as well as the sum of all angles involving the central hydrogen, which is expected to be 360° for a truly bifurcated system.

Nr	Type	Donor-H...Acceptor	ARU	D-H	H...A	D...A	D-H...A	A...H...A*	Sum
1	Intra	N(1) -H(1N) ...O(1)	[]	0.92	2.29	2.769(11)	112		
2	Intra	N(1) -H(1N) ...O(14)	[]	0.92	2.52	3.282(14)	141'	73'	326
3	Intra	N(2) -H(2N) ...O(18)	[]	0.92	2.39	2.830(8)	109		
4	Intra	N(2) -H(2N) ...O(32)	[]	0.92	2.18	3.095(9)	172'	78'	359
5	Inter	N(3) -H(3N) ...O(2)	[1454]	0.92	2.26	2.972(12)	134		
6	Intra	N(3) -H(3N) ...O(40)	[]	0.92	2.34	2.826(9)	112'	102'	348
7	Inter	O(6) -H(6H) ...O(42)	[1756]	0.84	2.11	2.819(10)	142		
8	Inter	O(13) -H(13H) ...O(61)	[]	0.84	1.88	2.701(13)	164		
9	Inter	O(14) -H(14H) ...O(71)	[]	0.84	2.26	2.766(18)	119		
10	Inter	O(16) -H(16H) ...O(76)	[]	0.84	1.91	2.54(3)	131		
11	Inter	O(36) -H(36H) ...O(42)	[1655]	0.84	1.95	2.773(7)	165		
12	Inter	O(44) -H(44H) ...O(52)	[1455]	0.84	2.11	2.900(9)	156		
13	Inter	O(50) -H(50S) ...O(44)	[1656]	0.84	2.08	2.845(8)	152		
14	Inter	O(50) -H(50T) ...O(70)	[1656]	0.84	1.94	2.766(9)	169		
15	Inter	O(51) -H(51S) ...O(20)	[2756]	0.84	2.51	2.796(14)	101		
16	Inter	O(51) -H(51T) ...O(60)	[2656]	0.82	2.32	3.141(15)	180		
17	Inter	O(52) -H(52S) ...O(19)	[]	0.84	2.15	2.947(10)	159		
18	Inter	O(52) -H(52T) ...O(37)	[1655]	0.83	2.28	2.839(10)	124		
19	Inter	O(52) -H(52T) ...O(39)	[1655]	0.83	2.42	3.093(9)	138'	66'	328
20	Inter	O(53) -H(53S) ...O(37)	[1655]	0.85	1.98	2.676(10)	138		
21	Inter	O(53) -H(53T) ...O(29)	[]	0.84	2.54	3.050(11)	120		
22	Inter	O(53) -H(53T) ...O(47)	[2655]	0.84	2.23	2.964(10)	147'	85'	352
23	Inter	O(54) -H(54S) ...O(73)	[]	0.84	2.25	2.850(17)	128		
24	Inter	O(54) -H(54T) ...O(60)	[1655]	0.84	2.60	3.007(12)	111		
25	Inter	O(54) -H(54T) ...O(61)	[1655]	0.84	2.41	3.199(13)	156'	90'	357
26	Inter	O(55) -H(55S) ...O(43)	[1655]	0.84	2.57	3.227(15)	136		
27	Inter	O(55) -H(55S) ...O(58)	[2655]	0.84	2.59	3.355(16)	152'	70'	358
28	Inter	O(55) -H(55T) ...O(70)	[1655]	0.84	2.05	2.765(15)	142		
29	Inter	O(56) -H(56S) ...O(42)	[1756]	0.84	2.12	2.884(10)	151		
30	Inter	O(56) -H(56T) ...O(38)	[1656]	0.84	2.22	2.970(11)	149		
31	Inter	O(57) -H(57S) ...O(20)	[2756]	0.84	2.16	2.784(15)	131		
32	Inter	O(57) -H(57T) ...O(79)	[2756]	0.84	2.48	3.11(4)	132		
33	Inter	O(58) -H(58S) ...O(38)	[2645]	0.84	1.92	2.753(11)	168		

34	Inter	O(58)	-H(58T)...	O(43)	[2545]	0.82	2.12	2.941(11)	180			
35	Inter	O(59)	-H(59S)...	O(49)	[1655]	0.84	1.93	2.762(10)	170			
36	Inter	O(59)	-H(59T)...	O(10)	[1454]	0.84	2.52	3.187(12)	137			
37	Inter	O(60)	-H(60S)...	O(37)	[]	0.84	2.01	2.816(12)	160			
38	Inter	O(60)	-H(60T)...	O(54)	[1455]	0.84	2.40	3.007(12)	129			
39	Inter	O(61)	-H(61S)...	O(75)	[]	0.84	2.00	2.81(2)	159			
40	Inter	O(61)	-H(61T)...	O(53)	[1455]	0.84	1.97	2.769(13)	158			
41	Inter	O(62)	-H(62S)...	O(76)	[]	0.84	1.99	2.81(3)	165			
42	Inter	O(62)	-H(62S)...	O(92)	[]	0.84	1.82	2.26(5)	111'	82'	358	
43	Inter	O(62)	-H(62T)...	O(74)	[]	0.84	1.97	2.72(3)	148			
44	Inter	O(63)	-H(63A)...	O(73)	[1455]	0.84	1.97	2.77(2)	159			
45	Inter	O(63)	-H(63C)...	O(51)	[2646]	0.84	2.37	3.18(3)	159			
46	Inter	O(64A)	-H(64S)...	O(78)	[2656]	0.84	1.90	2.66(5)	150			
47	Inter	O(64A)	-H(64T)...	O(72)	[2656]	0.85	2.21	3.04(5)	166			
48	Inter	O(65A)	-H(65S)...	O(29)	[1455]	0.84	2.37	3.00(2)	133			
49	Inter	O(65A)	-H(65T)...	O(11)	[2656]	0.84	2.20	2.90(2)	141			
50	Inter	O(66A)	-H(66S)...	O(77)	[2656]	0.84	1.74	2.56(6)	166			
51	Inter	O(66A)	-H(66T)...	O(4)	[]	0.85	2.59	2.87(6)	100			
52	Inter	O(66A)	-H(66T)...	O(14)	[]	0.85	2.16	2.95(5)	154'	105'	359	

ARU-Code expressed in equivalent positions

[1454] = $-1+x, y, -1+z$
 [1455] = $-1+x, y, z$
 [1655] = $1+x, y, z$
 [1656] = $1+x, y, 1+z$
 [1756] = $2+x, y, 1+z$
 [2545] = $-x, -1/2+y, -z$
 [2646] = $1-x, -1/2+y, 1-z$
 [2656] = $1-x, 1/2+y, 1-z$
 [2756] = $2-x, 1/2+y, 1-z$
 [2655] = $1-x, 1/2+y, -z$
 [2645] = $1-x, -1/2+y, -z$