Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 11:00 AM EDT

PDB ID	:	2ERM
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

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

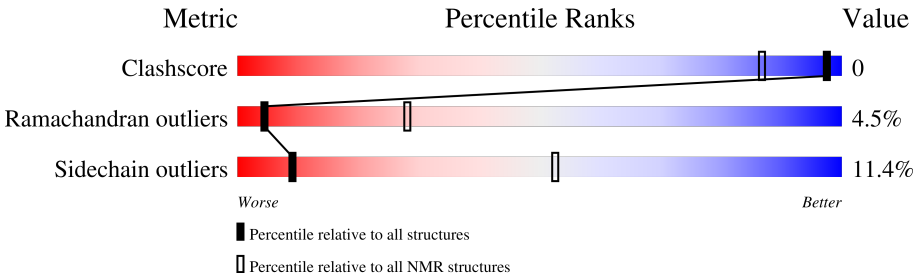
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	139	73% 11% • 11% •
2	B	6	100%

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

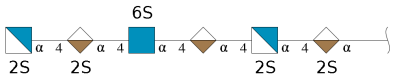
3 Entry composition

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.

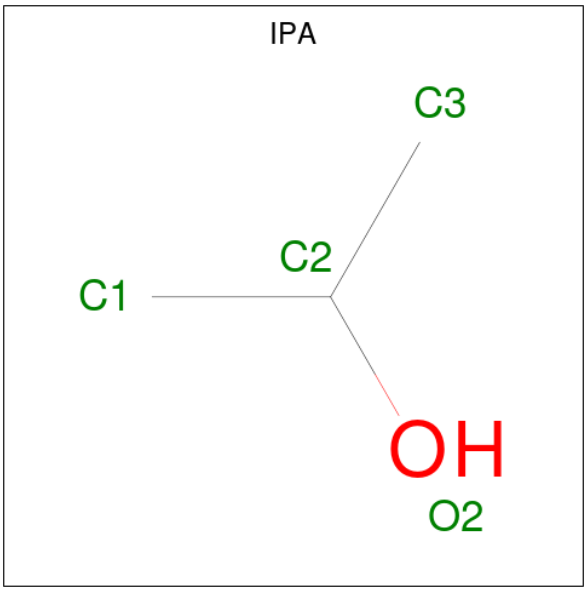
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	133	2108	671	1044	185	204	4	0

- 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 (three-letter code: IPA) (formula: C_3H_8O).



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

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

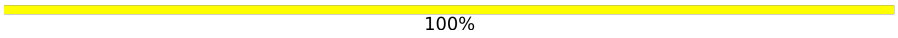
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• 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 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

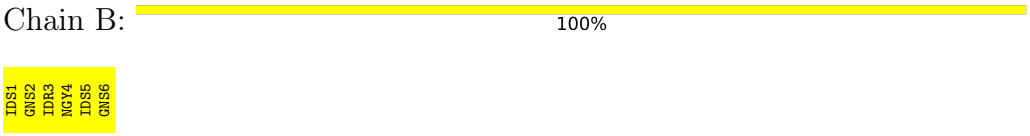
• Molecule 1: Heparin-binding growth factor 1

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-idopyranuron

ic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuron ic acid

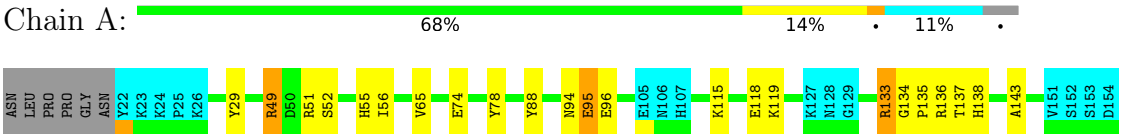
Chain B:



4.2.2 Score per residue for model 2 (medoid)

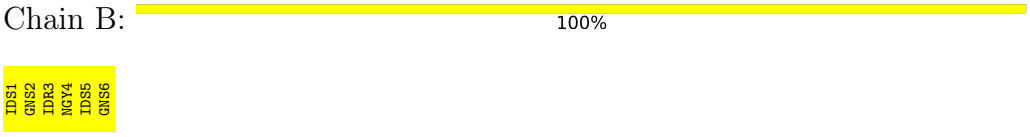
• Molecule 1: Heparin-binding growth factor 1

Chain A:



• Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranur onic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuron ic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuron ic acid

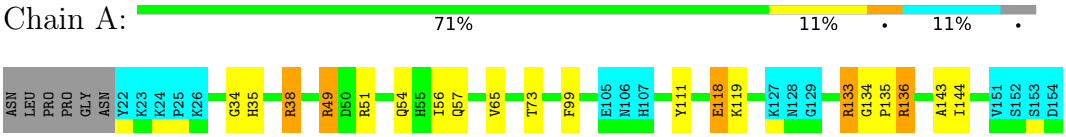
Chain B:



4.2.3 Score per residue for model 3

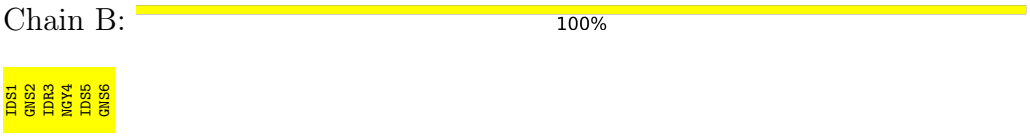
• Molecule 1: Heparin-binding growth factor 1

Chain A:



• Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranur onic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuron ic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuron ic acid

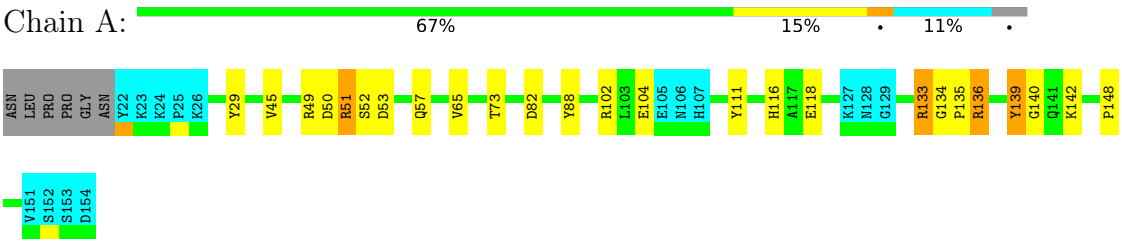
Chain B:



4.2.4 Score per residue for model 4

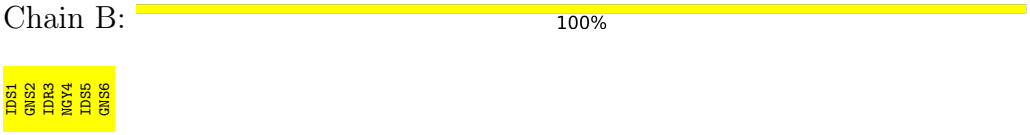
• Molecule 1: Heparin-binding growth factor 1

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

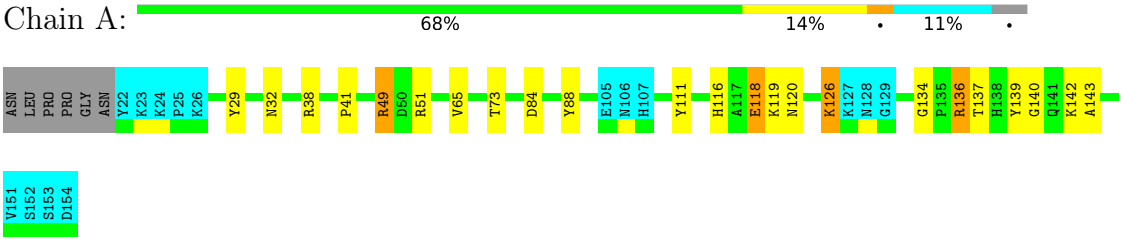
Chain B:



4.2.5 Score per residue for model 5

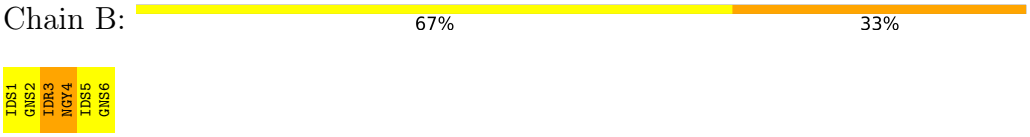
• Molecule 1: Heparin-binding growth factor 1

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

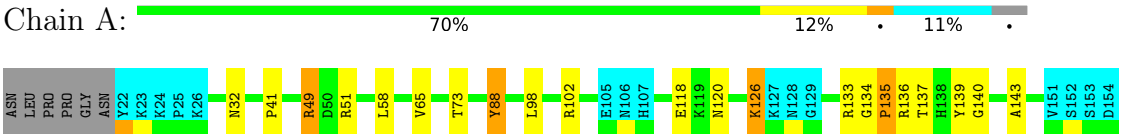
Chain B:



4.2.6 Score per residue for model 6

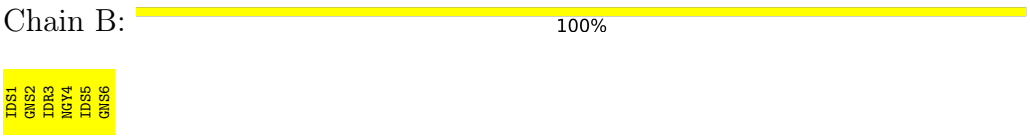
• Molecule 1: Heparin-binding growth factor 1

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

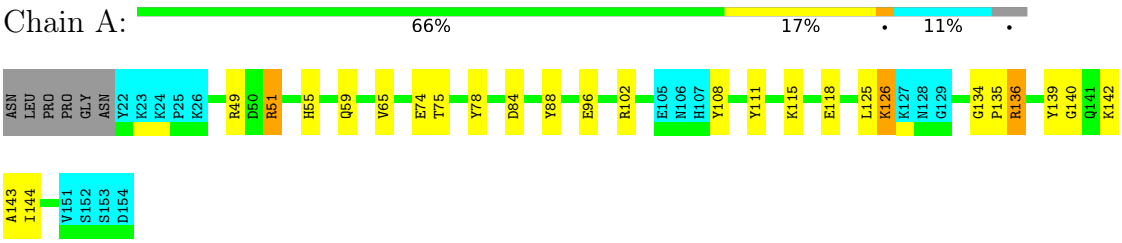
Chain B:



4.2.7 Score per residue for model 7

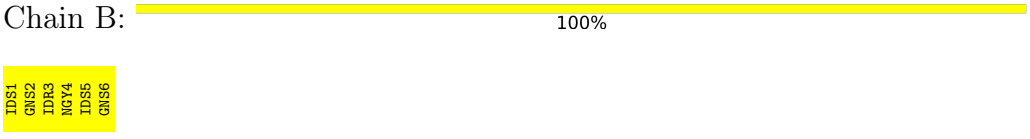
• Molecule 1: Heparin-binding growth factor 1

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

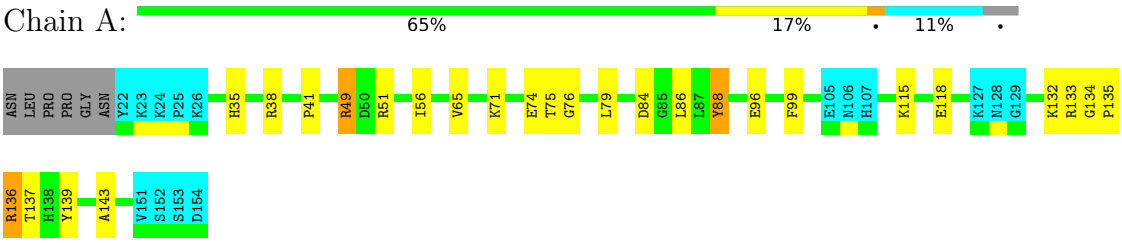
Chain B:



4.2.8 Score per residue for model 8

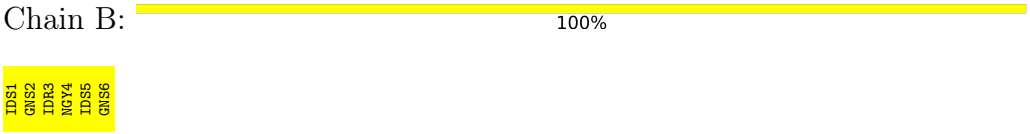
• Molecule 1: Heparin-binding growth factor 1

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

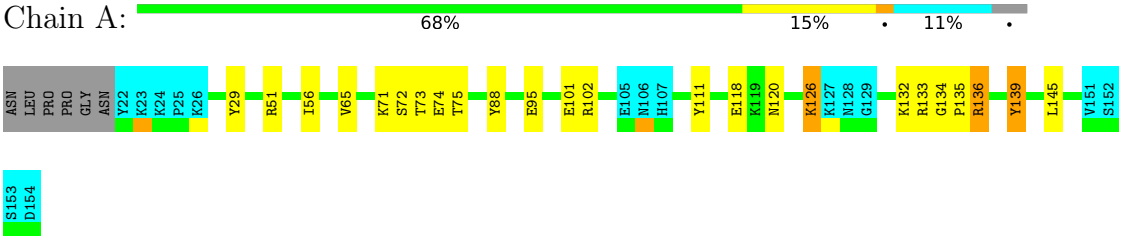
Chain B:



4.2.9 Score per residue for model 9

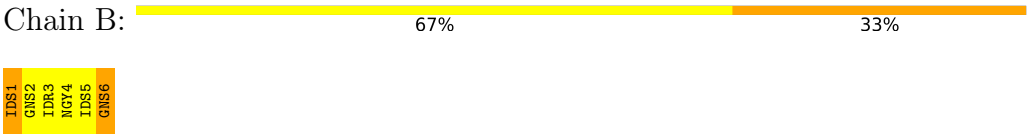
• Molecule 1: Heparin-binding growth factor 1

