wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 04:40 AM EDT

PDB ID	:	1KRF
Title	:	STRUCTURE OF P. CITRINUM ALPHA 1,2-MANNOSIDASE REVEALS THE BASIS FOR DIFFERENCES IN SPECIFICITY OF THE ER AND GOLGI CLASS I ENZYMES
Authors	:	Lobsanov, Y.D.; Vallee, F.; Imberty, A.; Yoshida, T.; Yip, P.; Herscovics, A.; Howell, P.L.
Deposited on	:	2002-01-09
Resolution	:	2.20 Å(reported)

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

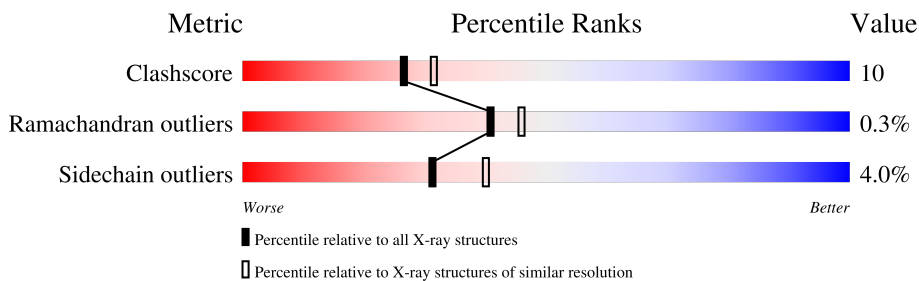|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		4.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	74% 17% • 7%
1	B	511	69% 23% • 7%
2	C	2	50% 50%
2	E	2	100%
2	F	2	100%
2	H	2	100%
3	D	5	80% 20%
3	G	5	40% 40% 20%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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
2	NAG	C	2	X	-	-	-
2	NAG	E	2	X	-	-	-
2	NAG	F	2	X	-	-	-
2	NAG	H	2	X	-	-	-
3	NAG	D	2	X	-	-	-
3	MAN	D	3	X	-	-	-
3	NAG	G	2	X	-	-	-
3	MAN	G	3	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7912 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 Mannosyl-oligosaccharide alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total 3724	C 2359	N 619	O 738	S 8	0	0	0
1	B	475	Total 3724	C 2359	N 619	O 738	S 8	0	0	0

- 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				ZeroOcc	AltConf	Trace
2	C	2	Total 28	C 16	N 2	O 10	0	0	0
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0	0
2	H	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
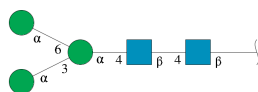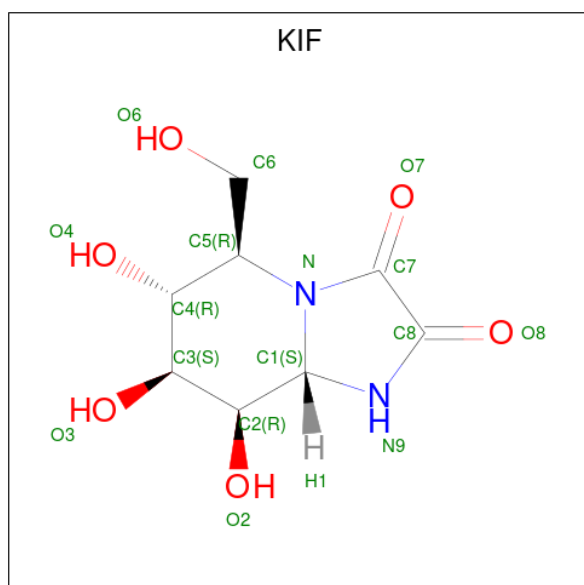
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total 61	C 34	N 2	O 25	0	0	0
3	G	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0

- Molecule 5 is KIFUNENSINE (three-letter code: KIF) (formula: $C_8H_{12}N_2O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 16	C 8	N 2	O 6	0	0
5	B	1	Total 16	C 8	N 2	O 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total 140	O 140	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	56	Total 56	O 56	0	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.

Note EDS was not executed.

• Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase
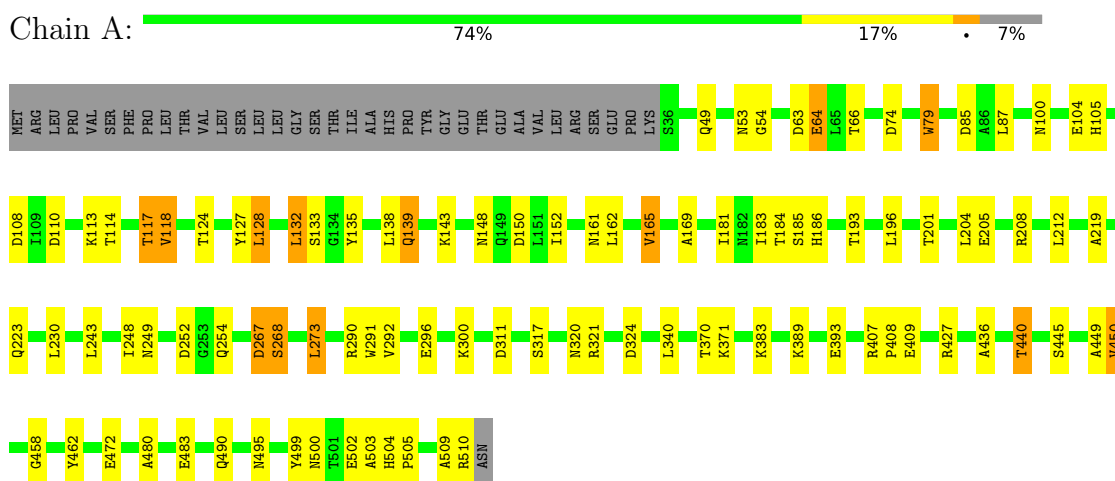
Chain A:

• Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase
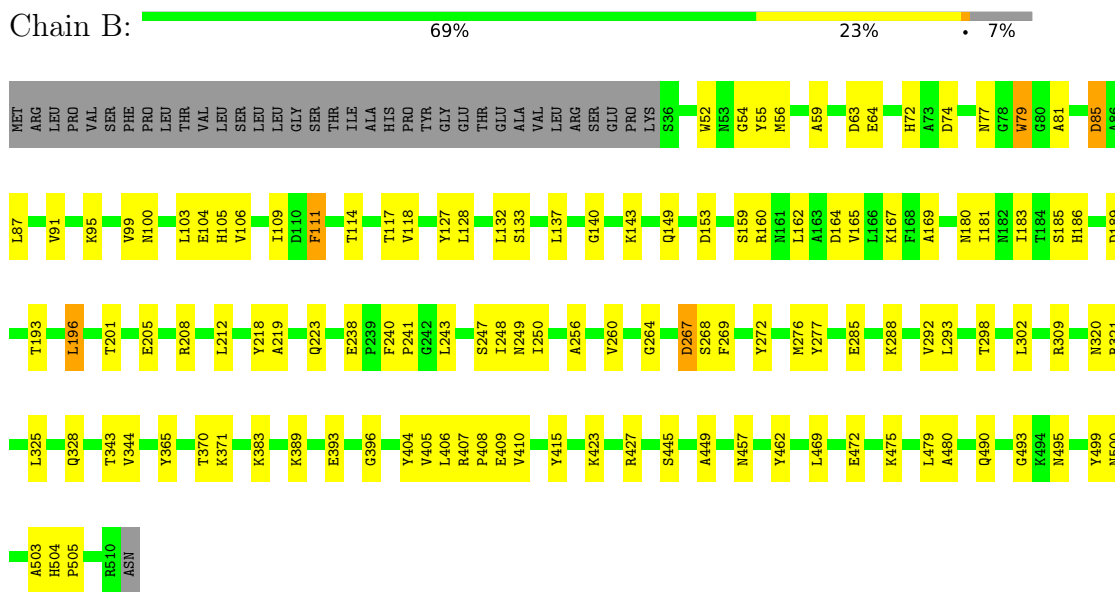
Chain B:

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

Chain C:
```
50%                    50%
```

NAG1 NAG2

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

Chain E:
```
100%
```

NAG1 NAG2

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

Chain F:
```
100%
```

NAG1 NAG2

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

Chain H:
```
100%
```

NAG1 NAG2

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain D:
```
80%                    20%
```

NAG1 NAG2 MAN3 MAN4 MAN5

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain G:
```
40%          40%          20%
```

NAG1 NAG2 MAN3 MAN4 MAN5

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.49Å 111.00Å 86.23Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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: NAG, KIF, MAN, CA

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	0/3819	0.60	1/5190 (0.0%)
1	B	0.30	0/3819	0.54	0/5190
All	All	0.33	0/7638	0.57	1/10380 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	THR	N-CA-C	-5.67	95.69	111.00

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	3724	0	3522	66	0
1	B	3724	0	3523	85	0
2	C	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	1	0
3	D	61	0	52	1	0
3	G	61	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	12	0	0
5	B	16	0	12	0	0
6	A	140	0	0	4	0
6	B	56	0	0	2	0
All	All	7912	0	7273	154	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 154 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:423:LYS:HE3	3:G:4:MAN:H61	1.53	0.90
1:A:490:GLN:H	1:A:495:ASN:HD21	1.22	0.87
1:B:77:ASN:ND2	1:B:118:VAL:HG12	1.90	0.86
1:A:436:ALA:O	1:A:440:THR:HG23	1.78	0.83
1:B:264:GLY:H	1:B:328:GLN:HE22	1.25	0.83

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	473/511 (93%)	458 (97%)	14 (3%)	1 (0%)	47	55
1	B	473/511 (93%)	447 (94%)	24 (5%)	2 (0%)	34	37
All	All	946/1022 (93%)	905 (96%)	38 (4%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASP
1	B	267	ASP
1	B	111	PHE

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	400/432 (93%)	378 (94%)	22 (6%)	21	26
1	B	400/432 (93%)	390 (98%)	10 (2%)	47	60
All	All	800/864 (93%)	768 (96%)	32 (4%)	31	40

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	293	LEU
1	B	393	GLU
1	A	243	LEU
1	A	204	LEU
1	B	408	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	149	GLN
1	B	251	ASN
1	B	495	ASN
1	B	249	ASN
1	B	305	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 ⓘ

18 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	C	1	2,1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	0.59	0
3	NAG	D	1	1,3	14,14,15	0.79	0	17,19,21	0.68	0
3	NAG	D	2	3	14,14,15	0.78	0	17,19,21	0.70	1 (5%)
3	MAN	D	3	3	11,11,12	0.62	0	15,15,17	0.41	0
3	MAN	D	4	3	11,11,12	0.47	0	15,15,17	0.58	0
3	MAN	D	5	3	11,11,12	0.46	0	15,15,17	0.56	0
2	NAG	E	1	2,1	14,14,15	0.46	0	17,19,21	0.66	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.71	0
2	NAG	F	1	2,1	14,14,15	0.49	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.74	0
3	NAG	G	1	1,3	14,14,15	0.63	0	17,19,21	0.70	0
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	0.67	0
3	MAN	G	3	3	11,11,12	0.59	0	15,15,17	0.34	0
3	MAN	G	4	3	11,11,12	0.47	0	15,15,17	0.59	1 (6%)
3	MAN	G	5	3	11,11,12	0.53	0	15,15,17	0.56	0
2	NAG	H	1	2,1	14,14,15	0.56	0	17,19,21	0.63	0
2	NAG	H	2	2	14,14,15	0.61	0	17,19,21	0.63	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
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	1/1/5/7	6/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/5/7	3/6/23/26	0/1/1/1
3	MAN	D	3	3	1/1/4/5	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	3/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	1/1/5/7	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C2-N2-C7	-2.19	119.79	122.90
3	G	4	MAN	C1-O5-C5	2.05	114.97	112.19
3	D	2	NAG	C2-N2-C7	-2.04	120.00	122.90

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	NAG	C1
2	E	2	NAG	C1
2	F	2	NAG	C1
2	H	2	NAG	C1
3	D	2	NAG	C1

5 of 41 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2

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| Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 7 short contacts:

| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	2	0
2	H	1	NAG	1	0
3	D	2	NAG	1	0
2	C	2	NAG	1	0
2	H	2	NAG	1	0
3	G	1	NAG	2	0
2	C	1	NAG	2	0
3	G	4	MAN	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles
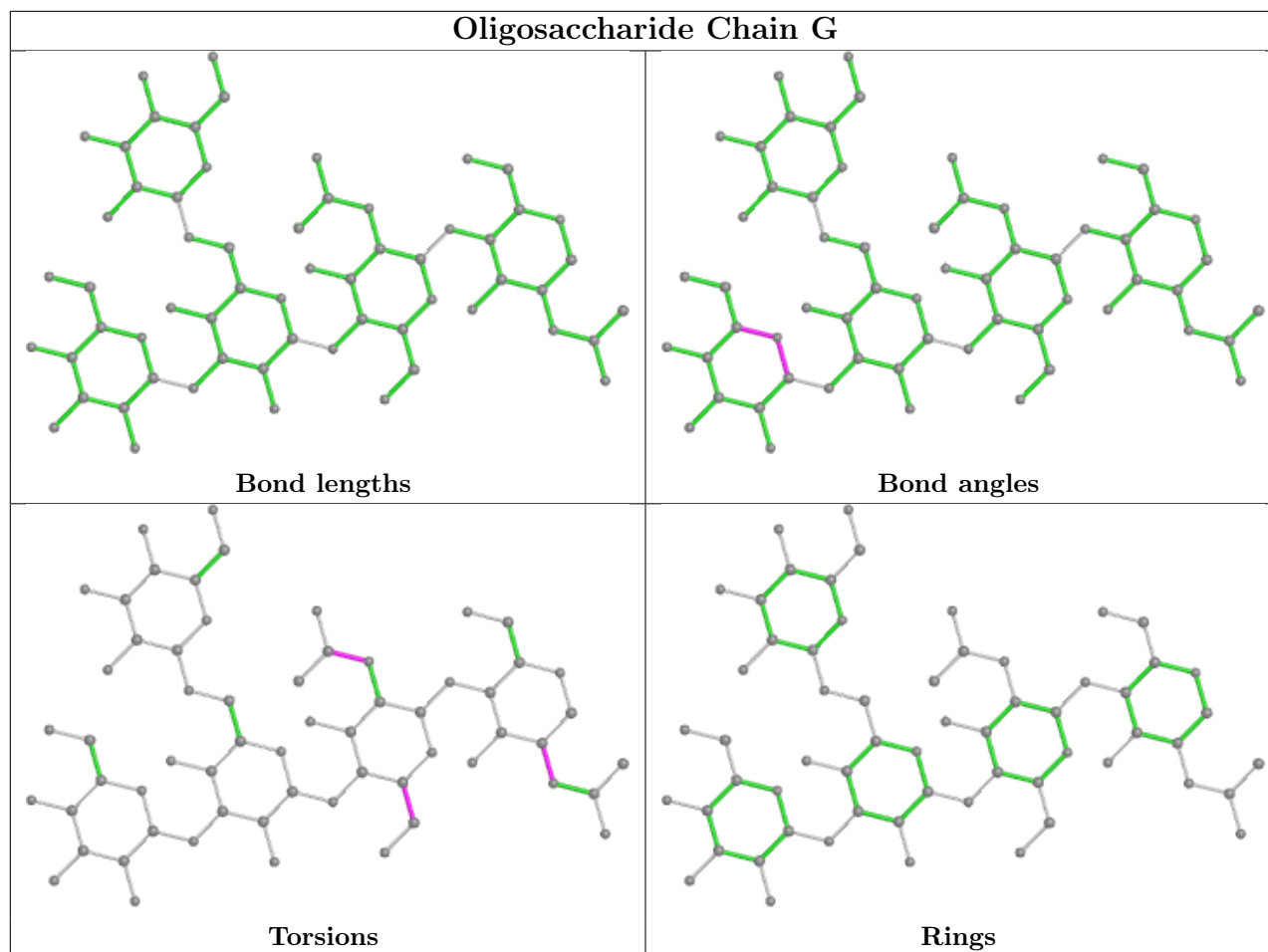

Torsions

Rings

Oligosaccharide Chain G
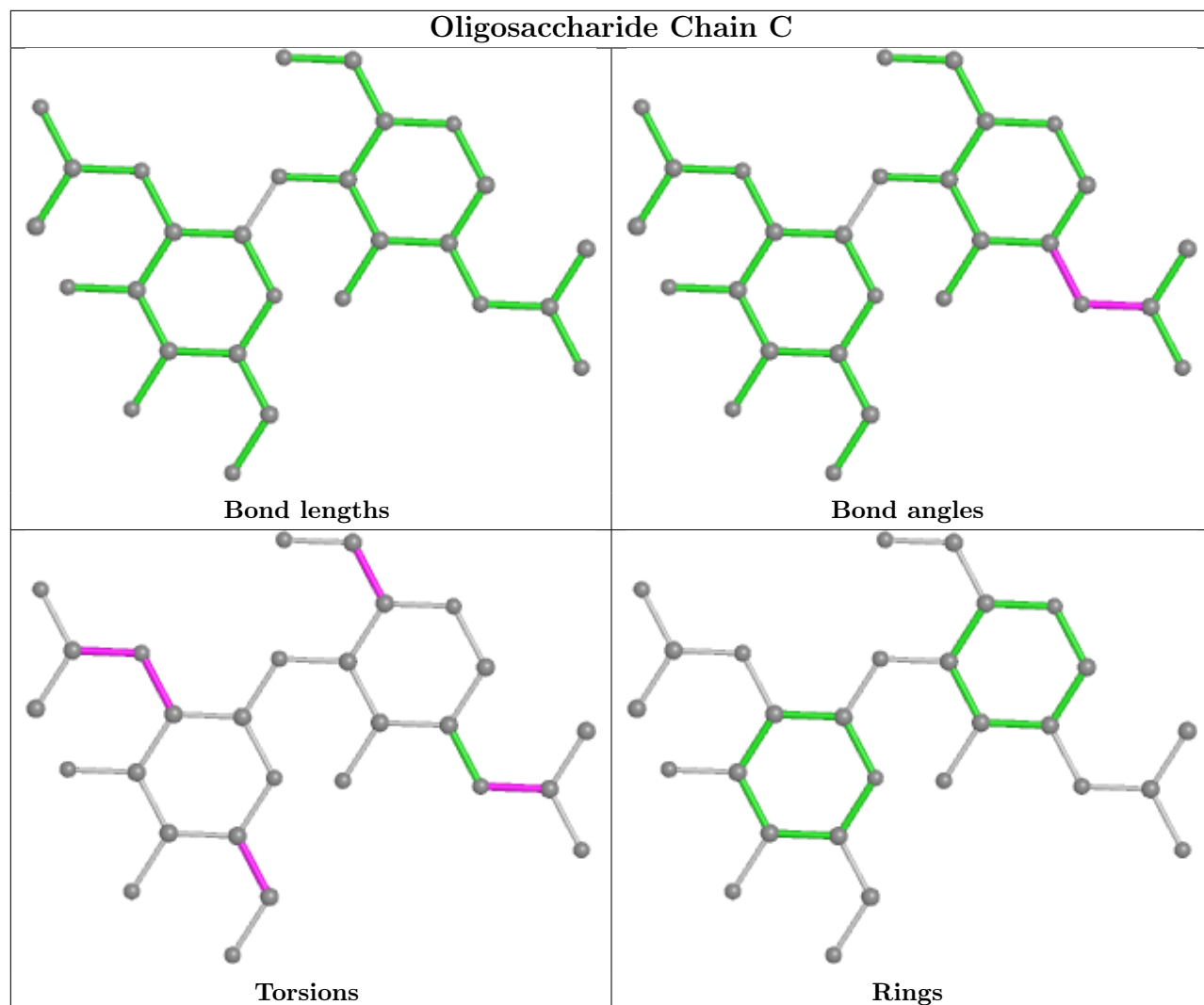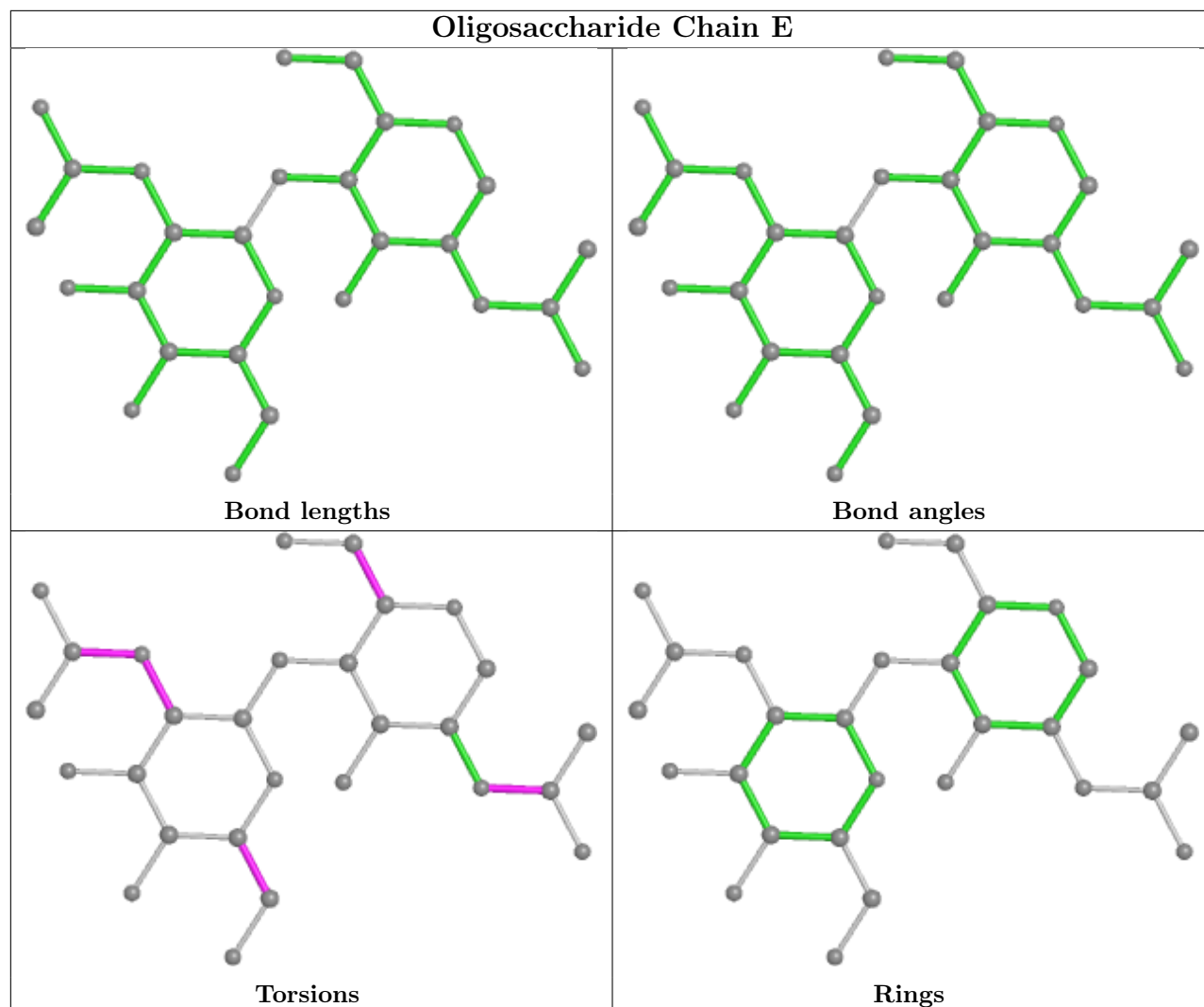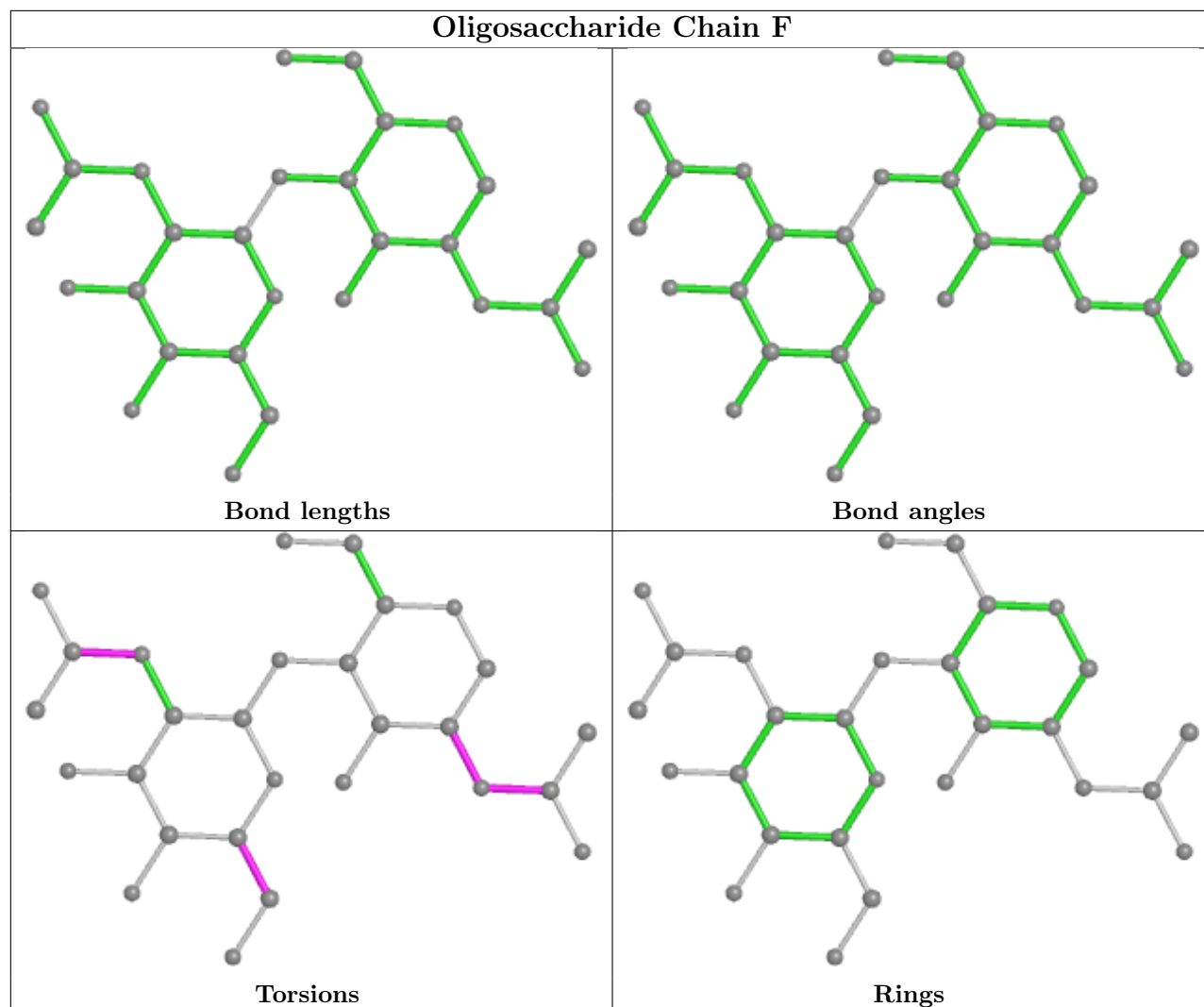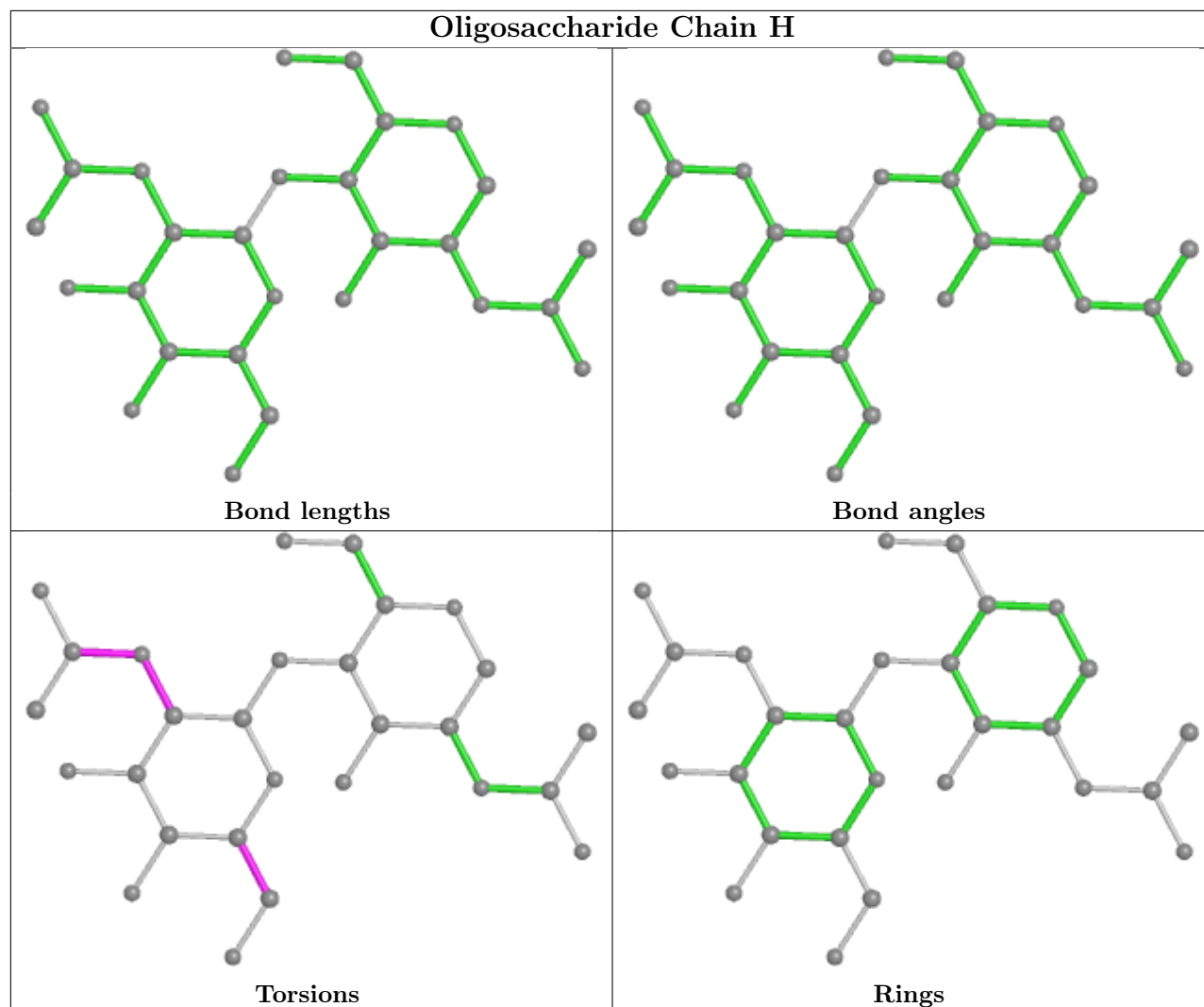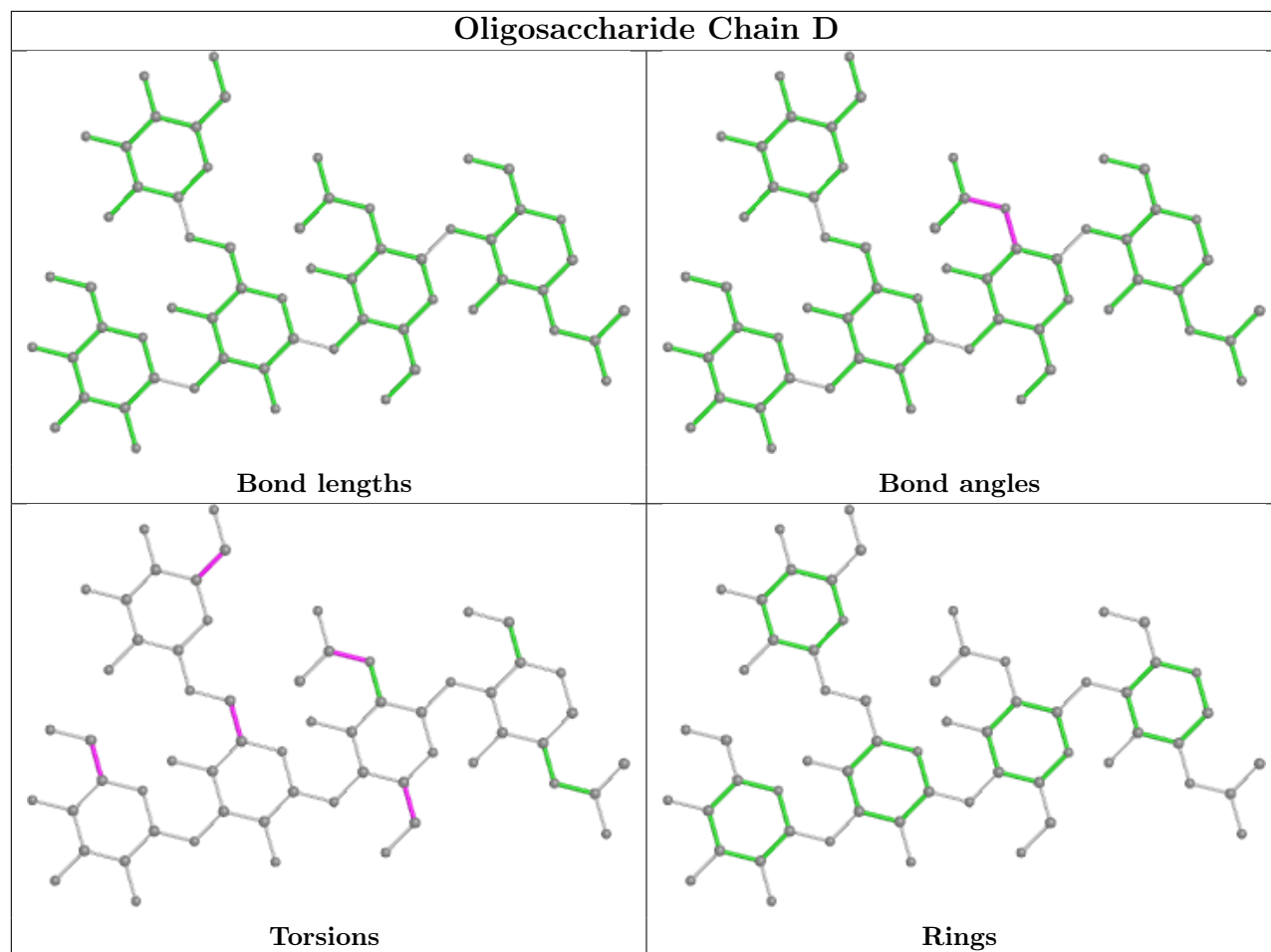
5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#|Z| > 2$
5	KIF	B	902	4	16,17,17	2.37	6 (37%)	15,26,26	4.06	4 (26%)
5	KIF	A	901	4	16,17,17	2.58	7 (43%)	15,26,26	4.07	5 (33%)

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	KIF	B	902	4	-	0/2/38/38	0/2/2/2
5	KIF	A	901	4	-	0/2/38/38	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	KIF	C5-N	6.12	1.58	1.48
5	B	902	KIF	C5-N	5.86	1.57	1.48
5	A	901	KIF	C1-N	-4.69	1.42	1.46
5	B	902	KIF	C1-N	-3.64	1.43	1.46
5	B	902	KIF	C3-C4	3.25	1.60	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	KIF	O6-C6-C5	13.79	141.00	111.42
5	A	901	KIF	O6-C6-C5	13.63	140.65	111.42
5	A	901	KIF	C7-C8-N9	5.30	110.42	105.42
5	B	902	KIF	C7-C8-N9	5.09	110.22	105.42
5	A	901	KIF	O4-C4-C5	-3.24	104.00	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.