



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 1SIE / pdb_00001sie
Title : MURINE POLYOMAVIRUS COMPLEXED WITH A DISIALYLATED OLIGOSACCHARIDE
Authors : Stehle, T.; Harrison, S.C.
Deposited on : 1995-12-12
Resolution : 3.65 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 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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

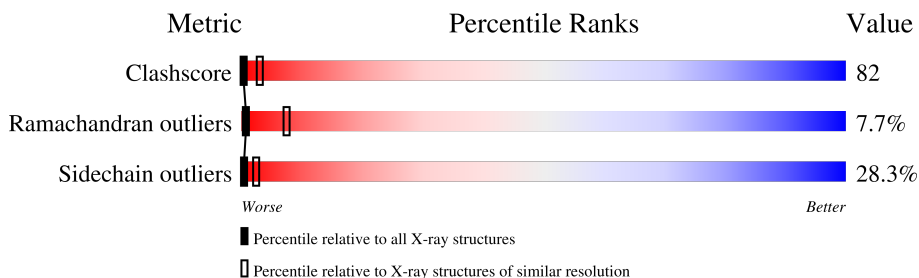
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)

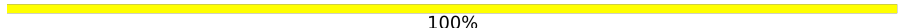


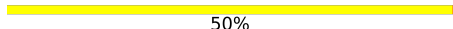
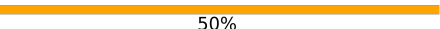
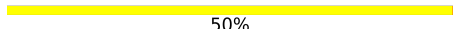
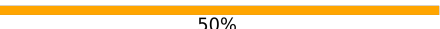
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	13% 46% 27% 9% .
1	B	383	16% 41% 32% 7% .
1	C	383	17% 41% 29% 7% 7%
1	D	383	15% 38% 28% 8% 11%
1	E	383	14% 39% 34% 9% .
1	F	383	15% 40% 27% 10% 8%
2	G	4	50% 50%
2	H	4	50% 50%

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Mol	Chain	Length	Quality of chain
2	I	4	 100%
2	J	4	 75%  25%
2	K	4	 50%  50%
2	L	4	 50%  50%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17141 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.

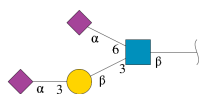
- Molecule 1 is a protein called POLYOMAVIRUS COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	Total 2849	C 1804	N 479	O 550	S 16	0	0	0
1	B	367	Total 2857	C 1808	N 481	O 552	S 16	0	0	0
1	C	357	Total 2784	C 1761	N 468	O 539	S 16	0	0	0
1	D	340	Total 2645	C 1674	N 445	O 511	S 15	0	0	0
1	E	367	Total 2857	C 1808	N 481	O 552	S 16	0	0	0
1	F	354	Total 2753	C 1740	N 461	O 536	S 16	0	0	0

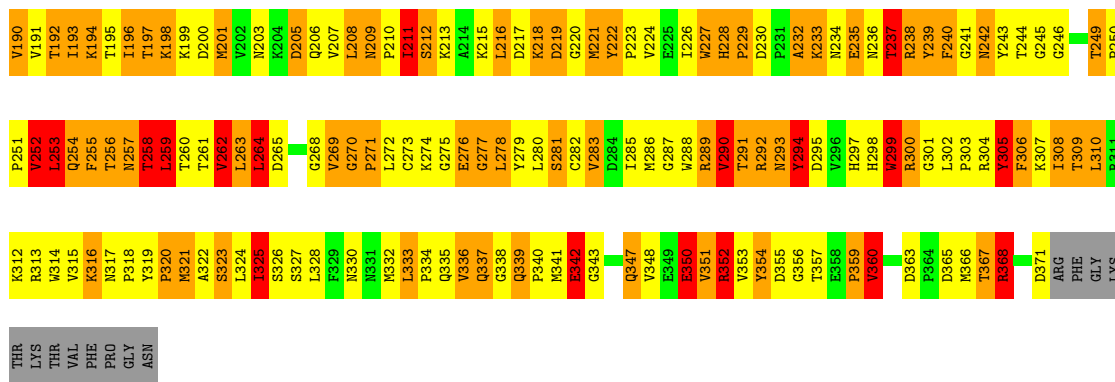
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	SER	conflict	UNP P49302
B	6	ALA	SER	conflict	UNP P49302
C	6	ALA	SER	conflict	UNP P49302
D	6	ALA	SER	conflict	UNP P49302
E	6	ALA	SER	conflict	UNP P49302
F	6	ALA	SER	conflict	UNP P49302

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



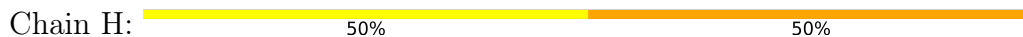
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	H	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	I	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	J	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	K	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	L	4	Total	C	N	O	0	0	0
			66	36	3	27			