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

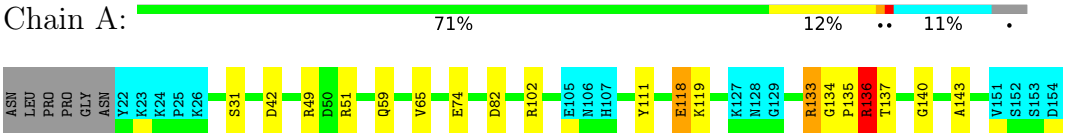
Chain B:



4.2.10 Score per residue for model 10

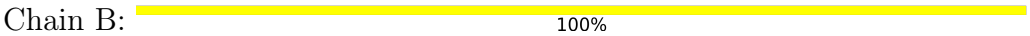
• Molecule 1: Heparin-binding growth factor 1

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

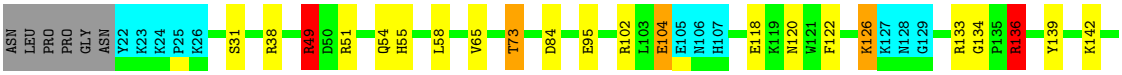
Chain B:



4.2.11 Score per residue for model 11

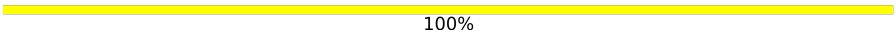
• Molecule 1: Heparin-binding growth factor 1

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:



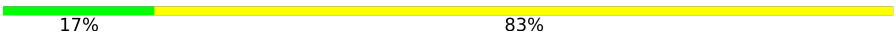
4.2.12 Score per residue for model 12

• 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

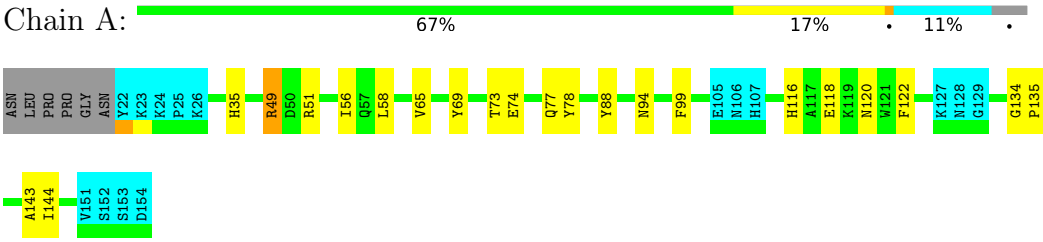
Chain B:



4.2.13 Score per residue for model 13

• Molecule 1: Heparin-binding growth factor 1

Chain A:



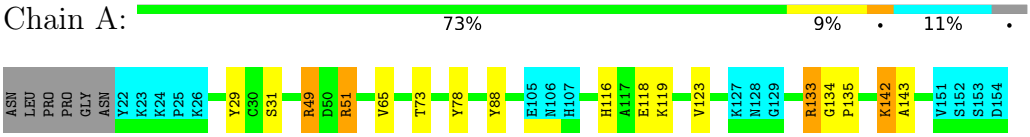
• Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain B:

4.2.14 Score per residue for model 14

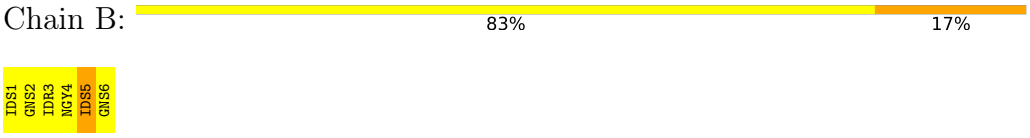
• Molecule 1: Heparin-binding growth factor 1

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

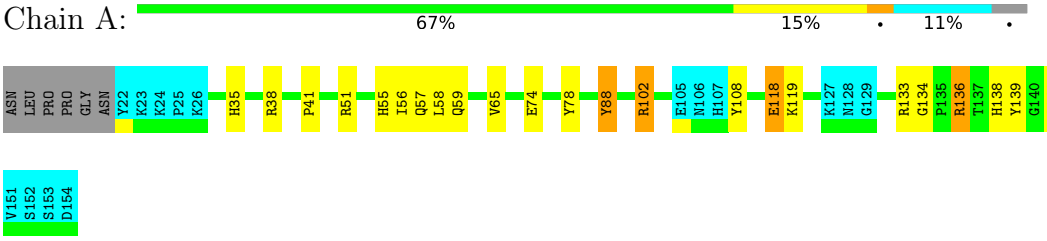
Chain B:



