



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 09:36 AM UTC

PDB ID : 2ERM / pdb\_00002erm  
Title : Solution structure of a biologically active human FGF-1 monomer, complexed to a hexasaccharide heparin-analogue  
Authors : Canales, A.; Lozano, R.; Nieto, P.M.; Martin-Lomas, M.; Gimenez-Gallego, G.; Jimenez-Barbero, J.  
Deposited on : 2005-10-25

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

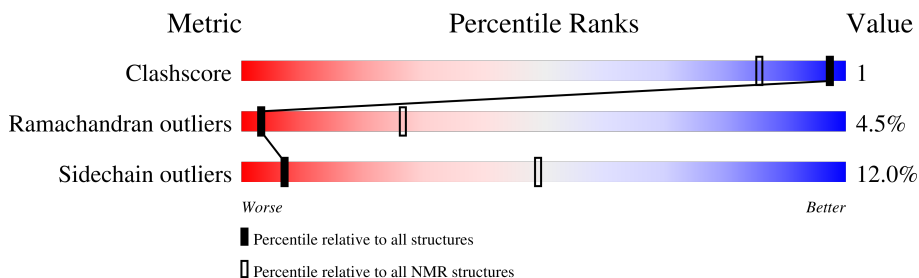
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	139	
2	B	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	B	GNS	2	2	-
2	B	IDR	3	1	-
2	B	IDS	5	3	-

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:27-A:104, A:108-A:126, A:130-A:150 (118)	0.88	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 7, 8, 9, 10, 12, 13, 14, 15, 16, 17, 19, 20
2	11, 18
Single-model clusters	4; 6

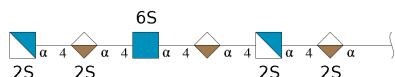
### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2263 atoms, of which 1103 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heparin-binding growth factor 1.

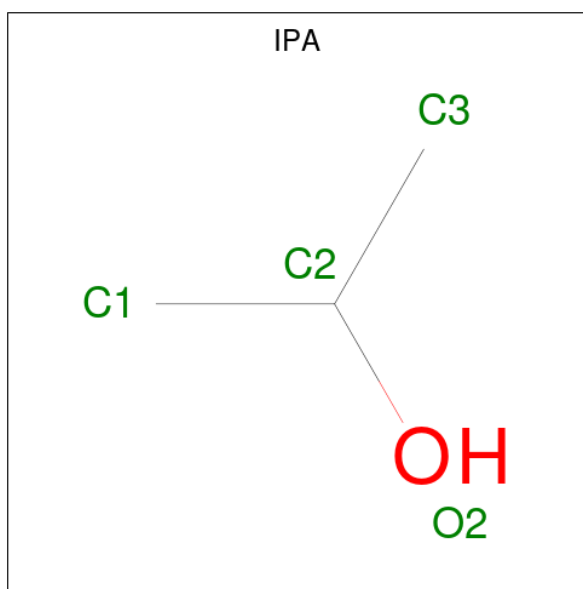
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	133	2108	671	1044	185	204	4	0

- Molecule 2 is an oligosaccharide called 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	6	144	38	52	3	46	5	0

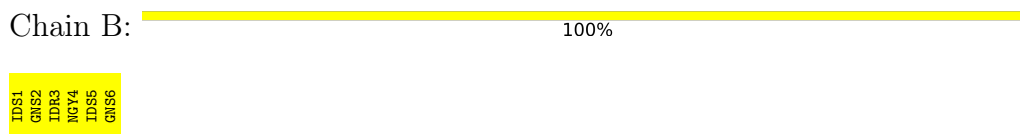
- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
3	A	1	11	3	7	1

