



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2024 – 09:59 pm BST

PDB ID : 2X1W  
Title : Crystal Structure of VEGF-C in Complex with Domains 2 and 3 of VEGFR2  
Authors : Leppanen, V.M.; Prota, A.E.; Jeltsch, M.; Anisimov, A.; Kalkkinen, N.; Strandin, T.; Lankinen, H.; Goldman, A.; Ballmer-Hofer, K.; Alitalo, K.  
Deposited on : 2010-01-08  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

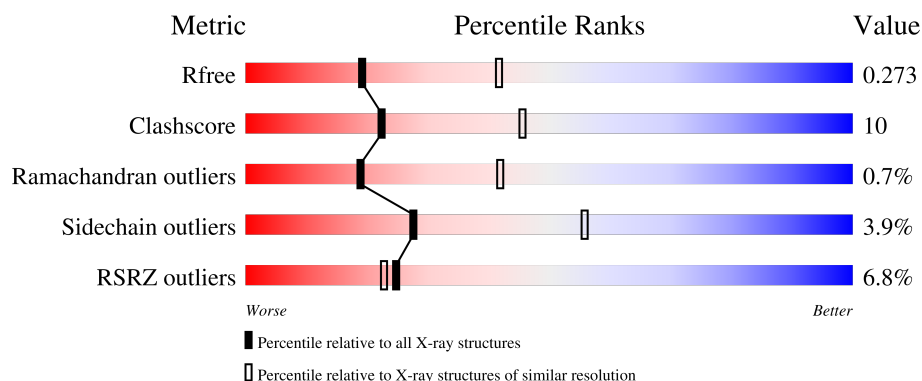
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	110	
1	B	110	
1	C	110	
1	D	110	
2	L	213	

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Mol	Chain	Length	Quality of chain
2	M	213	
2	N	213	
2	O	213	
3	E	3	
3	F	3	
3	G	3	
3	H	3	
3	I	3	
3	J	3	
3	K	3	
3	P	3	
3	S	3	
4	Q	2	
4	R	2	
4	T	2	
4	U	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	S	1	X	-	-	-
6	NAG	L	2401	X	-	-	-
6	NAG	O	2001	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9720 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 VASCULAR ENDOTHELIAL GROWTH FACTOR C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			750	468	127	144	11			
1	B	98	Total	C	N	O	S	0	0	0
			752	470	128	143	11			
1	C	97	Total	C	N	O	S	0	0	0
			743	465	127	140	11			
1	D	99	Total	C	N	O	S	0	0	0
			760	476	129	144	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	CYS	engineered mutation	UNP P49767
B	137	ALA	CYS	engineered mutation	UNP P49767
C	137	ALA	CYS	engineered mutation	UNP P49767
D	137	ALA	CYS	engineered mutation	UNP P49767

- Molecule 2 is a protein called VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	196	Total	C	N	O	S	0	0	0
			1535	977	261	287	10			
2	M	179	Total	C	N	O	S	0	0	0
			1402	894	236	262	10			
2	N	194	Total	C	N	O	S	0	0	0
			1522	969	255	288	10			
2	O	193	Total	C	N	O	S	0	0	0
			1516	967	256	283	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cs 1 1	0	0
5	C	1	Total Cs 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 14 8 1 5	0	0
6	L	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	O	1	Total C N O 14 8 1 5	0	0
6	O	1	Total C N O 14 8 1 5	0	0
6	O	1	Total C N O 14 8 1 5	0	0

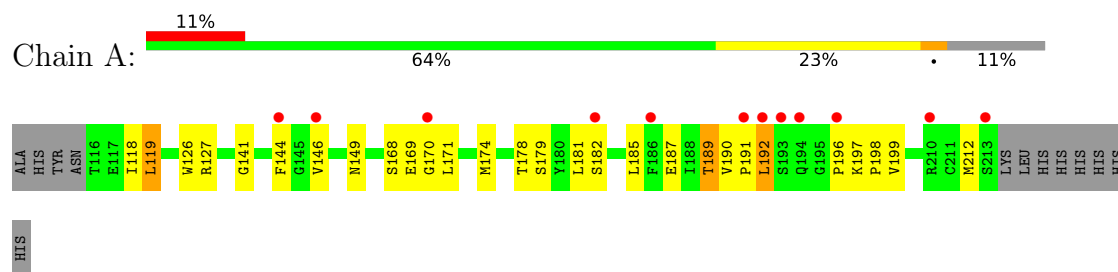
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total 14	O 14	0	0
7	B	11	Total 11	O 11	0	0
7	C	32	Total 32	O 32	0	0
7	D	19	Total 19	O 19	0	0
7	L	31	Total 31	O 31	0	0
7	M	12	Total 12	O 12	0	0
7	N	34	Total 34	O 34	0	0
7	O	24	Total 24	O 24	0	0

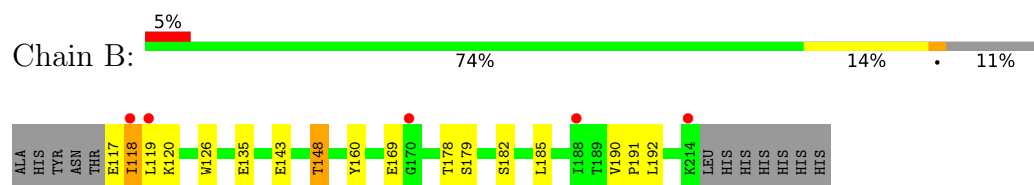
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

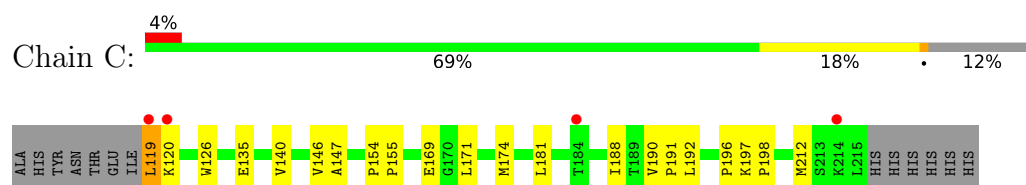
- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



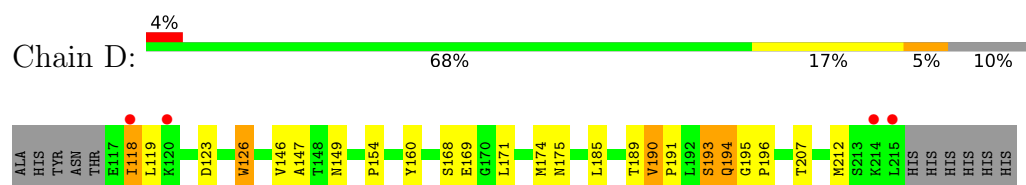
- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



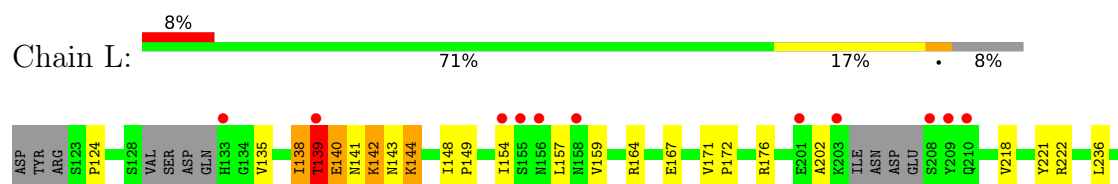
- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



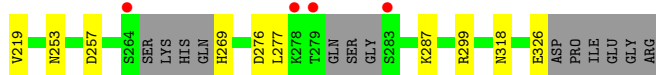
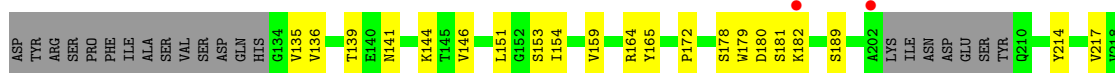
- Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



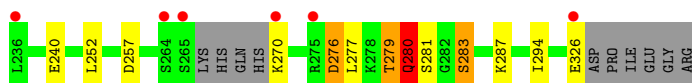
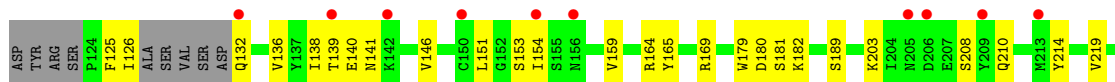




