



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2022 – 06:22 pm GMT

PDB ID : 7OGZ
Title : Plant peptide hormone receptor complex H1L3S1
Authors : Roman, A.O.; Jimenez-Sandoval, P.; Santiago, J.
Deposited on : 2021-05-07
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

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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.26

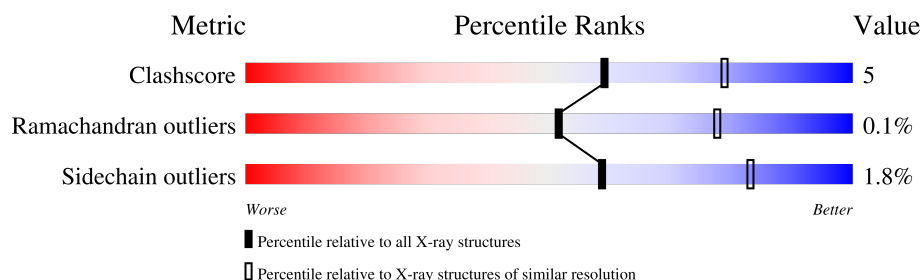
1 Overall quality at a glance

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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)


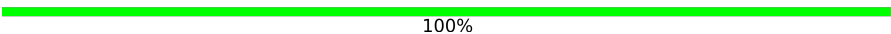

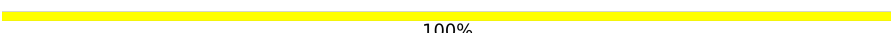
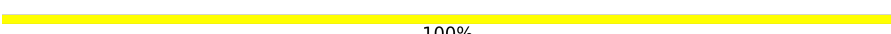
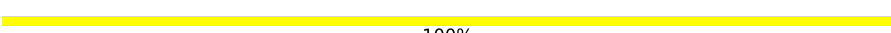




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	617	82% 14% .
1	DDD	617	83% 11% . 5%
2	BBB	201	84% 8% 8%
2	EEE	201	83% 9% 8%
3	CCC	12	83% 17%
3	FFF	12	92% 8%
4	AaA	2	50% 50%
4	AgA	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	AiA	2	 50% 50%
4	BaB	2	 100%
4	DbD	2	 50% 50%
4	DcD	2	 100%
4	DeD	2	 100%
4	DhD	2	 100%
4	DkD	2	 100%
4	EaE	2	 100%
5	AeA	3	 100%
5	DaD	3	 100%

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
4	NAG	AaA	2	X	-	-	-
4	NAG	AgA	2	X	-	-	-
4	NAG	AiA	2	X	-	-	-
4	NAG	BaB	1	X	-	-	-
4	NAG	DbD	2	X	-	-	-
4	NAG	DcD	2	X	-	-	-
4	NAG	DeD	2	X	-	-	-
4	NAG	DkD	2	X	-	-	-
4	NAG	EaE	2	X	-	-	-
5	NAG	AeA	2	X	-	-	-
5	BMA	AeA	3	X	-	-	-
5	NAG	DaD	2	X	-	-	-
5	BMA	DaD	3	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12054 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 Receptor-like protein kinase HSL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	591	Total	C	N	O	S	0	1	0
			4348	2750	714	868	16			
1	DDD	589	Total	C	N	O	S	0	1	0
			4350	2756	713	864	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	12	GLY	-	expression tag	UNP Q9SGP2
AAA	13	SER	-	expression tag	UNP Q9SGP2
AAA	14	SER	-	expression tag	UNP Q9SGP2
AAA	15	MET	-	expression tag	UNP Q9SGP2
AAA	16	ASP	-	expression tag	UNP Q9SGP2
AAA	619	LEU	-	expression tag	UNP Q9SGP2
AAA	620	GLU	-	expression tag	UNP Q9SGP2
AAA	621	GLY	-	expression tag	UNP Q9SGP2
AAA	622	SER	-	expression tag	UNP Q9SGP2
AAA	623	GLU	-	expression tag	UNP Q9SGP2
AAA	624	ASN	-	expression tag	UNP Q9SGP2
AAA	625	LEU	-	expression tag	UNP Q9SGP2
AAA	626	TYR	-	expression tag	UNP Q9SGP2
AAA	627	PHE	-	expression tag	UNP Q9SGP2
AAA	628	GLN	-	expression tag	UNP Q9SGP2
DDD	12	GLY	-	expression tag	UNP Q9SGP2
DDD	13	SER	-	expression tag	UNP Q9SGP2
DDD	14	SER	-	expression tag	UNP Q9SGP2
DDD	15	MET	-	expression tag	UNP Q9SGP2
DDD	16	ASP	-	expression tag	UNP Q9SGP2
DDD	619	LEU	-	expression tag	UNP Q9SGP2
DDD	620	GLU	-	expression tag	UNP Q9SGP2
DDD	621	GLY	-	expression tag	UNP Q9SGP2
DDD	622	SER	-	expression tag	UNP Q9SGP2
DDD	623	GLU	-	expression tag	UNP Q9SGP2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	624	ASN	-	expression tag	UNP Q9SGP2
DDD	625	LEU	-	expression tag	UNP Q9SGP2
DDD	626	TYR	-	expression tag	UNP Q9SGP2
DDD	627	PHE	-	expression tag	UNP Q9SGP2
DDD	628	GLN	-	expression tag	UNP Q9SGP2

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	185	Total	C	N	O	S	0	0	0
			1362	862	232	263	5			
2	EEE	185	Total	C	N	O	S	0	0	0
			1381	871	236	269	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	20	GLY	-	expression tag	UNP Q94AG2
BBB	21	SER	-	expression tag	UNP Q94AG2
BBB	22	SER	-	expression tag	UNP Q94AG2
BBB	23	MET	-	expression tag	UNP Q94AG2
BBB	214	LEU	-	expression tag	UNP Q94AG2
BBB	215	GLU	-	expression tag	UNP Q94AG2
BBB	216	ASN	-	expression tag	UNP Q94AG2
BBB	217	LEU	-	expression tag	UNP Q94AG2
BBB	218	TYR	-	expression tag	UNP Q94AG2
BBB	219	PHE	-	expression tag	UNP Q94AG2
BBB	220	GLN	-	expression tag	UNP Q94AG2
EEE	20	GLY	-	expression tag	UNP Q94AG2
EEE	21	SER	-	expression tag	UNP Q94AG2
EEE	22	SER	-	expression tag	UNP Q94AG2
EEE	23	MET	-	expression tag	UNP Q94AG2
EEE	214	LEU	-	expression tag	UNP Q94AG2
EEE	215	GLU	-	expression tag	UNP Q94AG2
EEE	216	ASN	-	expression tag	UNP Q94AG2
EEE	217	LEU	-	expression tag	UNP Q94AG2
EEE	218	TYR	-	expression tag	UNP Q94AG2
EEE	219	PHE	-	expression tag	UNP Q94AG2
EEE	220	GLN	-	expression tag	UNP Q94AG2

- Molecule 3 is a protein called Peptide hormone IDL3.

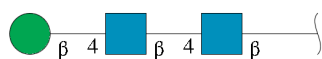
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	12	Total	C	N	O	0	0	0
			81	48	16	17			
3	FFF	12	Total	C	N	O	0	0	0
			81	48	16	17			

- 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	AaA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AgA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AiA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BaB	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DbD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DcD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DeD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DhD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DkD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	EaE	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	AeA	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	DaD	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
6	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
6	DDD	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	10	Total	O	0	0
			10	10		
7	BBB	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