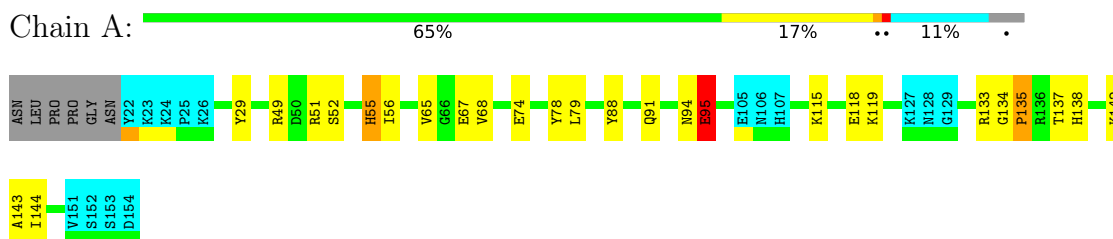


- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

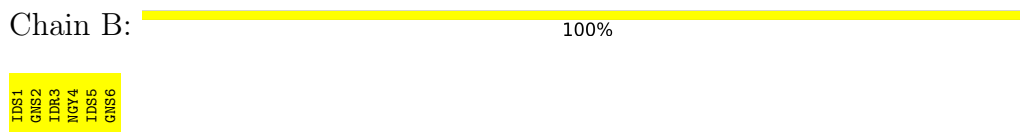


#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Heparin-binding growth factor 1

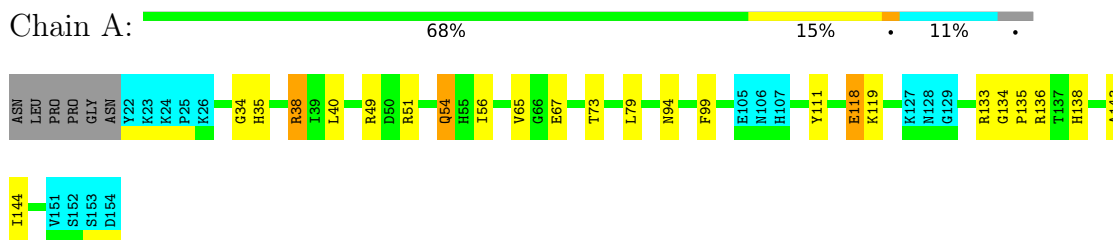


- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

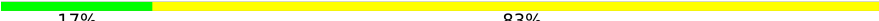


#### 4.2.3 Score per residue for model 3

- Molecule 1: Heparin-binding growth factor 1



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  17% 83%

IDS1  
GNS2  
IDR3  
NGY4  
IDS5  
GNS6

#### 4.2.4 Score per residue for model 4

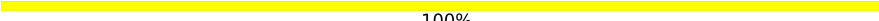
- Molecule 1: Heparin-binding growth factor 1

Chain A:  65% 19% 11%

ASN LEU PRO PRO GLY ASN Y22 K23 K24 P25 K26 Y29 P41 V45 R49 D60 R51 S52 D53 I56 Q57 V65 G66 E67 T73 D82 Y88 R102 E103 E104 N106 N107 Y111 H116 A117 E118 K126 K127 N128 G129 G134 P135 H138 Y139

G140 Q141 K142 A143 I144 P148 V151 S152 S153 D154

- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  100%

IDS1  
GNS2  
IDR3  
NGY4  
IDS5  
GNS6

#### 4.2.5 Score per residue for model 5


- Molecule 1: Heparin-binding growth factor 1

Chain A:  66% 17% 11%

ASN LEU PRO PRO GLY ASN Y22 K23 K24 P25 K26 Y29 N32 R38 P41 R49 D60 R51 V65 T73 D82 T83 D84 Y88 E105 M106 N107 Y111 H116 A117 E118 K119 N120 K126 K127 N128 G129 S130 G134 P135 R136 T137 H138 Y139 G140 Q141

K142 A143 V151 S152 S153 D154

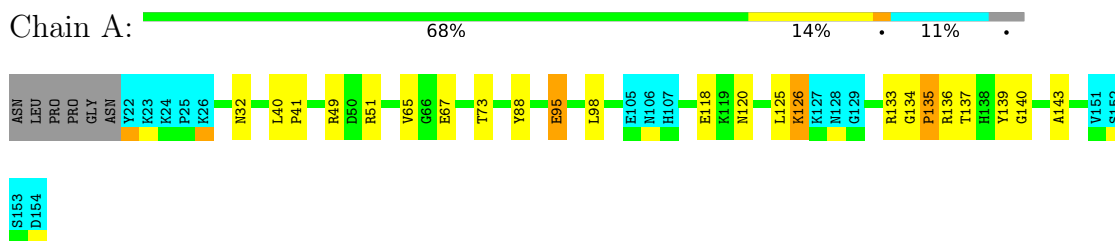
- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  83% 17%