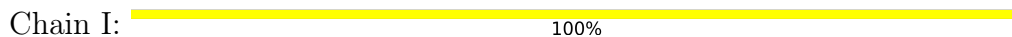
- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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Chain L:  50% 50%

MAG1
GAL2
STIA3
STIA4

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	570.00Å 570.00Å 570.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.65	Depositor
% Data completeness (in resolution range)	74.0 (12.00-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.244 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17141	wwPDB-VP
Average B, all atoms (Å ²)	82.0	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, SIA, GAL

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	1.33	20/2920 (0.7%)	1.83	110/3981 (2.8%)
1	B	1.34	19/2927 (0.6%)	1.83	98/3989 (2.5%)
1	C	1.31	16/2852 (0.6%)	1.83	114/3888 (2.9%)
1	D	1.33	14/2708 (0.5%)	1.87	93/3690 (2.5%)
1	E	1.30	12/2928 (0.4%)	1.87	112/3992 (2.8%)
1	F	1.33	18/2820 (0.6%)	1.85	102/3847 (2.7%)
All	All	1.32	99/17155 (0.6%)	1.85	629/23387 (2.7%)

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	5
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	2
1	F	0	2
All	All	0	18

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	336	VAL	C-N	-10.20	1.19	1.33
1	A	262	VAL	CA-CB	-10.04	1.42	1.54
1	B	130	VAL	CA-C	-8.19	1.43	1.52
1	F	262	VAL	CA-CB	-8.14	1.44	1.54
1	E	262	VAL	CA-CB	-7.90	1.44	1.53

The worst 5 of 629 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	VAL	O-C-N	-23.37	93.36	122.57
1	A	258	THR	N-CA-C	16.91	133.05	111.24
1	E	336	VAL	O-C-N	14.84	139.51	123.03
1	E	256	THR	N-CA-C	14.63	130.56	108.46
1	F	254	GLN	N-CA-C	14.62	129.16	108.54

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	305	TYR	Sidechain
1	A	336	VAL	Peptide,Mainchain
1	A	71	GLN	Mainchain
1	B	162	TYR	Sidechain

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	2849	0	2815	557	1
1	B	2857	0	2820	527	0
1	C	2784	0	2743	454	0
1	D	2645	0	2616	460	0
1	E	2857	0	2821	545	0
1	F	2753	0	2710	477	0
2	G	66	0	56	2	0
2	H	66	0	56	2	0
2	I	66	0	56	0	0
2	J	66	0	56	1	0
2	K	66	0	56	3	0
2	L	66	0	56	5	0
All	All	17141	0	16861	2797	1

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 82.

The worst 5 of 2797 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:336:VAL:CG2	1:A:337:GLN:HA	1.27	1.61
1:A:328:LEU:CD2	1:A:333:LEU:HD21	1.37	1.54
1:A:328:LEU:HD12	1:A:332:MET:CE	1.44	1.44
1:A:336:VAL:HG23	1:A:337:GLN:CA	0.98	1.44
1:A:328:LEU:CD1	1:A:332:MET:HE1	1.42	1.43

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:CD	1:A:328:LEU:O[2_555]	1.11	1.09

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	364/383 (95%)	254 (70%)	75 (21%)	35 (10%)	0	5
1	B	363/383 (95%)	278 (77%)	62 (17%)	23 (6%)	1	11
1	C	353/383 (92%)	279 (79%)	55 (16%)	19 (5%)	1	13
1	D	336/383 (88%)	257 (76%)	56 (17%)	23 (7%)	1	10
1	E	365/383 (95%)	264 (72%)	67 (18%)	34 (9%)	0	5
1	F	350/383 (91%)	263 (75%)	57 (16%)	30 (9%)	0	6
All	All	2131/2298 (93%)	1595 (75%)	372 (18%)	164 (8%)	1	7

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO

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Mol	Chain	Res	Type
1	A	148	VAL
1	A	183	THR
1	A	276	GLU
1	A	293	ASN

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 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	321/335 (96%)	235 (73%)	86 (27%)	0	3
1	B	322/335 (96%)	230 (71%)	92 (29%)	0	2
1	C	314/335 (94%)	231 (74%)	83 (26%)	0	3
1	D	298/335 (89%)	199 (67%)	99 (33%)	0	1
1	E	322/335 (96%)	230 (71%)	92 (29%)	0	2
1	F	311/335 (93%)	228 (73%)	83 (27%)	0	3
All	All	1888/2010 (94%)	1353 (72%)	535 (28%)	0	2

5 of 535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	79	ILE
1	F	135	LEU
1	F	77	ARG
1	F	330	ASN
1	C	99	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	139	HIS
1	F	142	ASN
1	E	206	GLN
1	E	339	GLN

