



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:57 AM UTC

PDB ID : 9C7R / pdb\_00009c7r  
EMDB ID : EMD-45285  
Title : Diheteromeric GluN1/GluN2A (M817V) in digitonin complexed with glycine, glutamate, and GNE-4123  
Authors : Jalali-Yazdi, F.; Kim, J.; Gouaux, E.  
Deposited on : 2024-06-11  
Resolution : 3.99 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](mailto: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>.

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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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

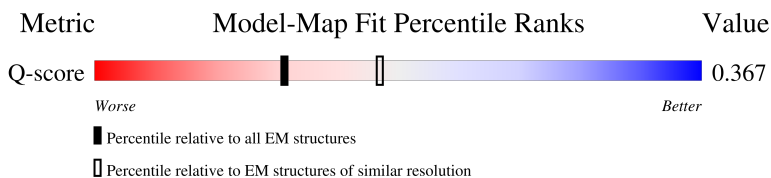
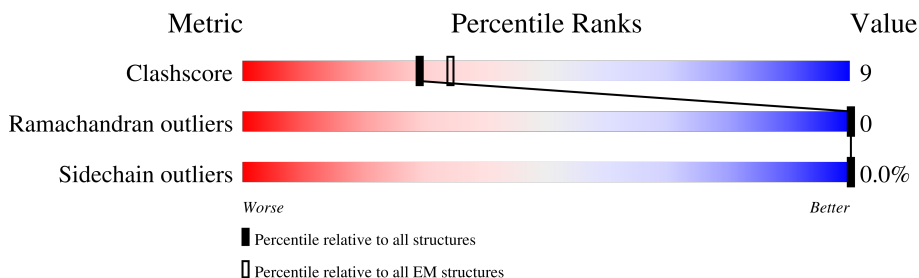
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.99 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.



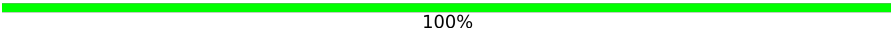


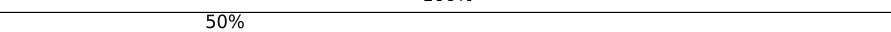
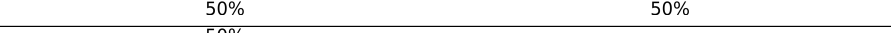
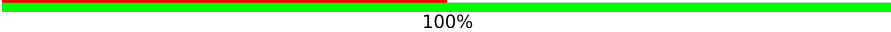


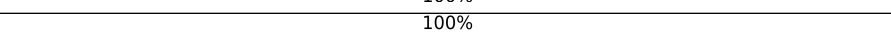
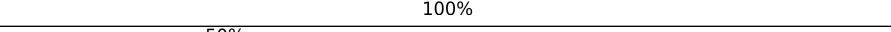



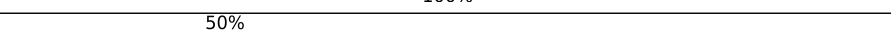
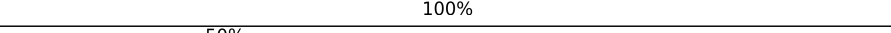
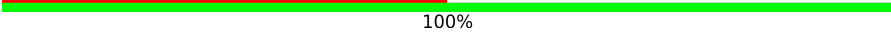


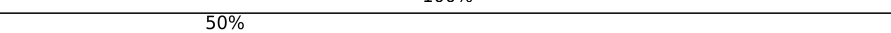
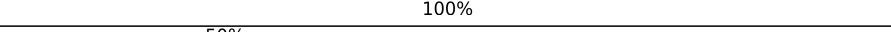
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7463 ( 3.49 - 4.49 )

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  $\geq 3$ , 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	1108	<div> <div>9%</div> <div>54%</div> <div>18%</div> <div>28%</div> </div>
1	C	1108	<div> <div>9%</div> <div>55%</div> <div>17%</div> <div>28%</div> </div>
2	B	1127	<div> <div>11%</div> <div>53%</div> <div>17%</div> <div>30%</div> </div>
2	D	1127	<div> <div>9%</div> <div>54%</div> <div>16%</div> <div>30%</div> </div>

