



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:01 PM UTC

PDB ID : 9CRH / pdb_00009crh
EMDB ID : EMD-45868
Title : Cryo-EM structure of SARS-CoV-2 Spike Proteins on intact virions: Delta (B.1.617.2) variant 3 closed RBDs
Authors : Ke, Z.; Briggs, J.A.G.
Deposited on : 2024-07-22
Resolution : 3.40 Å(reported)

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:

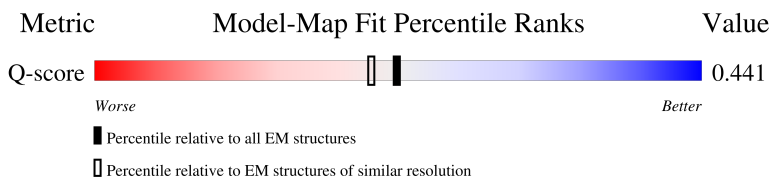
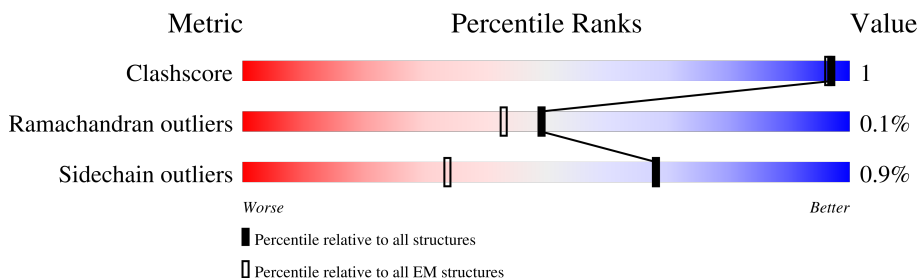
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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	1271	
1	B	1271	
1	C	1271	
2	D	2	

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 48189 atoms, of which 23805 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	994	Total	C	H	N	O	S	0	0
			15379	4977	7597	1291	1480	34		
1	C	994	Total	C	H	N	O	S	0	0
			15379	4977	7597	1291	1480	34		
1	B	994	Total	C	H	N	O	S	0	0
			15379	4977	7597	1291	1480	34		

There are 36 discrepancies between the modelled and reference sequences:

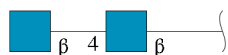
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	THR	variant	UNP P0DTC2
A	77	ARG	LYS	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	156	GLY	GLU	variant	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	222	VAL	ALA	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	950	ASN	ASP	variant	UNP P0DTC2
C	19	ARG	THR	variant	UNP P0DTC2
C	77	ARG	LYS	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	156	GLY	GLU	variant	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	222	VAL	ALA	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	950	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	ARG	THR	variant	UNP P0DTC2
B	77	ARG	LYS	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	156	GLY	GLU	variant	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	222	VAL	ALA	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	950	ASN	ASP	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.



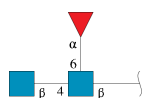
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	E	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	F	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	H	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	I	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	J	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	K	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	L	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	N	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	S	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	T	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	U	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	V	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	X	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	Y	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	Z	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	a	2	Total	C	H	N	O	0	0
			55	16	27	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	G	3	Total	C	H	N	O	0	0
			75	22	37	2	14		
3	O	3	Total	C	H	N	O	0	0
			75	22	37	2	14		
3	W	3	Total	C	H	N	O	0	0
			75	22	37	2	14		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

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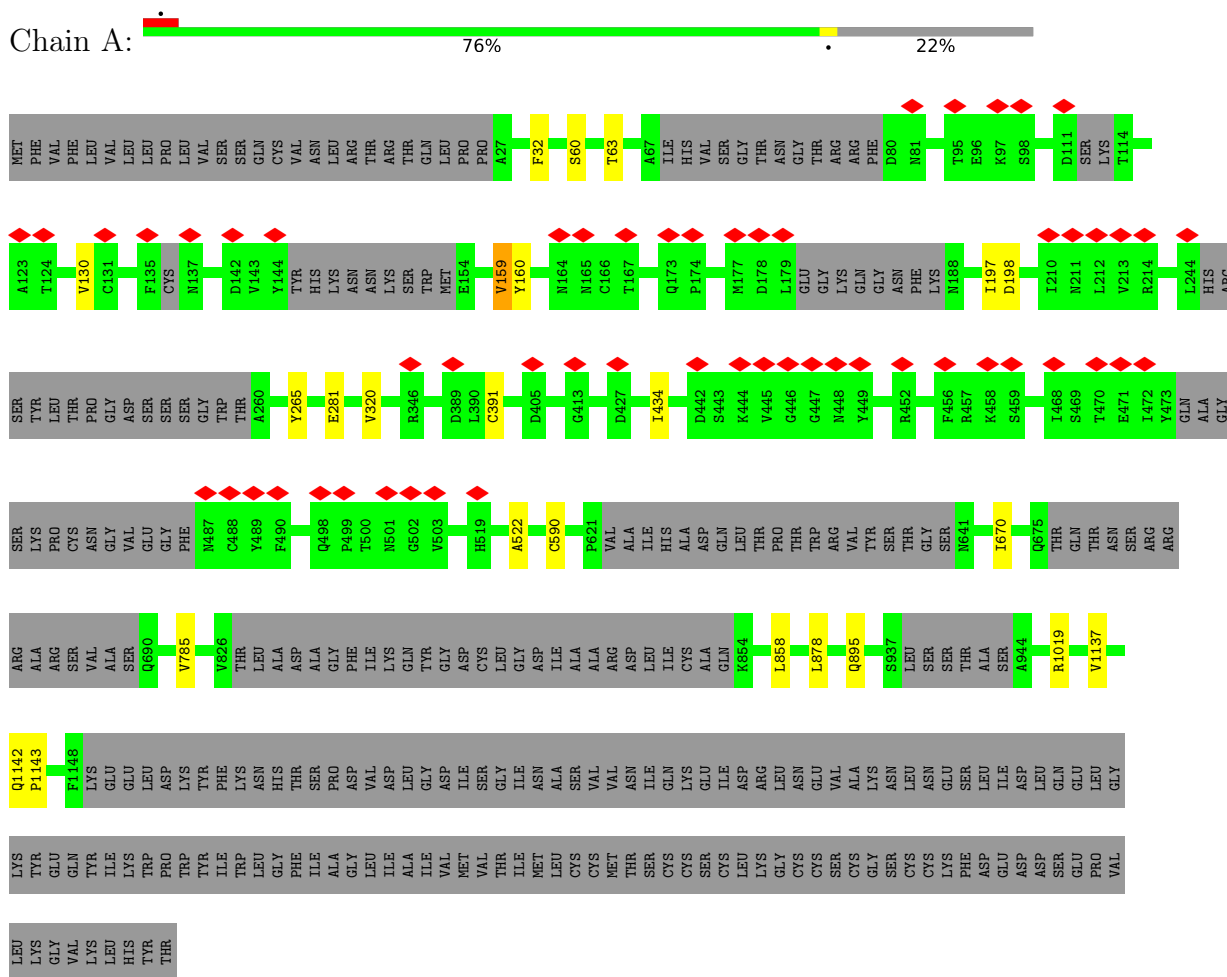
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Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	

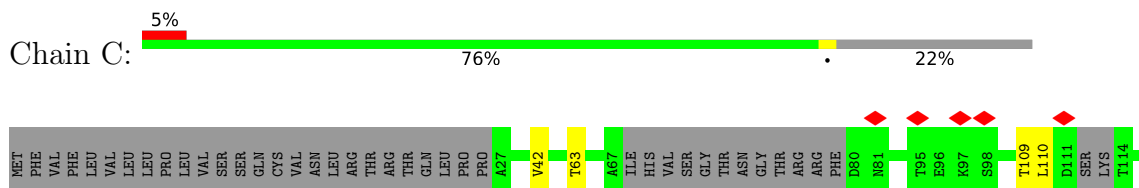
3 Residue-property plots

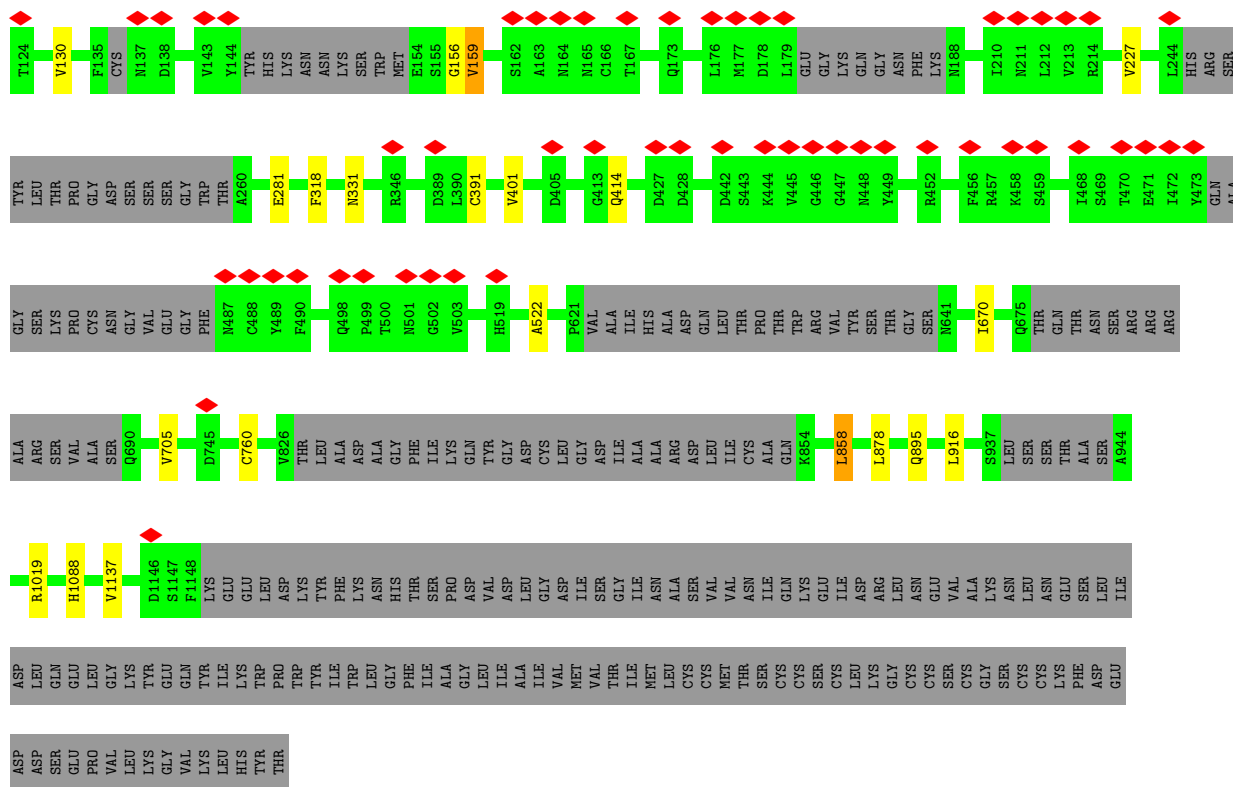
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

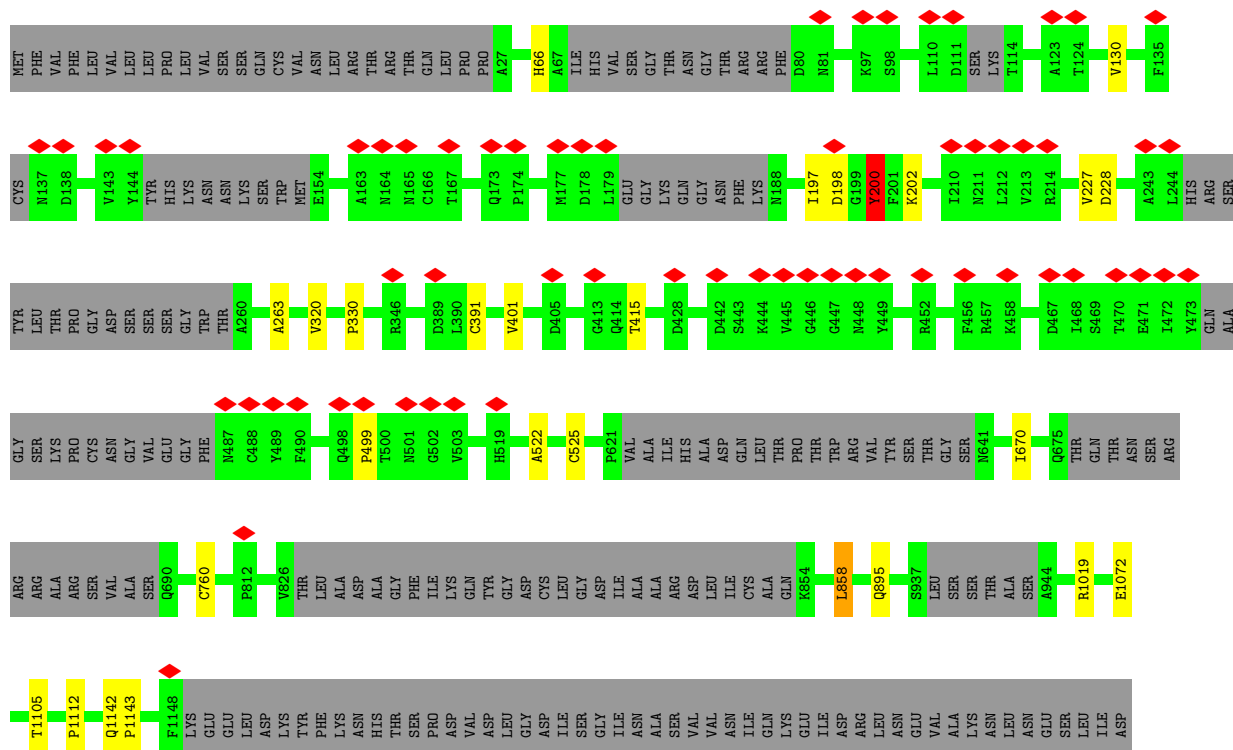
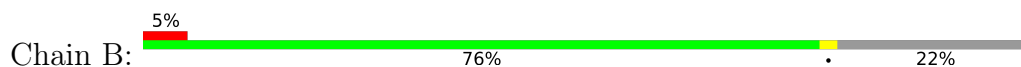


- Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



LEU GLN GLU LEU GLY LYS TYR GLN TYR ILE LYS LYS PRO TRP TRP TRP LEU GLY PHE ILE ILE GLY LEU ILE ALA VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS SER CYS LEU LYS GLY CYS SER CYS GLY SER CYS LYS PHE ASP GLU ASP

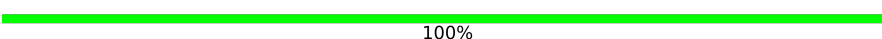
ASP SER GLU PRO VAL LEU LYS GLY VAL LYS LEU HIS TYR THR

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

Chain D: 



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

Chain E: 



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

Chain F: 



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

Chain H: 



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

Chain I: 



- 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 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



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- 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



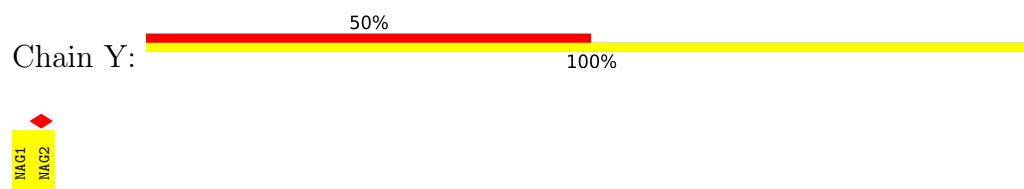
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



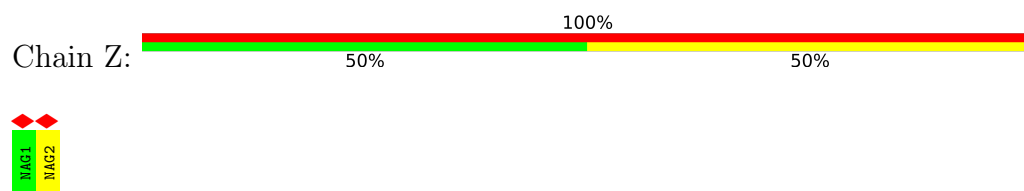
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



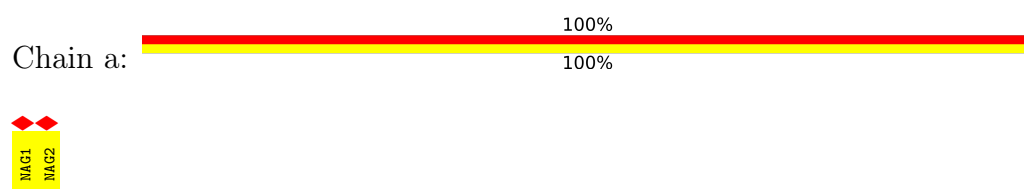
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



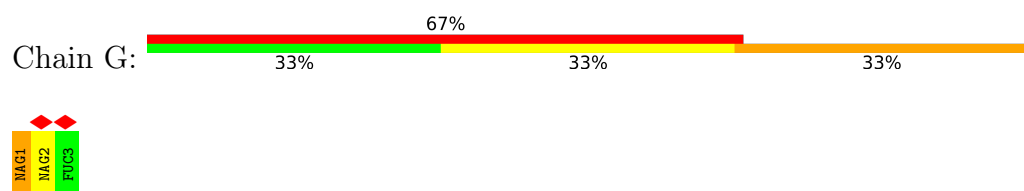
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



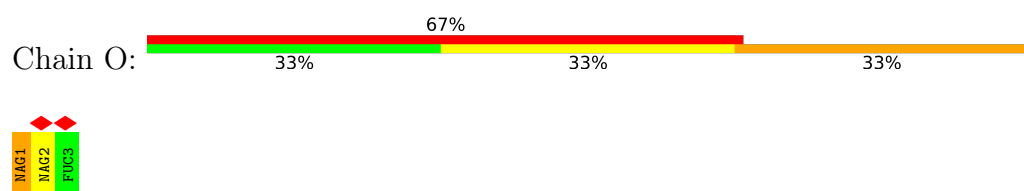
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	50656	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/7953	0.58	0/10815
1	B	0.26	0/7953	0.57	1/10815 (0.0%)
1	C	0.25	0/7953	0.57	0/10815
All	All	0.26	0/23859	0.57	1/32445 (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	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	TYR	CA-CB-CG	5.17	123.21	113.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	ARG	Sidechain
1	B	1019	ARG	Sidechain
1	B	499	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	C	1019	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7782	7597	7585	11	0
1	B	7782	7597	7585	14	0
1	C	7782	7597	7585	9	0
2	D	28	27	25	1	0
2	E	28	27	25	0	0
2	F	28	27	25	0	0
2	H	28	27	25	0	0
2	I	28	27	25	0	0
2	J	28	27	25	0	0
2	K	28	27	25	0	0
2	L	28	27	25	1	0
2	M	28	27	25	0	0
2	N	28	27	25	0	0
2	P	28	27	25	0	0
2	Q	28	27	25	0	0
2	R	28	27	25	0	0
2	S	28	27	25	0	0
2	T	28	27	25	0	0
2	U	28	27	25	0	0
2	V	28	27	25	0	0
2	X	28	27	25	0	0
2	Y	28	27	25	0	0
2	Z	28	27	25	0	0
2	a	28	27	25	0	0
3	G	38	37	34	1	0
3	O	38	37	34	1	0
3	W	38	37	34	2	0
4	A	112	112	104	0	0
4	B	112	112	104	0	0
4	C	112	112	104	0	0
All	All	24384	23805	23694	34	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 1.

