



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 PM UTC

PDB ID : 1BFB / pdb\_00001bfb  
Title : BASIC FIBROBLAST GROWTH FACTOR COMPLEXED WITH HEP-  
ARIN TETRAMER FRAGMENT  
Authors : Faham, S.; Rees, D.C.  
Deposited on : 1995-12-12  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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/XrayValidationReportHelp>

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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

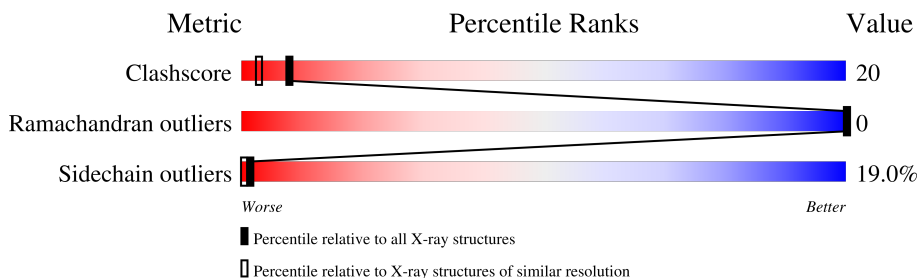
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	147	
2	B	4	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1070 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

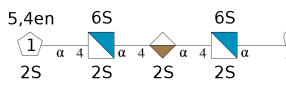
- Molecule 1 is a protein called BASIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	124	991	630	180	177	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	SER	CYS	engineered mutation	UNP P09038
A	88	SER	CYS	engineered mutation	UNP P09038

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	4	70	24	2	38	6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

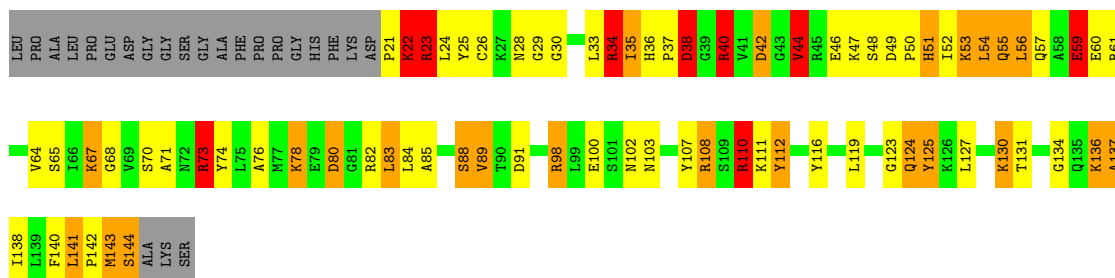
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR

Chain A: 



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

Chain B: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	32.02Å 41.80Å 85.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90	Depositor
% Data completeness (in resolution range)	93.9 (5.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SGN, UAP, IDS

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 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	1.06	1/1012 (0.1%)	1.82	16/1356 (1.2%)

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 outliers	#Planarity outliers
1	A	0	51

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CD2-NE2	-5.89	1.31	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH1	-18.91	102.59	121.50
1	A	40	ARG	CG-CD-NE	-8.93	92.36	112.00
1	A	40	ARG	NE-CZ-NH2	-8.36	111.67	119.20
1	A	108	ARG	NE-CZ-NH2	-7.56	112.39	119.20
1	A	110	ARG	NE-CZ-NH2	-7.08	112.83	119.20
1	A	38	ASP	O-C-N	-5.75	115.16	122.34
1	A	34	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	A	83	LEU	O-C-N	-5.47	116.81	123.27
1	A	23	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	A	40	ARG	CA-CB-CG	-5.24	103.62	114.10
1	A	76	ALA	CA-C-N	-5.14	115.81	123.11
1	A	76	ALA	C-N-CA	-5.14	115.81	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLU	CA-C-O	-5.11	113.30	119.27
1	A	98	ARG	O-C-N	-5.07	117.38	123.31
1	A	138	ILE	O-C-N	-5.04	117.16	122.20
1	A	116	TYR	CB-CA-C	-5.02	100.34	109.38