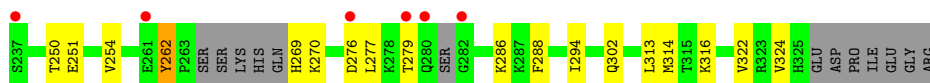
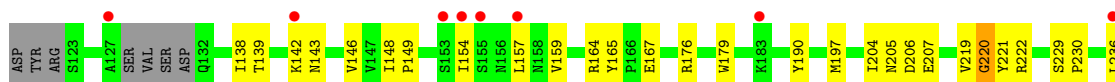
- Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



- Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



- Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 33% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 33% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  33% 67%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  33% 67%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50%  50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.75Å 123.83Å 211.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.96 – 2.70 52.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.96-2.70) 99.6 (52.96-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.227 , 0.280 0.222 , 0.273	Depositor DCC
$R_{free}$ test set	2747 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 70.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: NAG, CS, BMA

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	0.31	0/765	0.52	0/1035
1	B	0.34	0/767	0.54	0/1036
1	C	0.35	0/758	0.53	0/1024
1	D	0.34	0/775	0.53	0/1047
2	L	0.31	0/1565	0.48	0/2113
2	M	0.28	0/1426	0.47	0/1925
2	N	0.30	0/1550	0.47	0/2093
2	O	0.32	0/1544	0.50	0/2085
All	All	0.32	0/9150	0.50	0/12358

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	750	0	732	20	0
1	B	752	0	738	10	0
1	C	743	0	732	13	0
1	D	760	0	749	22	0
2	L	1535	0	1540	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1402	0	1415	24	0
2	N	1522	0	1526	37	0
2	O	1516	0	1518	33	0
3	E	39	0	34	1	0
3	F	39	0	34	2	0
3	G	39	0	34	1	0
3	H	39	0	34	3	0
3	I	39	0	34	0	0
3	J	39	0	34	1	0
3	K	39	0	34	1	0
3	P	39	0	34	4	0
3	S	39	0	34	2	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	L	28	0	26	0	0
6	N	28	0	26	0	0
6	O	42	0	39	3	0
7	A	14	0	0	0	0
7	B	11	0	0	1	0
7	C	32	0	0	1	0
7	D	19	0	0	1	0
7	L	31	0	0	0	0
7	M	12	0	0	0	0
7	N	34	0	0	0	0
7	O	24	0	0	0	0
All	All	9720	0	9447	198	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 10.

The worst 5 of 198 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)
2:N:280:GLN:HB2	2:N:281:SER:HA	1.22	1.14
2:N:280:GLN:CB	2:N:281:SER:HA	1.78	1.11
2:O:138:ILE:HG22	2:O:146:VAL:HG11	1.41	1.00
2:L:142:LYS:HG3	2:L:143:ASN:H	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:HA2	1:A:146:VAL:HG21	1.59	0.82

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	96/110 (87%)	92 (96%)	3 (3%)	1 (1%)	13	33
1	B	96/110 (87%)	95 (99%)	0	1 (1%)	13	33
1	C	95/110 (86%)	93 (98%)	2 (2%)	0	100	100
1	D	97/110 (88%)	89 (92%)	7 (7%)	1 (1%)	13	33
2	L	190/213 (89%)	175 (92%)	12 (6%)	3 (2%)	8	21
2	M	171/213 (80%)	156 (91%)	15 (9%)	0	100	100
2	N	188/213 (88%)	169 (90%)	18 (10%)	1 (0%)	25	49
2	O	185/213 (87%)	174 (94%)	10 (5%)	1 (0%)	25	49
All	All	1118/1292 (86%)	1043 (93%)	67 (6%)	8 (1%)	19	42

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	PHE
2	L	140	GLU
2	N	280	GLN
2	L	280	GLN
1	B	192	LEU

### 5.3.2 Protein sidechains ⓘ

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	89/100 (89%)	82 (92%)	7 (8%)	10	25
1	B	89/100 (89%)	82 (92%)	7 (8%)	10	25
1	C	88/100 (88%)	86 (98%)	2 (2%)	45	74
1	D	90/100 (90%)	86 (96%)	4 (4%)	24	51
2	L	176/192 (92%)	170 (97%)	6 (3%)	32	61
2	M	161/192 (84%)	157 (98%)	4 (2%)	42	72
2	N	175/192 (91%)	167 (95%)	8 (5%)	23	49
2	O	173/192 (90%)	170 (98%)	3 (2%)	56	81
All	All	1041/1168 (89%)	1000 (96%)	41 (4%)	27	56

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	269	HIS
2	N	280	GLN
2	M	276	ASP
2	N	257	ASP
2	N	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	141	ASN
2	N	132	GLN
2	N	280	GLN
2	O	280	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

35 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	$\# Z  > 2$
3	NAG	E	1	3,1	14,14,15	0.67	0	17,19,21	1.18	2 (11%)
3	NAG	E	2	3	14,14,15	0.50	0	17,19,21	0.79	0
3	BMA	E	3	3	11,11,12	0.65	0	15,15,17	0.88	0
3	NAG	F	1	3,1	14,14,15	0.63	0	17,19,21	1.02	0
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
3	BMA	F	3	3	11,11,12	0.71	0	15,15,17	0.58	0
3	NAG	G	1	3,1	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
3	NAG	G	2	3	14,14,15	0.48	0	17,19,21	0.82	1 (5%)
3	BMA	G	3	3	11,11,12	0.61	0	15,15,17	1.06	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.71	0	17,19,21	1.34	3 (17%)
3	NAG	H	2	3	14,14,15	0.60	0	17,19,21	1.05	1 (5%)
3	BMA	H	3	3	11,11,12	0.64	0	15,15,17	0.89	1 (6%)
3	NAG	I	1	3,1	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
3	NAG	I	2	3	14,14,15	0.55	0	17,19,21	0.82	0
3	BMA	I	3	3	11,11,12	0.64	0	15,15,17	0.97	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.64	0	17,19,21	1.23	3 (17%)
3	NAG	J	2	3	14,14,15	0.66	0	17,19,21	0.67	0
3	BMA	J	3	3	11,11,12	0.69	0	15,15,17	1.00	1 (6%)
3	NAG	K	1	3,1	14,14,15	0.51	0	17,19,21	1.37	1 (5%)
3	NAG	K	2	3	14,14,15	0.38	0	17,19,21	1.13	1 (5%)
3	BMA	K	3	3	11,11,12	0.61	0	15,15,17	0.84	0
3	NAG	P	1	3,1	14,14,15	0.47	0	17,19,21	1.19	4 (23%)
3	NAG	P	2	3	14,14,15	0.64	0	17,19,21	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	P	3	3	11,11,12	0.69	0	15,15,17	0.91	1 (6%)
4	NAG	Q	1	4,2	14,14,15	0.56	0	17,19,21	0.73	0
4	NAG	Q	2	4	14,14,15	0.55	0	17,19,21	0.76	0
4	NAG	R	1	4,2	14,14,15	0.54	0	17,19,21	0.82	0
4	NAG	R	2	4	14,14,15	0.54	0	17,19,21	0.79	0
3	NAG	S	1	3,2	14,14,15	0.60	0	17,19,21	1.64	3 (17%)
3	NAG	S	2	3	14,14,15	0.63	0	17,19,21	1.15	2 (11%)
3	BMA	S	3	3	11,11,12	0.61	0	15,15,17	1.21	2 (13%)
4	NAG	T	1	4,2	14,14,15	0.47	0	17,19,21	1.58	3 (17%)
4	NAG	T	2	4	14,14,15	0.48	0	17,19,21	1.19	3 (17%)
4	NAG	U	1	4,2	14,14,15	0.63	0	17,19,21	0.86	0
4	NAG	U	2	4	14,14,15	0.61	0	17,19,21	1.15	1 (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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
3	NAG	S	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	BMA	S	3	3	-	1/2/19/22	0/1/1/1
4	NAG	T	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1
4	NAG	U	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1	NAG	C3-C4-C5	-4.07	102.97	110.24
4	T	1	NAG	C1-O5-C5	3.43	116.83	112.19
3	J	1	NAG	O5-C1-C2	-3.42	105.89	111.29
3	K	1	NAG	C2-N2-C7	-3.34	118.15	122.90
3	H	1	NAG	C4-C3-C2	3.23	115.75	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	S	1	NAG	C1