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25867 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 Glutamate receptor ionotropic, NMDA 1, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			6295	4010	1091	1158	36		
1	C	795	Total	C	N	O	S	0	0
			6283	4003	1089	1155	36		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	848	LEU	-	linker	UNP P35439
A	849	VAL	-	linker	UNP P35439
A	850	PRO	-	linker	UNP P35439
A	851	ARG	-	linker	UNP P35439
A	852	GLY	-	linker	UNP P35439
A	853	SER	-	linker	UNP P35439
A	854	ALA	-	linker	UNP P35439
A	855	ALA	-	linker	UNP P35439
A	856	ALA	-	linker	UNP P35439
A	857	ALA	-	linker	UNP P35439
A	858	VAL	-	linker	UNP P35439
A	921	LEU	PHE	conflict	UNP P42212
A	922	THR	SER	conflict	UNP P42212
A	1063	LYS	ALA	conflict	UNP P42212
A	1088	LEU	HIS	conflict	UNP P42212
A	1096	SER	-	expression tag	UNP P42212
A	1097	GLY	-	expression tag	UNP P42212
A	1098	LEU	-	expression tag	UNP P42212
A	1099	ARG	-	expression tag	UNP P42212
A	1100	SER	-	expression tag	UNP P42212
A	1101	HIS	-	expression tag	UNP P42212
A	1102	HIS	-	expression tag	UNP P42212
A	1103	HIS	-	expression tag	UNP P42212
A	1104	HIS	-	expression tag	UNP P42212
A	1105	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1106	HIS	-	expression tag	UNP P42212
A	1107	HIS	-	expression tag	UNP P42212
A	1108	HIS	-	expression tag	UNP P42212
C	848	LEU	-	linker	UNP P35439
C	849	VAL	-	linker	UNP P35439
C	850	PRO	-	linker	UNP P35439
C	851	ARG	-	linker	UNP P35439
C	852	GLY	-	linker	UNP P35439
C	853	SER	-	linker	UNP P35439
C	854	ALA	-	linker	UNP P35439
C	855	ALA	-	linker	UNP P35439
C	856	ALA	-	linker	UNP P35439
C	857	ALA	-	linker	UNP P35439
C	858	VAL	-	linker	UNP P35439
C	921	LEU	PHE	conflict	UNP P42212
C	922	THR	SER	conflict	UNP P42212
C	1063	LYS	ALA	conflict	UNP P42212
C	1088	LEU	HIS	conflict	UNP P42212
C	1096	SER	-	expression tag	UNP P42212
C	1097	GLY	-	expression tag	UNP P42212
C	1098	LEU	-	expression tag	UNP P42212
C	1099	ARG	-	expression tag	UNP P42212
C	1100	SER	-	expression tag	UNP P42212
C	1101	HIS	-	expression tag	UNP P42212
C	1102	HIS	-	expression tag	UNP P42212
C	1103	HIS	-	expression tag	UNP P42212
C	1104	HIS	-	expression tag	UNP P42212
C	1105	HIS	-	expression tag	UNP P42212
C	1106	HIS	-	expression tag	UNP P42212
C	1107	HIS	-	expression tag	UNP P42212
C	1108	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	793	Total	C	N	O	S	0	0
			6282	4054	1025	1167	36		
2	D	788	Total	C	N	O	S	0	0
			6237	4027	1017	1158	35		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	758	THR	SER	conflict	UNP Q00959
B	817	VAL	MET	conflict	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	866	GLY	-	linker	UNP Q00959
B	867	LEU	-	linker	UNP Q00959
B	868	VAL	-	linker	UNP Q00959
B	869	PRO	-	linker	UNP Q00959
B	870	ARG	-	linker	UNP Q00959
B	871	GLY	-	linker	UNP Q00959
B	872	SER	-	linker	UNP Q00959
B	873	ALA	-	linker	UNP Q00959
B	874	ALA	-	linker	UNP Q00959
B	875	ALA	-	linker	UNP Q00959
B	876	ALA	-	linker	UNP Q00959
B	877	VAL	-	linker	UNP Q00959
B	940	LEU	PHE	conflict	UNP P42212
B	941	THR	SER	conflict	UNP P42212
B	1082	LYS	ALA	conflict	UNP P42212
B	1107	LEU	HIS	conflict	UNP P42212
B	1115	SER	-	expression tag	UNP P42212
B	1116	GLY	-	expression tag	UNP P42212
B	1117	LEU	-	expression tag	UNP P42212
B	1118	ARG	-	expression tag	UNP P42212
B	1119	SER	-	expression tag	UNP P42212
B	1120	TRP	-	expression tag	UNP P42212
B	1121	SER	-	expression tag	UNP P42212
B	1122	HIS	-	expression tag	UNP P42212
B	1123	PRO	-	expression tag	UNP P42212
B	1124	GLN	-	expression tag	UNP P42212
B	1125	PHE	-	expression tag	UNP P42212
B	1126	GLU	-	expression tag	UNP P42212
B	1127	LYS	-	expression tag	UNP P42212
D	758	THR	SER	conflict	UNP Q00959
D	817	VAL	MET	conflict	UNP Q00959
D	?	-	GLY	deletion	UNP Q00959
D	866	GLY	-	linker	UNP Q00959
D	867	LEU	-	linker	UNP Q00959
D	868	VAL	-	linker	UNP Q00959
D	869	PRO	-	linker	UNP Q00959
D	870	ARG	-	linker	UNP Q00959
D	871	GLY	-	linker	UNP Q00959
D	872	SER	-	linker	UNP Q00959
D	873	ALA	-	linker	UNP Q00959

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Chain	Residue	Modelled	Actual	Comment	Reference
D	874	ALA	-	linker	UNP Q00959
D	875	ALA	-	linker	UNP Q00959
D	876	ALA	-	linker	UNP Q00959
D	877	VAL	-	linker	UNP Q00959
D	940	LEU	PHE	conflict	UNP P42212
D	941	THR	SER	conflict	UNP P42212
D	1082	LYS	ALA	conflict	UNP P42212
D	1107	LEU	HIS	conflict	UNP P42212
D	1115	SER	-	expression tag	UNP P42212
D	1116	GLY	-	expression tag	UNP P42212
D	1117	LEU	-	expression tag	UNP P42212
D	1118	ARG	-	expression tag	UNP P42212
D	1119	SER	-	expression tag	UNP P42212
D	1120	TRP	-	expression tag	UNP P42212
D	1121	SER	-	expression tag	UNP P42212
D	1122	HIS	-	expression tag	UNP P42212
D	1123	PRO	-	expression tag	UNP P42212
D	1124	GLN	-	expression tag	UNP P42212
D	1125	PHE	-	expression tag	UNP P42212
D	1126	GLU	-	expression tag	UNP P42212
D	1127	LYS	-	expression tag	UNP P42212

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).





