



wwPDB EM Validation Summary Report ⓘ

Feb 26, 2025 – 12:23 am GMT

PDB ID : 8OQ3
EMDB ID : EMD-17103
Title : Structure of methylamine treated human complement C3
Authors : Gadeberg, T.A.F.; Andersen, G.R.
Deposited on : 2023-04-11
Resolution : 2.90 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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>.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

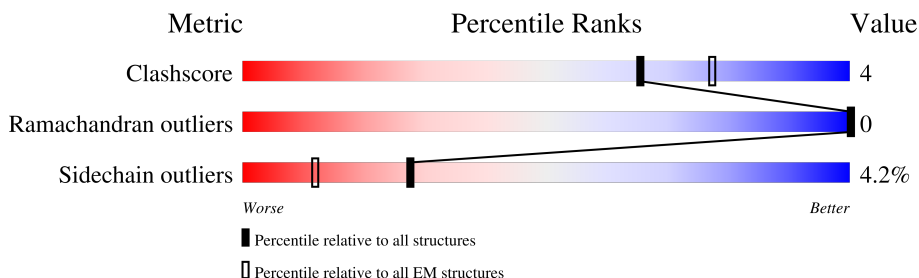
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1641	81% 12% • 5%
1	D	1641	83% 11% • 5%
2	C	129	75% 19% • 5%
2	F	129	78% 16% • 5%
3	G	3	67% 33%
3	H	3	33% 33% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

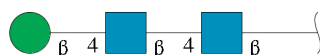
- Molecule 1 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1556	Total	C	N	O	S	0	0
			12307	7811	2077	2366	53		
1	D	1556	Total	C	N	O	S	0	0
			12307	7811	2077	2366	53		

- Molecule 2 is a protein called nanobody hC3Nb1 with mutation.

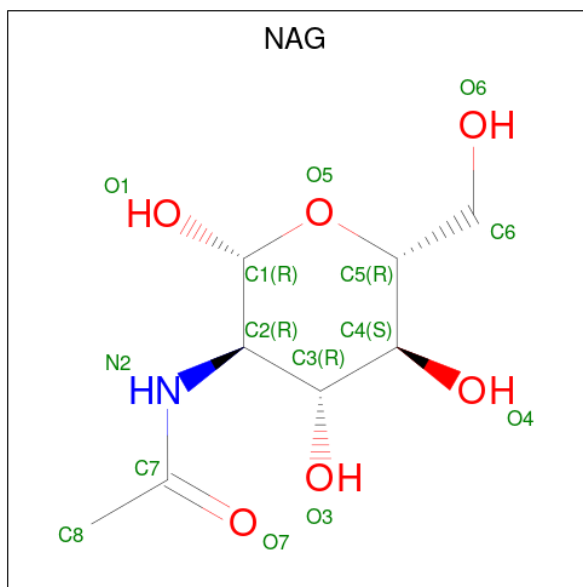
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	123	Total	C	N	O	S	0	0
			938	584	166	182	6		
2	F	123	Total	C	N	O	S	0	0
			938	584	166	182	6		

- 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				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