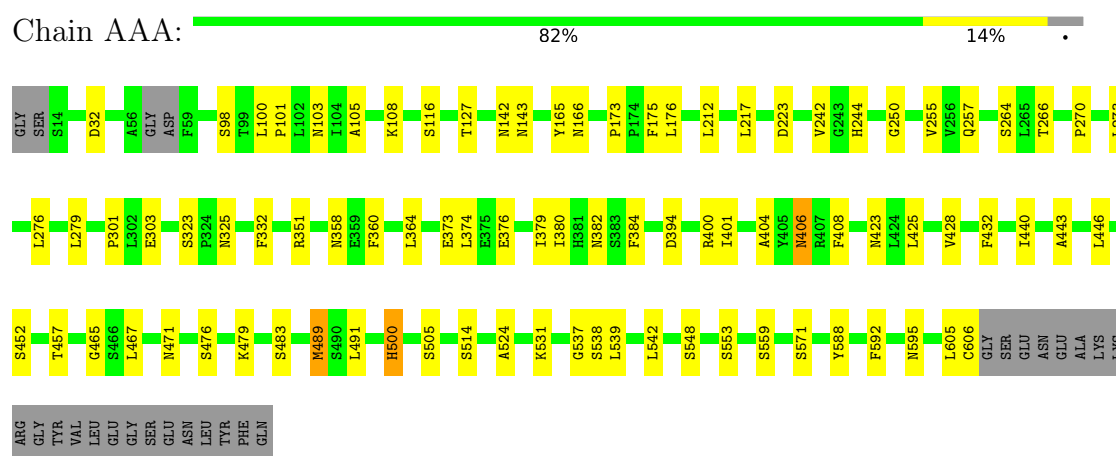
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total	O	0	0
			1	1		
7	DDD	7	Total	O	0	0
			7	7		
7	EEE	3	Total	O	0	0
			3	3		

3 Residue-property plots

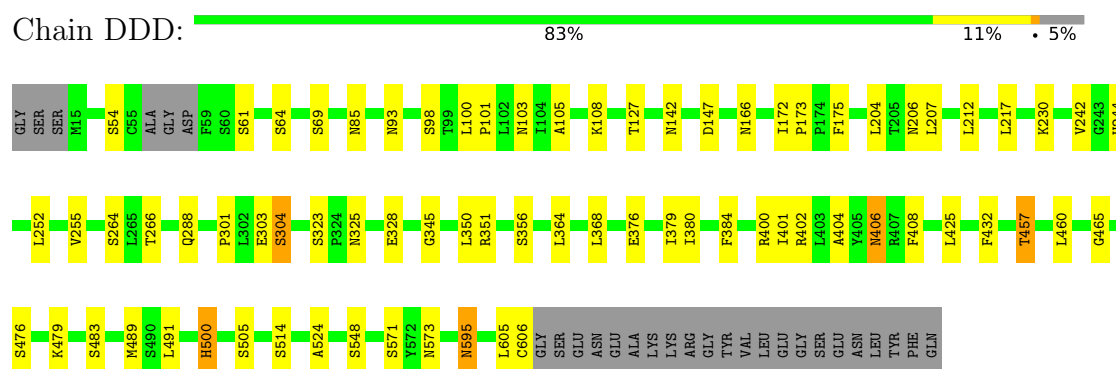
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

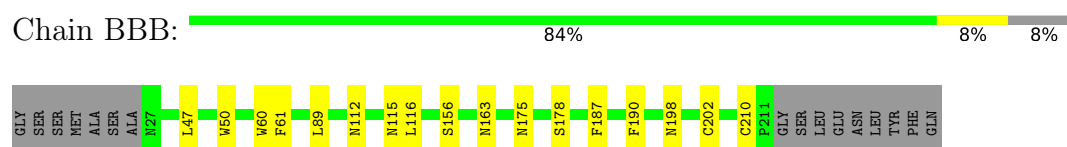
- Molecule 1: Receptor-like protein kinase HSL1




- Molecule 1: Receptor-like protein kinase HSL1



- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 2: Somatic embryogenesis receptor kinase 1

Chain EEE:  83% 9% 8%



- Molecule 3: Peptide hormone IDL3

Chain CCC:  83% 17%



- Molecule 3: Peptide hormone IDL3

Chain FFF:  92% 8%



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

Chain AaA:  50% 50%



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

Chain AgA:  100%



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

Chain AiA:  50% 50%



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

Chain BaB:  100%



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

Chain DbD:  50% 50%

MAG1
MAG2

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

Chain DcD:  100%

MAG1
MAG2

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

Chain DeD:  100%

MAG1
MAG2

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

Chain DhD:  100%

MAG1
MAG2

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

Chain DkD:  100%

MAG1
MAG2

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

Chain EaE:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AeA:  100%

MAG1
MAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DaD:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.84Å 144.50Å 168.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.70	Depositor
% Data completeness (in resolution range)	99.8 (47.66-2.70)	Depositor
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.353 , 0.371	Depositor
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.873	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12054	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7328e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, 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	AAA	0.65	0/4432	0.68	1/6056 (0.0%)
1	DDD	0.65	0/4432	0.68	0/6050
2	BBB	0.64	0/1391	0.72	0/1917
2	EEE	0.63	0/1410	0.72	0/1939
3	CCC	0.68	0/74	0.69	0/96
3	FFF	0.67	0/74	0.72	0/96
All	All	0.65	0/11813	0.69	1/16154 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	32	ASP	CB-CG-OD2	-5.64	113.22	118.30

There are no chirality outliers.

There are no planarity outliers.

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	AAA	4348	0	4115	47	0
1	DDD	4350	0	4157	46	0
2	BBB	1362	0	1284	10	0
2	EEE	1381	0	1324	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	81	0	66	1	0
3	FFF	81	0	66	0	0
4	AaA	28	0	25	0	0
4	AgA	28	0	25	0	0
4	AiA	28	0	25	0	0
4	BaB	28	0	25	0	0
4	DbD	28	0	25	0	0
4	DcD	28	0	25	0	0
4	DeD	28	0	25	0	0
4	DhD	28	0	25	0	0
4	DkD	28	0	25	0	0
4	EaE	28	0	25	0	0
5	AeA	39	0	34	0	0
5	DaD	39	0	34	0	0
6	AAA	42	0	39	0	0
6	DDD	28	0	26	0	0
7	AAA	10	0	0	0	0
7	BBB	2	0	0	0	0
7	CCC	1	0	0	0	0
7	DDD	7	0	0	0	0
7	EEE	3	0	0	0	0
All	All	12054	0	11395	111	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 5.

The worst 5 of 111 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:EEE:89:LEU:O	2:EEE:116:LEU:HD21	2.00	0.61
2:EEE:187:PHE:HA	2:EEE:190:PHE:HD2	1.64	0.60
1:DDD:206:ASN:HA	1:DDD:230:LYS:HD2	1.82	0.60
1:AAA:101:PRO:HB2	1:AAA:103:ASN:OD1	2.04	0.57
1:DDD:101:PRO:HB2	1:DDD:103:ASN:OD1	2.04	0.57

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	AAA	588/617 (95%)	577 (98%)	10 (2%)	1 (0%)	47	73
1	DDD	586/617 (95%)	576 (98%)	9 (2%)	1 (0%)	47	73
2	BBB	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
2	EEE	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
3	CCC	9/12 (75%)	9 (100%)	0	0	100	100
3	FFF	9/12 (75%)	9 (100%)	0	0	100	100
All	All	1558/1660 (94%)	1531 (98%)	25 (2%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	98	SER
1	DDD	98	SER

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	AAA	469/540 (87%)	457 (97%)	12 (3%)	46	75
1	DDD	473/540 (88%)	466 (98%)	7 (2%)	65	86
2	BBB	150/182 (82%)	149 (99%)	1 (1%)	84	94
2	EEE	157/182 (86%)	154 (98%)	3 (2%)	57	82
3	CCC	7/10 (70%)	7 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FFF	7/10 (70%)	7 (100%)	0	100	100
All	All	1263/1464 (86%)	1240 (98%)	23 (2%)	59	83

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	304	SER
1	DDD	457	THR
1	DDD	406	ASN
1	DDD	500	HIS
1	AAA	394	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	HYP	FFF	85	3	6,8,9	0.53	0	5,10,12	1.12	1 (20%)
3	HYP	CCC	85	3	6,8,9	0.57	0	5,10,12	1.05	1 (20%)

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	HYP	FFF	85	3	-	0/0/11/13	0/1/1/1
3	HYP	CCC	85	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FFF	85	HYP	O-C-CA	-2.14	119.18	124.78
3	CCC	85	HYP	O-C-CA	-2.07	119.34	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