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

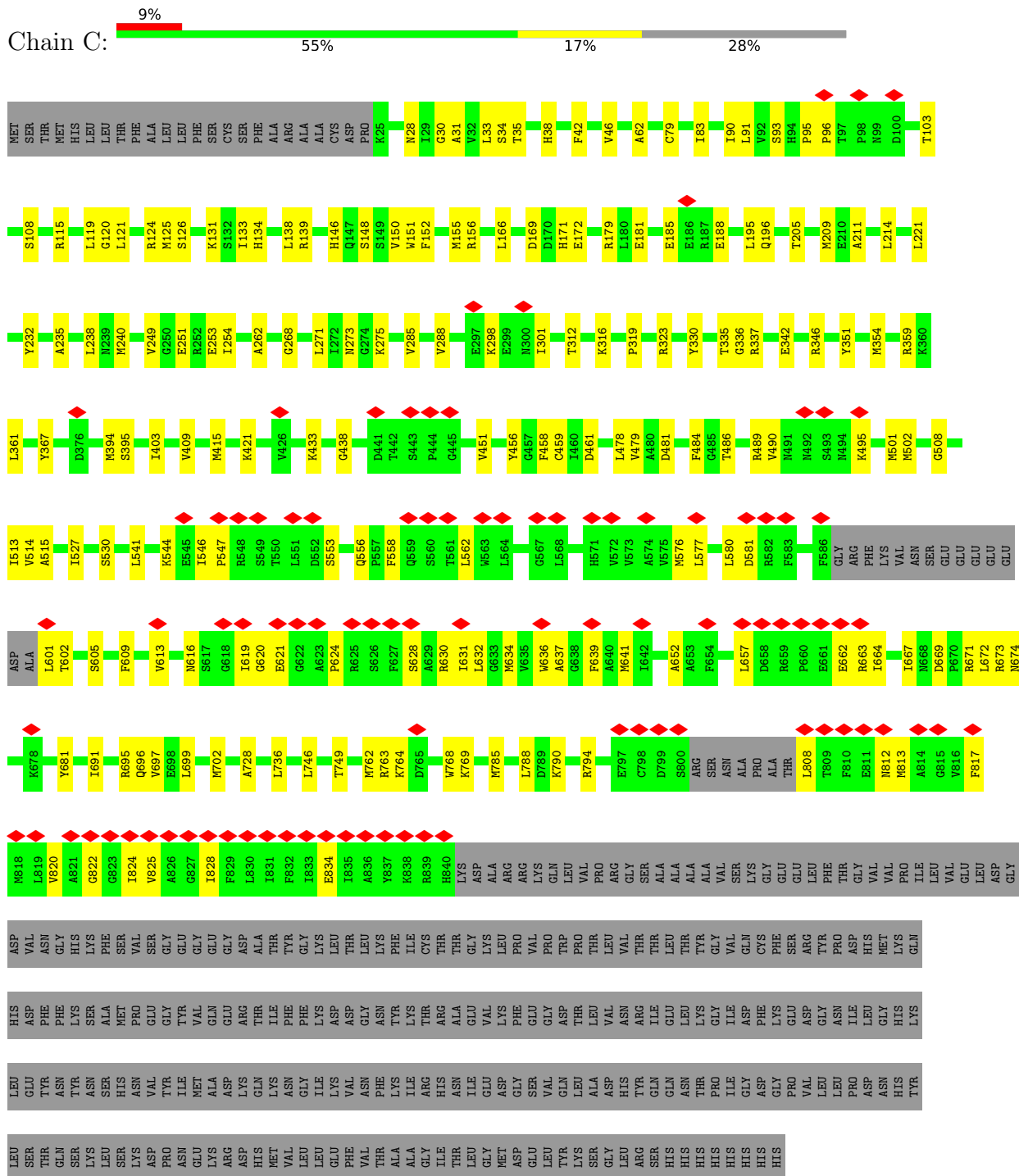
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	D	1	14	8	1	5	0



- Molecule 1: Glutamate receptor ionotropic, NMDA 1, Green fluorescent protein chimera



- Chain B: 





- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose







- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	431000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.215	Depositor
Minimum map value	-0.649	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.25	Depositor
Map size ( $\text{\AA}$ )	246.90001, 246.90001, 246.90001	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.823, 0.823, 0.823	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: 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	0.12	0/6436	0.35	0/8719
1	C	0.12	0/6424	0.32	0/8702
2	B	0.12	0/6436	0.33	0/8745
2	D	0.11	0/6390	0.32	0/8683
All	All	0.12	0/25686	0.33	0/34849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6295	0	6259	140	0
1	C	6283	0	6246	124	0
2	B	6282	0	6191	130	0
2	D	6237	0	6142	124	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	2	0
3	N	28	0	25	1	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	1	0
4	A	56	0	52	2	0
4	B	56	0	52	1	0
4	C	42	0	39	1	0
4	D	56	0	52	0	0
All	All	25867	0	25533	479	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 9.

All (479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:GLU:HB3	2:B:808:MET:HE1	1.57	0.86
2:B:560:MET:HA	2:B:564:MET:HE3	1.60	0.82
1:A:533:PHE:HB3	1:A:776:ILE:HD11	1.62	0.80
1:C:209:MET:HE3	1:C:238:LEU:HD13	1.65	0.79
2:B:535:VAL:HG22	2:B:729:ILE:HG12	1.66	0.78
1:A:218:VAL:HG12	1:A:246:VAL:HB	1.68	0.76
1:C:697:VAL:HG12	2:D:431:ARG:HG3	1.66	0.76
1:A:263:PRO:HD2	1:A:266:ILE:HD11	1.68	0.76
1:C:34:SER:HB2	1:C:96:PRO:HD3	1.70	0.73
2:B:561:MET:HA	2:B:565:LEU:HD12	1.71	0.72
1:C:93:SER:HB3	1:C:121:LEU:HD12	1.73	0.71
2:D:433:THR:HG22	2:D:457:LYS:HB3	1.71	0.71
2:B:784:GLY:HA3	1:C:695:ARG:HH12	1.55	0.70
1:A:554:PHE:O	1:A:647:TYR:OH	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ALA:HB1	2:B:614:ASN:HD22	1.57	0.69
1:C:205:THR:HG23	1:C:238:LEU:HD11	1.74	0.69
2:D:413:GLU:HG3	2:D:415:PRO:HD2	1.73	0.69
1:A:541:LEU:HD11	1:A:746:LEU:HB3	1.75	0.69
2:B:628:LYS:HA	2:B:631:VAL:HG22	1.75	0.68
2:B:58:GLU:HG3	2:B:60:ALA:H	1.57	0.68
2:B:782:PHE:HB3	2:B:788:MET:HE3	1.76	0.68
2:B:686:PRO:HD2	3:M:1:NAG:H82	1.77	0.67
1:A:337:ARG:NH2	1:A:339:GLU:OE2	2.26	0.67
2:B:48:GLU:HG2	2:B:71:ALA:HB3	1.76	0.67
1:A:113:PHE:HE1	2:B:106:GLN:HG2	1.59	0.66
2:B:785:ASP:OD1	1:C:695:ARG:NH2	2.27	0.66
1:A:695:ARG:NH2	2:D:785:ASP:OD1	2.29	0.66
1:A:489:ARG:HH11	1:A:494:ASN:H	1.42	0.66
2:B:419:VAL:HG12	2:B:456:CYS:HB3	1.78	0.66
2:D:279:VAL:HG12	2:D:363:VAL:HG22	1.77	0.66
1:A:195:LEU:HB3	1:A:207:LEU:HD12	1.77	0.65
1:A:619:ILE:O	2:D:621:ASN:ND2	2.29	0.65
1:C:616:ASN:HB2	2:D:615:ASN:HD21	1.61	0.65
1:A:28:ASN:ND2	1:A:85:SER:OG	2.28	0.65
2:B:781:GLN:NE2	2:B:785:ASP:OD2	2.29	0.65
1:C:577:LEU:HD21	1:C:632:LEU:HD22	1.79	0.64
1:A:441:ASP:O	1:A:448:ARG:NH1	2.31	0.64
2:D:759:THR:HG22	2:D:760:GLY:H	1.63	0.64
1:A:219:ILE:HD11	1:A:240:MET:HE2	1.81	0.63
1:C:530:SER:HA	1:C:769:LYS:HE2	1.79	0.63
2:D:161:ILE:HD13	2:D:383:LEU:HD21	1.79	0.63
2:D:521:VAL:HG12	2:D:522:VAL:HG13	1.80	0.63
1:A:699:LEU:HD12	1:A:702:MET:HG3	1.81	0.63
2:D:557:VAL:O	2:D:561:MET:HG3	1.99	0.63
1:A:502:MET:HE2	1:A:517:LEU:HD11	1.82	0.62
2:B:49:ARG:NH2	2:B:53:ASN:OD1	2.32	0.62
1:C:271:LEU:HD23	1:C:273:ASN:H	1.63	0.62
1:A:483:LYS:NZ	1:A:712:GLU:OE1	2.32	0.62
2:B:509:VAL:HG22	2:B:763:ILE:HD12	1.80	0.62
2:D:608:LEU:O	2:D:612:VAL:HG23	1.99	0.62
2:D:411:LEU:HB2	2:D:496:MET:HE2	1.81	0.62
1:C:115:ARG:NH1	2:D:106:GLN:OE1	2.31	0.62
1:A:685:LYS:HB2	1:A:710:ASN:HB3	1.82	0.62
2:D:686:PRO:HD2	3:X:1:NAG:H82	1.80	0.62
1:C:156:ARG:HH11	1:C:156:ARG:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HG22	1:A:268:GLY:H	1.63	0.62
2:D:373:GLU:OE2	2:D:386:ARG:NH1	2.33	0.62
1:A:499:ASN:ND2	1:A:686:GLN:OE1	2.33	0.61
2:D:39:LEU:HD23	2:D:72:LEU:HB3	1.82	0.61
1:A:115:ARG:NH1	2:B:106:GLN:OE1	2.32	0.61
2:B:75:ASN:OD1	2:B:76:ARG:N	2.33	0.61
2:B:279:VAL:HG12	2:B:363:VAL:HG22	1.82	0.61
2:D:209:SER:HB2	2:D:212:ASP:HB2	1.82	0.61
2:D:825:ALA:HA	2:D:828:MET:SD	2.40	0.61
1:A:407:PRO:HG3	1:A:735:VAL:HA	1.82	0.61
1:A:124:ARG:NH1	1:A:251:GLU:OE2	2.32	0.61
2:D:411:LEU:HD11	2:D:484:LYS:HD3	1.83	0.61
2:D:783:VAL:HA	2:D:788:MET:HG2	1.82	0.61
2:B:364:ILE:HG22	2:B:374:LYS:HA	1.83	0.61
1:C:211:ALA:HA	1:C:214:LEU:HD12	1.82	0.61
2:B:175:THR:HG22	2:B:176:ILE:H	1.66	0.60
1:A:131:LYS:NZ	1:A:137:PHE:O	2.35	0.60
2:B:508:ALA:HB3	2:B:764:ALA:HB3	1.82	0.60
2:B:759:THR:HG22	2:B:760:GLY:H	1.67	0.60
2:B:773:ARG:HH12	1:C:764:LYS:HZ2	1.50	0.60
1:C:669:ASP:HB3	1:C:672:LEU:HD23	1.82	0.60
3:H:2:NAG:H3	3:H:2:NAG:H83	1.84	0.60
1:A:140:THR:O	1:A:346:ARG:NH2	2.30	0.59
1:C:486:THR:HG23	1:C:691:ILE:HD11	1.84	0.59
2:D:702:HIS:O	2:D:706:THR:HG23	2.02	0.59
2:D:781:GLN:NE2	2:D:785:ASP:OD2	2.35	0.59
1:C:91:LEU:HD23	1:C:119:LEU:HB2	1.84	0.59
2:D:222:ILE:HG21	2:D:227:ILE:HD11	1.83	0.59
2:D:421:ASP:OD1	2:D:422:ILE:N	2.35	0.59
2:B:551:GLU:O	1:C:808:LEU:N	2.35	0.58
1:C:124:ARG:NH1	1:C:251:GLU:OE1	2.36	0.58
2:D:364:ILE:HG22	2:D:374:LYS:HA	1.84	0.58
1:C:639:PHE:HZ	2:D:823:MET:HG2	1.67	0.58
2:D:430:VAL:O	2:D:433:THR:OG1	2.22	0.58
2:D:607:LEU:HD13	2:D:619:VAL:HB	1.84	0.58
2:B:830:LEU:HA	2:B:833:ILE:HG12	1.87	0.57
1:C:546:ILE:HD12	1:C:547:PRO:HD2	1.86	0.57
1:A:790:LYS:HD3	1:A:794:ARG:HG3	1.87	0.57
2:D:288:LEU:HA	2:D:291:ARG:HD2	1.87	0.57
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.87	0.57
1:C:489:ARG:HB2	2:D:195:PHE:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:681:ARG:NH2	2:D:723:GLY:O	2.38	0.57
1:A:501:MET:SD	1:A:513:ILE:HD11	2.44	0.56
1:A:165:LEU:HD22	1:A:180:LEU:HD23	1.88	0.56
1:A:425:THR:OG1	1:A:429:ASP:OD1	2.22	0.56
1:C:298:LYS:HB2	1:C:301:ILE:HD11	1.86	0.56
2:D:536:MET:SD	2:D:747:LEU:HB3	2.45	0.56
2:B:285:ASP:OD2	2:B:374:LYS:NZ	2.37	0.56
2:B:612:VAL:HG22	2:B:634:TRP:HH2	1.70	0.56
1:C:762:MET:HE1	1:C:768:TRP:HB2	1.86	0.56
1:A:451:VAL:HG12	4:A:1203:NAG:H82	1.88	0.56
2:D:681:ARG:HB3	2:D:725:LEU:HD12	1.88	0.56
2:B:325:GLU:HG2	2:B:326:LYS:HG2	1.88	0.55
1:A:405:GLN:HE21	1:A:405:GLN:HA	1.72	0.55
4:B:1203:NAG:H3	4:B:1203:NAG:H83	1.89	0.55
1:A:695:ARG:HH12	2:D:784:GLY:HA3	1.71	0.55
4:A:1204:NAG:H3	4:A:1204:NAG:H83	1.88	0.55
1:C:312:THR:HG21	2:D:76:ARG:HE	1.72	0.55
2:D:686:PRO:HG3	2:D:709:ASN:HD21	1.71	0.55
2:D:343:TRP:CG	2:D:344:ASP:H	2.24	0.55
1:C:120:GLY:N	1:C:138:LEU:O	2.36	0.55
1:A:575:VAL:HA	1:A:578:TYR:CE1	2.41	0.55
2:B:207:ASP:OD1	2:B:208:THR:N	2.41	0.54
2:B:209:SER:OG	2:B:211:GLU:OE2	2.24	0.54
1:A:37:LYS:O	1:A:41:MET:HE3	2.08	0.54
2:D:233:LYS:NZ	2:D:262:SER:O	2.40	0.54
1:A:518:THR:O	1:A:523:ARG:NH1	2.37	0.54
1:C:262:ALA:O	1:C:359:ARG:NH1	2.41	0.54
2:D:127:ILE:HG23	2:D:291:ARG:HB3	1.89	0.54
2:B:536:MET:HE1	2:B:747:LEU:HB3	1.90	0.54
1:C:351:TYR:HB2	1:C:367:TYR:HD2	1.73	0.53
1:A:739:GLU:O	1:A:743:LYS:N	2.40	0.53
1:A:322:LYS:O	1:A:326:MET:HG2	2.08	0.53
1:A:668:ASN:HA	1:A:673:ARG:HH21	1.72	0.53
2:B:634:TRP:O	2:B:637:PHE:HB3	2.09	0.53
2:D:228:LEU:HD23	2:D:256:ILE:HB	1.90	0.53
1:A:573:VAL:HA	1:A:576:MET:HG3	1.91	0.53
1:A:602:THR:H	1:A:605:SER:HG	1.52	0.53
1:A:511:ASP:OD1	1:A:763:ARG:NH2	2.42	0.52
1:A:486:THR:HB	1:A:691:ILE:HD11	1.91	0.52
2:B:415:PRO:HB3	2:B:737:TYR:CG	2.45	0.52
1:C:148:SER:HA	1:C:151:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:N	1:A:253:GLU:OE1	2.42	0.52
1:A:209:MET:HE3	1:A:209:MET:HA	1.89	0.52
2:D:772:LYS:NZ	2:D:776:ASP:OD2	2.43	0.52
2:D:792:GLU:HG2	2:D:796:LEU:HB2	1.92	0.52
1:A:425:THR:OG1	1:A:427:ASN:OD1	2.26	0.52
2:D:344:ASP:OD1	2:D:345:GLY:N	2.42	0.52
1:A:576:MET:SD	1:A:632:LEU:HD21	2.50	0.52
1:A:677:ASP:OD1	1:A:678:LYS:N	2.43	0.52
1:A:558:PHE:CZ	1:A:647:TYR:HB2	2.45	0.51
1:A:148:SER:HA	1:A:151:TRP:CE3	2.44	0.51
1:A:404:HIS:CE1	1:A:411:VAL:HG22	2.45	0.51
1:A:462:LEU:HD13	1:A:785:MET:HE1	1.93	0.51
1:A:570:VAL:HG22	1:A:636:TRP:HZ2	1.75	0.51
1:C:31:ALA:HB1	1:C:33:LEU:HD23	1.91	0.51
1:A:31:ALA:O	1:A:64:SER:HA	2.09	0.51
1:A:577:LEU:HD13	1:A:632:LEU:HD23	1.92	0.51
2:B:557:VAL:HA	2:B:560:MET:HG3	1.91	0.51
1:C:620:GLY:O	1:C:621:GLU:HG3	2.10	0.51
2:B:563:VAL:O	2:B:567:ILE:HG12	2.11	0.51
2:B:153:GLN:NE2	2:B:356:GLN:O	2.43	0.51