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Sidechain
1	A	107	TYR	Sidechain
1	A	108	ARG	Sidechain
1	A	110	ARG	Sidechain
1	A	112	TYR	Mainchain
1	A	123	GLY	Mainchain
1	A	124	GLN	Mainchain
1	A	125	TYR	Mainchain,Sidechain
1	A	130	LYS	Mainchain
1	A	131	THR	Mainchain
1	A	134	GLY	Mainchain
1	A	137	ALA	Mainchain
1	A	141	LEU	Mainchain
1	A	142	PRO	Mainchain
1	A	143	MET	Mainchain
1	A	21	PRO	Mainchain
1	A	22	LYS	Mainchain
1	A	23	ARG	Mainchain,Sidechain
1	A	29	GLY	Mainchain
1	A	30	GLY	Mainchain
1	A	33	LEU	Mainchain
1	A	34	ARG	Sidechain
1	A	35	ILE	Mainchain
1	A	37	PRO	Mainchain
1	A	38	ASP	Mainchain
1	A	40	ARG	Mainchain,Sidechain
1	A	42	ASP	Mainchain
1	A	44	VAL	Mainchain
1	A	54	LEU	Mainchain
1	A	55	GLN	Mainchain
1	A	56	LEU	Mainchain
1	A	59	GLU	Mainchain
1	A	61	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	64	VAL	Mainchain
1	A	65	SER	Mainchain
1	A	68	GLY	Mainchain
1	A	70	SER	Mainchain
1	A	71	ALA	Mainchain
1	A	73	ARG	Mainchain,Sidechain
1	A	78	LYS	Mainchain
1	A	80	ASP	Sidechain
1	A	82	ARG	Mainchain
1	A	84	LEU	Mainchain
1	A	88	SER	Mainchain
1	A	89	VAL	Mainchain
1	A	91	ASP	Sidechain
1	A	98	ARG	Mainchain

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	991	0	999	41	0
2	B	70	0	23	0	0
3	A	9	0	0	0	0
All	All	1070	0	1022	41	0

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 20.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.09	1.10
1:A:127:LEU:HD12	1:A:130:LYS:HE3	1.39	1.03
1:A:38:ASP:OD2	1:A:40:ARG:HD3	1.65	0.94
1:A:38:ASP:CG	1:A:40:ARG:HD3	1.95	0.92
1:A:28:ASN:HA	1:A:136:LYS:HD3	1.52	0.89
1:A:110:ARG:HG2	1:A:110:ARG:NH1	1.84	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HD2	1:A:42:ASP:OD1	1.75	0.86
1:A:34:ARG:HD3	1:A:36:HIS:NE2	2.00	0.76
1:A:23:ARG:HD2	1:A:52:ILE:HD12	1.67	0.75
1:A:73:ARG:HB2	1:A:85:ALA:HB1	1.68	0.75
1:A:22:LYS:HB3	1:A:22:LYS:NZ	2.06	0.71
1:A:53:LYS:HE3	1:A:53:LYS:HA	1.70	0.71
1:A:67:LYS:HE2	1:A:74:TYR:CZ	2.31	0.64
1:A:53:LYS:HA	1:A:53:LYS:CE	2.26	0.63
1:A:36:HIS:HE1	1:A:42:ASP:OD2	1.81	0.62
1:A:23:ARG:HD2	1:A:52:ILE:CD1	2.29	0.61
1:A:22:LYS:HB3	1:A:22:LYS:HZ2	1.66	0.61
1:A:34:ARG:HD3	1:A:36:HIS:CD2	2.35	0.61
1:A:111:LYS:HE2	1:A:112:TYR:CZ	2.39	0.58
1:A:102:ASN:O	1:A:103:ASN:HB2	2.04	0.55
1:A:56:LEU:N	1:A:56:LEU:HD12	2.21	0.55
1:A:110:ARG:O	1:A:110:ARG:HG3	2.07	0.54
1:A:22:LYS:NZ	1:A:22:LYS:CB	2.72	0.53
1:A:26:CYS:HB2	1:A:140:PHE:CE2	2.44	0.53
1:A:119:LEU:HD23	1:A:125:TYR:HA	1.90	0.53
1:A:34:ARG:HD3	1:A:36:HIS:CE1	2.44	0.51
1:A:28:ASN:HB2	1:A:137:ALA:HA	1.95	0.48
1:A:34:ARG:NH2	1:A:44:VAL:HG11	2.29	0.48
1:A:49:ASP:O	1:A:52:ILE:HG12	2.14	0.47
1:A:110:ARG:HH11	1:A:110:ARG:CG	2.01	0.47
1:A:24:LEU:HG	1:A:54:LEU:HD12	1.96	0.47
1:A:34:ARG:CD	1:A:36:HIS:NE2	2.75	0.46
1:A:49:ASP:OD1	1:A:50:PRO:HD2	2.17	0.44
1:A:59:GLU:O	1:A:60:GLU:HG3	2.18	0.44
1:A:25:TYR:CB	1:A:143:MET:HE3	2.47	0.43
1:A:35:ILE:O	1:A:51:HIS:HB3	2.19	0.43
1:A:143:MET:C	1:A:144:SER:O	2.62	0.42
1:A:40:ARG:HE	1:A:40:ARG:HB2	1.17	0.41
1:A:111:LYS:HE2	1:A:112:TYR:OH	2.21	0.41
1:A:22:LYS:NZ	1:A:144:SER:HA	2.36	0.41
1:A:46:GLU:OE2	1:A:48:SER:OG	2.34	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	122/147 (83%)	115 (94%)	7 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	105/123 (85%)	85 (81%)	20 (19%)	1	0