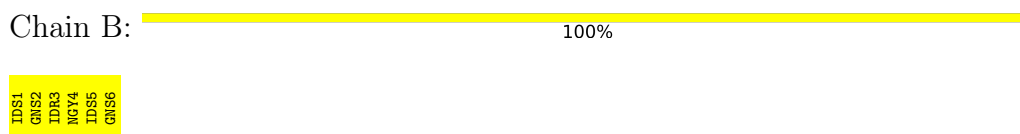
IDS1  
GNS2  
IDR3  
NGY4  
IDS5  
GNS6

### 4.2.6 Score per residue for model 6

- Molecule 1: Heparin-binding growth factor 1

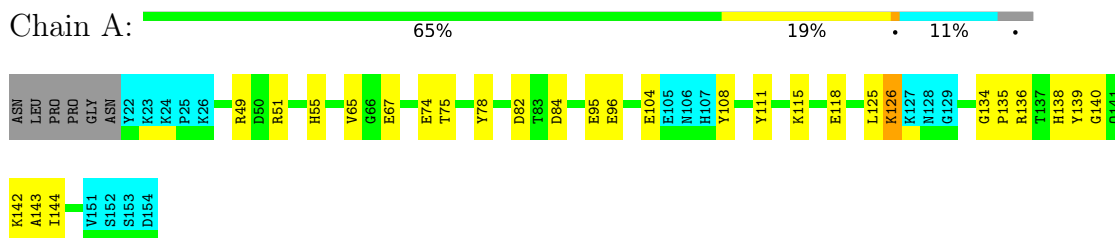


- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

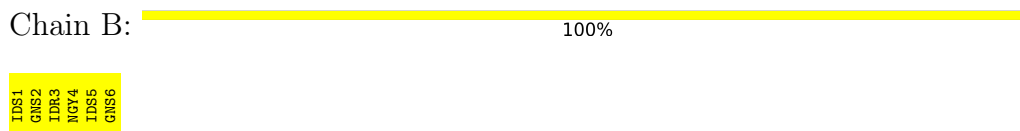


### 4.2.7 Score per residue for model 7

- Molecule 1: Heparin-binding growth factor 1



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid



### 4.2.8 Score per residue for model 8

- Molecule 1: Heparin-binding growth factor 1





- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

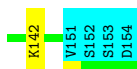
Chain B: 100%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Heparin-binding growth factor 1

Chain A: 68% 13% 11%



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B: 17% 83%



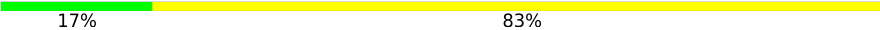
#### 4.2.12 Score per residue for model 12

- Molecule 1: Heparin-binding growth factor 1

Chain A: 70% 12% 11%



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  17% 83%

IDS1  
GNS2  
IDR3  
NGY4  
IDS5  
GNS6

#### 4.2.13 Score per residue for model 13

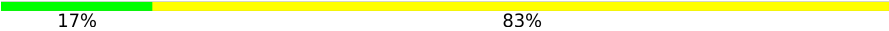
- Molecule 1: Heparin-binding growth factor 1

Chain A:  65% 19% 11%

ASN LEU PRO PRO GLY ASN Y22 K23 K24 P25 K26 H35 R49 D50 R51 I56 Q57 L58 V65 G66 E67 V68 Y69 T73 E74 Q77 Y78 Y88 N94 E95 F99 E105 M106 H107 K115 H116 A117 E118 K119 M120 F122 K127 M128 G129 G134 P135

R136 T137 H138 Y139 G140 A143 I144 V151 S152 S153 D154

- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  17% 83%

IDS1  
GNS2  
IDR3  
NGY4  
IDS5  
GNS6

#### 4.2.14 Score per residue for model 14

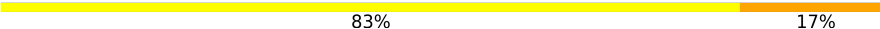
- Molecule 1: Heparin-binding growth factor 1

Chain A:  65% 19% 11%

ASN LEU PRO PRO GLY ASN Y22 K23 K24 P25 K26 Y29 C30 S31 L40 P41 V45 D46 R49 D50 E51 S52 D53 Q54 H55 V65 V68 T73 Y78 D82 Y88 N94 L98 E105 M106 H107 H116 A117 E118 K119 V123 K127 M128 G129