4.2.15 Score per residue for model 15

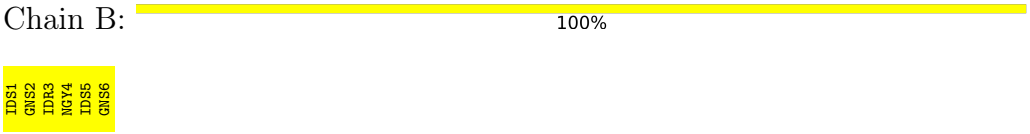
• Molecule 1: Heparin-binding growth factor 1

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

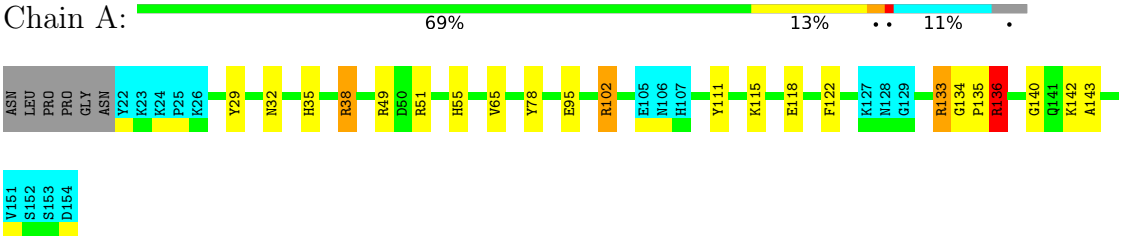
Chain B:



4.2.16 Score per residue for model 16

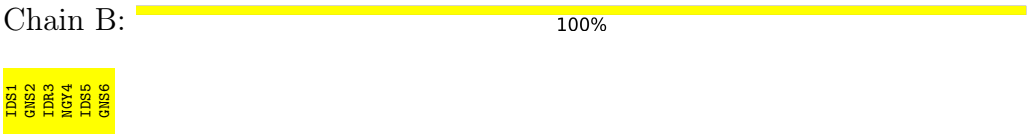
• Molecule 1: Heparin-binding growth factor 1

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

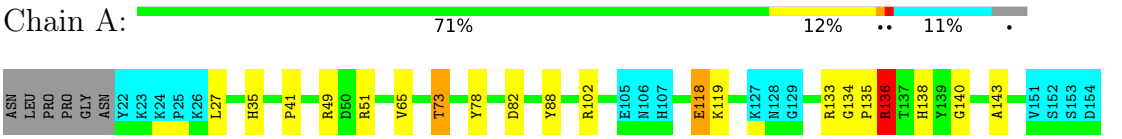
Chain B:



4.2.17 Score per residue for model 17

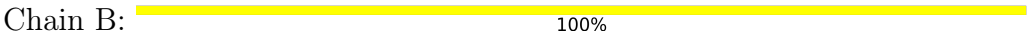
• Molecule 1: Heparin-binding growth factor 1

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

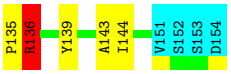
Chain B:



4.2.18 Score per residue for model 18

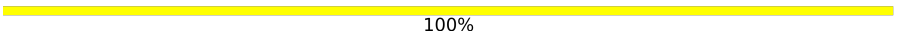
• Molecule 1: Heparin-binding growth factor 1

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

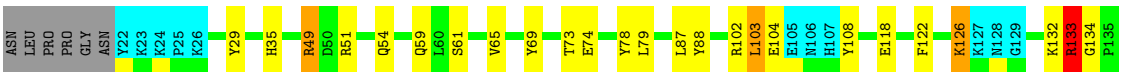
Chain B:



4.2.19 Score per residue for model 19

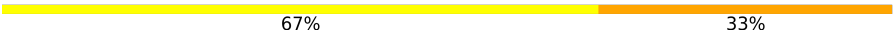
• Molecule 1: Heparin-binding growth factor 1

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

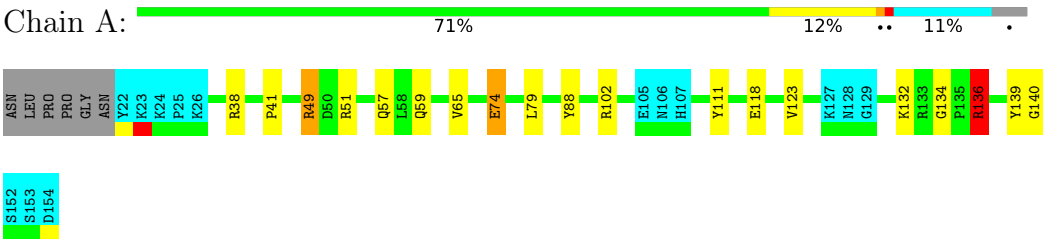
Chain B:



4.2.20 Score per residue for model 20

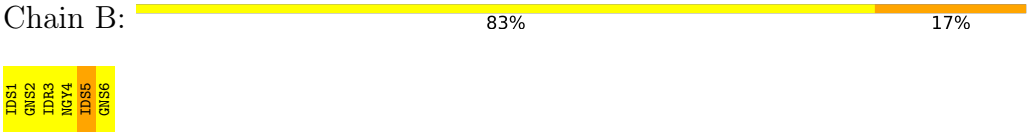
• Molecule 1: Heparin-binding growth factor 1

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:



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: NGY, IDS, IPA, IDR, 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	0.58±0.01	0±0/964 (0.0± 0.0%)	1.04±0.03	2±1/1304 (0.2± 0.1%)
All	All	0.58	0/19280 (0.0%)	1.05	50/26080 (0.2%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	136	ARG	NE-CZ-NH2	-9.99	115.31	120.30	8	4
1	A	133	ARG	NE-CZ-NH2	-9.91	115.34	120.30	9	5
1	A	133	ARG	NE-CZ-NH1	9.51	125.05	120.30	4	7
1	A	136	ARG	NE-CZ-NH1	9.13	124.87	120.30	11	12
1	A	49	ARG	NE-CZ-NH1	7.88	124.24	120.30	6	7
1	A	49	ARG	NE-CZ-NH2	-6.94	116.83	120.30	5	4
1	A	51	ARG	NE-CZ-NH1	6.69	123.65	120.30	7	3
1	A	51	ARG	NE-CZ-NH2	-6.23	117.19	120.30	14	1
1	A	88	TYR	CB-CG-CD2	-5.78	117.53	121.00	6	3
1	A	38	ARG	NE-CZ-NH1	5.50	123.05	120.30	11	2
1	A	49	ARG	CD-NE-CZ	5.35	131.09	123.60	5	1
1	A	38	ARG	NE-CZ-NH2	-5.14	117.73	120.30	11	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
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	20

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:132:LYS:NZ	2:B:6:GNS:O2S	0.43	2.51	9	1
1:A:118:GLU:OE2	1:A:119:LYS:NZ	0.41	2.52	17	6
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	4
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:142:LYS:NZ	2:B:5:IDS:O2S	0.41	2.53	14	1
1:A:71:LYS:NZ	1:A:74:GLU:OE1	0.41	2.54	9	1
1:A:133:ARG:NH2	2:B:2:GNS:O3S	0.40	2.54	19	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%)	4	28
All	All	2360/2780 (85%)	1908 (81%)	346 (15%)	106 (4%)	4	28

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

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Mol	Chain	Res	Type	Models (Total)
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
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 (89±2%)	12±3 (11±2%)	9 52
All	All	2060/2440 (84%)	1825 (89%)	235 (11%)	9 52

All 49 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	136	ARG	17
1	A	135	PRO	14
1	A	49	ARG	13

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Mol	Chain	Res	Type	Models (Total)
1	A	102	ARG	12
1	A	74	GLU	9
1	A	41	PRO	8
1	A	73	THR	7
1	A	133	ARG	6
1	A	138	HIS	6
1	A	56	ILE	6
1	A	142	LYS	6
1	A	126	LYS	6
1	A	59	GLN	6
1	A	35	HIS	6
1	A	58	LEU	5
1	A	55	HIS	4
1	A	38	ARG	4
1	A	144	ILE	4
1	A	116	HIS	4
1	A	84	ASP	4
1	A	88	TYR	4
1	A	120	ASN	4
1	A	119	LYS	3
1	A	57	GLN	3
1	A	104	GLU	3
1	A	79	LEU	3
1	A	78	TYR	2
1	A	94	ASN	2
1	A	95	GLU	2
1	A	132	LYS	2
1	A	54	GLN	2
1	A	82	ASP	2
1	A	103	LEU	2
1	A	45	VAL	1
1	A	52	SER	1
1	A	98	LEU	1
1	A	71	LYS	1
1	A	75	THR	1
1	A	101	GLU	1
1	A	139	TYR	1
1	A	77	GLN	1
1	A	141	GLN	1
1	A	115	LYS	1
1	A	27	LEU	1
1	A	63	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	91	GLN	1
1	A	87	LEU	1

