



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 01:07 AM EST

PDB ID : 6U2K
EMDB ID : EMD-20621
Title : EM structure of MPEG-1 (L425K, alpha conformation) soluble pre-pore complex
Authors : Pang, S.S.; Bayly-Jones, C.
Deposited on : 2019-08-20
Resolution : 2.93 Å(reported)

This is a Full wwPDB EM 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/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 : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

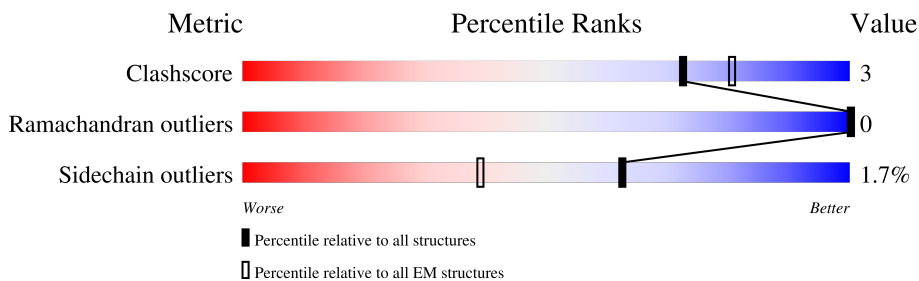
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	642	85% (green), 9% (yellow), 6% (orange), 0% (red), 0% (grey)
2	A	2	100% (green)
2	C	2	50% (green), 50% (yellow)

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4719 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 Macrophage-expressed gene 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	604	4663	2947	798	892	26	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	419F	LYS	LEU	engineered mutation	UNP Q2M385
B	622	HIS	-	expression tag	UNP Q2M385
B	623	HIS	-	expression tag	UNP Q2M385
B	624	HIS	-	expression tag	UNP Q2M385
B	625	HIS	-	expression tag	UNP Q2M385
B	626	HIS	-	expression tag	UNP Q2M385
B	627	HIS	-	expression tag	UNP Q2M385

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

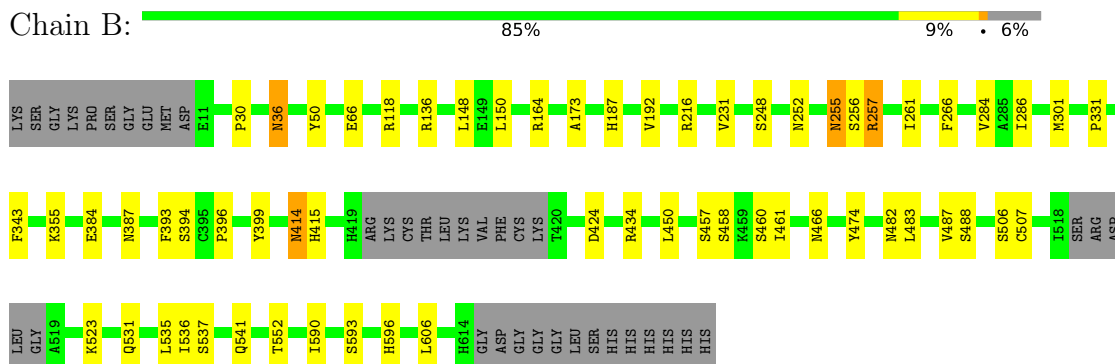


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	2	28	16	2	10	0	0
2	C	2	28	16	2	10	0	0

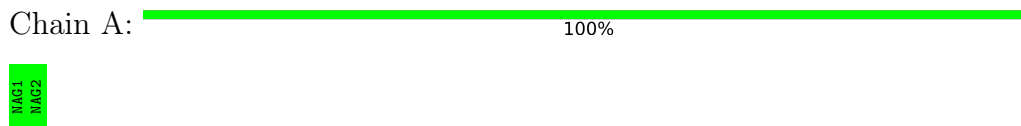
3 Residue-property plots [i](#)

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. 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: Macrophage-expressed gene 1 protein



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



- Molecule 2: 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, C1	Depositor
Number of particles used	527402	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 ($e^-/\text{\AA}^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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

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	B	0.49	0/4767	0.60	0/6480

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	B	4663	0	4520	32	0
2	A	28	0	25	0	0
2	C	28	0	25	0	0
All	All	4719	0	4570	32	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 3.