26 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	$\# Z > 2$
4	NAG	AaA	1	1,4	14,14,15	0.34	0	17,19,21	1.27	3 (17%)
4	NAG	AaA	2	4	14,14,15	0.32	0	17,19,21	0.75	0
5	NAG	AeA	1	1,5	14,14,15	0.35	0	17,19,21	1.07	2 (11%)
5	NAG	AeA	2	5	14,14,15	0.43	0	17,19,21	0.91	1 (5%)
5	BMA	AeA	3	5	11,11,12	0.33	0	15,15,17	0.78	1 (6%)
4	NAG	AgA	1	1,4	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
4	NAG	AgA	2	4	14,14,15	0.38	0	17,19,21	0.77	1 (5%)
4	NAG	AiA	1	1,4	14,14,15	0.44	0	17,19,21	1.39	2 (11%)
4	NAG	AiA	2	4	14,14,15	0.37	0	17,19,21	0.79	0
4	NAG	BaB	1	4,2	14,14,15	0.40	0	17,19,21	0.57	0
4	NAG	BaB	2	4	14,14,15	0.47	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	DaD	1	1,5	14,14,15	0.33	0	17,19,21	0.96	1 (5%)
5	NAG	DaD	2	5	14,14,15	0.50	0	17,19,21	1.15	1 (5%)
5	BMA	DaD	3	5	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
4	NAG	DbD	1	1,4	14,14,15	0.35	0	17,19,21	1.06	3 (17%)
4	NAG	DbD	2	4	14,14,15	0.36	0	17,19,21	0.68	0
4	NAG	DcD	1	1,4	14,14,15	0.46	0	17,19,21	1.22	1 (5%)
4	NAG	DcD	2	4	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
4	NAG	DeD	1	1,4	14,14,15	0.44	0	17,19,21	0.81	1 (5%)
4	NAG	DeD	2	4	14,14,15	0.32	0	17,19,21	10.12	5 (29%)
4	NAG	DhD	1	1,4	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
4	NAG	DhD	2	4	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
4	NAG	DkD	1	1,4	14,14,15	0.34	0	17,19,21	0.84	0
4	NAG	DkD	2	4	14,14,15	0.27	0	17,19,21	0.55	0
4	NAG	EaE	1	4,2	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
4	NAG	EaE	2	4	14,14,15	0.40	0	17,19,21	0.85	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
4	NAG	AaA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AaA	2	4	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	AeA	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	AeA	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	BMA	AeA	3	5	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	AgA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AgA	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	AiA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	AiA	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	BaB	1	4,2	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	BaB	2	4	-	1/6/23/26	0/1/1/1
5	NAG	DaD	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	DaD	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	BMA	DaD	3	5	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	DbD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	DbD	2	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	DcD	1	1,4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	DcD	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	DeD	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	DeD	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	DhD	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	DhD	2	4	-	0/6/23/26	0/1/1/1
4	NAG	DkD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	DkD	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	EaE	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	EaE	2	4	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DeD	2	NAG	C8-C7-N2	27.27	162.27	116.10
4	DeD	2	NAG	O7-C7-C8	-22.35	80.54	122.06
4	DeD	2	NAG	O7-C7-N2	-21.87	81.74	121.95
4	AiA	1	NAG	C1-O5-C5	3.84	117.39	112.19
4	AaA	1	NAG	C1-O5-C5	3.20	116.53	112.19

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AaA	2	NAG	C1
4	AgA	2	NAG	C1
4	AiA	2	NAG	C1
4	BaB	1	NAG	C1
4	DbD	2	NAG	C1

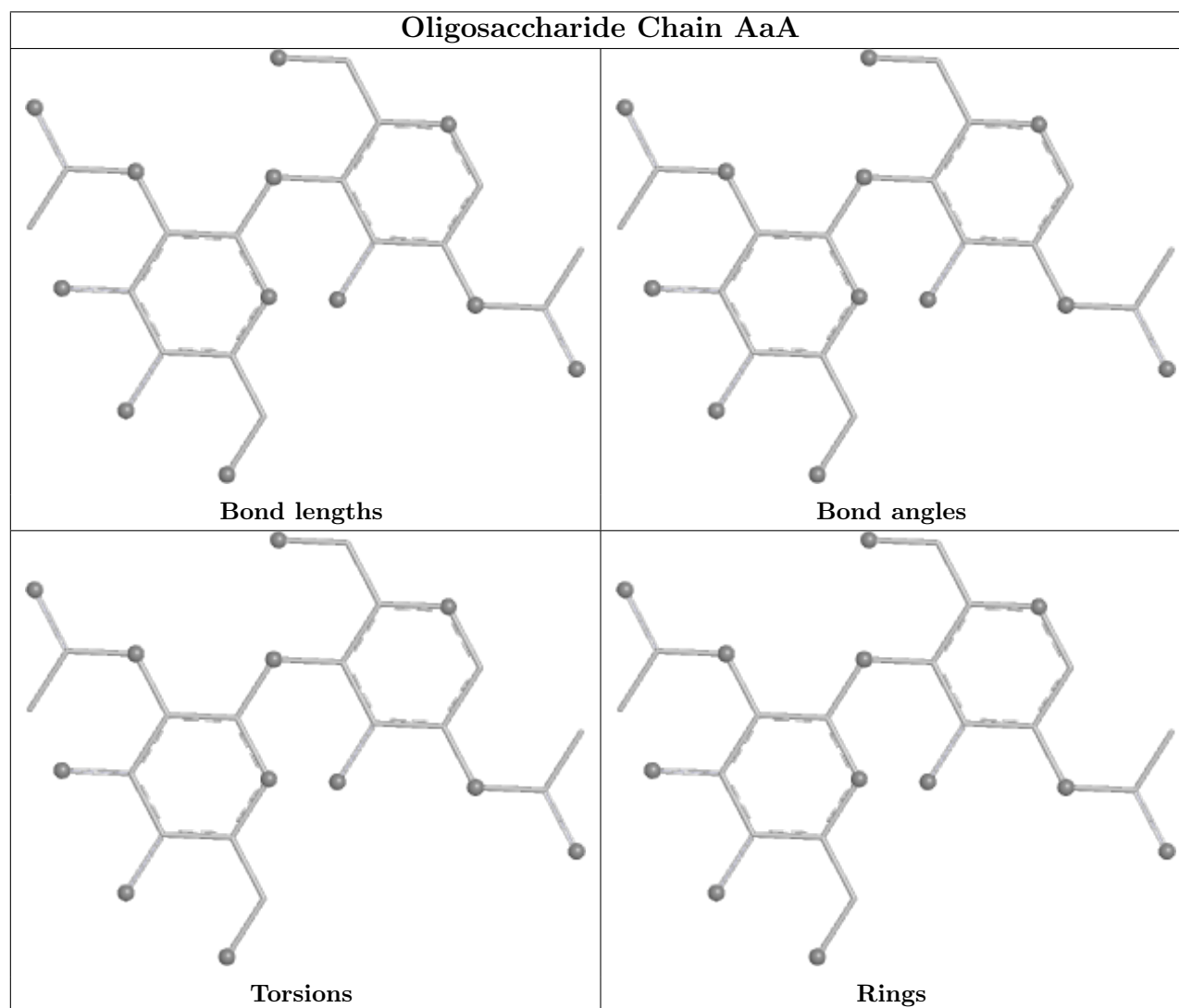
5 of 21 torsion outliers are listed below:

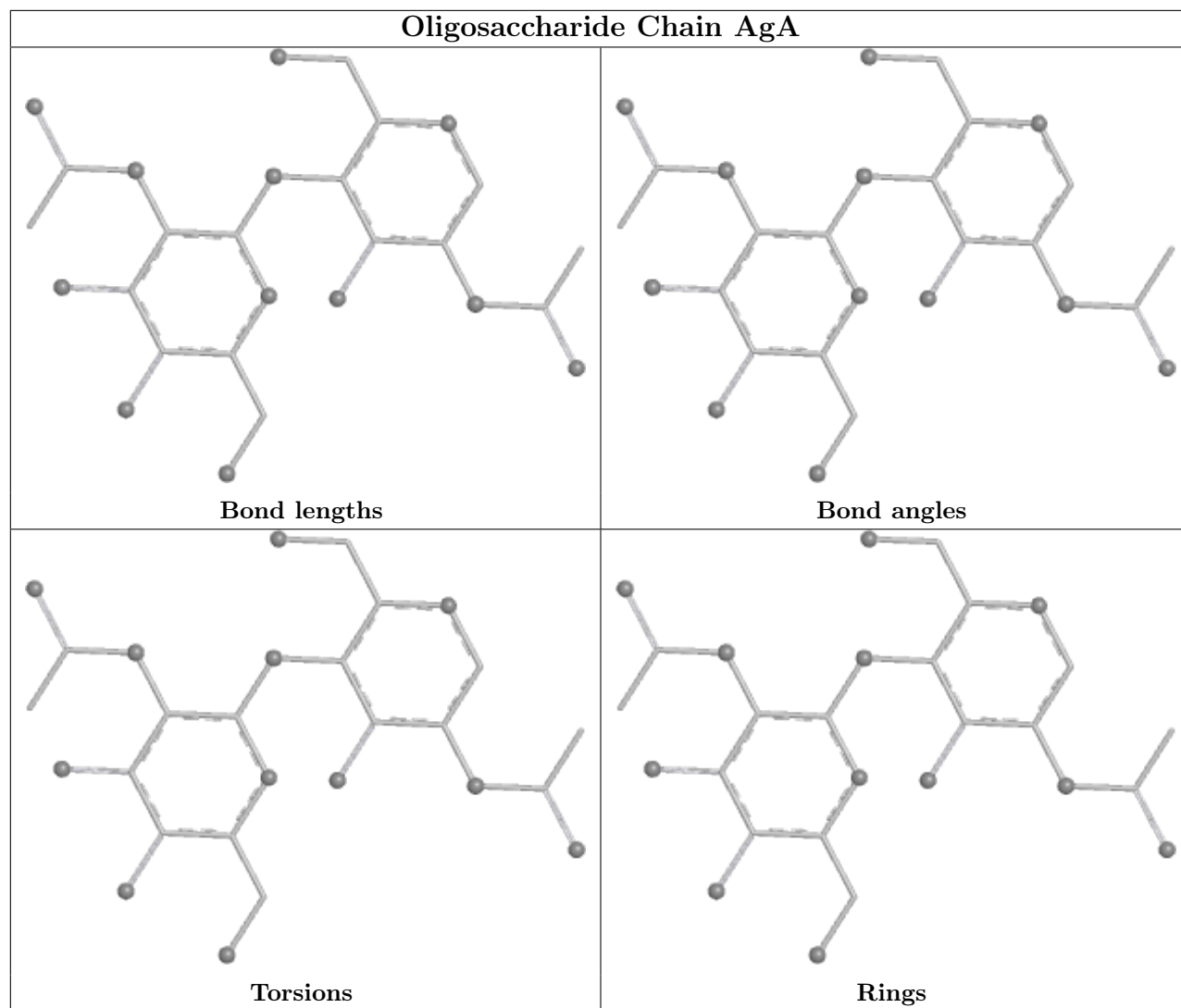
Mol	Chain	Res	Type	Atoms
4	DcD	1	NAG	O5-C5-C6-O6
4	AiA	1	NAG	O5-C5-C6-O6
4	AgA	2	NAG	O5-C5-C6-O6
4	DcD	1	NAG	C4-C5-C6-O6
4	DkD	2	NAG	O5-C5-C6-O6

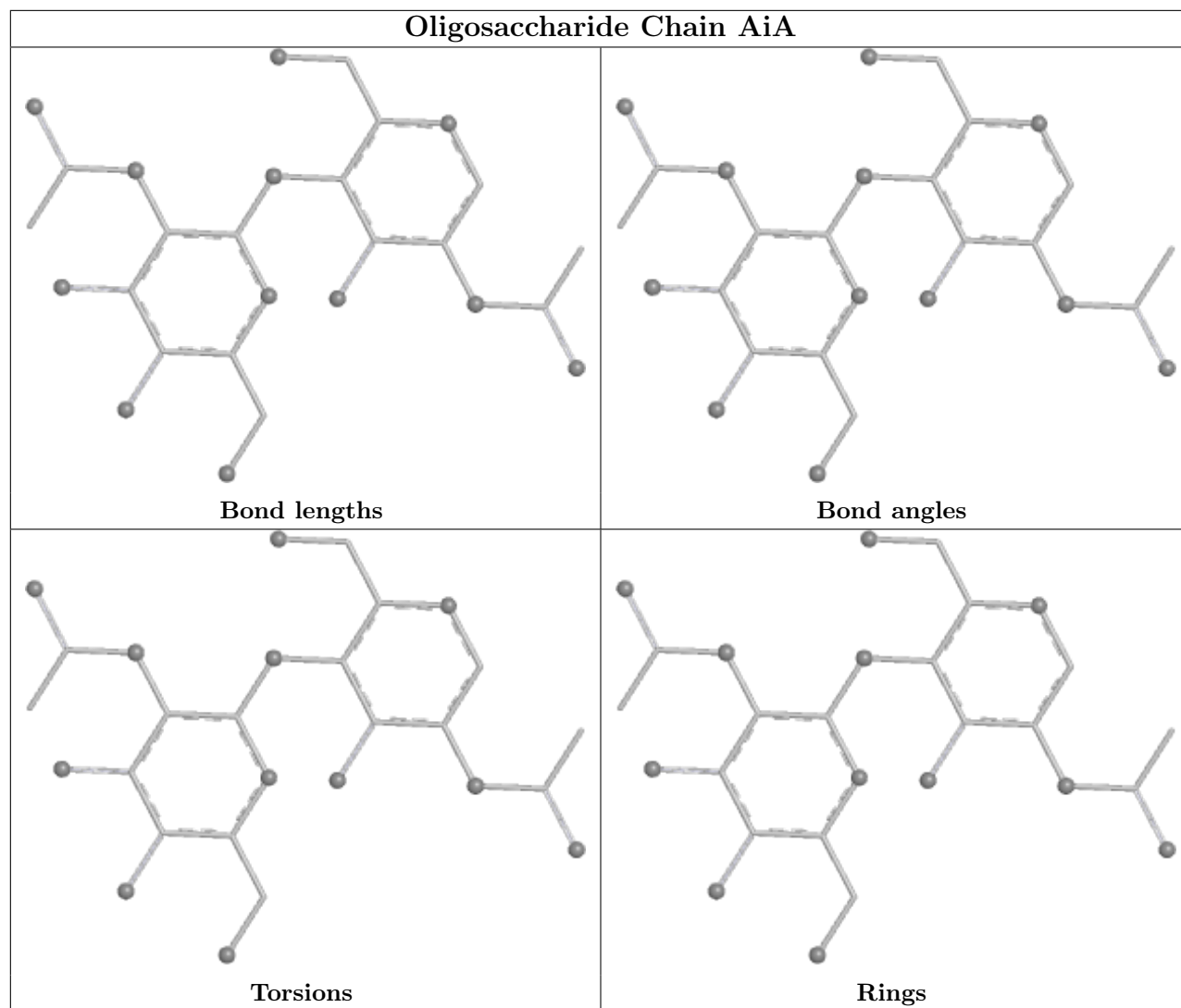
There are no ring outliers.