6.3.3 RNA (i)

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	1.23±0.05	1±1 (8±3%)
2	GNS	B	2	2	14,15,16	1.80±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	0.78±0.05	0±0 (0±0%)
2	IDS	B	5	2	16,16,17	1.20±0.07	1±0 (8±2%)
2	GNS	B	6	2	14,15,16	1.66±0.15	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	17,24,26	1.70±0.35	4±2 (20±9%)
2	GNS	B	2	2	17,22,24	1.89±0.25	5±1 (29±5%)
2	IDR	B	3	2	14,17,19	1.19±0.28	1±1 (10±6%)
2	NGY	B	4	2	22,26,28	1.50±0.20	4±1 (18±5%)
2	IDS	B	5	2	17,24,26	1.68±0.41	3±1 (16±7%)
2	GNS	B	6	2	17,22,24	1.65±0.34	3±1 (18±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	6.21	1.67	1.59	18	20
2	B	6	GNS	S1-N2	6.12	1.67	1.59	1	20
2	B	1	IDS	O2-C2	3.62	1.41	1.47	18	20
2	B	5	IDS	O2-C2	3.33	1.42	1.47	11	20
2	B	2	GNS	O2S-S1	3.02	1.45	1.42	2	8
2	B	2	GNS	O3S-S1	2.92	1.45	1.42	11	14
2	B	6	GNS	O2S-S1	2.61	1.45	1.42	6	6
2	B	5	IDS	C1-C2	2.54	1.55	1.51	13	6
2	B	1	IDS	C1-C2	2.50	1.55	1.51	5	6
2	B	6	GNS	C1-C2	2.31	1.55	1.52	1	1
2	B	1	IDS	C4-C5	2.26	1.57	1.53	18	1
2	B	6	GNS	O3S-S1	2.24	1.44	1.42	13	8
2	B	2	GNS	C1-C2	2.23	1.55	1.52	4	1
2	B	1	IDS	O2-S	2.10	1.63	1.57	5	1
2	B	5	IDS	O2-S	2.07	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(^{o})	Ideal(^{o})	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	5	IDS	C2-O2-S	6.87	126.86	117.91	7	20
2	B	1	IDS	O2-C2-C3	6.74	116.36	106.95	13	11
2	B	5	IDS	C1-C2-C3	6.54	119.18	109.40	12	4
2	B	6	GNS	C3-C2-N2	6.04	118.27	110.32	1	4
2	B	1	IDS	C2-O2-S	5.74	125.39	117.91	13	20
2	B	4	NGY	O6-C6-C5	5.30	117.50	107.62	7	12
2	B	6	GNS	O3S-S1-N2	5.20	99.38	108.87	1	18
2	B	6	GNS	O2S-S1-N2	5.14	99.50	108.87	14	19
2	B	3	IDR	C1-C2-C3	4.84	115.61	109.67	4	7
2	B	4	NGY	C2-N2-C7	4.80	129.74	122.90	14	1
2	B	2	GNS	O3S-S1-N2	4.62	100.43	108.87	20	18
2	B	2	GNS	C4-C3-C2	4.15	117.11	111.02	17	3
2	B	2	GNS	O2S-S1-N2	4.14	101.31	108.87	5	16
2	B	4	NGY	C3-C4-C5	4.08	102.96	110.24	16	8
2	B	4	NGY	O4-C4-C5	3.99	119.22	109.30	1	9
2	B	2	GNS	C1-C2-N2	3.97	117.11	110.27	9	1
2	B	2	GNS	O5-C1-C2	3.84	105.22	111.29	1	10
2	B	4	NGY	C6-C5-C4	3.80	120.02	112.09	18	13
2	B	4	NGY	C1-O5-C5	3.66	117.15	112.19	3	7
2	B	6	GNS	O2S-S1-O3S	3.58	111.70	120.16	12	14
2	B	1	IDS	C4-C3-C2	3.57	116.61	110.24	7	4
2	B	5	IDS	C4-C3-C2	3.54	116.56	110.24	2	3
2	B	1	IDS	O4-C4-C5	3.31	117.18	109.74	18	3
2	B	2	GNS	O4-C4-C5	3.30	101.11	109.30	14	8
2	B	6	GNS	O3-C3-C4	3.27	102.78	110.35	1	3
2	B	2	GNS	C3-C4-C5	3.18	115.92	110.24	18	2
2	B	2	GNS	O2S-S1-O3S	3.08	112.89	120.16	17	17
2	B	1	IDS	C3-C4-C5	3.05	114.47	109.25	14	2
2	B	1	IDS	O5-C5-C6	3.03	116.27	106.31	9	8
2	B	1	IDS	C1-C2-C3	3.02	113.92	109.40	7	2
2	B	2	GNS	C1-O5-C5	3.01	116.27	112.19	3	6
2	B	5	IDS	O5-C5-C6	3.00	116.17	106.31	13	7
2	B	3	IDR	O4-C4-C5	2.99	116.45	109.74	18	4
2	B	3	IDR	O5-C5-C6	2.98	116.12	106.31	7	16
2	B	4	NGY	O5-C5-C6	2.98	114.22	107.61	6	3
2	B	1	IDS	O5-C1-C2	2.78	115.03	109.41	9	1
2	B	4	NGY	O9-S-O8	2.67	117.78	108.49	8	8
2	B	2	GNS	O3-C3-C4	2.63	104.26	110.35	17	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	5	IDS	O5-C1-C2	2.58	114.63	109.41	6	1
2	B	4	NGY	O9-S-O7A	2.55	117.36	108.49	3	4
2	B	4	NGY	O6-S-O8	2.52	99.24	106.88	11	5
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	1	IDS	O3S-S-O1S	2.42	116.89	108.49	10	10
2	B	6	GNS	O5-C1-C2	2.35	107.58	111.29	2	2
2	B	1	IDS	O3S-S-O2S	2.34	116.61	108.49	9	10
2	B	5	IDS	O4-C4-C3	2.33	115.73	110.35	1	1
2	B	5	IDS	C3-C4-C5	2.27	113.14	109.25	2	1
2	B	6	GNS	C1-O5-C5	2.27	115.26	112.19	13	1
2	B	5	IDS	O3S-S-O1S	2.26	116.34	108.49	6	8
2	B	6	GNS	C4-C3-C2	2.24	107.74	111.02	2	3
2	B	2	GNS	O4-C4-C3	2.23	105.19	110.35	2	1
2	B	2	GNS	C6-C5-C4	2.21	107.82	113.00	16	2
2	B	5	IDS	O3S-S-O2S	2.17	116.03	108.49	9	5
2	B	4	NGY	O4-C4-C3	2.13	105.43	110.35	17	2
2	B	2	GNS	O5-C5-C6	2.11	110.52	107.20	5	1
2	B	3	IDR	O6B-C6-C5	2.05	121.17	113.65	2	1
2	B	4	NGY	O6-S-O7A	2.05	100.67	106.88	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