2:B:624:GLY:O	2:B:628:LYS:HG2	2.11	0.51
1:C:613:VAL:HG11	1:C:636:TRP:CD1	2.46	0.51
1:C:254:ILE:HD13	1:C:268:GLY:HA3	1.93	0.51
2:D:56:GLY:N	2:D:57:PRO:HD3	2.26	0.51
2:D:536:MET:HA	2:D:536:MET:HE2	1.92	0.51
2:B:406:LEU:HD22	2:B:506:VAL:HG11	1.92	0.51
2:B:677:SER:OG	2:B:678:PRO:HD3	2.10	0.51
1:C:133:ILE:HD11	2:D:136:ALA:HB3	1.91	0.51
2:D:191:VAL:HG23	2:D:198:TRP:HB3	1.93	0.51
1:A:153:GLU:HG3	1:A:367:TYR:HE1	1.76	0.51
1:A:354:MET:HE3	1:A:361:LEU:HB3	1.92	0.51
2:B:102:ASP:OD1	2:B:103:ASP:N	2.35	0.51
2:D:515:ASN:OD1	2:D:516:GLU:N	2.44	0.51
1:C:209:MET:HE2	1:C:209:MET:HA	1.93	0.51
1:C:541:LEU:HD11	1:C:746:LEU:HB3	1.93	0.51
1:A:557:PRO:HG2	1:A:651:LEU:HD23	1.92	0.50
2:B:306:MET:HE1	2:B:313:ILE:HG23	1.94	0.50
2:B:536:MET:HG2	2:B:735:LEU:HD12	1.94	0.50
1:C:126:SER:HA	1:C:139:ARG:HH22	1.75	0.50
2:B:538:SER:HA	2:B:747:LEU:HD13	1.94	0.50
1:C:609:PHE:O	1:C:613:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LEU:HD22	2:D:124:ILE:HG21	1.93	0.50
2:D:560:MET:O	2:D:564:MET:HG3	2.11	0.50
1:A:394:MET:HE2	1:A:768:TRP:NE1	2.27	0.50
1:C:681:TYR:HB3	1:C:728:ALA:HB3	1.94	0.50
2:D:466:LYS:HB3	2:D:782:PHE:CZ	2.47	0.50
1:A:662:GLU:O	1:A:663:ARG:HG2	2.11	0.50
1:C:150:VAL:HG22	1:C:367:TYR:CE2	2.47	0.50
1:C:628:SER:HA	1:C:631:ILE:HG12	1.93	0.50
2:D:37:ALA:HB2	2:D:95:ILE:HG21	1.93	0.50
1:A:50:ASN:ND2	1:A:59:GLN:OE1	2.45	0.50
1:C:95:PRO:HD3	1:C:103:THR:HG21	1.93	0.50
1:C:508:GLY:HA2	1:C:763:ARG:HH11	1.76	0.50
1:C:697:VAL:HB	2:D:432:ASN:HD22	1.77	0.50
2:D:210:PHE:O	2:D:215:THR:OG1	2.30	0.50
2:D:535:VAL:HG22	2:D:729:ILE:HG12	1.94	0.50
1:A:264:ASP:OD1	1:A:359:ARG:NH1	2.45	0.49
2:B:411:LEU:HD22	2:B:484:LYS:O	2.12	0.49
2:D:648:ASN:OD1	2:D:649:LEU:N	2.45	0.49
2:B:661:GLN:HG3	2:B:662:VAL:HG23	1.94	0.49
2:B:694:ILE:HG22	2:B:702:HIS:HB2	1.95	0.49
1:A:82:LEU:HB3	1:A:87:VAL:HG21	1.95	0.49
2:B:561:MET:HG3	2:B:562:PHE:CD1	2.48	0.49
2:D:637:PHE:HA	2:D:640:ILE:HG22	1.94	0.49
2:B:460:CYS:HB3	2:B:509:VAL:HG12	1.94	0.49
1:C:108:SER:OG	1:C:134:HIS:ND1	2.42	0.49
2:B:149:ALA:HB2	2:B:361:LEU:HD11	1.94	0.49
1:C:602:THR:N	1:C:605:SER:OG	2.45	0.49
1:C:30:GLY:O	1:C:90:ILE:HA	2.13	0.49
1:C:451:VAL:HG21	4:C:1202:NAG:H83	1.93	0.49
2:D:415:PRO:HB3	2:D:737:TYR:CG	2.47	0.49
1:C:152:PHE:O	1:C:155:MET:HB2	2.13	0.49
2:B:621:ASN:ND2	1:C:619:ILE:O	2.44	0.49
2:B:373:GLU:OE2	2:B:386:ARG:NH2	2.46	0.48
1:C:336:GLY:HA2	3:R:1:NAG:H61	1.94	0.48
1:A:364:VAL:HG11	1:A:379:ILE:HD13	1.93	0.48
1:A:505:LEU:HA	1:A:510:ALA:HB3	1.95	0.48
2:B:286:TYR:OH	2:B:294:ASP:OD2	2.27	0.48
2:B:612:VAL:HG22	2:B:634:TRP:CH2	2.48	0.48
1:A:513:ILE:HG22	1:A:761:GLY:O	2.14	0.48
1:A:722:ARG:HG3	1:A:746:LEU:HD11	1.96	0.48
2:B:99:VAL:HG21	2:B:296:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:MET:HE2	1:C:361:LEU:HD13	1.94	0.48
1:C:335:THR:HG23	1:C:346:ARG:HH12	1.77	0.48
1:C:702:MET:HE2	1:C:702:MET:HB3	1.78	0.48
1:A:411:VAL:HG11	1:A:478:LEU:HD21	1.96	0.48
2:B:459:PHE:O	2:B:463:ILE:HG12	2.14	0.48
1:C:620:GLY:HA2	2:D:617:VAL:HG22	1.96	0.48
1:A:645:ALA:HB1	2:B:646:THR:HG22	1.95	0.48
2:D:104:THR:HG23	2:D:106:GLN:H	1.78	0.48
1:C:251:GLU:OE2	1:C:275:LYS:NZ	2.39	0.47
2:D:83:ILE:HD11	2:D:112:MET:HE1	1.96	0.47
2:D:684:THR:HG22	2:D:705:MET:HE3	1.96	0.47
1:C:125:MET:O	1:C:139:ARG:NH1	2.46	0.47
1:C:576:MET:O	1:C:580:LEU:HG	2.13	0.47
1:A:411:VAL:HG12	1:A:455:CYS:SG	2.54	0.47
1:A:789:ASP:OD2	1:A:794:ARG:NH2	2.47	0.47
2:B:441:LYS:HD2	2:B:446:THR:HG23	1.94	0.47
2:B:553:PHE:HD1	1:C:813:MET:HE3	1.79	0.47
2:D:54:LEU:HD21	2:D:289:GLU:HG3	1.96	0.47
2:B:191:VAL:HG23	2:B:198:TRP:HB2	1.96	0.47
2:D:182:ASP:OD2	2:D:182:ASP:N	2.44	0.47
1:A:155:MET:HA	1:A:155:MET:HE2	1.95	0.47
1:A:404:HIS:ND1	1:A:411:VAL:HG22	2.30	0.47
2:D:612:VAL:HG22	2:D:634:TRP:HE1	1.77	0.47
2:B:38:VAL:HG22	2:B:99:VAL:HB	1.96	0.47
2:D:326:LYS:HG2	2:D:327:PRO:HD2	1.97	0.47
2:D:531:THR:HG21	2:D:761:TYR:CD1	2.50	0.47
1:A:483:LYS:HD2	1:A:686:GLN:HB3	1.96	0.47
1:A:502:MET:HE1	1:A:523:ARG:CD	2.45	0.47
2:B:99:VAL:HG12	2:B:99:VAL:O	2.14	0.47
2:B:116:ILE:O	2:B:120:THR:OG1	2.26	0.47
2:B:740:GLY:HA3	2:B:798:GLY:HA3	1.96	0.47
1:C:489:ARG:NH2	2:D:425:LEU:O	2.48	0.47
1:C:527:ILE:HB	1:C:762:MET:O	2.14	0.47
2:D:442:ILE:H	2:D:442:ILE:HD12	1.80	0.47
1:A:663:ARG:HA	1:A:663:ARG:NE	2.30	0.47
1:C:35:THR:OG1	1:C:38:HIS:ND1	2.46	0.47
2:D:523:ASP:OD2	2:D:524:PHE:N	2.48	0.47
1:A:217:ARG:HA	1:A:217:ARG:HD3	1.67	0.47
2:B:625:THR:HA	2:B:628:LYS:HE2	1.97	0.47
1:C:541:LEU:HB2	1:C:736:LEU:HD22	1.96	0.47
1:C:696:GLN:HB2	1:C:699:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:VAL:HG11	2:D:116:ILE:HG21	1.96	0.47
2:B:600:THR:HG22	2:B:602:GLY:H	1.80	0.47
2:B:118:SER:HB3	2:B:142:SER:HB2	1.96	0.46
1:C:409:VAL:HG22	1:C:459:CYS:HB2	1.98	0.46
1:A:699:LEU:O	1:A:702:MET:HB2	2.14	0.46
1:A:829:PHE:O	1:A:833:ILE:HG12	2.15	0.46
2:D:406:LEU:HB3	2:D:506:VAL:HG11	1.97	0.46
2:B:433:THR:HA	2:B:457:LYS:HB3	1.97	0.46
1:C:438:GLY:HA3	1:C:478:LEU:HB2	1.97	0.46
2:D:830:LEU:HA	2:D:833:ILE:HG12	1.97	0.46
1:A:813:MET:O	1:A:816:VAL:HG22	2.16	0.46
1:C:674:ASN:HD21	2:D:741:ARG:HG3	1.79	0.46
1:A:39:GLU:HG2	1:A:64:SER:HB3	1.97	0.46
1:A:696:GLN:HE22	1:A:698:GLU:HB3	1.80	0.46
1:C:342:GLU:HG3	2:D:176:ILE:HD11	1.97	0.46
1:C:558:PHE:HB3	1:C:562:LEU:HD13	1.98	0.46
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.97	0.46
1:A:351:TYR:HB2	1:A:367:TYR:HB3	1.98	0.46
1:A:521:ASN:O	1:A:525:GLN:HG3	2.16	0.46
1:A:576:MET:HA	1:A:579:LEU:HB3	1.98	0.46
1:A:790:LYS:HA	1:A:794:ARG:HB2	1.98	0.46
2:B:169:VAL:HA	2:B:199:ASP:HB3	1.98	0.46
2:B:681:ARG:NH2	2:B:723:GLY:O	2.49	0.46
2:B:738:LYS:HA	2:B:738:LYS:HD3	1.71	0.46
1:A:636:TRP:CZ3	2:B:824:LEU:HD21	2.51	0.46
1:A:659:ARG:HE	1:A:660:PRO:HD2	1.81	0.46
1:A:754:PHE:HE1	2:D:784:GLY:HA2	1.80	0.46
2:B:379:GLU:O	2:B:382:THR:OG1	2.26	0.46
1:C:667:ILE:HG13	1:C:673:ARG:HH12	1.80	0.46
2:D:487:LYS:HE3	2:D:687:ASN:HA	1.98	0.46
1:A:519:ILE:HG22	2:D:780:LEU:HD11	1.97	0.46
1:C:235:ALA:HB1	1:C:240:MET:HB2	1.97	0.46
1:C:657:LEU:HD12	1:C:657:LEU:O	2.16	0.46
1:C:822:GLY:HA2	1:C:825:VAL:HG12	1.97	0.46
1:C:624:PRO:HG2	1:C:630:ARG:HG2	1.97	0.45
1:C:817:PHE:HA	1:C:820:VAL:HG12	1.97	0.45
1:A:217:ARG:CZ	1:A:393:GLN:HE22	2.29	0.45
2:D:645:TYR:O	2:D:649:LEU:HD13	2.16	0.45
2:B:90:MET:HE3	2:B:316:ALA:HB1	1.99	0.45
1:A:117:PRO:HA	1:A:136:SER:HB2	1.98	0.45
2:B:59:GLN:O	2:B:61:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:HIS:ND1	2:D:137:ASP:OD2	2.47	0.45
1:A:99:ASN:HD22	1:A:101:HIS:CE1	2.34	0.45
1:A:636:TRP:HZ3	2:B:824:LEU:HD21	1.81	0.45
1:C:181:GLU:O	1:C:185:GLU:HG2	2.16	0.45
1:C:553:SER:HA	1:C:556:GLN:HE22	1.81	0.45
2:D:720:LEU:HD22	2:D:725:LEU:HB3	1.98	0.45
2:B:533:ILE:HG12	2:B:757:ALA:HB2	1.98	0.45
2:D:134:ILE:HA	2:D:146:GLN:OE1	2.16	0.45
1:A:113:PHE:CE1	2:B:106:GLN:HG2	2.48	0.45
1:C:169:ASP:OD1	1:C:196:GLN:HB3	2.17	0.45
1:A:535:TYR:HB3	2:D:530:GLU:HG2	1.98	0.45
2:D:817:VAL:HG12	2:D:817:VAL:O	2.16	0.45
2:B:662:VAL:HG11	2:B:670:PHE:HE2	1.82	0.45
2:D:410:THR:HB	2:D:477:LEU:HD21	1.99	0.45
2:D:421:ASP:OD1	2:D:422:ILE:HD12	2.16	0.45