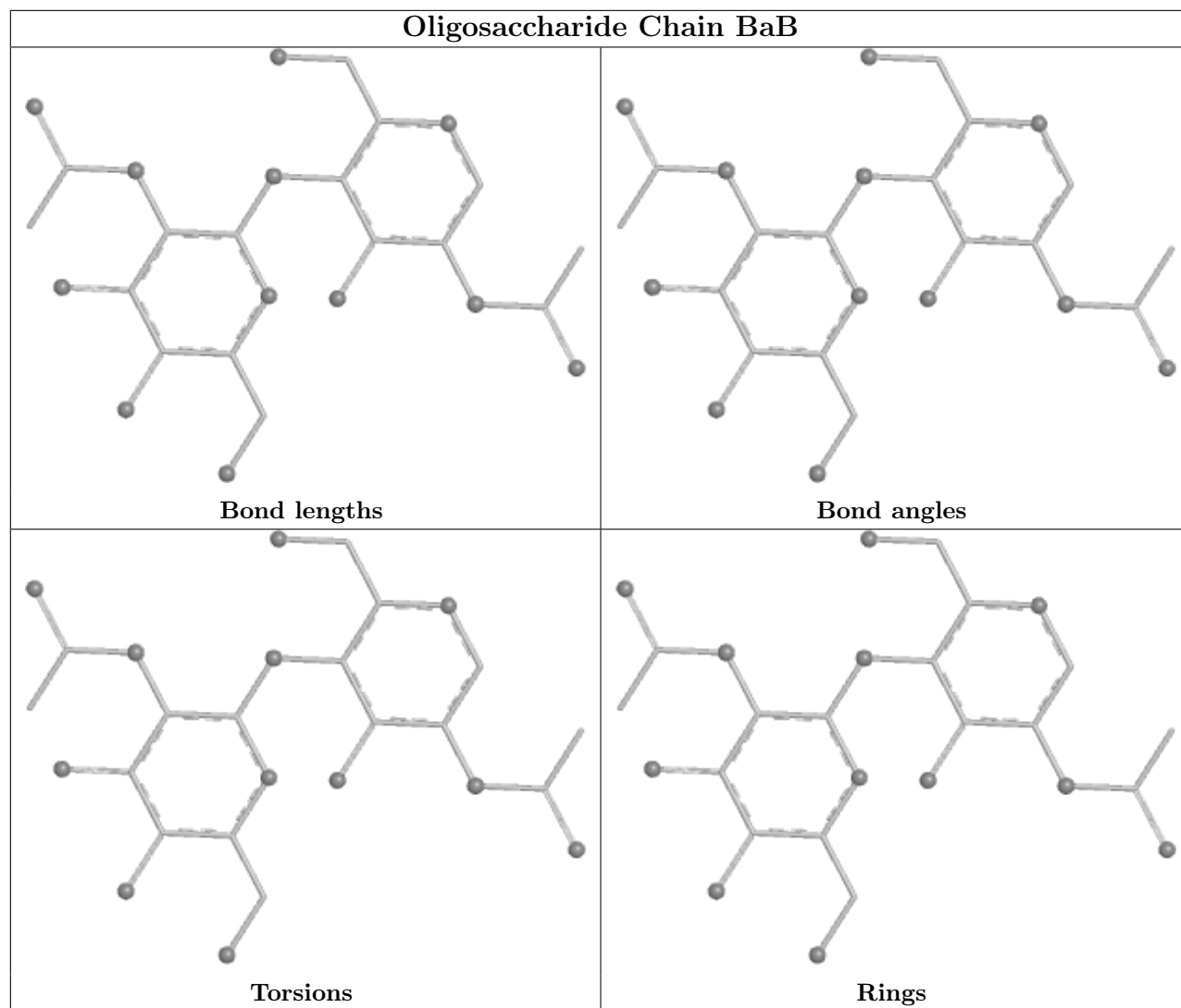
No monomer is involved in short contacts.

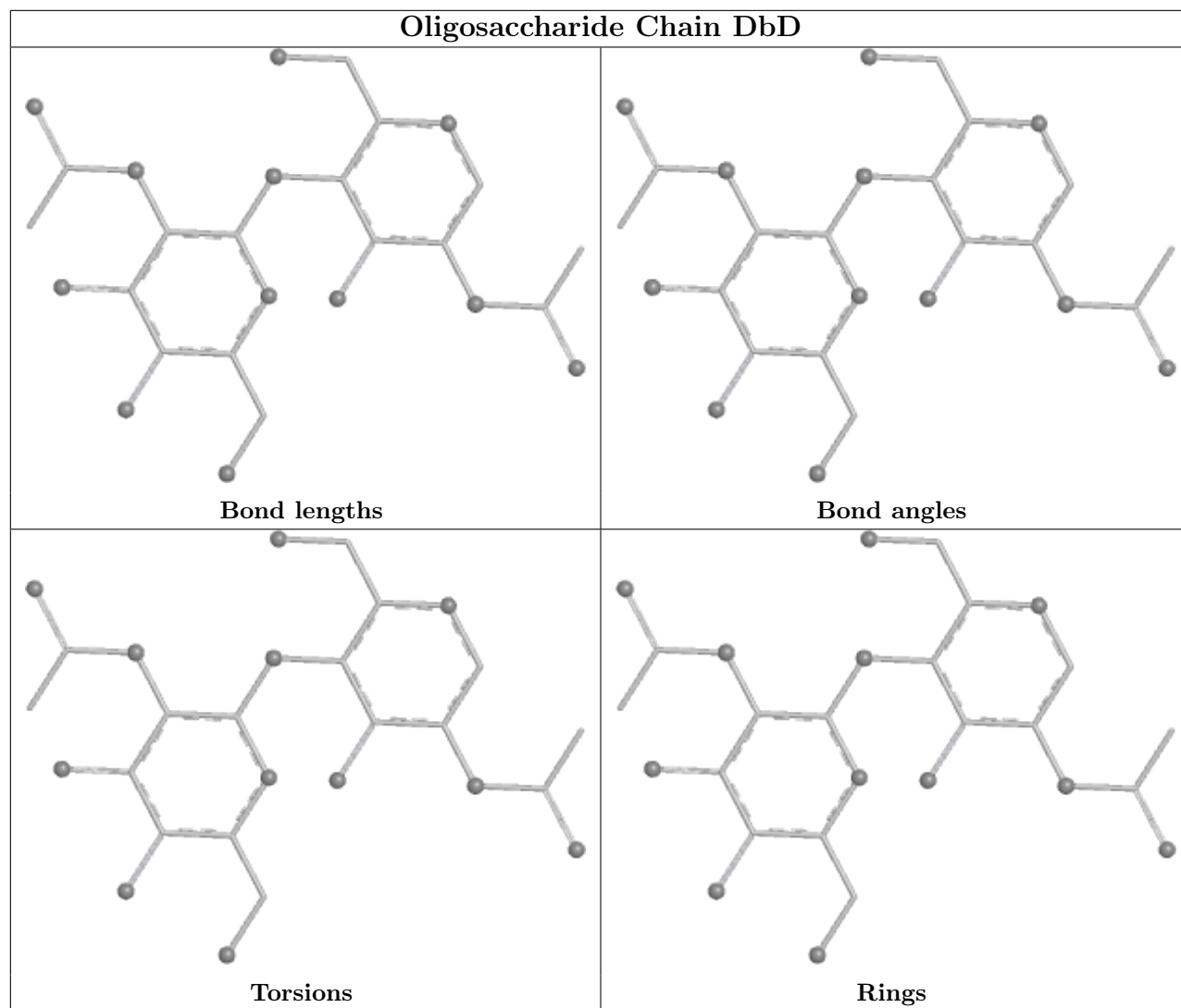
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

