



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:41 PM UTC

PDB ID : 7TO4 / pdb_00007to4
EMDB ID : EMD-26029
Title : Structural and functional impact by SARS-CoV-2 Omicron spike mutations
Authors : Zhang, J.; Xiao, T.S.; Cai, Y.F.; Peng, H.Q.; Volloch, S.R.; Chen, B.
Deposited on : 2022-01-22
Resolution : 3.40 Å (reported)
Based on initial model : 7KRR

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

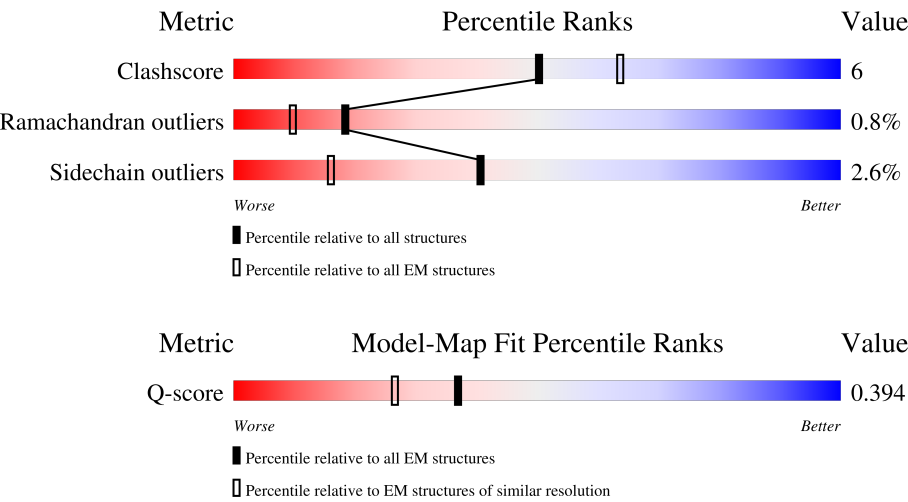
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



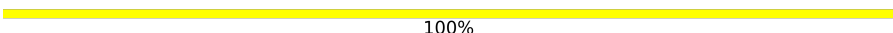
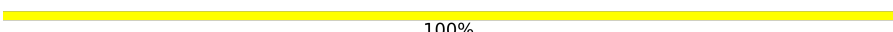
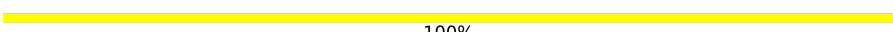
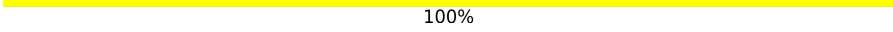
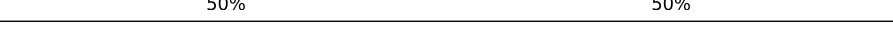
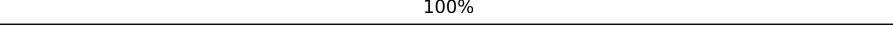
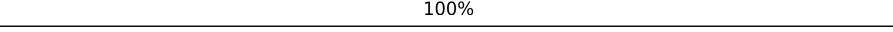
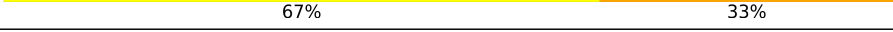
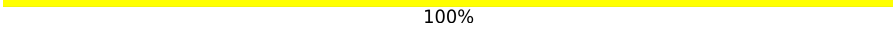
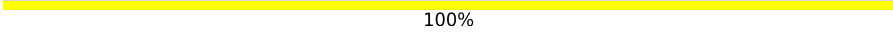
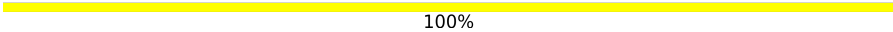
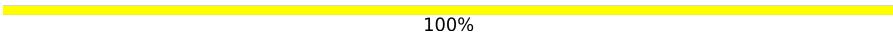
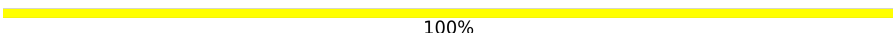
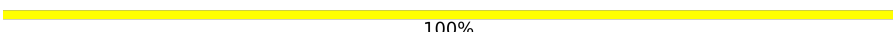
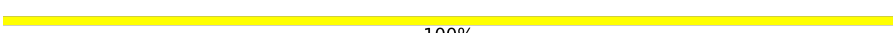
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1270	80%7%12%
1	B	1270	80%8%12%
1	C	1270	79%8%12%
2	D	2	50% 100%

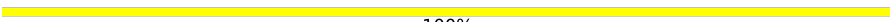
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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%
2	L	2	 50% 50%
2	N	2	 100%
2	P	2	 50% 50%
2	V	2	 50% 50%
2	X	2	 50% 50%
2	a	2	 100%
3	I	3	 100%
3	S	3	 67% 33%
3	d	3	 33% 67%
4	J	3	 100%
4	K	3	 100%
4	M	3	 100%
4	O	3	 100%
4	Q	3	 100%
4	R	3	 100%
4	T	3	 33% 67%
4	U	3	 100%
4	W	3	 33% 67%
4	Y	3	 100%
4	Z	3	 100%
4	b	3	 100%

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Mol	Chain	Length	Quality of chain
4	c	3	 100%
4	e	3	 100%
4	f	3	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27672 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1112	Total	C	N	O	S	0	0
			8737	5593	1458	1646	40		
1	B	1119	Total	C	N	O	S	0	0
			8789	5624	1466	1659	40		
1	C	1119	Total	C	N	O	S	0	0
			8789	5624	1466	1659	40		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	144	PHE	TYR	variant	UNP P0DTC2
A	145	ASP	TYR	variant	UNP P0DTC2
A	212	ILE	-	insertion	UNP P0DTC2
A	213	VAL	-	insertion	UNP P0DTC2
A	214	ARG	ASN	variant	UNP P0DTC2
A	214A	GLU	LEU	variant	UNP P0DTC2
A	214B	PRO	VAL	variant	UNP P0DTC2
A	214C	GLU	ARG	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	144	PHE	TYR	variant	UNP P0DTC2
B	145	ASP	TYR	variant	UNP P0DTC2
B	212	ILE	-	insertion	UNP P0DTC2
B	213	VAL	-	insertion	UNP P0DTC2
B	214	ARG	ASN	variant	UNP P0DTC2
B	214A	GLU	LEU	variant	UNP P0DTC2
B	214B	PRO	VAL	variant	UNP P0DTC2
B	214C	GLU	ARG	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	144	PHE	TYR	variant	UNP P0DTC2
C	145	ASP	TYR	variant	UNP P0DTC2
C	212	ILE	-	insertion	UNP P0DTC2
C	213	VAL	-	insertion	UNP P0DTC2
C	214	ARG	ASN	variant	UNP P0DTC2
C	214A	GLU	LEU	variant	UNP P0DTC2
C	214B	PRO	VAL	variant	UNP P0DTC2
C	214C	GLU	ARG	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2

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



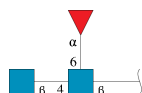
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		

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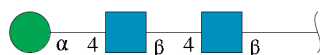
Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			38	22	2	14		
3	S	3	Total	C	N	O	0	0
			38	22	2	14		
3	d	3	Total	C	N	O	0	0
			38	22	2	14		

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



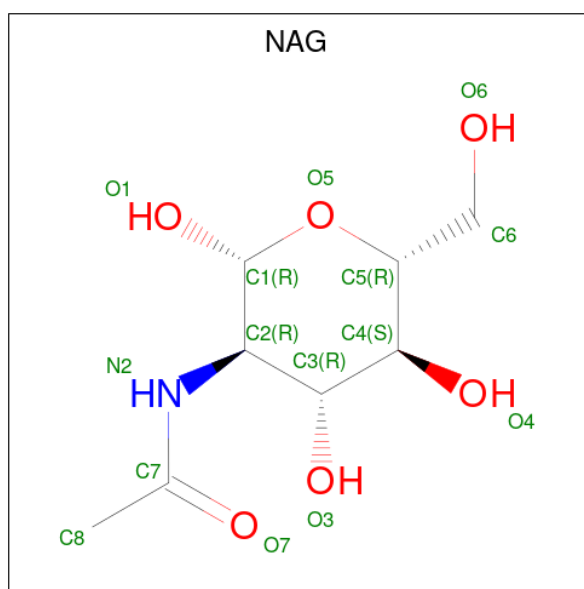
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	O	3	Total	C	N	O	0	0
			39	22	2	15		
4	Q	3	Total	C	N	O	0	0
			39	22	2	15		
4	R	3	Total	C	N	O	0	0
			39	22	2	15		
4	T	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	3	Total	C	N	O	0	0
			39	22	2	15		
4	W	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		
4	Z	3	Total	C	N	O	0	0
			39	22	2	15		
4	b	3	Total	C	N	O	0	0
			39	22	2	15		
4	c	3	Total	C	N	O	0	0
			39	22	2	15		
4	e	3	Total	C	N	O	0	0
			39	22	2	15		
4	f	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

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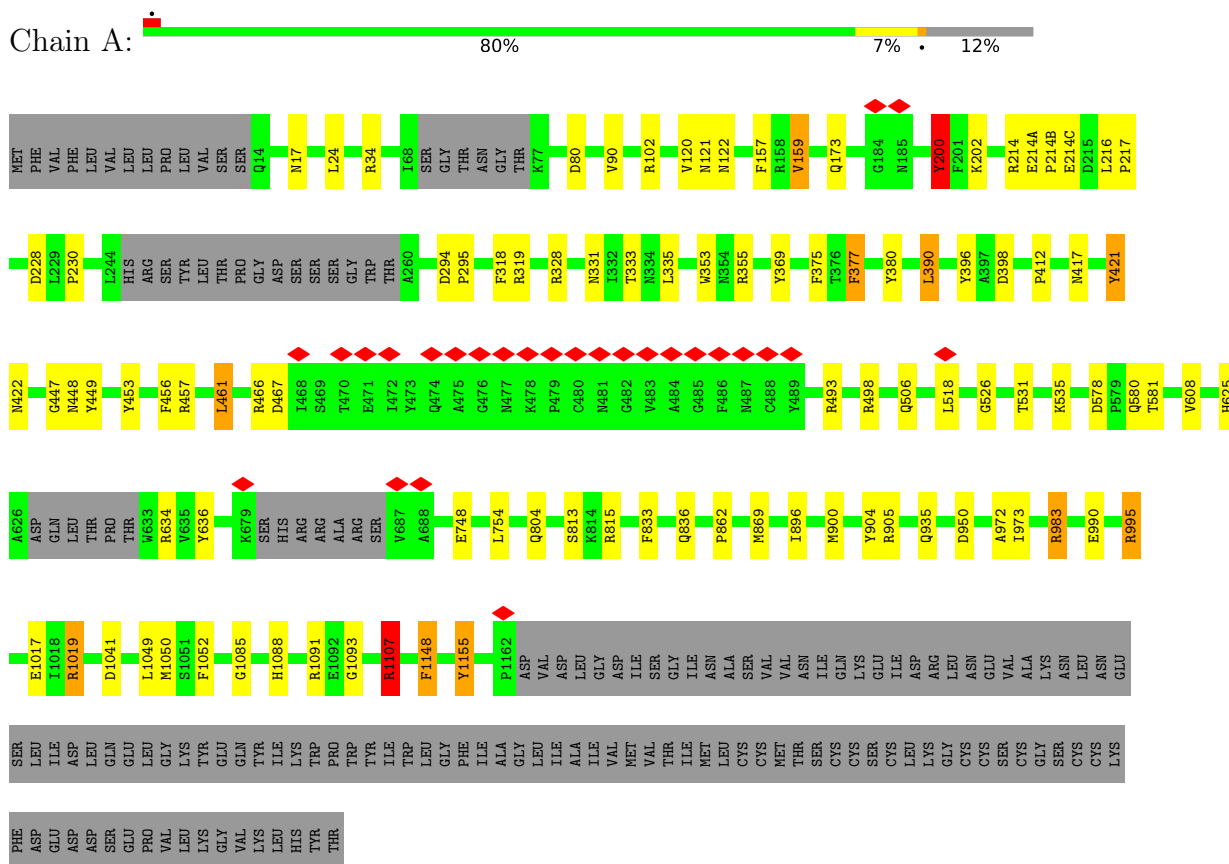
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	14	8	1	5	0

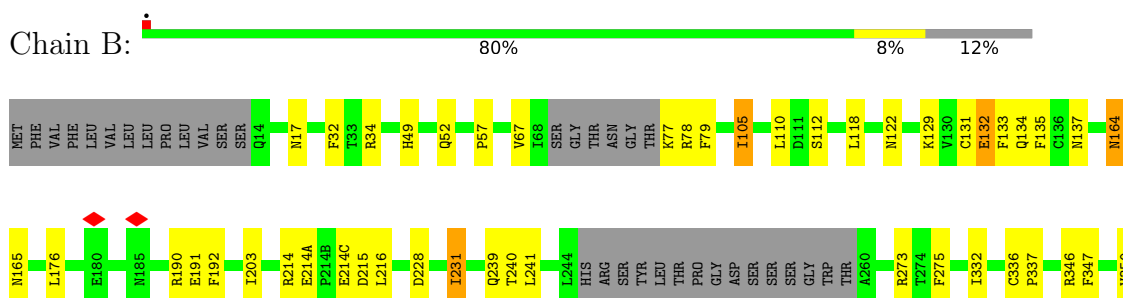
3 Residue-property plots

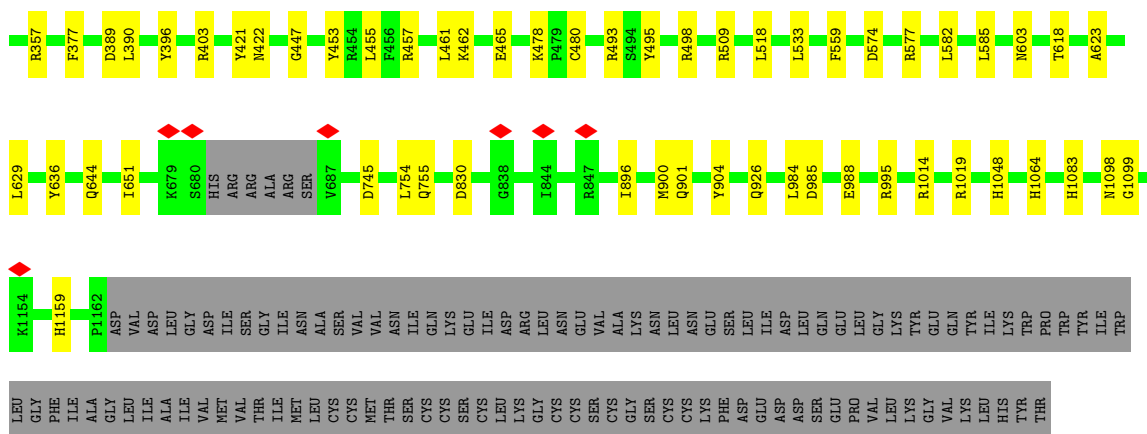
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein

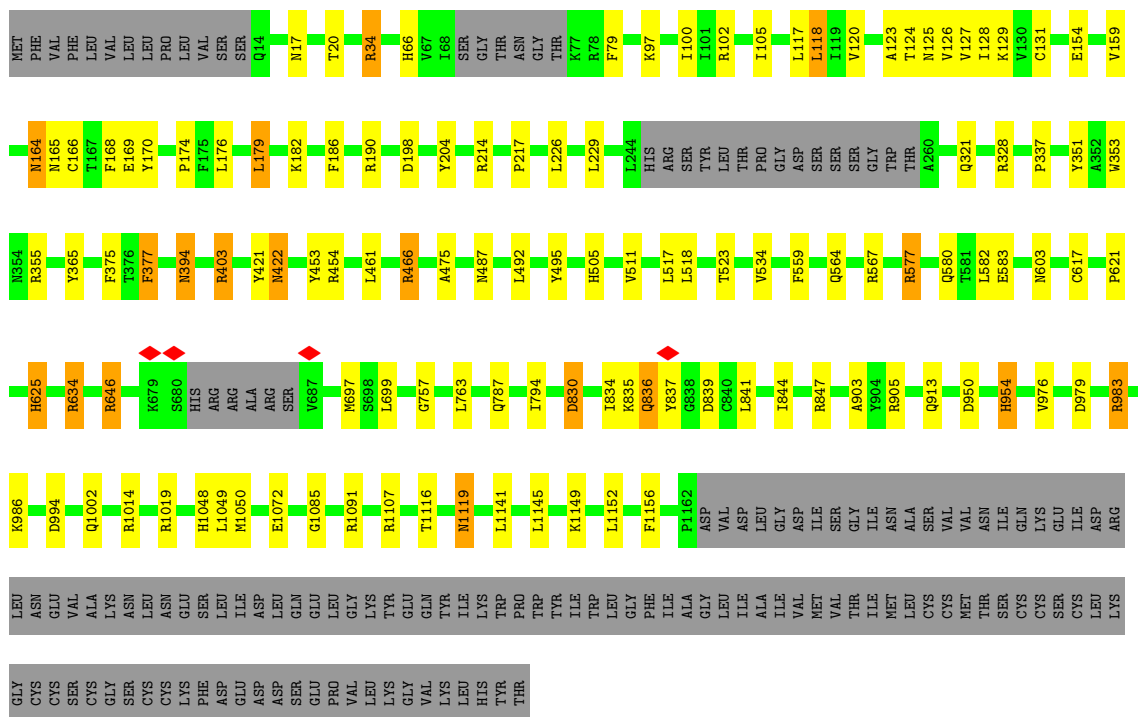
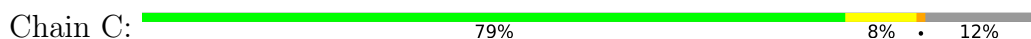


• Molecule 1: Spike glycoprotein





- Molecule 1: Spike glycoprotein



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

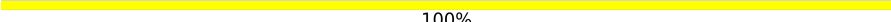


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

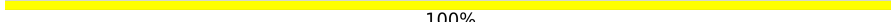
NAG1
NAG2

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

Chain F:  100%

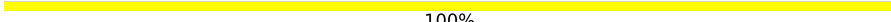
NAG1
NAG2

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

Chain G:  100%

NAG1
NAG2

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

Chain H:  100%

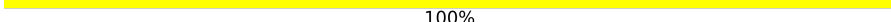
NAG1
NAG2

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

Chain L:  50% 50% 50%


NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

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

Chain P:  50% 50%



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



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



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



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



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



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



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

Chain J:  100%

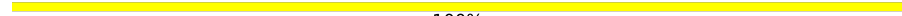
MAG1
MAG2
MAN3

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

Chain K:  100%

MAG1
MAG2
MAN3

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

Chain M:  100%

MAG1
MAG2
MAN3

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

Chain O:  100%

MAG1
MAG2
MAN3

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

Chain Q:  100%

MAG1
MAG2
MAN3

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

Chain R:  100%

MAG1
MAG2
MAN3

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

Chain T:  33% 67%



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

Chain U:  100%



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

Chain W:  33% 67%



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

Chain Y:  100%



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

Chain Z:  100%

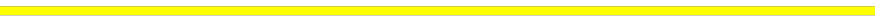


- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%



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

Chain c:  100%



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

Chain e:  100%

MAG1
MAG2
MAM3

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

Chain f:  100%

MAG1
MAG2
MAM3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87330	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.592	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.063	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, FUC

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	0.77	2/8942 (0.0%)	1.31	25/12156 (0.2%)
1	B	0.75	1/8996 (0.0%)	1.32	21/12233 (0.2%)
1	C	0.77	1/8996 (0.0%)	1.30	26/12233 (0.2%)
All	All	0.76	4/26934 (0.0%)	1.31	72/36622 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	LEU	CA-C	8.26	1.62	1.52
1	A	983	ARG	C-O	-7.14	1.16	1.24
1	B	1014	ARG	C-O	-5.07	1.17	1.24
1	A	1019	ARG	C-O	-5.07	1.18	1.24

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASN	N-CA-C	11.14	123.12	110.97
1	A	1091	ARG	N-CA-C	-7.86	102.31	111.03
1	A	421	TYR	N-CA-C	7.29	122.46	113.50
1	B	389	ASP	CA-CB-CG	7.18	119.78	112.60
1	C	834	ILE	N-CA-C	7.13	118.64	109.30
1	C	567	ARG	N-CA-C	7.09	119.95	109.24
1	C	198	ASP	CA-CB-CG	6.68	119.28	112.60
1	C	559	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	80	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	215	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	321	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	C	118	LEU	N-CA-C	6.23	119.11	108.02
1	C	983	ARG	N-CA-C	6.18	124.03	114.64
1	B	132	GLU	N-CA-C	-6.17	100.71	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1119	ASN	CA-CB-CG	6.02	118.62	112.60
1	C	403	ARG	N-CA-C	-6.01	100.94	109.96
1	C	950	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	52	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	1085	GLY	CA-C-N	5.82	128.98	120.71
1	A	1085	GLY	C-N-CA	5.82	128.98	120.71
1	A	375	PHE	CA-CB-CG	5.80	119.60	113.80
1	C	214	ARG	N-CA-C	-5.76	100.61	109.76
1	C	118	LEU	CA-C-N	5.73	129.53	122.37
1	C	118	LEU	C-N-CA	5.73	129.53	122.37
1	A	200	TYR	CB-CA-C	-5.68	104.38	111.43
1	C	1091	ARG	N-CA-C	-5.64	104.82	110.97
1	A	804	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	390	LEU	N-CA-C	5.57	117.65	109.24
1	B	228	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	122	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	745	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	422	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	1148	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	377	PHE	CA-CB-CG	5.49	119.29	113.80
1	C	377	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	456	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	1107	ARG	N-CA-C	5.40	122.30	110.80
1	A	526	GLY	CA-C-N	-5.38	114.19	119.99
1	A	526	GLY	C-N-CA	-5.38	114.19	119.99
1	B	478	LYS	CA-C-N	5.36	125.37	119.90
1	B	478	LYS	C-N-CA	5.36	125.37	119.90
1	A	294	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	1155	TYR	N-CA-C	-5.33	105.38	111.14
1	B	1159	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	862	PRO	N-CA-CB	5.30	105.98	103.22
1	C	394	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	475	ALA	CA-C-N	5.28	125.12	120.10
1	C	475	ALA	C-N-CA	5.28	125.12	120.10
1	A	950	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	1088	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	B	49	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	448	ASN	CA-C-N	5.22	131.51	121.54
1	A	448	ASN	C-N-CA	5.22	131.51	121.54
1	B	164	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	C	1048	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	B	403	ARG	N-CA-C	-5.17	102.03	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	B	1083	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	B	926	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	17	ASN	CB-CG-ND2	-5.14	108.69	116.40
1	B	231	ILE	N-CA-C	5.13	115.86	110.62
1	A	625	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	A	398	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	1085	GLY	CA-C-N	5.05	127.94	120.82
1	C	1085	GLY	C-N-CA	5.05	127.94	120.82
1	B	1048	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	B	1064	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	B	336	CYS	CA-C-N	5.02	126.12	119.84
1	B	336	CYS	C-N-CA	5.02	126.12	119.84
1	A	836	GLN	N-CA-C	5.02	120.30	113.37
1	C	787	GLN	OE1-CD-NE2	-5.01	117.58	122.60
1	C	954	HIS	CB-CG-CD2	-5.01	124.69	131.20

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	A	8737	0	8544	99	0
1	B	8789	0	8591	111	0
1	C	8789	0	8592	124	0
2	D	28	0	25	0	0
2	E	28	0	25	3	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	L	28	0	25	0	0
2	N	28	0	25	1	0
2	P	28	0	25	2	0
2	V	28	0	25	1	0
2	X	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	28	0	25	0	0
3	I	38	0	34	0	0
3	S	38	0	34	1	0
3	d	38	0	34	0	0
4	J	39	0	34	0	0
4	K	39	0	34	0	0
4	M	39	0	34	0	0
4	O	39	0	34	0	0
4	Q	39	0	34	0	0
4	R	39	0	34	0	0
4	T	39	0	34	1	0
4	U	39	0	34	0	0
4	W	39	0	34	4	0
4	Y	39	0	34	3	0
4	Z	39	0	34	0	0
4	b	39	0	34	0	0
4	c	39	0	34	0	0
4	e	39	0	34	0	0
4	f	39	0	34	0	0
5	A	140	0	130	0	0
5	B	112	0	104	1	0
5	C	98	0	91	0	0
All	All	27672	0	26939	307	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 6.