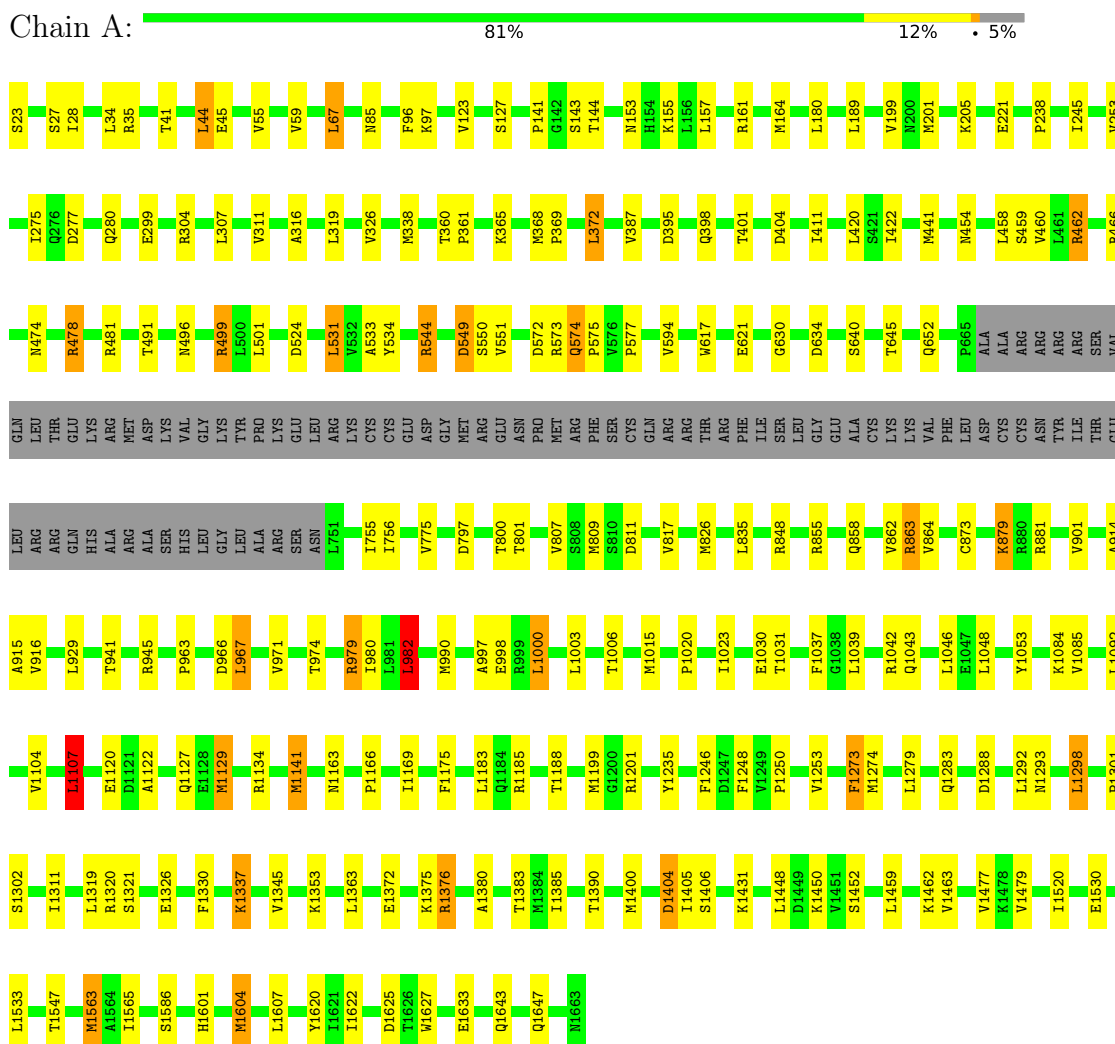


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0
4	D	1	14	8	1	5	0

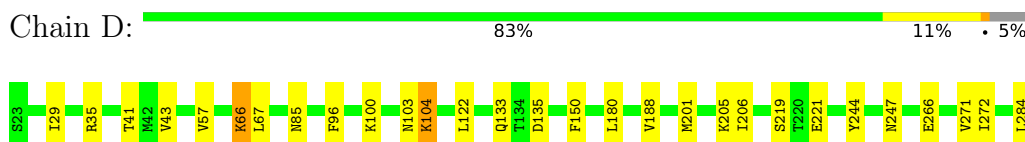
3 Residue-property plots

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.