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Mol	Chain	Res	Type
1	F	331	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](#)

24 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	G	1	2	15,15,15	1.35	1 (6%)	21,21,21	1.52	4 (19%)
2	GAL	G	2	2	11,11,12	0.47	0	15,15,17	1.30	1 (6%)
2	SIA	G	3	2	20,20,21	1.19	2 (10%)	21,28,31	0.92	1 (4%)
2	SIA	G	4	2	20,20,21	1.65	4 (20%)	21,28,31	1.06	1 (4%)
2	NAG	H	1	2	15,15,15	1.65	2 (13%)	21,21,21	2.15	5 (23%)
2	GAL	H	2	2	11,11,12	0.45	0	15,15,17	1.48	1 (6%)
2	SIA	H	3	2	20,20,21	1.02	2 (10%)	21,28,31	1.10	2 (9%)
2	SIA	H	4	2	20,20,21	1.85	5 (25%)	21,28,31	0.97	1 (4%)
2	NAG	I	1	2	15,15,15	1.49	1 (6%)	21,21,21	1.90	5 (23%)
2	GAL	I	2	2	11,11,12	0.39	0	15,15,17	1.18	1 (6%)
2	SIA	I	3	2	20,20,21	0.76	0	21,28,31	1.00	2 (9%)
2	SIA	I	4	2	20,20,21	1.72	4 (20%)	21,28,31	1.00	1 (4%)
2	NAG	J	1	2	15,15,15	0.87	1 (6%)	21,21,21	0.90	1 (4%)
2	GAL	J	2	2	11,11,12	0.48	0	15,15,17	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	J	3	2	20,20,21	1.28	3 (15%)	21,28,31	1.15	3 (14%)
2	SIA	J	4	2	20,20,21	1.73	5 (25%)	21,28,31	0.84	1 (4%)
2	NAG	K	1	2	15,15,15	1.78	1 (6%)	21,21,21	2.37	5 (23%)
2	GAL	K	2	2	11,11,12	0.30	0	15,15,17	1.47	1 (6%)
2	SIA	K	3	2	20,20,21	0.75	0	21,28,31	1.11	1 (4%)
2	SIA	K	4	2	20,20,21	1.88	5 (25%)	21,28,31	0.87	1 (4%)
2	NAG	L	1	2	15,15,15	1.52	2 (13%)	21,21,21	1.79	4 (19%)
2	GAL	L	2	2	11,11,12	0.40	0	15,15,17	1.68	1 (6%)
2	SIA	L	3	2	20,20,21	0.97	2 (10%)	21,28,31	1.00	1 (4%)
2	SIA	L	4	2	20,20,21	1.79	4 (20%)	21,28,31	0.95	1 (4%)

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	G	1	2	-	2/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	5/18/34/38	0/1/1/1
2	SIA	G	4	2	-	1/18/34/38	0/1/1/1
2	NAG	H	1	2	-	2/6/26/26	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	SIA	H	3	2	-	6/18/34/38	0/1/1/1
2	SIA	H	4	2	-	2/18/34/38	0/1/1/1
2	NAG	I	1	2	-	2/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	1/18/34/38	0/1/1/1
2	SIA	I	4	2	-	1/18/34/38	0/1/1/1
2	NAG	J	1	2	-	4/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	4/18/34/38	0/1/1/1
2	SIA	J	4	2	-	1/18/34/38	0/1/1/1
2	NAG	K	1	2	-	2/6/26/26	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	SIA	K	3	2	-	5/18/34/38	0/1/1/1
2	SIA	K	4	2	-	3/18/34/38	0/1/1/1
2	NAG	L	1	2	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1
2	SIA	L	3	2	-	5/18/34/38	0/1/1/1
2	SIA	L	4	2	-	0/18/34/38	0/1/1/1

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C1-C2	6.03	1.60	1.52
2	H	1	NAG	C1-C2	5.33	1.59	1.52
2	I	1	NAG	C1-C2	5.01	1.58	1.52
2	L	1	NAG	C1-C2	4.97	1.58	1.52
2	I	4	SIA	C2-C1	4.50	1.57	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	O5-C1-C2	6.79	116.34	109.52
2	H	1	NAG	O5-C1-C2	5.82	115.36	109.52
2	L	2	GAL	C1-C2-C3	-5.68	101.38	109.64
2	K	1	NAG	C3-C4-C5	-5.57	100.13	110.23
2	H	2	GAL	C1-C2-C3	-5.25	102.00	109.64

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	SIA	O7-C7-C8-C9
2	H	3	SIA	C5-C6-C7-O7
2	H	3	SIA	O6-C6-C7-O7
2	H	4	SIA	C7-C8-C9-O9
2	H	4	SIA	O8-C8-C9-O9

There are no ring outliers.

9 monomers are involved in 13 short contacts:

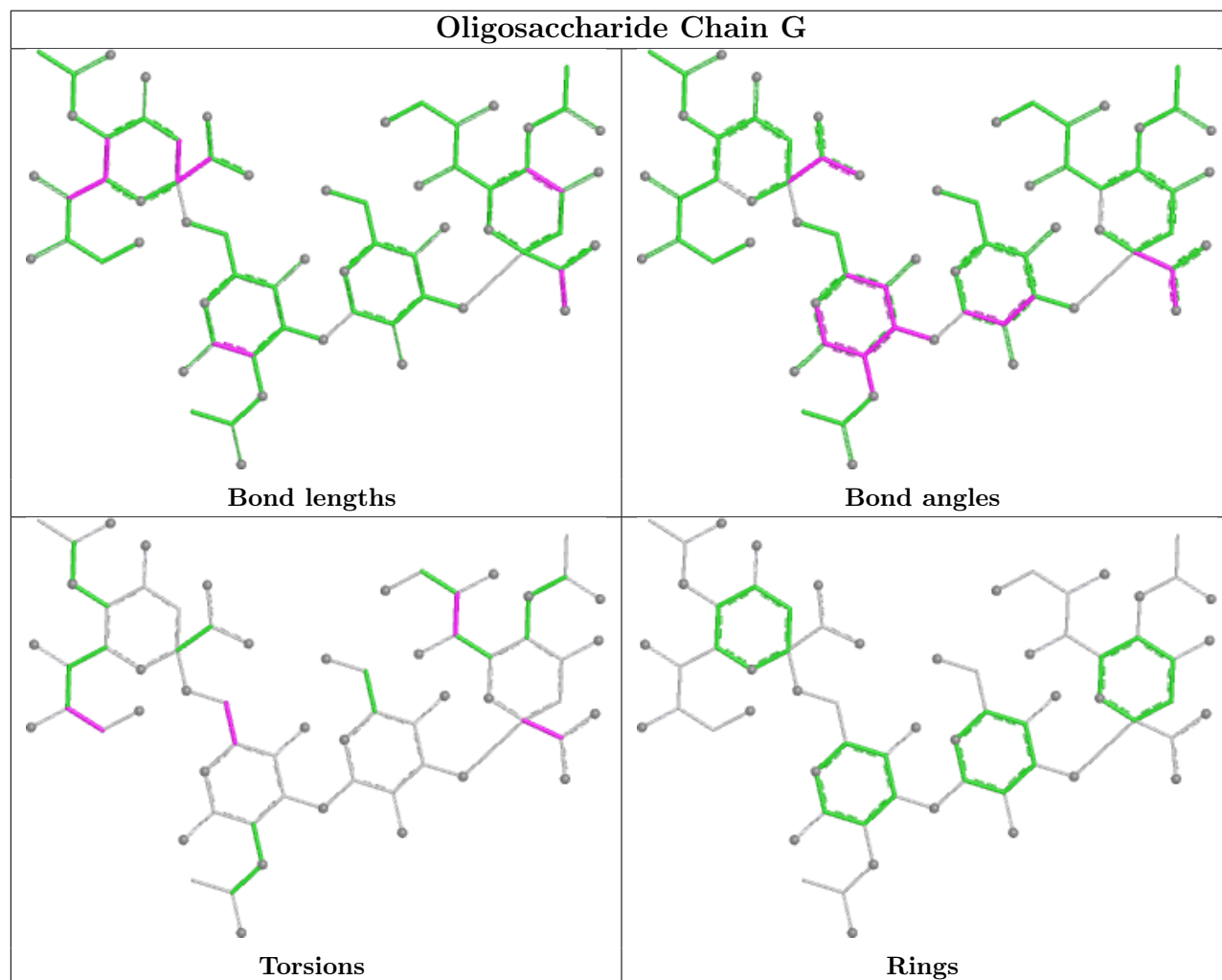
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	SIA	2	0
2	K	2	GAL	3	0
2	J	3	SIA	1	0
2	G	2	GAL	2	0
2	L	2	GAL	4	0

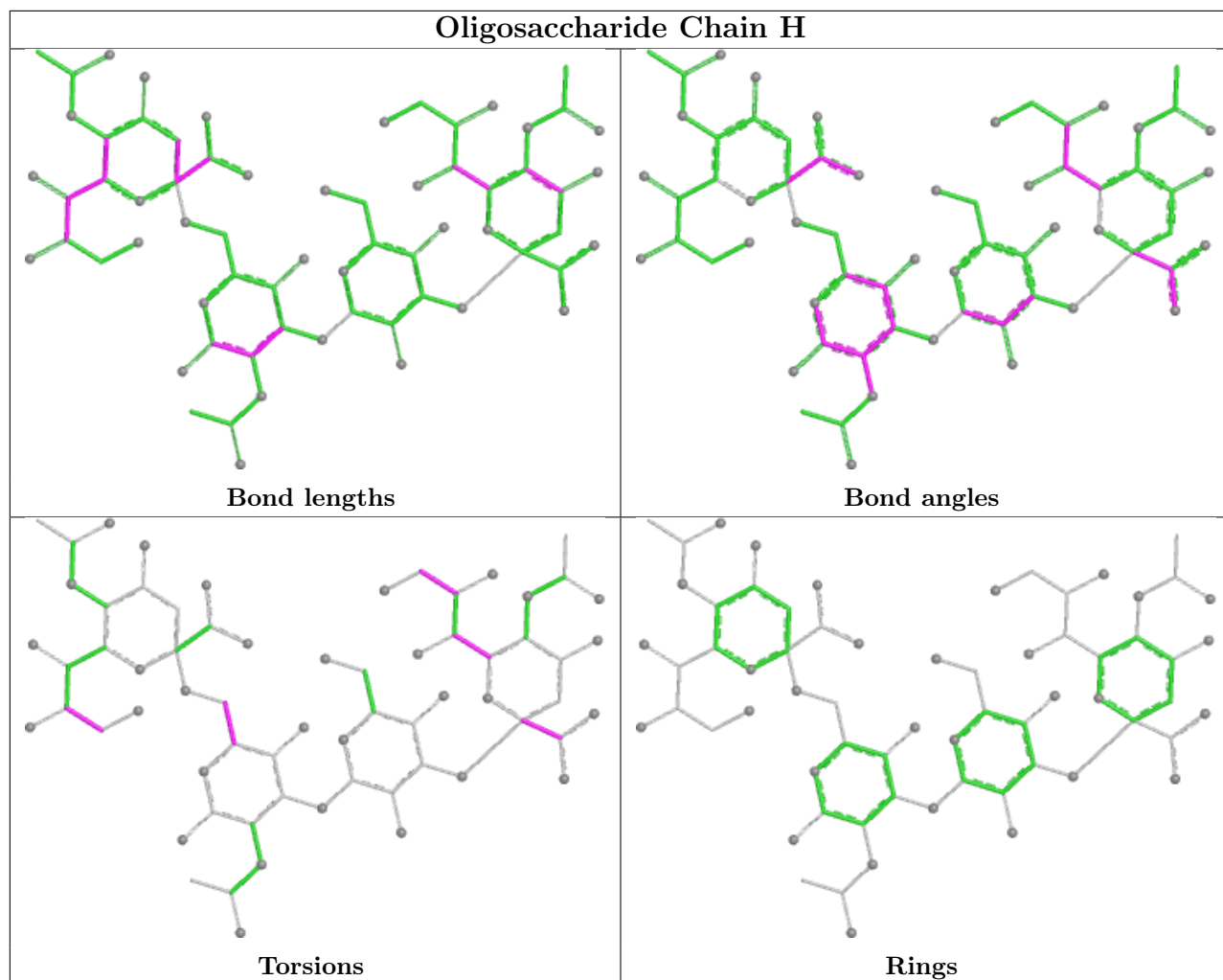
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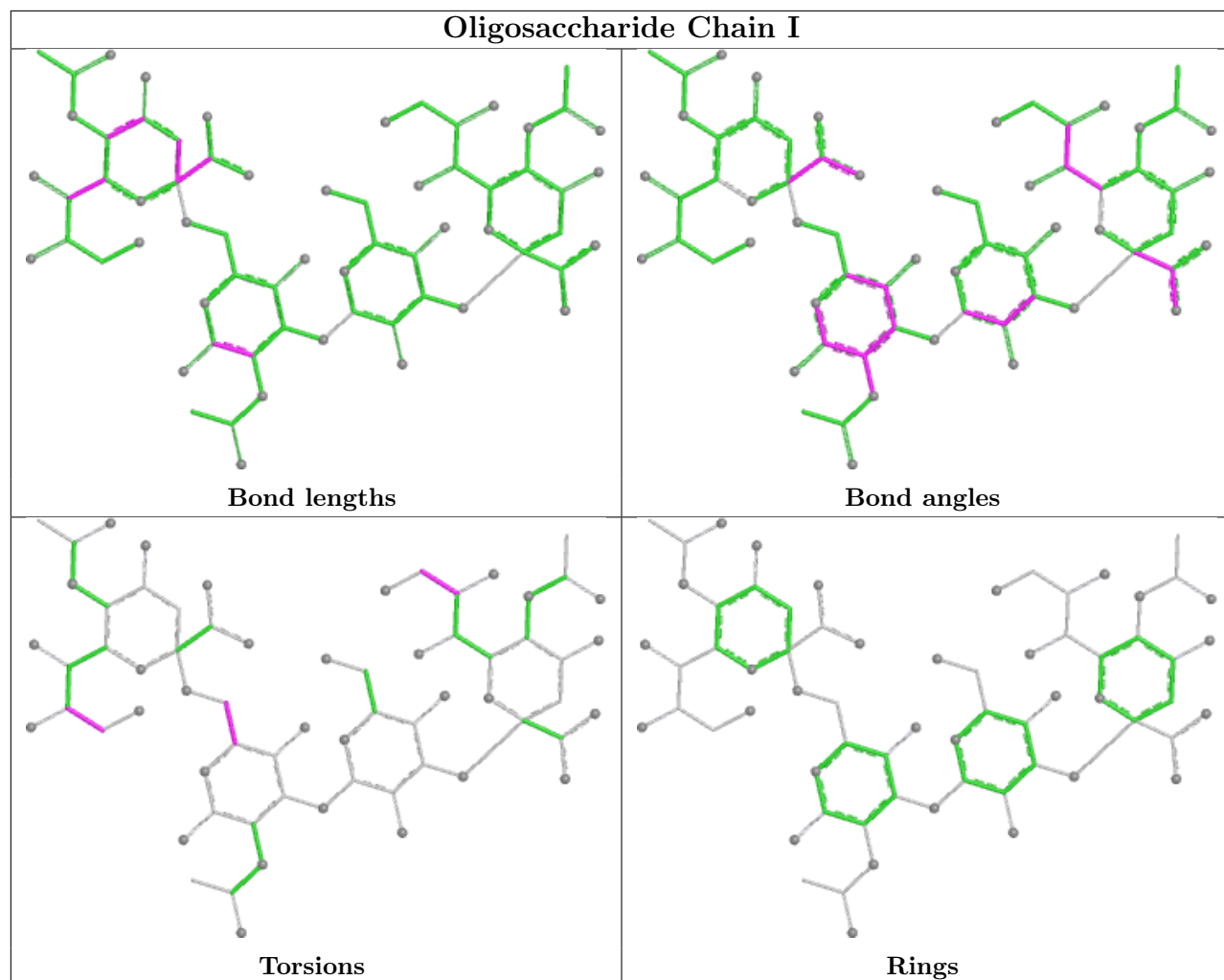
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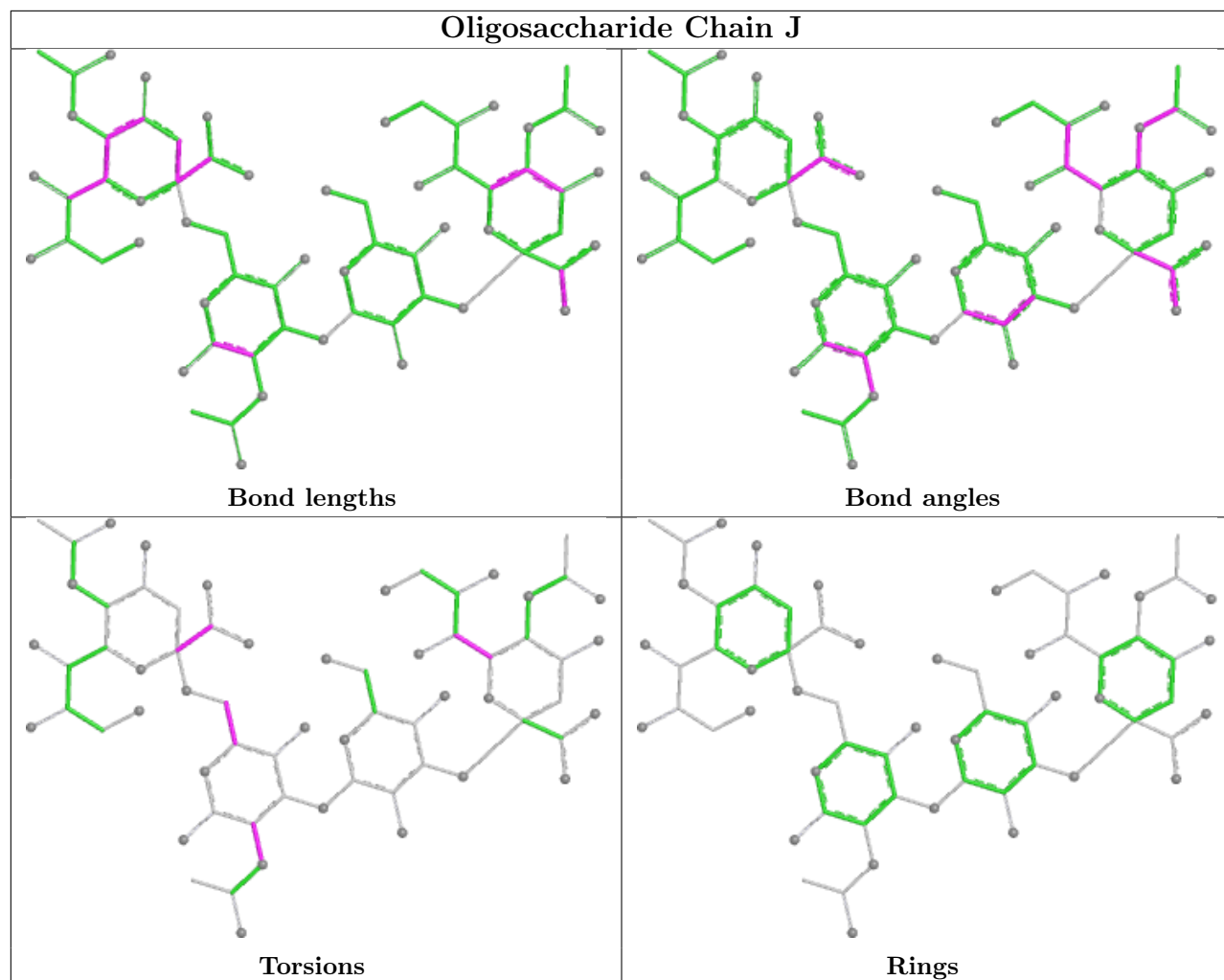
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	3	SIA	1	0
2	H	2	GAL	1	0
2	G	3	SIA	1	0
2	L	3	SIA	2	0