G134 P135 H138 K142 A143 V151 S152 S153 D154

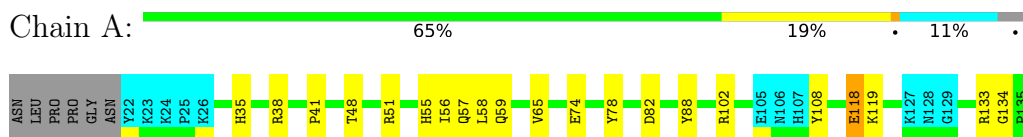
- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  83% 17%

IDS1  
GNS2  
IDR3  
NGY4  
IDS5  
GNS6

#### 4.2.15 Score per residue for model 15

- Molecule 1: Heparin-binding growth factor 1

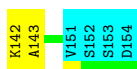
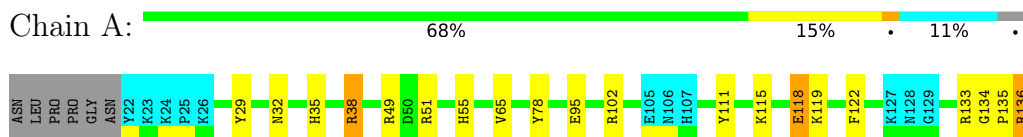


- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

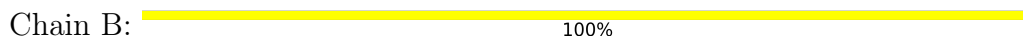


#### 4.2.16 Score per residue for model 16

- Molecule 1: Heparin-binding growth factor 1



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid



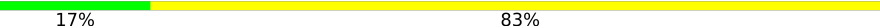
#### 4.2.17 Score per residue for model 17

- Molecule 1: Heparin-binding growth factor 1

Chain A: 



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

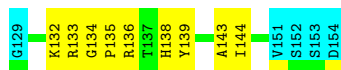
Chain B: 



#### 4.2.18 Score per residue for model 18

- Molecule 1: Heparin-binding growth factor 1

Chain A: 



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

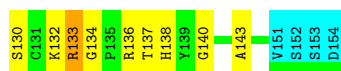
Chain B: 



#### 4.2.19 Score per residue for model 19

- Molecule 1: Heparin-binding growth factor 1

Chain A: 



- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  67% 33%



#### 4.2.20 Score per residue for model 20

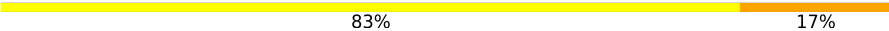
- Molecule 1: Heparin-binding growth factor 1

Chain A:  70% 14% 11%





- Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:  83% 17%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated annealing, restrained molecular dynamics*.

Of the 30 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	5.0

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, NGY, IDR, IDS, GNS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.68±0.01	0±0/964 ( 0.0± 0.0%)	1.35±0.03	4±3/1304 ( 0.3± 0.2%)
All	All	0.68	0/19280 ( 0.0%)	1.35	90/26080 ( 0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	6.0±2.1
All	All	0	119