All (32) 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:B:414:ASN:HD21	1:B:424:ASP:HB2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASN:ND2	1:B:394:SER:O	2.36	0.58
1:B:483:LEU:HB2	1:B:535:LEU:HD13	1.89	0.55
1:B:590:ILE:HD11	1:B:606:LEU:HB3	1.89	0.54
1:B:507:CYS:O	1:B:523:LYS:NZ	2.40	0.53
1:B:118:ARG:HH11	1:B:257:ARG:HH12	1.57	0.52
1:B:343:PHE:H	1:B:552:THR:HG23	1.75	0.52
1:B:414:ASN:ND2	1:B:415:HIS:O	2.43	0.52
1:B:255:ASN:HD22	1:B:256:SER:H	1.59	0.51
1:B:482:ASN:HB2	1:B:535:LEU:HD11	1.95	0.49
1:B:457:SER:OG	1:B:458:SER:N	2.46	0.49
1:B:261:ILE:HG22	1:B:284:VAL:HG21	1.93	0.48
1:B:136:ARG:HD2	1:B:286:ILE:HD12	1.96	0.47
1:B:231:VAL:HG23	1:B:266:PHE:HE1	1.81	0.46
1:B:66:GLU:HG3	1:B:148:LEU:HD13	1.98	0.46
1:B:450:LEU:HD13	1:B:487:VAL:HG11	1.98	0.46
1:B:506:SER:OG	1:B:507:CYS:N	2.49	0.45
1:B:118:ARG:NH1	1:B:257:ARG:HH12	2.15	0.45
1:B:535:LEU:HD23	1:B:537:SER:HB3	1.98	0.45
1:B:248:SER:OG	1:B:252:ASN:OD1	2.35	0.44
1:B:150:LEU:HD13	1:B:301:MET:HB3	2.00	0.43
1:B:536:ILE:HG12	1:B:541:GLN:HB3	2.00	0.43
1:B:331:PRO:HD2	1:B:531:GLN:HE21	1.84	0.42
1:B:384:GLU:OE2	1:B:393:PHE:HZ	2.03	0.42
1:B:30:PRO:HG3	1:B:192:VAL:HG22	1.99	0.42
1:B:396:PRO:HG2	1:B:399:TYR:CD2	2.55	0.41
1:B:36:ASN:HB2	1:B:187:HIS:HD2	1.85	0.41
1:B:424:ASP:OD1	1:B:424:ASP:N	2.54	0.41
1:B:474:TYR:HA	1:B:488:SER:HB2	2.01	0.41
1:B:593:SER:O	1:B:596:HIS:ND1	2.46	0.41
1:B:460:SER:OG	1:B:461:ILE:N	2.54	0.40
1:B:164:ARG:HB2	1:B:173:ALA:HB2	2.03	0.40

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	B	598/642 (93%)	540 (90%)	58 (10%)	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 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	B	518/562 (92%)	509 (98%)	9 (2%)	60	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	ASN
1	B	50	TYR
1	B	216	ARG
1	B	255	ASN
1	B	257	ARG
1	B	355	LYS
1	B	414	ASN
1	B	434	ARG
1	B	466	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	ASN
1	B	255	ASN
1	B	281	ASN
1	B	370	GLN
1	B	414	ASN
1	B	466	ASN

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	NAG	A	1	1,2	14,14,15	0.27	0	17,19,21	0.57	0
2	NAG	A	2	2	14,14,15	0.39	0	17,19,21	0.49	0
2	NAG	C	1	1,2	14,14,15	0.34	0	17,19,21	0.59	0
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	0.96	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
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	2.99	127.16	122.90

There are no chirality outliers.