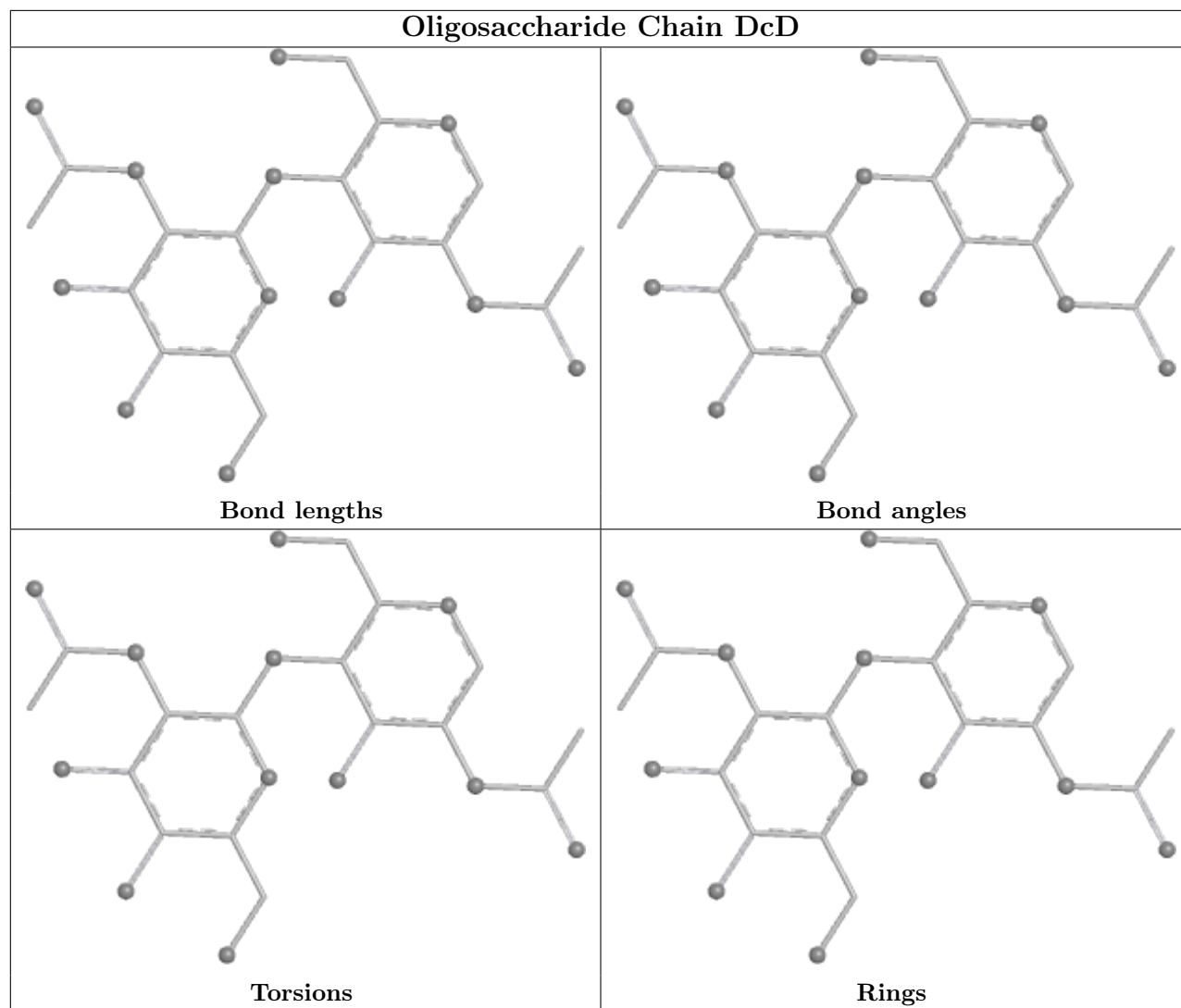




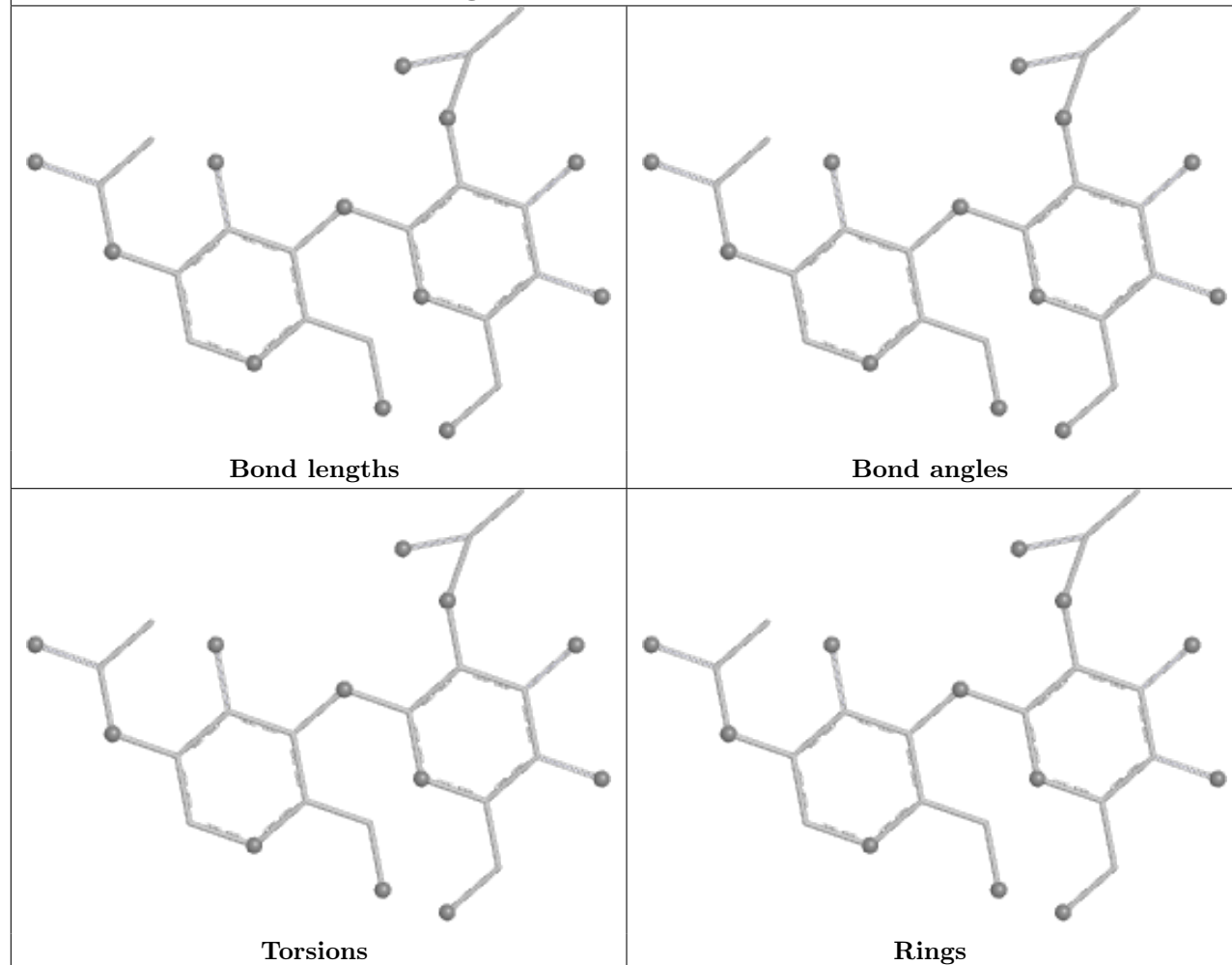


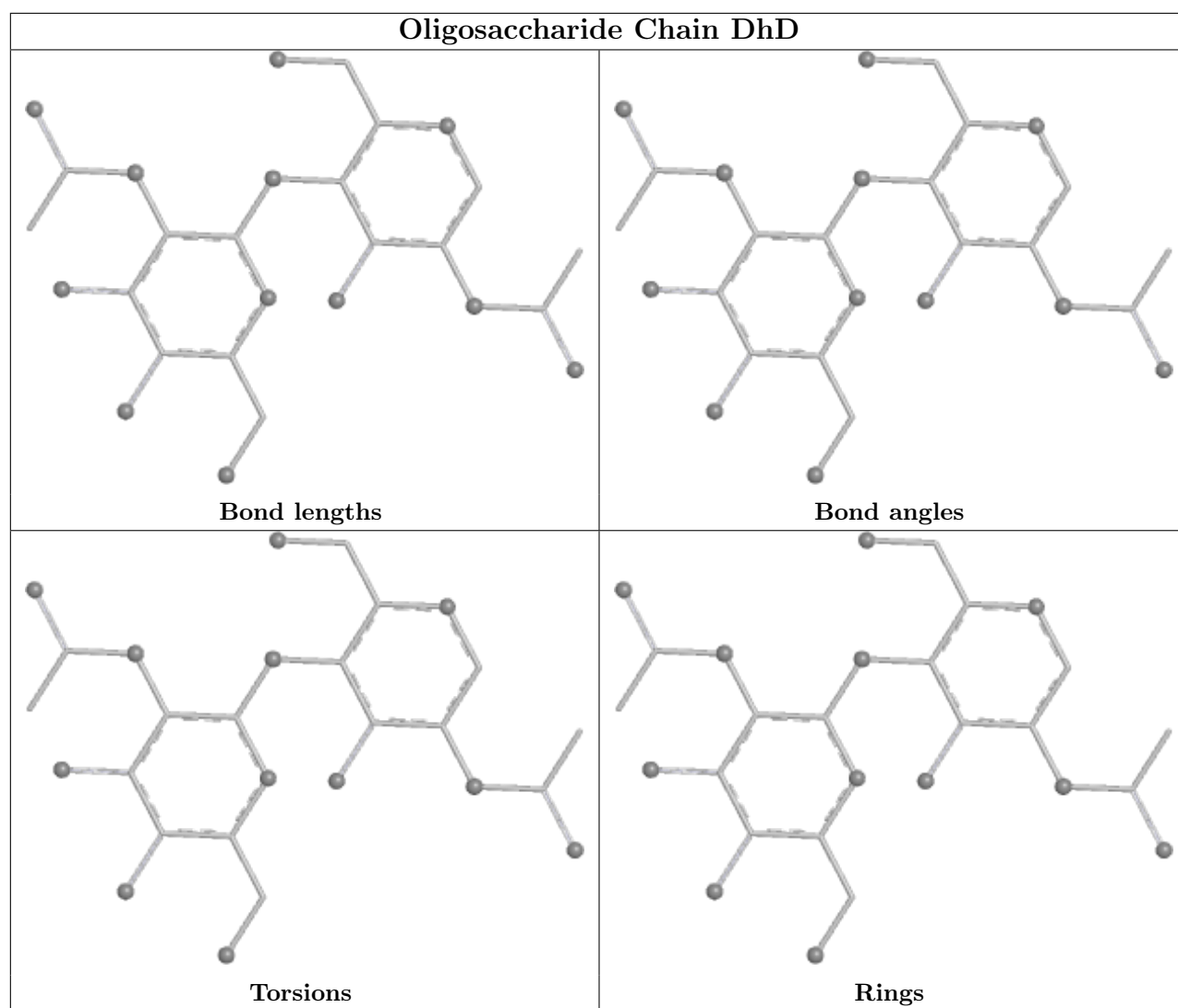


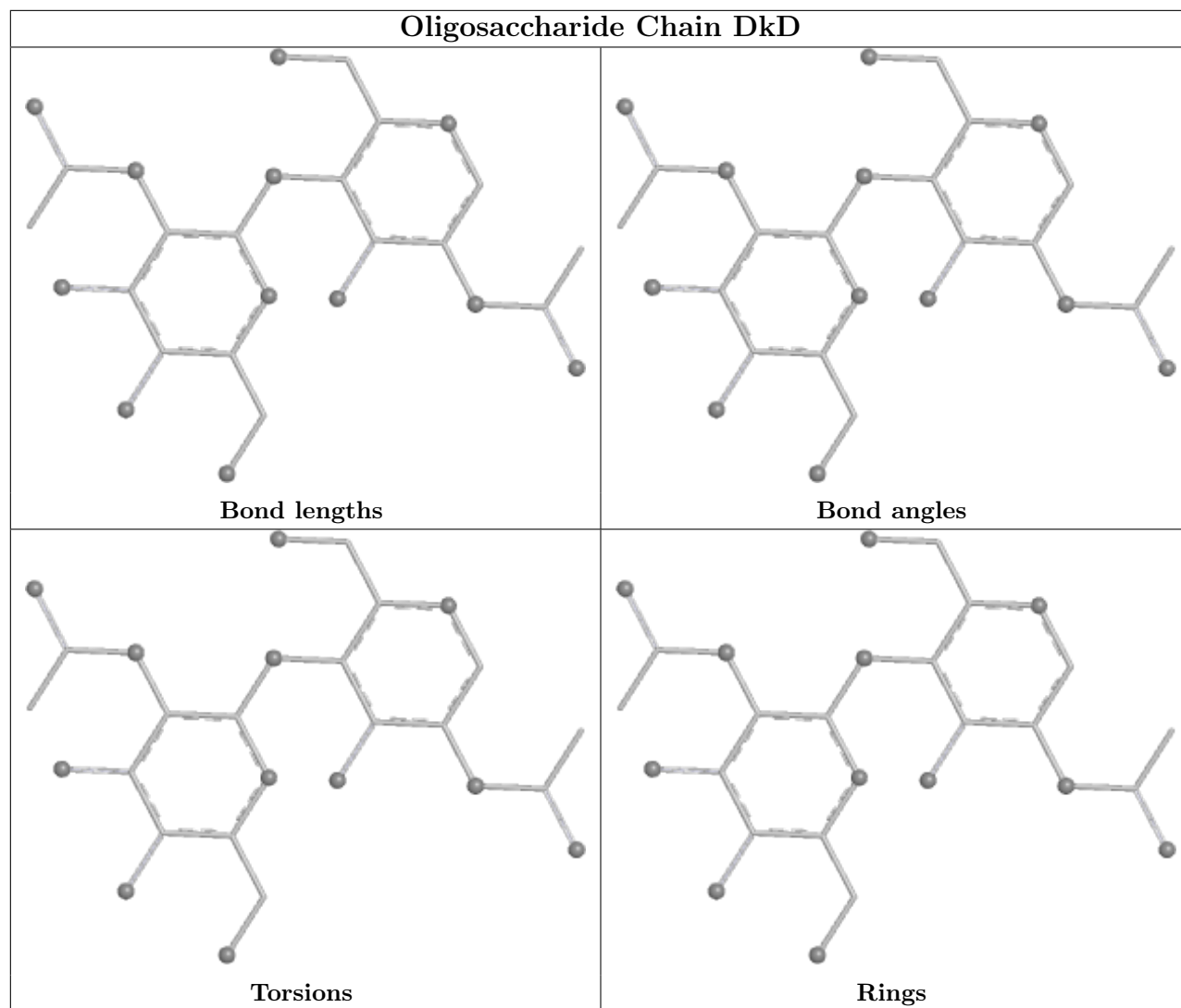


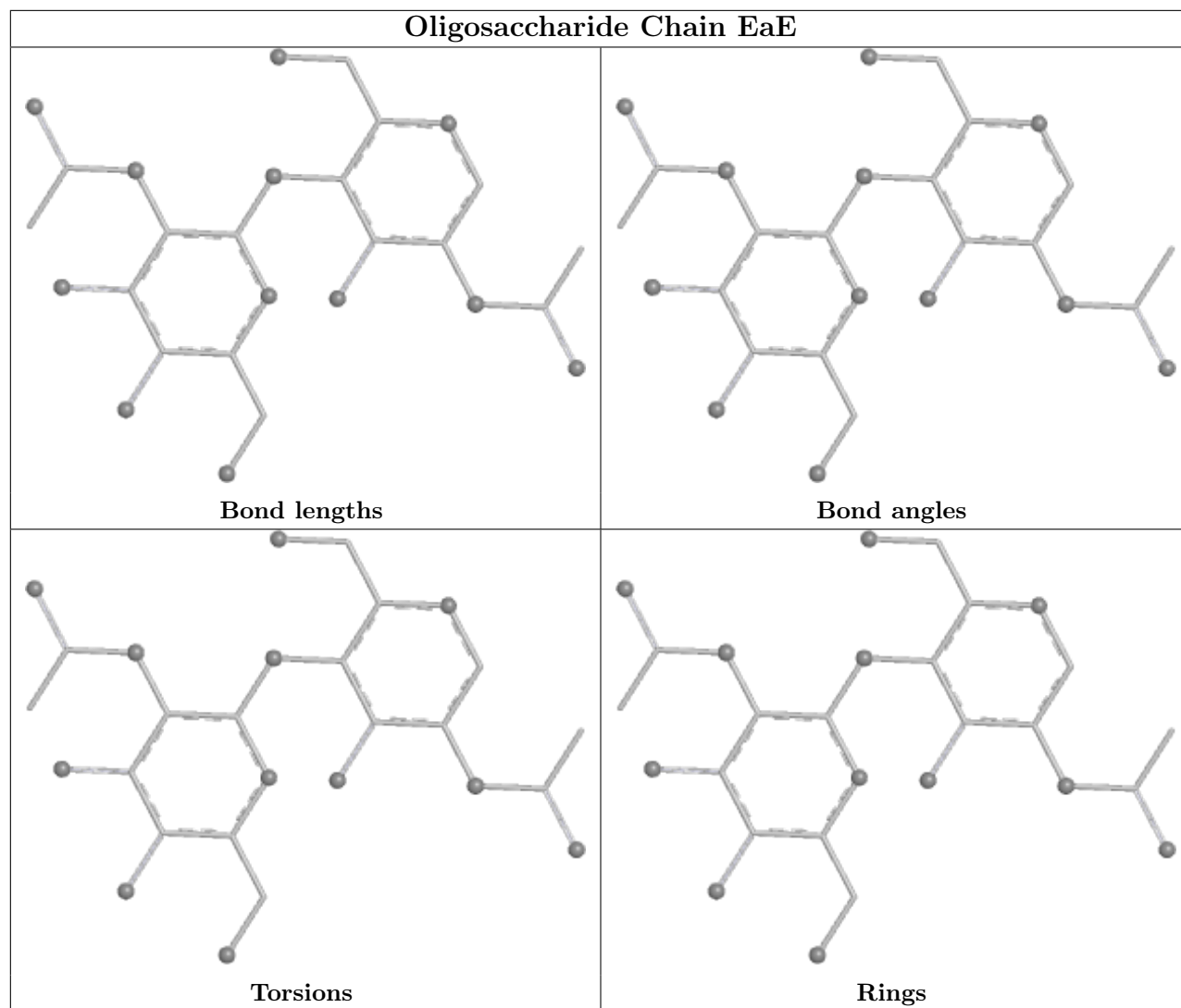


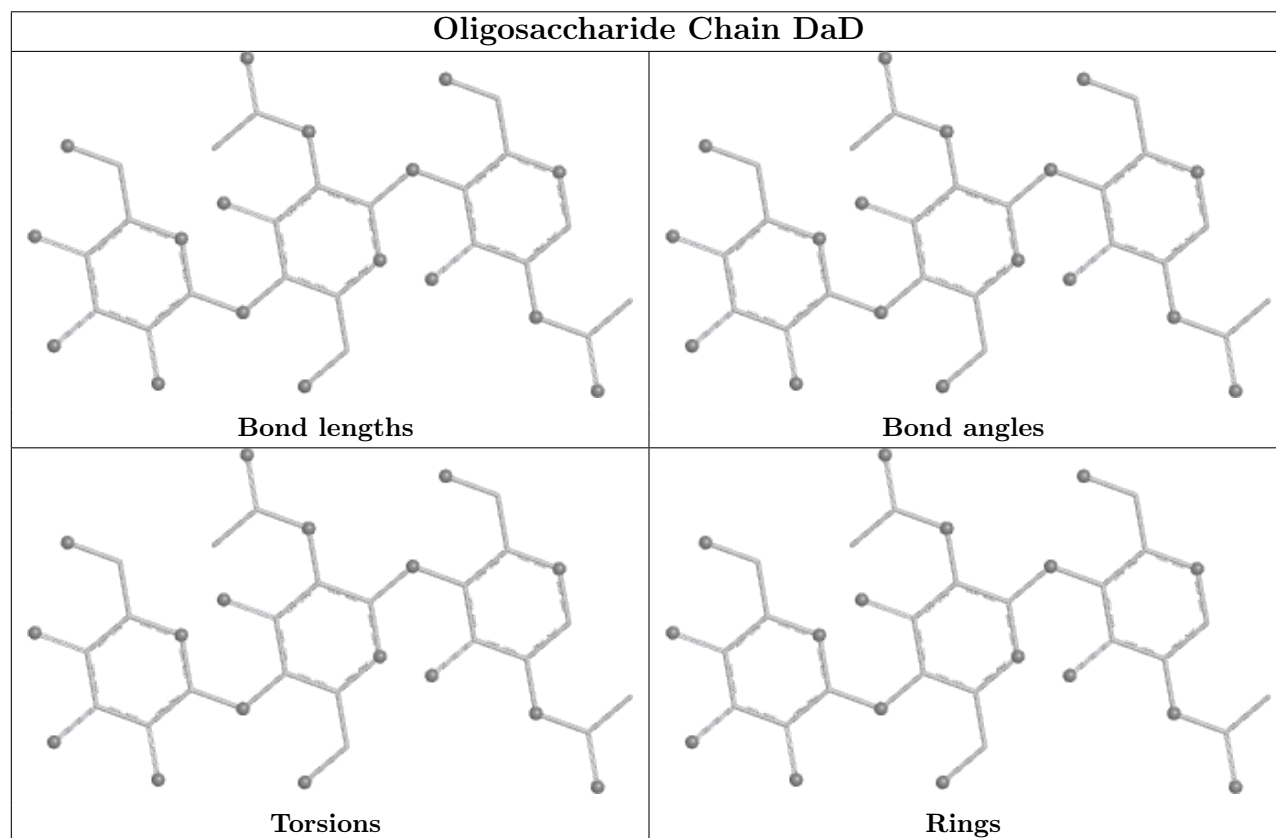
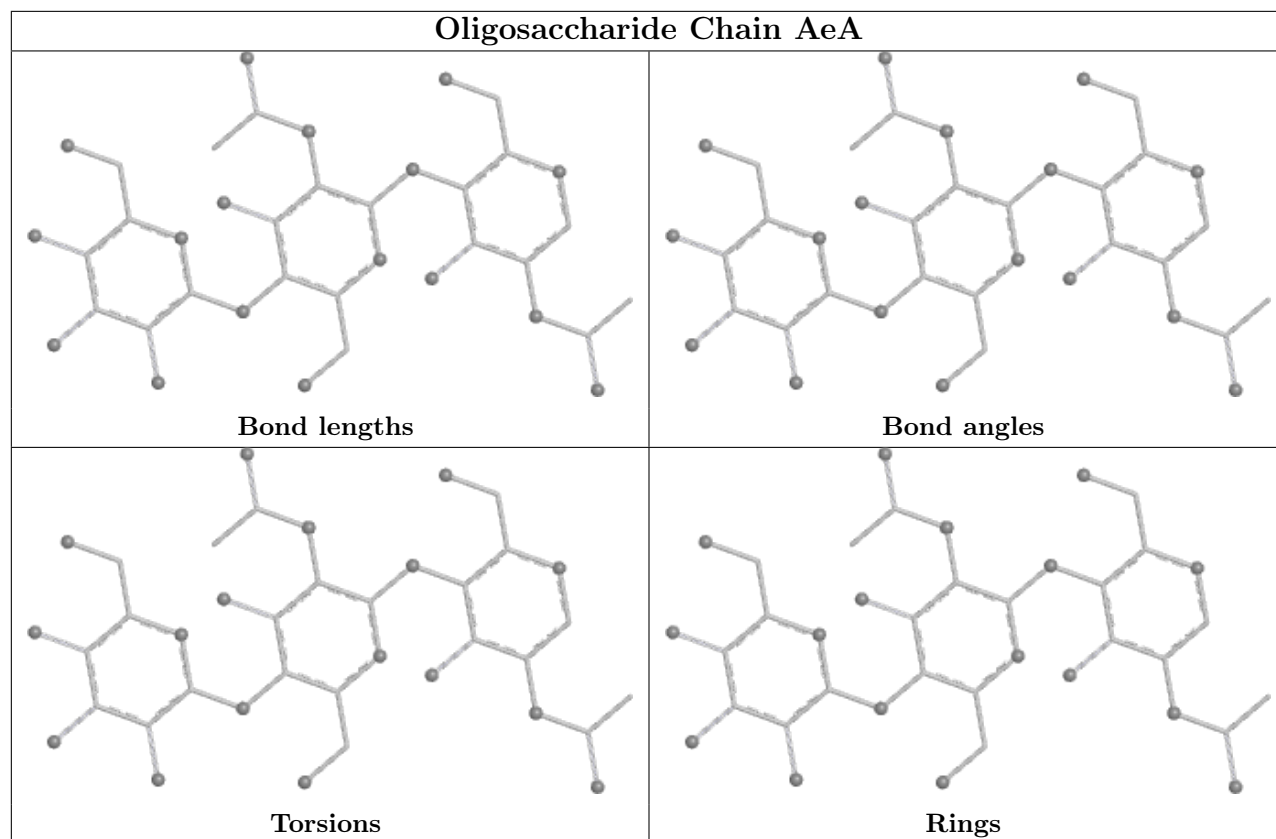
Oligosaccharide Chain DeD











5.6 Ligand geometry

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	$\# Z > 2$
6	NAG	AAA	701	1	14,14,15	0.45	0	17,19,21	1.25	4 (23%)
