



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 03:48 PM BST

PDB ID : 1NQL
Title : Structure of the extracellular domain of human epidermal growth factor (EGF) receptor in an inactive (low pH) complex with EGF.
Authors : Ferguson, K.M.; Lemmon, M.A.
Deposited on : 2003-01-21
Resolution : 2.80 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

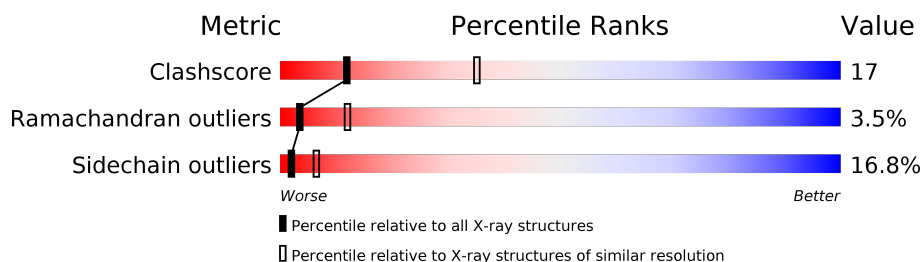
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	624	
2	B	53	
3	C	3	
3	D	3	
4	E	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
5	NAG	A	4201	X	-	-	-
5	NAG	A	5791	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5150 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.

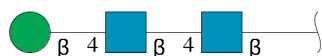
- Molecule 1 is a protein called epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	10	0	0
			4597	2836	817	885	59			

- Molecule 2 is a protein called epidermal growth factor.

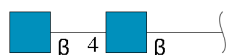
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	48	Total	C	N	O	S	0	0	0
			377	235	62	73	7			

- 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	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



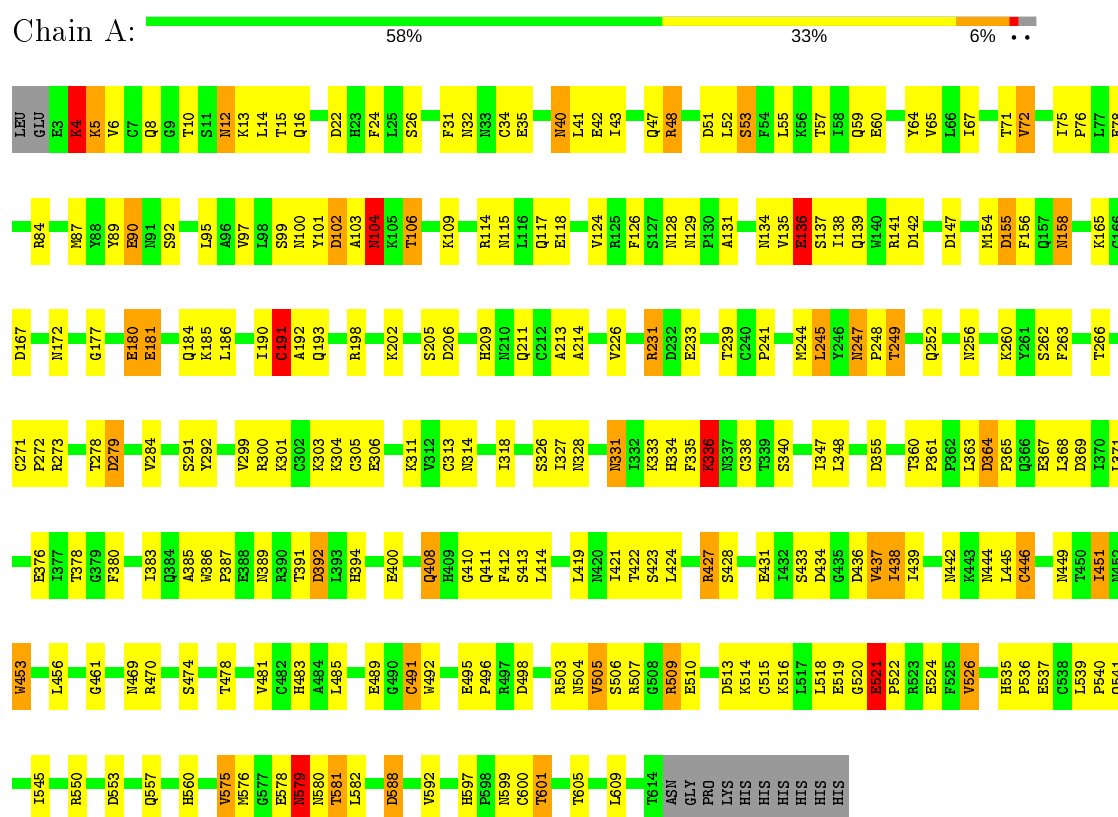
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

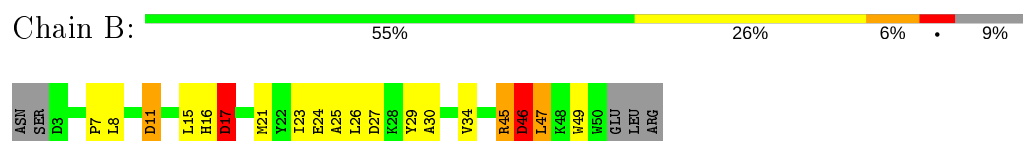
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: epidermal growth factor receptor



- Molecule 2: epidermal growth factor



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



MAG1
MAG2
B/M3

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

Chain D:  33% 67%

MAG1
MAG2
B/M3

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

Chain E:  100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 103.66Å 101.49Å 90.00° 119.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.241 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: BMA, NAG

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	0.85	4/4688 (0.1%)	0.98	22/6365 (0.3%)
2	B	0.57	0/386	0.92	3/523 (0.6%)
All	All	0.83	4/5074 (0.1%)	0.97	25/6888 (0.4%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	LYS	C-N	-35.46	0.52	1.34
1	A	4	LYS	CB-CG	-9.44	1.27	1.52
1	A	244	MET	CG-SD	7.65	2.01	1.81
1	A	90	GLU	CD-OE2	6.72	1.33	1.25

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	O-C-N	17.58	150.83	122.70
1	A	4	LYS	CA-C-N	-15.53	83.04	117.20
1	A	4	LYS	CB-CG-CD	-10.81	83.50	111.60
1	A	4	LYS	CA-CB-CG	10.07	135.56	113.40
1	A	142	ASP	CB-CG-OD2	8.02	125.52	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide
1	A	578	GLU	Peptide

5.2 Too-close contacts

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	4597	0	4316	166	0
2	B	377	0	328	10	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
4	E	28	0	25	0	0
5	A	70	0	65	13	0
All	All	5150	0	4802	172	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 17.

The worst 5 of 172 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:516:LYS:HB3	1:A:520:GLY:HA3	1.33	1.05
1:A:576:MET:SD	5:A:5791:NAG:O3	2.15	1.05
1:A:576:MET:CG	5:A:5791:NAG:H4	2.05	0.86
1:A:256:ASN:HD21	5:A:5791:NAG:C6	1.89	0.85
1:A:541:GLN:HE22	1:A:557:GLN:HE21	1.24	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	610/624 (98%)	514 (84%)	73 (12%)	23 (4%)	3	10
2	B	46/53 (87%)	37 (80%)	9 (20%)	0	100	100
All	All	656/677 (97%)	551 (84%)	82 (12%)	23 (4%)	3	12

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LYS
1	A	104	ASN
1	A	191	CYS
1	A	521	GLU

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	507/545 (93%)	424 (84%)	83 (16%)	2	7
2	B	40/47 (85%)	31 (78%)	9 (22%)	1	2
All	All	547/592 (92%)	455 (83%)	92 (17%)	2	6

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	ILE
1	A	391	THR
2	B	15	LEU
1	A	327	ILE
1	A	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	210	ASN
1	A	560	HIS
1	A	134	ASN
1	A	597	HIS

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 ⓘ

8 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	C	1	1,3	14,14,15	0.70	0	17,19,21	1.54	3 (17%)
3	NAG	C	2	3	14,14,15	0.66	0	17,19,21	1.56	4 (23%)
3	BMA	C	3	3	11,11,12	0.68	0	15,15,17	1.28	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.67	0	17,19,21	1.37	3 (17%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	1.20	2 (11%)
3	BMA	D	3	3	11,11,12	0.71	0	15,15,17	0.78	0
4	NAG	E	1	1,4	14,14,15	0.69	0	17,19,21	2.65	8 (47%)
4	NAG	E	2	4	14,14,15	0.57	0	17,19,21	1.37	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	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	8.21	123.32	112.19
4	E	2	NAG	C1-O5-C5	4.49	118.28	112.19
3	D	1	NAG	C4-C3-C2	3.96	116.83	111.02
3	C	2	NAG	C2-N2-C7	-3.46	117.98	122.90
3	C	3	BMA	C1-C2-C3	3.35	113.79	109.67

There are no chirality outliers.

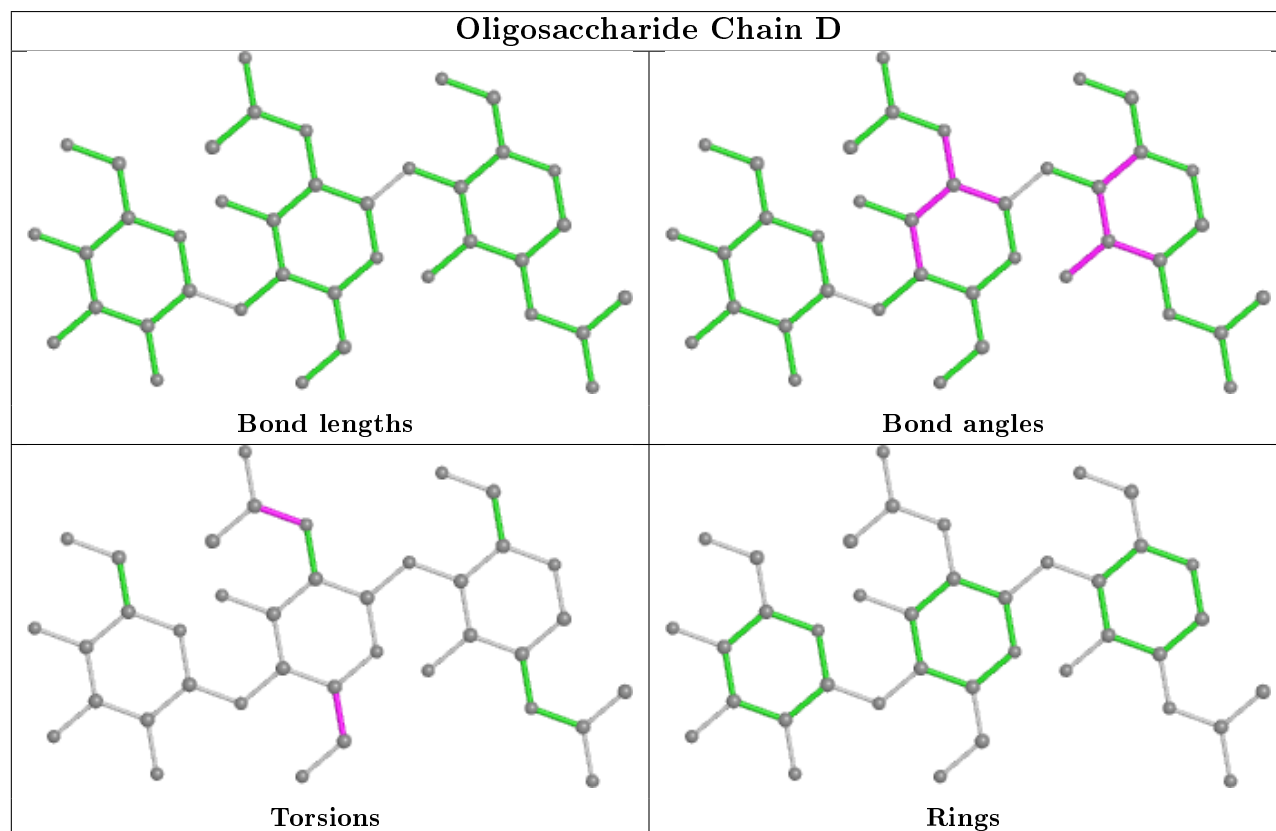
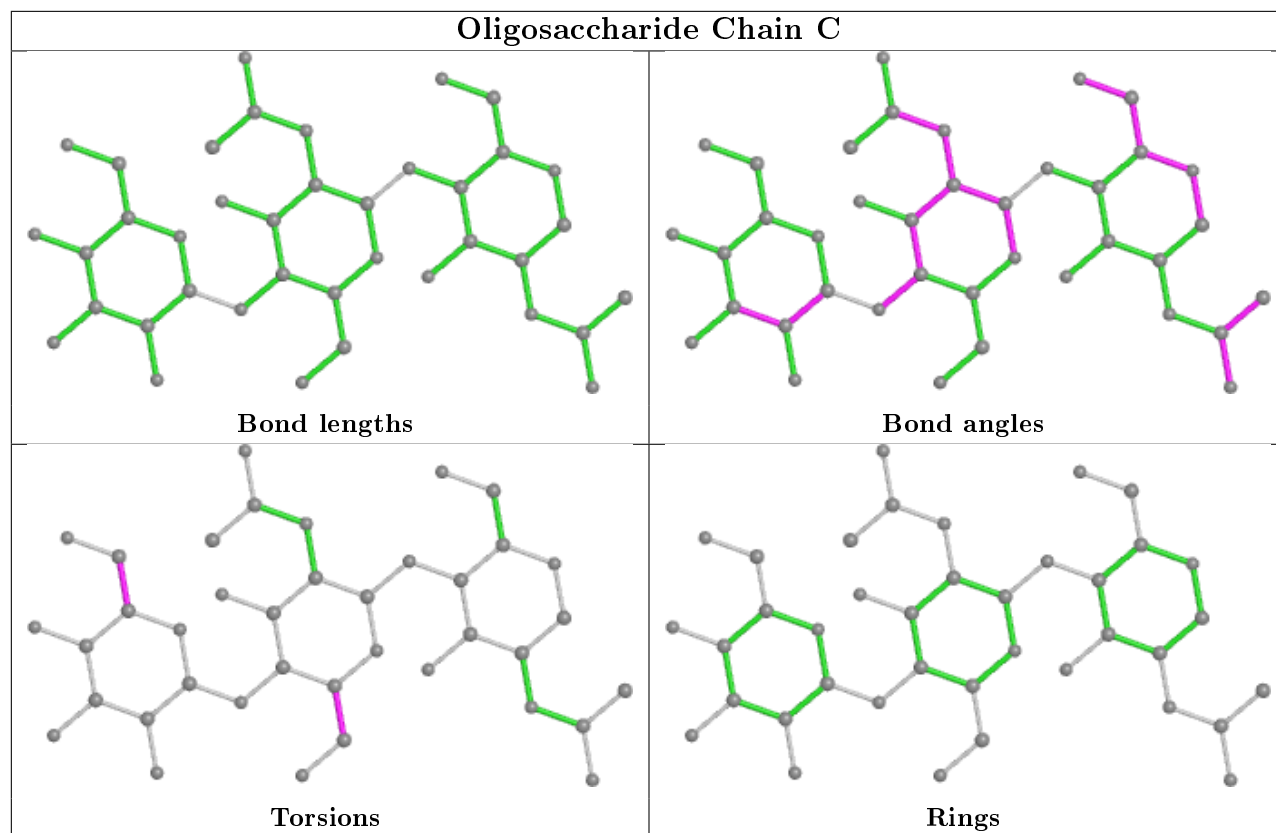
5 of 11 torsion outliers are listed below:

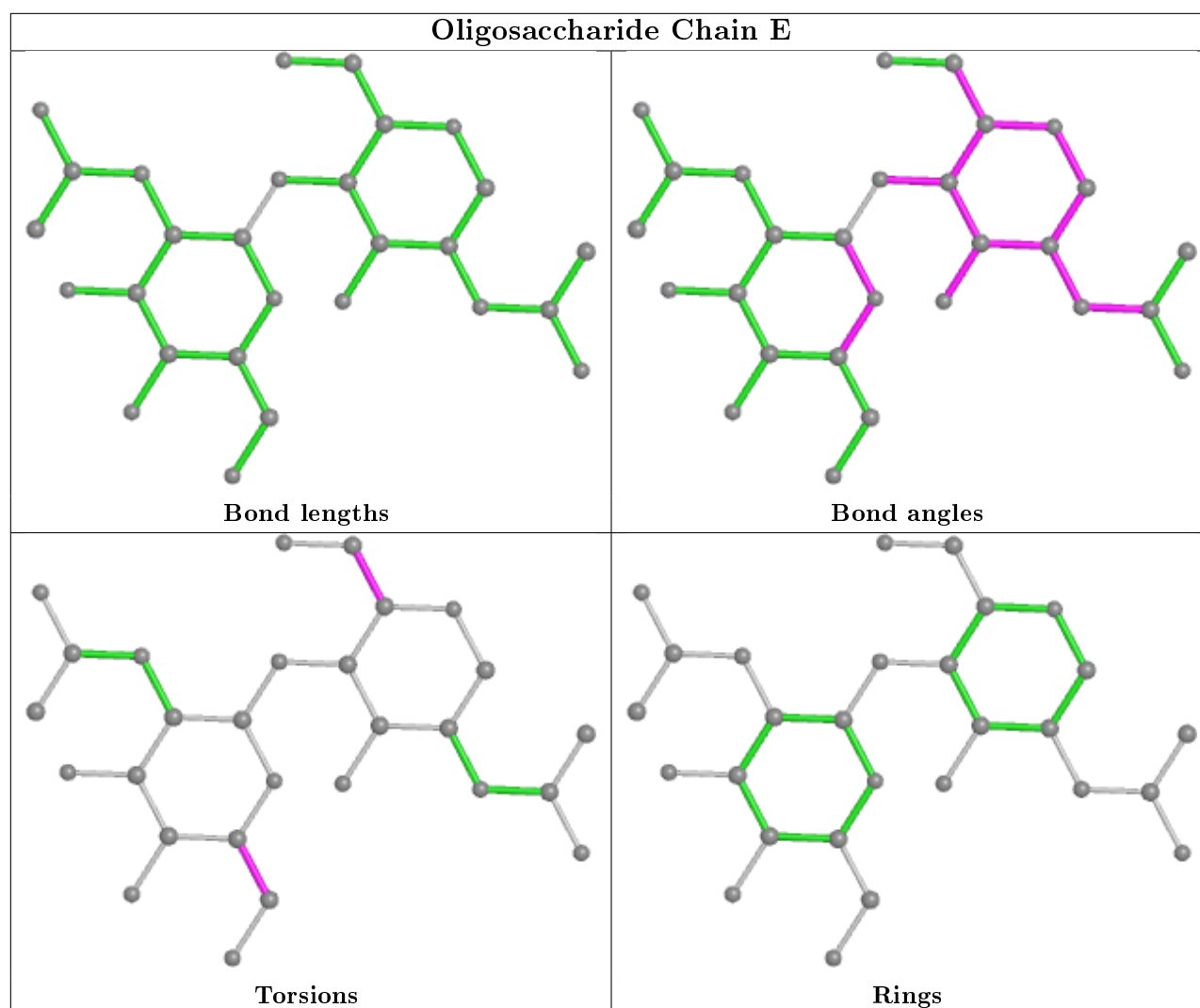
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