All (307) 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:904:TYR:CE2	1:C:1107:ARG:HD3	1.40	1.53
1:B:57:PRO:HB3	1:B:273:ARG:NH2	1.39	1.38
1:C:905:ARG:NH1	1:C:1050:MET:HB3	1.47	1.27
1:B:110:LEU:HB2	1:B:135:PHE:CD2	1.70	1.25
1:B:105:ILE:HD11	1:B:118:LEU:CD1	1.65	1.25
1:A:904:TYR:CD2	1:C:1107:ARG:HD3	1.73	1.24
1:B:176:LEU:HD12	1:B:190:ARG:NH2	1.55	1.20
1:A:417:ASN:HA	1:A:421:TYR:CE2	1.80	1.16
1:A:904:TYR:CE2	1:C:1107:ARG:CD	2.29	1.16
1:A:904:TYR:HE2	1:C:1107:ARG:CD	1.59	1.14
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	1.83	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ILE:HD11	1:B:904:TYR:CE1	1.84	1.11
1:A:1107:ARG:HD3	1:B:904:TYR:HE2	1.14	1.11
1:C:105:ILE:CD1	1:C:118:LEU:HD12	1.81	1.11
1:B:105:ILE:CD1	1:B:118:LEU:CD1	2.30	1.08
1:B:214:ARG:HG2	1:B:214(C):GLU:HB2	1.30	1.08
1:B:176:LEU:HD12	1:B:190:ARG:HH21	0.91	1.05
1:B:105:ILE:HD11	1:B:118:LEU:HD13	1.07	1.04
1:C:403:ARG:HD2	1:C:505:HIS:HA	1.37	1.04
1:C:128:ILE:HD11	1:C:170:TYR:CD2	1.93	1.03
1:B:896:ILE:HD11	1:B:904:TYR:HE1	1.17	1.03
1:B:105:ILE:CD1	1:B:118:LEU:HD12	1.87	1.01
1:B:176:LEU:CD1	1:B:190:ARG:HH21	1.72	1.01
1:A:995:ARG:HH11	1:A:995:ARG:HG2	1.27	1.00
1:C:905:ARG:HH12	1:C:1050:MET:CB	1.74	0.99
1:B:453:TYR:CD1	1:B:495:TYR:CE2	2.51	0.97
1:B:105:ILE:HD13	1:B:118:LEU:HD12	1.41	0.97
1:B:453:TYR:HD1	1:B:495:TYR:CE2	1.83	0.95
1:A:457:ARG:HE	1:A:457:ARG:HA	1.31	0.94
1:A:369:TYR:HE1	1:C:487:ASN:HD21	1.09	0.93
1:B:110:LEU:CB	1:B:135:PHE:CD2	2.51	0.93
1:B:453:TYR:CD1	1:B:495:TYR:CZ	2.58	0.92
1:B:57:PRO:HB3	1:B:273:ARG:HH22	1.23	0.92
1:A:417:ASN:HA	1:A:421:TYR:HE2	1.34	0.91
1:A:1107:ARG:CD	1:B:904:TYR:HE2	1.84	0.90
1:B:105:ILE:HG12	1:B:241:LEU:HD11	1.53	0.90
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.35	0.90
1:C:168:PHE:HE2	1:C:229:LEU:HD12	1.36	0.89
1:B:57:PRO:CB	1:B:273:ARG:NH2	2.33	0.89
1:A:369:TYR:HE1	1:C:487:ASN:ND2	1.69	0.89
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.53	0.88
1:A:421:TYR:HB3	1:A:457:ARG:CG	2.04	0.88
1:C:905:ARG:HH12	1:C:1050:MET:HB3	1.13	0.88
1:B:357:ARG:HB2	1:B:396:TYR:CE1	2.08	0.87
1:B:110:LEU:HB2	1:B:135:PHE:HD2	1.29	0.87
1:B:176:LEU:CD1	1:B:190:ARG:NH2	2.33	0.86
1:B:1019:ARG:HG3	1:B:1019:ARG:HH11	1.39	0.86
1:A:904:TYR:HE2	1:C:1107:ARG:CG	1.87	0.86
1:B:896:ILE:CD1	1:B:904:TYR:CE1	2.59	0.85
1:C:105:ILE:HD11	1:C:118:LEU:HD12	1.56	0.85
1:B:105:ILE:CD1	1:B:118:LEU:HD13	1.95	0.85
1:A:417:ASN:CA	1:A:421:TYR:CE2	2.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:GLN:HG2	2:P:1:NAG:H82	1.57	0.84
1:B:190:ARG:NE	1:B:192:PHE:CZ	2.45	0.84
1:A:390:LEU:HD11	1:A:518:LEU:HD21	1.60	0.84
1:A:421:TYR:HB3	1:A:457:ARG:HG2	1.59	0.84
1:C:128:ILE:HD11	1:C:170:TYR:CG	2.11	0.84
1:C:179:LEU:HD23	1:C:179:LEU:H	1.40	0.84
1:B:214:ARG:CG	1:B:214(C):GLU:HB2	2.09	0.83
2:E:1:NAG:H62	2:E:2:NAG:H82	1.60	0.82
1:B:176:LEU:HB2	1:B:190:ARG:NH2	1.94	0.82
1:C:128:ILE:CD1	1:C:170:TYR:CD2	2.62	0.82
1:C:453:TYR:CD1	1:C:495:TYR:CZ	2.67	0.82
1:A:369:TYR:HE2	1:A:377:PHE:HB3	1.43	0.82
1:A:417:ASN:CA	1:A:421:TYR:HE2	1.92	0.81
1:B:176:LEU:HB2	1:B:190:ARG:HH22	1.46	0.80
1:B:421:TYR:CD1	1:B:457:ARG:HB2	2.17	0.80
1:C:453:TYR:HD1	1:C:495:TYR:CE2	2.00	0.80
1:C:954:HIS:HB3	1:C:1014:ARG:NH1	1.95	0.79
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.65	0.79
1:A:904:TYR:HE2	1:C:1107:ARG:HD3	1.01	0.78
1:C:128:ILE:HG12	1:C:170:TYR:O	1.83	0.78
1:A:457:ARG:HA	1:A:457:ARG:NE	1.99	0.77
1:B:17:ASN:OD1	1:B:17:ASN:O	2.01	0.77
1:A:353:TRP:CE2	1:A:466:ARG:HB3	2.19	0.77
1:C:128:ILE:CG1	1:C:170:TYR:HB3	2.15	0.76
1:B:453:TYR:HB3	1:B:495:TYR:OH	1.84	0.76
1:C:466:ARG:HB3	1:C:466:ARG:NH1	2.00	0.76
1:A:369:TYR:CE2	1:A:377:PHE:HB3	2.21	0.76
1:B:110:LEU:CB	1:B:135:PHE:HD2	1.95	0.76
1:C:128:ILE:HG13	1:C:170:TYR:HB3	1.68	0.75
1:A:896:ILE:HD11	1:A:904:TYR:CE1	2.22	0.75
1:B:462:LYS:HG2	4:Y:1:NAG:C8	2.17	0.74
1:C:905:ARG:NH1	1:C:1050:MET:CB	2.34	0.74
1:A:417:ASN:CB	1:A:421:TYR:HE2	1.99	0.73
1:A:421:TYR:HD1	1:A:457:ARG:HB2	1.51	0.73
1:C:836:GLN:N	1:C:836:GLN:OE1	2.21	0.73
1:A:417:ASN:O	1:A:421:TYR:CD2	2.42	0.72
1:C:179:LEU:H	1:C:179:LEU:CD2	2.02	0.72
1:A:905:ARG:NH1	1:A:1050:MET:HB3	2.04	0.72
1:C:129:LYS:HE2	1:C:166:CYS:HB3	1.71	0.72
1:A:896:ILE:HD11	1:A:904:TYR:HE1	1.54	0.72
1:C:127:VAL:HG11	4:W:1:NAG:O6	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:ARG:CD	1:B:904:TYR:CE2	2.63	0.71
1:C:131:CYS:HA	1:C:165:ASN:O	1.90	0.71
1:C:453:TYR:CD1	1:C:495:TYR:CE2	2.79	0.71
1:B:110:LEU:CA	1:B:135:PHE:HD2	2.04	0.71
1:A:578:ASP:HB3	1:A:581:THR:O	1.93	0.69
1:A:904:TYR:CD2	1:C:1107:ARG:CD	2.66	0.69
1:C:179:LEU:HD23	1:C:179:LEU:N	2.07	0.69
1:A:1107:ARG:HD3	1:B:904:TYR:CD2	2.28	0.68
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.25	0.68
1:B:190:ARG:HG2	1:B:192:PHE:CE1	2.28	0.68
1:C:128:ILE:CD1	1:C:170:TYR:HB3	2.23	0.68
1:B:190:ARG:NE	1:B:192:PHE:CE1	2.61	0.68
1:A:833:PHE:CE2	1:C:646:ARG:CZ	2.77	0.68
1:B:559:PHE:CB	1:B:577:ARG:HH21	2.07	0.68
1:C:128:ILE:HD11	1:C:170:TYR:HB3	1.75	0.68
1:B:190:ARG:CZ	1:B:192:PHE:HZ	2.07	0.68
1:B:1019:ARG:HG3	1:B:1019:ARG:NH1	1.99	0.68
1:A:331:ASN:HB3	1:A:580:GLN:HG2	1.76	0.68
1:C:168:PHE:HE2	1:C:229:LEU:CD1	2.07	0.67
1:B:190:ARG:NE	1:B:192:PHE:HZ	1.90	0.67
1:A:973:ILE:HD12	1:A:983:ARG:HH21	1.59	0.67
1:B:176:LEU:CG	1:B:190:ARG:NH2	2.57	0.66
1:B:78:ARG:HA	1:B:78:ARG:NE	2.10	0.66
1:C:17:ASN:OD1	1:C:17:ASN:O	2.14	0.66
1:A:102:ARG:NH2	1:A:121:ASN:O	2.29	0.66
1:C:100:ILE:O	1:C:102:ARG:HG3	1.96	0.65
1:B:131:CYS:HA	1:B:165:ASN:O	1.97	0.65
1:A:1155:TYR:CD2	1:C:1152:LEU:HD21	2.32	0.65
1:B:453:TYR:CB	1:B:495:TYR:OH	2.44	0.65
1:C:466:ARG:HH11	1:C:466:ARG:HG2	1.61	0.65
1:B:462:LYS:HG2	4:Y:1:NAG:H82	1.78	0.65
1:C:34:ARG:NH1	1:C:217:PRO:O	2.30	0.64
1:B:447:GLY:CA	1:B:498:ARG:HG2	2.28	0.64
1:A:833:PHE:CZ	1:C:646:ARG:CZ	2.81	0.64
1:C:466:ARG:HB3	1:C:466:ARG:CZ	2.28	0.63
1:A:995:ARG:HG2	1:A:995:ARG:NH1	2.03	0.63
1:A:353:TRP:CZ2	1:A:466:ARG:HB3	2.33	0.63
1:A:905:ARG:CZ	1:A:1050:MET:HB3	2.29	0.63
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.32	0.63
1:B:78:ARG:HA	1:B:78:ARG:HE	1.63	0.63
1:B:465:GLU:OE1	4:Y:1:NAG:H81	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:CB	1:B:190:ARG:NH2	2.62	0.62
1:C:125:ASN:HA	1:C:174:PRO:HB3	1.79	0.62
1:B:453:TYR:CG	1:B:495:TYR:CZ	2.87	0.61
1:B:455:LEU:HD12	1:B:493:ARG:HD2	1.82	0.61
1:C:128:ILE:HD11	1:C:170:TYR:CB	2.28	0.61
1:C:466:ARG:HH11	1:C:466:ARG:CG	2.13	0.61
1:B:190:ARG:CD	1:B:192:PHE:HE1	2.13	0.61
1:C:105:ILE:CD1	1:C:118:LEU:CD1	2.69	0.61
1:C:105:ILE:HD12	1:C:118:LEU:HD12	1.78	0.61
1:A:995:ARG:HH11	1:A:995:ARG:CG	2.09	0.60
1:A:200:TYR:HB3	1:A:202:LYS:NZ	2.17	0.60
1:C:634:ARG:HD3	1:C:634:ARG:N	2.16	0.60
1:C:105:ILE:HD11	1:C:118:LEU:CD1	2.29	0.59
1:C:17:ASN:ND2	2:V:1:NAG:O7	2.36	0.59
1:C:403:ARG:CD	1:C:505:HIS:HA	2.21	0.59
1:C:128:ILE:HG13	1:C:128:ILE:O	2.01	0.59
1:C:168:PHE:CE2	1:C:229:LEU:HD12	2.28	0.59
1:C:127:VAL:HG21	4:W:2:NAG:H82	1.83	0.59
1:B:110:LEU:CA	1:B:135:PHE:CD2	2.83	0.58
1:C:646:ARG:NH1	1:C:646:ARG:HG3	2.18	0.58
1:B:900:MET:O	1:B:904:TYR:CD1	2.56	0.58
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.38	0.58
1:A:417:ASN:HB2	1:A:421:TYR:HE2	1.68	0.58
1:A:200:TYR:HB3	1:A:202:LYS:HZ3	1.67	0.58
1:A:1093:GLY:HA2	1:A:1107:ARG:HG3	1.85	0.58
1:B:17:ASN:HB3	1:B:137:ASN:HB3	1.86	0.58
1:C:176:LEU:HD23	1:C:176:LEU:C	2.29	0.58
1:C:403:ARG:HD2	1:C:505:HIS:CA	2.23	0.58
1:B:176:LEU:C	1:B:176:LEU:HD23	2.29	0.58
3:S:1:NAG:O4	3:S:2:NAG:O7	2.21	0.57
1:C:617:CYS:O	1:C:621:PRO:HD3	2.04	0.57
1:A:580:GLN:O	2:E:1:NAG:H83	2.04	0.57
1:B:132:GLU:HB2	1:B:164:ASN:HB3	1.85	0.57
1:C:129:LYS:HG3	1:C:169:GLU:HB3	1.87	0.57
1:A:421:TYR:CD1	1:A:457:ARG:HB2	2.36	0.56
1:A:869:MET:HE2	1:C:699:LEU:HD21	1.87	0.56
1:A:1017:GLU:OE2	1:B:1019:ARG:HD3	2.04	0.56
1:B:190:ARG:CD	1:B:192:PHE:CE1	2.88	0.56
1:A:34:ARG:NH2	1:A:217:PRO:HG2	2.21	0.56
1:A:896:ILE:CD1	1:A:904:TYR:CE1	2.88	0.56
1:B:190:ARG:NH1	1:B:192:PHE:HZ	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:CE1	1:A:228:ASP:HB2	2.41	0.56
1:C:403:ARG:HH11	1:C:505:HIS:CD2	2.24	0.55
1:A:904:TYR:CE2	1:C:1107:ARG:CG	2.78	0.55
1:C:124:THR:H	4:W:1:NAG:H82	1.72	0.55
1:B:453:TYR:CB	1:B:495:TYR:HH	2.20	0.54
1:C:646:ARG:HG3	1:C:646:ARG:HH11	1.73	0.54
1:C:128:ILE:CD1	1:C:170:TYR:HD2	2.15	0.54
1:A:833:PHE:CE2	1:C:646:ARG:NH2	2.75	0.54
1:C:979:ASP:OD2	1:C:983:ARG:NH1	2.40	0.54
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.35	0.54
1:B:453:TYR:HB3	1:B:495:TYR:CZ	2.43	0.53
1:B:636:TYR:O	1:B:651:ILE:HG21	2.08	0.53
1:C:466:ARG:NH1	1:C:466:ARG:CG	2.71	0.53
1:A:328:ARG:NH1	1:A:531:THR:O	2.40	0.53
1:B:57:PRO:HB3	1:B:273:ARG:HH21	1.58	0.53
1:A:369:TYR:CE1	1:C:487:ASN:ND2	2.62	0.53
1:C:466:ARG:CZ	1:C:466:ARG:CB	2.86	0.53
1:A:634:ARG:HD3	1:A:634:ARG:N	2.22	0.52
1:A:900:MET:O	1:A:904:TYR:HD1	1.91	0.52
1:B:984:LEU:HD13	1:B:988:GLU:HG3	1.91	0.52
1:B:577:ARG:HD3	1:B:582:LEU:HD12	1.91	0.52
1:C:830:ASP:OD1	1:C:835:LYS:NZ	2.40	0.52
1:A:331:ASN:CB	1:A:580:GLN:HG2	2.40	0.52
1:B:453:TYR:HD1	1:B:495:TYR:CD2	2.26	0.51
1:C:954:HIS:CB	1:C:1014:ARG:NH1	2.72	0.51
1:C:830:ASP:OD2	1:C:835:LYS:NZ	2.43	0.51
1:C:328:ARG:NH2	1:C:580:GLN:HB2	2.27	0.50
1:C:353:TRP:CD1	1:C:466:ARG:HD3	2.46	0.50
1:A:417:ASN:HB2	1:A:421:TYR:CE2	2.44	0.50
1:B:110:LEU:C	1:B:135:PHE:HD2	2.19	0.50
1:A:331:ASN:OD1	2:E:1:NAG:N2	2.45	0.50
4:T:1:NAG:H61	4:T:2:NAG:HN2	1.76	0.50
1:C:905:ARG:HH11	1:C:1050:MET:HB3	1.64	0.50
1:C:466:ARG:NH1	1:C:466:ARG:CB	2.71	0.50
1:C:976:VAL:HB	1:C:979:ASP:HB2	1.94	0.50
1:C:129:LYS:HG3	1:C:169:GLU:CB	2.42	0.50
1:A:904:TYR:HE2	1:C:1107:ARG:HG2	1.76	0.49
1:C:830:ASP:CG	1:C:835:LYS:NZ	2.70	0.49
1:A:173:GLN:CD	1:A:173:GLN:H	2.21	0.49
1:C:634:ARG:HD3	1:C:634:ARG:H	1.76	0.49
1:A:972:ALA:CA	1:A:995:ARG:HD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:TYR:HB3	1:B:495:TYR:CE2	2.47	0.49
1:A:1155:TYR:HB3	1:C:1156:PHE:CZ	2.48	0.49
1:A:421:TYR:HB3	1:A:457:ARG:HG3	1.88	0.49
1:A:608:VAL:HG23	1:A:636:TYR:OH	2.12	0.49
1:B:239:GLN:NE2	1:B:240:THR:H	2.11	0.49
1:C:839:ASP:OD2	1:C:839:ASP:N	2.44	0.49
1:A:102:ARG:CZ	1:A:121:ASN:O	2.61	0.49
1:A:355:ARG:NH2	1:A:396:TYR:CG	2.73	0.49
1:A:369:TYR:HE1	1:C:487:ASN:CG	2.21	0.49
1:C:118:LEU:HD21	1:C:120:VAL:CG1	2.42	0.48
1:A:972:ALA:HB2	1:A:995:ARG:HD2	1.95	0.48
1:C:179:LEU:HD12	1:C:186:PHE:CD1	2.48	0.48
1:B:346:ARG:HA	1:B:509:ARG:HH21	1.78	0.48
1:B:453:TYR:CE1	1:B:493:ARG:O	2.66	0.48
1:C:403:ARG:HD3	1:C:505:HIS:O	2.13	0.48
1:B:347:PHE:CD1	1:B:509:ARG:HG2	2.49	0.47
1:A:295:PRO:HG2	1:A:636:TYR:CE1	2.49	0.47
1:B:190:ARG:CG	1:B:192:PHE:CE1	2.96	0.47
1:C:128:ILE:CG1	1:C:170:TYR:O	2.59	0.47
1:C:403:ARG:CD	1:C:505:HIS:O	2.62	0.47
1:B:190:ARG:CZ	1:B:192:PHE:CZ	2.91	0.47
1:A:417:ASN:O	1:A:421:TYR:HD2	1.94	0.47
1:A:1107:ARG:NH1	1:B:904:TYR:CD2	2.83	0.47
1:C:351:TYR:CE1	1:C:492:LEU:CD2	2.98	0.47
1:C:421:TYR:O	1:C:454:ARG:HD2	2.15	0.47
1:C:634:ARG:HG2	1:C:634:ARG:O	2.14	0.47
1:A:421:TYR:CA	1:A:457:ARG:HG3	2.46	0.46
1:A:813:SER:HB2	1:A:815:ARG:NH1	2.30	0.46
1:B:77:LYS:HG3	1:B:78:ARG:NH2	2.30	0.46
1:B:603:ASN:OD1	1:B:603:ASN:O	2.32	0.46
1:A:380:TYR:CE2	1:A:412:PRO:HG2	2.51	0.46
1:C:564:GLN:NE2	1:C:577:ARG:HG2	2.30	0.46
1:A:390:LEU:CD1	1:A:518:LEU:HD21	2.36	0.46
1:B:129:LYS:HD3	1:B:133:PHE:HZ	1.80	0.46
1:B:164:ASN:OD1	2:N:1:NAG:H62	2.15	0.46
1:C:617:CYS:O	1:C:621:PRO:CD	2.63	0.46
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.15	0.46
1:B:34:ARG:HD3	1:B:191:GLU:OE2	2.15	0.46
1:B:110:LEU:CB	1:B:135:PHE:CE2	2.98	0.46
1:B:453:TYR:CG	1:B:495:TYR:OH	2.69	0.46
1:B:559:PHE:HB2	1:B:577:ARG:NH2	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:MET:O	1:B:904:TYR:HD1	1.96	0.46
1:B:453:TYR:CD1	1:B:493:ARG:O	2.69	0.45
1:A:447:GLY:H	1:A:498:ARG:HG2	1.81	0.45
1:B:110:LEU:HD12	1:B:110:LEU:O	2.17	0.45
1:B:453:TYR:CD1	1:B:495:TYR:CD2	3.03	0.45
1:C:903:ALA:HB1	1:C:913:GLN:HE21	1.82	0.45
2:P:1:NAG:H62	2:P:2:NAG:H82	1.99	0.45
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.51	0.45
1:B:559:PHE:CB	1:B:577:ARG:NH2	2.77	0.45
1:C:453:TYR:CD1	1:C:495:TYR:OH	2.69	0.44
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.50	0.44
1:B:421:TYR:CD1	1:B:457:ARG:CB	2.96	0.44
1:A:833:PHE:CD1	1:C:646:ARG:HD2	2.53	0.44
1:B:78:ARG:NE	1:B:78:ARG:CA	2.80	0.44
1:A:34:ARG:HH21	1:A:217:PRO:HG2	1.82	0.44
1:C:127:VAL:HG13	1:C:127:VAL:O	2.18	0.44
1:B:901:GLN:HA	1:B:904:TYR:HD1	1.83	0.44
1:C:836:GLN:O	1:C:836:GLN:HG2	2.17	0.44
1:B:67:VAL:HG12	1:B:79:PHE:HA	2.00	0.43
1:C:179:LEU:CD1	1:C:186:PHE:CD1	3.02	0.43
1:C:634:ARG:N	1:C:634:ARG:CD	2.81	0.43
1:A:905:ARG:NH1	1:A:1050:MET:CB	2.76	0.43
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.99	0.43
1:A:453:TYR:CD1	1:A:493:ARG:O	2.72	0.43
5:B:1307:NAG:H83	1:C:794:ILE:HD11	2.01	0.43
1:B:110:LEU:HA	1:B:135:PHE:CD2	2.52	0.43
1:A:904:TYR:HD2	1:C:1107:ARG:HD3	1.64	0.42
1:C:176:LEU:HG	1:C:190:ARG:NE	2.35	0.42
1:C:625:HIS:CD2	1:C:634:ARG:HH22	2.38	0.42
1:C:844:ILE:HG22	1:C:847:ARG:NH2	2.35	0.42
1:A:157:PHE:CZ	1:A:159:VAL:HG22	2.55	0.42
1:A:904:TYR:CE2	1:C:1107:ARG:HG2	2.52	0.42
1:C:353:TRP:CE2	1:C:466:ARG:HD3	2.55	0.41
1:A:230:PRO:HB2	1:C:355:ARG:HD3	2.02	0.41
1:A:421:TYR:O	1:A:457:ARG:HG3	2.20	0.41
1:A:995:ARG:NH1	1:A:995:ARG:CG	2.73	0.41
1:B:57:PRO:CB	1:B:273:ARG:HH22	2.12	0.41
1:C:403:ARG:NH1	1:C:505:HIS:CD2	2.88	0.41
1:A:422:ASN:HA	1:A:461:LEU:HD21	2.01	0.41
1:B:110:LEU:O	1:B:135:PHE:HB2	2.20	0.41
1:A:102:ARG:HH22	1:A:122:ASN:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:O	1:C:102:ARG:CG	2.64	0.41
1:C:176:LEU:C	1:C:176:LEU:CD2	2.93	0.41
1:C:129:LYS:HD2	4:W:2:NAG:H81	2.02	0.41
1:A:417:ASN:CB	1:A:421:TYR:CE2	2.88	0.41
1:A:1050:MET:HE2	1:A:1052:PHE:CE1	2.55	0.41
1:B:995:ARG:HH22	1:C:994:ASP:CG	2.28	0.41
1:A:355:ARG:NE	1:A:396:TYR:CD2	2.83	0.40
1:C:176:LEU:HG	1:C:190:ARG:CZ	2.52	0.40
1:C:118:LEU:HD23	1:C:118:LEU:C	2.46	0.40

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1102/1270 (87%)	1015 (92%)	82 (7%)	5 (0%)	24	54
1	B	1111/1270 (88%)	1030 (93%)	73 (7%)	8 (1%)	18	47
1	C	1111/1270 (88%)	1014 (91%)	84 (8%)	13 (1%)	10	35
All	All	3324/3810 (87%)	3059 (92%)	239 (7%)	26 (1%)	18	44

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	449	TYR
1	B	32	PHE
1	C	830	ASP
1	A	333	THR
1	B	112	SER
1	B	134	GLN
1	C	836	GLN
1	C	837	TYR

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Mol	Chain	Res	Type
1	A	1107	ARG
1	C	20	THR
1	A	216	LEU
1	A	1041	ASP
1	B	216	LEU
1	B	337	PRO
1	B	623	ALA
1	B	830	ASP
1	C	123	ALA
1	C	375	PHE
1	B	214(A)	GLU
1	C	182	LYS
1	C	337	PRO
1	C	518	LEU
1	C	582	LEU
1	C	986	LYS
1	C	625	HIS
1	C	757	GLY

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	971/1112 (87%)	948 (98%)	23 (2%)	43	62
1	B	978/1112 (88%)	961 (98%)	17 (2%)	53	67
1	C	978/1112 (88%)	942 (96%)	36 (4%)	30	55
All	All	2927/3336 (88%)	2851 (97%)	76 (3%)	41	61

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	90	VAL
1	A	120	VAL
1	A	159	VAL

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Mol	Chain	Res	Type
1	A	200	TYR
1	A	214	ARG
1	A	214(A)	GLU
1	A	214(B)	PRO
1	A	214(C)	GLU
1	A	318	PHE
1	A	319	ARG
1	A	335	LEU
1	A	377	PHE
1	A	461	LEU
1	A	506	GLN
1	A	535	LYS
1	A	748	GLU
1	A	754	LEU
1	A	935	GLN
1	A	990	GLU
1	A	995	ARG
1	A	1019	ARG
1	A	1148	PHE
1	B	105	ILE
1	B	203	ILE
1	B	231	ILE
1	B	275	PHE
1	B	332	ILE
1	B	350	VAL
1	B	390	LEU
1	B	422	ASN
1	B	461	LEU
1	B	480	CYS
1	B	518	LEU
1	B	574	ASP
1	B	618	THR
1	B	629	LEU
1	B	754	LEU
1	B	755	GLN
1	B	985	ASP
1	C	34	ARG
1	C	79	PHE
1	C	97	LYS
1	C	117	LEU
1	C	154	GLU
1	C	159	VAL

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Mol	Chain	Res	Type
1	C	164	ASN
1	C	179	LEU
1	C	204	TYR
1	C	226	LEU
1	C	365	TYR
1	C	377	PHE
1	C	394	ASN
1	C	422	ASN
1	C	461	LEU
1	C	466	ARG
1	C	511	VAL
1	C	517	LEU
1	C	523	THR
1	C	534	VAL
1	C	577	ARG
1	C	583	GLU
1	C	603	ASN
1	C	634	ARG
1	C	646	ARG
1	C	697	MET
1	C	763	LEU
1	C	841	LEU
1	C	1002	GLN
1	C	1019	ARG
1	C	1072	GLU
1	C	1116	THR
1	C	1119	ASN
1	C	1141	LEU
1	C	1145	LEU
1	C	1149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	388	ASN
1	A	394	ASN
1	A	505	HIS
1	A	613	GLN
1	A	690	GLN
1	A	914	ASN
1	A	925	ASN