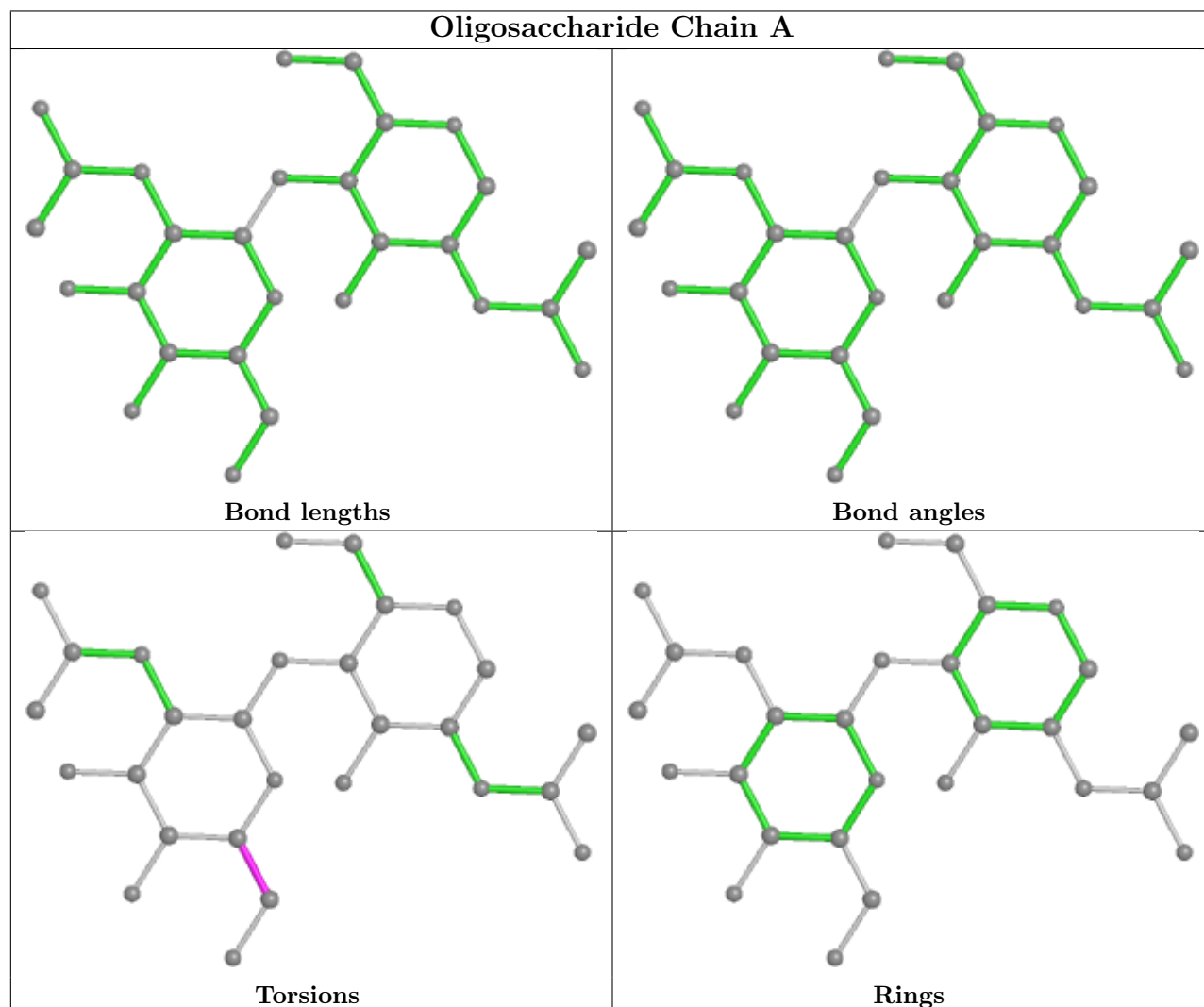
All (6) torsion outliers are listed below:

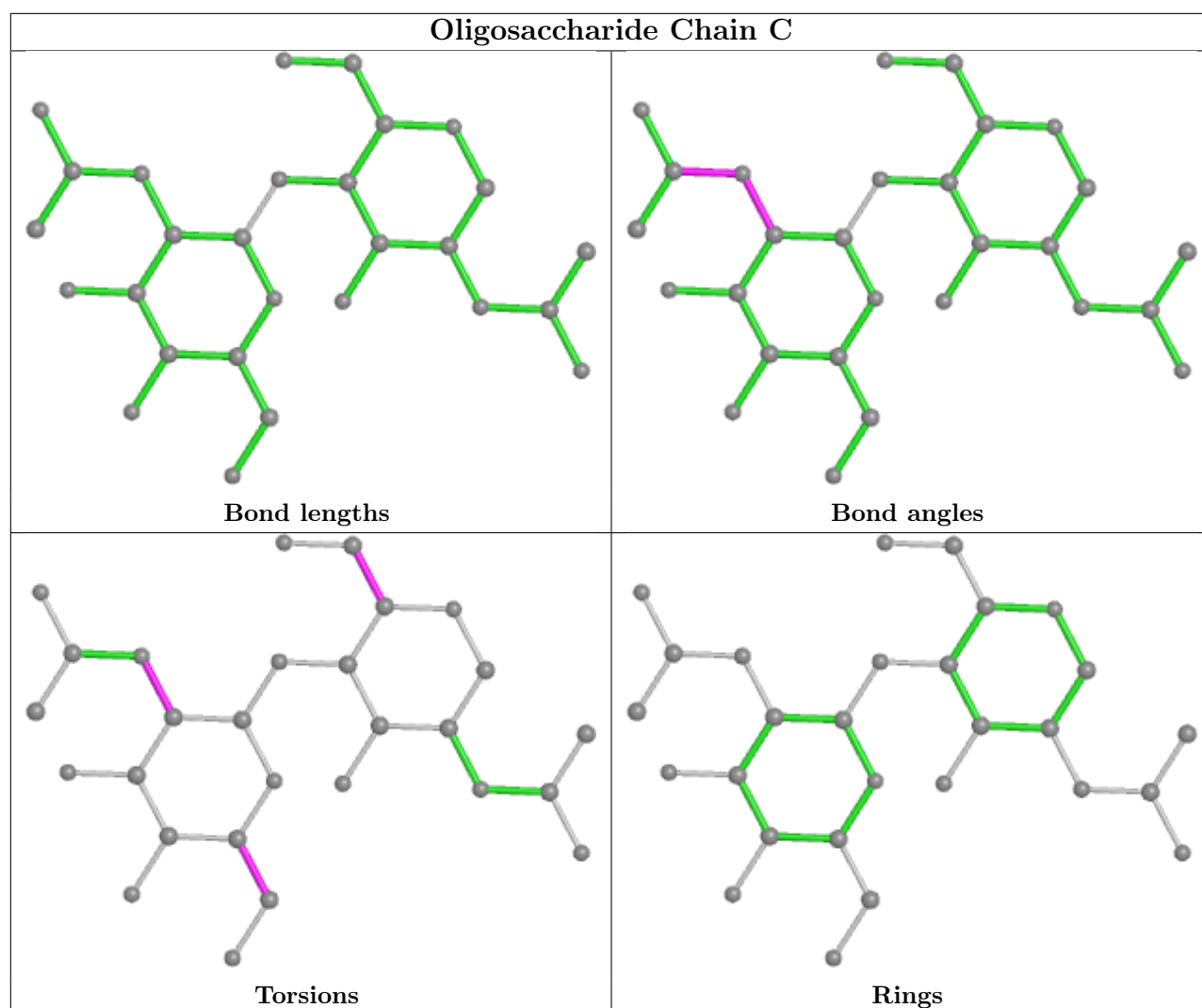
Mol	Chain	Res	Type	Atoms
2	A	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	A	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-20621. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.