All (34) 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:159:VAL:HG13	1:A:160:TYR:H	1.55	0.70
1:C:895:GLN:OE1	3:W:1:NAG:H82	1.91	0.69
1:B:1072:GLU:OE1	3:W:1:NAG:H81	2.07	0.55
1:C:391:CYS:SG	1:C:522:ALA:HB1	2.49	0.52
1:B:895:GLN:OE1	3:G:1:NAG:H82	2.11	0.51
1:B:200:TYR:OH	1:B:202:LYS:HE2	2.13	0.49
1:A:391:CYS:SG	1:A:522:ALA:HB1	2.53	0.48
1:C:156:GLY:O	1:C:159:VAL:HG22	2.14	0.47
1:B:391:CYS:SG	1:B:522:ALA:HB1	2.54	0.47
1:A:281:GLU:HB3	2:D:1:NAG:H82	1.97	0.47
1:B:197:ILE:HG22	1:B:198:ASP:N	2.30	0.47
1:C:858:LEU:HD22	1:C:858:LEU:H	1.80	0.46
1:A:858:LEU:H	1:A:858:LEU:HD22	1.80	0.46
1:B:858:LEU:H	1:B:858:LEU:HD22	1.81	0.46
1:B:66:HIS:HA	1:B:263:ALA:O	2.16	0.46
1:B:330:PRO:HD2	1:B:525:CYS:SG	2.57	0.45
1:A:1142:GLN:HB3	1:A:1143:PRO:HD3	1.97	0.45
1:B:670:ILE:N	1:B:670:ILE:HD12	2.32	0.45
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.99	0.45
1:A:197:ILE:HG22	1:A:198:ASP:N	2.32	0.44
1:C:1088:HIS:CE1	1:C:1137:VAL:HG21	2.53	0.44
1:B:320:VAL:O	1:B:320:VAL:HG13	2.18	0.44
1:A:670:ILE:HD12	1:A:670:ILE:N	2.32	0.43
1:A:785:VAL:HG13	1:A:785:VAL:O	2.16	0.43
1:A:895:GLN:OE1	3:O:1:NAG:H82	2.18	0.43
1:C:670:ILE:HD12	1:C:670:ILE:N	2.33	0.43
1:A:32:PHE:CE2	1:A:60:SER:O	2.73	0.42
1:A:320:VAL:HG13	1:A:590:CYS:SG	2.60	0.41
1:B:227:VAL:HG22	1:B:228:ASP:N	2.35	0.41
1:C:130:VAL:O	1:C:130:VAL:HG12	2.20	0.41
1:B:130:VAL:O	1:B:130:VAL:CG1	2.68	0.41
1:C:109:THR:HG22	1:C:110:LEU:N	2.35	0.41
1:C:281:GLU:HB3	2:L:1:NAG:H82	2.02	0.41
1:B:1105:THR:HG22	1:B:1112:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	970/1271 (76%)	906 (93%)	63 (6%)	1 (0%)	48	78
1	B	970/1271 (76%)	912 (94%)	58 (6%)	0	100	100
1	C	970/1271 (76%)	905 (93%)	64 (7%)	1 (0%)	48	78
All	All	2910/3813 (76%)	2723 (94%)	185 (6%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	VAL
1	C	159	VAL

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	869/1110 (78%)	863 (99%)	6 (1%)	76	78
1	B	869/1110 (78%)	864 (99%)	5 (1%)	78	80
1	C	869/1110 (78%)	857 (99%)	12 (1%)	59	70
All	All	2607/3330 (78%)	2584 (99%)	23 (1%)	68	76

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR

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Mol	Chain	Res	Type
1	A	130	VAL
1	A	265	TYR
1	A	434	ILE
1	A	878	LEU
1	A	1137	VAL
1	C	42	VAL
1	C	63	THR
1	C	227	VAL
1	C	318	PHE
1	C	331	ASN
1	C	401	VAL
1	C	414	GLN
1	C	705	VAL
1	C	760	CYS
1	C	858	LEU
1	C	878	LEU
1	C	916	LEU
1	B	200	TYR
1	B	401	VAL
1	B	415	THR
1	B	760	CYS
1	B	858	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	370	ASN
1	A	536	ASN
1	A	540	ASN
1	A	544	ASN
1	A	564	GLN
1	A	641	ASN
1	A	655	HIS
1	A	777	ASN
1	A	804	GLN
1	A	919	ASN
1	A	935	GLN
1	A	1058	HIS
1	C	196	ASN
1	C	460	ASN
1	C	536	ASN

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Mol	Chain	Res	Type
1	C	540	ASN
1	C	544	ASN
1	C	564	GLN
1	C	613	GLN
1	C	675	GLN
1	C	777	ASN
1	C	787	GLN
1	C	804	GLN
1	C	919	ASN
1	C	935	GLN
1	B	121	ASN
1	B	164	ASN
1	B	196	ASN
1	B	370	ASN
1	B	460	ASN
1	B	536	ASN
1	B	540	ASN
1	B	564	GLN
1	B	655	HIS
1	B	762	GLN
1	B	777	ASN
1	B	919	ASN
1	B	1058	HIS
1	B	1083	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

51 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	0.25	0	17,19,21	0.69	1 (5%)
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.76	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.54	0	17,19,21	0.59	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.48	0
2	NAG	F	1	2,1	14,14,15	0.28	0	17,19,21	0.62	0
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
3	NAG	G	1	3,1	14,14,15	1.44	2 (14%)	17,19,21	1.22	1 (5%)
3	NAG	G	2	3	14,14,15	0.55	0	17,19,21	0.71	1 (5%)
3	FUC	G	3	3	10,10,11	0.65	0	14,14,16	0.61	0
2	NAG	H	1	2,1	14,14,15	0.20	0	17,19,21	0.60	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.61	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.61	0	17,19,21	0.75	1 (5%)
2	NAG	I	2	2	14,14,15	0.18	0	17,19,21	0.53	0
2	NAG	J	1	2,1	14,14,15	0.47	0	17,19,21	0.83	1 (5%)
2	NAG	J	2	2	14,14,15	0.24	0	17,19,21	0.84	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.49	0	17,19,21	0.61	0
2	NAG	K	2	2	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	L	2	2	14,14,15	0.26	0	17,19,21	0.80	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.61	0	17,19,21	0.63	0
2	NAG	M	2	2	14,14,15	0.24	0	17,19,21	0.53	0
2	NAG	N	1	2,1	14,14,15	0.48	0	17,19,21	0.54	0
2	NAG	N	2	2	14,14,15	0.37	0	17,19,21	0.70	1 (5%)
3	NAG	O	1	3,1	14,14,15	1.56	2 (14%)	17,19,21	1.22	1 (5%)
3	NAG	O	2	3	14,14,15	0.59	0	17,19,21	0.77	1 (5%)
3	FUC	O	3	3	10,10,11	0.72	0	14,14,16	0.60	0
2	NAG	P	1	2,1	14,14,15	0.37	0	17,19,21	0.55	0
2	NAG	P	2	2	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	Q	1	2,1	14,14,15	0.58	0	17,19,21	0.75	1 (5%)
2	NAG	Q	2	2	14,14,15	0.23	0	17,19,21	0.52	0
2	NAG	R	1	2,1	14,14,15	0.61	0	17,19,21	1.02	1 (5%)
2	NAG	R	2	2	14,14,15	0.24	0	17,19,21	0.59	0
2	NAG	S	1	2,1	14,14,15	0.44	0	17,19,21	0.91	1 (5%)
2	NAG	S	2	2	14,14,15	0.18	0	17,19,21	0.60	0
2	NAG	T	1	2,1	14,14,15	0.46	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	T	2	2	14,14,15	0.22	0	17,19,21	0.73	1 (5%)
2	NAG	U	1	2,1	14,14,15	0.23	0	17,19,21	0.57	0
2	NAG	U	2	2	14,14,15	0.21	0	17,19,21	0.54	0
2	NAG	V	1	2,1	14,14,15	0.42	0	17,19,21	0.51	0
2	NAG	V	2	2	14,14,15	0.33	0	17,19,21	0.75	1 (5%)
3	NAG	W	1	3,1	14,14,15	1.54	2 (14%)	17,19,21	1.24	1 (5%)
3	NAG	W	2	3	14,14,15	0.60	0	17,19,21	0.74	1 (5%)
3	FUC	W	3	3	10,10,11	0.72	0	14,14,16	0.61	0
2	NAG	X	1	2,1	14,14,15	0.32	0	17,19,21	0.64	0
2	NAG	X	2	2	14,14,15	0.21	0	17,19,21	0.61	1 (5%)
2	NAG	Y	1	2,1	14,14,15	0.64	0	17,19,21	0.68	1 (5%)
2	NAG	Y	2	2	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
2	NAG	Z	1	2,1	14,14,15	0.75	0	17,19,21	0.79	0
2	NAG	Z	2	2	14,14,15	0.19	0	17,19,21	0.65	1 (5%)
2	NAG	a	1	2,1	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
2	NAG	a	2	2	14,14,15	0.28	0	17,19,21	0.76	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/6/23/26	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
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	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
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	1	NAG	C1-C2	4.83	1.58	1.52
3	O	1	NAG	C1-C2	4.81	1.58	1.52
3	G	1	NAG	C1-C2	4.25	1.58	1.52
3	G	1	NAG	O5-C1	3.02	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	NAG	O5-C1	2.91	1.48	1.43
3	W	1	NAG	O5-C1	2.65	1.48	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	4.31	117.96	112.19
3	W	1	NAG	C1-O5-C5	4.17	117.78	112.19
3	O	1	NAG	C1-O5-C5	3.97	117.50	112.19
2	R	1	NAG	C1-O5-C5	3.52	116.90	112.19
2	S	1	NAG	C1-O5-C5	3.38	116.72	112.19
2	J	2	NAG	C1-O5-C5	3.17	116.44	112.19
2	L	2	NAG	C1-O5-C5	2.86	116.03	112.19
2	a	2	NAG	C1-O5-C5	2.83	115.97	112.19
3	O	2	NAG	C1-O5-C5	2.83	115.97	112.19
2	a	1	NAG	C1-O5-C5	2.80	115.94	112.19
2	V	2	NAG	C1-O5-C5	2.79	115.92	112.19
2	I	1	NAG	C1-O5-C5	2.79	115.92	112.19
2	Q	1	NAG	C1-O5-C5	2.79	115.92	112.19
2	D	2	NAG	C1-O5-C5	2.70	115.80	112.19
3	W	2	NAG	C1-O5-C5	2.68	115.78	112.19
2	T	2	NAG	C1-O5-C5	2.67	115.76	112.19
2	F	2	NAG	C1-O5-C5	2.65	115.73	112.19
3	G	2	NAG	C1-O5-C5	2.57	115.64	112.19
2	N	2	NAG	C1-O5-C5	2.51	115.55	112.19
2	J	1	NAG	C1-O5-C5	2.50	115.54	112.19
2	K	2	NAG	C1-O5-C5	2.49	115.52	112.19
2	Y	1	NAG	C1-O5-C5	2.40	115.41	112.19
2	Y	2	NAG	C1-O5-C5	2.29	115.25	112.19
2	D	1	NAG	C1-O5-C5	2.26	115.22	112.19
2	Z	2	NAG	C1-O5-C5	2.19	115.11	112.19
2	H	2	NAG	C1-O5-C5	2.06	114.95	112.19
2	X	2	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C1-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	Y	1	NAG	C1-C2-N2-C7

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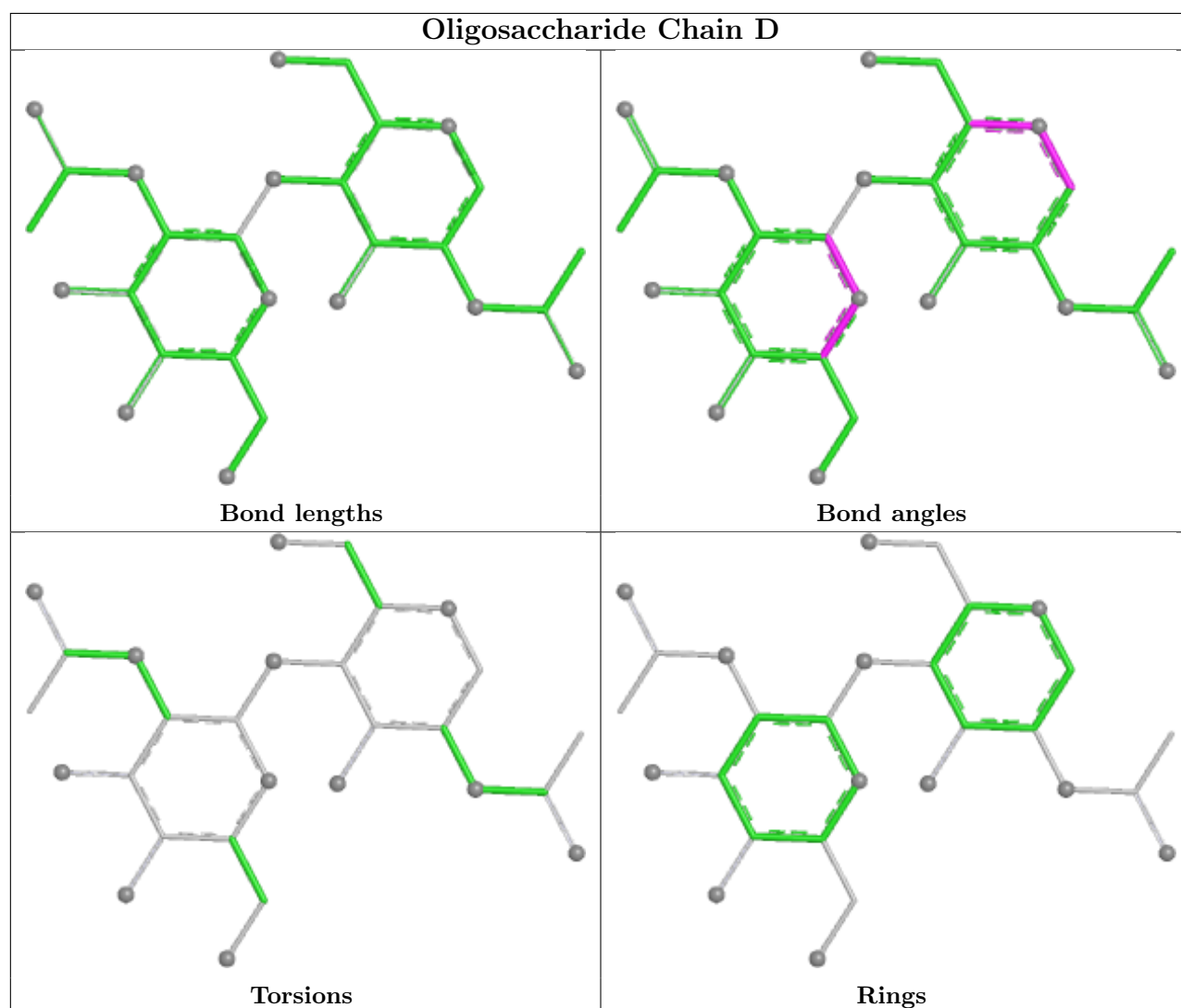
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C4-C5-C6-O6

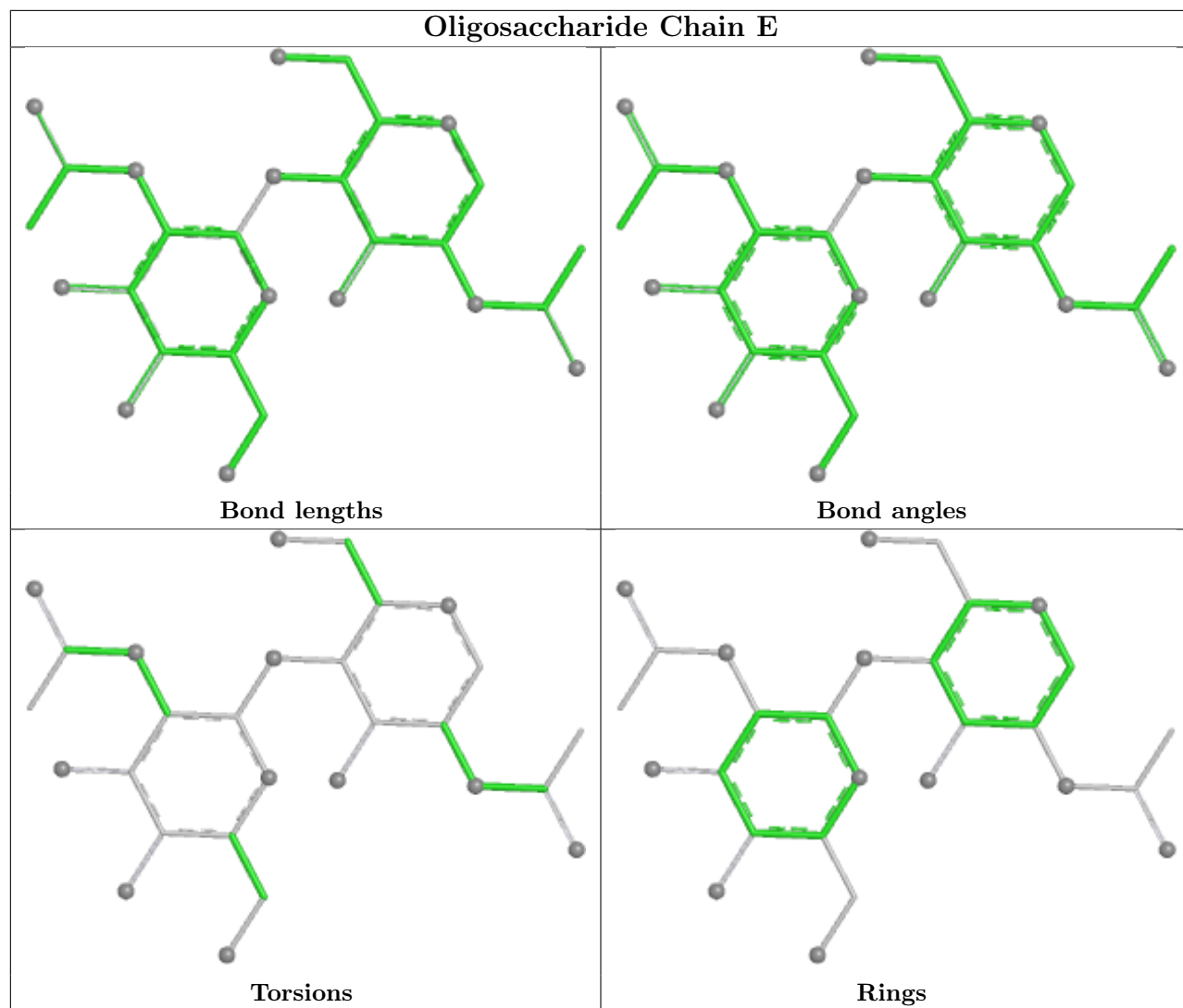
There are no ring outliers.

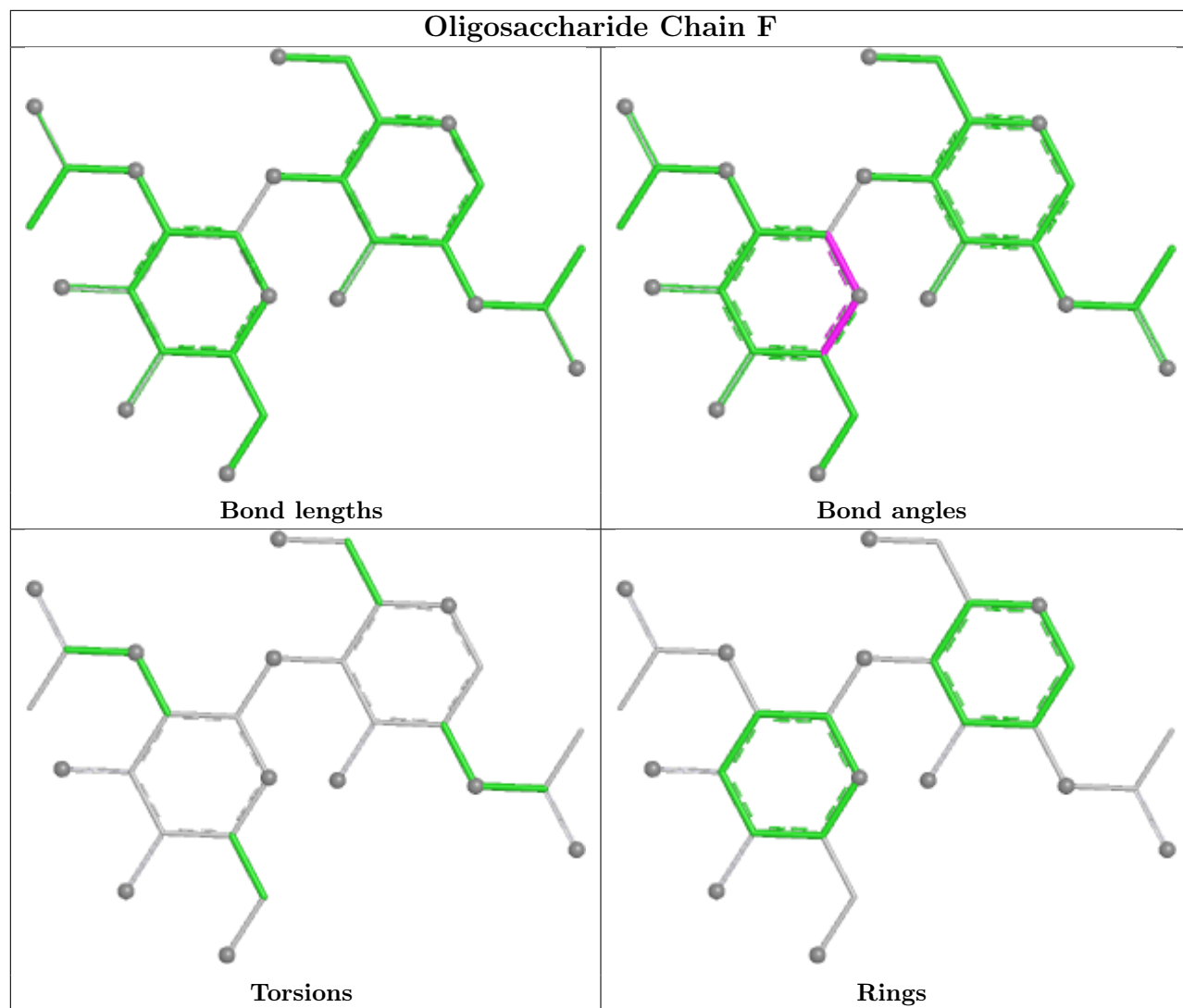
5 monomers are involved in 6 short contacts:

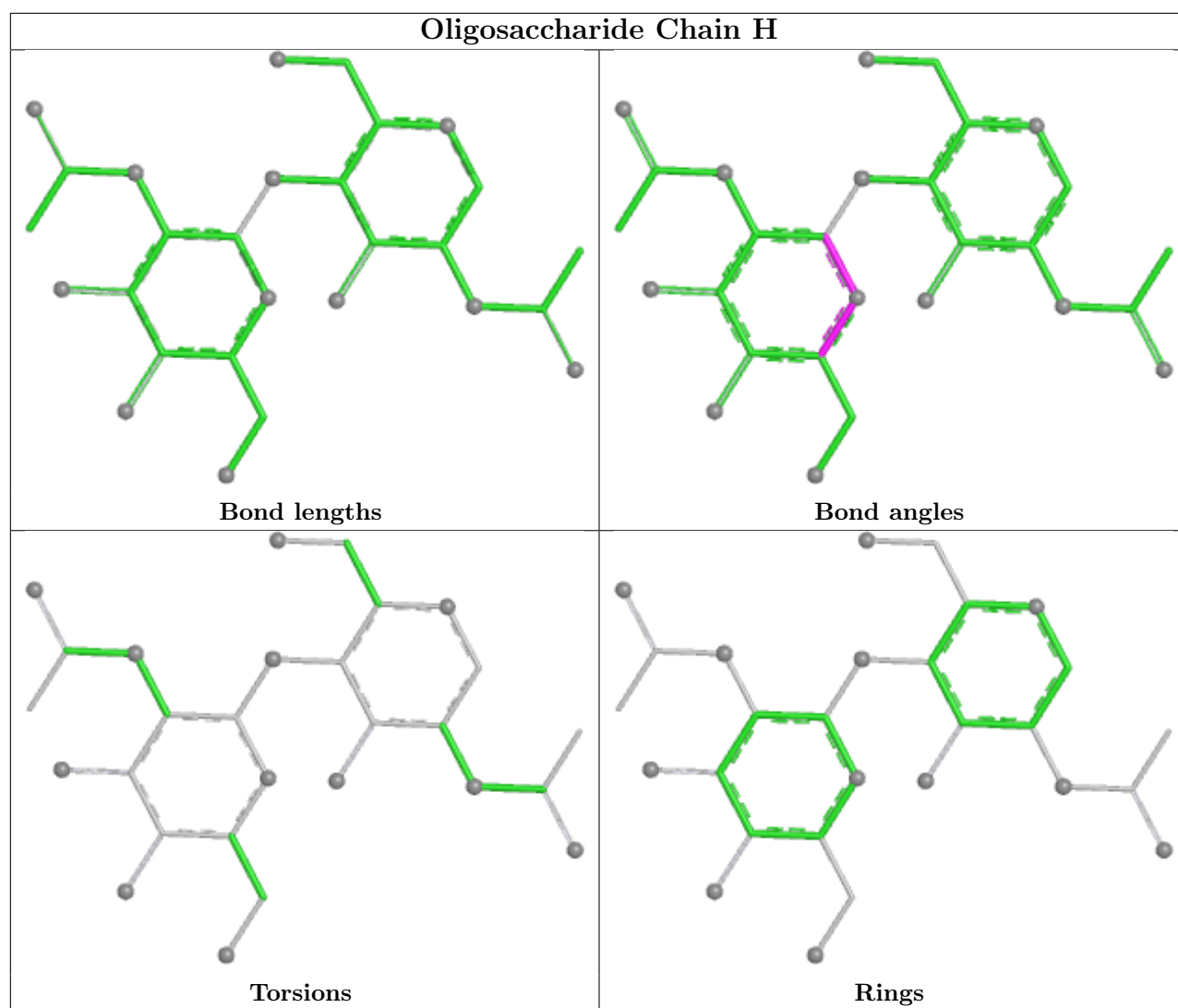
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	W	1	NAG	2	0
2	L	1	NAG	1	0
3	O	1	NAG	1	0
2	D	1	NAG	1	0

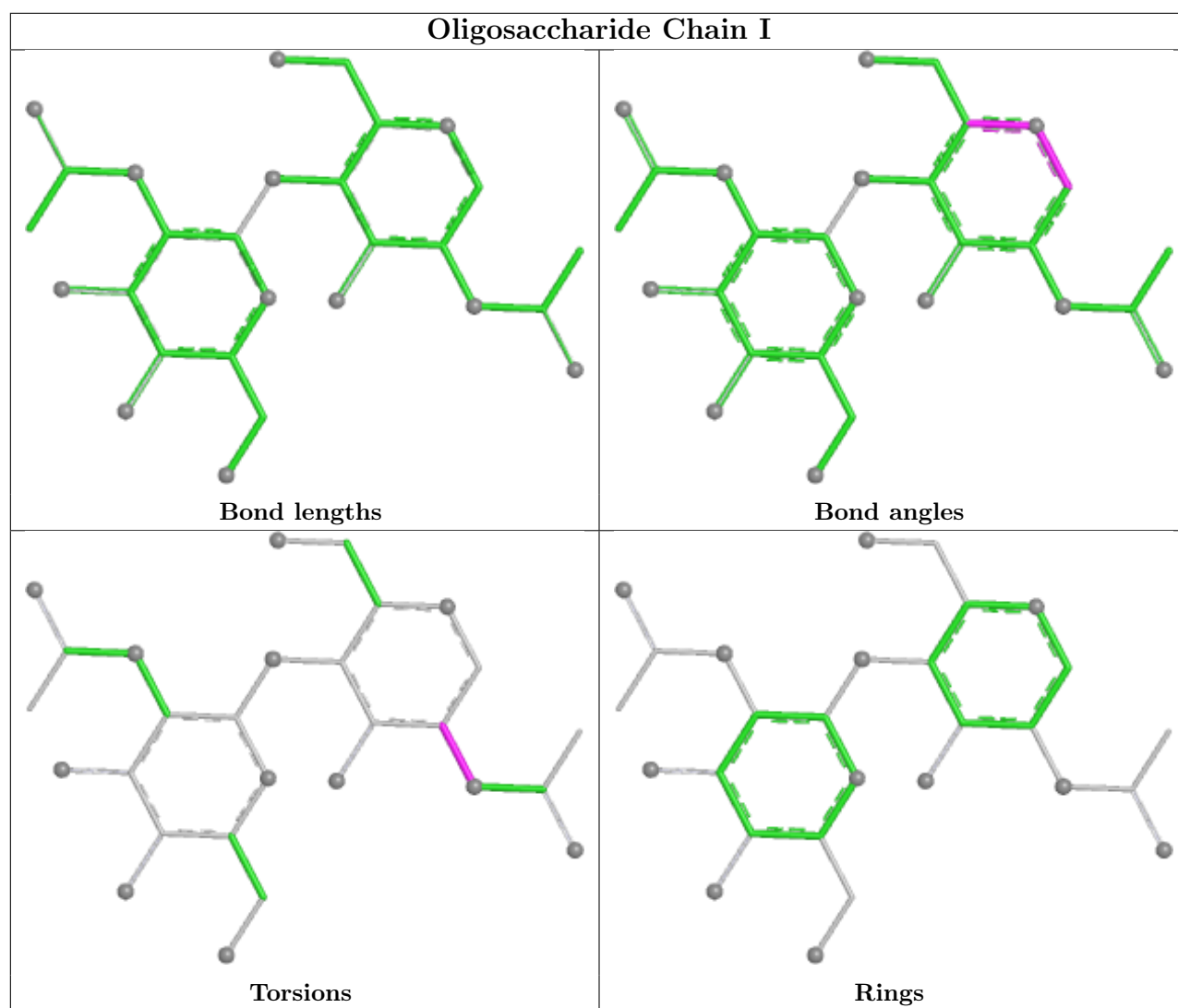
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

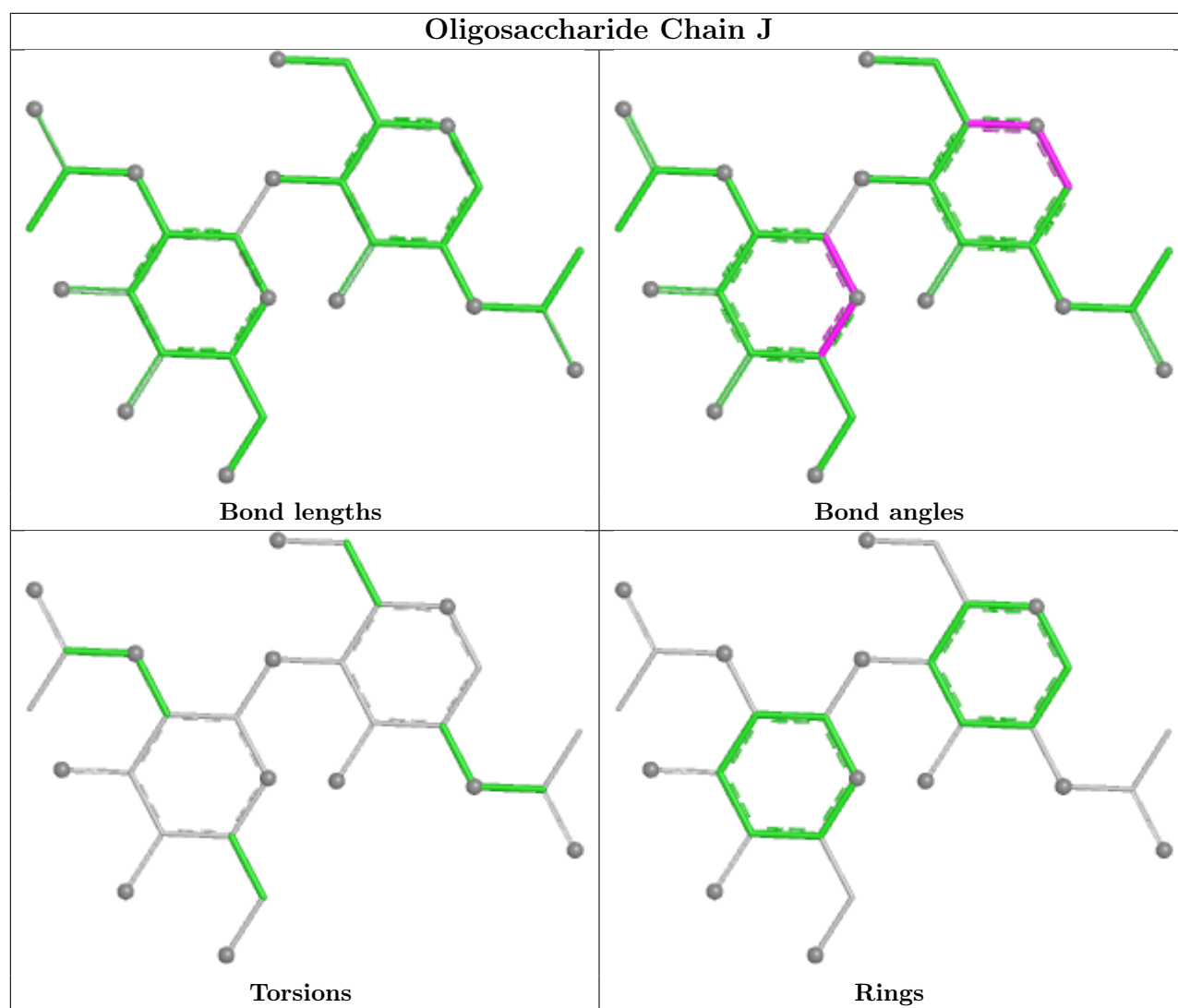


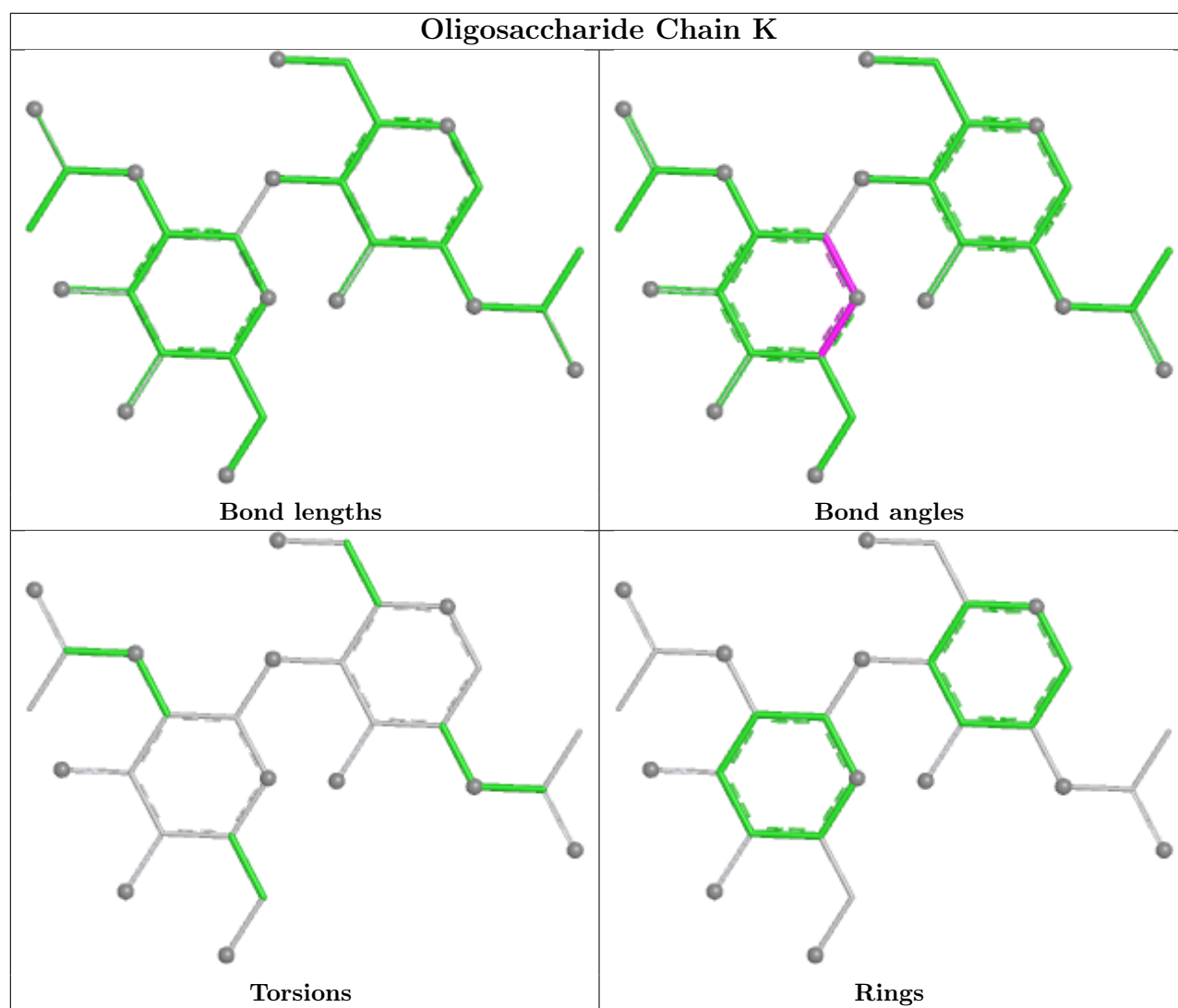


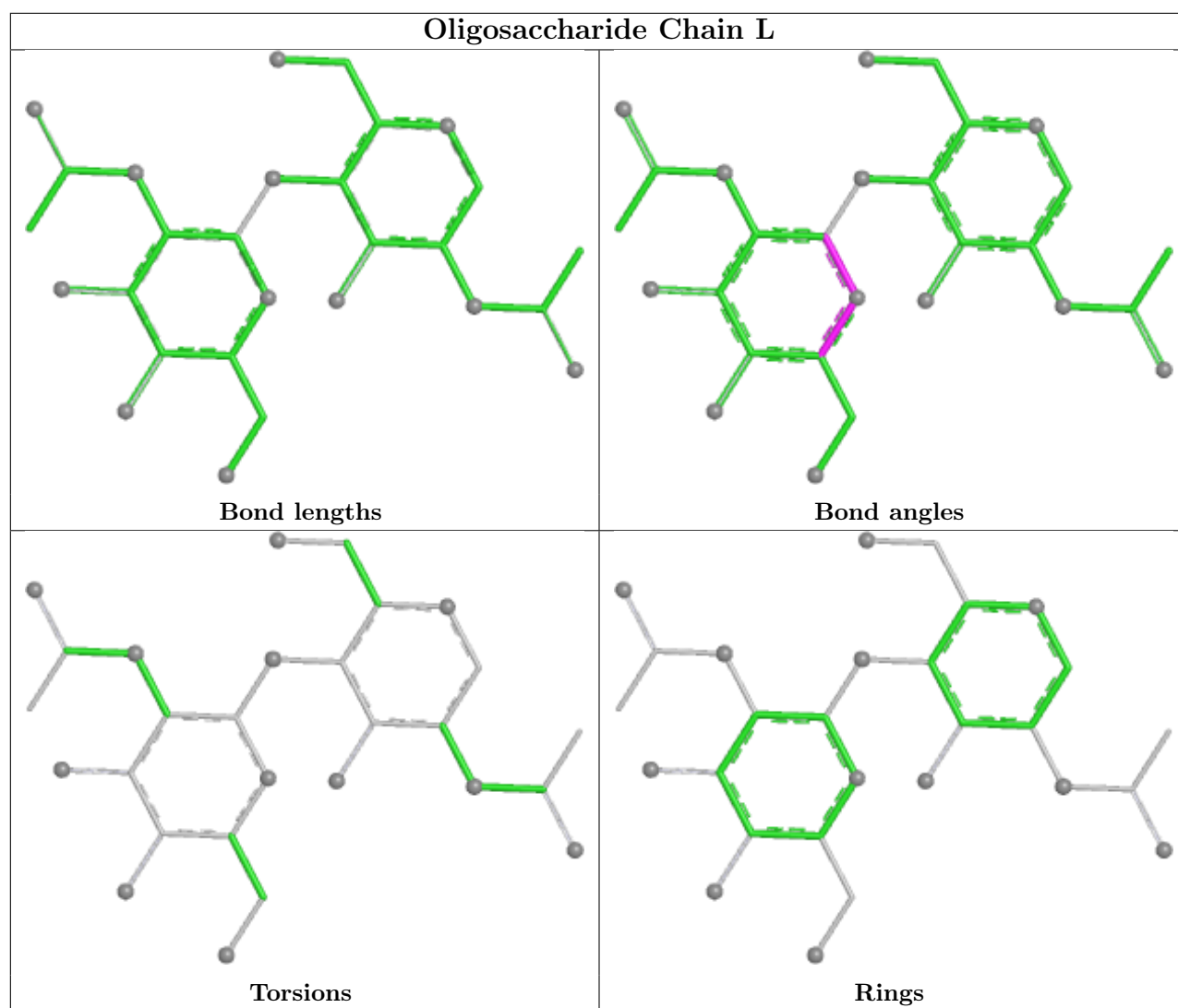


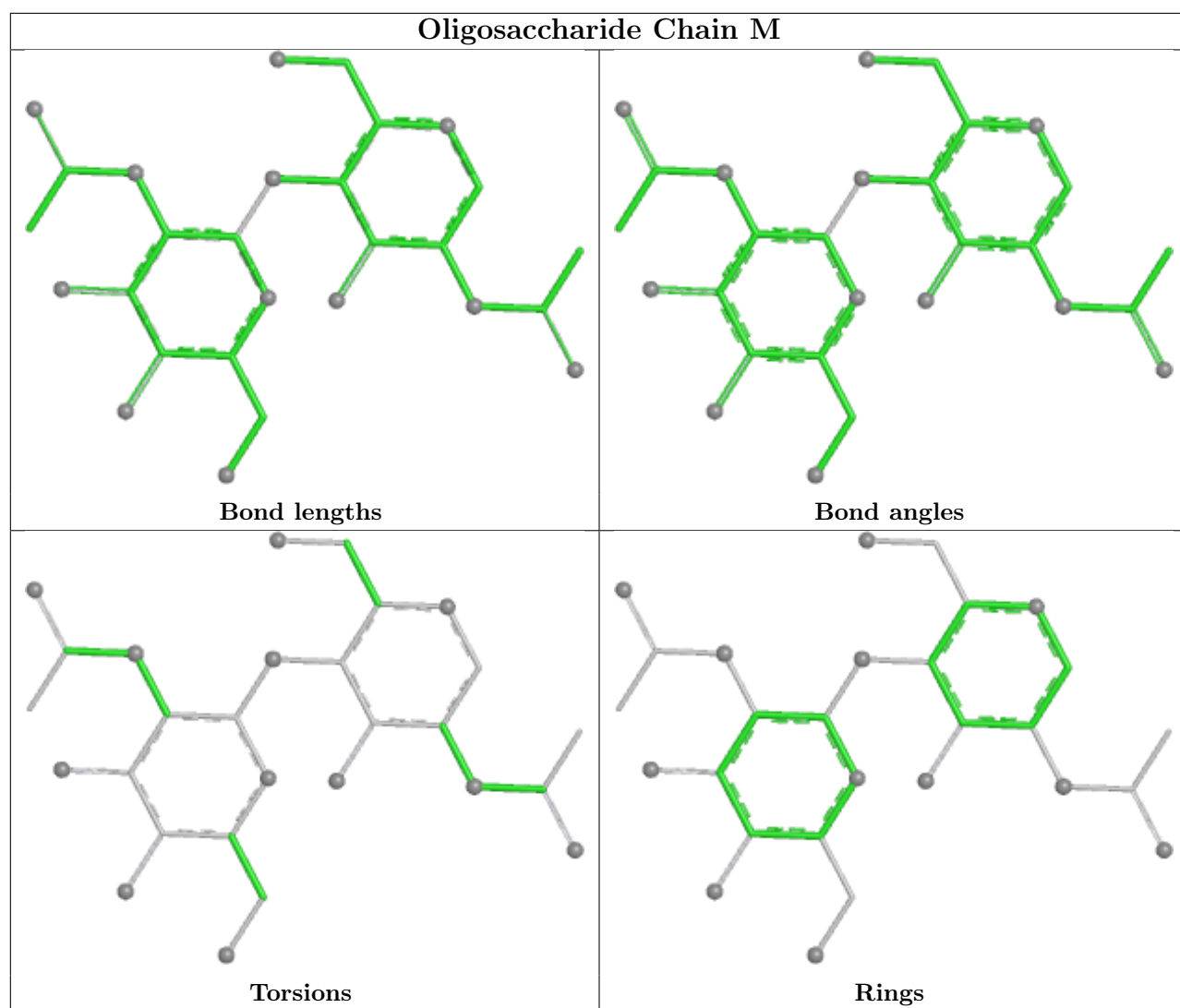


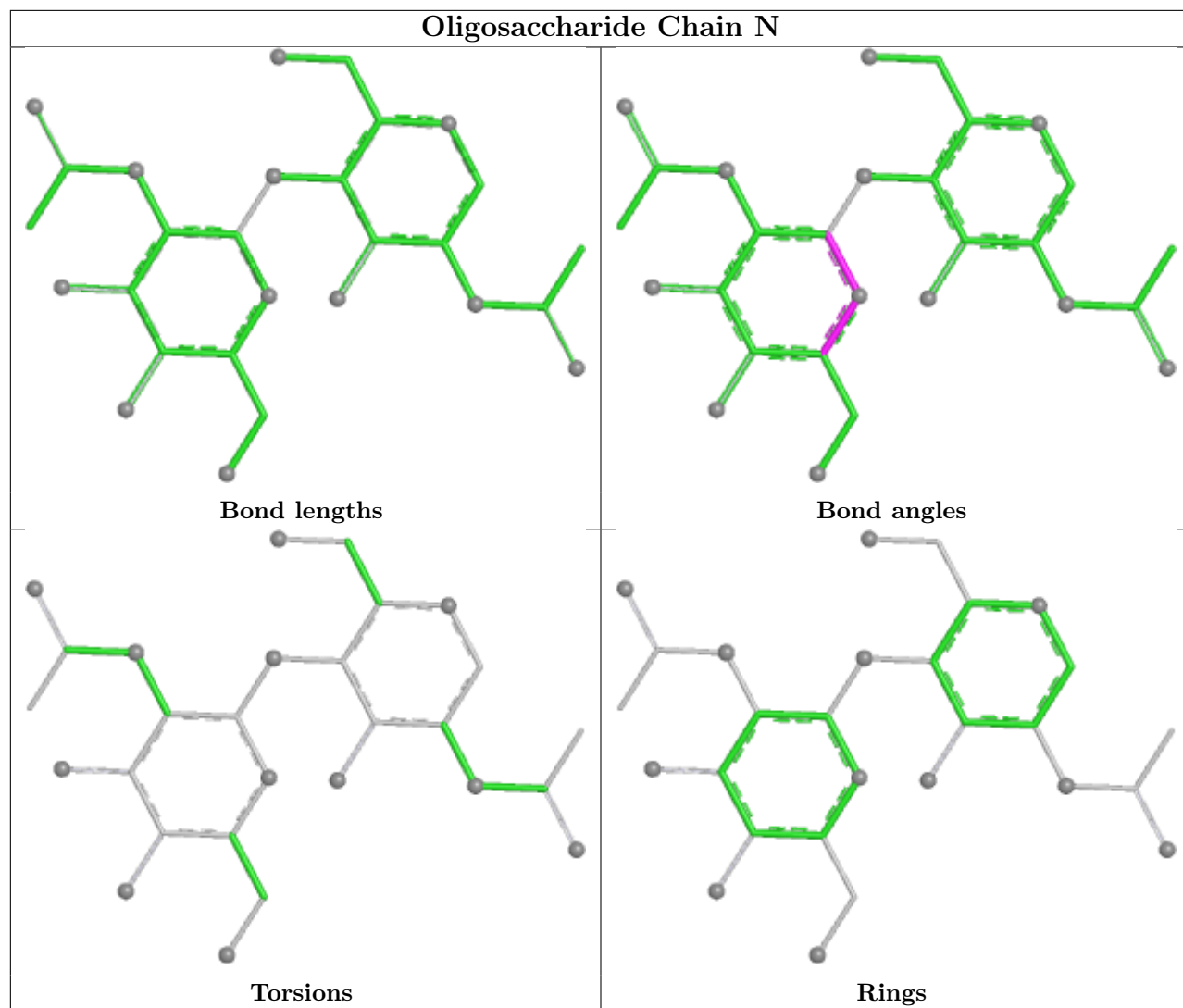


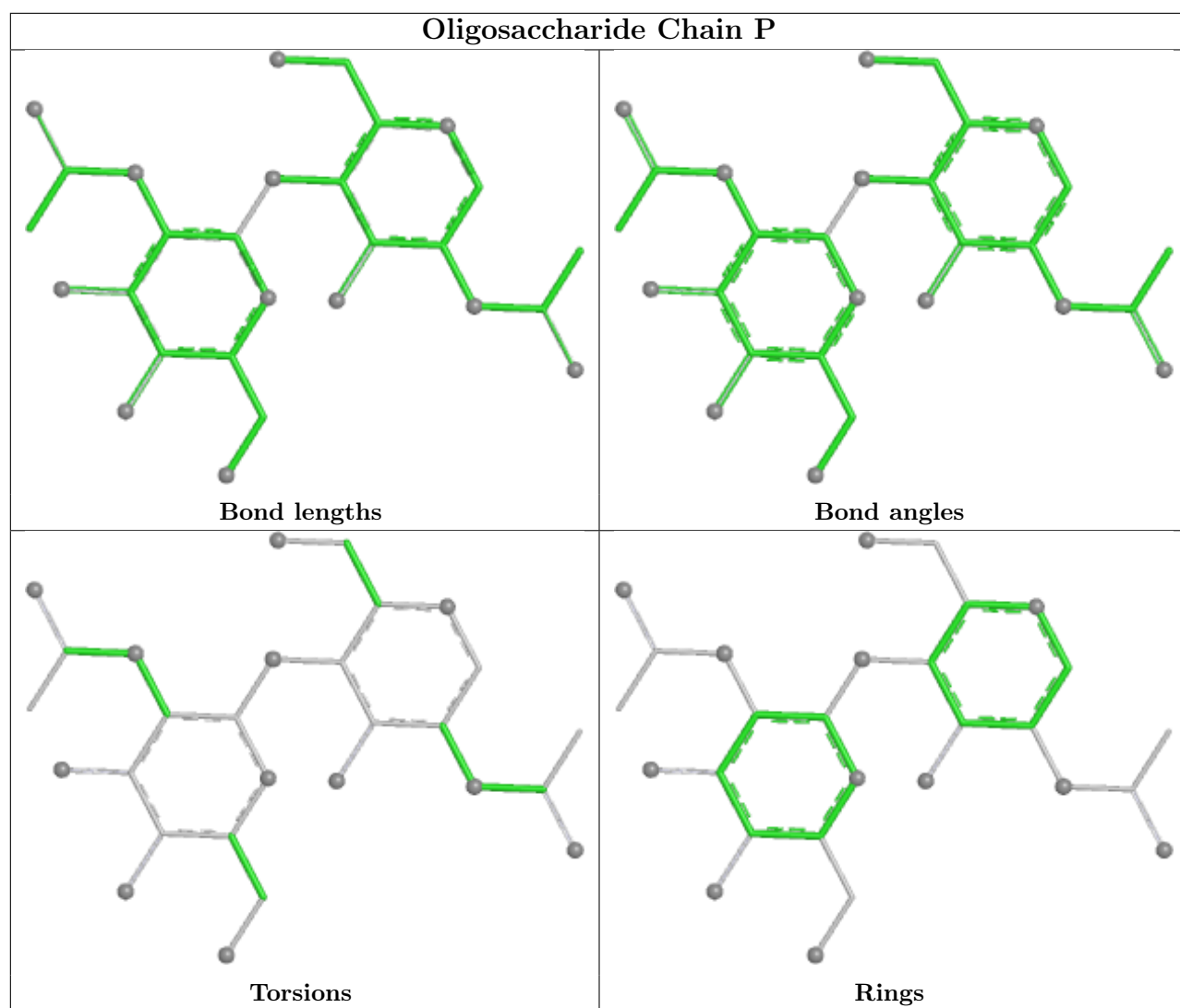


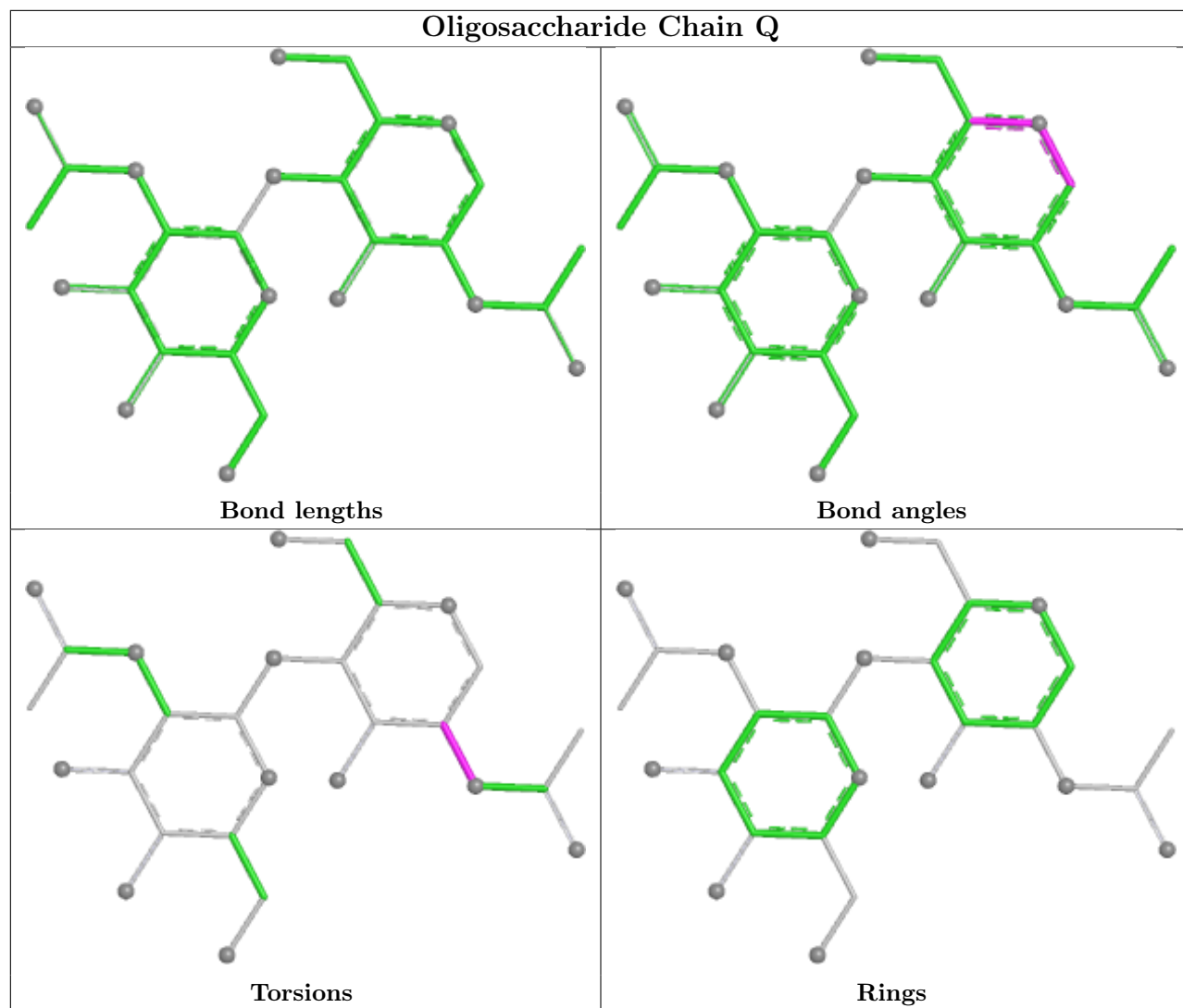


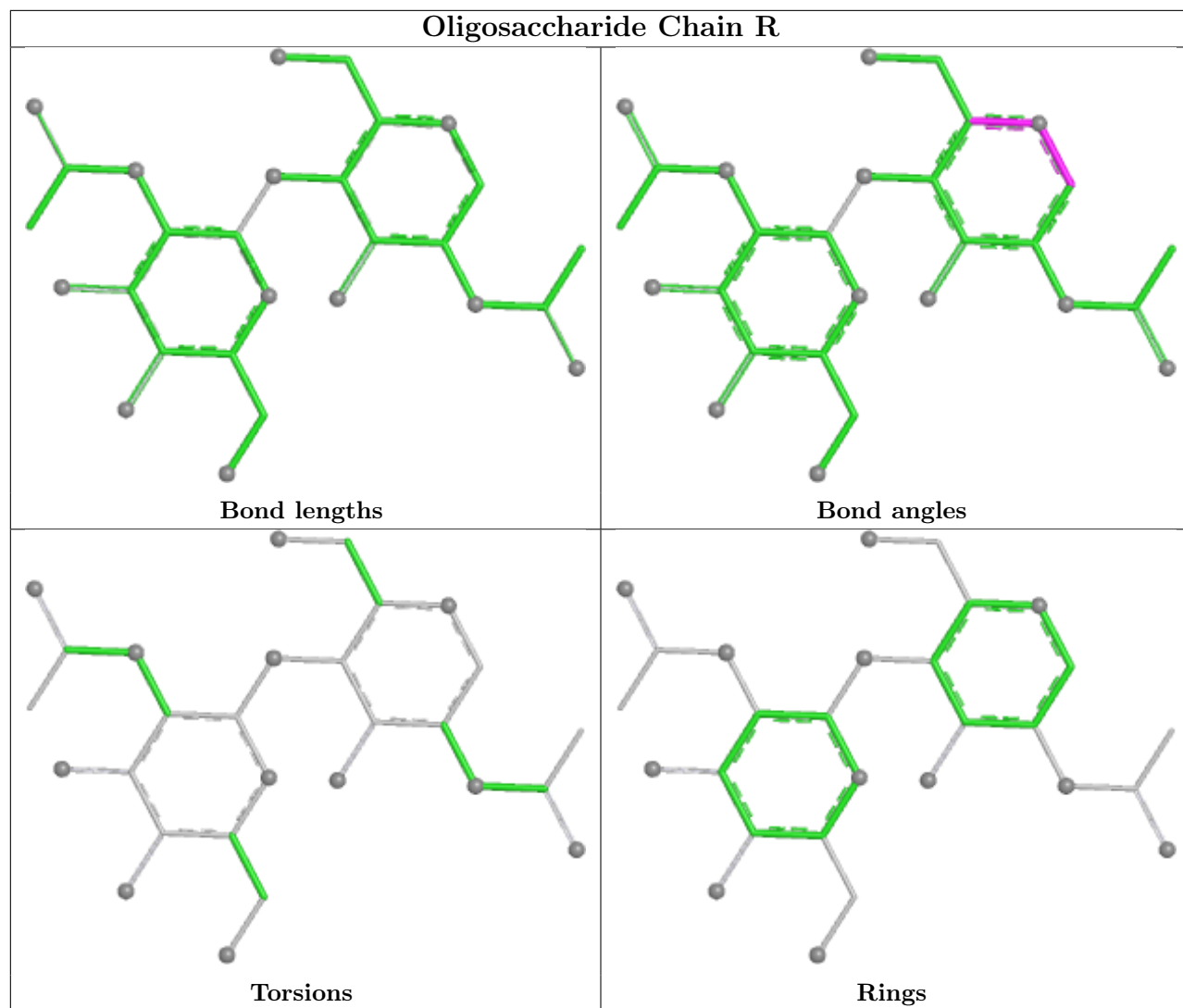


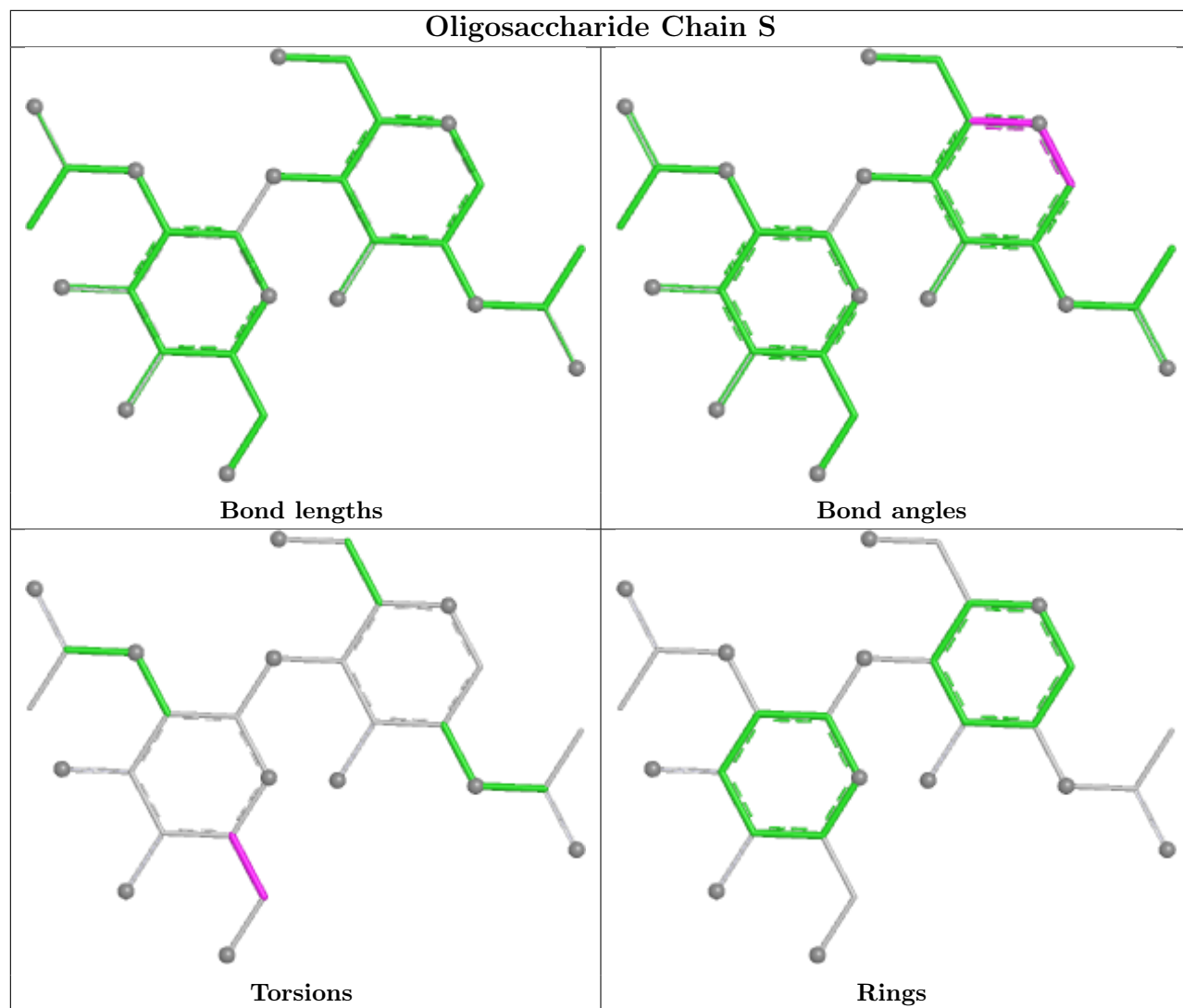


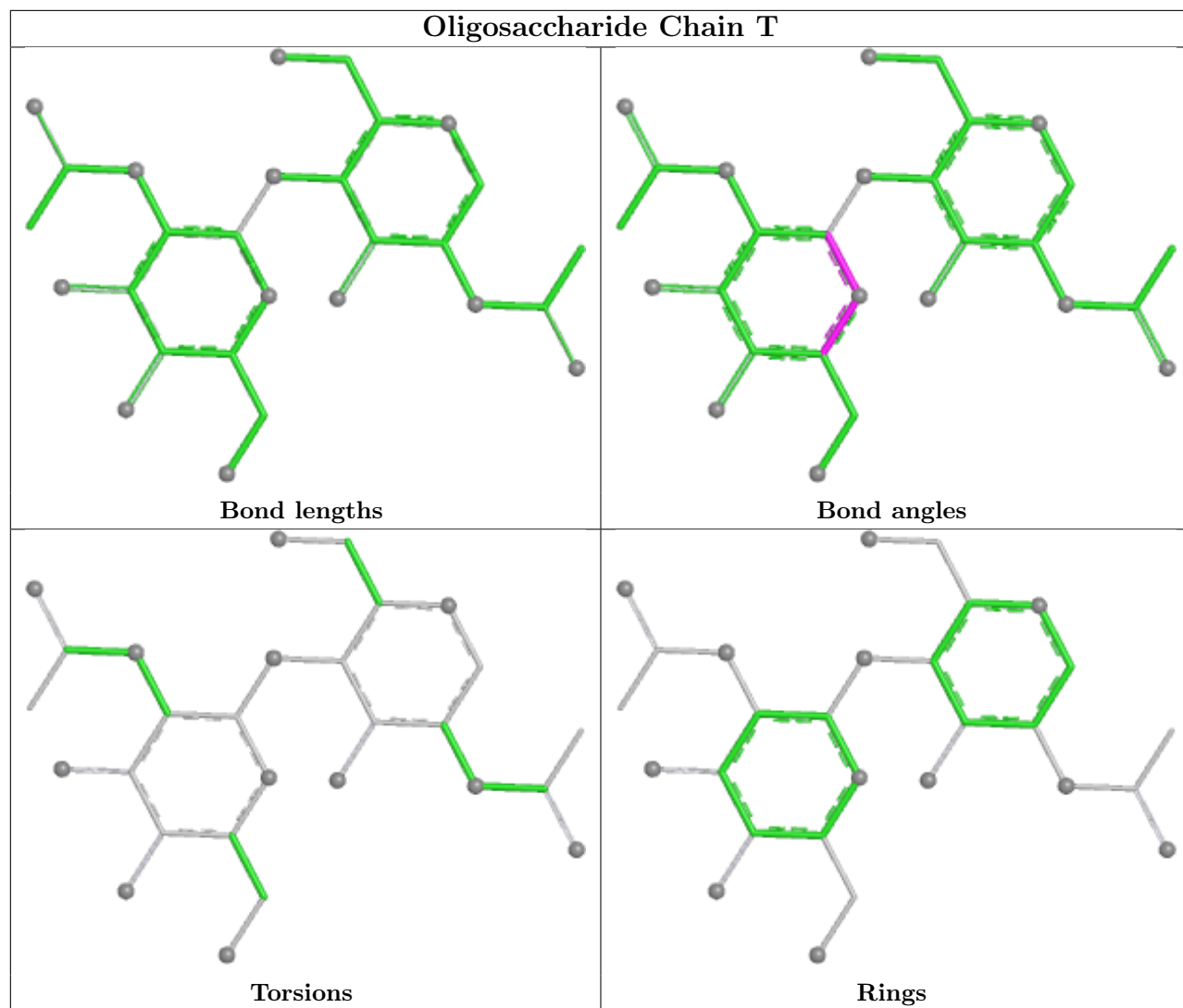


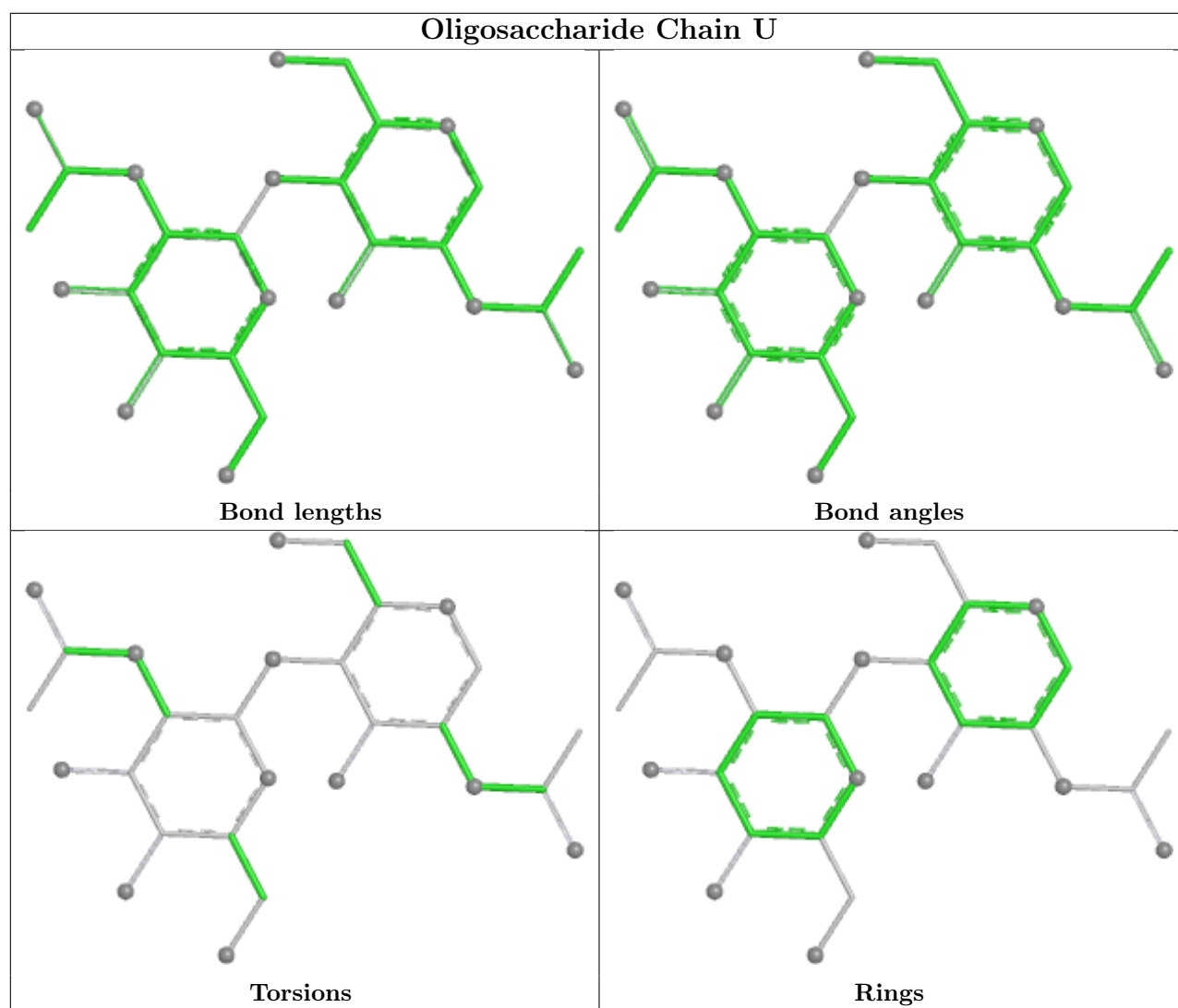


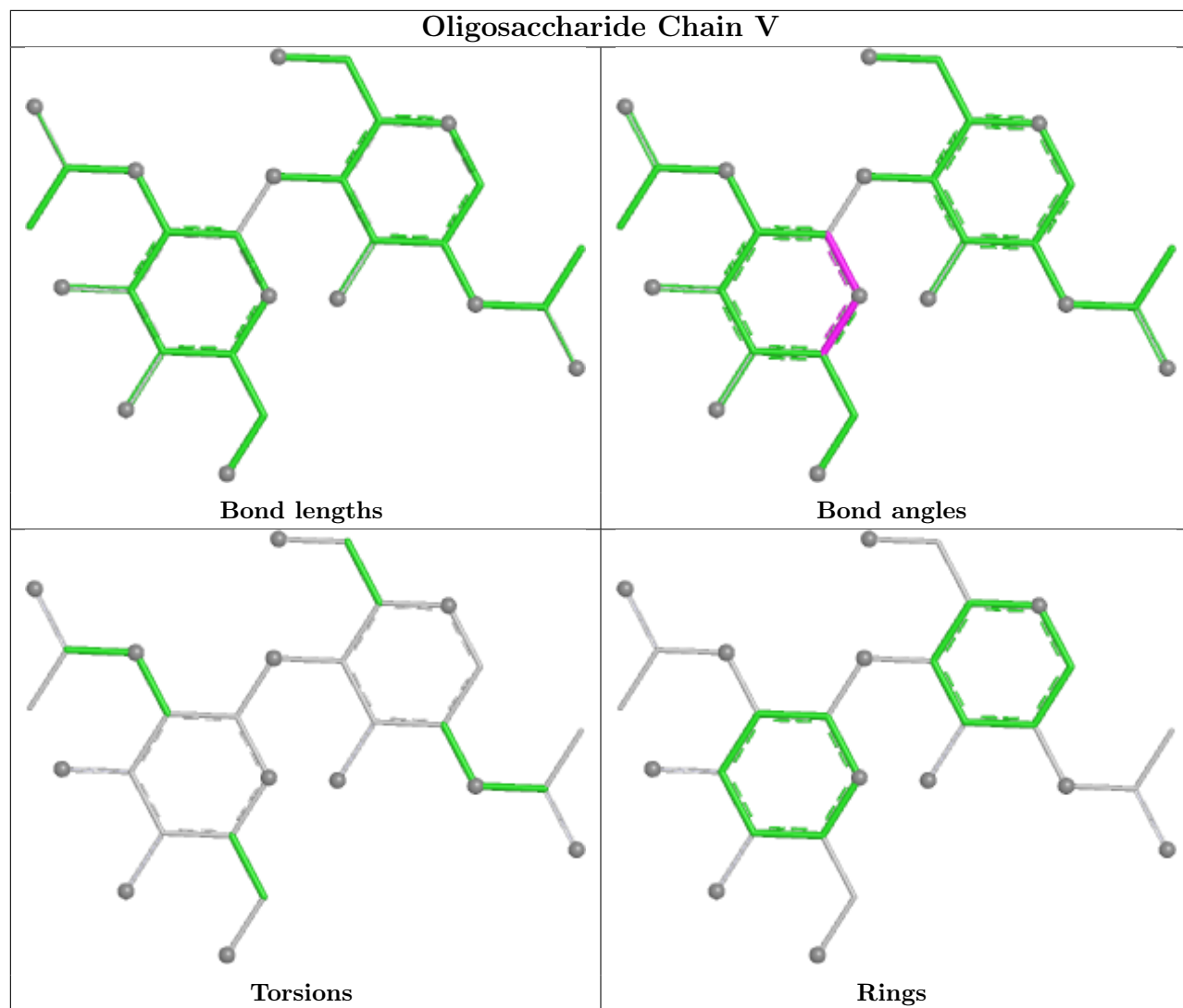


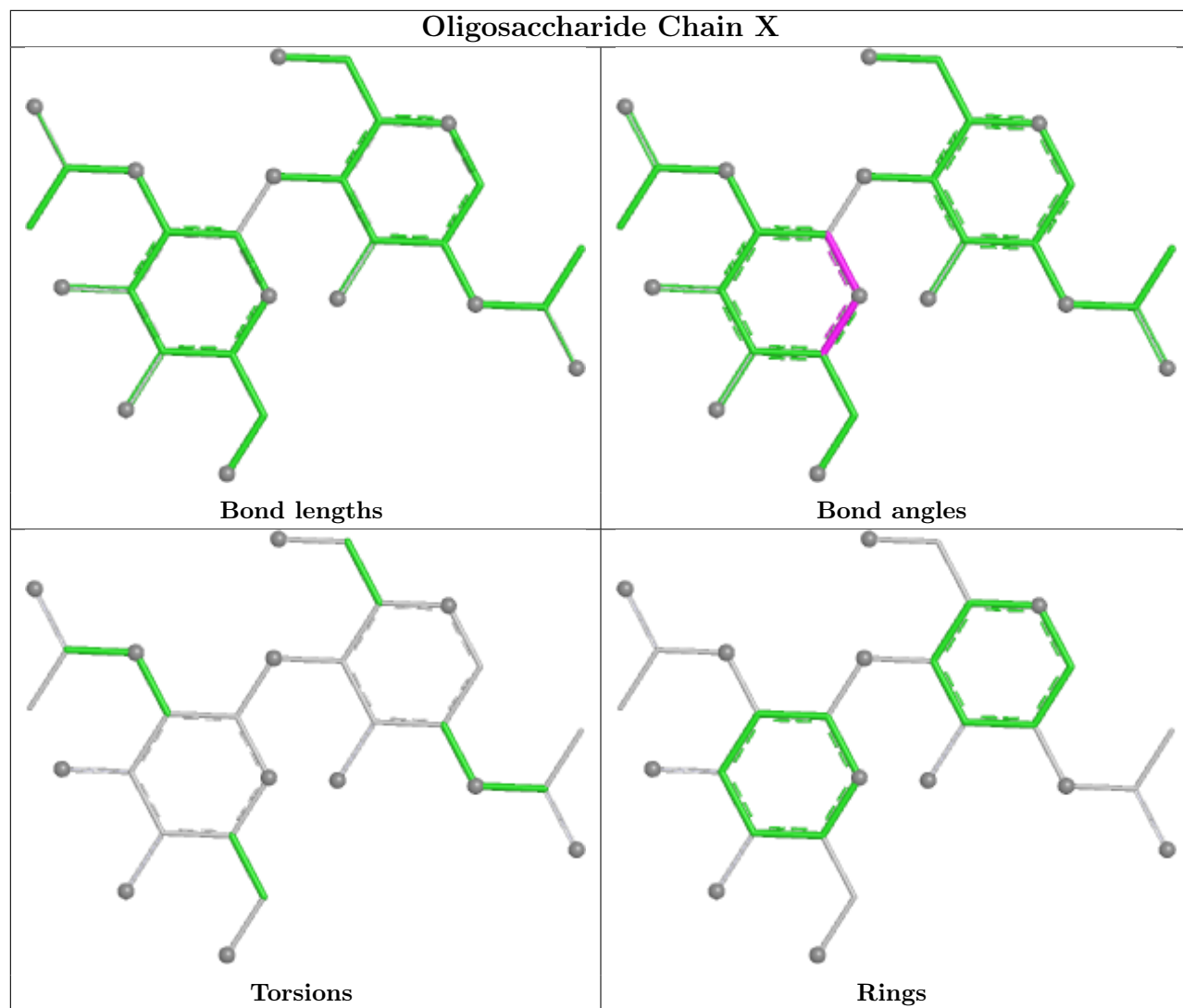


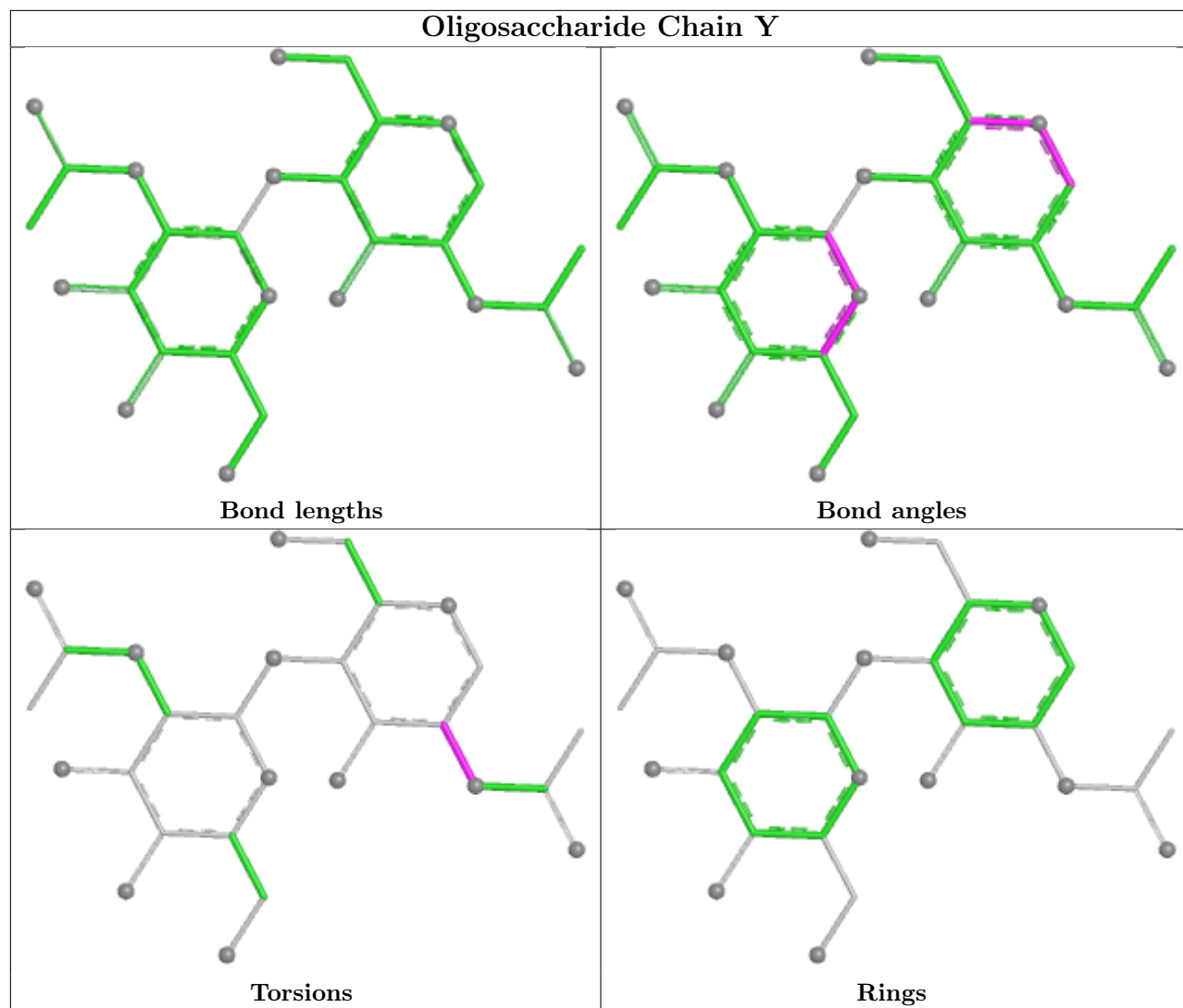


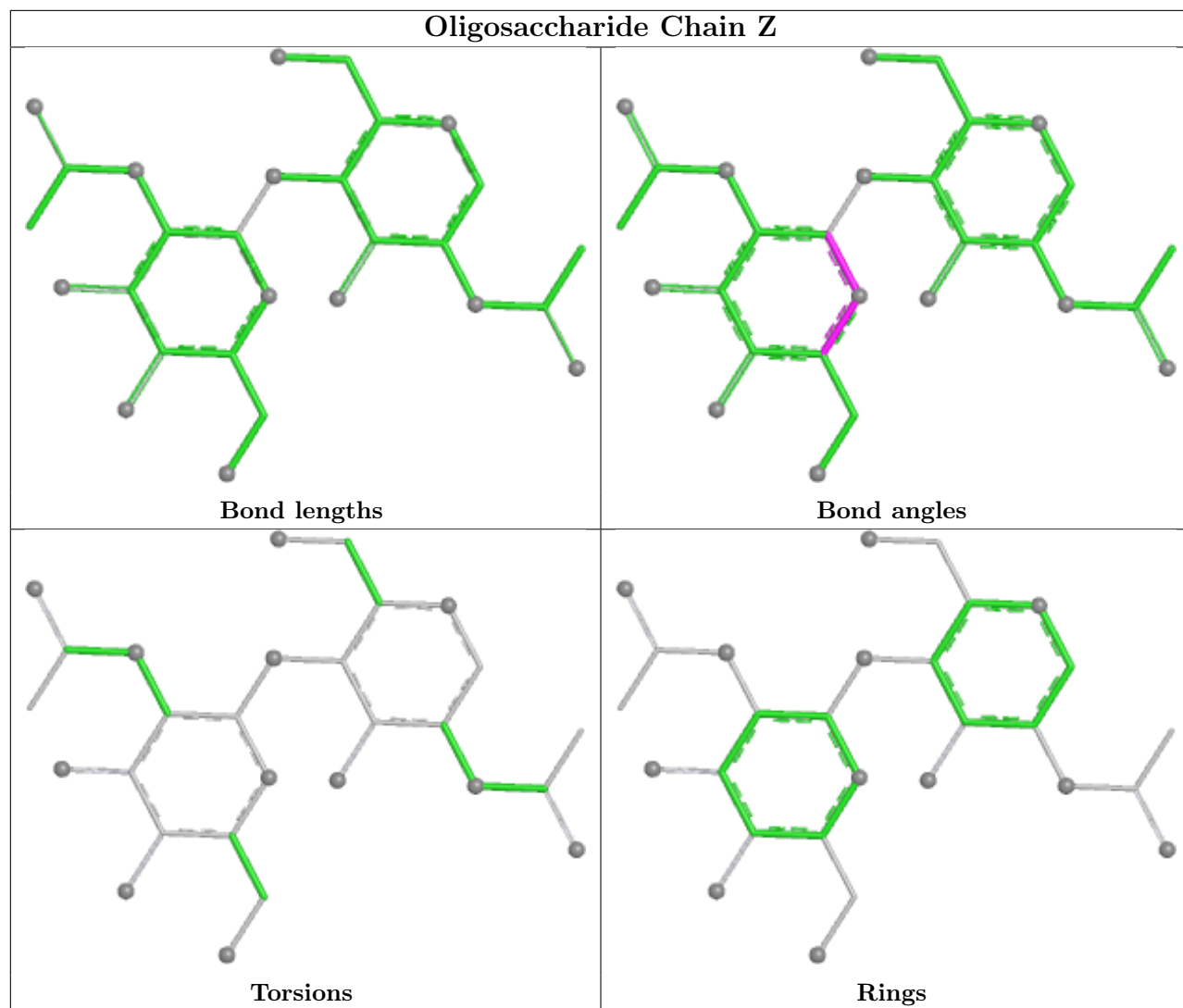


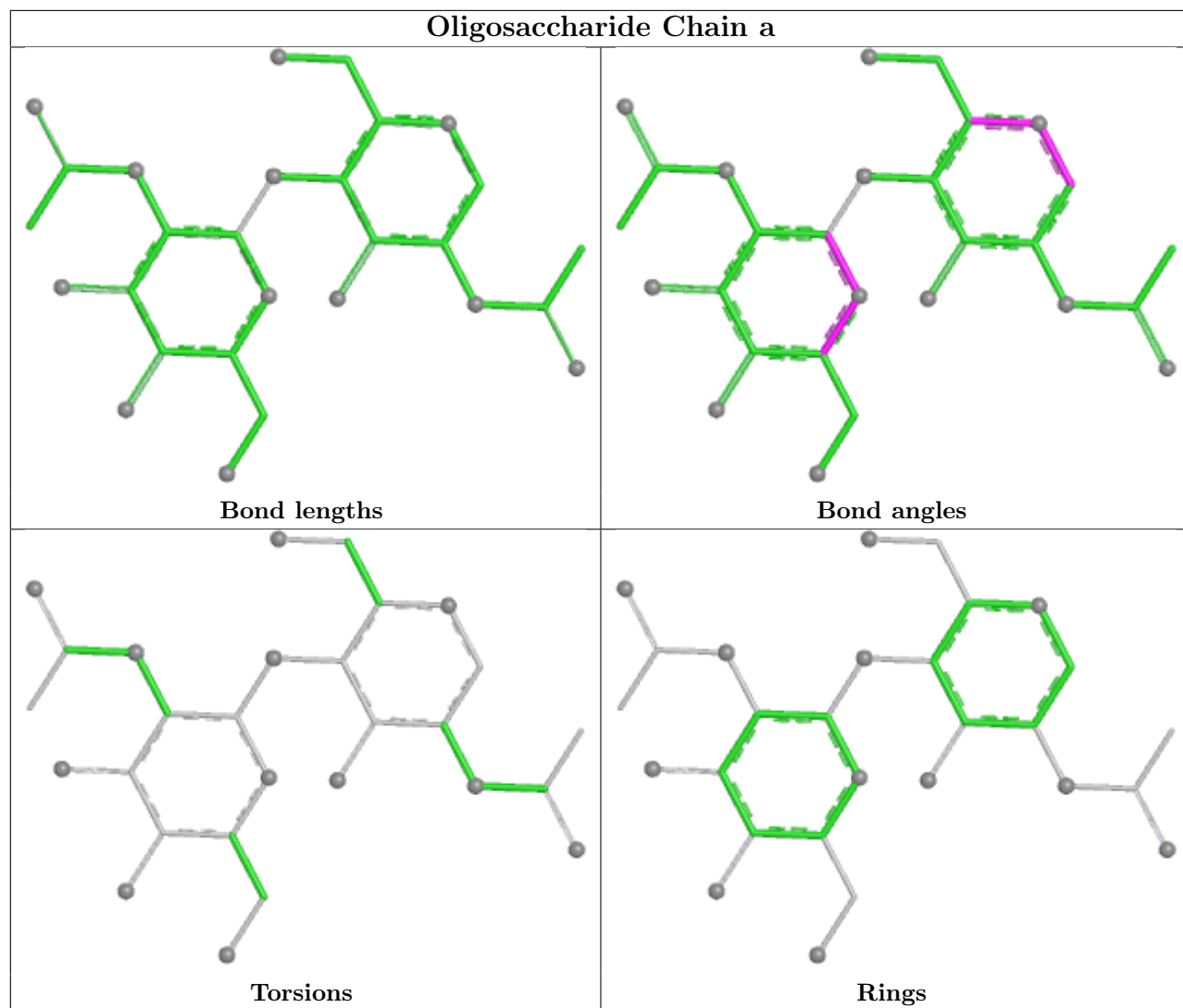


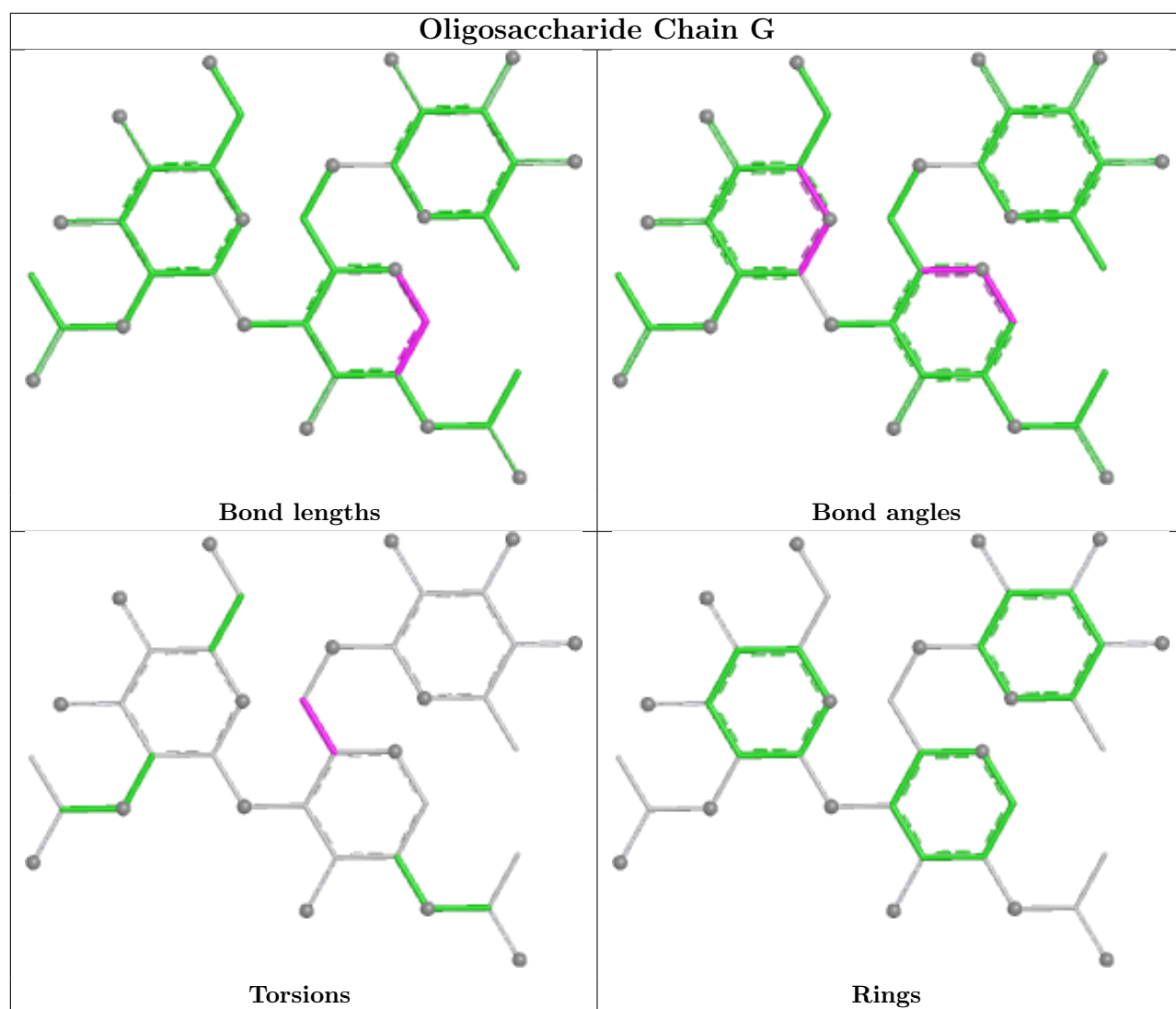


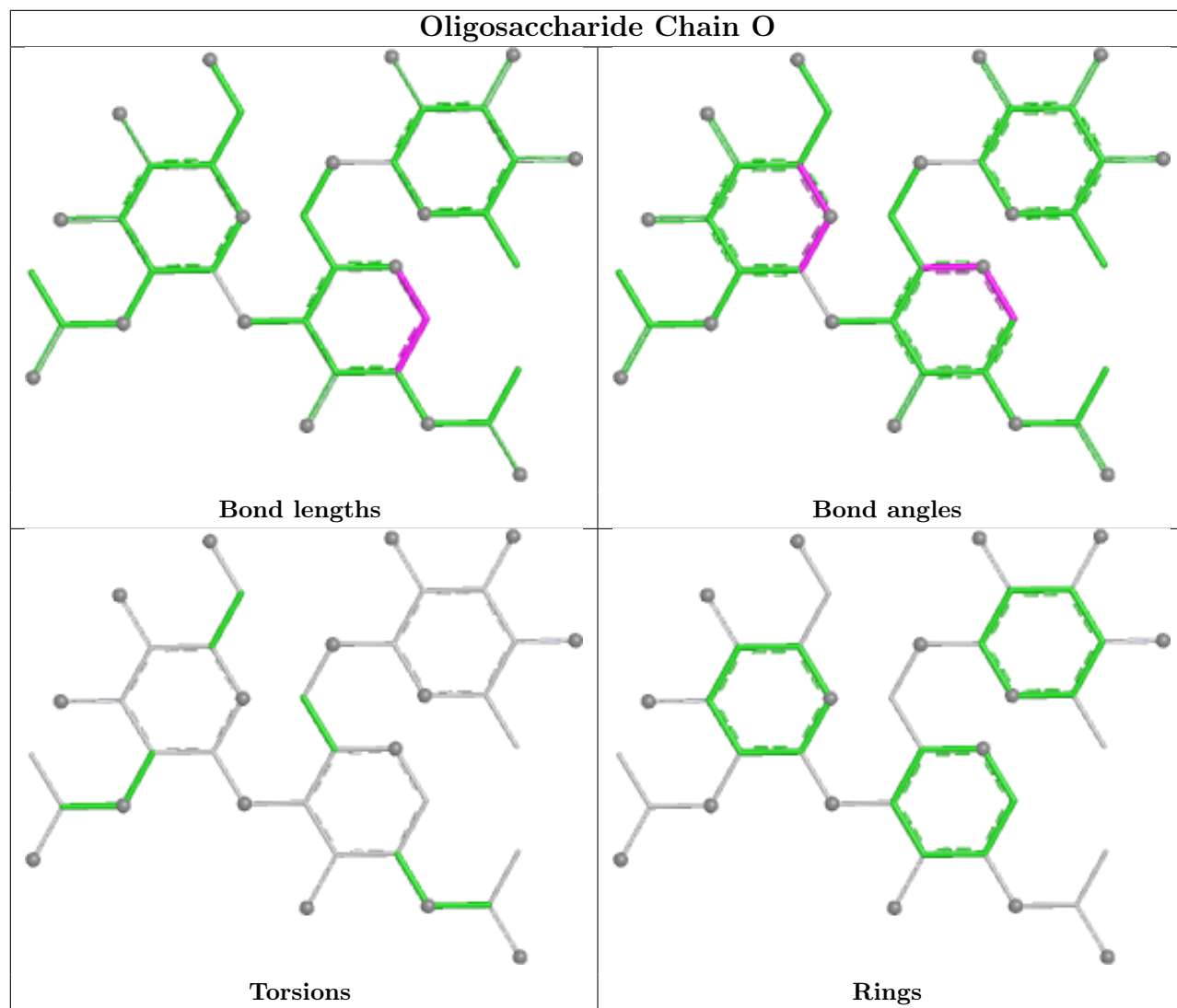


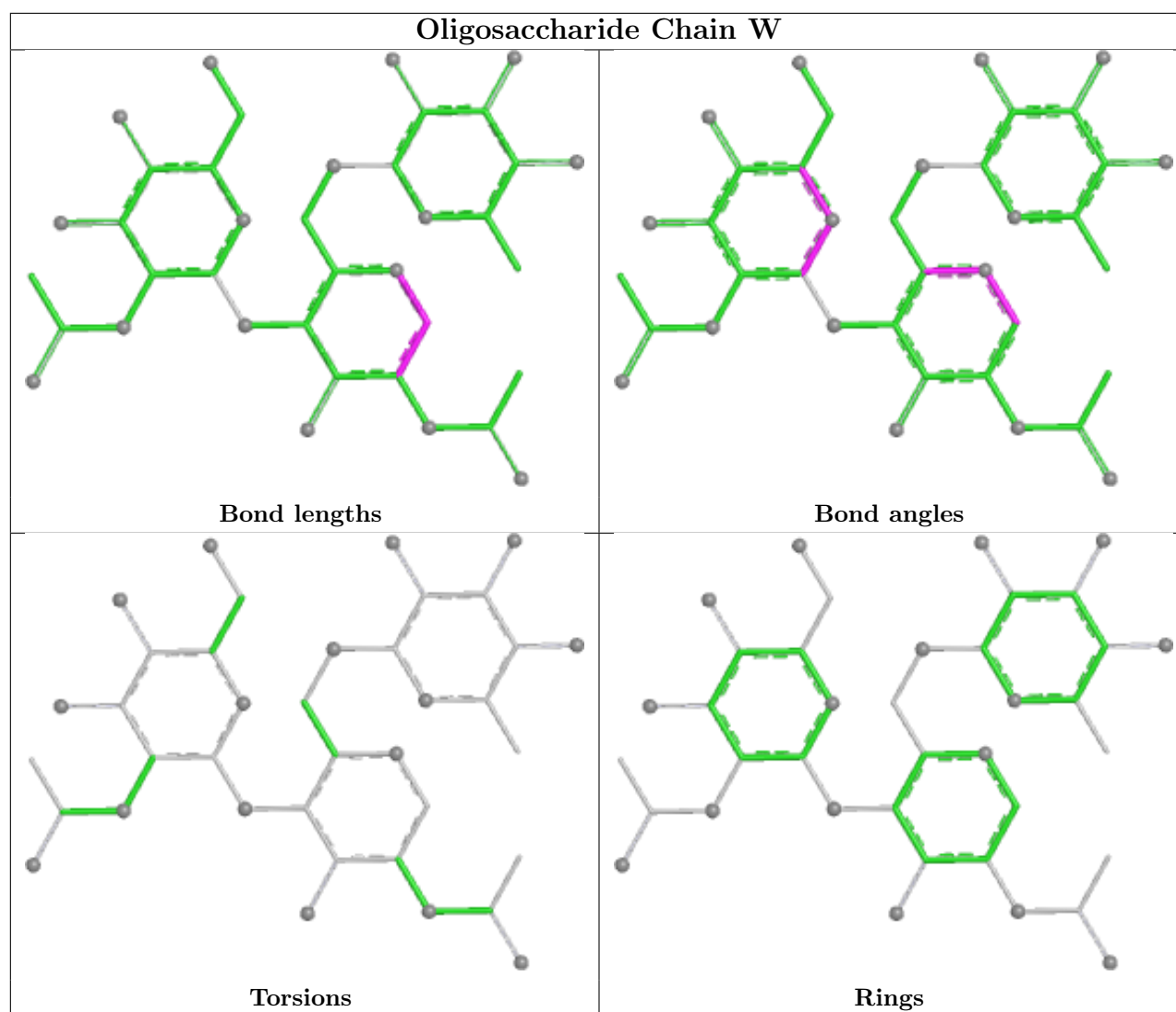












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
4	NAG	C	2008	1	14,14,15	0.17	0	17,19,21	0.60	0
4	NAG	C	2007	1	14,14,15	0.55	0	17,19,21	0.41	0
4	NAG	B	2002	1	14,14,15	0.63	0	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2005	1	14,14,15	0.91	2 (14%)	17,19,21	0.83	1 (5%)
4	NAG	B	2008	1	14,14,15	0.20	0	17,19,21	0.60	0
4	NAG	C	2005	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
4	NAG	A	2001	1	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
4	NAG	C	2006	1	14,14,15	0.60	0	17,19,21	0.71	1 (5%)
4	NAG	B	2007	1	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	B	2003	1	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	A	2003	1	14,14,15	0.64	0	17,19,21	0.54	0
4	NAG	A	2004	1	14,14,15	0.59	0	17,19,21	0.71	1 (5%)
4	NAG	C	2004	1	14,14,15	0.34	0	17,19,21	0.59	0
4	NAG	A	2006	1	14,14,15	0.31	0	17,19,21	0.54	0
4	NAG	B	2001	1	14,14,15	0.59	0	17,19,21	0.75	1 (5%)
4	NAG	B	2005	1	14,14,15	0.84	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	C	2003	1	14,14,15	0.39	0	17,19,21	0.43	0
4	NAG	C	2002	1	14,14,15	0.57	0	17,19,21	0.83	1 (5%)
4	NAG	A	2002	1	14,14,15	0.64	0	17,19,21	0.92	1 (5%)
4	NAG	B	2004	1	14,14,15	0.63	0	17,19,21	0.65	1 (5%)
4	NAG	B	2006	1	14,14,15	0.49	0	17,19,21	0.68	1 (5%)
4	NAG	A	2008	1	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
4	NAG	C	2001	1	14,14,15	0.67	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	A	2007	1	14,14,15	0.40	0	17,19,21	0.35	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
4	NAG	C	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2007	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2005	NAG	O5-C1	2.47	1.47	1.43
4	B	2005	NAG	O5-C1	2.39	1.47	1.43
4	A	2005	NAG	C1-C2	2.26	1.55	1.52
4	C	2001	NAG	C1-C2	2.21	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	NAG	C1-O5-C5	3.41	116.76	112.19
4	A	2002	NAG	C1-O5-C5	3.38	116.71	112.19
4	A	2005	NAG	C1-O5-C5	3.27	116.56	112.19
4	B	2005	NAG	C1-O5-C5	3.19	116.46	112.19
4	B	2002	NAG	C1-O5-C5	2.98	116.18	112.19
4	C	2002	NAG	C1-O5-C5	2.97	116.16	112.19
4	B	2001	NAG	C1-O5-C5	2.77	115.89	112.19
4	A	2004	NAG	C1-O5-C5	2.59	115.66	112.19
4	C	2006	NAG	C1-O5-C5	2.52	115.57	112.19
4	A	2008	NAG	C1-O5-C5	2.50	115.54	112.19
4	B	2006	NAG	C1-O5-C5	2.41	115.42	112.19
4	B	2004	NAG	C1-O5-C5	2.32	115.30	112.19
4	C	2005	NAG	C1-O5-C5	2.10	115.00	112.19
4	A	2001	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	NAG	O5-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	C	2008	NAG	C1-C2-N2-C7
4	B	2008	NAG	C1-C2-N2-C7
4	B	2001	NAG	O5-C5-C6-O6
4	A	2002	NAG	C3-C2-N2-C7
4	A	2008	NAG	C3-C2-N2-C7
4	C	2002	NAG	C3-C2-N2-C7
4	B	2002	NAG	C3-C2-N2-C7
4	B	2008	NAG	C3-C2-N2-C7
4	A	2002	NAG	C1-C2-N2-C7
4	A	2008	NAG	C1-C2-N2-C7
4	C	2002	NAG	C1-C2-N2-C7
4	B	2002	NAG	C1-C2-N2-C7
4	C	2001	NAG	C3-C2-N2-C7
4	C	2008	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

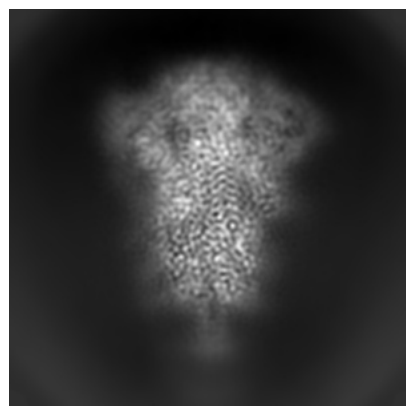
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45868. These allow visual inspection of the internal detail of the map and identification of artifacts.

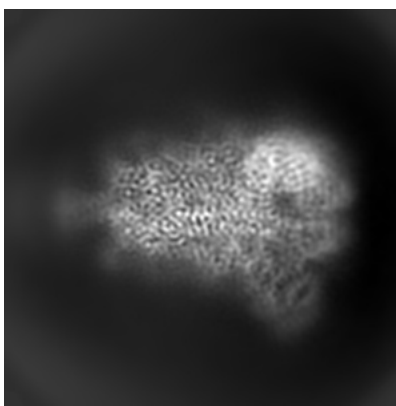
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

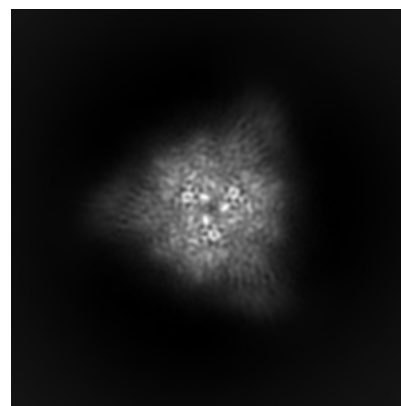
6.1.1 Primary map



X

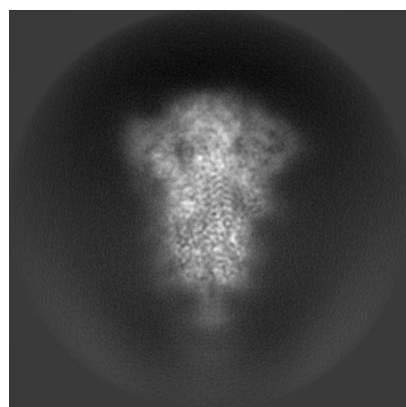


Y

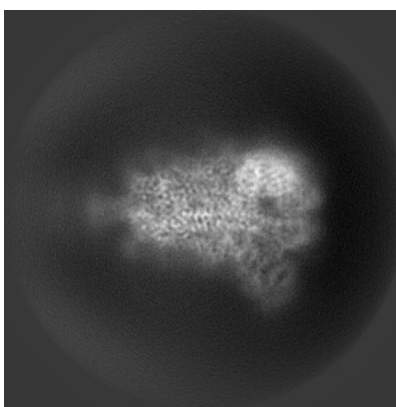


Z

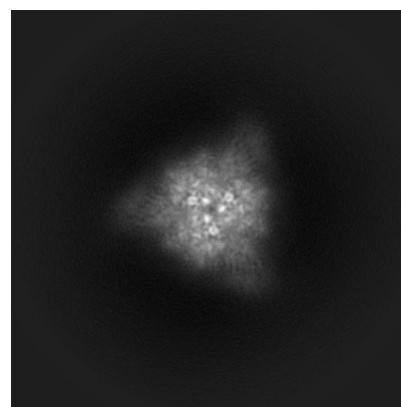
6.1.2 Raw map



X



Y

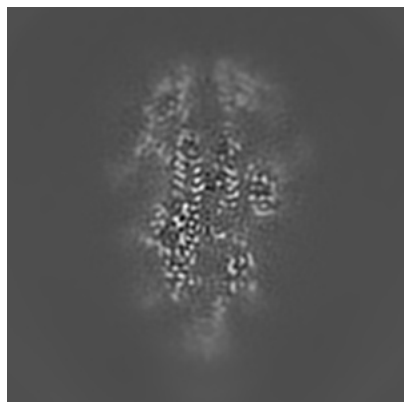


Z

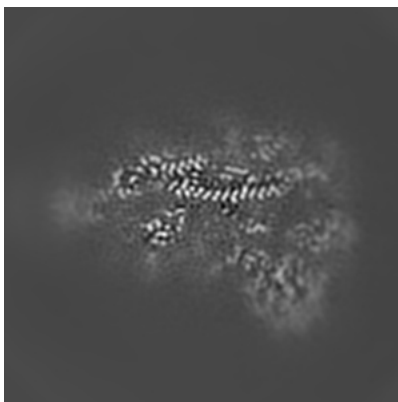
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

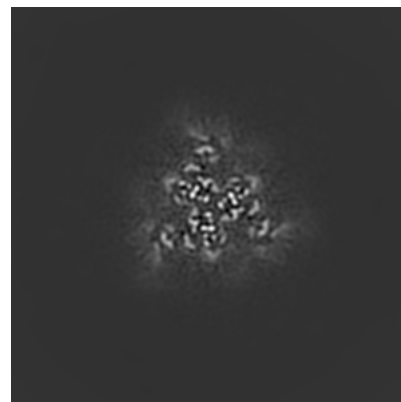
6.2.1 Primary map



X Index: 128

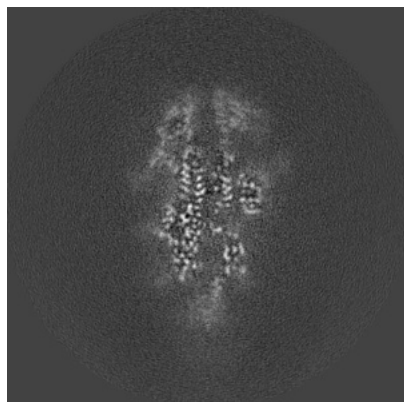


Y Index: 128

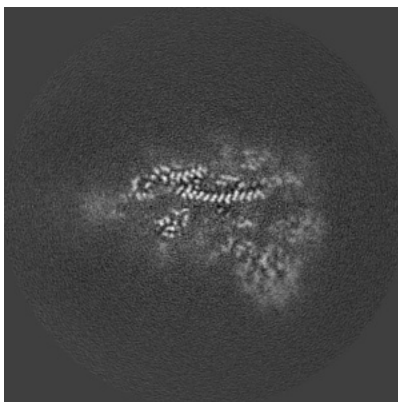


Z Index: 128

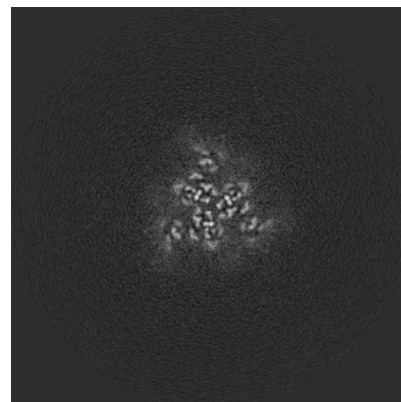
6.2.2 Raw map



X Index: 162



Y Index: 162

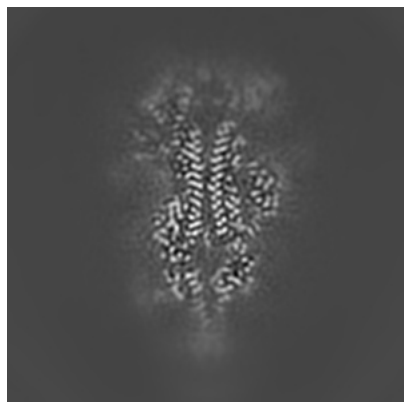


Z Index: 162

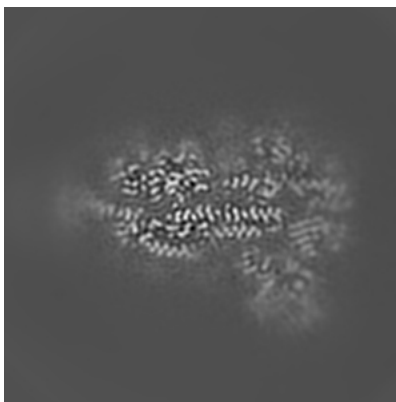
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

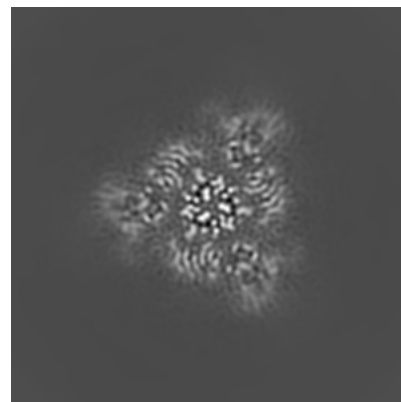
6.3.1 Primary map



X Index: 124

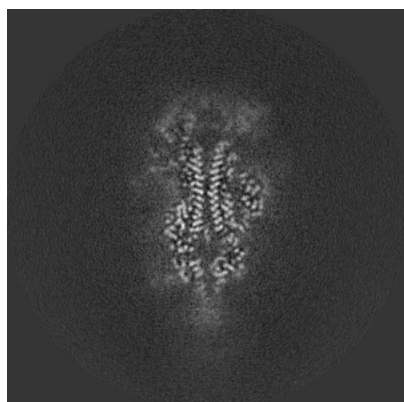


Y Index: 136

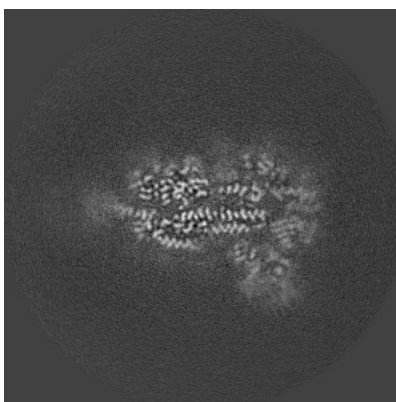


Z Index: 164

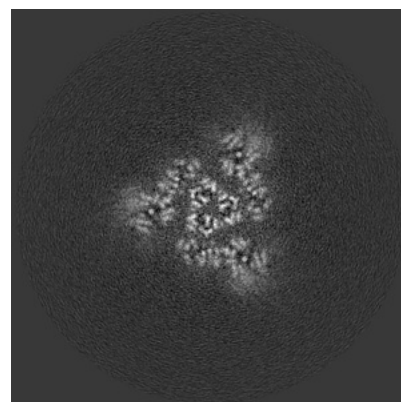
6.3.2 Raw map



X Index: 158



Y Index: 170

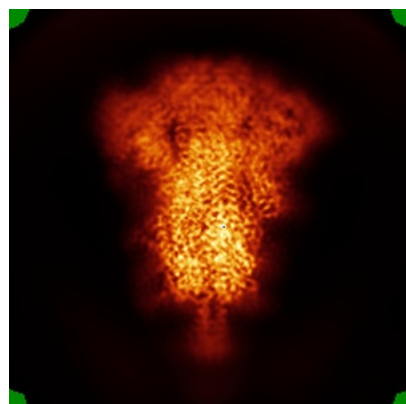


Z Index: 202

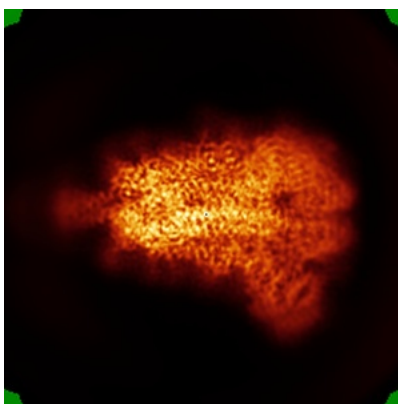
The images above show the largest variance slices of the map in three orthogonal directions.

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

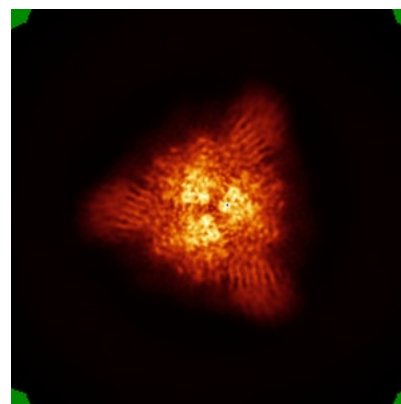
6.4.1 Primary map



X

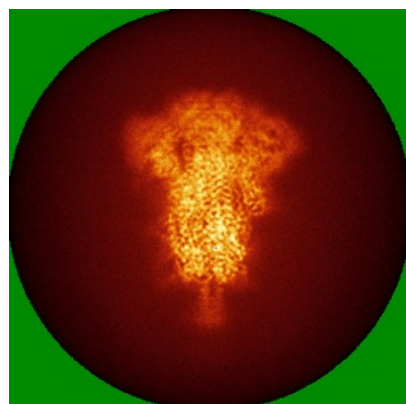


Y

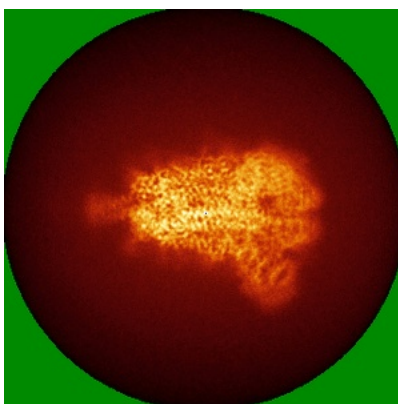


Z

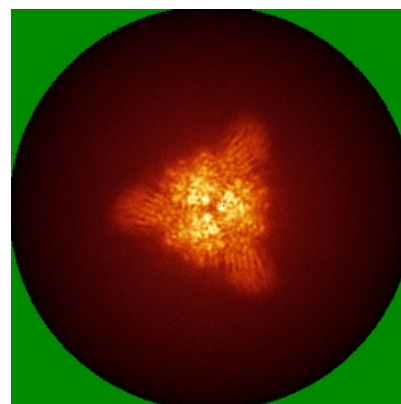
6.4.2 Raw map



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](#)

This section was not generated.

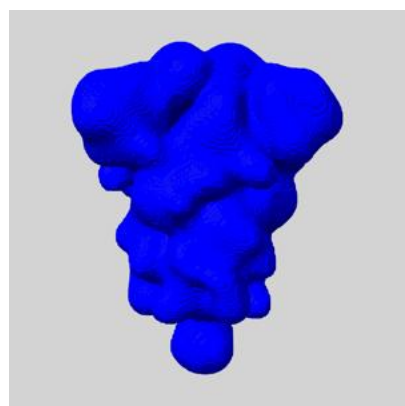
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

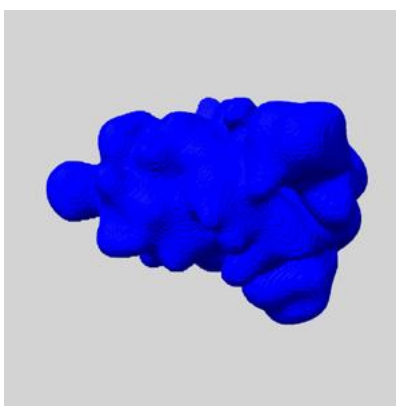
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

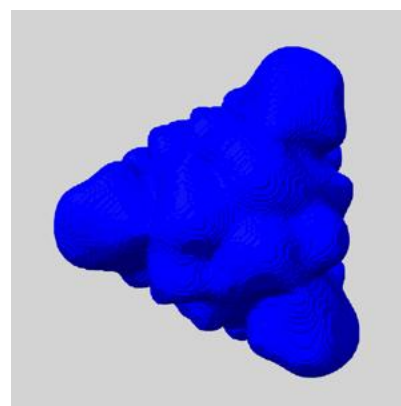
6.6.1 emd_45868_msk_1.map [i](#)



X



Y

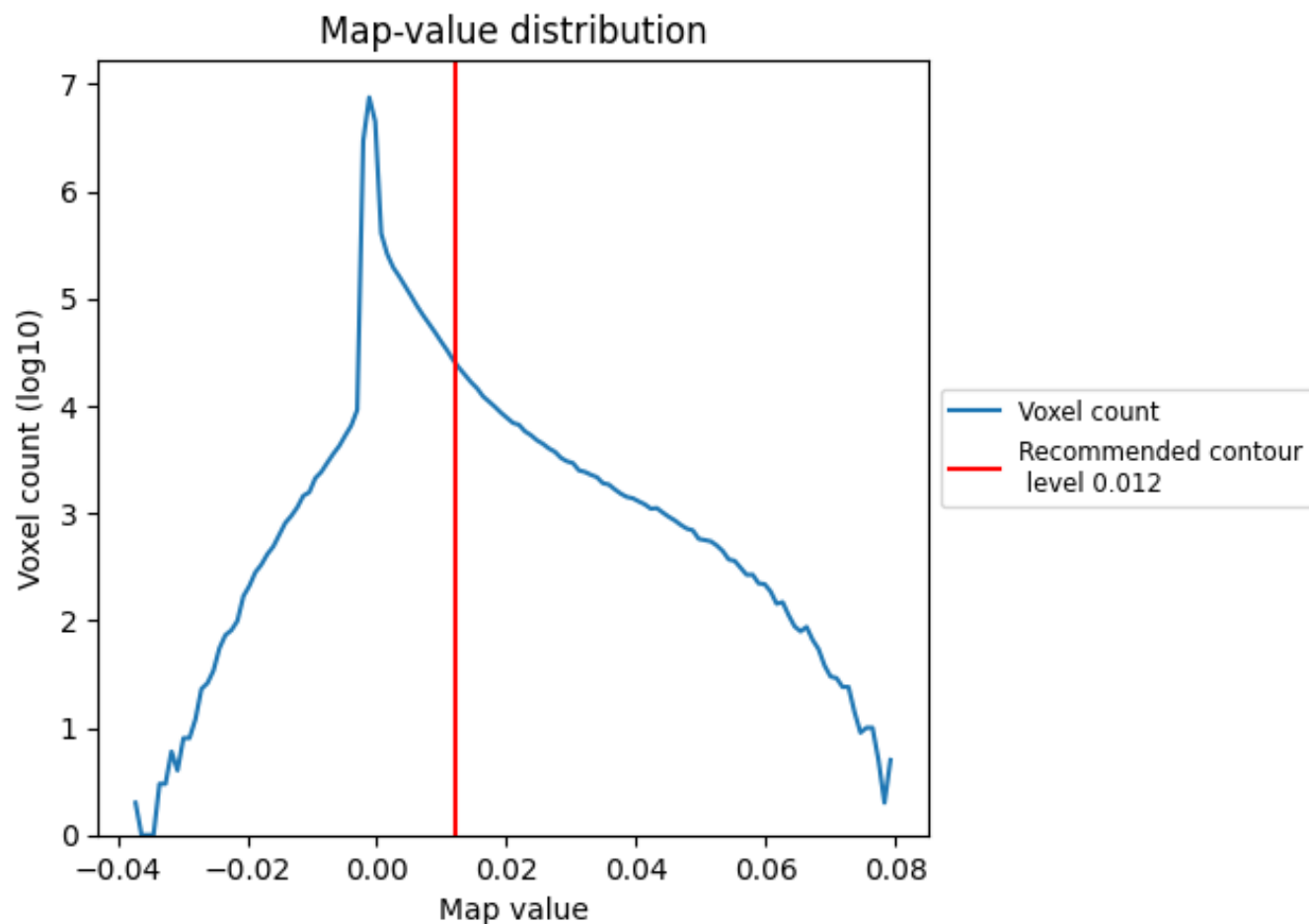


Z

7 Map analysis [i](#)

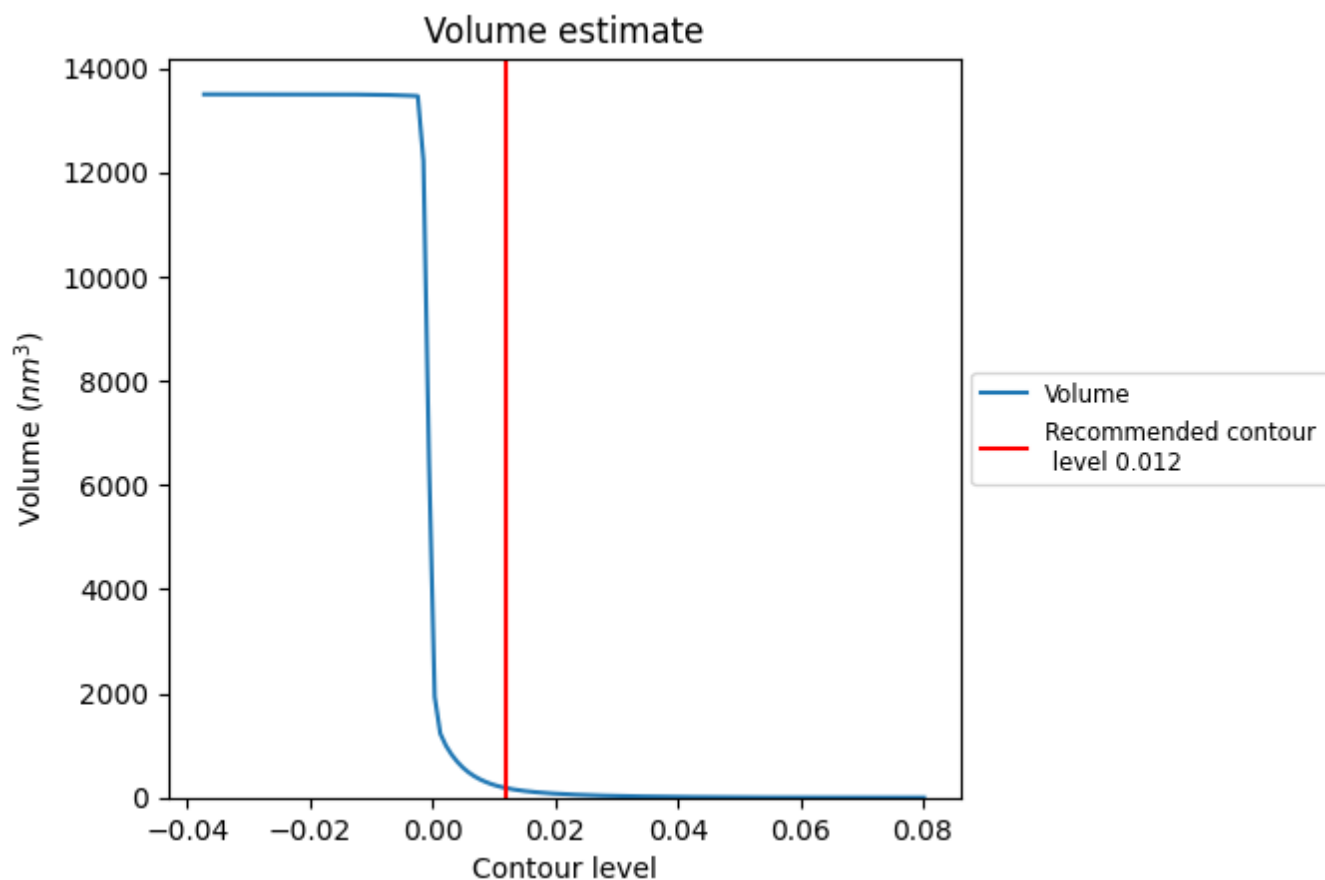
This section contains the results of statistical analysis of the map.

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.

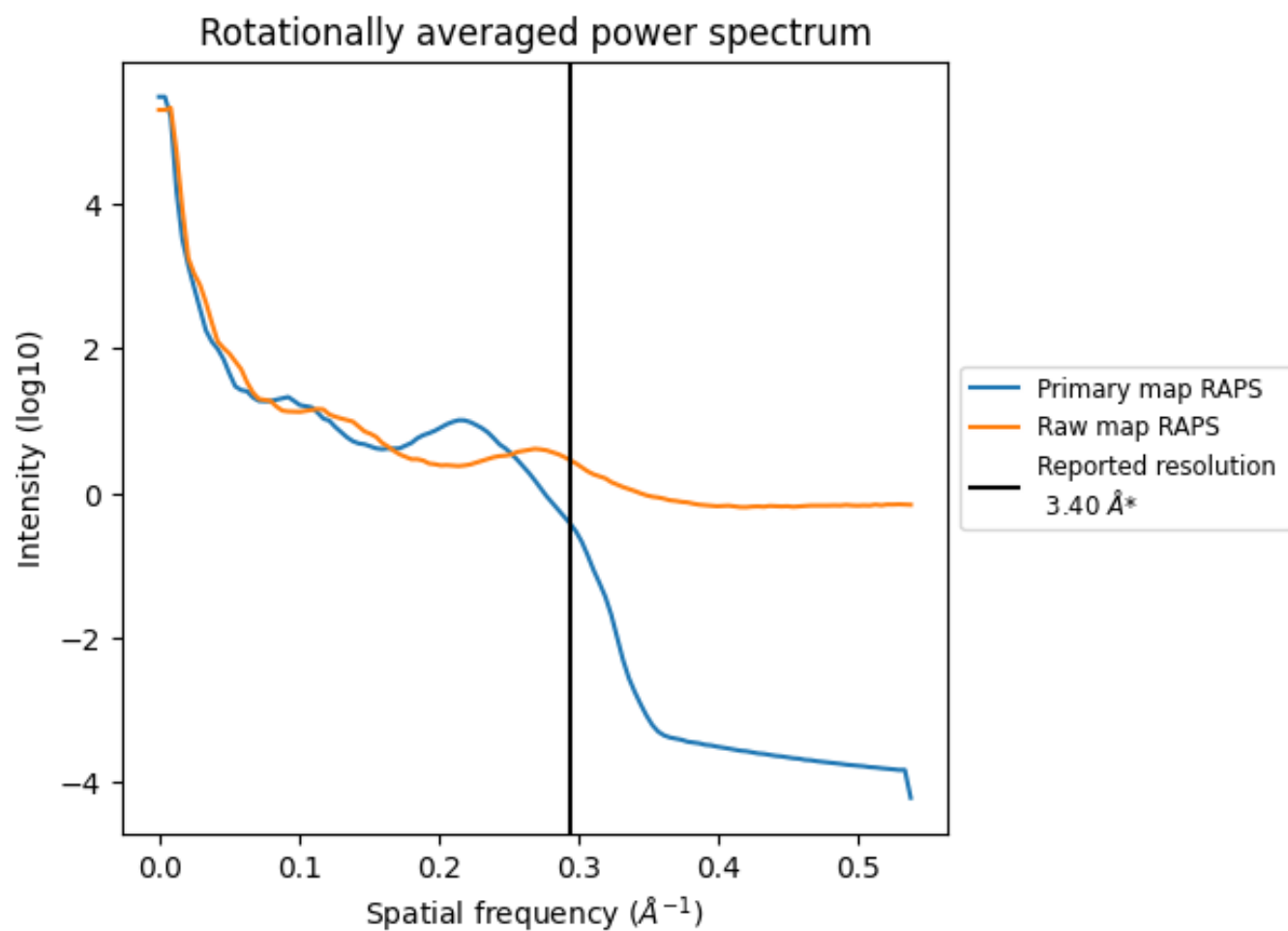
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

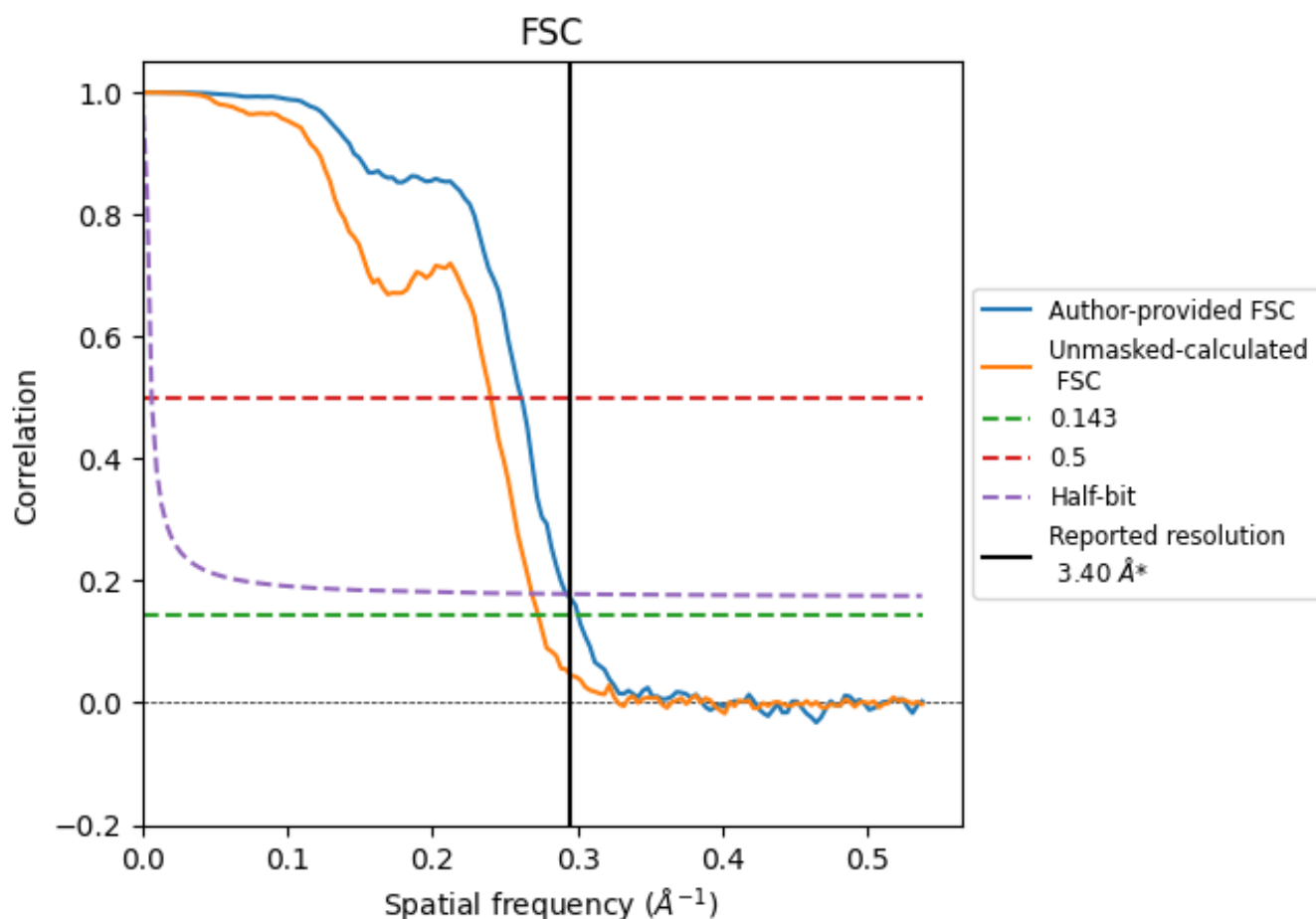


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

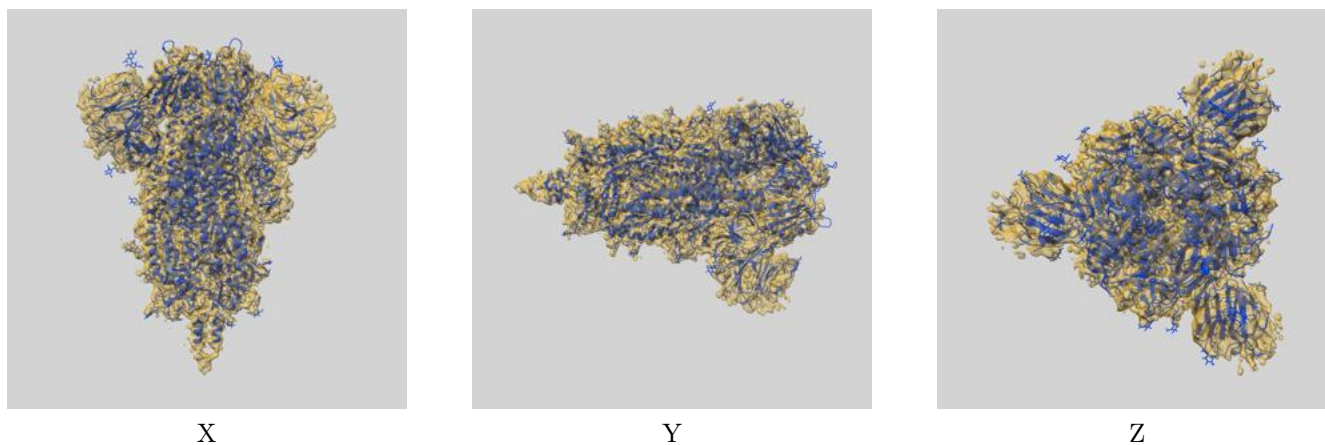
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.33	3.83	3.42
Unmasked-calculated*	3.66	4.16	3.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

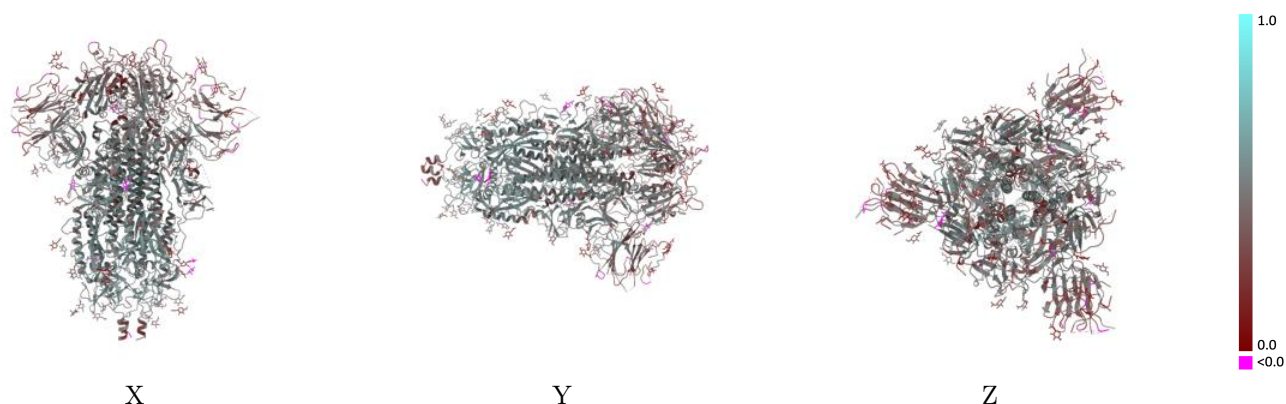
This section contains information regarding the fit between EMDB map EMD-45868 and PDB model 9CRH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.012 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](#)

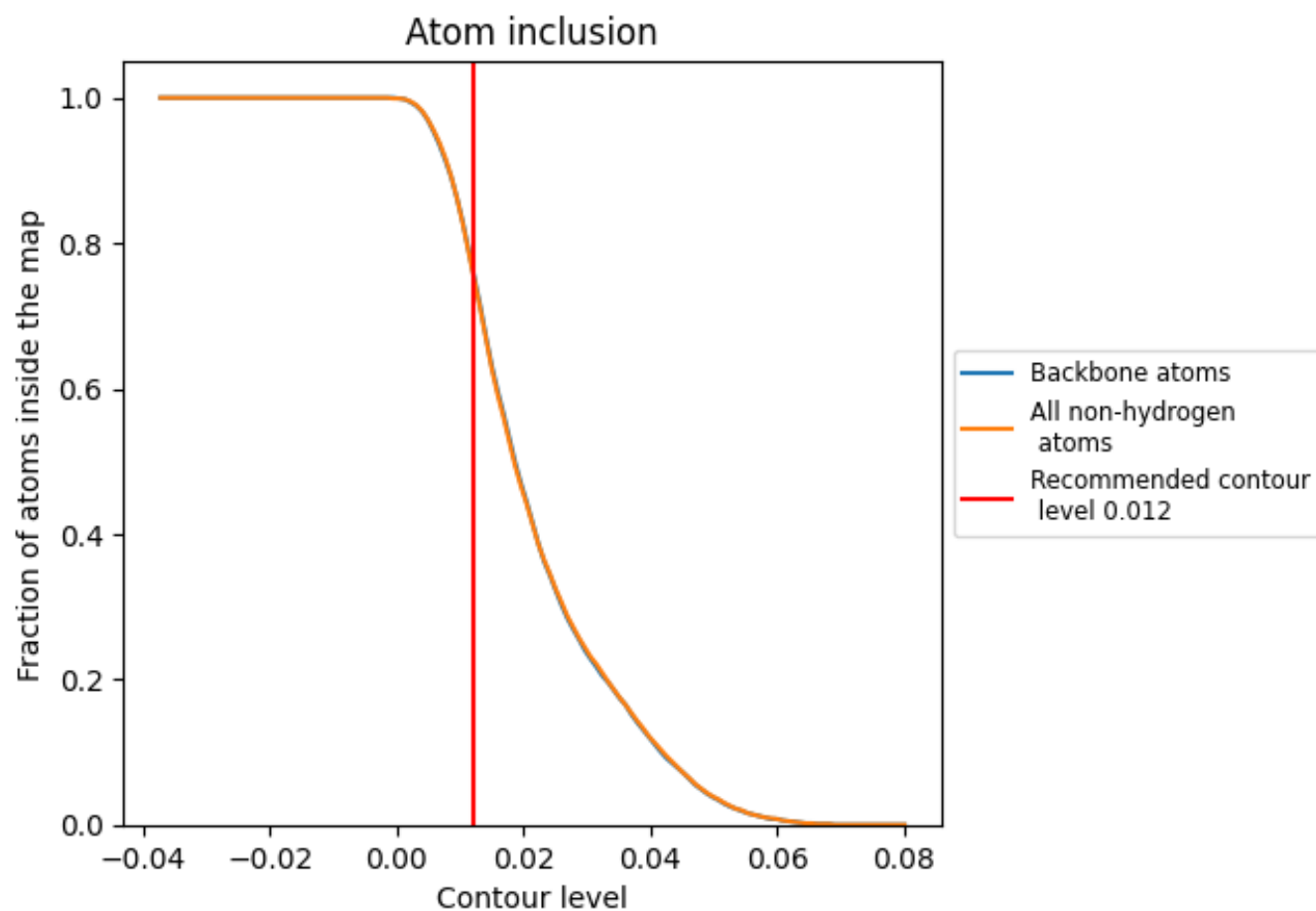


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.4410
A	 0.7790	 0.4460
B	 0.7770	 0.4450
C	 0.7770	 0.4470
D	 0.3210	 0.2710
E	 0.6790	 0.3530
F	 0.5710	 0.2530
G	 0.2100	 0.0070
H	 0.5710	 0.2830
I	 0.6070	 0.4120
J	 0.1430	 0.2100
K	 0.0360	 0.2670
L	 0.3570	 0.4070
M	 0.6790	 0.3820
N	 0.5710	 0.2980
O	 0.2370	 0.1570
P	 0.6070	 0.3880
Q	 0.5710	 0.4160
R	 0.1430	 0.2930
S	 0.0000	 0.1310
T	 0.1430	 0.1570
U	 0.8210	 0.4650
V	 0.5360	 0.3010
W	 0.2100	 0.0990
X	 0.6790	 0.3680
Y	 0.5710	 0.3940
Z	 0.1790	 0.1630
a	 0.0710	 0.0730