6	NAG	AAA	702	1	14,14,15	0.43	0	17,19,21	0.78	0
6	NAG	DDD	702	1	14,14,15	0.42	0	17,19,21	1.18	2 (11%)
6	NAG	AAA	703	1	14,14,15	0.37	0	17,19,21	0.79	0
6	NAG	DDD	701	1	14,14,15	0.34	0	17,19,21	0.93	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	AAA	701	1	-	0/6/23/26	0/1/1/1
6	NAG	AAA	702	1	-	2/6/23/26	0/1/1/1
6	NAG	DDD	702	1	-	2/6/23/26	0/1/1/1
6	NAG	AAA	703	1	-	2/6/23/26	0/1/1/1
6	NAG	DDD	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	DDD	702	NAG	O5-C5-C6	3.27	112.33	107.20
6	AAA	701	NAG	C1-O5-C5	2.47	115.53	112.19
6	AAA	701	NAG	O5-C1-C2	-2.17	107.86	111.29
6	AAA	701	NAG	C4-C3-C2	-2.16	107.85	111.02
6	DDD	701	NAG	O5-C5-C6	2.09	110.48	107.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	DDD	702	NAG	O5-C5-C6-O6
6	DDD	702	NAG	C4-C5-C6-O6
6	AAA	703	NAG	C4-C5-C6-O6
6	AAA	703	NAG	O5-C5-C6-O6
6	AAA	702	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.