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	135	PRO	CB-CA-C	7.28	118.15	110.00	12	2
1	A	82	ASP	CA-C-N	7.20	130.24	120.38	17	6
1	A	82	ASP	C-N-CA	7.20	130.24	120.38	17	6
1	A	95	GLU	CA-C-N	7.01	129.68	120.28	17	10
1	A	95	GLU	C-N-CA	7.01	129.68	120.28	17	10
1	A	55	HIS	CB-CG-CD2	-6.27	123.05	131.20	15	6
1	A	104	GLU	CA-C-N	6.09	132.67	121.70	7	1
1	A	104	GLU	C-N-CA	6.09	132.67	121.70	7	1
1	A	138	HIS	CB-CG-CD2	-5.80	123.66	131.20	12	15
1	A	35	HIS	CB-CG-CD2	-5.75	123.72	131.20	19	2
1	A	120	ASN	CA-CB-CG	5.58	118.18	112.60	9	1
1	A	73	THR	CA-C-N	5.55	129.14	120.82	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	THR	C-N-CA	5.55	129.14	120.82	12	1
1	A	68	VAL	N-CA-C	5.52	116.31	108.42	18	1
1	A	120	ASN	CB-CA-C	5.47	118.83	111.82	9	1
1	A	125	LEU	CA-C-N	5.39	131.83	121.54	6	1
1	A	125	LEU	C-N-CA	5.39	131.83	121.54	6	1
1	A	46	ASP	CA-C-N	5.33	127.26	122.20	18	2
1	A	46	ASP	C-N-CA	5.33	127.26	122.20	18	2
1	A	40	LEU	CA-C-N	5.29	126.45	119.84	6	3
1	A	40	LEU	C-N-CA	5.29	126.45	119.84	6	3
1	A	132	LYS	CA-C-N	5.26	128.18	120.71	18	1
1	A	132	LYS	C-N-CA	5.26	128.18	120.71	18	1
1	A	94	ASN	CA-C-N	5.24	128.03	120.38	8	1
1	A	94	ASN	C-N-CA	5.24	128.03	120.38	8	1
1	A	55	HIS	N-CA-C	5.18	117.47	110.06	2	1
1	A	53	ASP	CA-C-N	5.12	127.65	120.28	18	2
1	A	53	ASP	C-N-CA	5.12	127.65	120.28	18	2
1	A	130	SER	CA-C-N	5.12	128.48	120.75	5	2
1	A	130	SER	C-N-CA	5.12	128.48	120.75	5	2
1	A	55	HIS	CA-CB-CG	5.08	118.88	113.80	15	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	134	GLY	Peptide	19
1	A	88	TYR	Sidechain	11
1	A	111	TYR	Sidechain	10
1	A	29	TYR	Sidechain	9
1	A	133	ARG	Peptide,Sidechain	9
1	A	139	TYR	Sidechain	8
1	A	78	TYR	Sidechain	8
1	A	49	ARG	Sidechain,Peptide	6
1	A	108	TYR	Sidechain	5
1	A	122	PHE	Sidechain	5
1	A	38	ARG	Sidechain	4
1	A	99	PHE	Sidechain	4
1	A	102	ARG	Sidechain	4
1	A	69	TYR	Sidechain	3
1	A	136	ARG	Sidechain	3
1	A	142	LYS	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	50	ASP	Peptide	1
1	A	148	PRO	Peptide	1
1	A	125	LEU	Peptide	1
1	A	72	SER	Peptide	1
1	A	55	HIS	Peptide	1
1	A	104	GLU	Peptide	1
1	A	138	HIS	Sidechain	1
1	A	35	HIS	Peptide	1

## 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	942	925	925	1±1
2	B	92	52	37	0±1
All	All	20760	19680	19380	26

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ASP:CG	1:A:83:THR:N	0.45	2.74	18	2
1:A:136:ARG:HH12	2:B:3:IDR:C6	0.45	2.23	5	1
1:A:136:ARG:HH22	2:B:5:IDS:C6	0.44	2.25	20	1
1:A:98:LEU:HD13	1:A:98:LEU:C	0.44	2.36	14	1
1:A:96:GLU:H	1:A:96:GLU:CD	0.43	2.21	20	1
1:A:132:LYS:NZ	2:B:6:GNS:O2S	0.43	2.51	9	1
1:A:74:GLU:N	1:A:74:GLU:CD	0.42	2.77	12	1
1:A:118:GLU:OE2	1:A:119:LYS:NZ	0.41	2.52	17	7
1:A:95:GLU:OE2	1:A:115:LYS:NZ	0.41	2.54	2	1
1:A:96:GLU:OE2	1:A:115:LYS:NZ	0.41	2.53	1	3
1:A:142:LYS:NZ	2:B:4:NGY:O7A	0.41	2.53	5	1
1:A:132:LYS:NZ	2:B:4:NGY:O9	0.41	2.53	19	1
1:A:71:LYS:NZ	1:A:74:GLU:OE1	0.41	2.54	9	1
1:A:74:GLU:CD	1:A:74:GLU:H	0.40	2.25	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ARG:NH2	2:B:2:GNS:O3S	0.40	2.54	19	1
1:A:142:LYS:NZ	2:B:5:IDS:O2S	0.40	2.53	14	1
1:A:136:ARG:HE	2:B:3:IDR:C6	0.40	2.29	20	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	118/139 (85%)	95±3 (81±3%)	17±3 (15±2%)	5±1 (4±1%)	3	27
All	All	2360/2780 (85%)	1908 (81%)	346 (15%)	106 (4%)	3	27