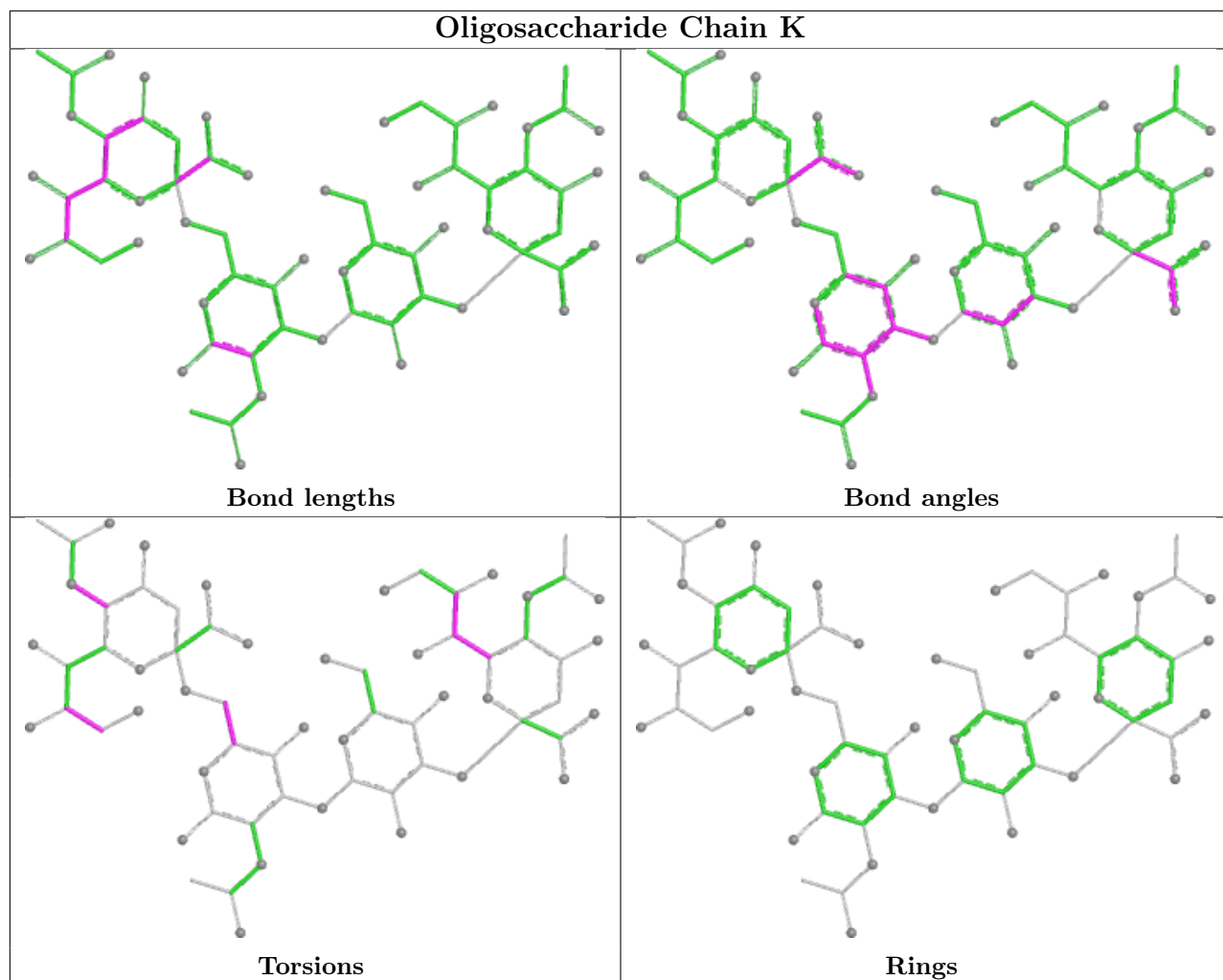
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