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	34	ARG
1	A	40	ARG
1	A	44	VAL
1	A	47	LYS
1	A	53	LYS
1	A	55	GLN
1	A	57	GLN
1	A	67	LYS
1	A	73	ARG
1	A	78	LYS
1	A	80	ASP
1	A	83	LEU

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Mol	Chain	Res	Type
1	A	88	SER
1	A	89	VAL
1	A	110	ARG
1	A	124	GLN
1	A	136	LYS
1	A	141	LEU
1	A	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	57	GLN
1	A	135	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SGN	B	1	2	20,20,20	3.94	2 (10%)	25,31,31	1.44	3 (12%)
2	IDS	B	2	2	16,16,17	2.04	2 (12%)	16,24,26	0.93	0
2	SGN	B	3	2	19,19,20	3.64	4 (21%)	23,29,31	1.83	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UAP	B	4	2	15,15,16	3.19	5 (33%)	18,22,24	1.67	3 (16%)

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	SGN	B	1	2	-	5/11/31/31	0/1/1/1
2	IDS	B	2	2	-	0/9/26/29	0/1/1/1
2	SGN	B	3	2	-	0/11/28/31	0/1/1/1
2	UAP	B	4	2	-	0/9/22/25	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SGN	S1-N2	15.50	1.79	1.59
2	B	3	SGN	S1-N2	13.22	1.76	1.59
2	B	1	SGN	O6-S2	7.61	1.77	1.56
2	B	4	UAP	C5-C6	-7.37	1.32	1.48
2	B	3	SGN	O6-S2	7.01	1.75	1.56
2	B	4	UAP	C3-C4	-5.76	1.43	1.50
2	B	4	UAP	O2-S	5.58	1.74	1.57
2	B	2	IDS	O2-C2	-5.50	1.39	1.47
2	B	2	IDS	O2-S	4.91	1.72	1.57
2	B	4	UAP	O2-C2	-4.56	1.40	1.47
2	B	3	SGN	O1S-S1	3.17	1.45	1.42
2	B	4	UAP	O6B-C6	-2.49	1.23	1.30
2	B	3	SGN	C2-N2	-2.46	1.43	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SGN	O1S-S1-O2S	-5.78	107.49	120.36
2	B	1	SGN	O1S-S1-O2S	-4.70	109.91	120.36
2	B	4	UAP	O5-C5-C6	4.47	120.08	111.85
2	B	4	UAP	C4-C5-C6	-3.58	115.81	123.56
2	B	3	SGN	C1-C2-N2	-2.89	105.65	110.22
2	B	4	UAP	O5-C1-C2	-2.76	108.13	111.10
2	B	1	SGN	C3-C4-C5	-2.63	105.46	110.23
2	B	1	SGN	O1-C1-C2	2.52	114.45	109.22
2	B	3	SGN	C4-C3-C2	-2.31	107.63	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SGN	O4-C4-C3	-2.30	104.96	110.38
2	B	3	SGN	C3-C2-N2	-2.18	107.46	110.32
2	B	3	SGN	O5-C5-C4	-2.06	105.82	110.83