• Molecule 1: Complement C3



• Molecule 1: Complement C3





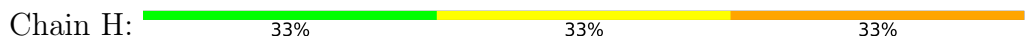
- Molecule 2: nanobody hC3Nb1 with mutation



- 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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197438	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.5	Depositor
Minimum defocus (nm)	170	Depositor
Maximum defocus (nm)	2438	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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, 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	0.36	0/12555	0.70	20/17025 (0.1%)
1	D	0.35	0/12555	0.67	15/17025 (0.1%)
2	C	0.47	0/958	0.91	4/1295 (0.3%)
2	F	0.45	0/958	0.92	3/1295 (0.2%)
All	All	0.36	0/27026	0.70	42/36640 (0.1%)

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	D	0	2

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	73	ASP	CB-CG-OD2	11.24	128.42	118.30
1	D	1499	ASP	CB-CG-OD2	11.03	128.22	118.30
2	C	73	ASP	CB-CG-OD1	9.27	126.64	118.30
1	A	1404	ASP	CB-CG-OD2	8.84	126.25	118.30
1	A	1000	LEU	CA-CB-CG	8.36	134.53	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1018	MET	Peptide

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Mol	Chain	Res	Type	Group
1	D	662	CYS	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	12307	0	12288	101	0
1	D	12307	0	12288	81	0
2	C	938	0	895	9	0
2	F	938	0	895	10	0
3	G	39	0	34	1	0
3	H	39	0	34	1	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
All	All	26596	0	26460	200	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 4.

The worst 5 of 200 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:1293:ASN:HA	1:A:1311:ILE:O	1.77	0.85
1:A:1042:ARG:HH21	1:A:1046:LEU:HD21	1.58	0.69
2:C:12:VAL:O	2:C:121:VAL:HA	1.97	0.65
1:A:1039:LEU:O	1:A:1042:ARG:HB3	1.98	0.63
1:D:459:SER:HB2	1:D:474:ASN:HB2	1.82	0.62

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 PDB entries followed by that with respect to all EM

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	1552/1641 (95%)	1500 (97%)	52 (3%)	0	100	100
1	D	1552/1641 (95%)	1503 (97%)	49 (3%)	0	100	100
2	C	121/129 (94%)	115 (95%)	6 (5%)	0	100	100
2	F	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
All	All	3346/3540 (94%)	3234 (97%)	112 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM 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	1375/1450 (95%)	1311 (95%)	64 (5%)	22	55
1	D	1375/1450 (95%)	1326 (96%)	49 (4%)	30	65
2	C	97/103 (94%)	91 (94%)	6 (6%)	15	43
2	F	97/103 (94%)	92 (95%)	5 (5%)	19	50
All	All	2944/3106 (95%)	2820 (96%)	124 (4%)	27	59

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1450	LYS
1	D	1341	THR
1	D	57	VAL
1	D	1293	ASN
1	D	1604	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	474	ASN
1	D	1198	GLN
1	D	1136	ASN
1	D	1289	HIS
1	A	496	ASN

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 ⓘ

6 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	G	1	3,1	14,14,15	0.42	0	17,19,21	0.82	1 (5%)
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
3	BMA	G	3	3	11,11,12	1.16	1 (9%)	15,15,17	0.99	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
3	NAG	H	2	3	14,14,15	0.62	0	17,19,21	0.61	0
3	BMA	H	3	3	11,11,12	1.12	2 (18%)	15,15,17	1.22	1 (6%)

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	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	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	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	BMA	C2-C3	2.36	1.56	1.52
3	H	3	BMA	C2-C3	2.17	1.55	1.52
3	H	3	BMA	C1-C2	2.00	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	3.40	116.80	112.19
3	G	2	NAG	C1-O5-C5	2.61	115.72	112.19
3	G	3	BMA	C1-O5-C5	2.47	115.54	112.19
3	G	1	NAG	C1-O5-C5	2.24	115.23	112.19
3	H	1	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6