All 29 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	65	VAL	20
1	A	143	ALA	16
1	A	140	GLY	11
1	A	137	THR	8
1	A	126	LYS	6
1	A	73	THR	5
1	A	123	VAL	4
1	A	139	TYR	4
1	A	136	ARG	4
1	A	32	ASN	3
1	A	31	SER	3
1	A	82	ASP	2
1	A	120	ASN	2
1	A	75	THR	2
1	A	95	GLU	2
1	A	34	GLY	1
1	A	35	HIS	1
1	A	54	GLN	1
1	A	51	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	53	ASP	1
1	A	135	PRO	1
1	A	76	GLY	1
1	A	86	LEU	1
1	A	145	LEU	1
1	A	42	ASP	1
1	A	104	GLU	1
1	A	55	HIS	1
1	A	103	LEU	1
1	A	57	GLN	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/122 (84%)	91±3 (88±3%)	12±3 (12±3%)	7	49
All	All	2060/2440 (84%)	1812 (88%)	248 (12%)	7	49

All 50 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	51	ARG	20
1	A	118	GLU	20
1	A	135	PRO	14
1	A	41	PRO	12
1	A	67	GLU	12
1	A	136	ARG	11
1	A	49	ARG	11
1	A	74	GLU	9
1	A	142	LYS	8
1	A	144	ILE	8
1	A	73	THR	8
1	A	56	ILE	7
1	A	79	LEU	6
1	A	102	ARG	6
1	A	126	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	68	VAL	5
1	A	94	ASN	5
1	A	54	GLN	5
1	A	35	HIS	5
1	A	95	GLU	4
1	A	45	VAL	4
1	A	116	HIS	4
1	A	84	ASP	4
1	A	120	ASN	4
1	A	103	LEU	4
1	A	115	LYS	4
1	A	58	LEU	3
1	A	119	LYS	3
1	A	133	ARG	3
1	A	38	ARG	3
1	A	104	GLU	3
1	A	88	TYR	3
1	A	59	GLN	3
1	A	55	HIS	2
1	A	78	TYR	2
1	A	57	GLN	2
1	A	132	LYS	2
1	A	91	GLN	1
1	A	98	LEU	1
1	A	71	LYS	1
1	A	75	THR	1
1	A	101	GLU	1
1	A	138	HIS	1
1	A	77	GLN	1
1	A	48	THR	1
1	A	141	GLN	1
1	A	27	LEU	1
1	A	63	GLU	1
1	A	82	ASP	1
1	A	87	LEU	1