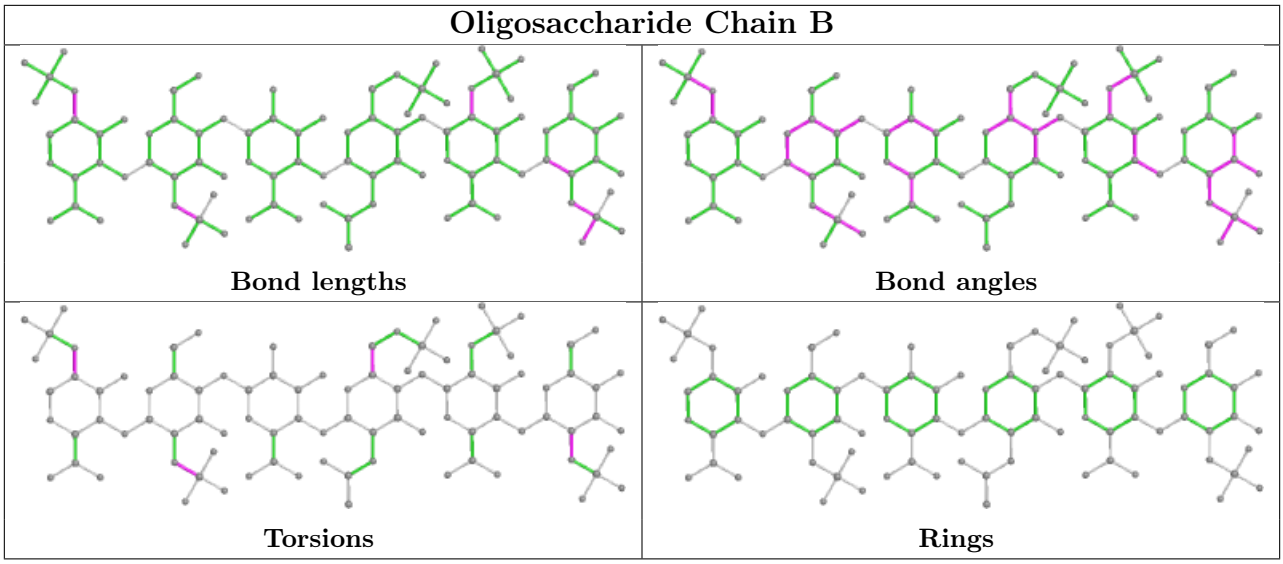
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

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