5 of 54 torsion outliers are listed below:

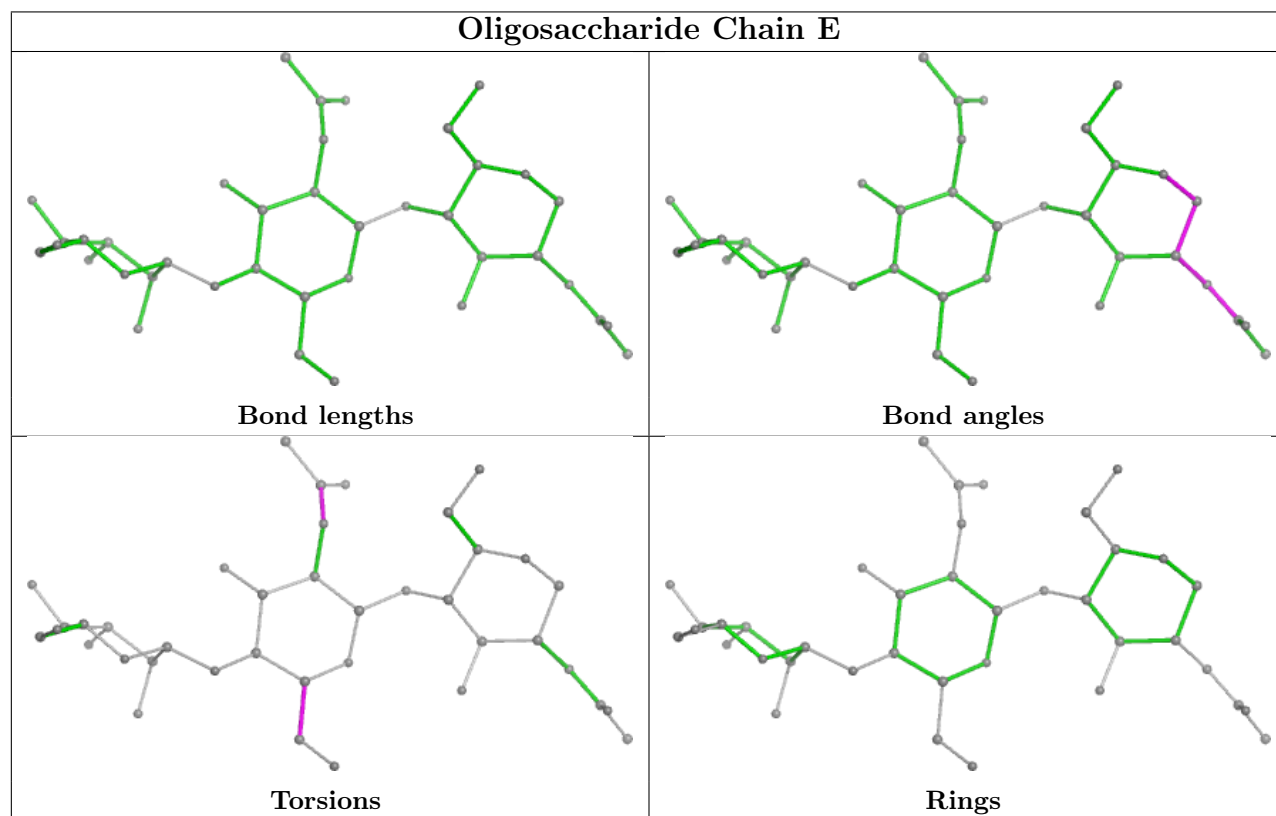
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2

There are no ring outliers.

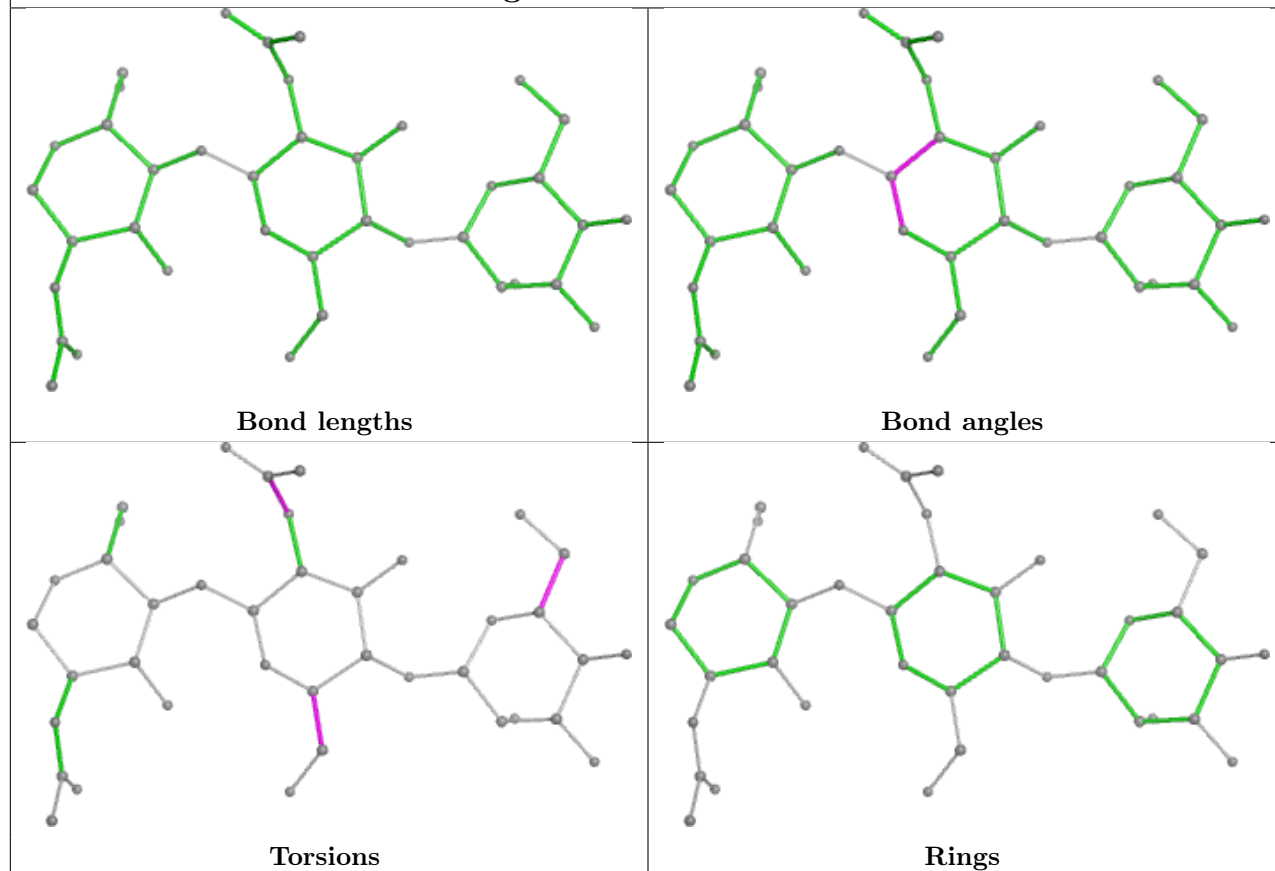
12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	3	0
3	E	2	NAG	1	0
3	S	1	NAG	2	0
3	H	2	NAG	2	0
3	K	1	NAG	1	0
3	S	2	NAG	1	0
3	J	1	NAG	1	0
3	P	2	NAG	1	0
3	E	3	BMA	1	0
3	G	2	NAG	1	0
3	P	1	NAG	4	0
3	F	1	NAG	2	0