### 6.3.3 RNA

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	IDS	B	1	2	16,16,17	1.24±0.05	2±1 (9±3%)
2	GNS	B	2	2	15,15,16	1.85±0.18	2±1 (15±4%)
2	IDR	B	3	2	12,12,13	0.88±0.05	0±0 (0±0%)
2	NGY	B	4	2	18,18,19	0.80±0.05	0±0 (0±0%)
2	IDS	B	5	2	16,16,17	1.21±0.07	1±0 (8±2%)
2	GNS	B	6	2	15,15,16	1.72±0.16	2±1 (12±4%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	IDS	B	1	2	16,24,26	1.41±0.34	3±2 (15±10%)
2	GNS	B	2	2	17,22,24	1.95±0.24	5±1 (30±5%)
2	IDR	B	3	2	14,17,19	1.09±0.26	1±1 (7±6%)
2	NGY	B	4	2	23,26,28	1.52±0.19	4±1 (18±5%)
2	IDS	B	5	2	16,24,26	1.35±0.34	2±1 (9±7%)
2	GNS	B	6	2	17,22,24	1.74±0.34	4±1 (20±5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IDS	B	1	2	-	0±0,9,26,29	0±0,1,1,1
2	GNS	B	2	2	-	0±0,7,24,27	0±0,1,1,1
2	IDR	B	3	2	-	0±0,4,21,24	0±0,1,1,1
2	NGY	B	4	2	-	0±0,10,27,30	0±0,1,1,1
2	IDS	B	5	2	-	0±0,9,26,29	0±0,1,1,1
2	GNS	B	6	2	-	1±0,7,24,27	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	2	GNS	S1-N2	6.70	1.67	1.59	18	20
2	B	6	GNS	S1-N2	6.60	1.67	1.59	1	20
2	B	1	IDS	O2-C2	3.74	1.41	1.47	18	20
2	B	5	IDS	O2-C2	3.43	1.42	1.47	11	20
2	B	2	GNS	O2S-S1	3.06	1.45	1.42	2	9
2	B	2	GNS	O3S-S1	2.96	1.45	1.42	11	14
2	B	6	GNS	O2S-S1	2.66	1.45	1.42	6	6
2	B	5	IDS	C1-C2	2.57	1.55	1.51	13	6
2	B	6	GNS	C1-C2	2.53	1.55	1.52	1	3
2	B	1	IDS	C1-C2	2.52	1.55	1.51	5	8
2	B	2	GNS	C1-C2	2.44	1.55	1.52	4	3
2	B	1	IDS	C4-C5	2.31	1.57	1.53	18	1
2	B	6	GNS	O3S-S1	2.28	1.44	1.42	13	8
2	B	1	IDS	O2-S	2.05	1.63	1.57	5	1
2	B	5	IDS	O2-S	2.02	1.63	1.57	6	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	5	IDS	O2-C2-C3	7.04	116.78	106.95	7	7
2	B	2	GNS	C3-C2-N2	7.03	119.57	110.32	14	10
2	B	1	IDS	O2-C2-C3	6.74	116.36	106.95	13	11
2	B	6	GNS	C3-C2-N2	6.04	118.27	110.32	1	4
2	B	6	GNS	O3S-S1-N2	5.68	99.38	108.88	1	19
2	B	6	GNS	O2S-S1-N2	5.61	99.50	108.88	14	20
2	B	4	NGY	O6-C6-C5	5.57	117.50	107.57	7	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	4	NGY	C2-N2-C7	5.10	129.74	122.90	14	1
2	B	2	GNS	O3S-S1-N2	5.05	100.43	108.88	20	19
2	B	2	GNS	O2S-S1-N2	4.53	101.31	108.88	5	17
2	B	2	GNS	C1-C2-N2	4.36	117.11	110.22	9	4
2	B	2	GNS	C4-C3-C2	4.15	117.11	111.02	17	3
2	B	3	IDR	C1-C2-C3	4.10	115.61	109.64	4	5
2	B	4	NGY	O4-C4-C5	4.02	119.22	109.32	1	9
2	B	4	NGY	C3-C4-C5	4.01	102.96	110.23	16	8
2	B	2	GNS	O5-C1-C2	3.92	105.22	111.29	1	11
2	B	6	GNS	O2S-S1-O3S	3.90	111.70	120.36	12	17
2	B	4	NGY	C6-C5-C4	3.79	120.02	112.07	18	13
2	B	4	NGY	C1-O5-C5	3.71	117.15	112.19	3	7
2	B	1	IDS	O3S-S-O2	3.64	98.02	106.37	4	6
2	B	1	IDS	C4-C3-C2	3.51	116.61	110.23	7	4
2	B	5	IDS	C4-C3-C2	3.49	116.56	110.23	2	3
2	B	2	GNS	O2S-S1-O3S	3.36	112.89	120.36	17	17
2	B	2	GNS	O4-C4-C5	3.34	101.11	109.32	14	8
2	B	1	IDS	O4-C4-C5	3.25	117.18	109.76	18	3
2	B	6	GNS	O3-C3-C4	3.22	102.78	110.38	1	3
2	B	2	GNS	C3-C4-C5	3.14	115.92	110.23	18	2
2	B	4	NGY	O9-S-O6	3.13	99.18	106.37	5	5
2	B	4	NGY	O5-C5-C6	3.07	114.22	107.59	6	3
2	B	2	GNS	C1-O5-C5	3.05	116.27	112.19	3	6
2	B	1	IDS	C3-C4-C5	3.01	114.47	109.30	14	2
2	B	5	IDS	O3S-S-O2	2.99	99.49	106.37	9	4
2	B	3	IDR	O4-C4-C5	2.93	116.45	109.76	18	3
2	B	1	IDS	O5-C1-C2	2.73	115.03	109.51	9	1
2	B	1	IDS	O5-C5-C6	2.71	116.27	106.59	9	5
2	B	5	IDS	O5-C5-C6	2.68	116.17	106.59	13	3
2	B	3	IDR	O5-C5-C6	2.67	116.12	106.59	7	12
2	B	4	NGY	O9-S-O8	2.63	117.78	108.56	8	6
2	B	2	GNS	O3-C3-C4	2.59	104.26	110.38	17	4
2	B	5	IDS	O5-C1-C2	2.53	114.63	109.51	6	1
2	B	4	NGY	O9-S-O7A	2.52	117.36	108.56	3	4
2	B	4	NGY	O6-S-O8	2.52	99.24	106.92	11	4
2	B	4	NGY	C4-C3-C2	2.50	107.36	111.02	12	4
2	B	4	NGY	O5-C5-C4	2.45	104.87	110.83	10	5
2	B	6	GNS	O5-C1-C2	2.40	107.58	111.29	2	2
2	B	1	IDS	O3S-S-O1S	2.38	116.89	108.56	10	10
2	B	1	IDS	O3S-S-O2S	2.30	116.61	108.56	9	9
2	B	6	GNS	C1-O5-C5	2.30	115.26	112.19	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	5	IDS	O4-C4-C3	2.27	115.73	110.38	1	1
2	B	6	GNS	C4-C3-C2	2.24	107.74	111.02	2	3
2	B	5	IDS	C3-C4-C5	2.23	113.14	109.30	2	1
2	B	5	IDS	O3S-S-O1S	2.22	116.34	108.56	6	7
2	B	2	GNS	O4-C4-C3	2.20	105.19	110.38	2	1
2	B	5	IDS	O3S-S-O2S	2.13	116.03	108.56	9	4
2	B	2	GNS	C6-C5-C4	2.12	107.82	113.02	16	2
2	B	4	NGY	O4-C4-C3	2.10	105.43	110.38	17	1
2	B	3	IDR	O6B-C6-C5	2.09	121.17	113.64	2	1
2	B	4	NGY	O6-S-O7A	2.05	100.67	106.92	20	1
2	B	2	GNS	O5-C5-C4	2.00	115.70	110.83	1	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