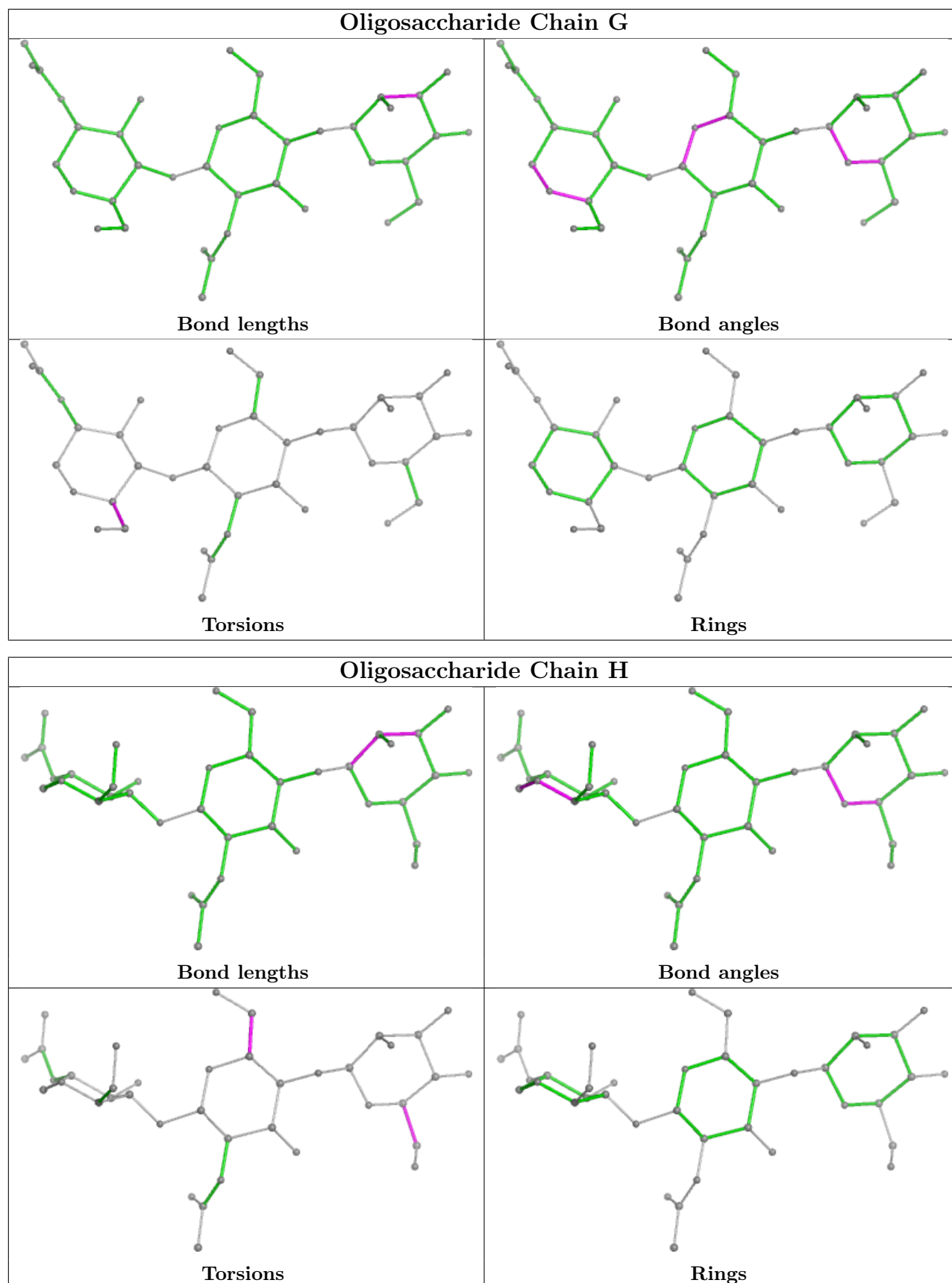
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	H	1	NAG	1	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.



5.6 Ligand geometry

2 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
4	NAG	D	1701	1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)
4	NAG	A	1701	1	14,14,15	1.11	2 (14%)	17,19,21	0.54	0

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
4	NAG	D	1701	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1701	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1701	NAG	O5-C1	3.42	1.49	1.43
4	A	1701	NAG	C1-C2	2.14	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1701	NAG	C1-O5-C5	2.31	115.33	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1701	NAG	O5-C5-C6-O6
4	A	1701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	1701	NAG	C4-C5-C6-O6
4	A	1701	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.