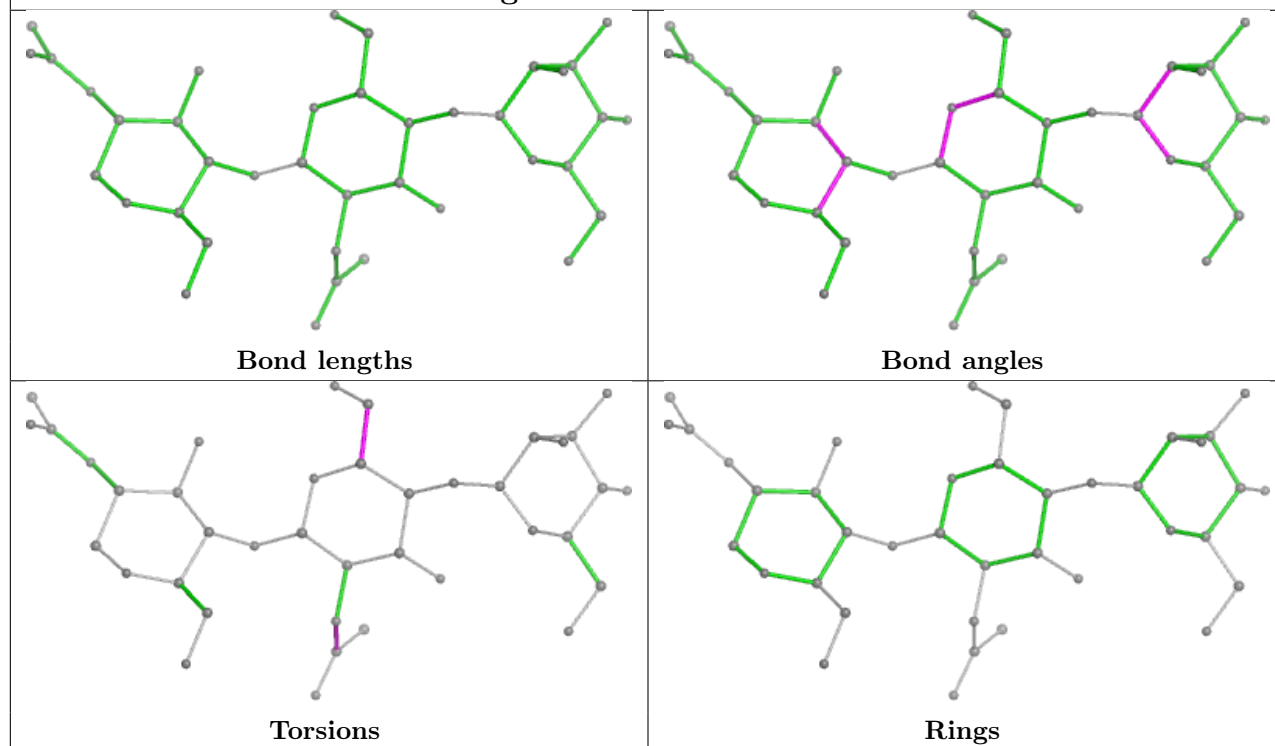
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



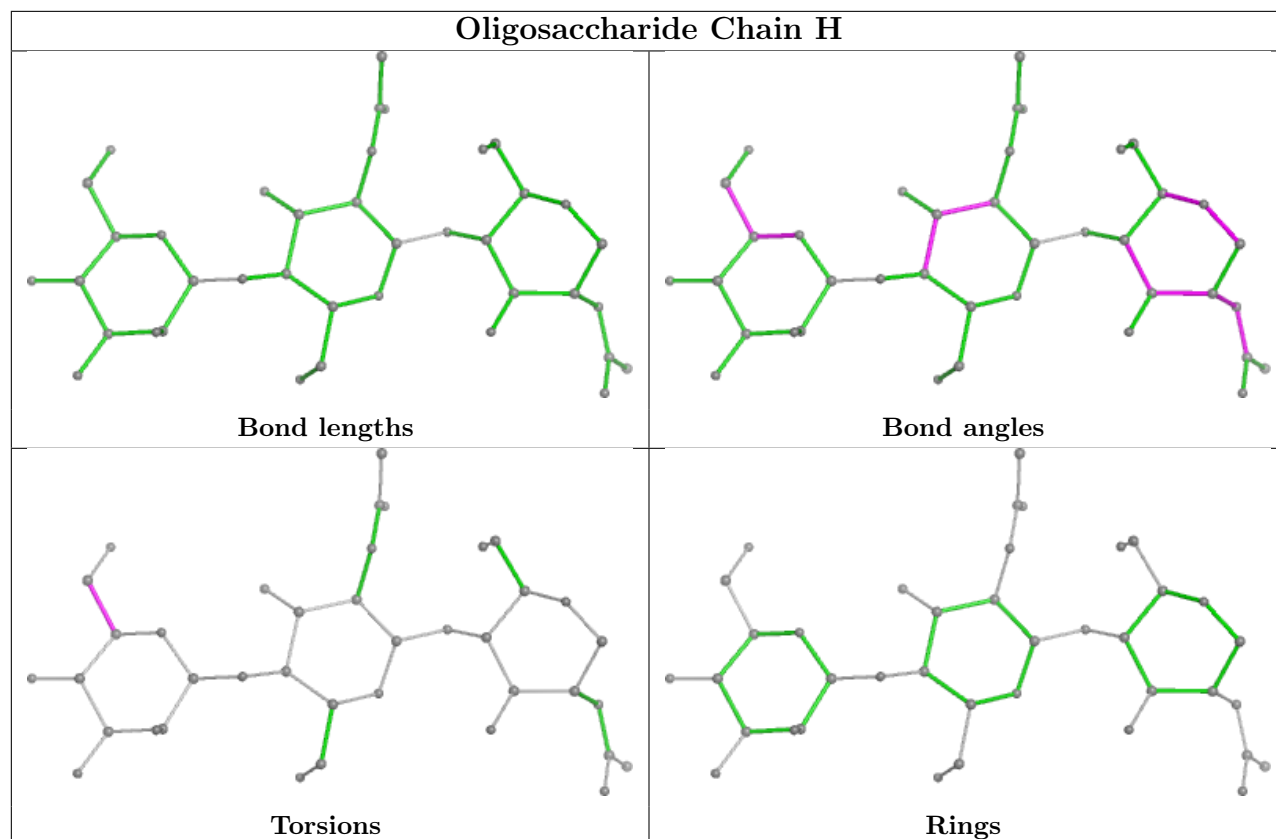
## Oligosaccharide Chain F



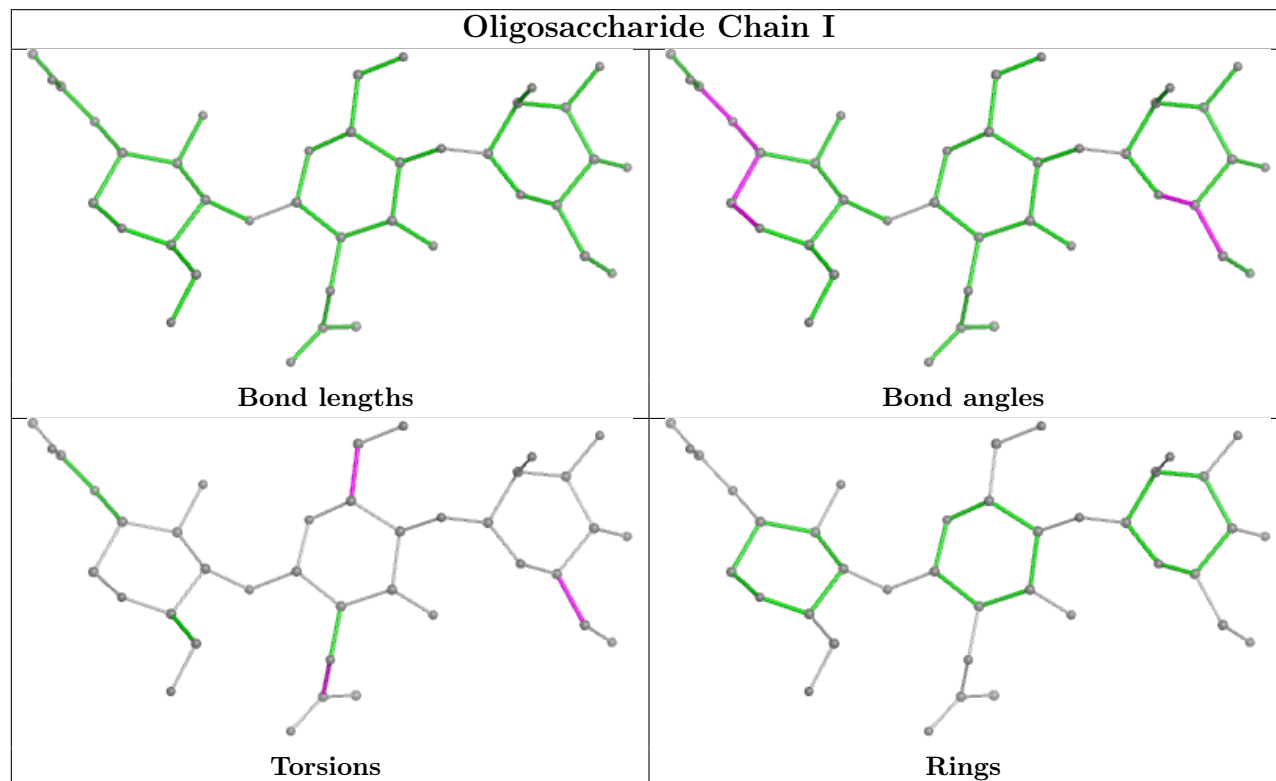
## Oligosaccharide Chain G



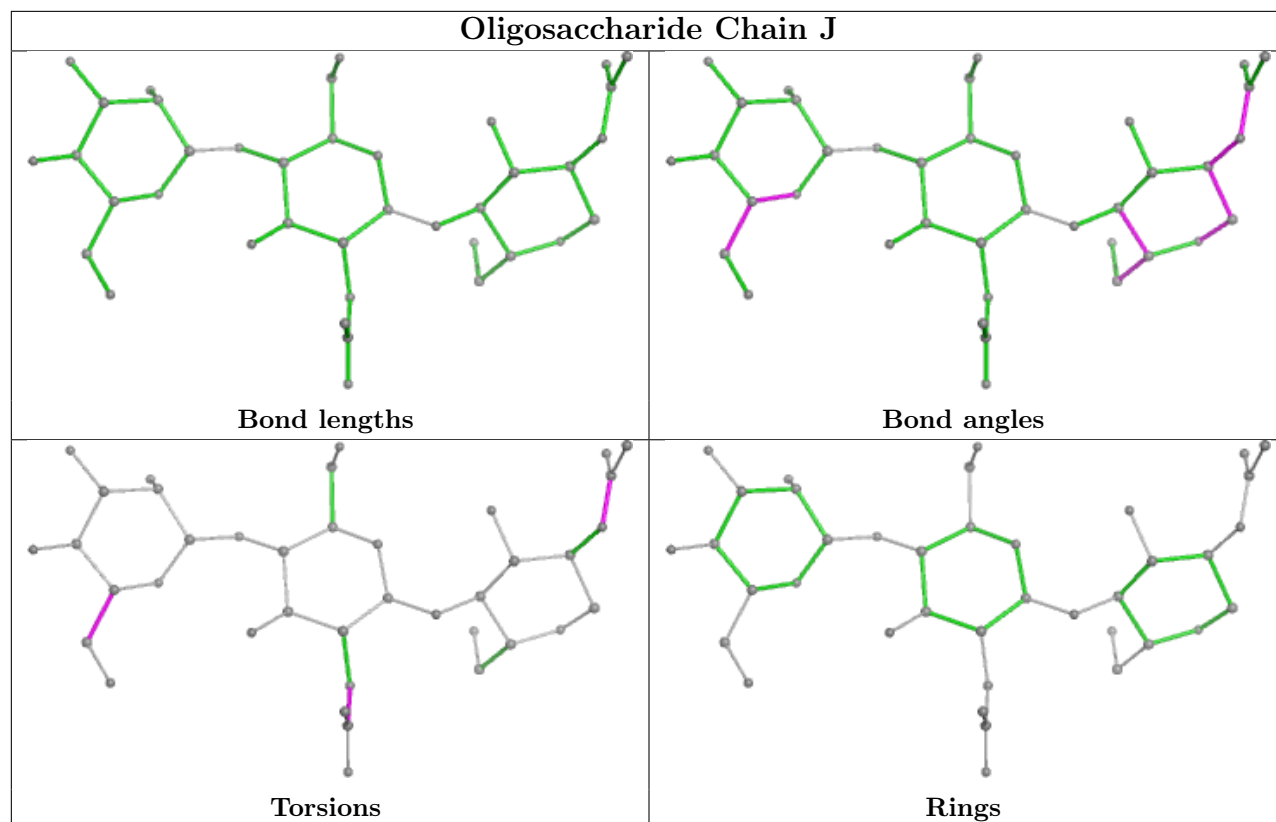
## Oligosaccharide Chain H



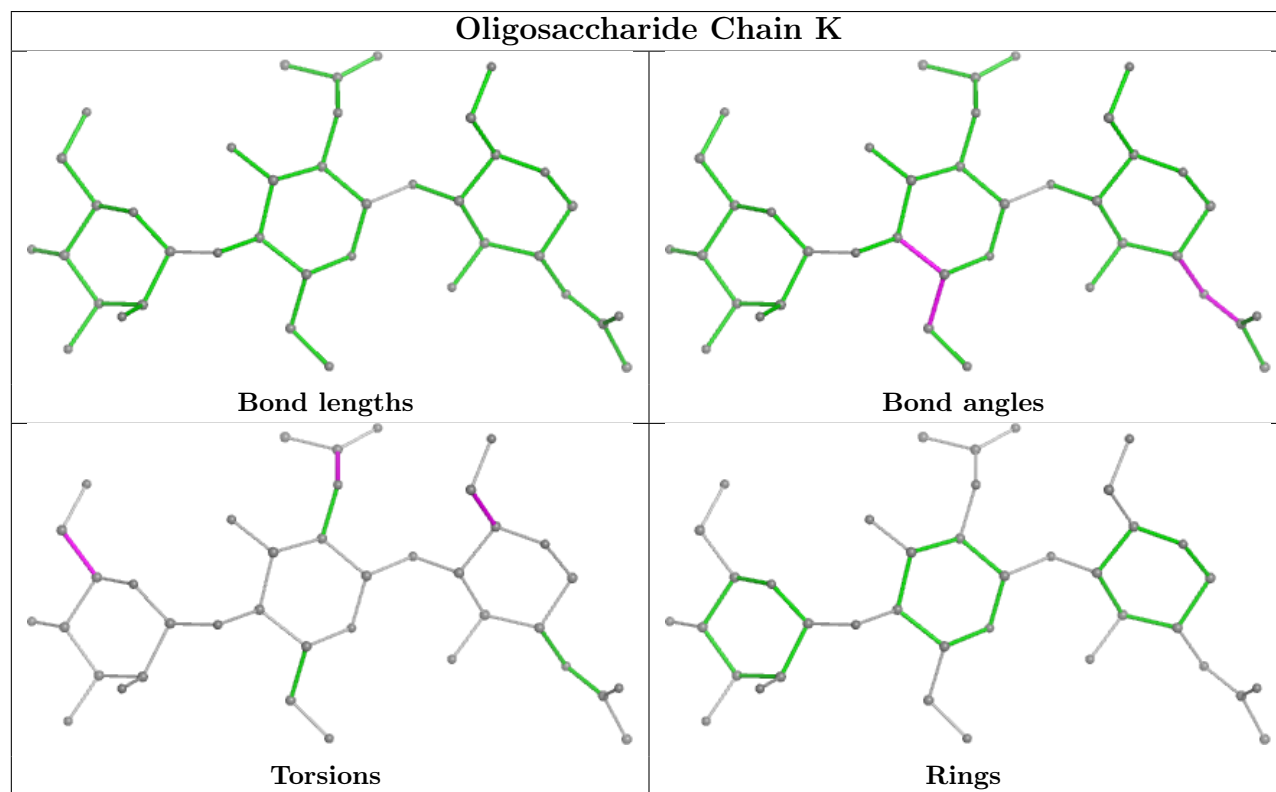
## Oligosaccharide Chain I



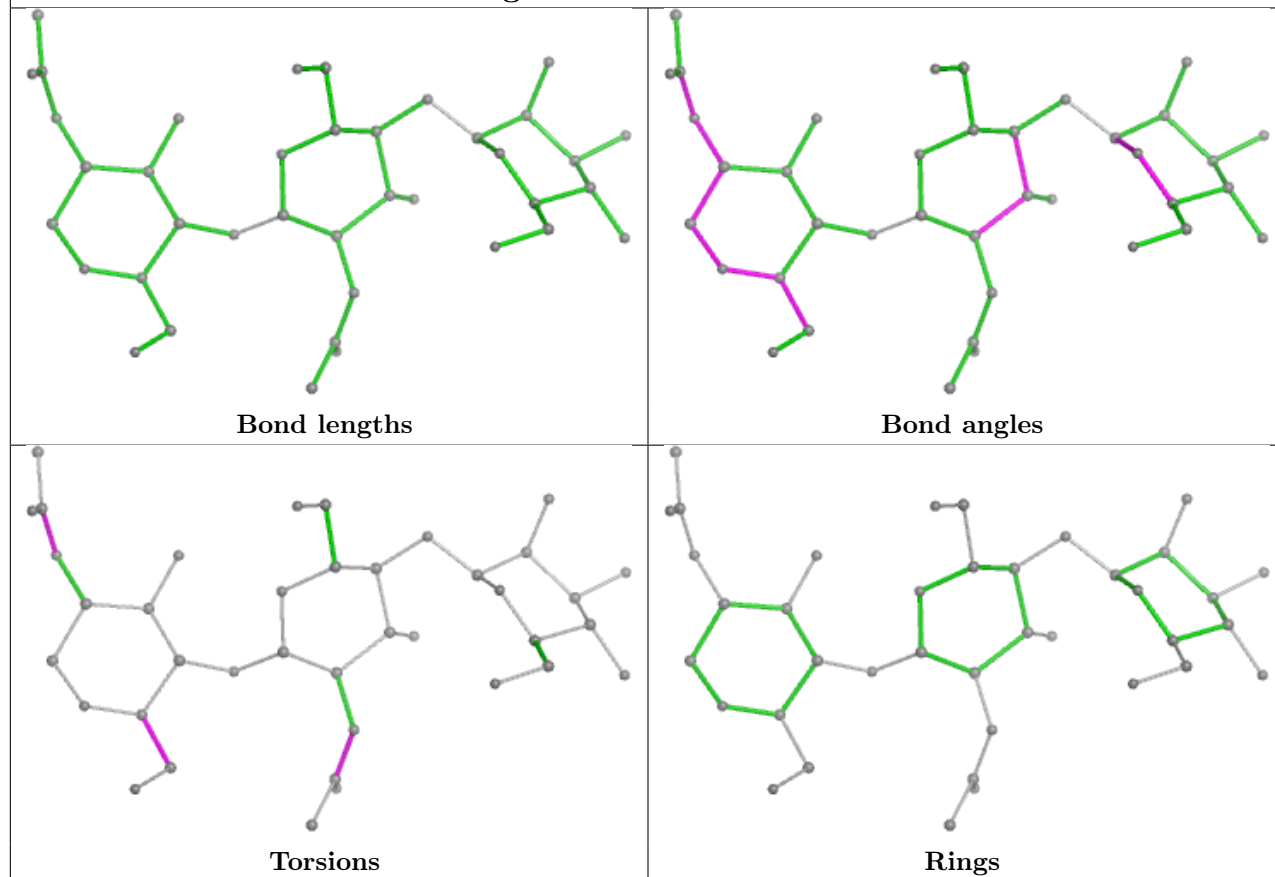
## Oligosaccharide Chain J



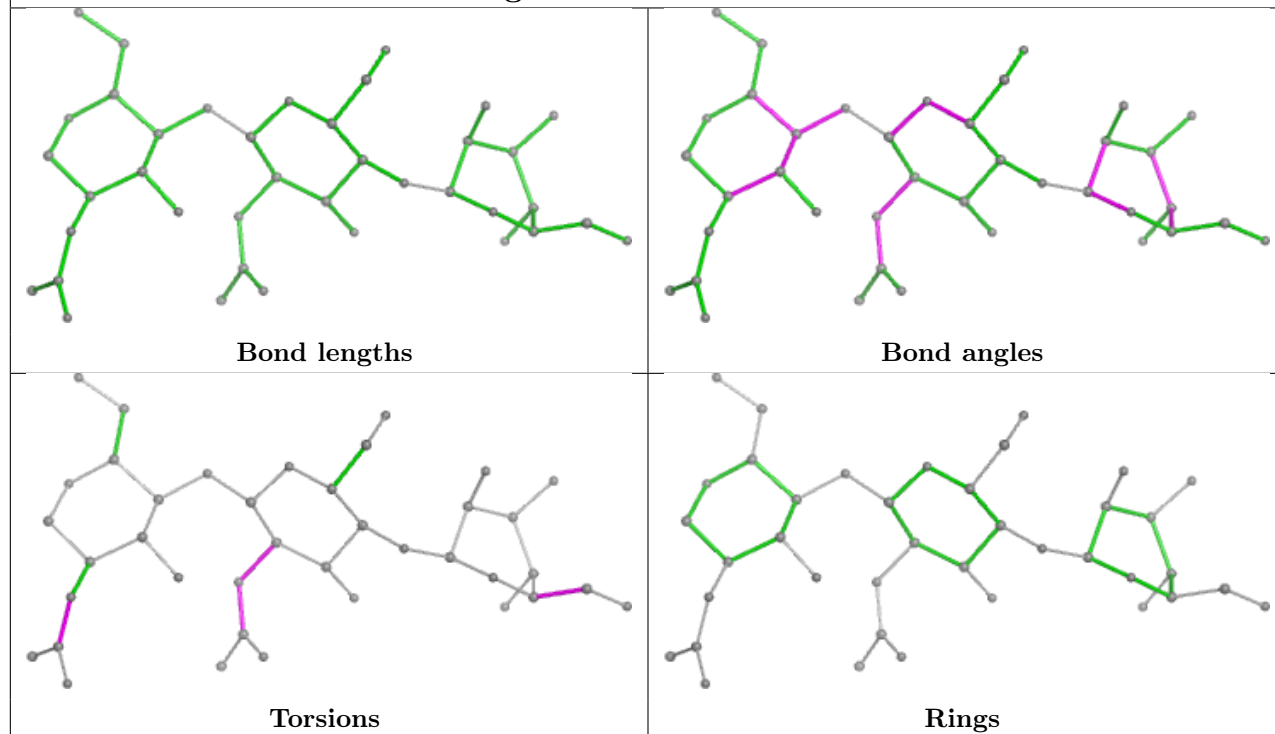
## Oligosaccharide Chain K



## Oligosaccharide Chain P

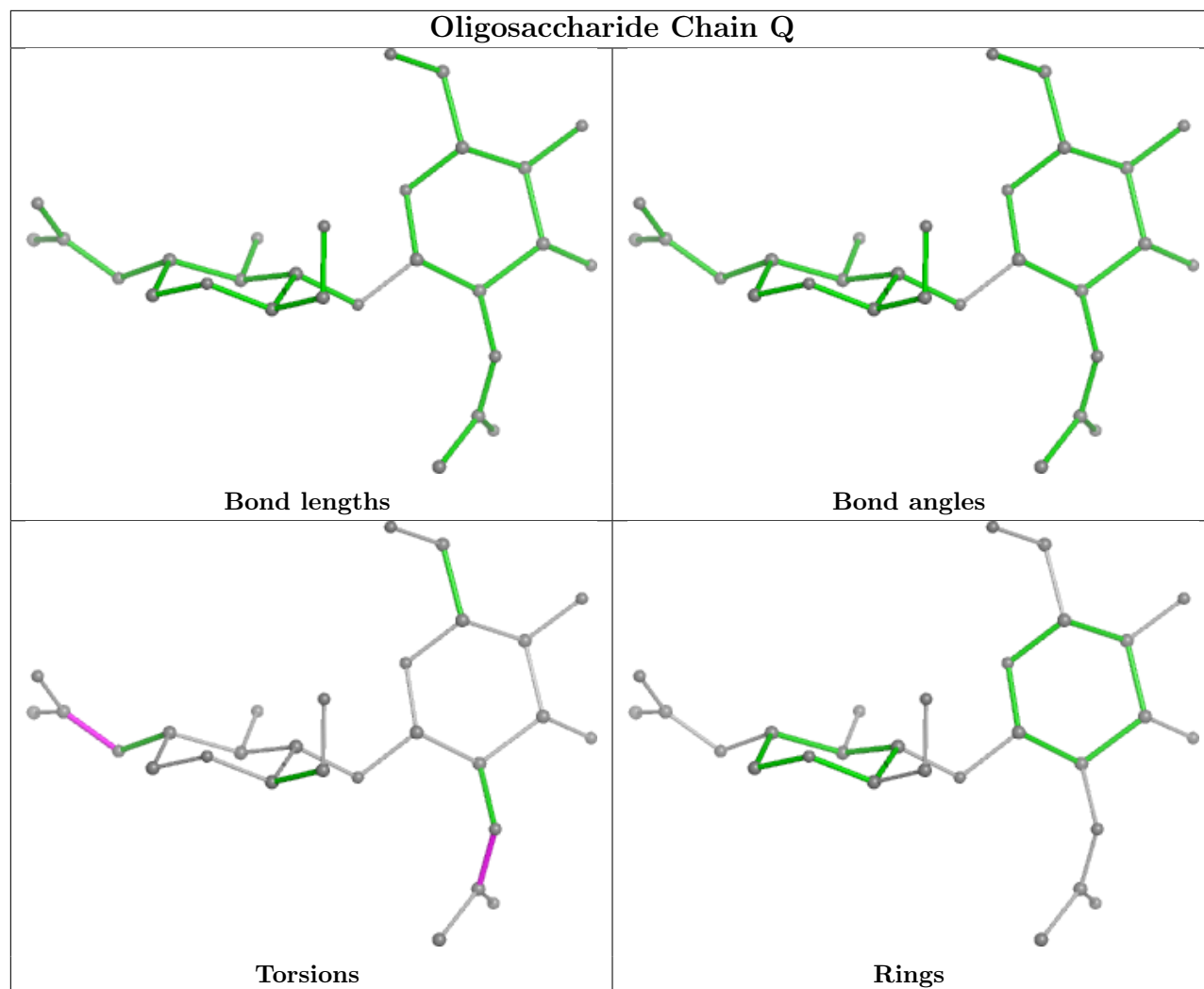


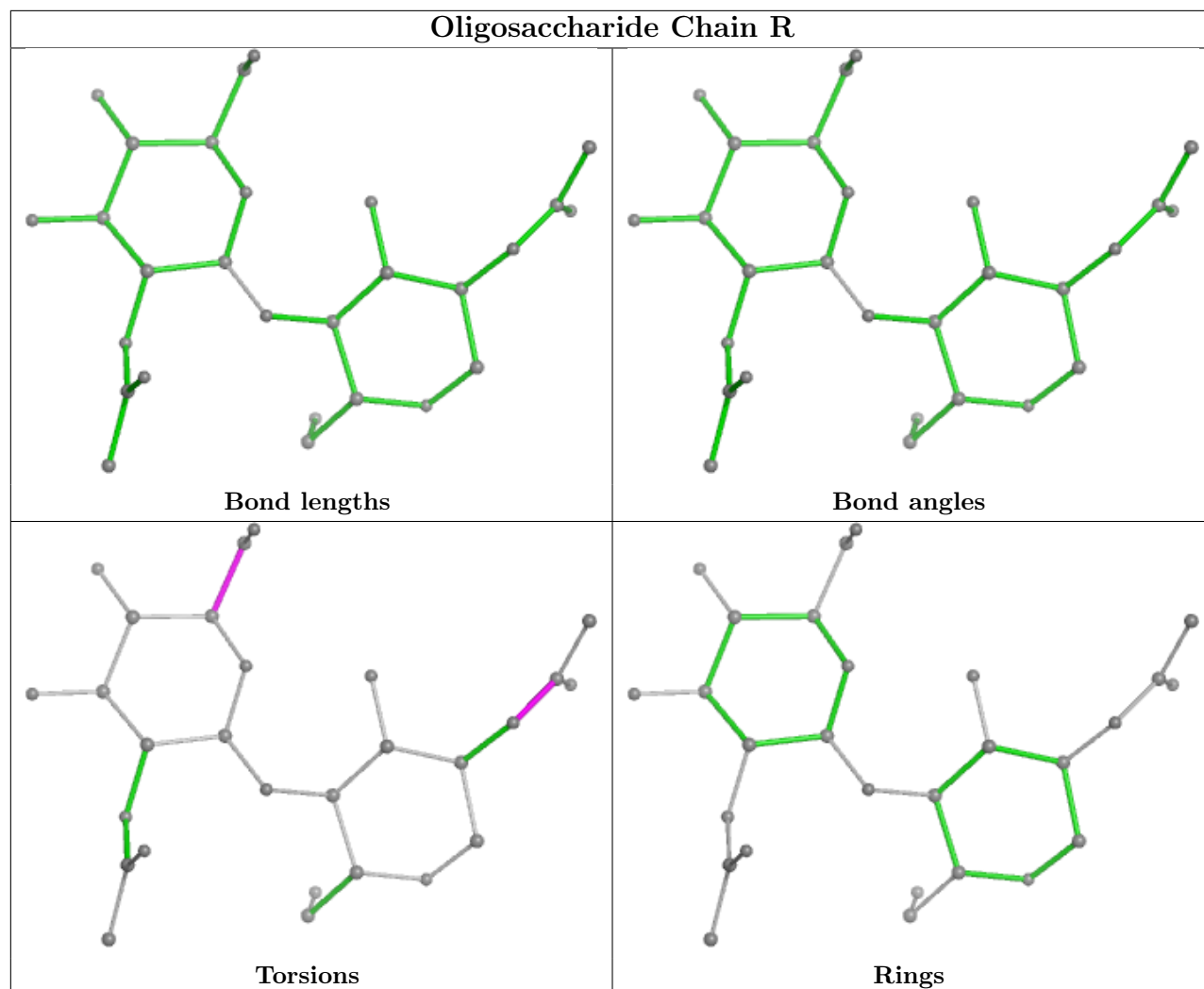
## Oligosaccharide Chain S



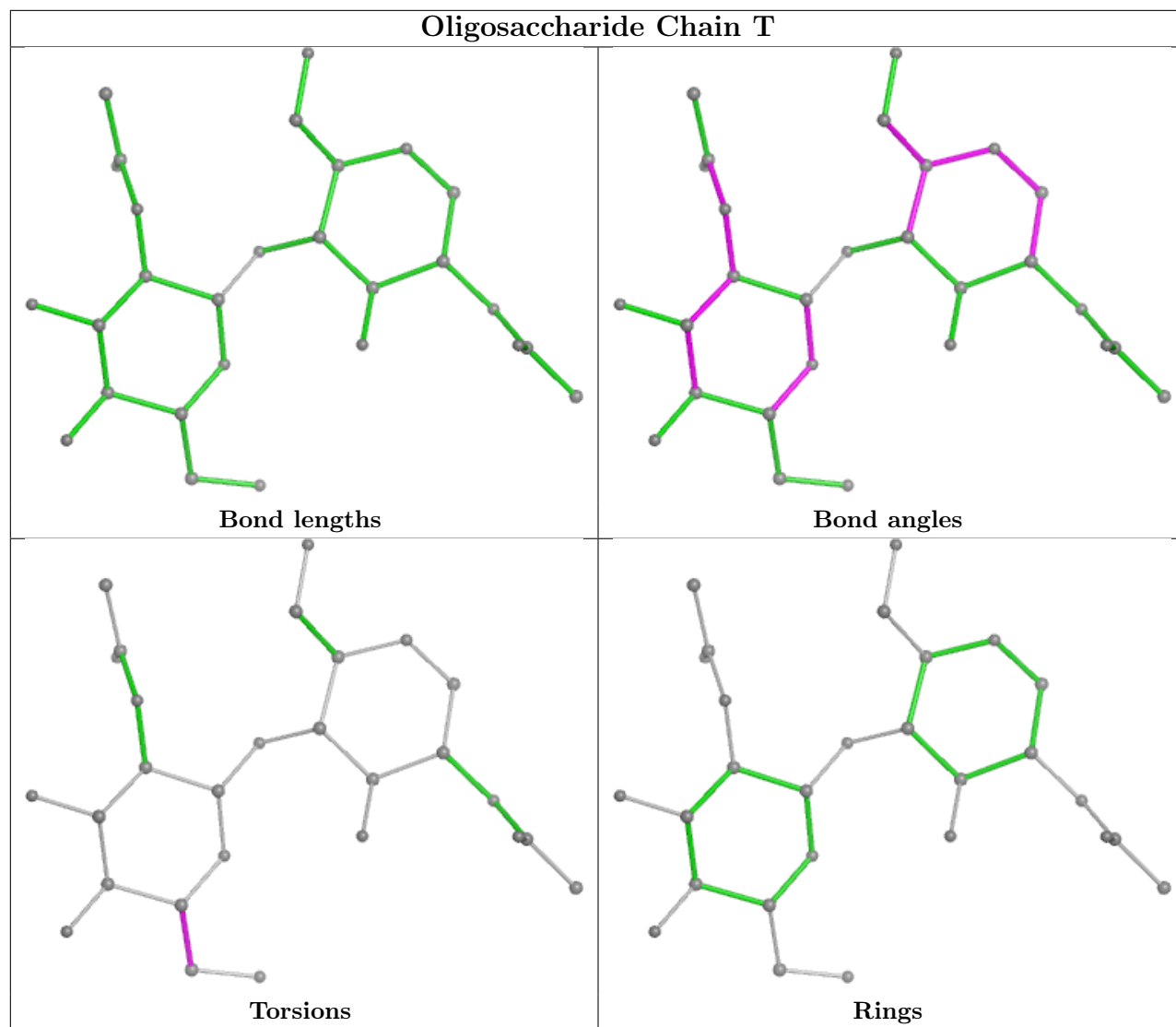


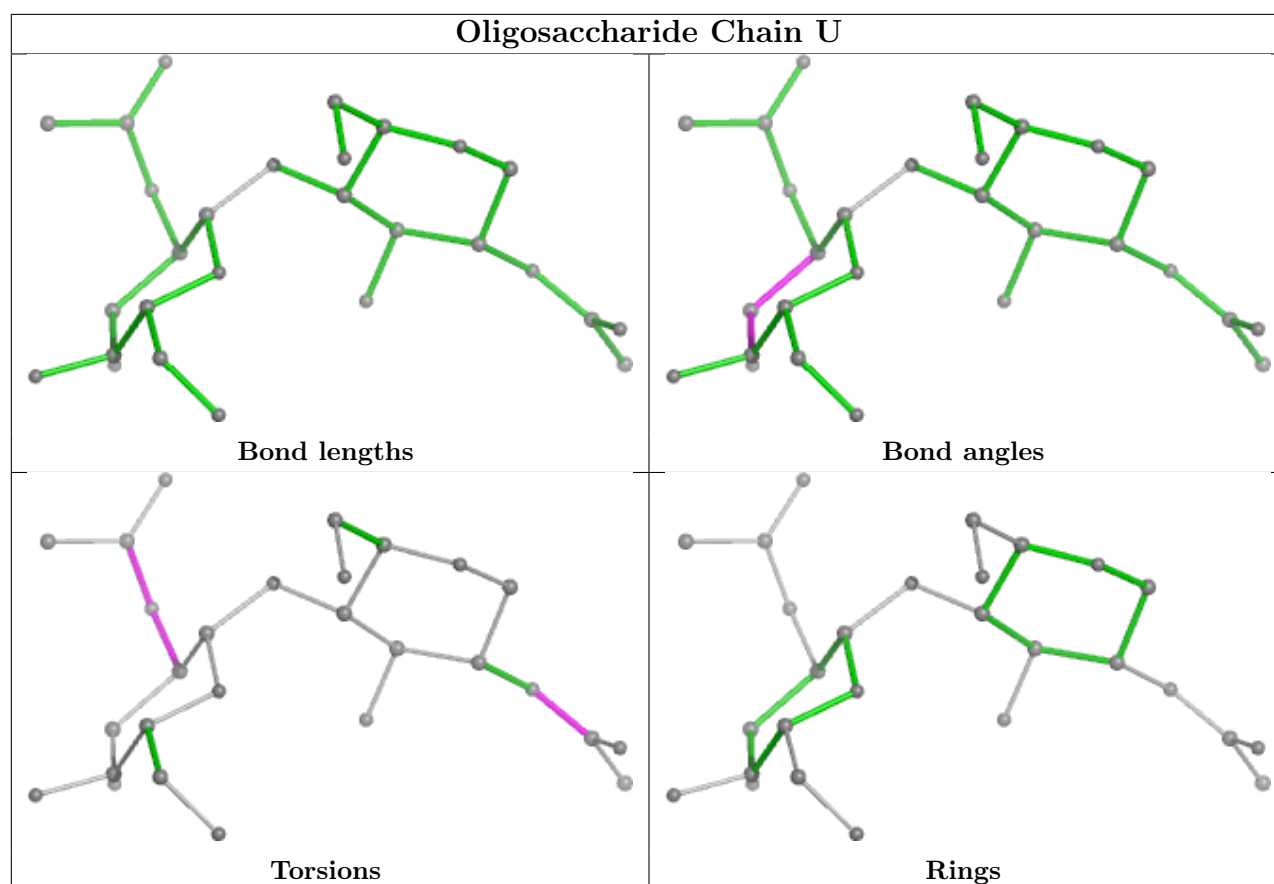
## Oligosaccharide Chain Q





## Oligosaccharide Chain T





## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
6	NAG	N	1401	2	14,14,15	0.59	0	17,19,21	0.95	0
6	NAG	L	2701	2	14,14,15	0.45	0	17,19,21	1.39	2 (11%)
6	NAG	N	1601	2	14,14,15	0.50	0	17,19,21	1.20	1 (5%)
6	NAG	O	2301	2	14,14,15	0.44	0	17,19,21	1.01	1 (5%)
6	NAG	O	2101	2	14,14,15	0.45	0	17,19,21	1.05	2 (11%)
6	NAG	O	2001	2	14,14,15	0.55	0	17,19,21	1.57	3 (17%)
6	NAG	L	2401	2	14,14,15	0.46	0	17,19,21	0.89	1 (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
6	NAG	N	1401	2	-	4/6/23/26	0/1/1/1
6	NAG	L	2701	2	-	2/6/23/26	0/1/1/1
6	NAG	N	1601	2	-	0/6/23/26	0/1/1/1
6	NAG	O	2301	2	-	0/6/23/26	0/1/1/1
6	NAG	O	2101	2	-	3/6/23/26	0/1/1/1
6	NAG	O	2001	2	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	L	2401	2	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	2001	NAG	C1-O5-C5	4.33	118.06	112.19
6	L	2701	NAG	O5-C5-C6	4.21	113.80	107.20
6	N	1601	NAG	O5-C1-C2	-3.70	105.45	111.29
6	O	2101	NAG	O5-C5-C6	2.62	111.31	107.20