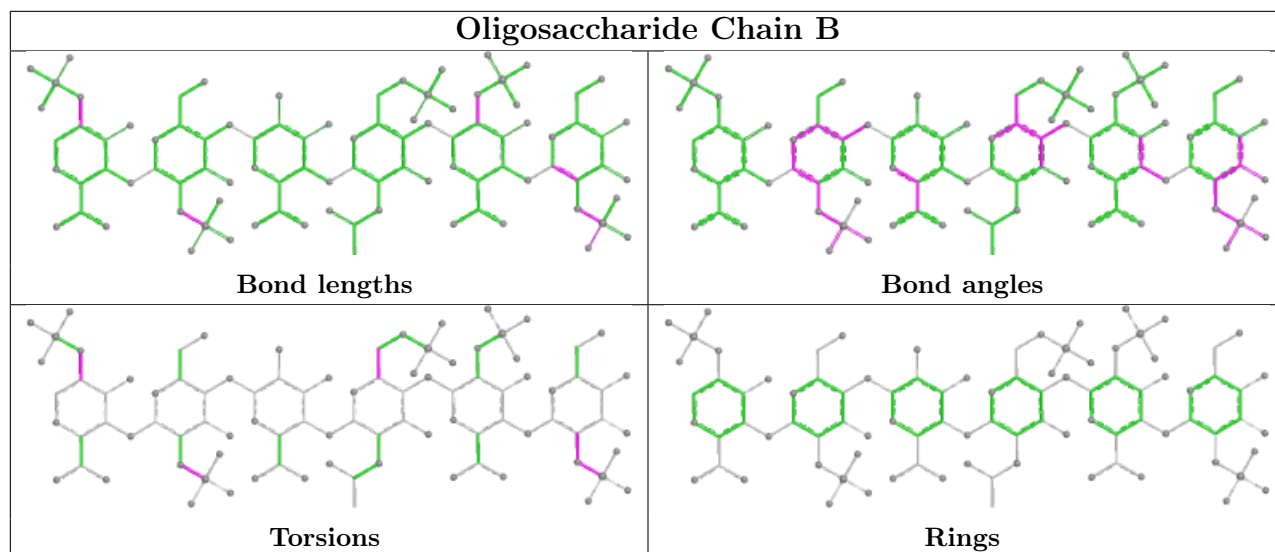
Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	5	IDS	C1	3
2	B	2	GNS	C1	2
2	B	3	IDR	C1	1

All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	6	GNS	C3-C2-N2-S1	2
2	B	2	GNS	C3-C2-N2-S1	1
2	B	5	IDS	C3-C2-O2-S	1
2	B	5	IDS	C1-C2-O2-S	1

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	IPA	A	15	-	3,3,3	0.65±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	IPA	A	15	-	3,3,3	0.39±0.05	0±0 (0±0%)

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided