



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 04:22 AM EDT

PDB ID : 3MUU
Title : Crystal structure of the Sindbis virus E2-E1 heterodimer at low pH
Authors : Li, L.; Jose, J.; Xiang, Y.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : 2010-05-03
Resolution : 3.29 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

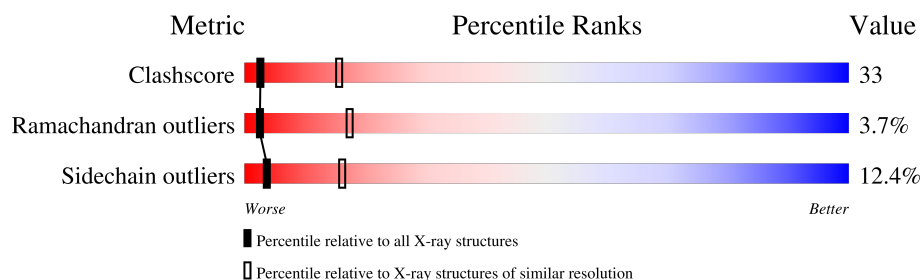
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)




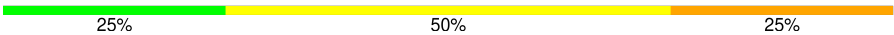

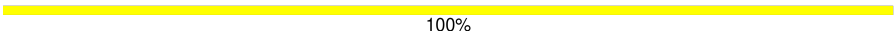

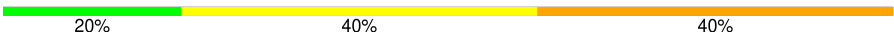


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	A	750	39% 36% 7% 17%
1	B	750	37% 38% 7% 17%
1	C	750	38% 37% 7% 17%
1	D	750	39% 36% 8% 17%
1	E	750	40% 35% 7% 17%
1	F	750	39% 36% 7% 18%
2	G	4	25% 75%
2	I	4	25% 75%

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Mol	Chain	Length	Quality of chain
2	J	4	
2	K	4	
2	L	4	
2	M	4	
2	O	4	
2	Q	4	
3	H	5	
3	P	5	
3	R	5	
4	N	3	

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	G	1	X	-	-	-
2	NAG	Q	1	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29159 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 Structural polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	Se	0	0	0
			4767	3015	808	910	24	10			
1	B	622	Total	C	N	O	S	Se	0	0	0
			4761	3013	808	906	24	10			
1	C	622	Total	C	N	O	S	Se	0	0	0
			4761	3012	807	908	24	10			
1	D	622	Total	C	N	O	S	Se	0	0	0
			4760	3009	807	910	24	10			
1	E	623	Total	C	N	O	S	Se	0	0	0
			4761	3012	808	907	24	10			
1	F	618	Total	C	N	O	S	Se	0	0	0
			4727	2990	801	902	24	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	GLY	-	linker	UNP P03316
A	346	GLY	-	linker	UNP P03316
A	347	GLY	-	linker	UNP P03316
A	348	SER	-	linker	UNP P03316
A	349	TRP	-	linker	UNP P03316
A	350	SER	-	linker	UNP P03316
A	351	HIS	-	linker	UNP P03316
A	352	PRO	-	linker	UNP P03316
A	353	GLN	-	linker	UNP P03316
A	354	PHE	-	linker	UNP P03316
A	355	GLU	-	linker	UNP P03316
A	356	LYS	-	linker	UNP P03316
A	357	GLY	-	linker	UNP P03316
A	358	GLY	-	linker	UNP P03316
A	359	GLY	-	linker	UNP P03316
A	360	GLY	-	linker	UNP P03316
A	435	GLY	ASP	engineered mutation	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	GLY	-	linker	UNP P03316
B	346	GLY	-	linker	UNP P03316
B	347	GLY	-	linker	UNP P03316
B	348	SER	-	linker	UNP P03316
B	349	TRP	-	linker	UNP P03316
B	350	SER	-	linker	UNP P03316
B	351	HIS	-	linker	UNP P03316
B	352	PRO	-	linker	UNP P03316
B	353	GLN	-	linker	UNP P03316
B	354	PHE	-	linker	UNP P03316
B	355	GLU	-	linker	UNP P03316
B	356	LYS	-	linker	UNP P03316
B	357	GLY	-	linker	UNP P03316
B	358	GLY	-	linker	UNP P03316
B	359	GLY	-	linker	UNP P03316
B	360	GLY	-	linker	UNP P03316
B	435	GLY	ASP	engineered mutation	UNP P03316
C	345	GLY	-	linker	UNP P03316
C	346	GLY	-	linker	UNP P03316
C	347	GLY	-	linker	UNP P03316
C	348	SER	-	linker	UNP P03316
C	349	TRP	-	linker	UNP P03316
C	350	SER	-	linker	UNP P03316
C	351	HIS	-	linker	UNP P03316
C	352	PRO	-	linker	UNP P03316
C	353	GLN	-	linker	UNP P03316
C	354	PHE	-	linker	UNP P03316
C	355	GLU	-	linker	UNP P03316
C	356	LYS	-	linker	UNP P03316
C	357	GLY	-	linker	UNP P03316
C	358	GLY	-	linker	UNP P03316
C	359	GLY	-	linker	UNP P03316
C	360	GLY	-	linker	UNP P03316
C	435	GLY	ASP	engineered mutation	UNP P03316
D	345	GLY	-	linker	UNP P03316
D	346	GLY	-	linker	UNP P03316
D	347	GLY	-	linker	UNP P03316
D	348	SER	-	linker	UNP P03316
D	349	TRP	-	linker	UNP P03316
D	350	SER	-	linker	UNP P03316
D	351	HIS	-	linker	UNP P03316
D	352	PRO	-	linker	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
D	353	GLN	-	linker	UNP P03316
D	354	PHE	-	linker	UNP P03316
D	355	GLU	-	linker	UNP P03316
D	356	LYS	-	linker	UNP P03316
D	357	GLY	-	linker	UNP P03316
D	358	GLY	-	linker	UNP P03316
D	359	GLY	-	linker	UNP P03316
D	360	GLY	-	linker	UNP P03316
D	435	GLY	ASP	engineered mutation	UNP P03316
E	345	GLY	-	linker	UNP P03316
E	346	GLY	-	linker	UNP P03316
E	347	GLY	-	linker	UNP P03316
E	348	SER	-	linker	UNP P03316
E	349	TRP	-	linker	UNP P03316
E	350	SER	-	linker	UNP P03316
E	351	HIS	-	linker	UNP P03316
E	352	PRO	-	linker	UNP P03316
E	353	GLN	-	linker	UNP P03316
E	354	PHE	-	linker	UNP P03316
E	355	GLU	-	linker	UNP P03316
E	356	LYS	-	linker	UNP P03316
E	357	GLY	-	linker	UNP P03316
E	358	GLY	-	linker	UNP P03316
E	359	GLY	-	linker	UNP P03316
E	360	GLY	-	linker	UNP P03316
E	435	GLY	ASP	engineered mutation	UNP P03316
F	345	GLY	-	linker	UNP P03316
F	346	GLY	-	linker	UNP P03316
F	347	GLY	-	linker	UNP P03316
F	348	SER	-	linker	UNP P03316
F	349	TRP	-	linker	UNP P03316
F	350	SER	-	linker	UNP P03316
F	351	HIS	-	linker	UNP P03316
F	352	PRO	-	linker	UNP P03316
F	353	GLN	-	linker	UNP P03316
F	354	PHE	-	linker	UNP P03316
F	355	GLU	-	linker	UNP P03316
F	356	LYS	-	linker	UNP P03316
F	357	GLY	-	linker	UNP P03316
F	358	GLY	-	linker	UNP P03316
F	359	GLY	-	linker	UNP P03316
F	360	GLY	-	linker	UNP P03316

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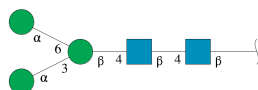
Chain	Residue	Modelled	Actual	Comment	Reference
F	435	GLY	ASP	engineered mutation	UNP P03316

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	L	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



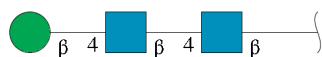
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 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.



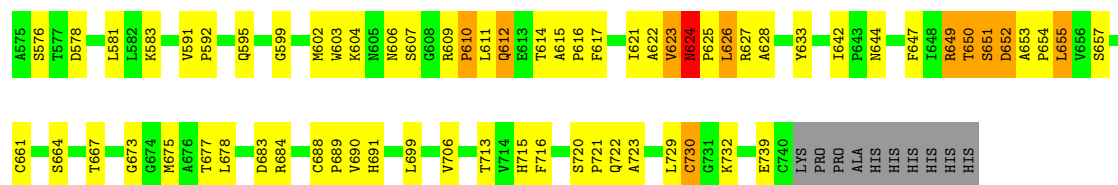
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

Response	Percentage
Yes, the U.S. should take action to protect the environment	37%
No, the U.S. should focus on the economy	38%
Both	7%
Don't know	17%

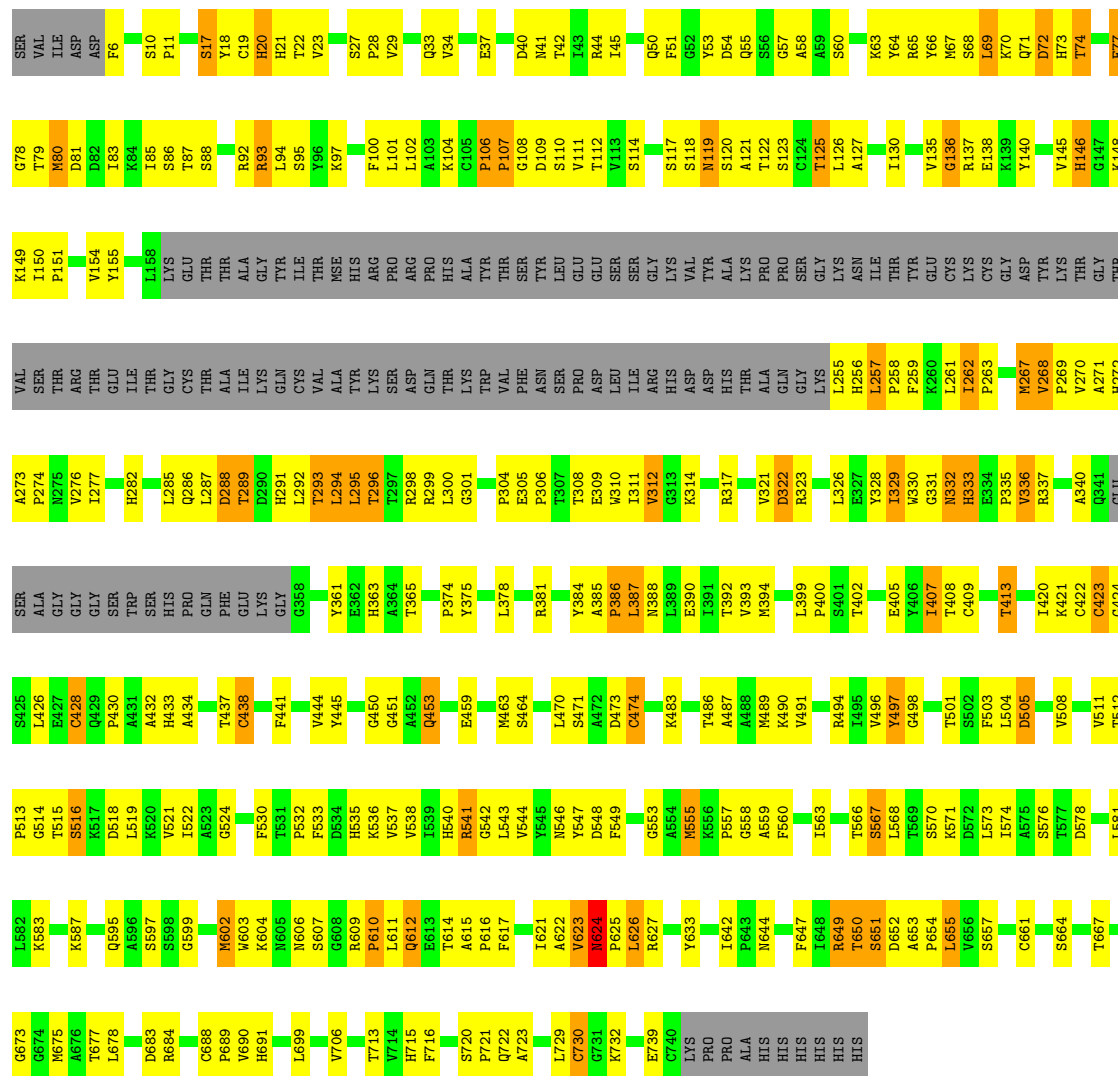


Response	Percentage
Doing a good job	38%
Not doing a good job	37%
Don't know	7%
Refuse to answer	1%
Other	17%

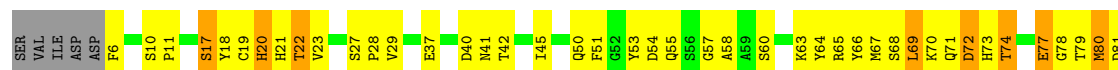


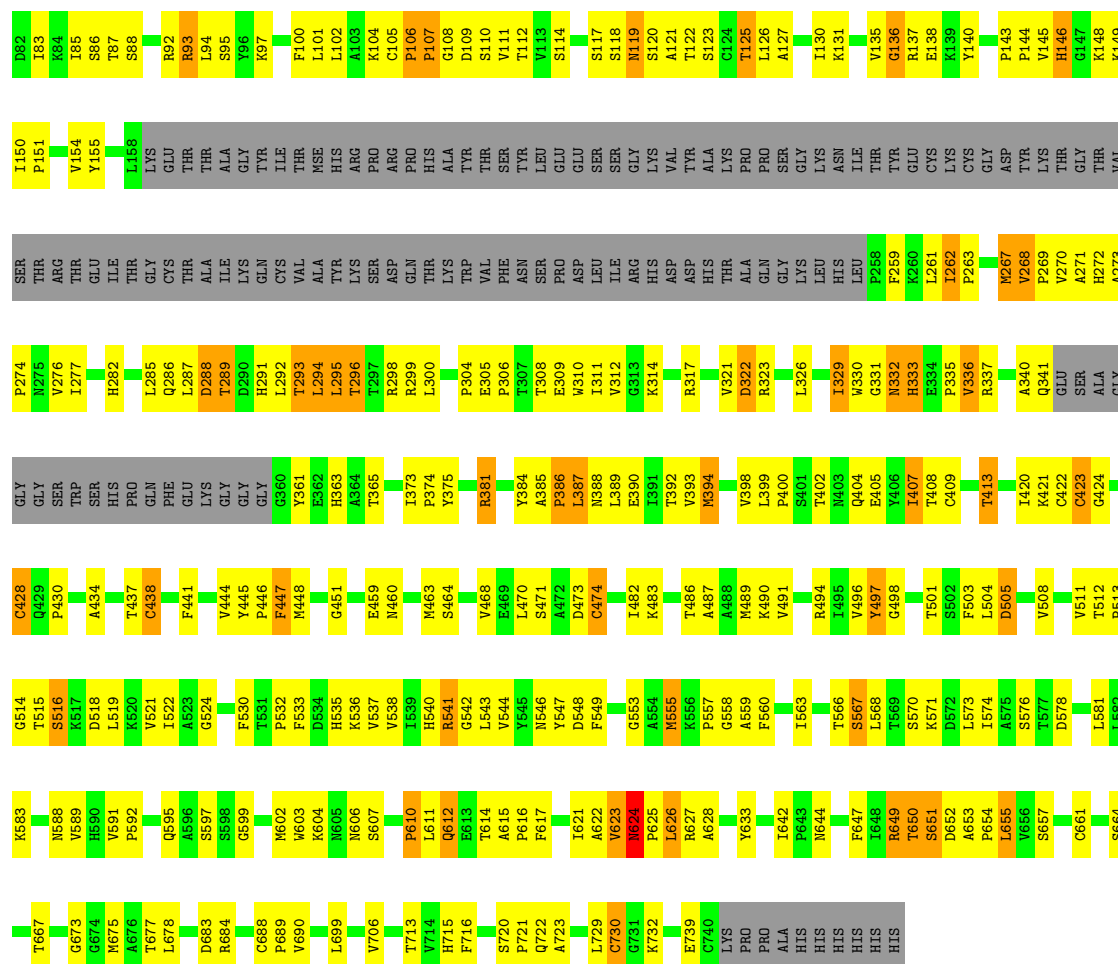


• Molecule 1: Structural polypeptide



• Molecule 1: Structural polypeptide





- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

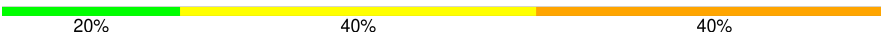


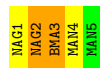
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



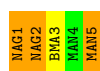
- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain P: 



- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain R: 



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

Chain N: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.48Å 158.43Å 160.68Å 60.42° 89.80° 89.65°	Depositor
Resolution (Å)	60.72 – 3.29	Depositor
% Data completeness (in resolution range)	92.4 (60.72-3.29)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.239 , 0.252	Depositor
Wilson B-factor (Å ²)	87.2	Xtriage
Anisotropy	0.703	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,k-l,k 0.033 for h,l,-k+l 0.297 for h,-l,k-l 0.297 for h,-k+l,-k 0.037 for h,-k,-l 0.408 for -h,k,k-l 0.289 for -h,-l,-k 0.033 for -h,k-l,-l 0.309 for -h,-k+l,l 0.039 for -h,-k,-k+l 0.033 for -h,l,k	Xtriage
Total number of atoms	29159	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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: BMA, NAG, MAN

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	0.35	0/4876	0.58	0/6624
1	B	0.35	0/4870	0.60	1/6615 (0.0%)
1	C	0.38	1/4870 (0.0%)	0.60	1/6617 (0.0%)
1	D	0.35	0/4869	0.58	0/6615
1	E	0.35	0/4870	0.58	0/6616
1	F	0.36	0/4835	0.67	3/6568 (0.0%)
All	All	0.36	1/29190 (0.0%)	0.60	5/39655 (0.0%)

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	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	653	ALA	C-N	7.00	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	381	ARG	NE-CZ-NH1	-19.90	110.35	120.30
1	F	381	ARG	NE-CZ-NH2	17.34	128.97	120.30
1	B	94	LEU	CA-CB-CG	-7.54	97.95	115.30
1	F	381	ARG	CD-NE-CZ	7.40	133.97	123.60
1	C	255	LEU	CB-CG-CD2	5.25	119.92	111.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	VAL	Peptide
1	A	624	ASN	Peptide
1	B	254	LYS	Peptide
1	B	623	VAL	Peptide
1	B	624	ASN	Peptide

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	4767	0	4659	316	0
1	B	4761	0	4661	335	0
1	C	4761	0	4651	329	0
1	D	4760	0	4645	320	0
1	E	4761	0	4653	311	0
1	F	4727	0	4619	304	0
2	G	50	0	42	2	0
2	I	50	0	43	0	0
2	J	50	0	43	2	0
2	K	50	0	42	2	0
2	L	50	0	43	2	0
2	M	50	0	42	1	0
2	O	50	0	42	0	0
2	Q	50	0	43	0	0
3	H	61	0	52	3	0
3	P	61	0	52	2	0
3	R	61	0	52	6	0
4	N	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29159	0	28418	1903	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 33.

The worst 5 of 1903 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:D:22:THR:HG21	1:E:104:LYS:HD2	1.29	1.14
1:B:507:TYR:CE1	1:D:625:PRO:HG2	1.88	1.09
1:D:88:SER:HB3	1:D:107:PRO:HG3	1.10	1.09
1:B:255:LEU:HG	1:B:256:HIS:H	1.14	1.08
1:B:88:SER:HB3	1:B:107:PRO:HG3	1.09	1.08

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	617/750 (82%)	501 (81%)	92 (15%)	24 (4%)	2	16
1	B	616/750 (82%)	499 (81%)	96 (16%)	21 (3%)	3	19
1	C	616/750 (82%)	500 (81%)	92 (15%)	24 (4%)	2	16
1	D	616/750 (82%)	502 (82%)	92 (15%)	22 (4%)	3	18
1	E	617/750 (82%)	505 (82%)	90 (15%)	22 (4%)	3	18
1	F	612/750 (82%)	503 (82%)	87 (14%)	22 (4%)	3	18
All	All	3694/4500 (82%)	3010 (82%)	549 (15%)	135 (4%)	2	17

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	117	SER
1	A	434	ALA
1	A	650	THR
1	A	730	CYS

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	534/630 (85%)	468 (88%)	66 (12%)	4	16
1	B	533/630 (85%)	466 (87%)	67 (13%)	3	16
1	C	533/630 (85%)	466 (87%)	67 (13%)	3	16
1	D	533/630 (85%)	469 (88%)	64 (12%)	4	17
1	E	532/630 (84%)	466 (88%)	66 (12%)	4	16
1	F	529/630 (84%)	464 (88%)	65 (12%)	4	16
All	All	3194/3780 (84%)	2799 (88%)	395 (12%)	4	16

5 of 395 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	387	LEU
1	E	293	THR
1	D	428	CYS
1	D	649	ARG
1	E	407	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	62	ASN
1	F	146	HIS
1	E	291	HIS
1	E	612	GLN

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Mol	Chain	Res	Type
1	F	540	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 ⓘ

50 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	2,1	14,14,15	0.41	0	17,19,21	2.09	2 (11%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	2.05	5 (29%)
2	BMA	G	3	2	11,11,12	1.71	2 (18%)	15,15,17	4.14	10 (66%)
2	MAN	G	4	2	11,11,12	0.89	1 (9%)	15,15,17	2.00	4 (26%)
3	NAG	H	1	1,3	14,14,15	0.71	0	17,19,21	1.35	2 (11%)
3	NAG	H	2	3	14,14,15	0.48	0	17,19,21	1.15	1 (5%)
3	BMA	H	3	3	11,11,12	2.11	4 (36%)	15,15,17	3.03	9 (60%)
3	MAN	H	4	3	11,11,12	0.41	0	15,15,17	1.54	2 (13%)
3	MAN	H	5	3	11,11,12	0.50	0	15,15,17	1.40	1 (6%)
2	NAG	I	1	2,1	14,14,15	0.76	0	17,19,21	1.01	0
2	NAG	I	2	2	14,14,15	0.83	0	17,19,21	1.96	3 (17%)
2	BMA	I	3	2	11,11,12	2.20	5 (45%)	15,15,17	2.89	7 (46%)
2	MAN	I	4	2	11,11,12	0.52	0	15,15,17	1.05	1 (6%)
2	NAG	J	1	2,1	14,14,15	0.55	0	17,19,21	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	2	2	14,14,15	0.59	0	17,19,21	1.53	3 (17%)
2	BMA	J	3	2	11,11,12	1.82	3 (27%)	15,15,17	3.54	9 (60%)
2	MAN	J	4	2	11,11,12	0.61	0	15,15,17	0.69	0
2	NAG	K	1	2,1	14,14,15	0.69	0	17,19,21	1.18	1 (5%)
2	NAG	K	2	2	14,14,15	0.63	0	17,19,21	1.00	2 (11%)
2	BMA	K	3	2	11,11,12	2.04	4 (36%)	15,15,17	3.66	10 (66%)
2	MAN	K	4	2	11,11,12	0.77	1 (9%)	15,15,17	1.79	5 (33%)
2	NAG	L	1	2,1	14,14,15	0.46	0	17,19,21	1.97	4 (23%)
2	NAG	L	2	2	14,14,15	0.49	0	17,19,21	2.90	5 (29%)
2	BMA	L	3	2	11,11,12	1.82	3 (27%)	15,15,17	3.30	8 (53%)
2	MAN	L	4	2	11,11,12	0.44	0	15,15,17	1.71	1 (6%)
2	NAG	M	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	2.21	6 (35%)
2	NAG	M	2	2	14,14,15	0.58	0	17,19,21	1.67	4 (23%)
2	BMA	M	3	2	11,11,12	1.89	4 (36%)	15,15,17	3.29	12 (80%)
2	MAN	M	4	2	11,11,12	0.55	0	15,15,17	0.91	0
4	NAG	N	1	1,4	14,14,15	0.39	0	17,19,21	2.14	2 (11%)
4	NAG	N	2	4	14,14,15	0.52	0	17,19,21	1.25	2 (11%)
4	BMA	N	3	4	11,11,12	2.00	4 (36%)	15,15,17	3.29	9 (60%)
2	NAG	O	1	2,1	14,14,15	0.62	0	17,19,21	0.85	0
2	NAG	O	2	2	14,14,15	0.67	0	17,19,21	1.88	4 (23%)
2	BMA	O	3	2	11,11,12	1.95	4 (36%)	15,15,17	3.65	10 (66%)
2	MAN	O	4	2	11,11,12	0.65	0	15,15,17	0.63	0
3	NAG	P	1	1,3	14,14,15	0.52	0	17,19,21	2.22	4 (23%)
3	NAG	P	2	3	14,14,15	0.66	1 (7%)	17,19,21	2.53	5 (29%)
3	BMA	P	3	3	11,11,12	1.81	3 (27%)	15,15,17	3.74	8 (53%)
3	MAN	P	4	3	11,11,12	0.57	0	15,15,17	1.07	1 (6%)
3	MAN	P	5	3	11,11,12	0.61	0	15,15,17	0.50	0
2	NAG	Q	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	1.83	2 (11%)
2	NAG	Q	2	2	14,14,15	0.48	0	17,19,21	3.23	5 (29%)
2	BMA	Q	3	2	11,11,12	2.05	4 (36%)	15,15,17	4.14	10 (66%)
2	MAN	Q	4	2	11,11,12	0.51	0	15,15,17	1.33	2 (13%)
3	NAG	R	1	1,3	14,14,15	0.43	0	17,19,21	1.94	3 (17%)
3	NAG	R	2	3	14,14,15	0.45	0	17,19,21	2.23	3 (17%)
3	BMA	R	3	3	11,11,12	2.09	4 (36%)	15,15,17	1.99	6 (40%)
3	MAN	R	4	3	11,11,12	0.60	0	15,15,17	0.60	0
3	MAN	R	5	3	11,11,12	0.46	0	15,15,17	1.51	4 (26%)

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	2,1	1/1/5/7	6/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	1/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	2/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	1/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	BMA	M	3	2	-	2/2/19/22	0/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
2	NAG	O	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	2/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	MAN	P	4	3	-	0/2/19/22	1/1/1/1
3	MAN	P	5	3	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	2,1	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	2/2/19/22	1/1/1/1
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	BMA	R	3	3	-	1/2/19/22	0/1/1/1
3	MAN	R	4	3	-	1/2/19/22	0/1/1/1
3	MAN	R	5	3	-	2/2/19/22	1/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	3	BMA	C4-C5	4.32	1.62	1.53
2	I	3	BMA	C4-C5	4.25	1.62	1.53
3	H	3	BMA	C4-C5	4.08	1.61	1.53
4	N	3	BMA	C4-C5	3.99	1.61	1.53
3	R	3	BMA	C4-C5	3.88	1.61	1.53

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	2	NAG	C4-C3-C2	-10.25	96.00	111.02
2	Q	3	BMA	C1-O5-C5	-9.65	99.26	112.19
2	L	2	NAG	C1-O5-C5	8.34	123.36	112.19
3	H	3	BMA	C1-O5-C5	-8.11	101.31	112.19
2	O	3	BMA	C1-O5-C5	-7.76	101.78	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1

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Mol	Chain	Res	Type	Atom
2	Q	1	NAG	C1

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	4	MAN	C1-C2-C3-C4-C5-O5
3	P	4	MAN	C1-C2-C3-C4-C5-O5
3	R	5	MAN	C1-C2-C3-C4-C5-O5
3	H	5	MAN	C1-C2-C3-C4-C5-O5
2	Q	4	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 20 short contacts:

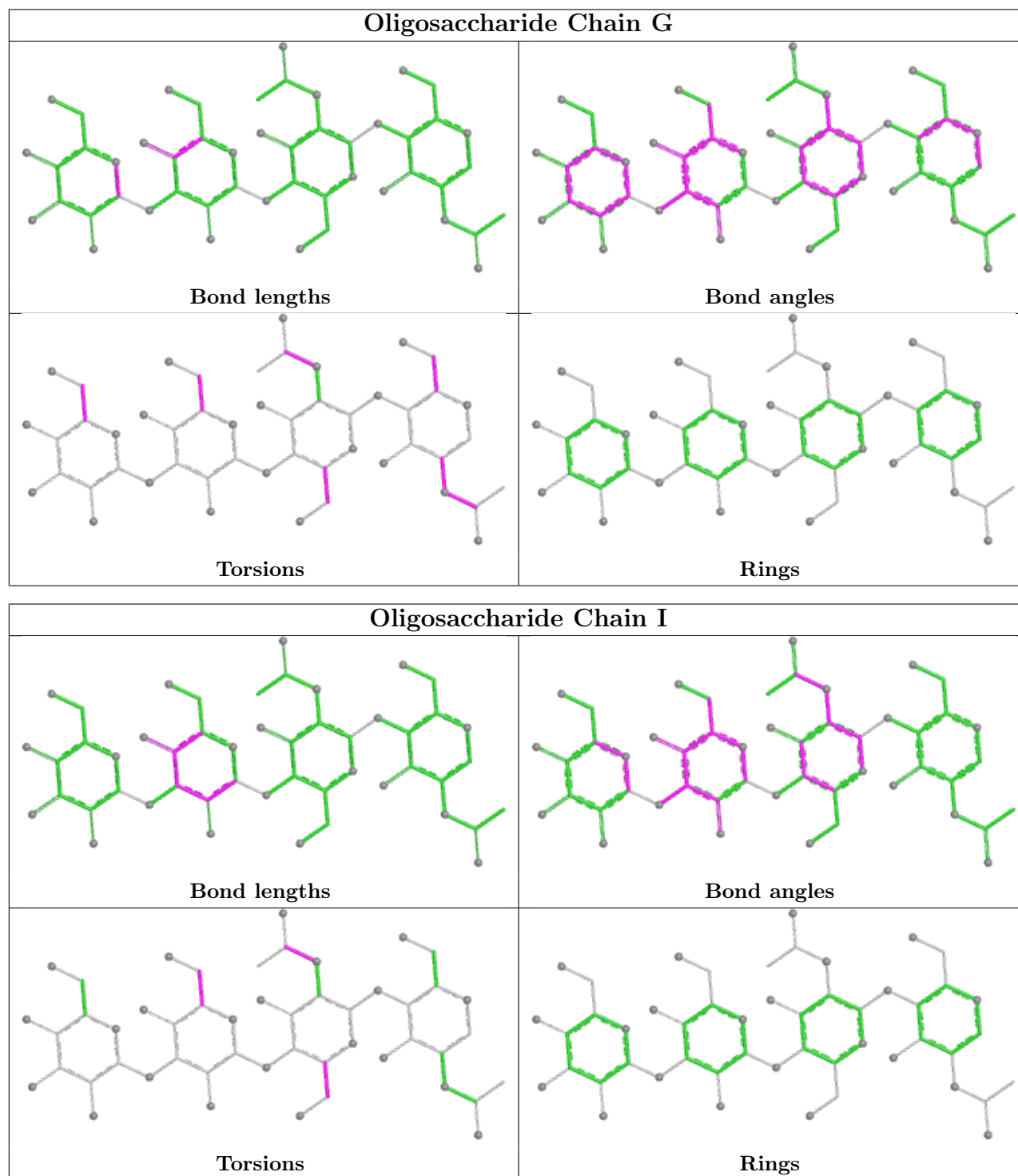
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	NAG	4	0
2	M	2	NAG	1	0
4	N	1	NAG	2	0
2	G	1	NAG	1	0
2	G	3	BMA	1	0
2	L	3	BMA	1	0
3	H	4	MAN	1	0
3	P	3	BMA	1	0
2	J	3	BMA	2	0
2	J	4	MAN	2	0
3	H	3	BMA	2	0
3	H	2	NAG	1	0
4	N	2	NAG	1	0
2	K	1	NAG	2	0
3	R	1	NAG	4	0
3	P	2	NAG	1	0
2	G	4	MAN	1	0
2	L	2	NAG	1	0
2	L	1	NAG	1	0

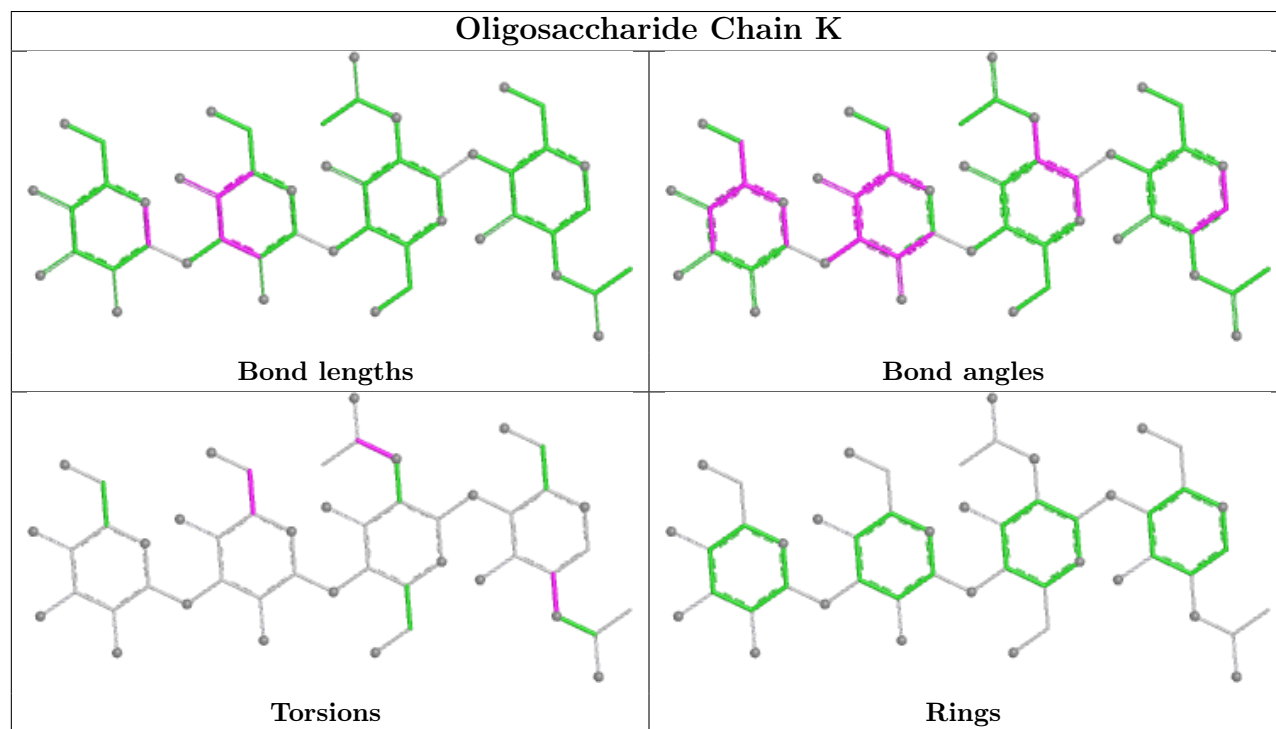
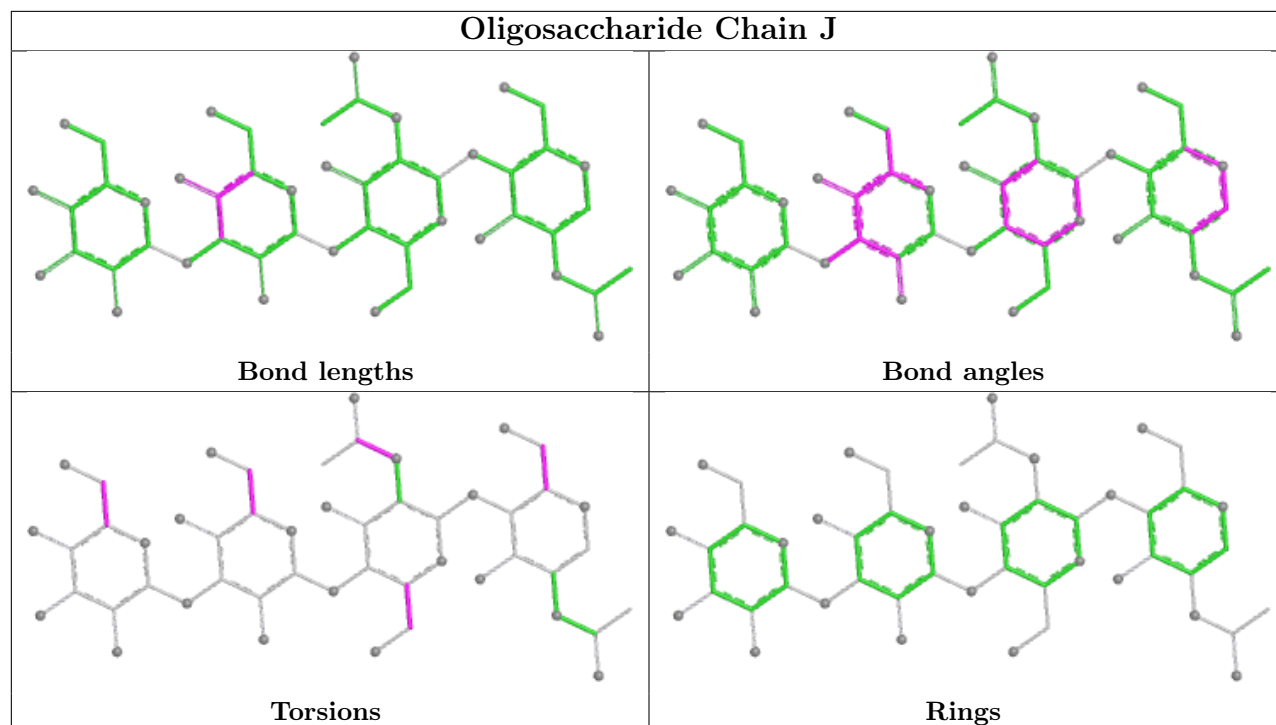
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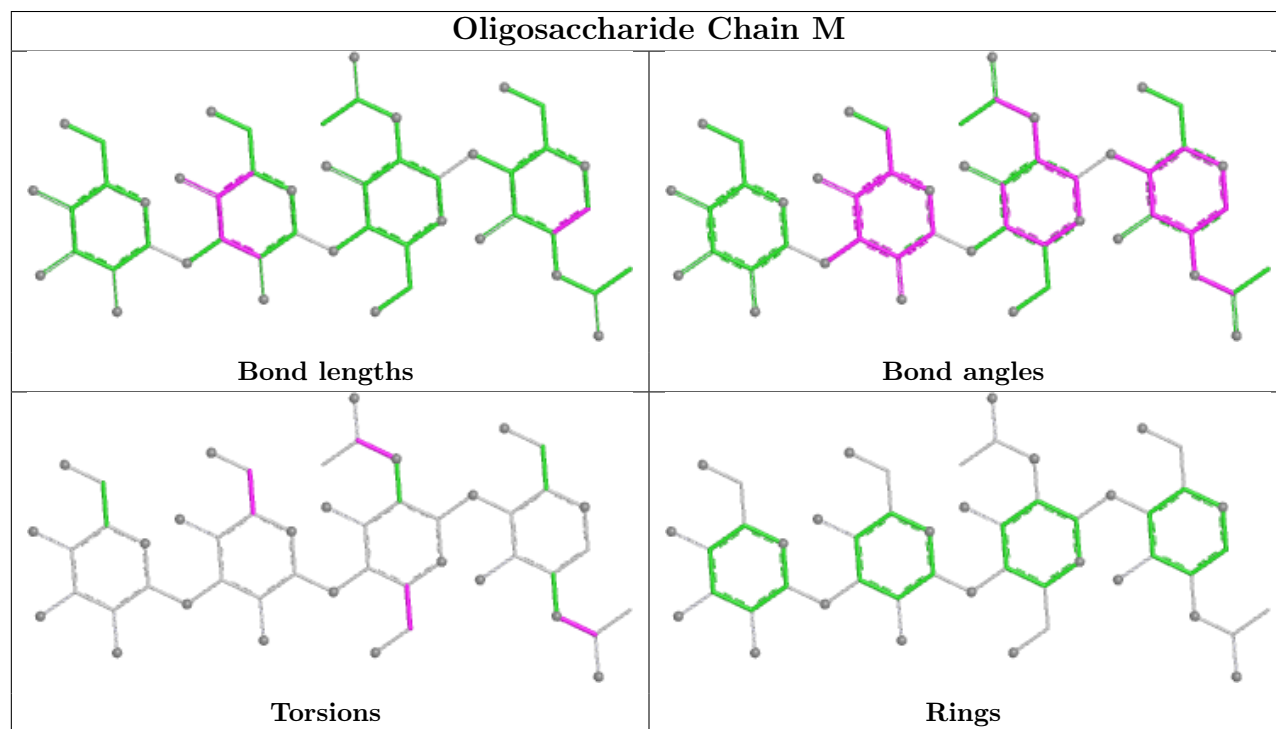
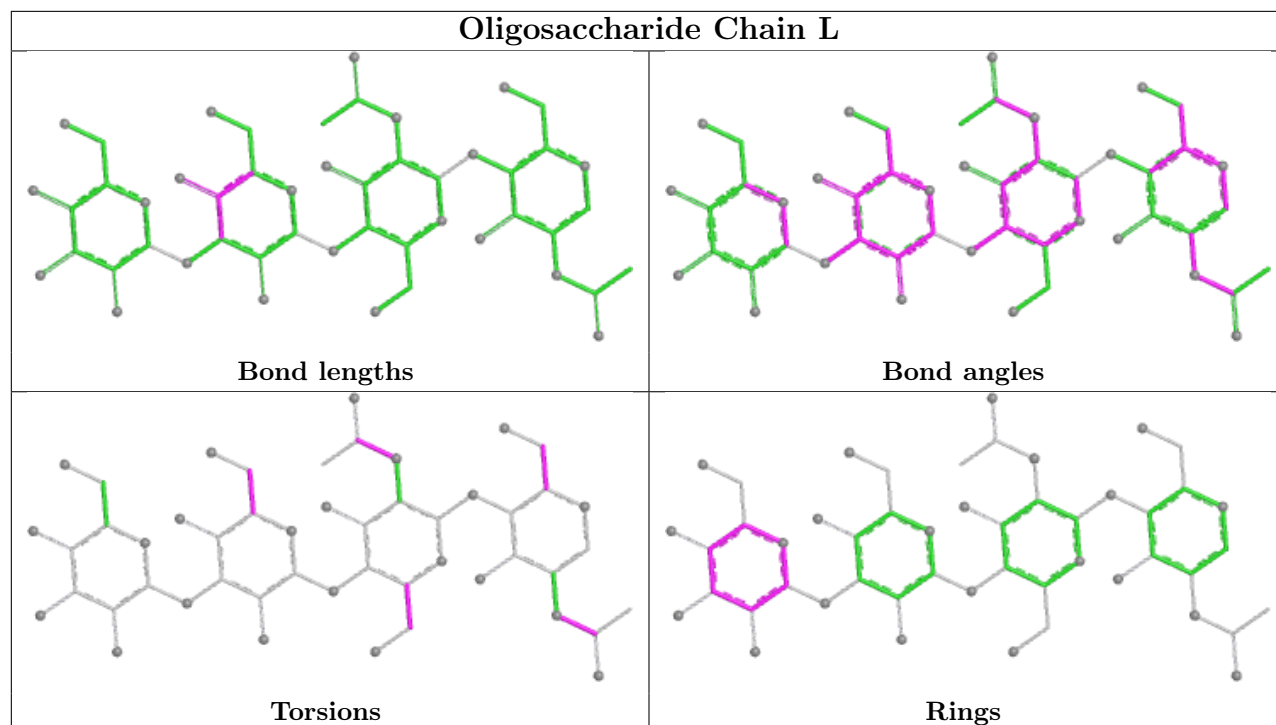
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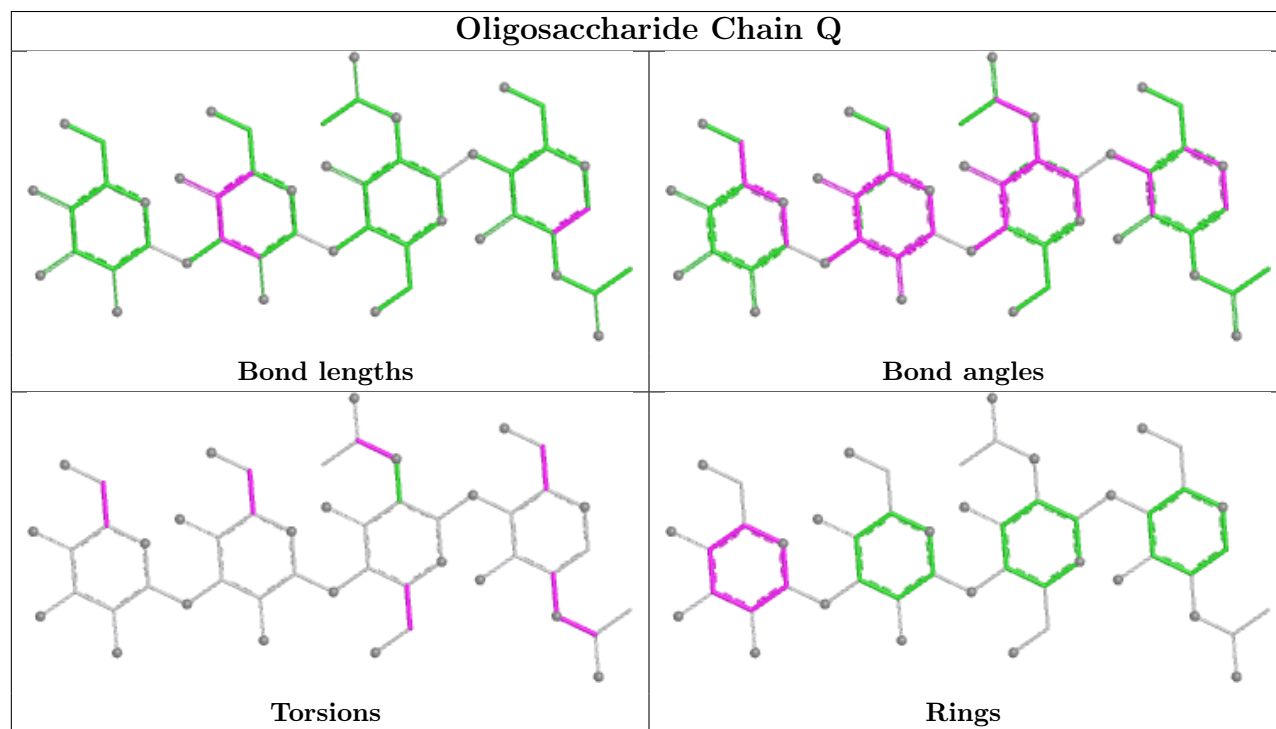
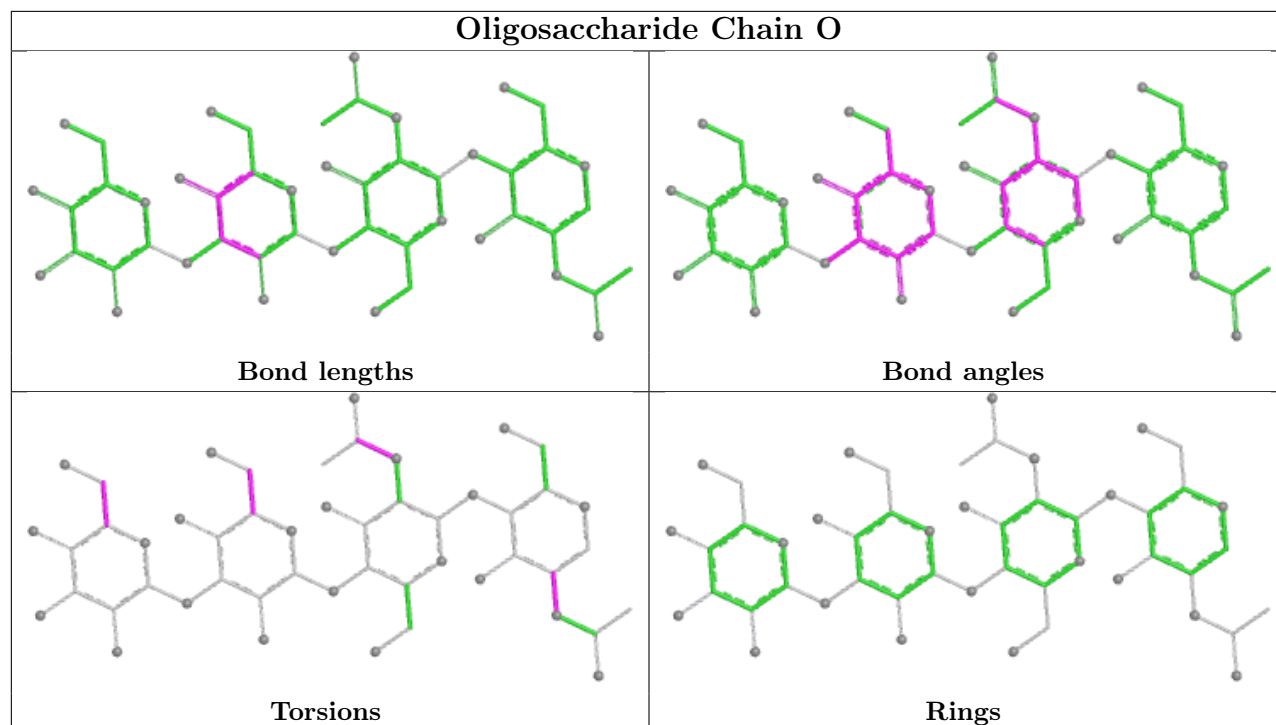
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	NAG	2	0
3	R	5	MAN	2	0
3	H	5	MAN	1	0

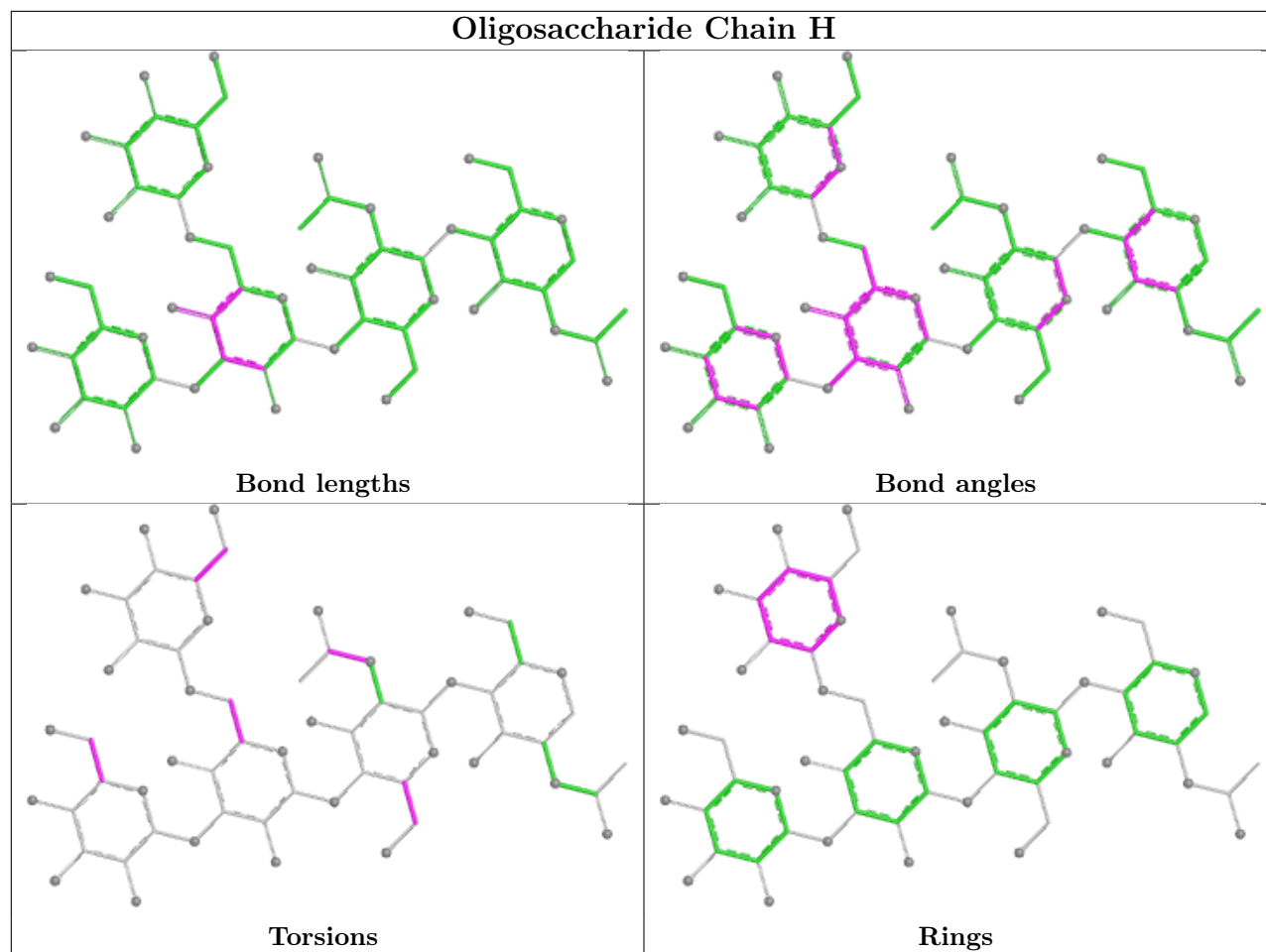
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

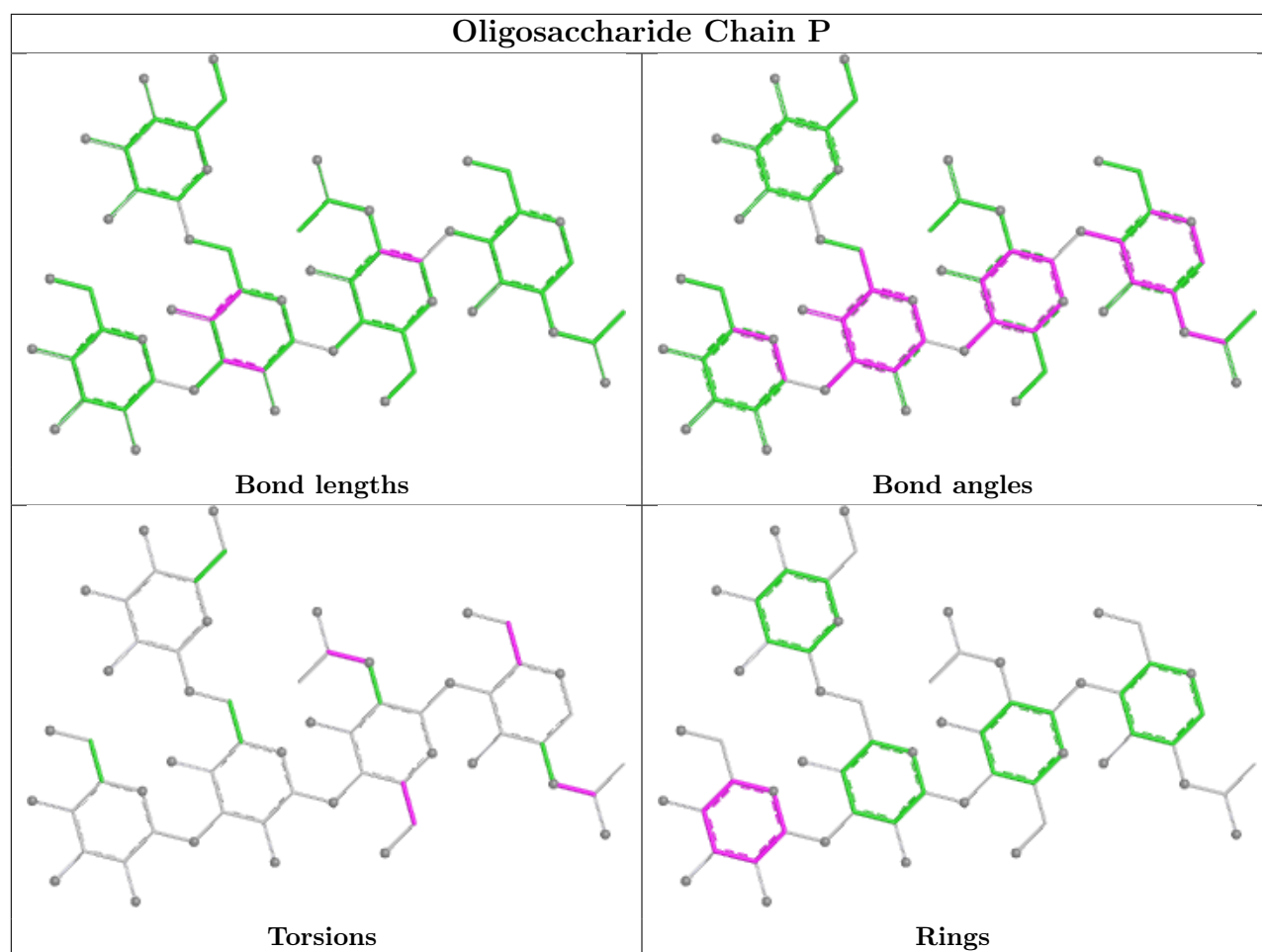




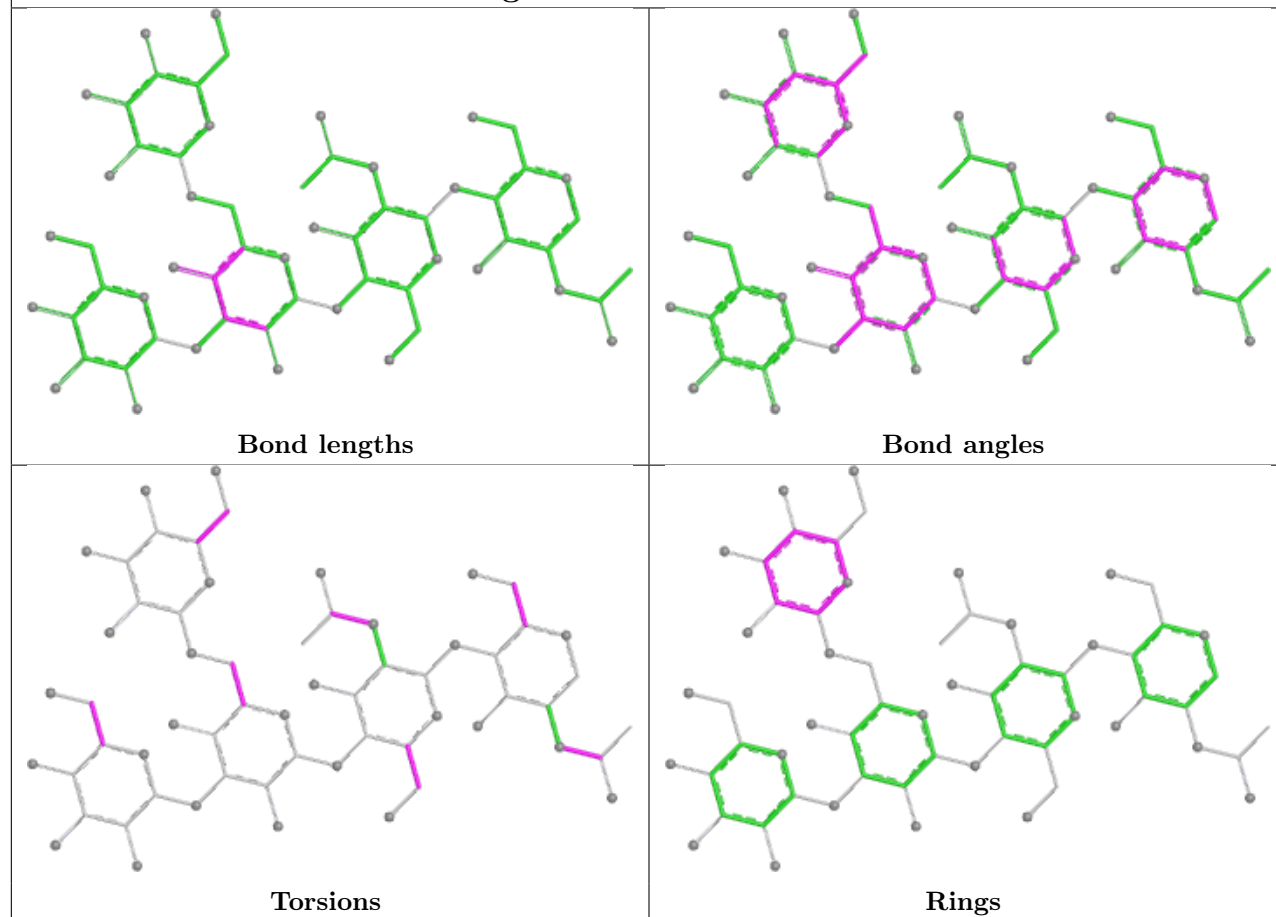




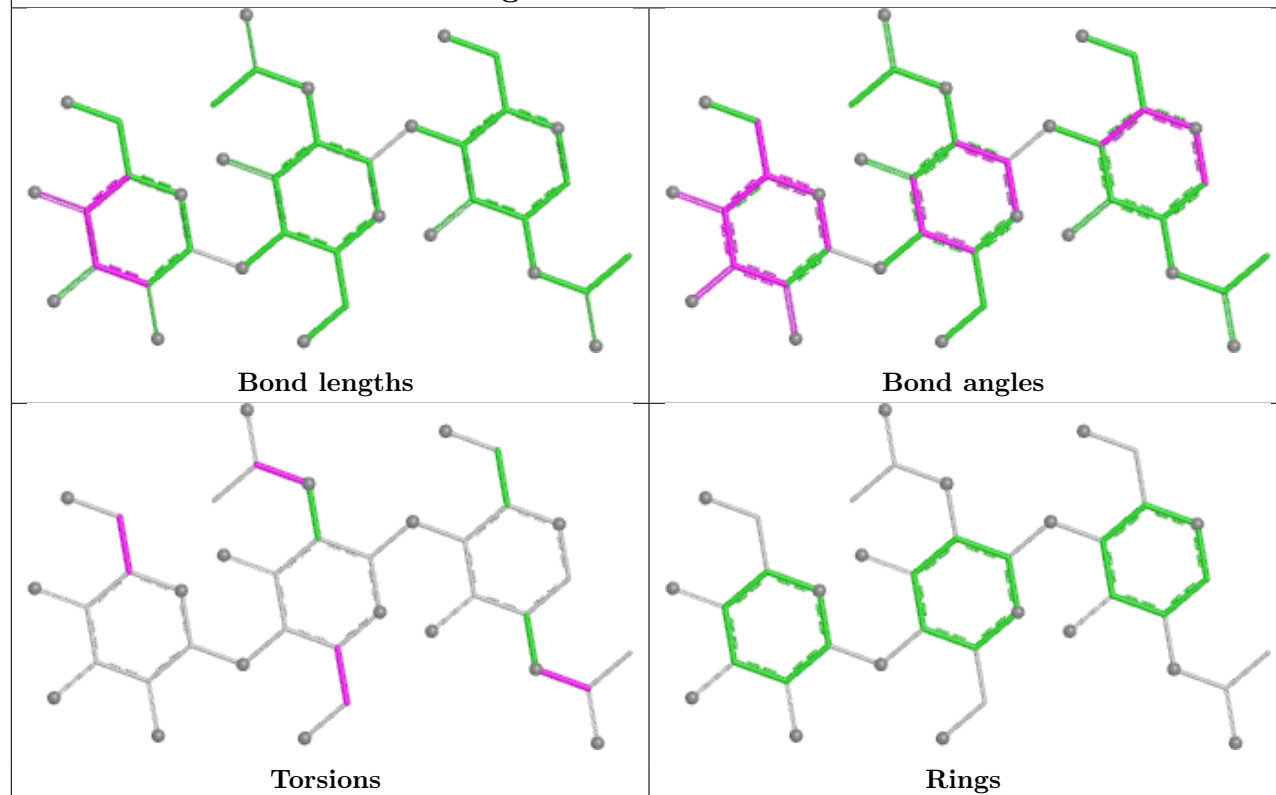




Oligosaccharide Chain R



Oligosaccharide Chain N



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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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