There are no chirality outliers.

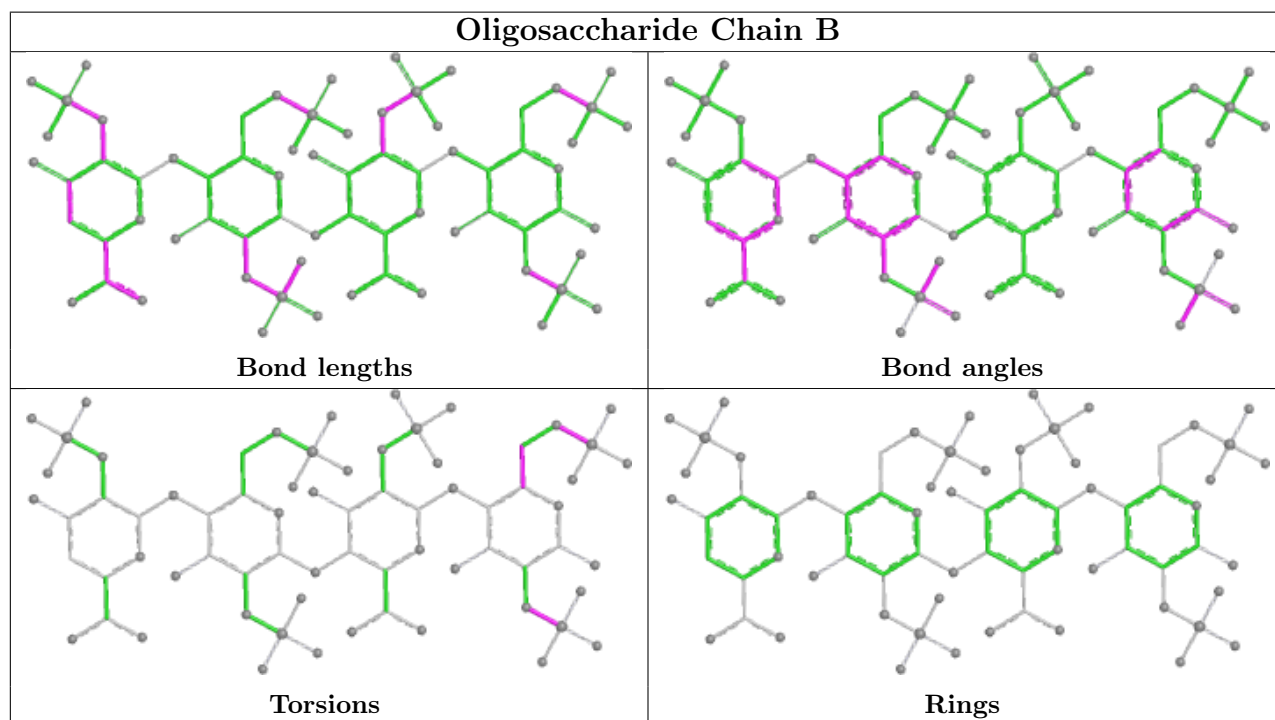
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	SGN	O5-C5-C6-O6
2	B	1	SGN	C2-N2-S1-O1S
2	B	1	SGN	C6-O6-S2-O6S
2	B	1	SGN	C6-O6-S2-O4S
2	B	1	SGN	C6-O6-S2-O5S

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.