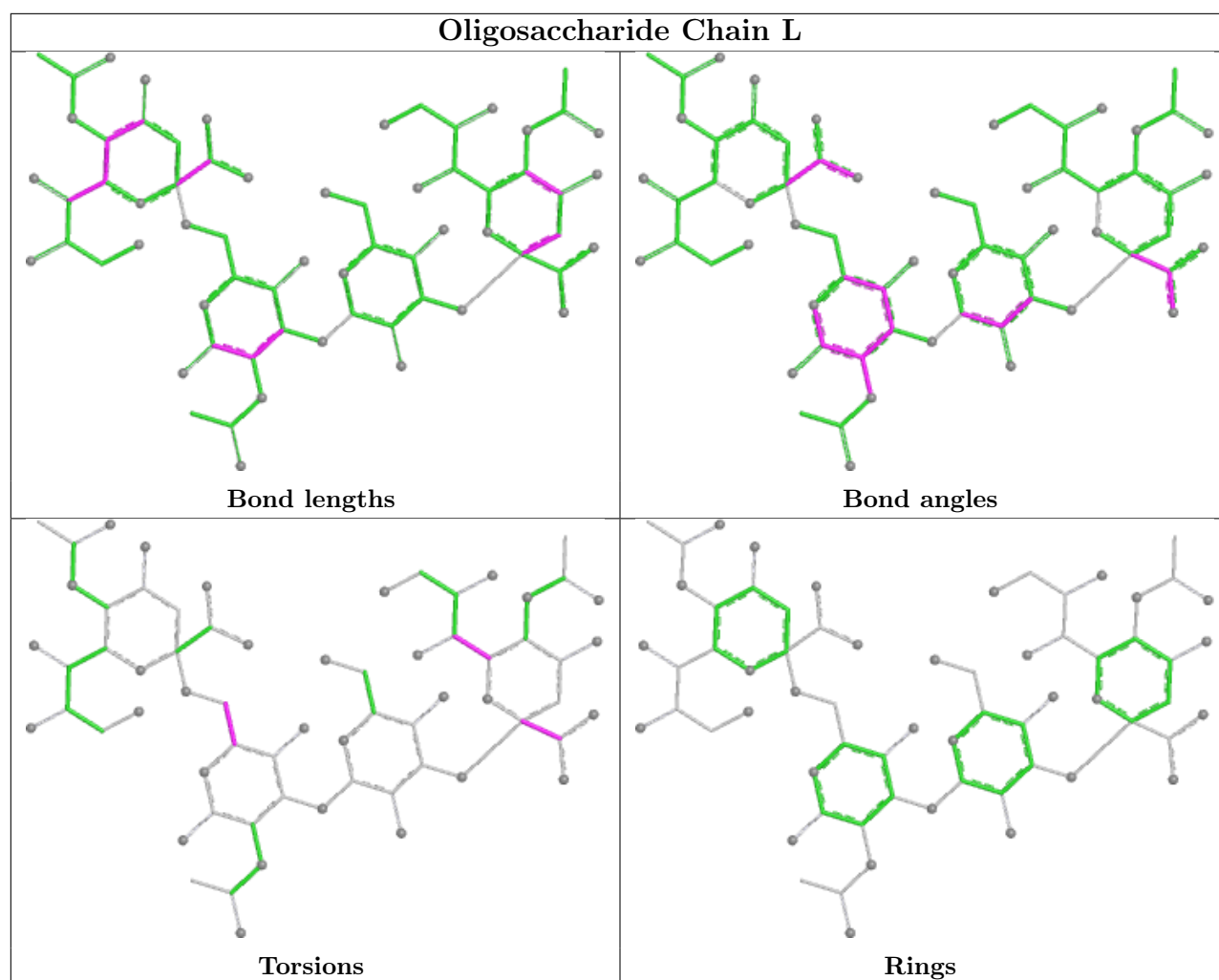












5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	F	1
1	C	1

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Mol	Chain	Number of breaks
1	B	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	336:VAL	C	337:GLN	N	4.77
1	F	336:VAL	C	337:GLN	N	4.21
1	C	336:VAL	C	337:GLN	N	3.33
1	B	336:VAL	C	337:GLN	N	3.13
1	E	336:VAL	C	337:GLN	N	1.19

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.