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Mol	Chain	Res	Type
1	A	935	GLN
1	A	955	ASN
1	A	1010	GLN
1	B	30	ASN
1	B	134	GLN
1	B	137	ASN
1	B	207	HIS
1	B	239	GLN
1	B	370	ASN
1	B	409	GLN
1	B	450	ASN
1	B	460	ASN
1	B	505	HIS
1	B	784	GLN
1	B	953	ASN
1	B	960	ASN
1	B	1002	GLN
1	B	1058	HIS
1	C	164	ASN
1	C	334	ASN
1	C	394	ASN
1	C	505	HIS
1	C	544	ASN
1	C	556	ASN
1	C	564	GLN
1	C	613	GLN
1	C	625	HIS
1	C	677	GLN
1	C	690	GLN
1	C	762	GLN
1	C	913	GLN
1	C	1002	GLN
1	C	1005	GLN
1	C	1058	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 ⓘ

76 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	D	1	2,1	14,14,15	1.35	3 (21%)	17,19,21	1.20	1 (5%)
2	NAG	D	2	2	14,14,15	1.17	2 (14%)	17,19,21	0.90	0
2	NAG	E	1	2,1	14,14,15	1.21	1 (7%)	17,19,21	1.02	1 (5%)
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	F	1	2,1	14,14,15	1.26	3 (21%)	17,19,21	1.06	1 (5%)
2	NAG	F	2	2	14,14,15	1.38	2 (14%)	17,19,21	0.80	1 (5%)
2	NAG	G	1	2,1	14,14,15	1.23	2 (14%)	17,19,21	0.86	0
2	NAG	G	2	2	14,14,15	1.19	2 (14%)	17,19,21	0.81	1 (5%)
2	NAG	H	1	2,1	14,14,15	1.02	1 (7%)	17,19,21	0.79	0
2	NAG	H	2	2	14,14,15	1.34	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	I	1	1,3	14,14,15	1.32	1 (7%)	17,19,21	0.85	0
3	NAG	I	2	3	14,14,15	1.23	1 (7%)	17,19,21	0.86	1 (5%)
3	FUC	I	3	3	10,10,11	1.55	2 (20%)	14,14,16	1.15	2 (14%)
4	NAG	J	1	4,1	14,14,15	1.17	1 (7%)	17,19,21	1.02	2 (11%)
4	NAG	J	2	4	14,14,15	1.12	1 (7%)	17,19,21	0.77	1 (5%)
4	MAN	J	3	4	11,11,12	1.61	2 (18%)	15,15,17	0.77	0
4	NAG	K	1	4,1	14,14,15	1.05	1 (7%)	17,19,21	0.92	0
4	NAG	K	2	4	14,14,15	1.16	1 (7%)	17,19,21	0.93	1 (5%)
4	MAN	K	3	4	11,11,12	1.57	2 (18%)	15,15,17	1.18	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	L	2	2	14,14,15	1.12	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	M	1	4,1	14,14,15	1.37	2 (14%)	17,19,21	0.95	1 (5%)
4	NAG	M	2	4	14,14,15	1.45	3 (21%)	17,19,21	1.12	1 (5%)
4	MAN	M	3	4	11,11,12	1.40	2 (18%)	15,15,17	1.31	1 (6%)
2	NAG	N	1	2,1	14,14,15	0.27	0	17,19,21	0.39	0
2	NAG	N	2	2	14,14,15	1.13	1 (7%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	O	1	4,1	14,14,15	1.40	2 (14%)	17,19,21	1.83	2 (11%)
4	NAG	O	2	4	14,14,15	1.33	2 (14%)	17,19,21	0.94	1 (5%)
4	MAN	O	3	4	11,11,12	1.57	2 (18%)	15,15,17	0.91	1 (6%)
2	NAG	P	1	2,1	14,14,15	0.17	0	17,19,21	0.49	0
2	NAG	P	2	2	14,14,15	1.03	1 (7%)	17,19,21	0.75	0
4	NAG	Q	1	4,1	14,14,15	1.23	2 (14%)	17,19,21	1.03	0
4	NAG	Q	2	4	14,14,15	1.30	2 (14%)	17,19,21	1.00	1 (5%)
4	MAN	Q	3	4	11,11,12	1.57	2 (18%)	15,15,17	1.32	1 (6%)
4	NAG	R	1	4,1	14,14,15	1.04	2 (14%)	17,19,21	0.58	0
4	NAG	R	2	4	14,14,15	1.26	1 (7%)	17,19,21	1.07	2 (11%)
4	MAN	R	3	4	11,11,12	1.37	1 (9%)	15,15,17	0.80	0
3	NAG	S	1	1,3	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	S	2	3	14,14,15	1.10	1 (7%)	17,19,21	1.04	1 (5%)
3	FUC	S	3	3	10,10,11	1.33	1 (10%)	14,14,16	1.13	2 (14%)
4	NAG	T	1	4,1	14,14,15	1.41	2 (14%)	17,19,21	1.16	1 (5%)
4	NAG	T	2	4	14,14,15	1.30	2 (14%)	17,19,21	0.96	1 (5%)
4	MAN	T	3	4	11,11,12	1.52	2 (18%)	15,15,17	1.26	2 (13%)
4	NAG	U	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	0.67	0
4	NAG	U	2	4	14,14,15	1.31	3 (21%)	17,19,21	1.01	1 (5%)
4	MAN	U	3	4	11,11,12	1.71	2 (18%)	15,15,17	1.12	1 (6%)
2	NAG	V	1	2,1	14,14,15	1.25	2 (14%)	17,19,21	1.04	1 (5%)
2	NAG	V	2	2	14,14,15	1.34	2 (14%)	17,19,21	1.17	1 (5%)
4	NAG	W	1	4,1	14,14,15	1.06	1 (7%)	17,19,21	1.84	2 (11%)
4	NAG	W	2	4	14,14,15	1.34	3 (21%)	17,19,21	1.18	1 (5%)
4	MAN	W	3	4	11,11,12	1.40	2 (18%)	15,15,17	0.97	1 (6%)
2	NAG	X	1	2,1	14,14,15	0.17	0	17,19,21	0.48	0
2	NAG	X	2	2	14,14,15	1.22	1 (7%)	17,19,21	0.84	0
4	NAG	Y	1	4,1	14,14,15	0.35	0	17,19,21	0.53	0
4	NAG	Y	2	4	14,14,15	1.10	2 (14%)	17,19,21	0.95	1 (5%)
4	MAN	Y	3	4	11,11,12	1.51	2 (18%)	15,15,17	0.90	1 (6%)
4	NAG	Z	1	4,1	14,14,15	1.35	3 (21%)	17,19,21	0.80	0
4	NAG	Z	2	4	14,14,15	1.39	3 (21%)	17,19,21	0.95	2 (11%)
4	MAN	Z	3	4	11,11,12	1.68	2 (18%)	15,15,17	0.84	0
2	NAG	a	1	2,1	14,14,15	1.34	2 (14%)	17,19,21	0.82	0
2	NAG	a	2	2	14,14,15	1.33	1 (7%)	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	b	1	4,1	14,14,15	1.25	3 (21%)	17,19,21	0.99	2 (11%)
4	NAG	b	2	4	14,14,15	1.32	2 (14%)	17,19,21	0.65	0
4	MAN	b	3	4	11,11,12	1.61	2 (18%)	15,15,17	1.34	1 (6%)
4	NAG	c	1	4,1	14,14,15	1.10	1 (7%)	17,19,21	0.66	0
4	NAG	c	2	4	14,14,15	1.37	3 (21%)	17,19,21	0.98	1 (5%)
4	MAN	c	3	4	11,11,12	1.33	1 (9%)	15,15,17	0.87	0
3	NAG	d	1	1,3	14,14,15	0.35	0	17,19,21	0.47	0
3	NAG	d	2	3	14,14,15	1.05	1 (7%)	17,19,21	0.81	1 (5%)
3	FUC	d	3	3	10,10,11	1.45	2 (20%)	14,14,16	1.31	2 (14%)
4	NAG	e	1	4,1	14,14,15	1.11	1 (7%)	17,19,21	1.10	2 (11%)
4	NAG	e	2	4	14,14,15	1.28	2 (14%)	17,19,21	1.00	2 (11%)
4	MAN	e	3	4	11,11,12	1.40	2 (18%)	15,15,17	1.05	2 (13%)
4	NAG	f	1	4,1	14,14,15	1.33	3 (21%)	17,19,21	0.75	0
4	NAG	f	2	4	14,14,15	1.29	2 (14%)	17,19,21	0.69	0
4	MAN	f	3	4	11,11,12	1.65	2 (18%)	15,15,17	1.16	2 (13%)

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	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	MAN	J	3	4	-	1/2/19/22	1/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	MAN	K	3	4	-	1/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	MAN	M	3	4	-	1/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	MAN	O	3	4	-	0/2/19/22	1/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	MAN	Q	3	4	-	0/2/19/22	1/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	MAN	R	3	4	-	1/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	FUC	S	3	3	-	-	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	MAN	T	3	4	-	1/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	MAN	U	3	4	-	0/2/19/22	1/1/1/1
2	NAG	V	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	MAN	W	3	4	-	1/2/19/22	0/1/1/1
2	NAG	X	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	MAN	Y	3	4	-	0/2/19/22	1/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	Z	3	4	-	0/2/19/22	1/1/1/1
2	NAG	a	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	1/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	MAN	b	3	4	-	0/2/19/22	1/1/1/1
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	MAN	c	3	4	-	1/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	0/6/23/26	0/1/1/1
3	FUC	d	3	3	-	-	0/1/1/1
4	NAG	e	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	MAN	e	3	4	-	0/2/19/22	1/1/1/1
4	NAG	f	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
4	MAN	f	3	4	-	0/2/19/22	1/1/1/1

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-4.59	1.36	1.43
2	E	1	NAG	O5-C1	-4.12	1.36	1.43
2	X	2	NAG	O5-C5	3.82	1.50	1.43
4	f	3	MAN	O5-C5	3.58	1.50	1.43
4	Z	3	MAN	O5-C5	3.55	1.50	1.43
4	U	3	MAN	O5-C5	3.50	1.50	1.43
4	J	3	MAN	O5-C5	3.43	1.50	1.43
4	K	3	MAN	O5-C5	3.37	1.50	1.43
4	T	2	NAG	O5-C5	3.31	1.49	1.43
2	H	2	NAG	O5-C5	3.31	1.49	1.43
4	Z	3	MAN	O5-C1	3.28	1.49	1.43
4	M	1	NAG	O5-C5	3.24	1.49	1.43
4	b	3	MAN	O5-C5	3.24	1.49	1.43
2	V	2	NAG	O5-C5	3.24	1.49	1.43
4	O	3	MAN	O5-C5	3.23	1.49	1.43
3	S	2	NAG	O5-C5	3.22	1.49	1.43
2	V	1	NAG	O5-C5	3.20	1.49	1.43
4	Y	3	MAN	O5-C5	3.14	1.49	1.43
4	Q	3	MAN	O5-C5	3.14	1.49	1.43
2	F	2	NAG	O5-C5	3.13	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	3	FUC	O5-C5	3.07	1.49	1.43
2	a	2	NAG	O5-C5	3.04	1.49	1.43
2	a	1	NAG	O5-C5	3.01	1.49	1.43
4	e	3	MAN	O5-C5	2.98	1.49	1.43
4	O	2	NAG	O5-C5	2.96	1.49	1.43
4	c	3	MAN	O5-C5	2.93	1.49	1.43
4	b	2	NAG	O4-C4	2.92	1.50	1.43
4	M	2	NAG	O4-C4	2.89	1.50	1.43
4	W	3	MAN	O5-C5	2.88	1.49	1.43
4	c	2	NAG	O5-C5	2.85	1.49	1.43
4	T	3	MAN	O5-C1	2.84	1.48	1.43
4	f	3	MAN	O5-C1	2.81	1.48	1.43
3	I	3	FUC	O5-C5	2.80	1.49	1.43
4	J	3	MAN	O5-C1	2.80	1.48	1.43
4	Q	2	NAG	O5-C5	2.77	1.48	1.43
4	e	2	NAG	O5-C5	2.75	1.48	1.43
4	M	3	MAN	O5-C5	2.74	1.48	1.43
4	b	3	MAN	O5-C1	2.74	1.48	1.43
3	I	2	NAG	O5-C5	2.74	1.48	1.43
4	T	3	MAN	O5-C5	2.73	1.48	1.43
4	Z	1	NAG	C1-C2	2.73	1.56	1.52
4	W	3	MAN	O5-C1	2.72	1.48	1.43
3	I	1	NAG	O5-C5	2.70	1.48	1.43
2	G	2	NAG	O5-C5	2.70	1.48	1.43
4	R	3	MAN	O5-C5	2.70	1.48	1.43
2	P	2	NAG	O5-C5	2.67	1.48	1.43
4	Q	1	NAG	O5-C5	2.66	1.48	1.43
3	d	2	NAG	O5-C5	2.65	1.48	1.43
4	Z	2	NAG	O5-C5	2.64	1.48	1.43
4	O	1	NAG	O5-C5	2.64	1.48	1.43
4	f	1	NAG	O5-C5	2.62	1.48	1.43
4	K	3	MAN	O5-C1	2.60	1.48	1.43
2	D	2	NAG	O5-C5	2.59	1.48	1.43
4	O	1	NAG	C8-C7	2.58	1.55	1.50
4	f	1	NAG	O5-C1	2.57	1.48	1.43
4	Y	2	NAG	O5-C5	2.54	1.48	1.43
4	T	2	NAG	O4-C4	2.54	1.49	1.43
2	G	1	NAG	O5-C5	2.53	1.48	1.43
4	O	3	MAN	O5-C1	2.52	1.47	1.43
4	Q	2	NAG	O4-C4	2.51	1.49	1.43
4	b	1	NAG	O5-C5	2.49	1.48	1.43
4	U	3	MAN	O5-C1	2.47	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C5	2.46	1.48	1.43
4	W	2	NAG	O5-C1	2.43	1.47	1.43
2	H	1	NAG	O5-C5	2.42	1.48	1.43
4	K	1	NAG	O5-C5	2.42	1.48	1.43
2	D	1	NAG	O5-C5	2.42	1.48	1.43
4	U	1	NAG	O5-C5	2.41	1.48	1.43
4	R	2	NAG	O5-C5	2.41	1.48	1.43
4	f	2	NAG	O5-C5	2.41	1.48	1.43
3	I	3	FUC	O5-C1	2.40	1.47	1.43
4	W	1	NAG	O5-C5	2.39	1.48	1.43
4	e	3	MAN	O5-C1	2.36	1.47	1.43
4	U	2	NAG	O5-C5	2.36	1.48	1.43
3	S	3	FUC	O5-C5	2.35	1.48	1.43
2	N	2	NAG	O5-C5	2.35	1.48	1.43
2	L	2	NAG	O5-C5	2.33	1.48	1.43
4	T	1	NAG	C1-C2	-2.33	1.49	1.52
4	Z	1	NAG	O4-C4	2.32	1.48	1.43
4	J	1	NAG	O5-C5	2.31	1.47	1.43
4	R	1	NAG	O5-C5	2.31	1.47	1.43
2	H	2	NAG	C8-C7	2.30	1.55	1.50
4	W	2	NAG	O5-C5	2.29	1.47	1.43
4	W	2	NAG	C1-C2	2.26	1.55	1.52
2	F	1	NAG	O5-C5	2.26	1.47	1.43
2	D	2	NAG	O5-C1	2.26	1.47	1.43
4	M	2	NAG	O5-C5	2.26	1.47	1.43
4	U	2	NAG	O4-C4	2.25	1.48	1.43
4	c	1	NAG	O5-C5	2.24	1.47	1.43
4	b	1	NAG	O5-C1	2.22	1.47	1.43
4	c	2	NAG	O4-C4	2.21	1.48	1.43
2	V	1	NAG	C8-C7	2.20	1.55	1.50
4	Z	2	NAG	O4-C4	2.19	1.48	1.43
4	Z	2	NAG	O5-C1	2.19	1.47	1.43
4	M	3	MAN	O5-C1	2.18	1.47	1.43
4	f	2	NAG	O4-C4	2.17	1.48	1.43
4	e	2	NAG	O5-C1	2.16	1.47	1.43
4	U	2	NAG	C8-C7	2.16	1.55	1.50
2	G	1	NAG	O4-C4	2.15	1.48	1.43
2	a	1	NAG	O4-C4	2.14	1.48	1.43
4	c	2	NAG	O5-C1	2.14	1.47	1.43
4	Q	3	MAN	O5-C1	2.13	1.47	1.43
4	O	2	NAG	O4-C4	2.12	1.48	1.43
4	K	2	NAG	O5-C5	2.11	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	1	NAG	O5-C5	2.10	1.47	1.43
2	F	2	NAG	O5-C1	2.10	1.47	1.43
4	Y	2	NAG	O4-C4	2.10	1.48	1.43
4	b	1	NAG	C1-C2	2.09	1.55	1.52
3	d	3	FUC	C2-C3	2.09	1.55	1.52
2	F	1	NAG	O4-C4	2.08	1.48	1.43
4	M	1	NAG	C1-C2	2.06	1.55	1.52
4	b	2	NAG	O5-C5	2.06	1.47	1.43
2	D	1	NAG	O4-C4	2.06	1.48	1.43
4	Q	1	NAG	C1-C2	2.05	1.55	1.52
2	D	1	NAG	C1-C2	2.05	1.55	1.52
4	R	1	NAG	O4-C4	2.05	1.48	1.43
4	e	1	NAG	O5-C5	2.03	1.47	1.43
2	V	2	NAG	C8-C7	2.02	1.54	1.50
2	F	1	NAG	C1-C2	2.01	1.55	1.52
2	G	2	NAG	C8-C7	2.01	1.54	1.50
4	M	2	NAG	O5-C1	2.01	1.47	1.43
4	Y	3	MAN	O5-C1	2.01	1.47	1.43
4	f	1	NAG	O4-C4	2.00	1.47	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	1	NAG	C1-O5-C5	6.45	120.83	112.19
4	O	1	NAG	C1-O5-C5	6.34	120.69	112.19
4	b	3	MAN	C1-O5-C5	4.45	118.15	112.19
4	Q	3	MAN	C1-O5-C5	4.30	117.95	112.19
2	V	2	NAG	C1-O5-C5	3.76	117.23	112.19
4	W	2	NAG	C4-C3-C2	-3.62	105.72	111.02
4	T	1	NAG	C3-C4-C5	3.51	116.60	110.23
4	M	3	MAN	C1-O5-C5	3.35	116.68	112.19
4	R	2	NAG	C1-O5-C5	3.22	116.51	112.19
3	d	3	FUC	C1-C2-C3	3.21	114.32	109.64
4	T	2	NAG	C1-O5-C5	3.20	116.47	112.19
4	c	2	NAG	C1-O5-C5	3.16	116.42	112.19
4	f	3	MAN	C1-O5-C5	3.07	116.29	112.19
3	S	2	NAG	C1-O5-C5	2.97	116.17	112.19
4	U	3	MAN	C1-O5-C5	2.91	116.08	112.19
4	K	2	NAG	C1-O5-C5	2.88	116.04	112.19
4	Q	2	NAG	O5-C1-C2	-2.79	106.97	111.29
4	U	2	NAG	C1-O5-C5	2.78	115.91	112.19
4	Y	2	NAG	C1-O5-C5	2.78	115.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	3	MAN	C1-O5-C5	2.77	115.89	112.19
4	O	2	NAG	C1-O5-C5	2.76	115.89	112.19
4	K	3	MAN	C1-C2-C3	2.75	113.65	109.64
2	E	1	NAG	C3-C4-C5	2.70	115.13	110.23
2	F	1	NAG	C1-O5-C5	2.65	115.73	112.19
3	d	3	FUC	O5-C5-C4	2.65	114.31	109.55
2	a	2	NAG	C1-O5-C5	2.63	115.71	112.19
4	O	3	MAN	C1-O5-C5	2.60	115.67	112.19
4	R	2	NAG	C4-C3-C2	-2.59	107.22	111.02
4	J	1	NAG	C1-O5-C5	2.58	115.64	112.19
4	Y	3	MAN	C1-O5-C5	2.53	115.57	112.19
2	F	2	NAG	C1-O5-C5	2.53	115.57	112.19
4	e	2	NAG	C1-O5-C5	2.49	115.52	112.19
2	H	2	NAG	C1-O5-C5	2.43	115.45	112.19
4	b	1	NAG	C1-O5-C5	2.42	115.44	112.19
2	V	1	NAG	C1-O5-C5	2.42	115.43	112.19
2	L	2	NAG	C1-O5-C5	2.41	115.42	112.19
3	S	3	FUC	C1-O5-C5	2.40	118.64	112.97
2	N	2	NAG	C1-O5-C5	2.39	115.39	112.19
4	M	2	NAG	C1-O5-C5	2.38	115.37	112.19
4	Z	2	NAG	C4-C3-C2	-2.35	107.57	111.02
4	T	3	MAN	C1-O5-C5	2.29	115.25	112.19
3	I	3	FUC	C6-C5-C4	2.28	117.25	113.08
4	e	1	NAG	C3-C4-C5	2.26	114.33	110.23
2	D	1	NAG	C3-C4-C5	2.25	114.32	110.23
3	I	3	FUC	C1-C2-C3	2.25	112.92	109.64
4	J	1	NAG	C3-C4-C5	2.25	114.31	110.23
4	O	1	NAG	C3-C4-C5	2.24	114.30	110.23
4	M	1	NAG	C1-O5-C5	2.23	115.17	112.19
2	G	2	NAG	O5-C1-C2	-2.21	107.87	111.29
4	W	1	NAG	C2-N2-C7	-2.20	119.95	122.90
4	e	3	MAN	O5-C5-C6	2.16	111.86	107.66
4	Z	2	NAG	C1-O5-C5	2.15	115.07	112.19
3	I	2	NAG	O5-C1-C2	-2.15	107.97	111.29
4	J	2	NAG	O5-C1-C2	-2.14	107.98	111.29
4	W	3	MAN	C1-O5-C5	2.14	115.05	112.19
4	e	1	NAG	O4-C4-C3	-2.14	105.34	110.38
3	S	3	FUC	C1-C2-C3	2.12	112.73	109.64
3	d	2	NAG	C1-O5-C5	2.10	115.01	112.19
4	e	2	NAG	C4-C3-C2	-2.09	107.95	111.02
4	f	3	MAN	C1-C2-C3	2.07	112.67	109.64
4	b	1	NAG	O4-C4-C3	-2.06	105.52	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	3	MAN	C3-C4-C5	2.05	113.95	110.23

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	1	NAG	C1-C2-N2-C7
3	I	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
4	M	3	MAN	O5-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
4	J	3	MAN	O5-C5-C6-O6
4	W	3	MAN	O5-C5-C6-O6
4	T	3	MAN	O5-C5-C6-O6
4	c	3	MAN	O5-C5-C6-O6
4	R	3	MAN	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
2	P	2	NAG	C1-C2-N2-C7
2	a	2	NAG	C1-C2-N2-C7
3	S	2	NAG	C1-C2-N2-C7
4	U	1	NAG	C1-C2-N2-C7
4	Y	1	NAG	C1-C2-N2-C7
4	b	1	NAG	C1-C2-N2-C7
2	V	1	NAG	C3-C2-N2-C7
3	S	2	NAG	C3-C2-N2-C7
4	M	1	NAG	O5-C5-C6-O6
4	K	3	MAN	O5-C5-C6-O6

All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	3	MAN	C1-C2-C3-C4-C5-O5
4	U	3	MAN	C1-C2-C3-C4-C5-O5
4	Z	3	MAN	C1-C2-C3-C4-C5-O5

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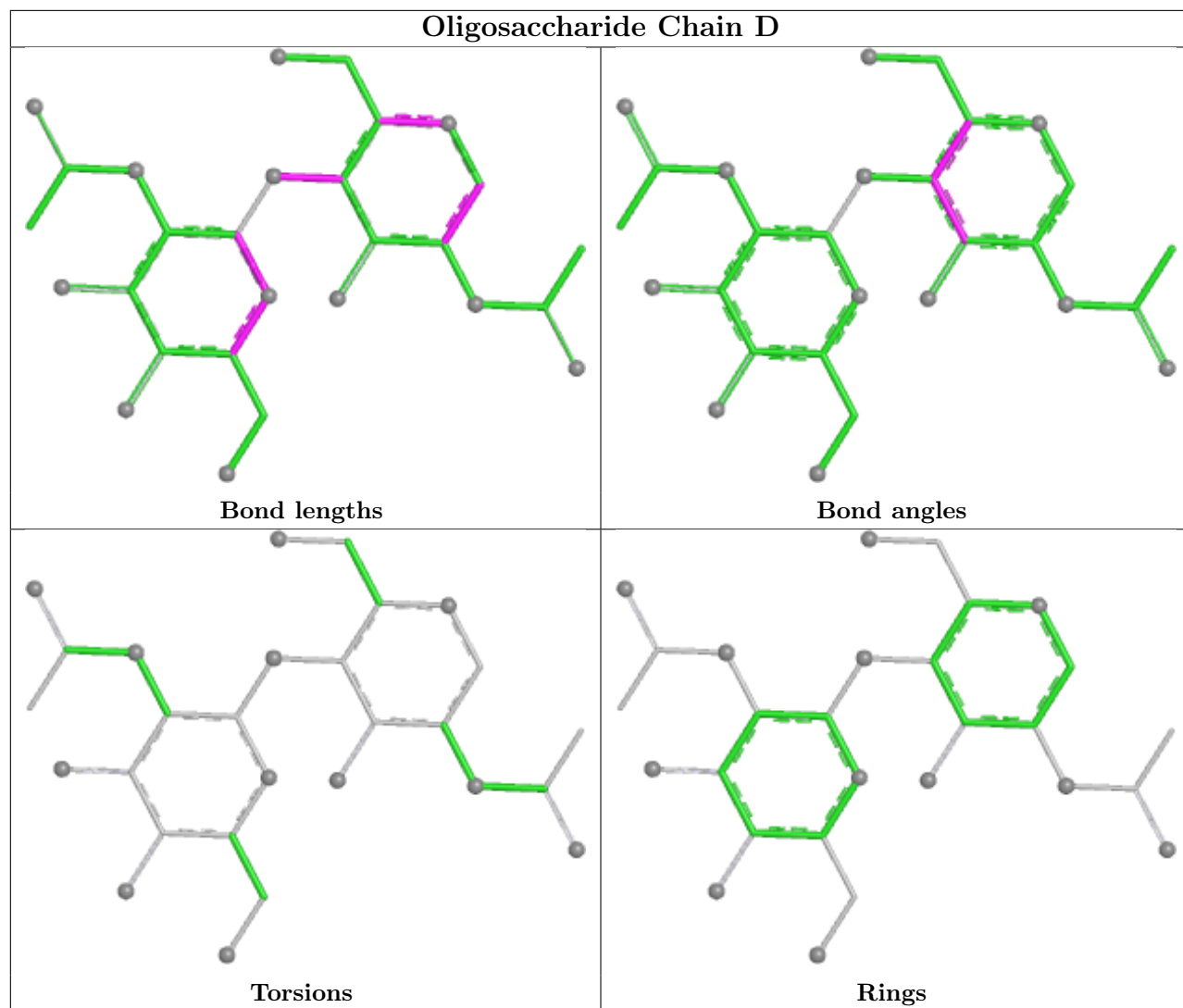
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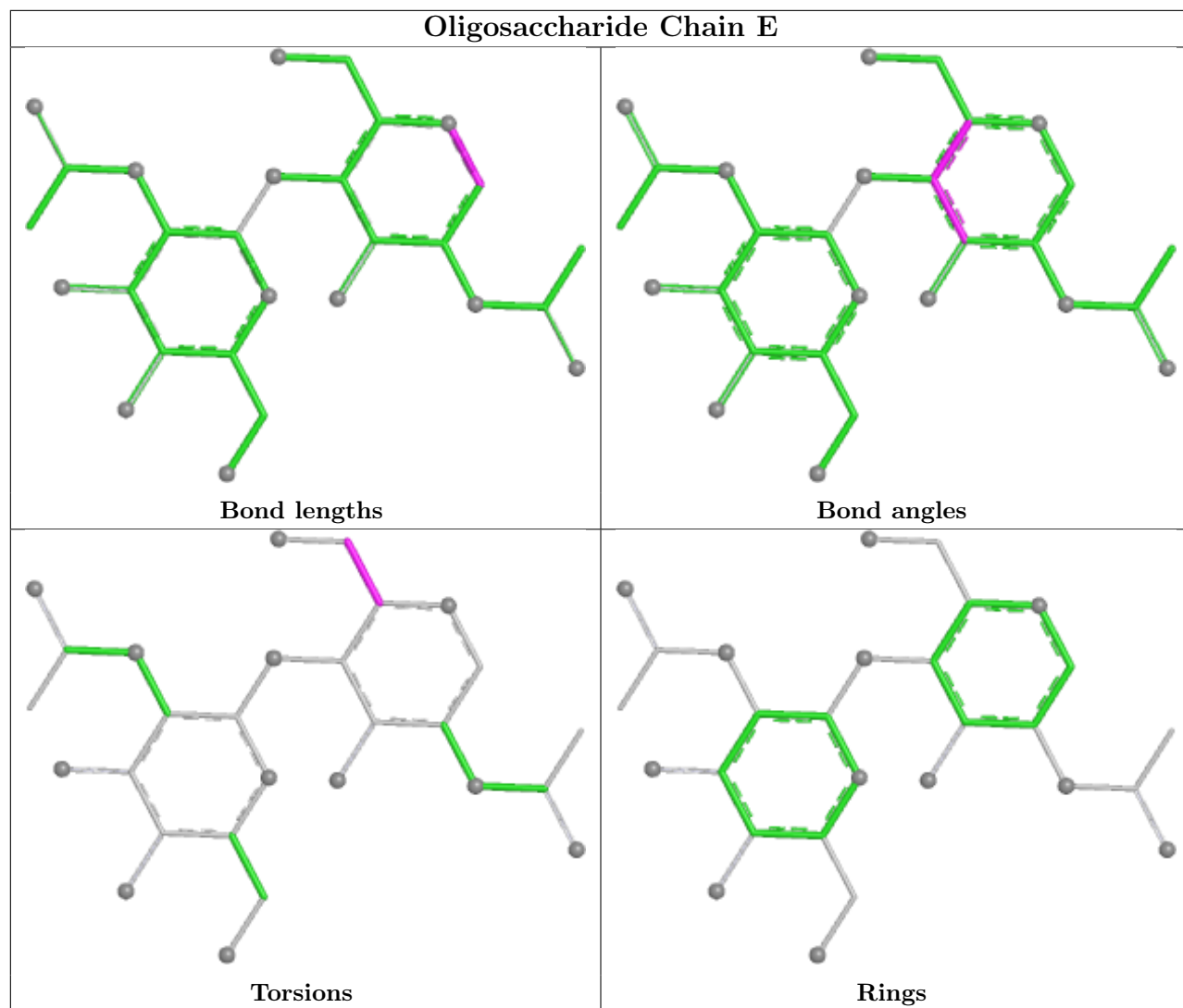
Mol	Chain	Res	Type	Atoms
4	Q	3	MAN	C1-C2-C3-C4-C5-O5
4	f	3	MAN	C1-C2-C3-C4-C5-O5
4	J	3	MAN	C1-C2-C3-C4-C5-O5
4	e	3	MAN	C1-C2-C3-C4-C5-O5
4	b	3	MAN	C1-C2-C3-C4-C5-O5
4	O	3	MAN	C1-C2-C3-C4-C5-O5

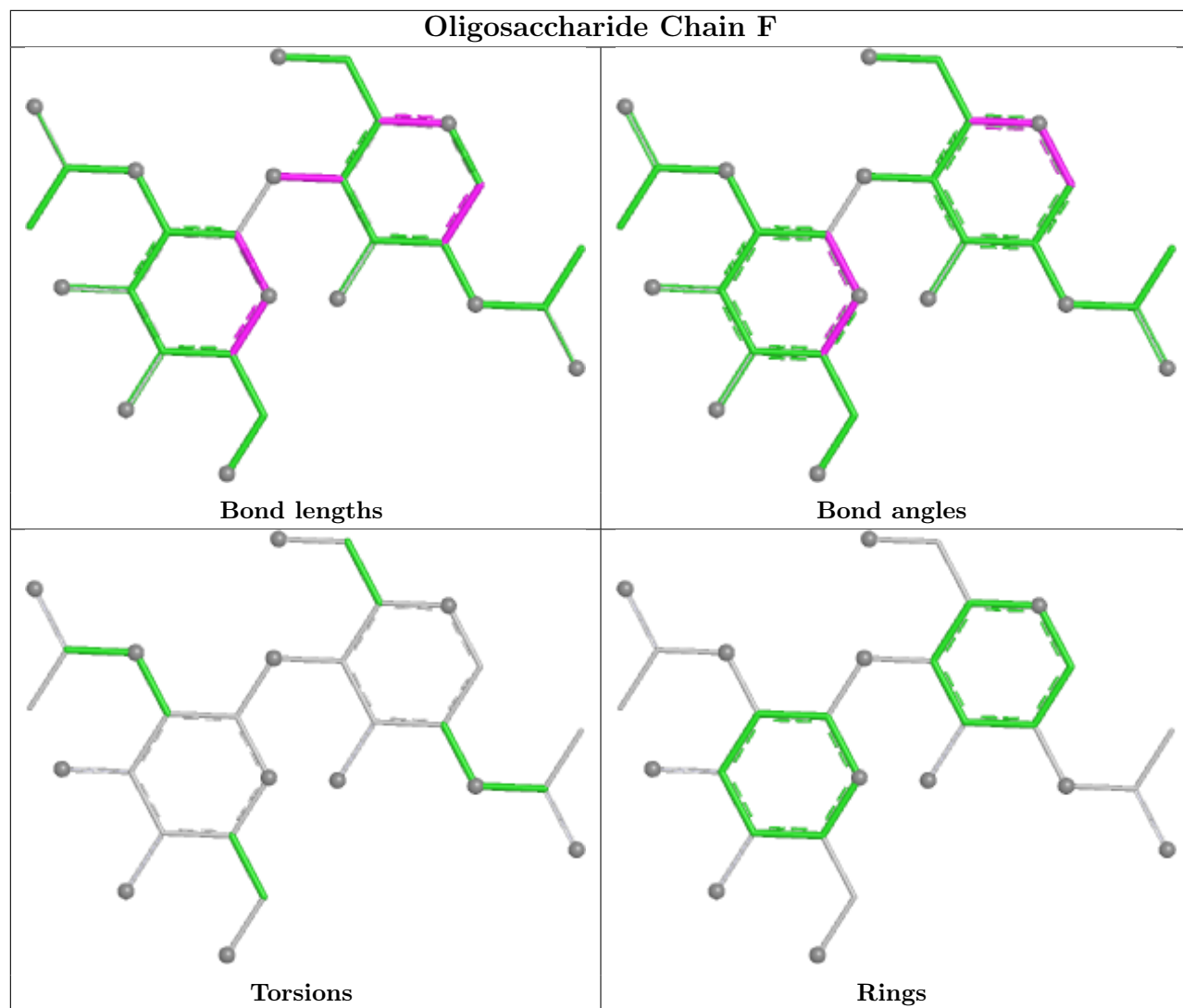
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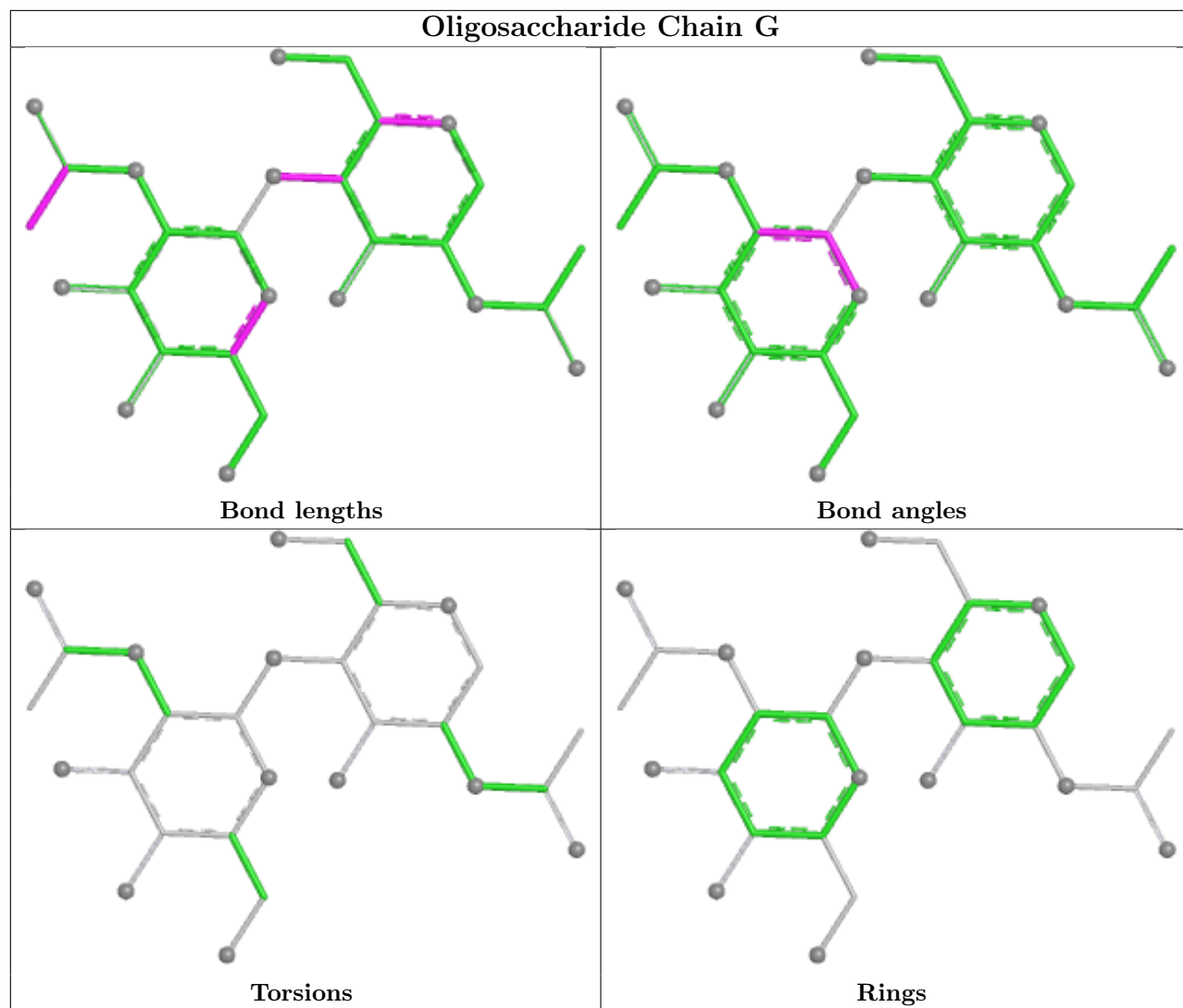
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	2	NAG	2	0
2	P	1	NAG	2	0
2	P	2	NAG	1	0
2	E	1	NAG	3	0
3	S	1	NAG	1	0
2	V	1	NAG	1	0
4	T	1	NAG	1	0
4	W	1	NAG	2	0
2	N	1	NAG	1	0
4	Y	1	NAG	3	0
2	E	2	NAG	1	0
3	S	2	NAG	1	0
4	T	2	NAG	1	0

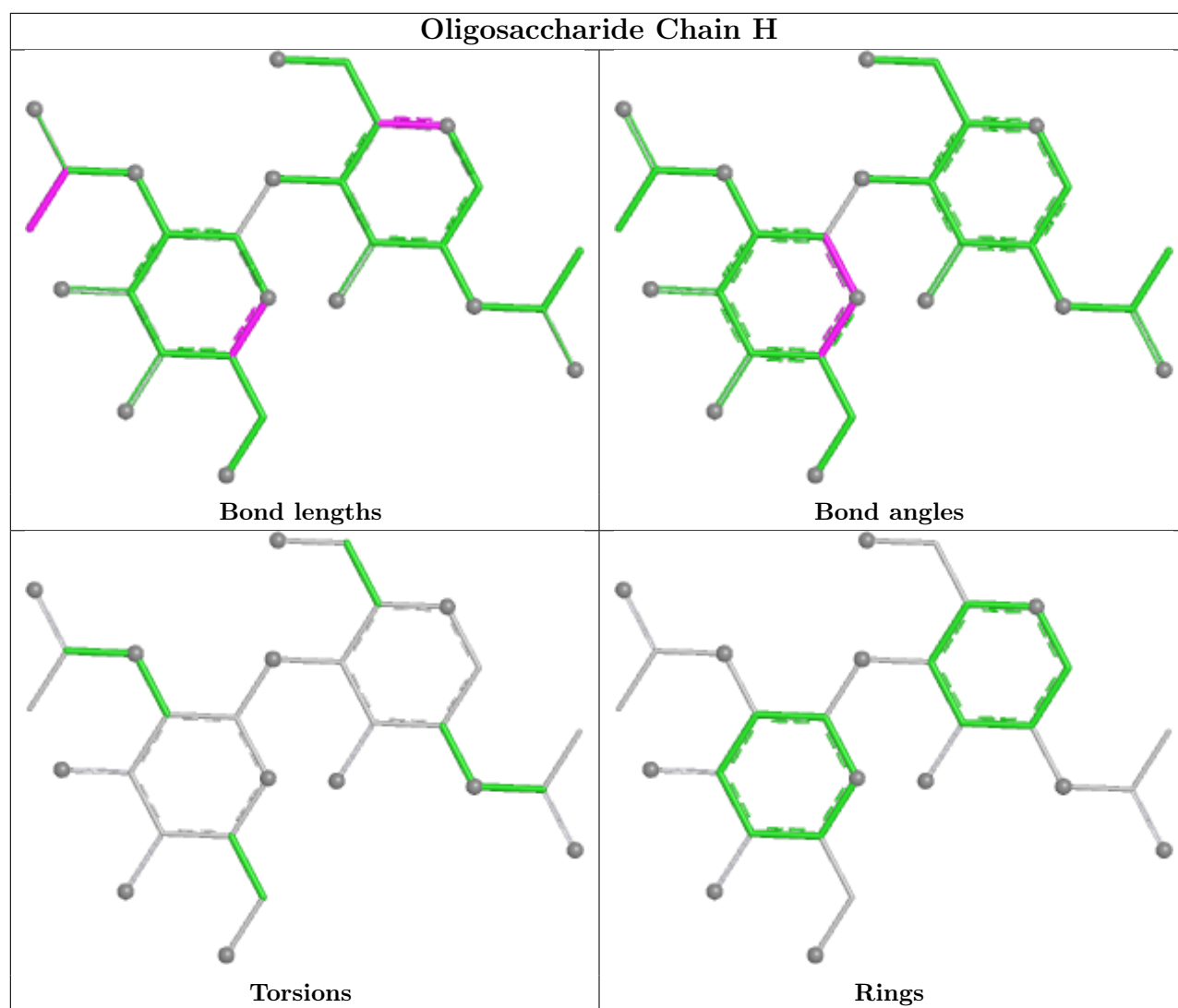
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

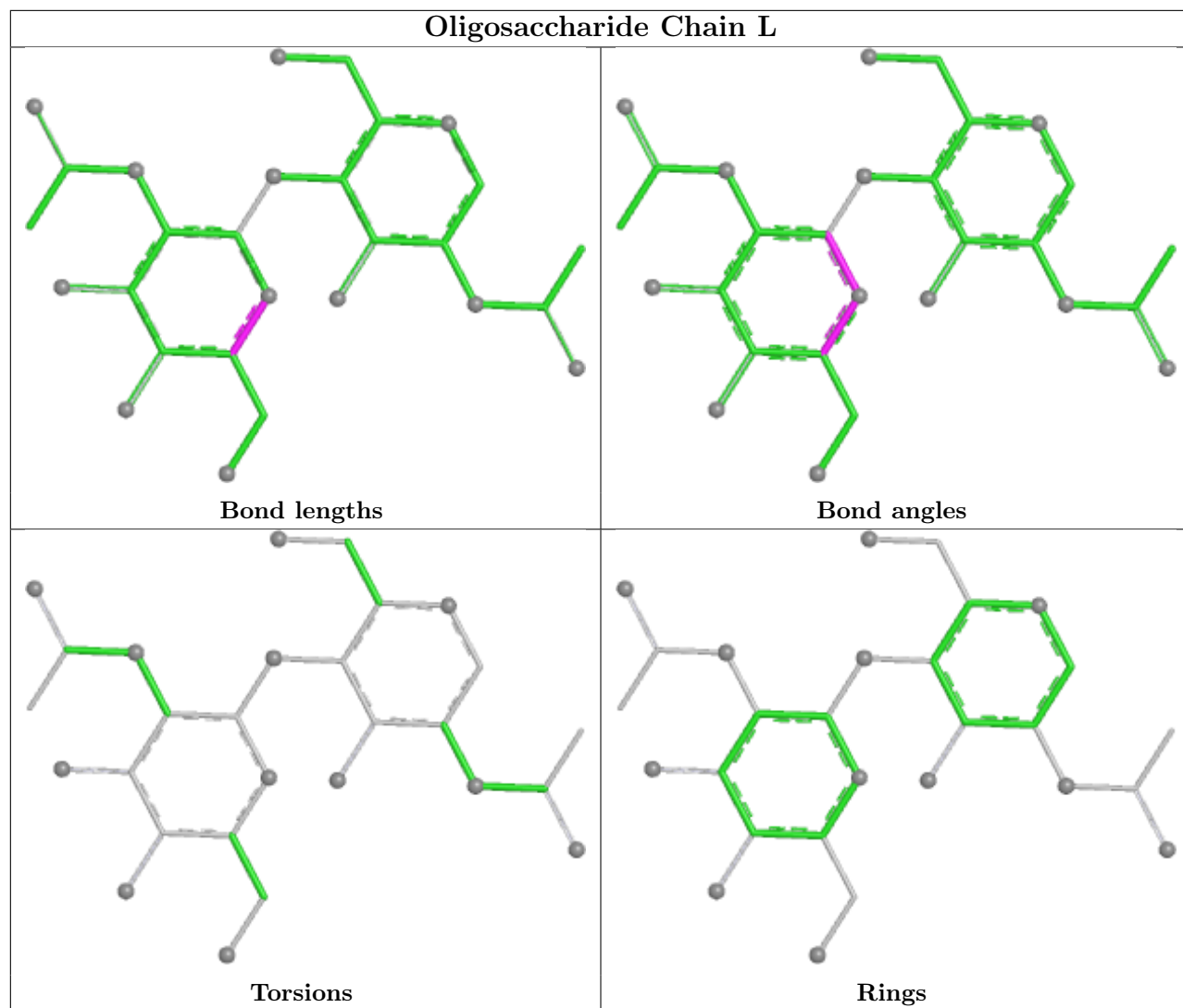


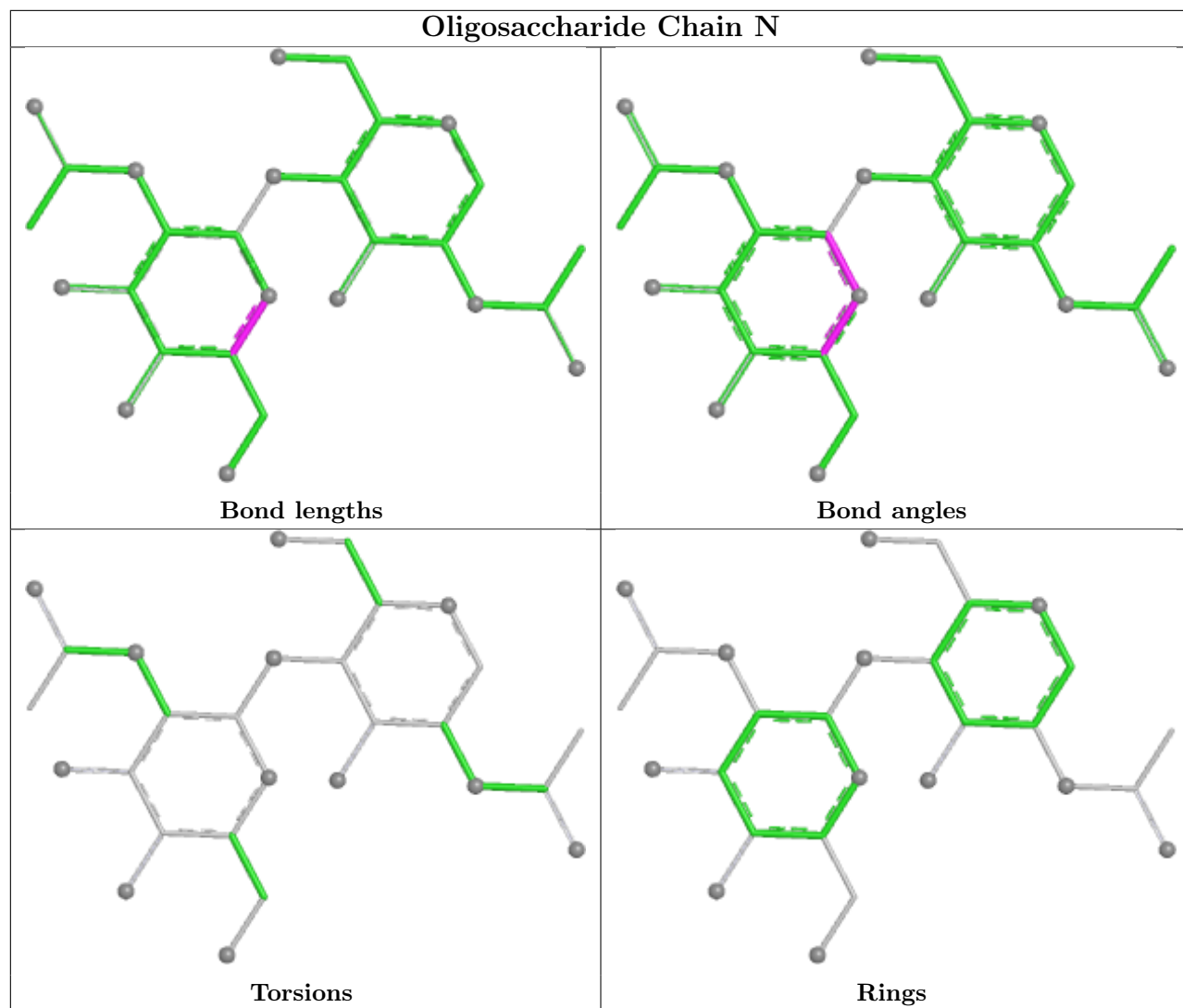


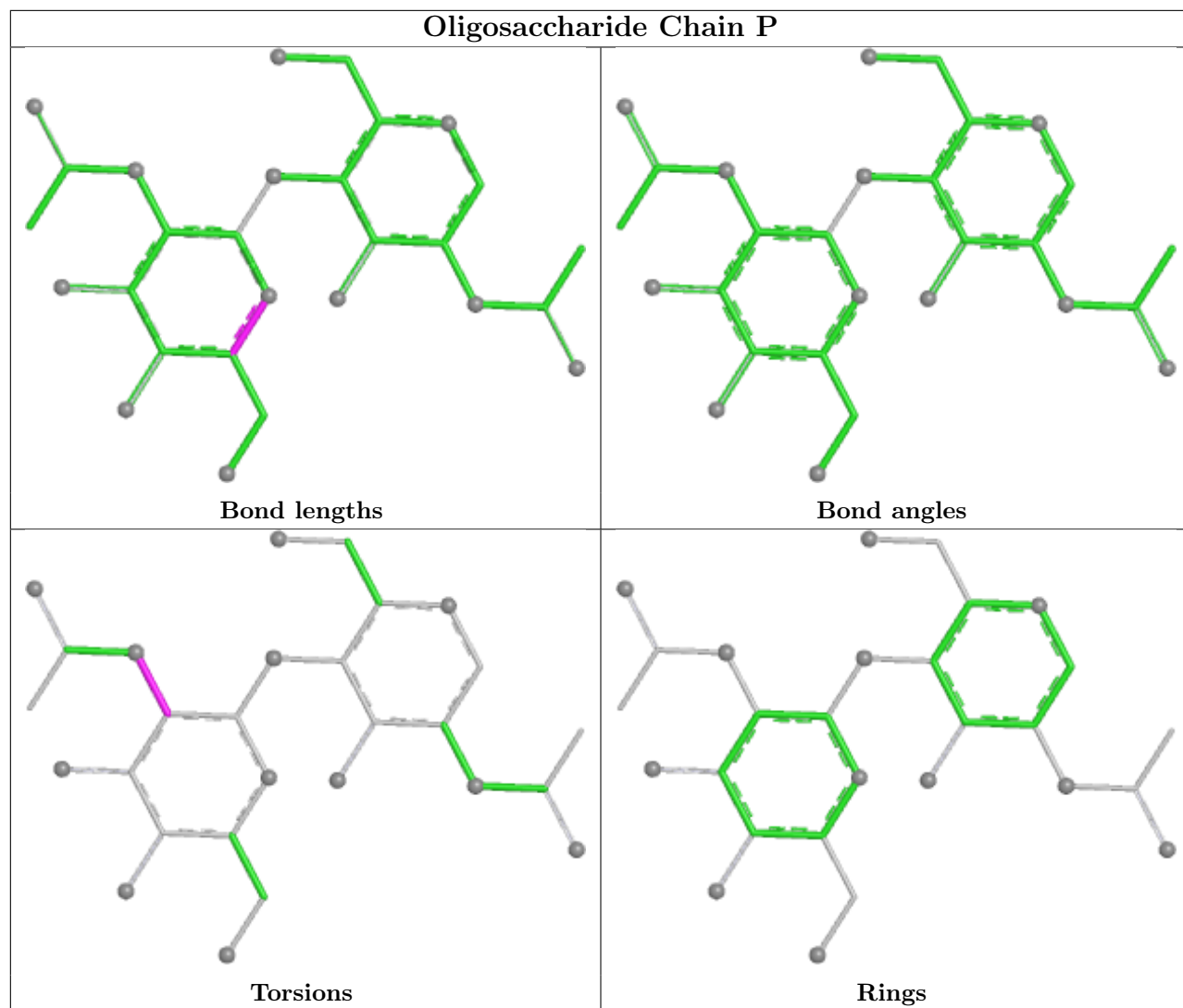


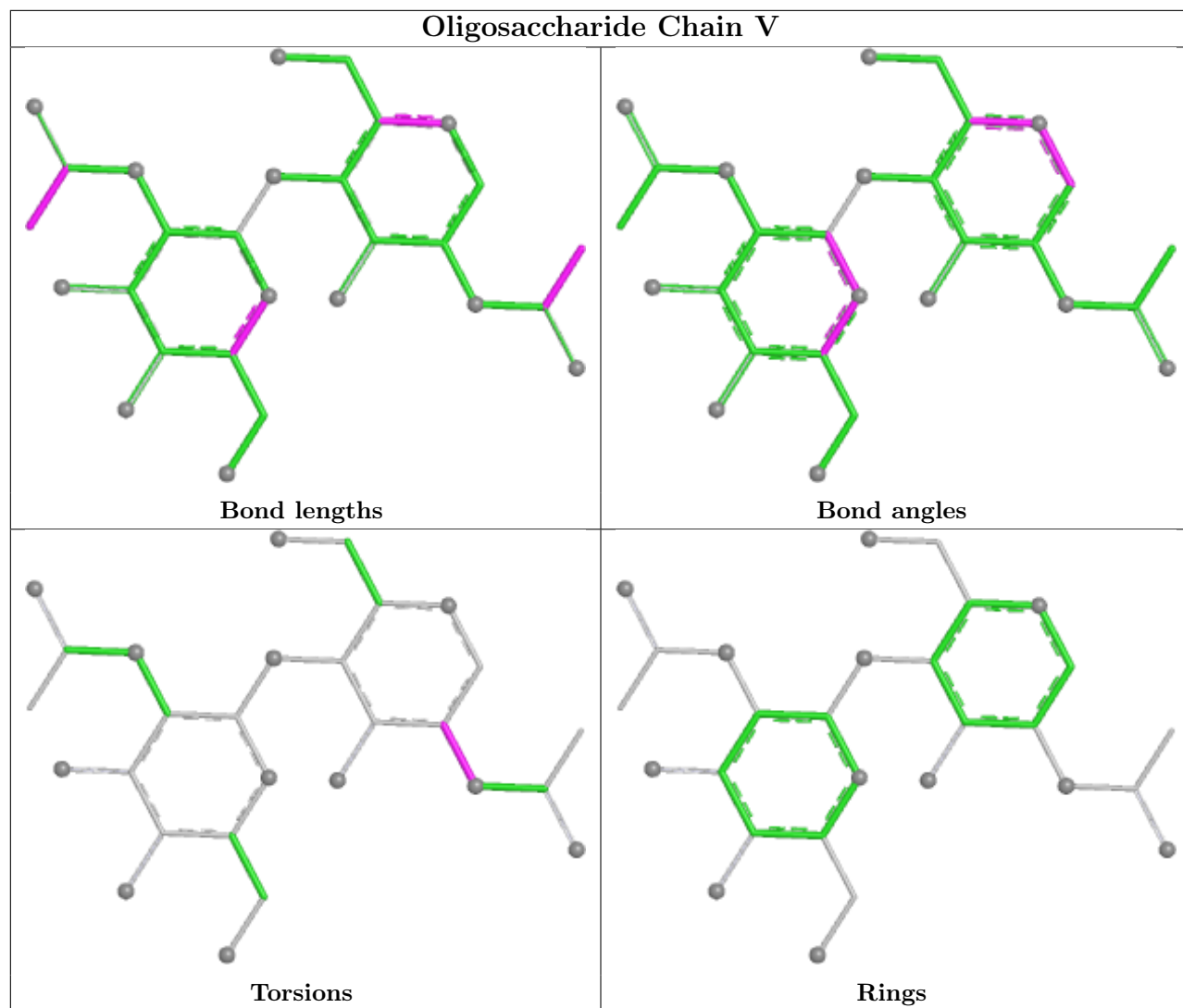


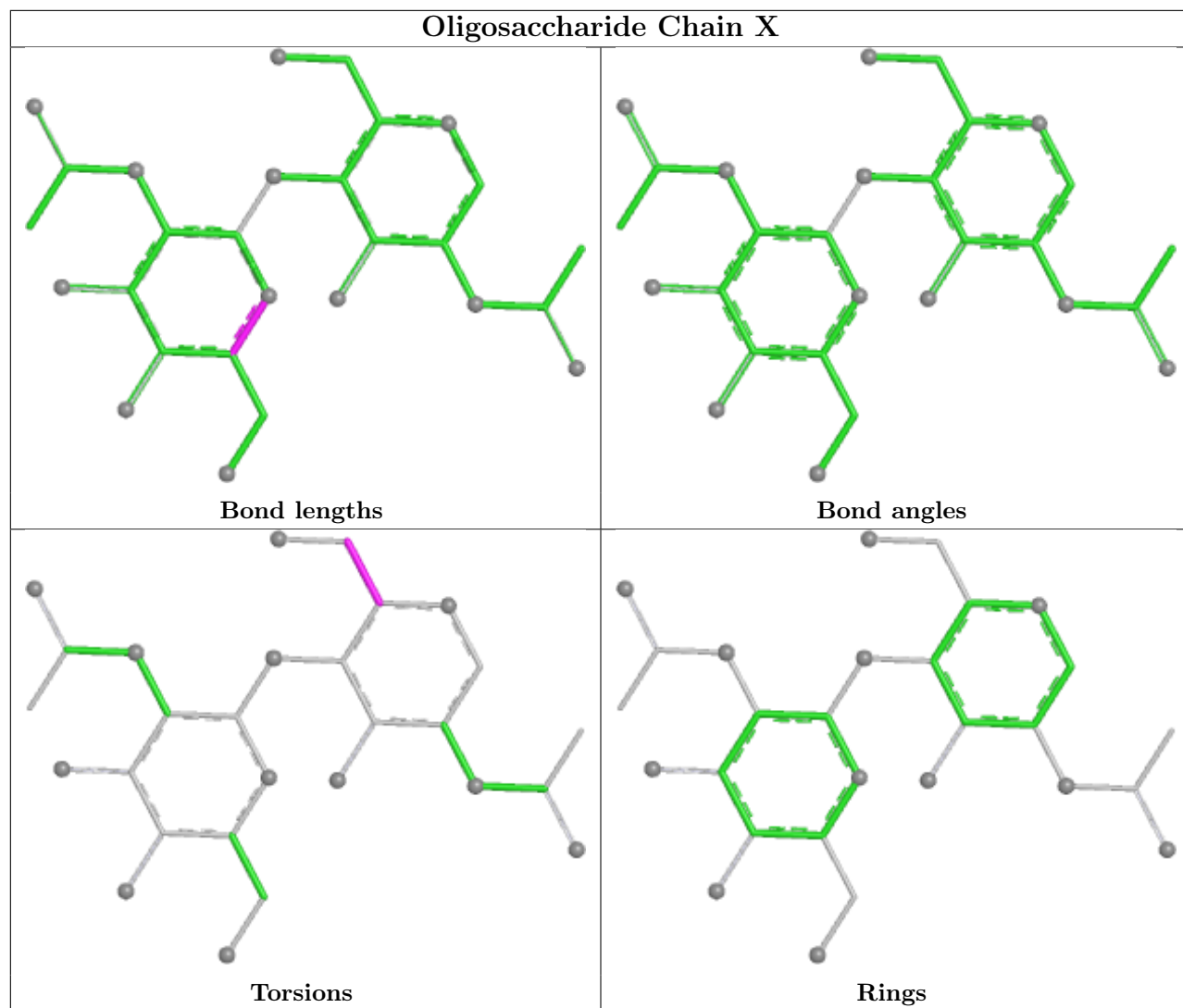


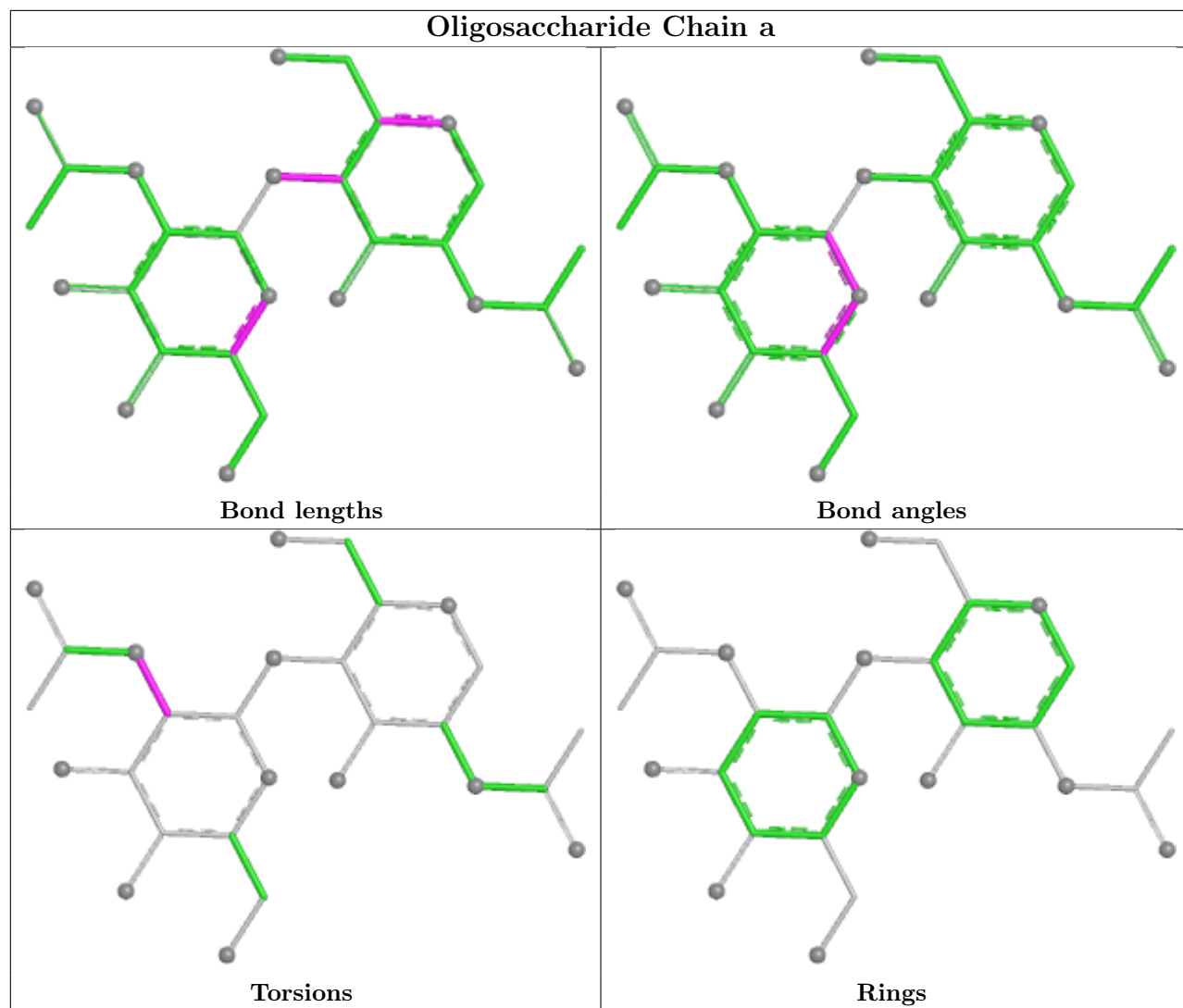


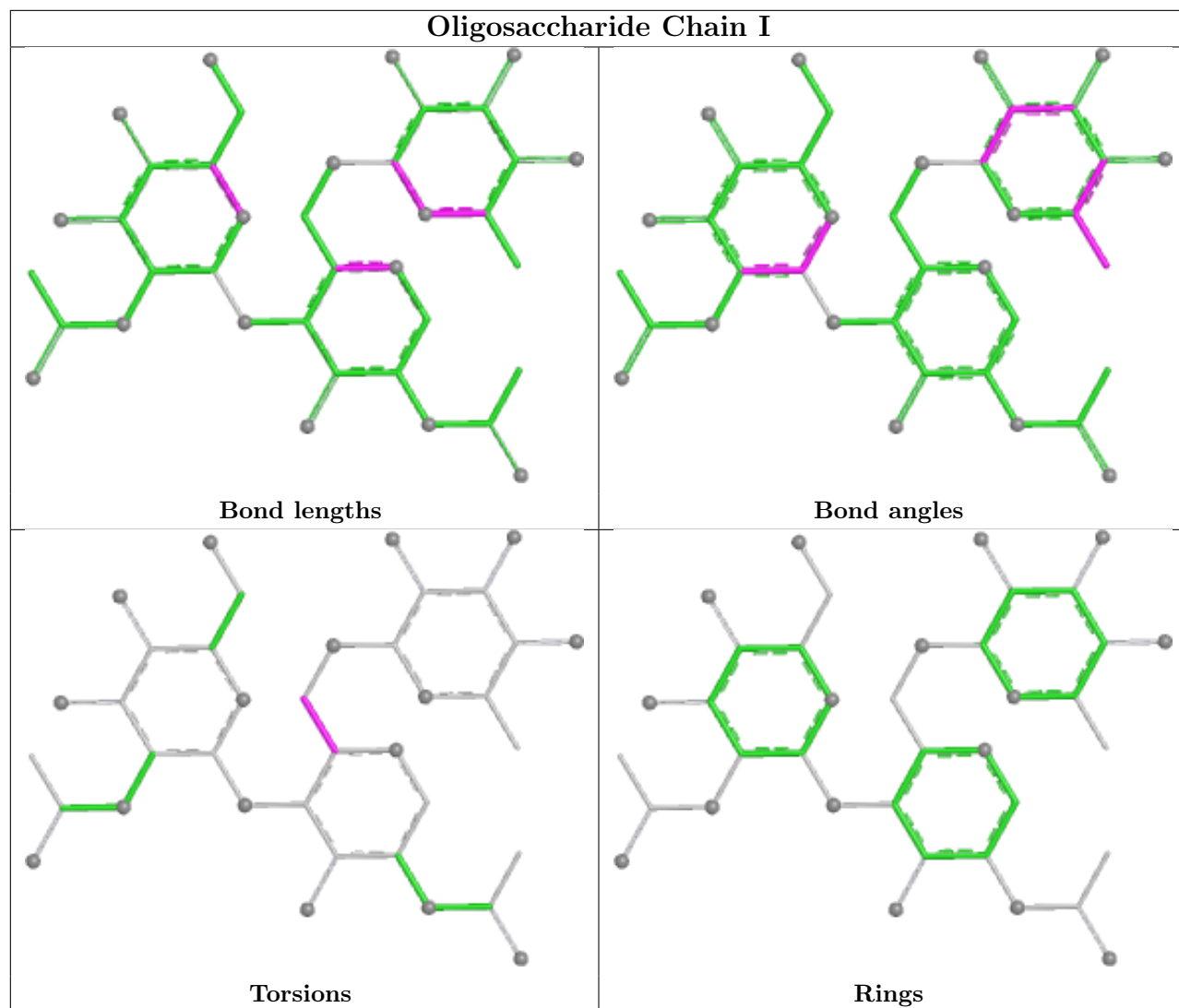


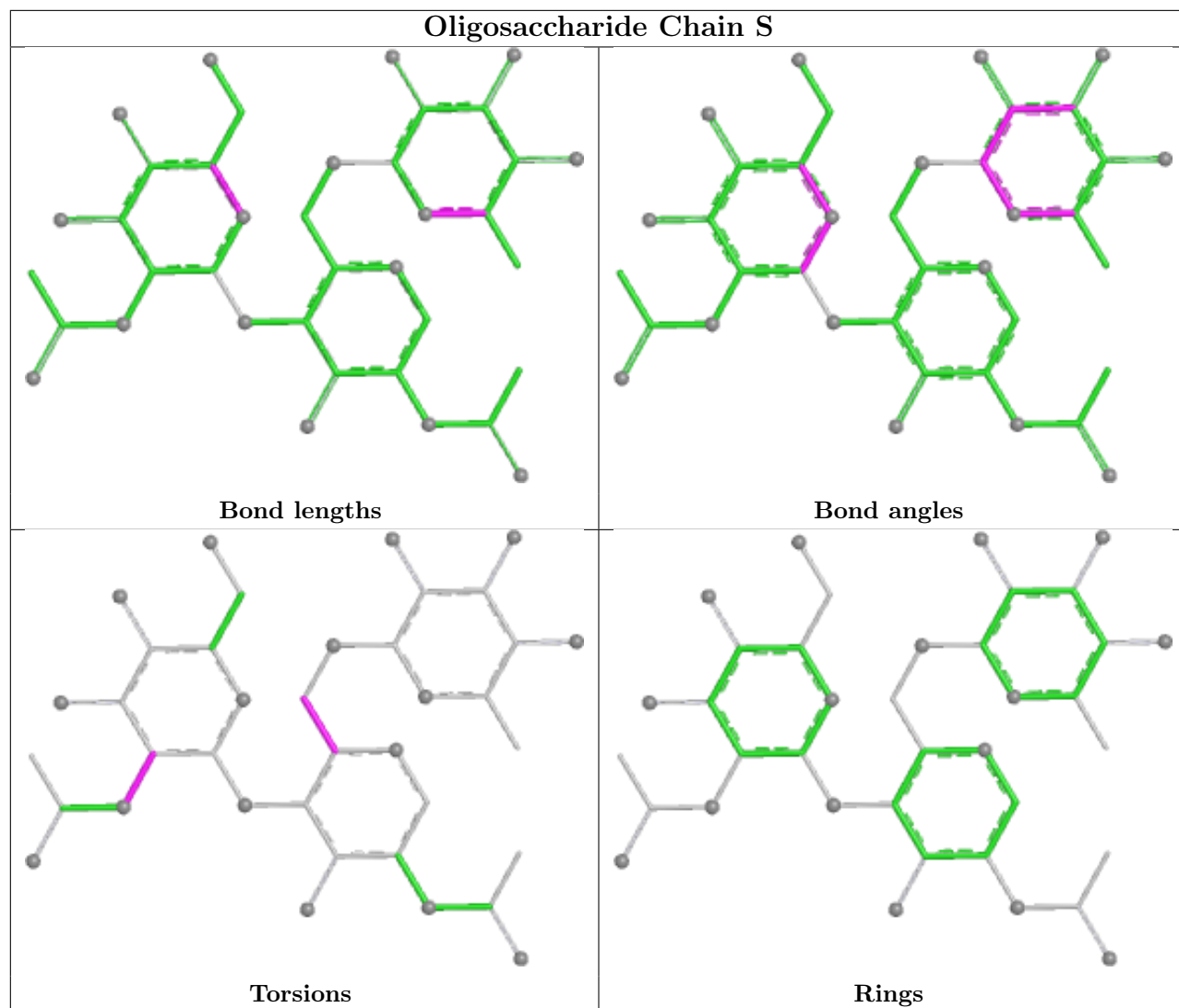


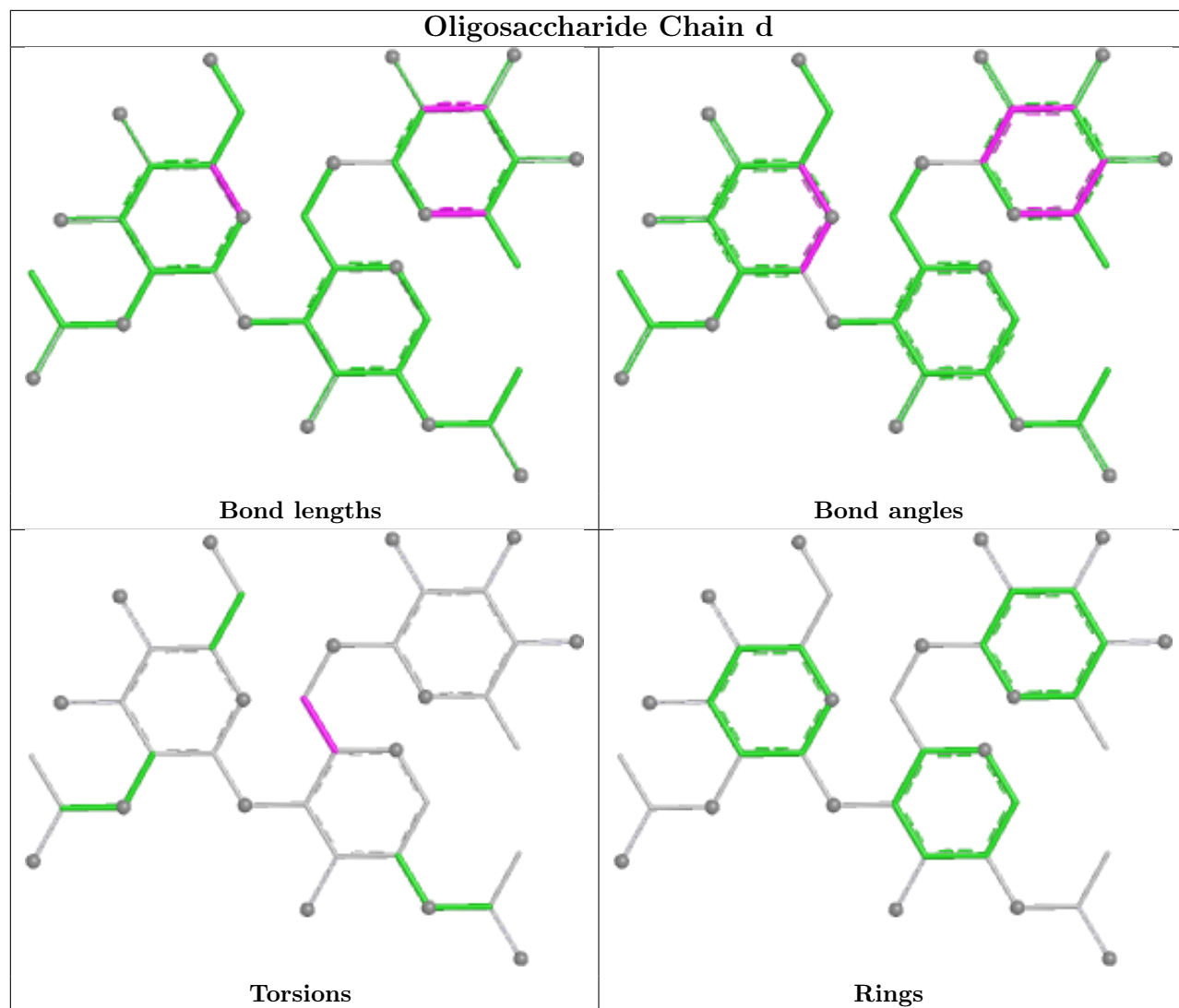


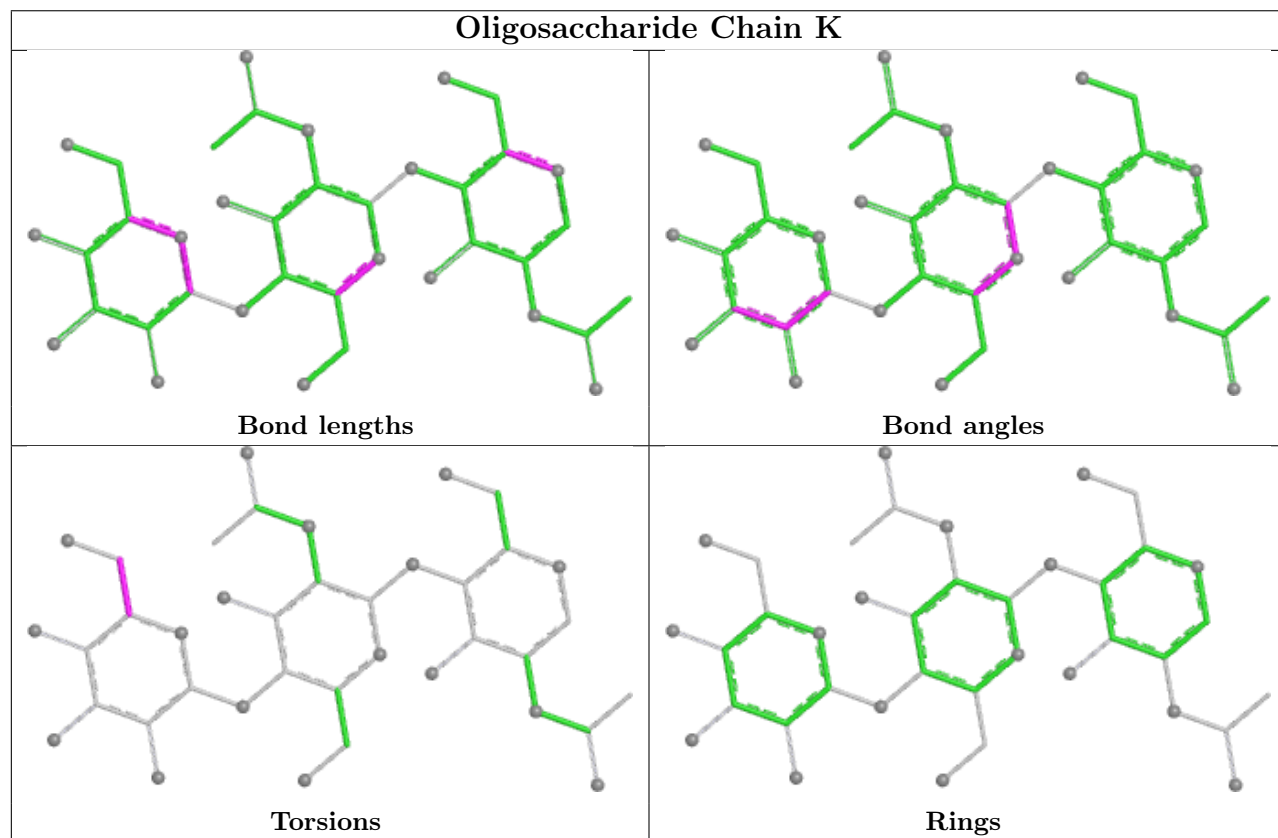
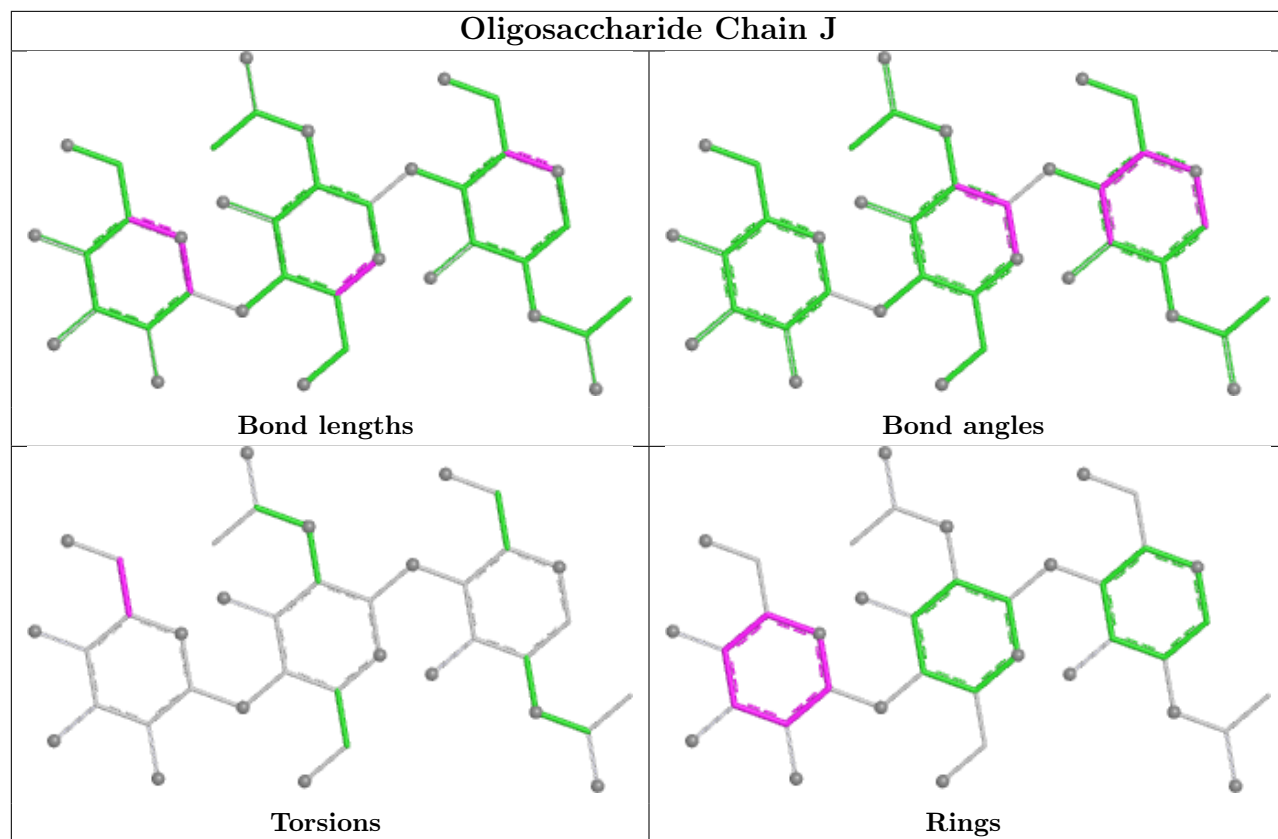


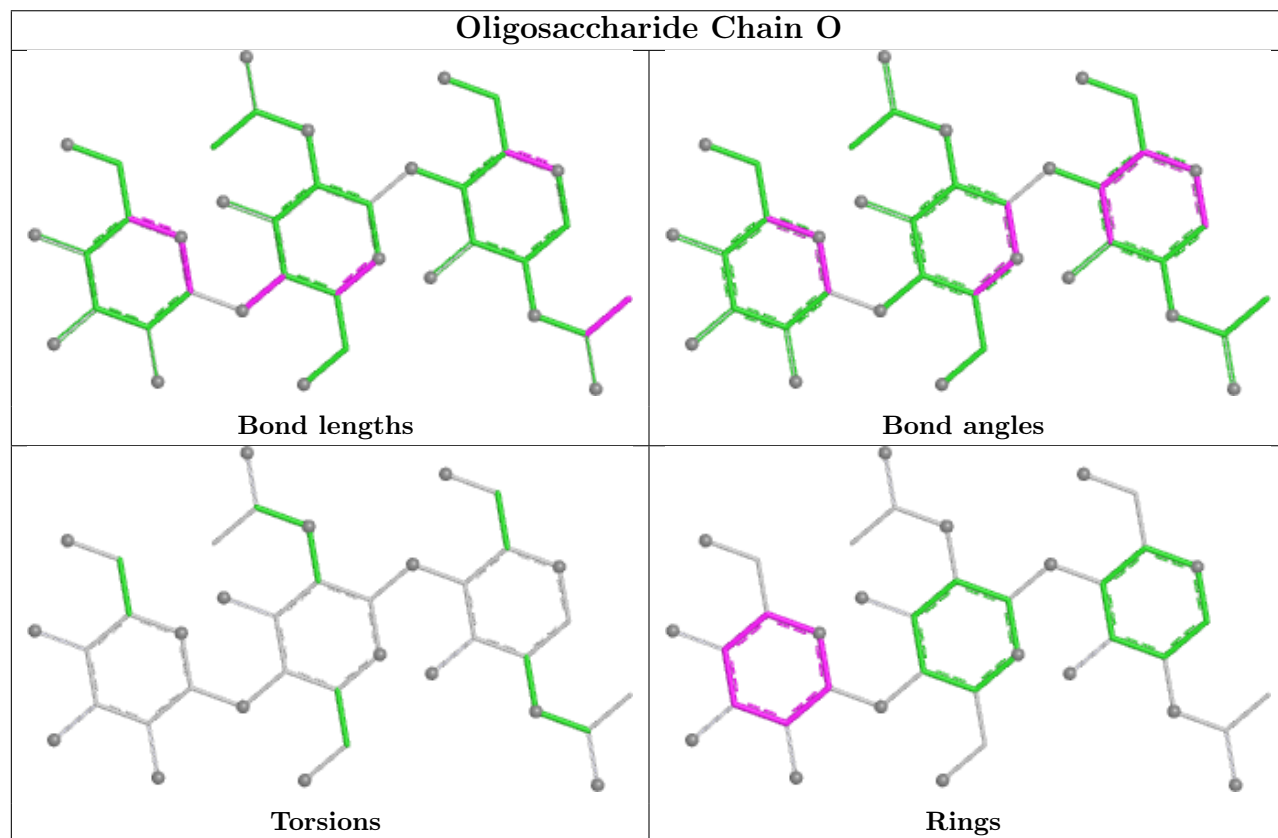
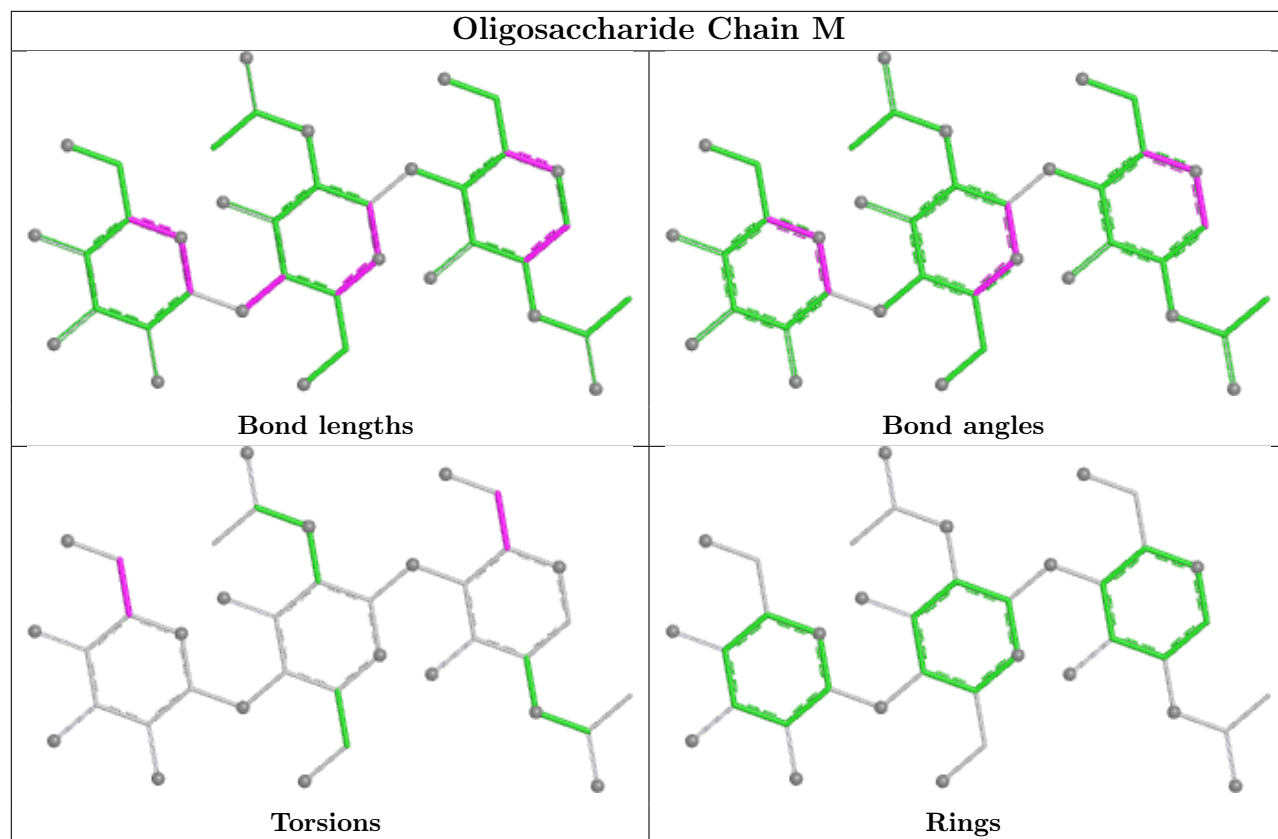


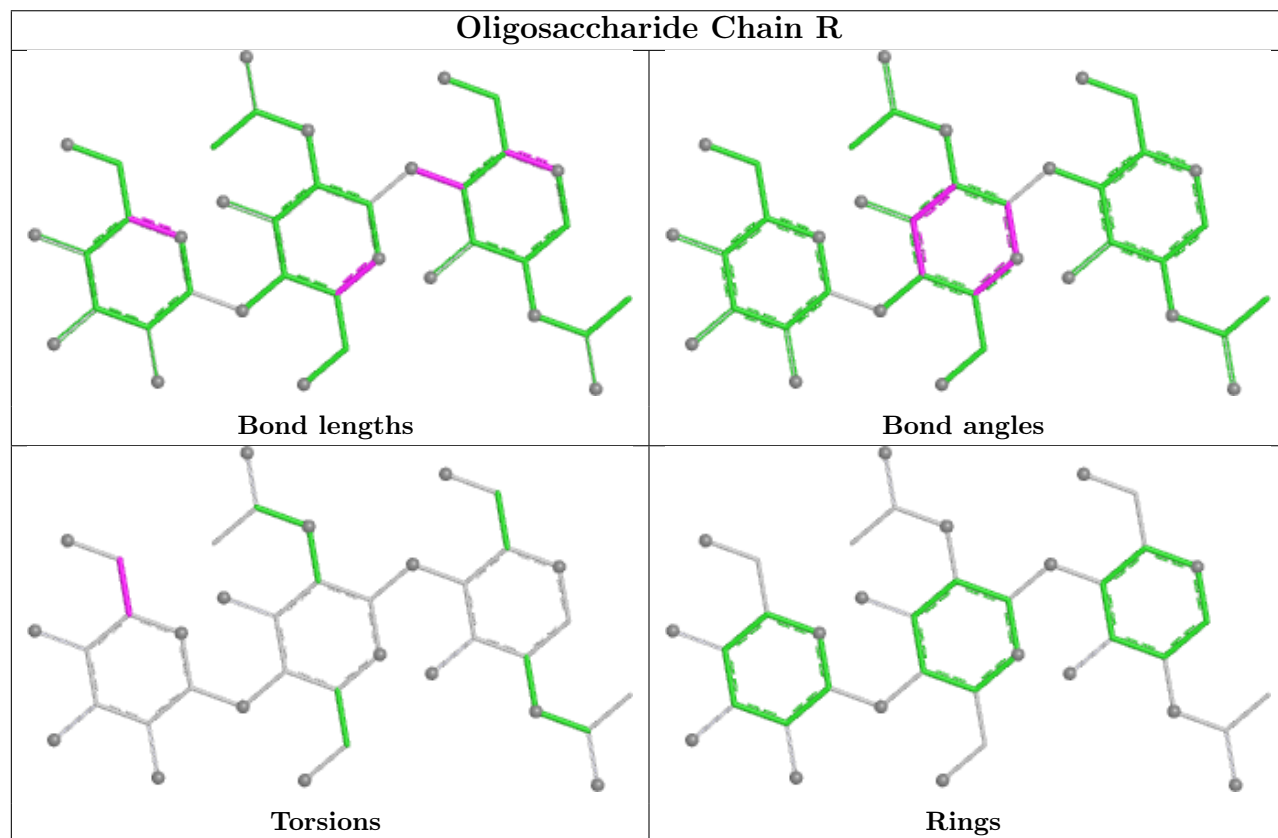
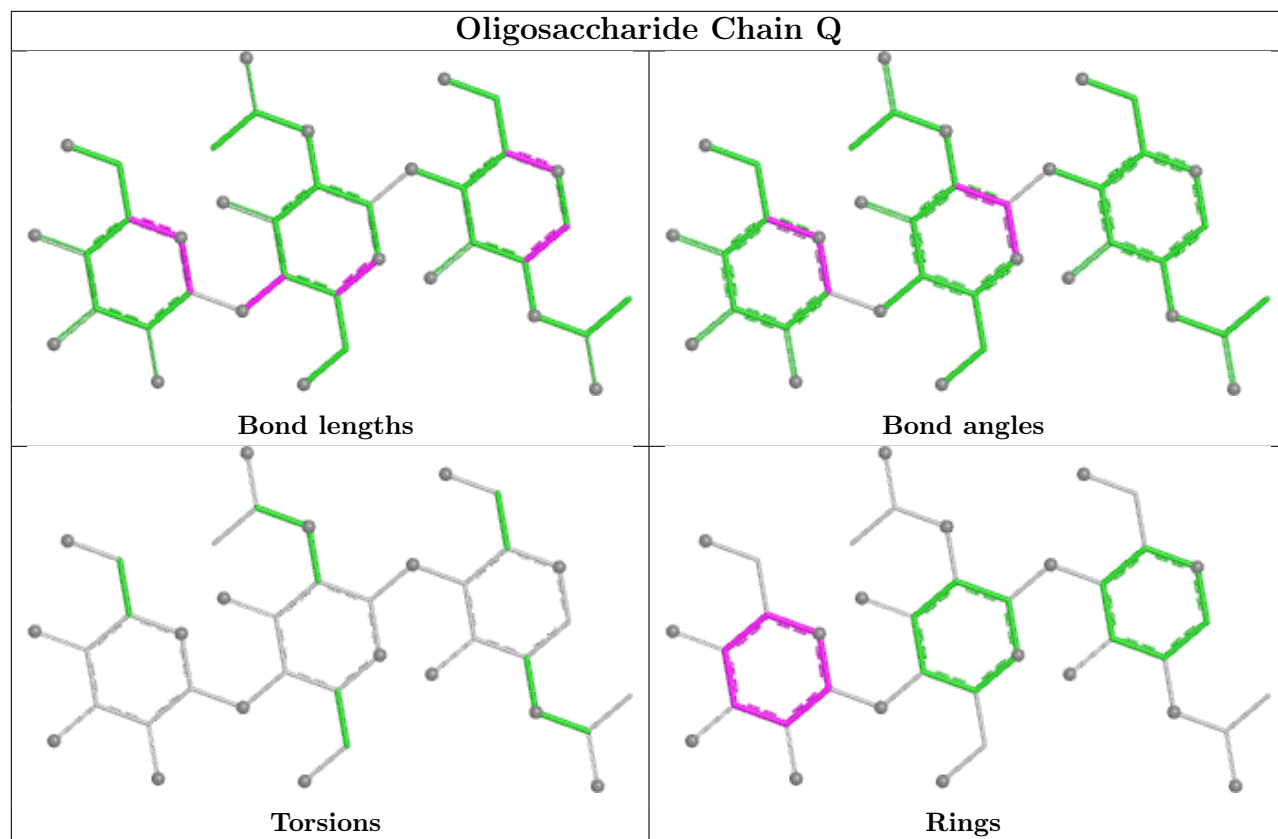


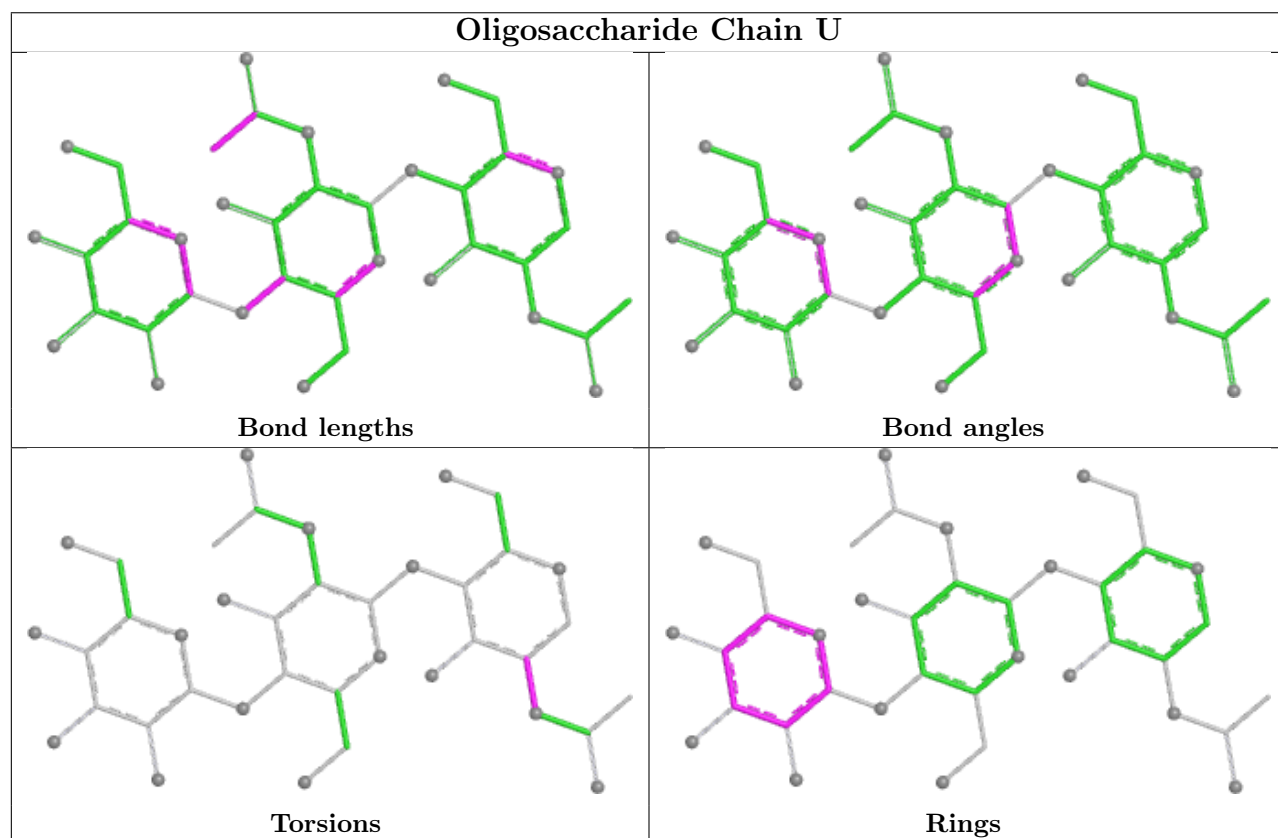
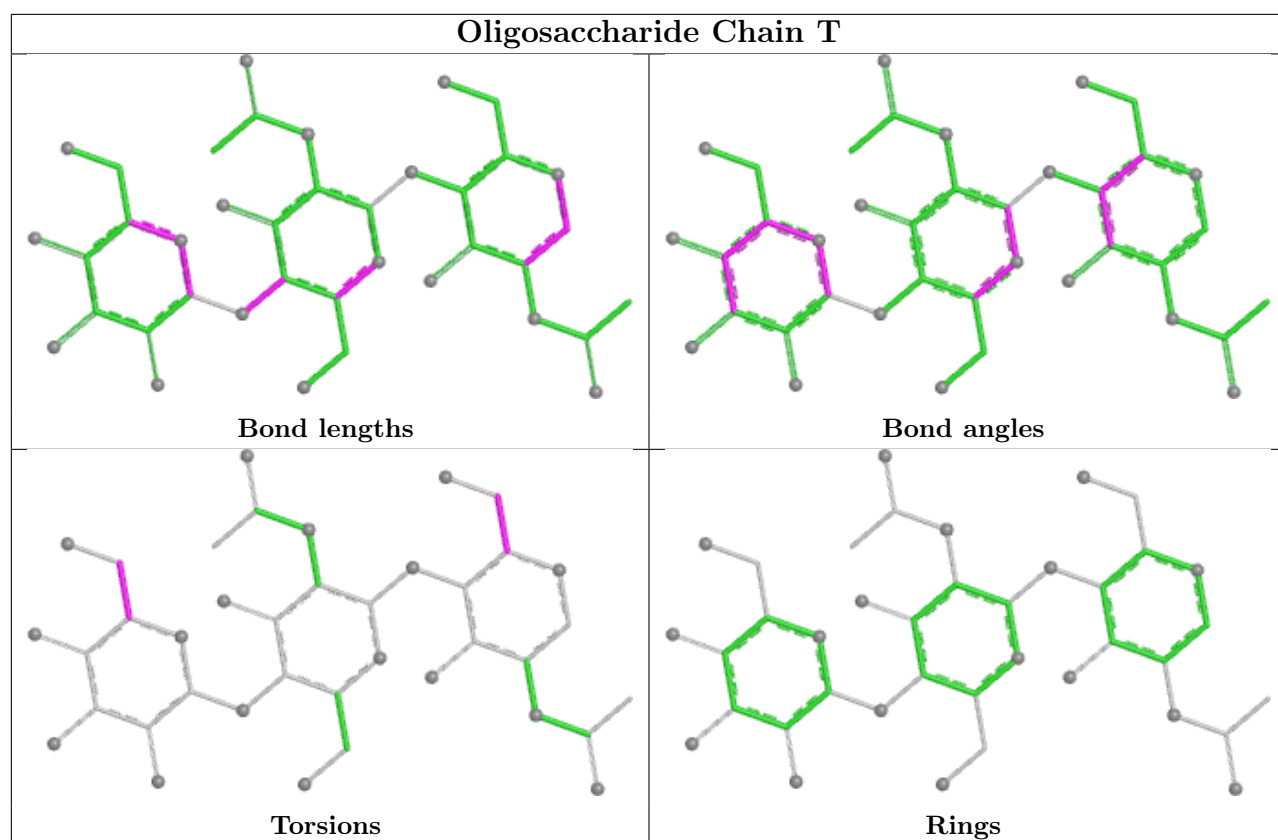


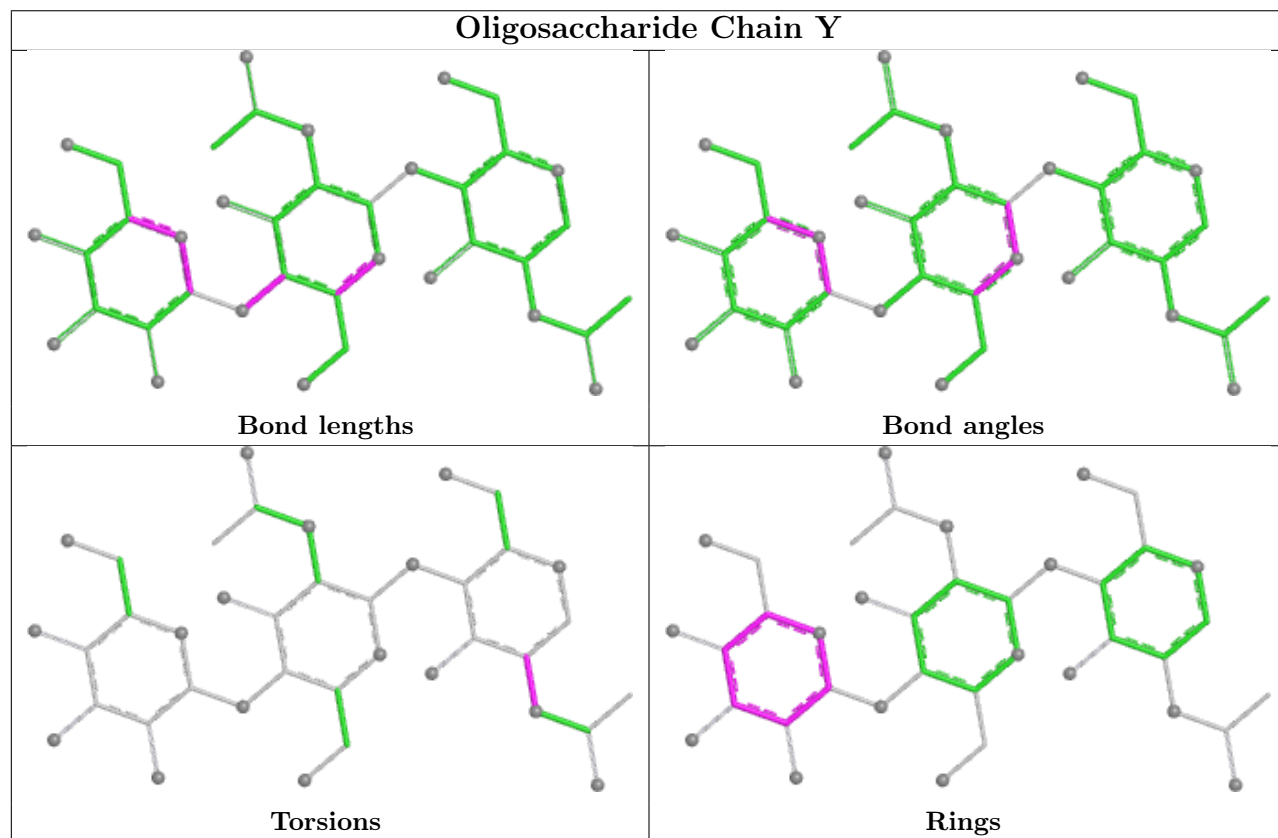
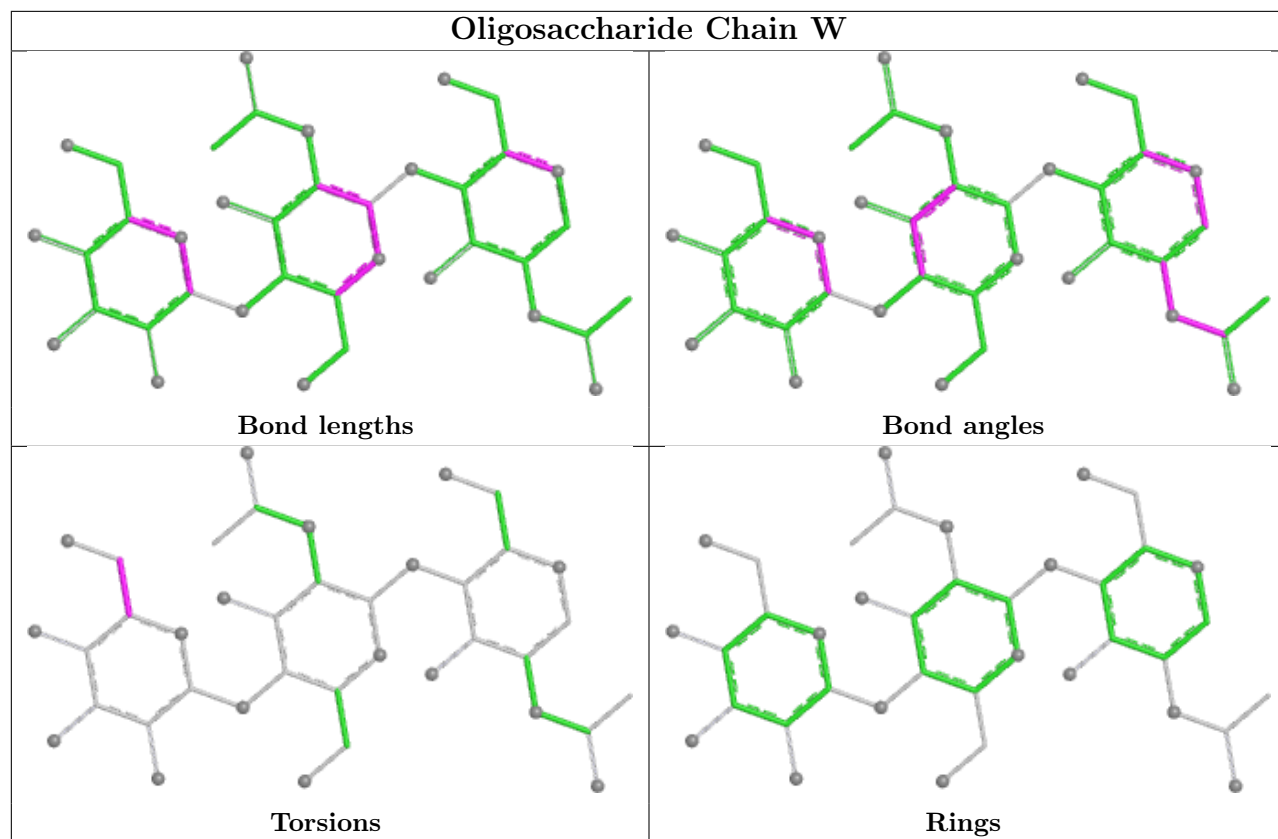


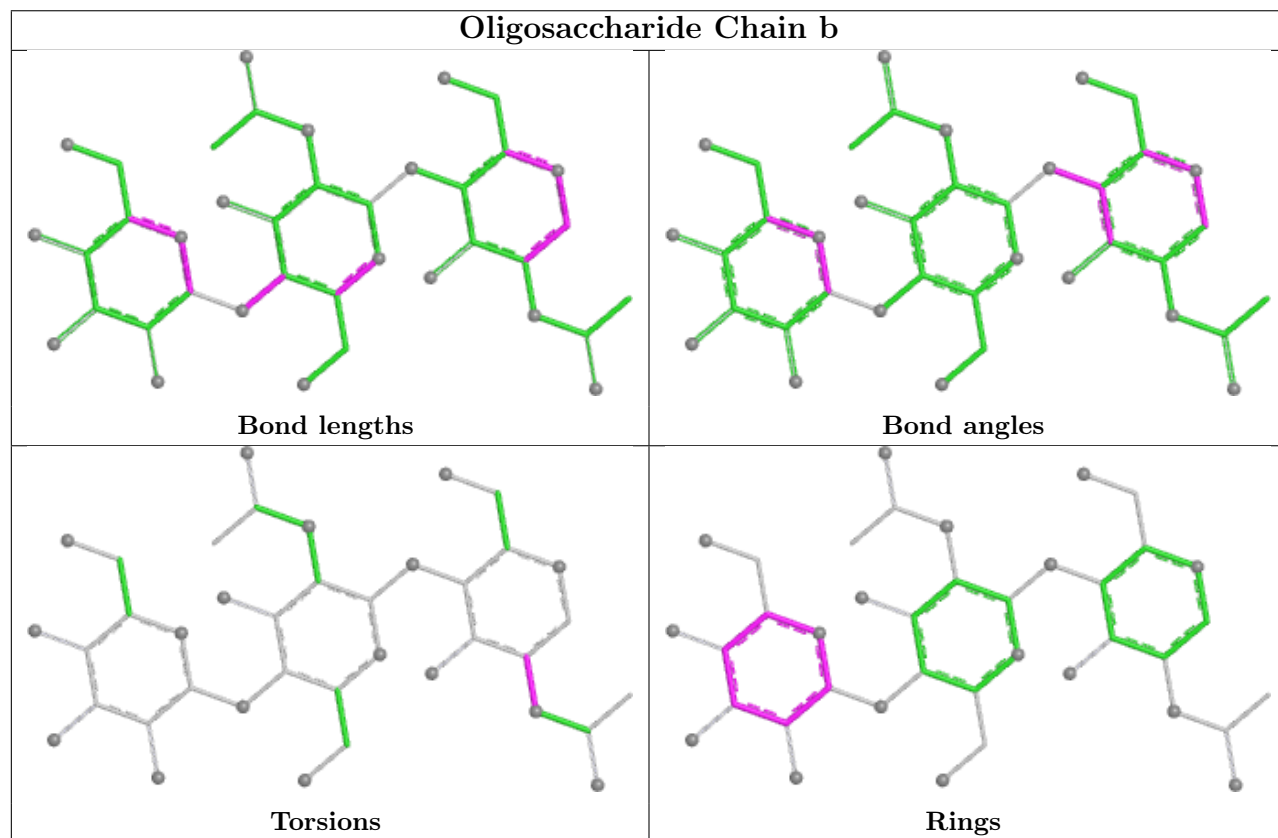
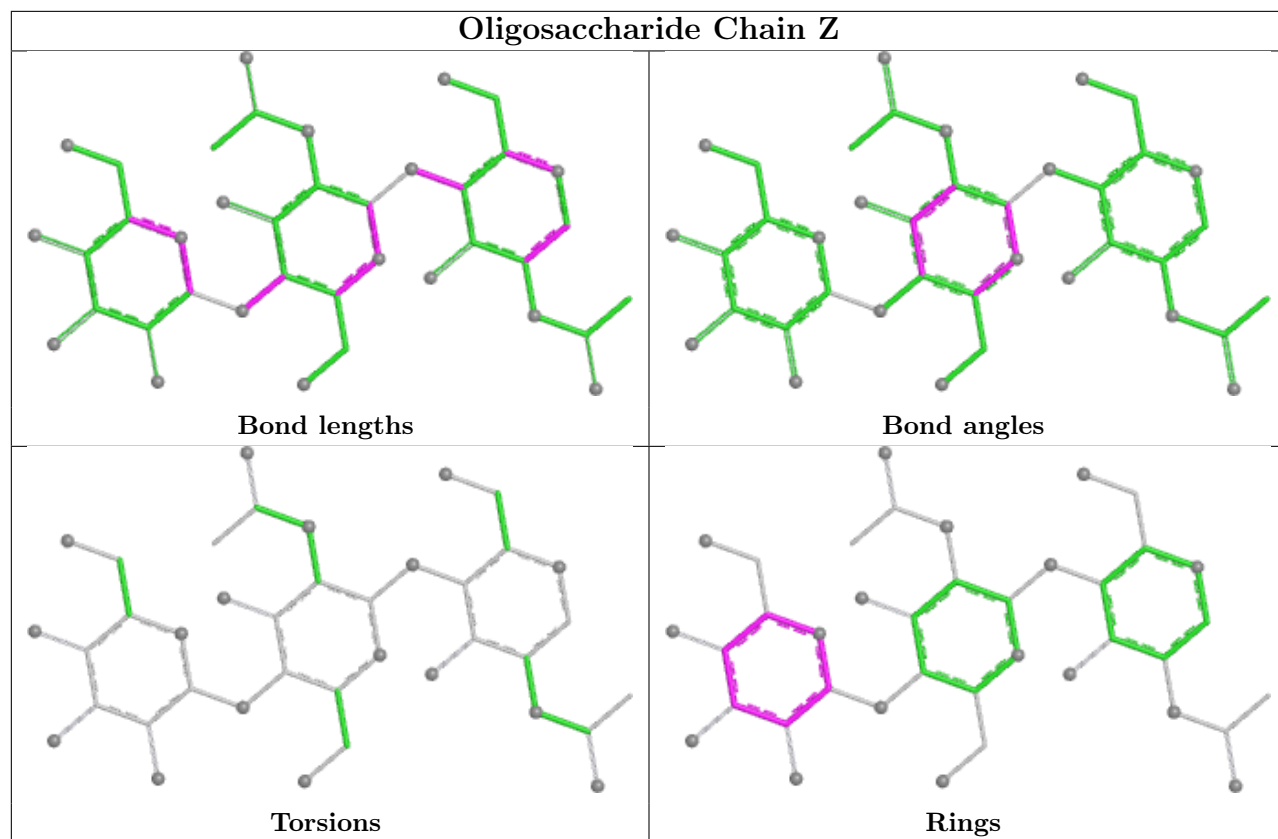


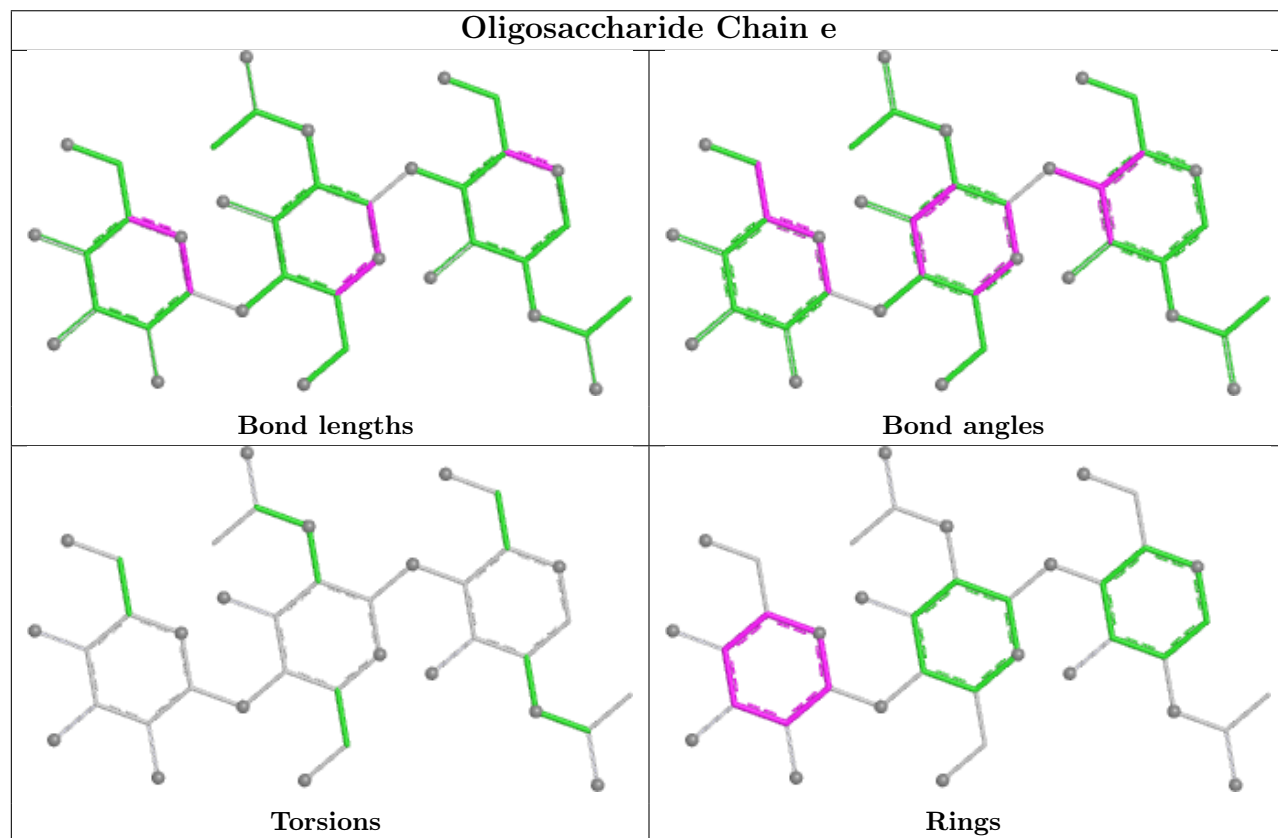
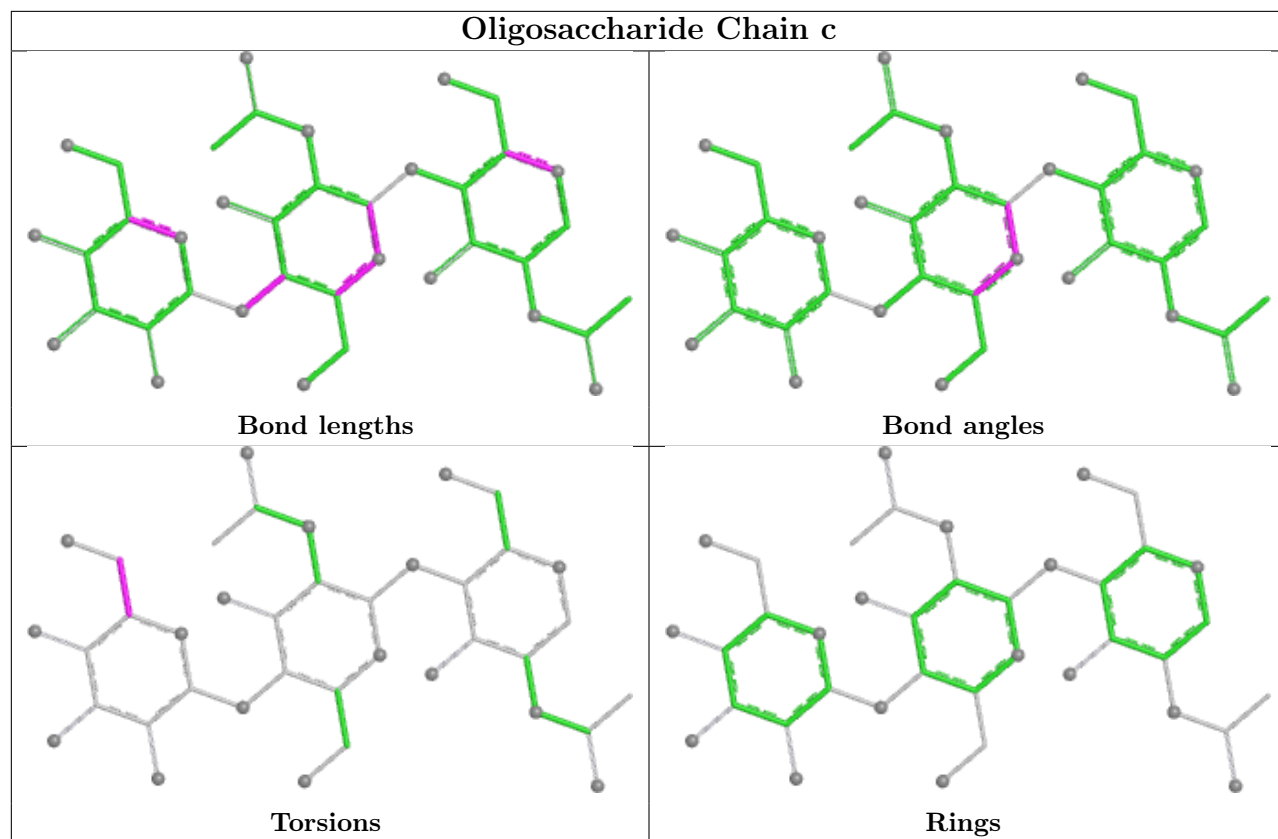


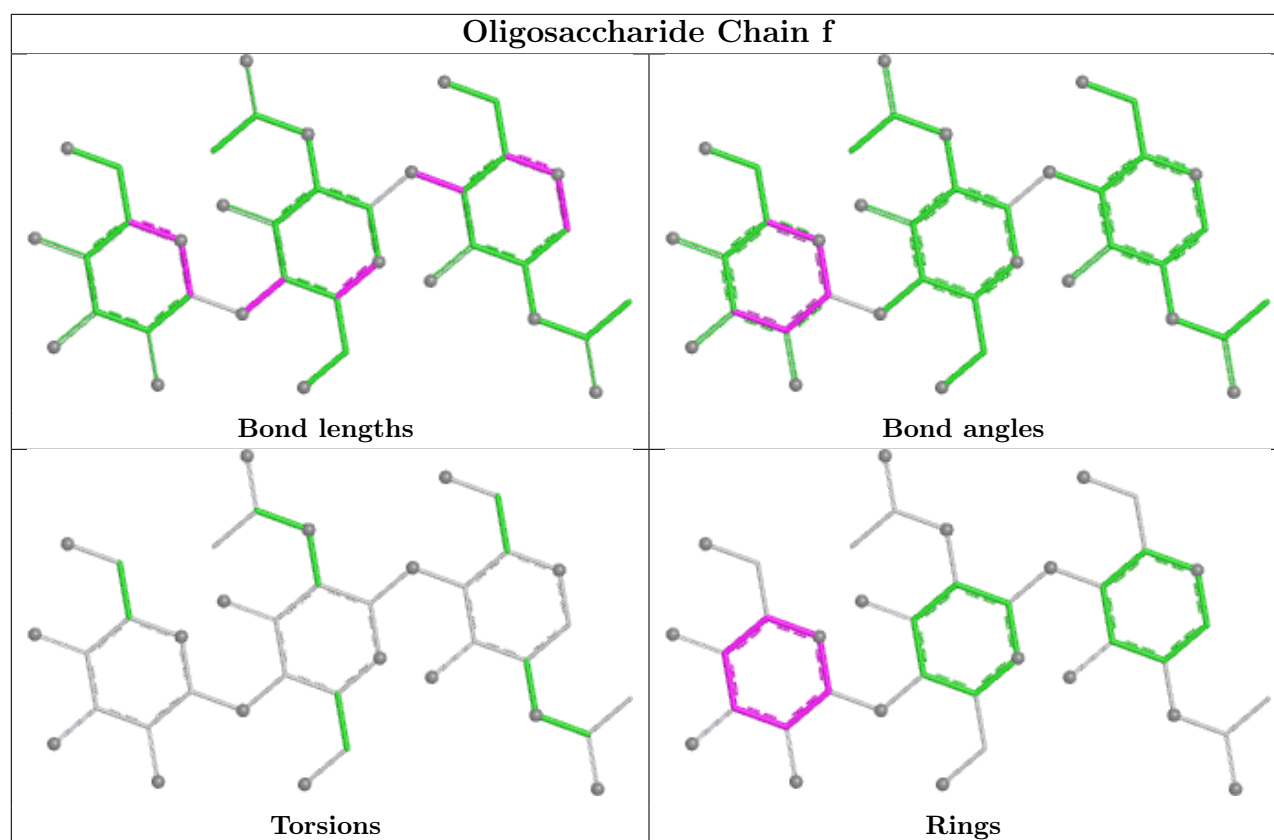












5.6 Ligand geometry [i](#)

25 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	$\# Z > 2$
5	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	C	1303	1	14,14,15	1.34	3 (21%)	17,19,21	0.94	0
5	NAG	A	1307	1	14,14,15	1.29	2 (14%)	17,19,21	0.60	0
5	NAG	B	1303	1	14,14,15	1.38	2 (14%)	17,19,21	1.07	1 (5%)
5	NAG	A	1308	1	14,14,15	1.30	3 (21%)	17,19,21	0.56	0
5	NAG	A	1304	1	14,14,15	1.24	2 (14%)	17,19,21	0.64	0
5	NAG	C	1306	1	14,14,15	1.24	2 (14%)	17,19,21	0.94	1 (5%)
5	NAG	A	1302	1	14,14,15	1.28	1 (7%)	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1307	1	14,14,15	1.27	1 (7%)	17,19,21	0.94	0
5	NAG	B	1304	1	14,14,15	1.18	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	A	1309	1	14,14,15	0.36	0	17,19,21	0.36	0
5	NAG	A	1310	1	14,14,15	1.44	3 (21%)	17,19,21	0.72	0
5	NAG	B	1308	1	14,14,15	1.41	3 (21%)	17,19,21	1.16	1 (5%)
5	NAG	C	1304	1	14,14,15	1.41	3 (21%)	17,19,21	1.13	1 (5%)
5	NAG	C	1307	1	14,14,15	1.28	2 (14%)	17,19,21	0.73	0
5	NAG	A	1303	1	14,14,15	1.31	3 (21%)	17,19,21	0.65	0
5	NAG	A	1305	1	14,14,15	1.33	2 (14%)	17,19,21	0.88	0
5	NAG	B	1306	1	14,14,15	1.19	1 (7%)	17,19,21	0.83	0
5	NAG	C	1301	1	14,14,15	1.32	3 (21%)	17,19,21	0.90	1 (5%)
5	NAG	A	1306	1	14,14,15	1.33	1 (7%)	17,19,21	0.72	0
5	NAG	C	1305	1	14,14,15	1.17	1 (7%)	17,19,21	0.72	0
5	NAG	A	1301	1	14,14,15	1.42	3 (21%)	17,19,21	0.81	0
5	NAG	B	1301	1	14,14,15	1.37	2 (14%)	17,19,21	1.47	2 (11%)
5	NAG	C	1302	1	14,14,15	1.10	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.43	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
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	NAG	O5-C5	4.07	1.51	1.43
5	C	1306	NAG	O5-C5	3.33	1.49	1.43
5	B	1303	NAG	O5-C5	3.29	1.49	1.43
5	B	1301	NAG	O5-C5	3.12	1.49	1.43
5	A	1302	NAG	O5-C5	3.10	1.49	1.43
5	A	1307	NAG	O5-C5	3.06	1.49	1.43
5	A	1310	NAG	O5-C5	3.00	1.49	1.43
5	A	1306	NAG	O5-C5	2.97	1.49	1.43
5	C	1304	NAG	O5-C5	2.96	1.49	1.43
5	A	1301	NAG	O5-C5	2.91	1.49	1.43
5	A	1305	NAG	O5-C5	2.86	1.49	1.43
5	C	1301	NAG	O5-C5	2.81	1.48	1.43
5	C	1303	NAG	O5-C5	2.80	1.48	1.43
5	B	1308	NAG	O5-C5	2.77	1.48	1.43
5	C	1305	NAG	O5-C5	2.75	1.48	1.43
5	B	1306	NAG	O5-C5	2.74	1.48	1.43
5	C	1307	NAG	O5-C5	2.72	1.48	1.43
5	A	1301	NAG	C1-C2	2.71	1.56	1.52
5	A	1308	NAG	O5-C5	2.70	1.48	1.43
5	C	1302	NAG	O5-C5	2.67	1.48	1.43
5	B	1303	NAG	C1-C2	2.58	1.55	1.52
5	A	1303	NAG	O5-C5	2.57	1.48	1.43
5	A	1308	NAG	C1-C2	2.52	1.55	1.52
5	A	1310	NAG	C1-C2	2.52	1.55	1.52
5	A	1305	NAG	O5-C1	2.50	1.47	1.43
5	A	1304	NAG	O5-C5	2.48	1.48	1.43
5	B	1304	NAG	C1-C2	2.42	1.55	1.52
5	B	1308	NAG	O5-C1	2.42	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1303	NAG	O5-C1	2.37	1.47	1.43
5	C	1304	NAG	C1-C2	2.37	1.55	1.52
5	B	1308	NAG	C1-C2	2.34	1.55	1.52
5	A	1310	NAG	O5-C1	2.32	1.47	1.43
5	C	1303	NAG	C1-C2	2.29	1.55	1.52
5	C	1301	NAG	C1-C2	2.20	1.55	1.52
5	C	1307	NAG	C1-C2	2.16	1.55	1.52
5	A	1303	NAG	O5-C1	2.16	1.47	1.43
5	C	1306	NAG	C8-C7	2.13	1.55	1.50
5	C	1301	NAG	O5-C1	2.12	1.47	1.43
5	B	1301	NAG	O5-C1	2.12	1.47	1.43
5	A	1304	NAG	O5-C1	2.11	1.47	1.43
5	A	1303	NAG	C1-C2	2.10	1.55	1.52
5	A	1301	NAG	C8-C7	2.10	1.54	1.50
5	A	1307	NAG	O5-C1	2.08	1.47	1.43
5	C	1304	NAG	C8-C7	2.03	1.54	1.50
5	A	1308	NAG	O5-C1	2.01	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1301	NAG	C1-O5-C5	4.69	118.47	112.19
5	C	1304	NAG	C1-O5-C5	3.19	116.46	112.19
5	B	1303	NAG	C1-O5-C5	2.85	116.00	112.19
5	B	1304	NAG	C1-O5-C5	2.73	115.85	112.19
5	C	1302	NAG	C1-O5-C5	2.65	115.74	112.19
5	B	1308	NAG	C1-O5-C5	2.65	115.73	112.19
5	C	1301	NAG	C1-O5-C5	2.44	115.46	112.19
5	C	1306	NAG	O5-C5-C6	2.31	112.15	107.66
5	B	1301	NAG	C4-C3-C2	-2.29	107.66	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	C	1301	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1307	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

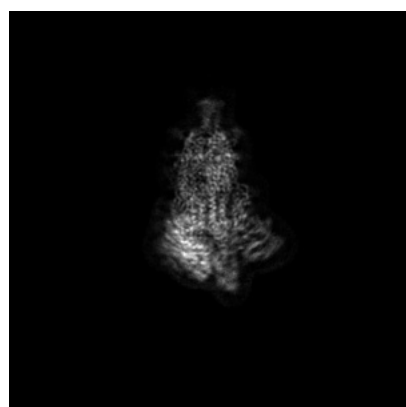
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26029. These allow visual inspection of the internal detail of the map and identification of artifacts.

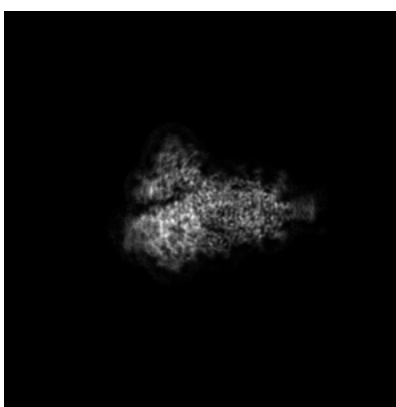
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

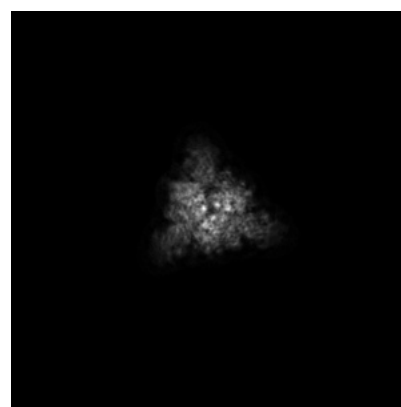
6.1.1 Primary map



X



Y



Z

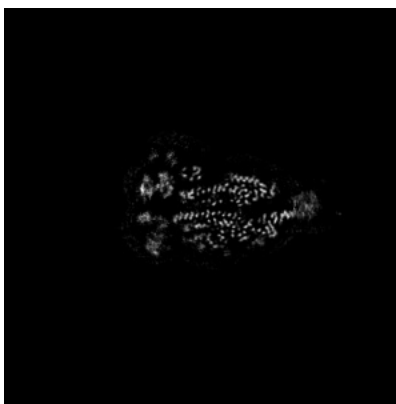
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 231



Y Index: 230

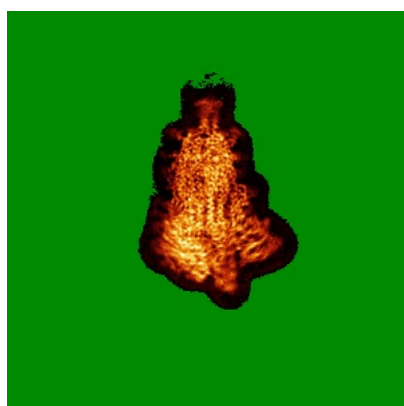


Z Index: 188

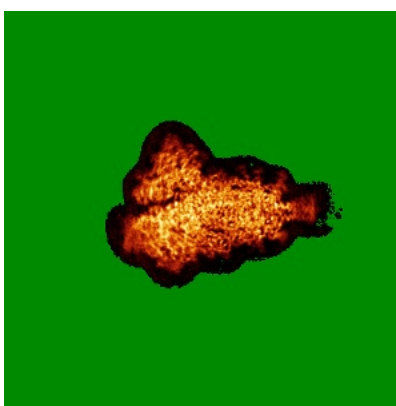
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

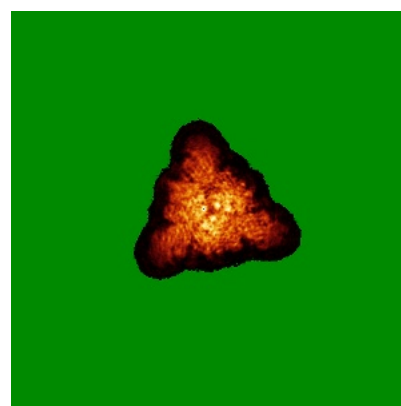
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

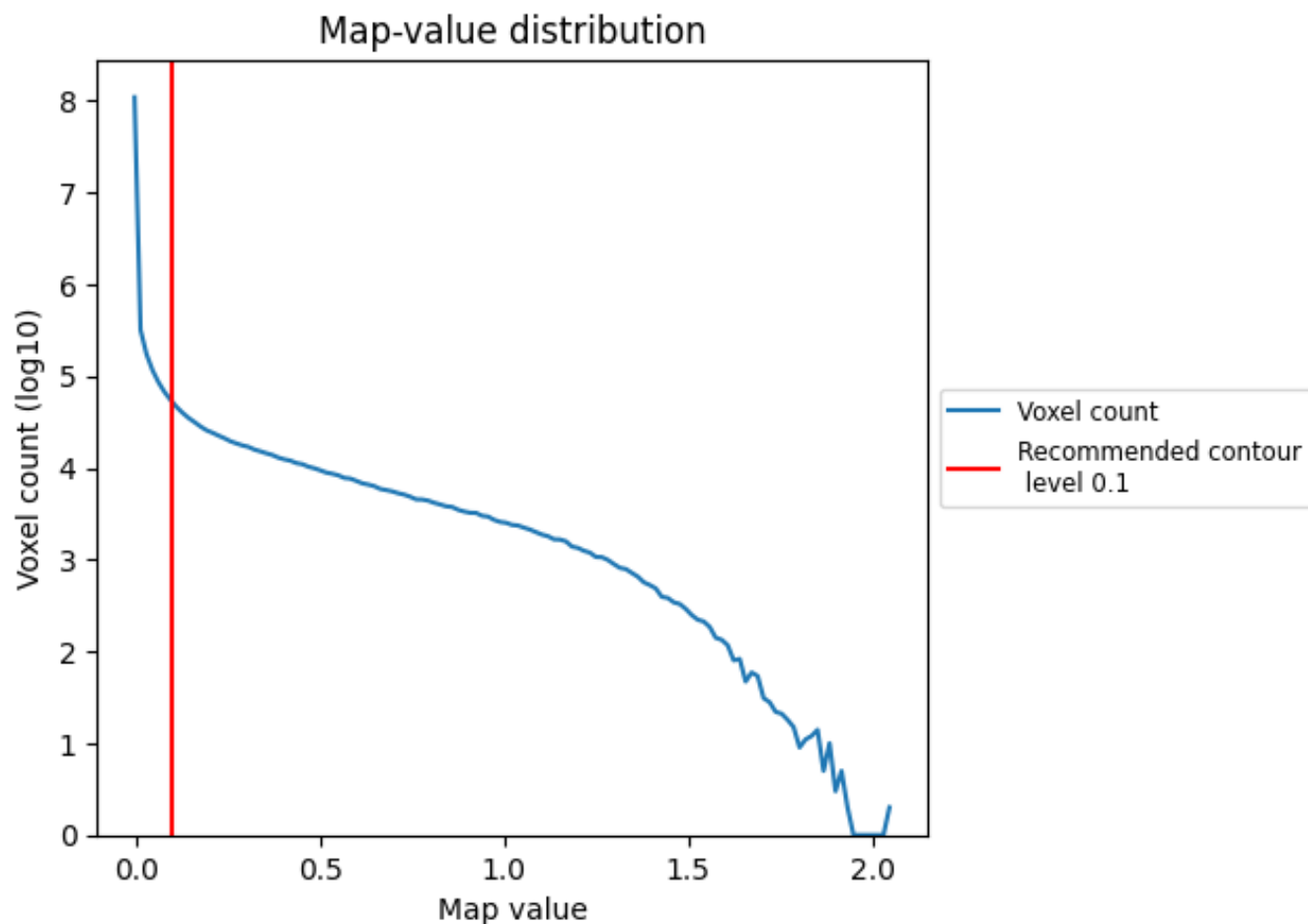
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

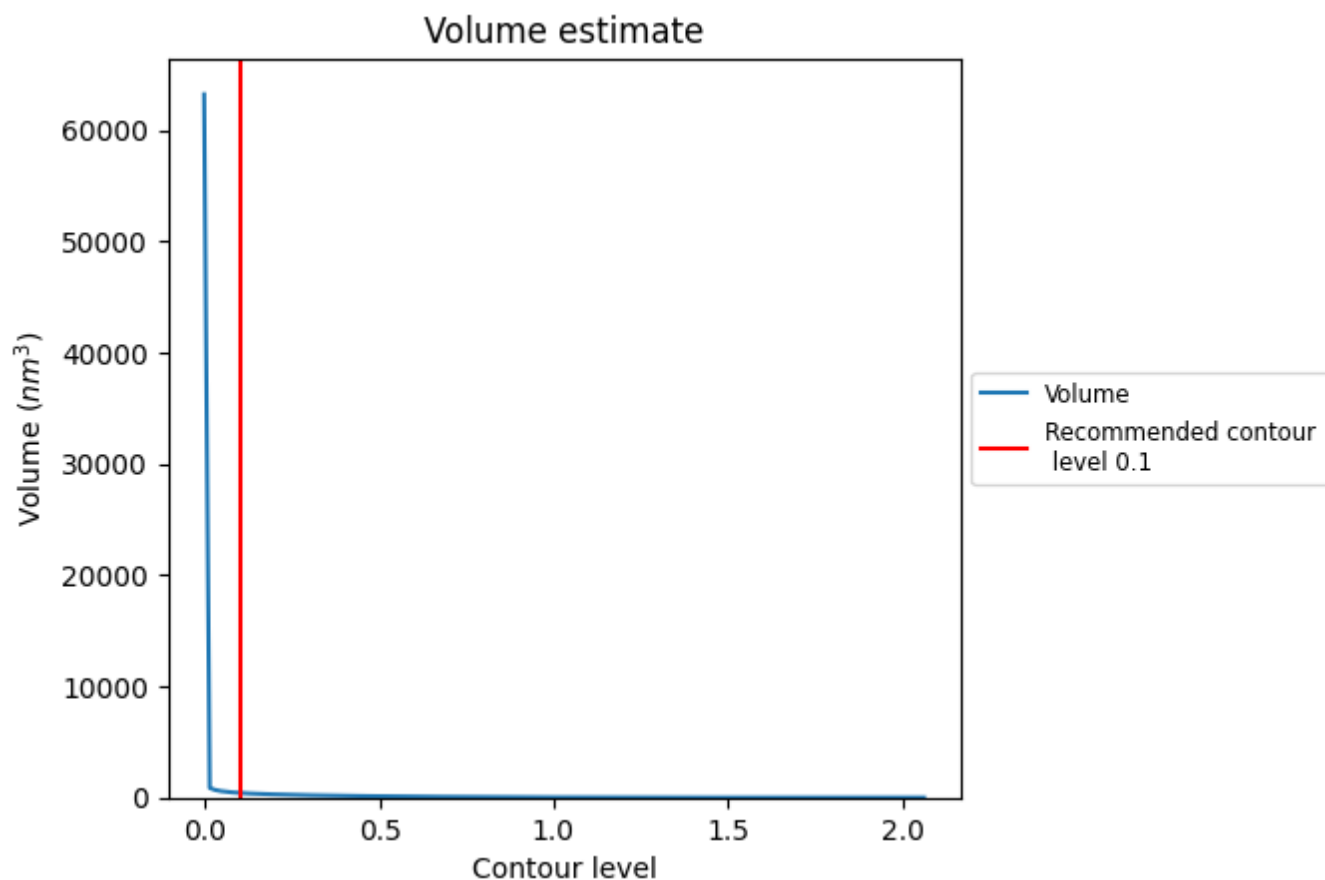
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

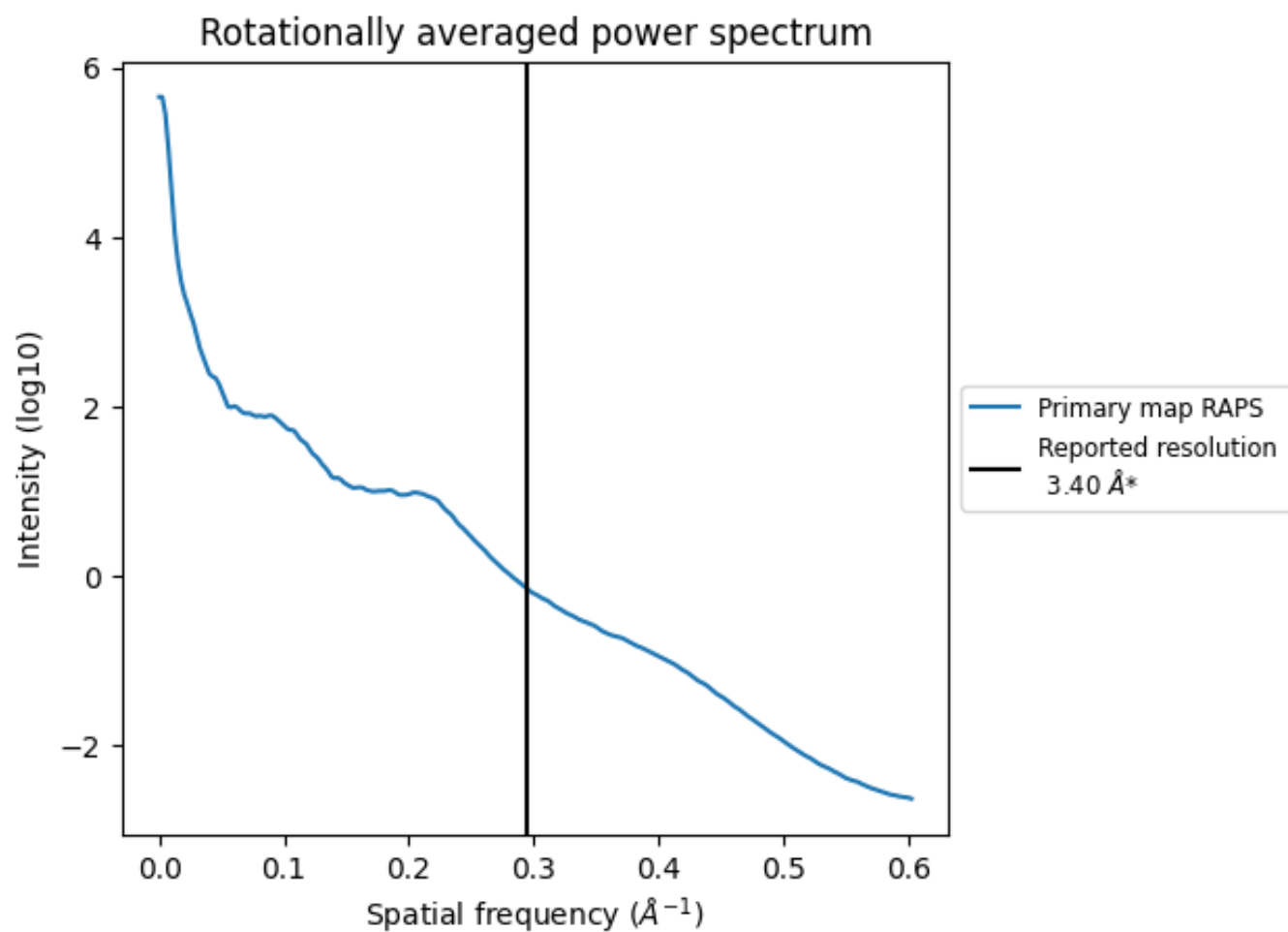
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

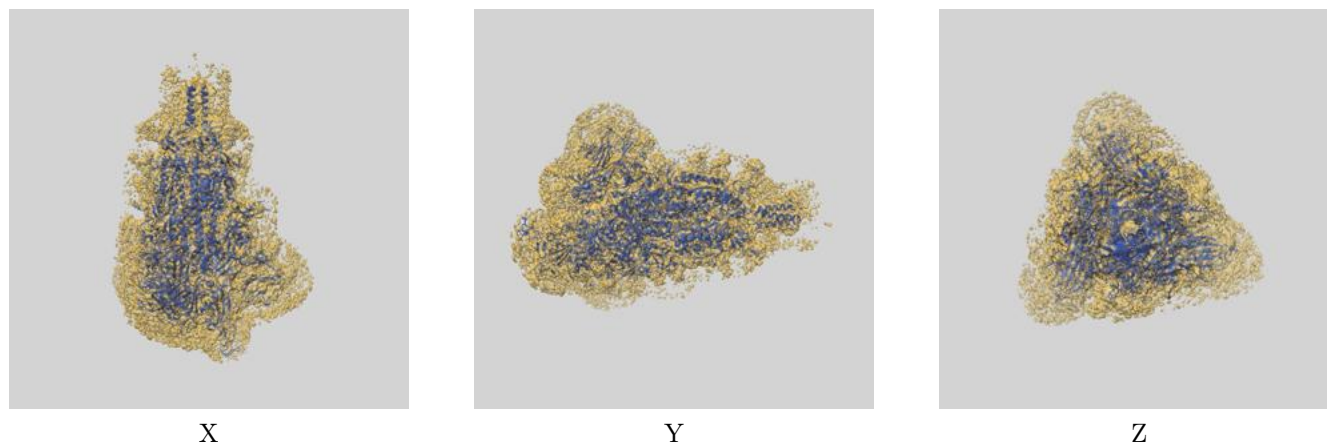
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

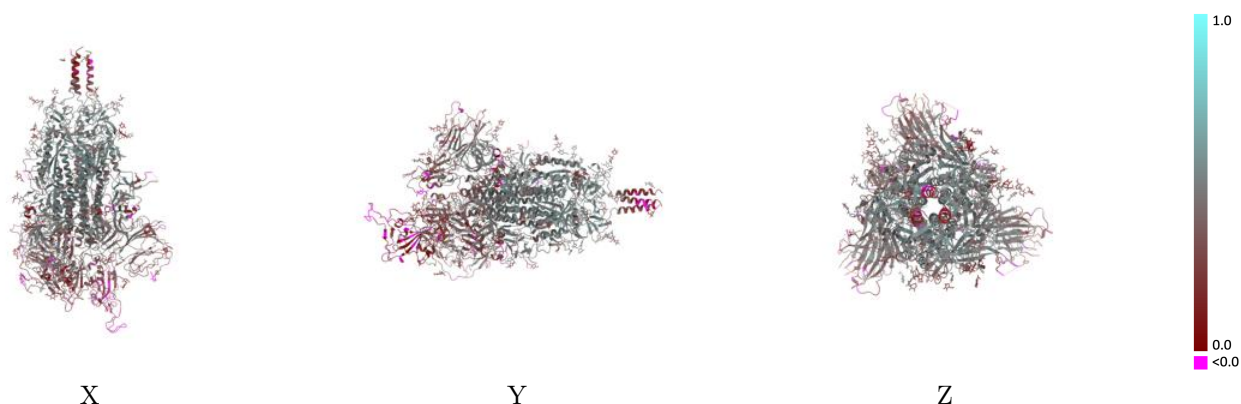
This section contains information regarding the fit between EMDB map EMD-26029 and PDB model 7TO4. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



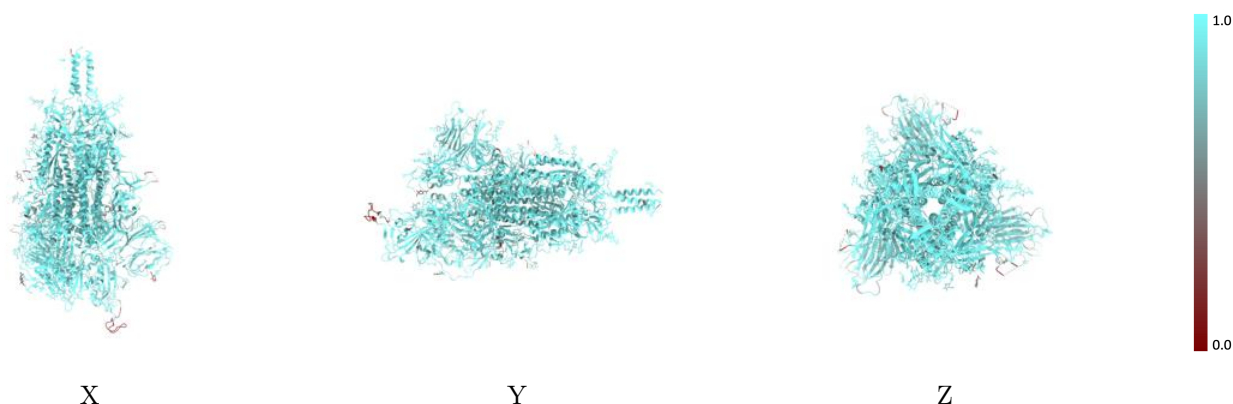
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



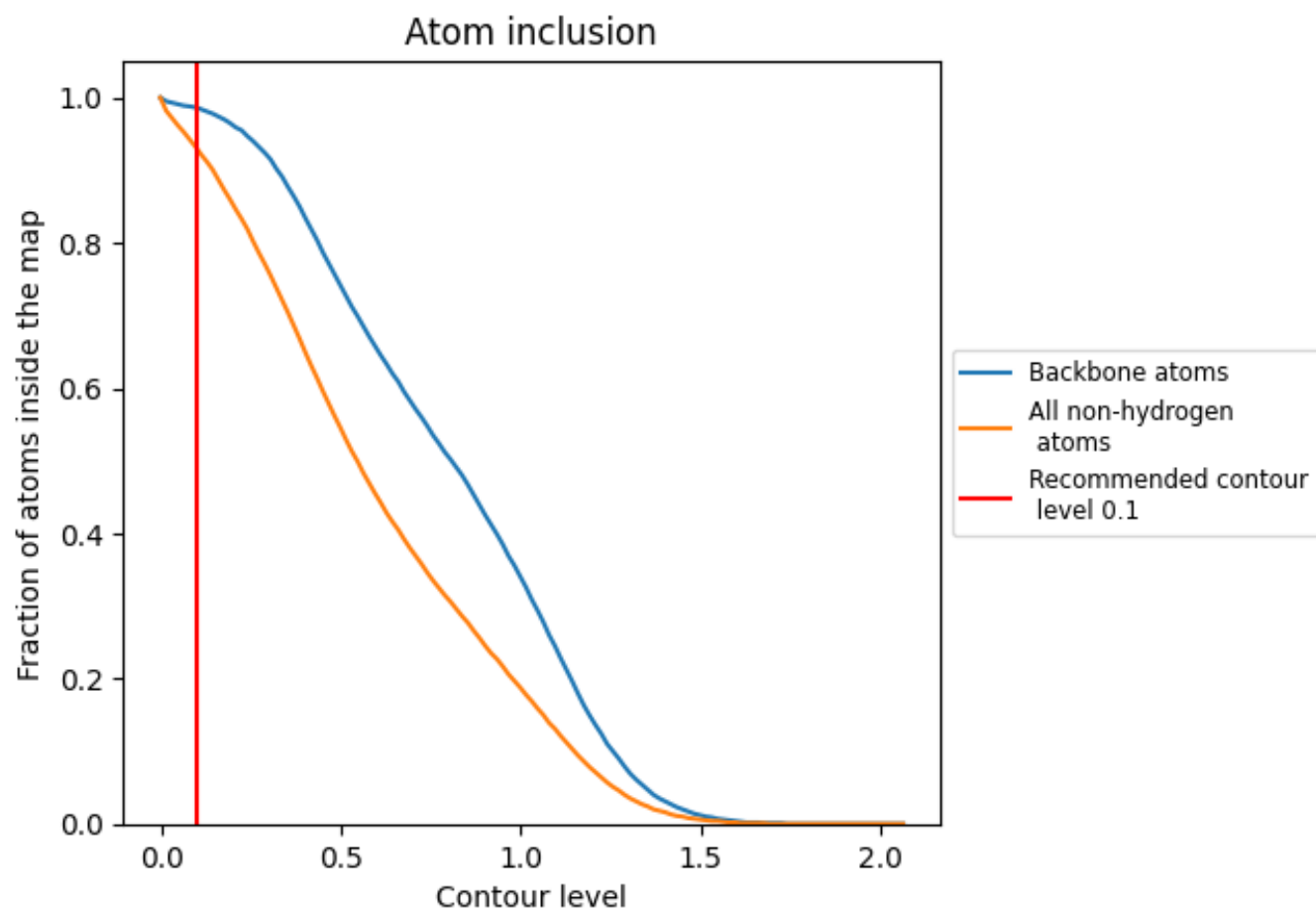
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.3940
A	 0.9220	 0.3690
B	 0.9330	 0.4000
C	 0.9370	 0.4220
D	 0.6430	 0.1890
E	 0.9290	 0.3280
F	 0.9290	 0.3950
G	 0.9290	 0.4310
H	 0.9640	 0.4060
I	 0.9470	 0.4560
J	 0.9490	 0.3920
K	 1.0000	 0.3920
L	 0.6070	 0.1020
M	 0.9490	 0.3190
N	 0.7140	 0.0840
O	 0.9490	 0.3520
P	 0.9290	 0.3020
Q	 0.9740	 0.4460
R	 0.9490	 0.3530
S	 0.7630	 0.0610
T	 0.9740	 0.3670
U	 0.9740	 0.3420
V	 0.5000	 0.0550
W	 0.8720	 0.1490
X	 0.8930	 0.2320
Y	 0.8720	 0.2920
Z	 0.9490	 0.2920
a	 0.8570	 0.2810
b	 0.9490	 0.4230
c	 0.9230	 0.3560
d	 0.7630	 0.2840
e	 0.9230	 0.3830
f	 0.8970	 0.3310