6	O	2001	NAG	C3-C4-C5	-2.49	105.80	110.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	2401	NAG	C1
6	O	2001	NAG	C1

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	1401	NAG	C8-C7-N2-C2
6	N	1401	NAG	O7-C7-N2-C2
6	O	2001	NAG	C8-C7-N2-C2
6	L	2401	NAG	C8-C7-N2-C2
6	L	2401	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	2001	NAG	3	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	98/110 (89%)	0.53	12 (12%) 10 9	43, 69, 129, 148	0
1	B	98/110 (89%)	0.31	5 (5%) 34 32	44, 65, 109, 125	0
1	C	97/110 (88%)	0.03	4 (4%) 42 40	35, 53, 93, 137	0
1	D	99/110 (90%)	0.19	4 (4%) 43 41	35, 57, 118, 142	0
2	L	196/213 (92%)	0.25	17 (8%) 17 16	40, 61, 120, 166	0
2	M	179/213 (84%)	0.35	6 (3%) 48 46	42, 68, 130, 150	0
2	N	194/213 (91%)	0.44	16 (8%) 19 17	37, 67, 125, 143	0
2	O	193/213 (90%)	0.29	14 (7%) 22 20	35, 62, 114, 159	0
All	All	1154/1292 (89%)	0.31	78 (6%) 25 23	35, 62, 121, 166	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	LEU	5.8
2	O	153	SER	5.8
1	A	192	LEU	5.4
1	B	118	ILE	5.4
2	O	282	GLY	5.3

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

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

### 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	L	2401	14/15	0.44	0.20	111,164,183,184	0
6	NAG	N	1401	14/15	0.53	0.13	99,119,126,128	0
6	NAG	O	2101	14/15	0.64	0.14	88,114,133,134	0
6	NAG	O	2001	14/15	0.68	0.23	72,132,193,197	0
6	NAG	L	2701	14/15	0.88	0.12	55,72,90,100	0
5	CS	C	1216	1/1	0.90	0.13	135,135,135,135	0
6	NAG	N	1601	14/15	0.90	0.10	34,61,71,78	0
6	NAG	O	2301	14/15	0.90	0.09	49,71,78,90	0
5	CS	B	1215	1/1	0.96	0.06	85,85,85,85	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.