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](#)

5 ligands 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	$\# Z > 2$
5	NAG	A	625	-	14,14,15	0.65	0	17,19,21	1.02	2 (11%)
5	NAG	A	5791	1	14,14,15	0.90	1 (7%)	17,19,21	1.74	2 (11%)
5	NAG	A	4201	1	14,14,15	0.66	0	17,19,21	1.29	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	4202	-	14,14,15	0.59	0	17,19,21	1.76	4 (23%)
5	NAG	A	5041	1	14,14,15	0.57	0	17,19,21	2.35	2 (11%)

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
5	NAG	A	625	-	-	3/6/23/26	0/1/1/1
5	NAG	A	5791	1	-	6/6/23/26	0/1/1/1
5	NAG	A	4201	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	4202	-	-	2/6/23/26	0/1/1/1
5	NAG	A	5041	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5791	NAG	O5-C5	-2.04	1.39	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5041	NAG	C1-O5-C5	8.29	123.43	112.19
5	A	5791	NAG	C1-O5-C5	-6.05	103.99	112.19
5	A	4202	NAG	C3-C4-C5	4.09	117.53	110.24
5	A	4202	NAG	O5-C1-C2	-3.14	106.33	111.29
5	A	4201	NAG	O5-C5-C6	2.74	111.50	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	4201	NAG	C1

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5041	NAG	C8-C7-N2-C2
5	A	5041	NAG	O7-C7-N2-C2
5	A	5791	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	5791	NAG	O7-C7-N2-C2
5	A	625	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	625	NAG	1	0
5	A	5791	NAG	11	0
5	A	5041	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4:LYS	C	5:LYS	N	0.52

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.