2:D:533:ILE:HG22	2:D:690:THR:HG22	1.98	0.45
1:A:405:GLN:HG3	1:A:407:PRO:HD2	1.99	0.45
2:B:48:GLU:OE1	2:B:52:ARG:NH2	2.50	0.45
2:B:113:LEU:HD22	2:B:124:ILE:HG21	1.98	0.45
2:B:167:TRP:HB3	2:B:226:VAL:HG21	1.98	0.45
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.98	0.45
2:D:378:TRP:HE3	2:D:383:LEU:HB2	1.81	0.44
2:B:230:TYR:HD1	2:B:258:PRO:HG3	1.82	0.44
1:C:484:PHE:HA	1:C:501:MET:HE1	1.99	0.44
1:C:813:MET:SD	1:C:813:MET:N	2.91	0.44
2:B:603:LYS:HA	2:B:606:TRP:CE2	2.52	0.44
1:C:172:GLU:HA	1:C:172:GLU:OE1	2.17	0.44
1:C:479:VAL:HG12	1:C:481:ASP:H	1.82	0.44
2:D:787:GLU:HA	2:D:790:GLU:OE2	2.16	0.44
2:B:518:ARG:HB3	2:B:524:PHE:CZ	2.53	0.44
2:B:730:TYR:HB3	2:B:735:LEU:CD2	2.48	0.44
2:B:755:ILE:HG22	2:B:758:THR:H	1.82	0.44
1:C:285:VAL:HA	1:C:288:VAL:HG12	2.00	0.44
2:D:738:LYS:HD3	2:D:738:LYS:HA	1.74	0.44
2:D:780:LEU:HA	2:D:783:VAL:HG12	2.00	0.44
1:A:399:LYS:HE3	1:A:509:GLN:O	2.16	0.44
1:A:624:PRO:HG2	1:A:630:ARG:HD2	1.98	0.44
1:A:181:GLU:O	1:A:185:GLU:HG2	2.18	0.44
2:B:681:ARG:NH2	2:B:726:ASP:OD1	2.50	0.44
2:D:34:LEU:HB2	2:D:65:LEU:HD12	1.99	0.44
2:D:206:LEU:HD22	2:D:215:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:ARG:HG3	2:B:708:PHE:CD1	2.53	0.44
1:C:502:MET:HE1	1:C:527:ILE:HD11	2.00	0.44
2:D:552:PRO:HB3	2:D:648:ASN:ND2	2.33	0.44
1:A:35:THR:HG23	1:A:37:LYS:HG2	2.00	0.44
1:C:825:VAL:O	1:C:828:ILE:HG22	2.18	0.44
2:D:824:LEU:HG	2:D:828:MET:HE1	2.00	0.44
1:A:398:LEU:HD13	1:A:472:PHE:CD2	2.53	0.44
2:B:37:ALA:HB2	2:B:95:ILE:HG21	1.99	0.43
2:B:426:THR:HG22	2:B:428:THR:HG22	1.99	0.43
1:A:702:MET:HB3	1:A:702:MET:HE3	1.69	0.43
1:C:664:ILE:O	1:C:749:THR:OG1	2.31	0.43
1:A:26:ILE:HD11	1:A:61:ASN:HB2	2.00	0.43
2:B:208:THR:HG21	2:B:214:LYS:HB3	1.99	0.43
2:B:647:ALA:HB1	1:C:652:ALA:HA	2.00	0.43
1:C:316:LYS:HD3	1:C:316:LYS:HA	1.60	0.43
1:A:90:ILE:HD12	1:A:111:ALA:HB2	2.00	0.43
2:B:449:GLY:O	2:B:450:MET:HE2	2.18	0.43
1:C:31:ALA:HB1	1:C:33:LEU:CD2	2.49	0.43
2:B:608:LEU:O	2:B:612:VAL:HG23	2.18	0.43
1:C:319:PRO:O	1:C:323:ARG:NE	2.47	0.43
2:B:626:THR:HB	1:C:834:GLU:HG3	2.01	0.43
1:C:461:ASP:HB3	1:C:788:LEU:HD11	1.99	0.43
2:D:161:ILE:HD11	2:D:363:VAL:HG21	2.01	0.43
1:A:354:MET:HB3	1:A:361:LEU:HD12	2.01	0.43
1:A:308:CYS:HB3	2:B:79:PRO:HD2	2.00	0.43
1:C:188:GLU:OE2	1:C:188:GLU:HA	2.19	0.43
2:B:76:ARG:HD2	2:B:76:ARG:HA	1.69	0.43
2:B:487:LYS:HD2	2:B:687:ASN:HA	2.01	0.43
1:C:415:MET:HE1	1:C:421:LYS:N	2.34	0.43
1:C:544:LYS:O	1:C:663:ARG:NH1	2.51	0.43
1:A:808:LEU:HD12	2:D:648:ASN:HD22	1.83	0.42
1:A:816:VAL:O	1:A:820:VAL:HG23	2.19	0.42
2:B:484:LYS:NZ	3:M:1:NAG:O7	2.52	0.42
2:B:518:ARG:HA	2:B:521:VAL:HG12	2.01	0.42
1:C:79:CYS:HA	1:C:83:ILE:HB	2.01	0.42
2:B:533:ILE:HG13	2:B:693:ASN:HD22	1.84	0.42
2:B:700:TYR:HA	2:B:703:GLN:HG2	2.01	0.42
2:D:298:ILE:HD11	2:D:348:LEU:HB3	2.00	0.42
1:A:235:ALA:HB1	1:A:240:MET:HB3	2.01	0.42
2:B:432:ASN:OD1	2:B:433:THR:N	2.52	0.42
2:D:415:PRO:HG2	2:D:416:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:SER:O	2:B:631:VAL:HG13	2.19	0.42
1:C:394:MET:HE3	1:C:395:SER:H	1.85	0.42
2:D:544:VAL:HG12	2:D:659:VAL:HB	2.01	0.42
1:A:248:LEU:HD23	1:A:267:ILE:HB	2.01	0.42
1:A:700:SER:O	1:A:703:TYR:HB3	2.19	0.42
1:A:812:ASN:C	1:A:812:ASN:HD22	2.27	0.42
1:A:835:ILE:O	1:A:839:ARG:HG2	2.19	0.42
2:B:358:HIS:HD2	2:B:380:ASN:HA	1.84	0.42
2:B:557:VAL:HG12	2:B:561:MET:CE	2.50	0.42
1:C:330:TYR:O	1:C:337:ARG:NH2	2.53	0.42
1:C:501:MET:HB3	1:C:513:ILE:HD13	2.01	0.42
1:A:484:PHE:HA	1:A:501:MET:HE2	2.01	0.42
1:A:659:ARG:NE	1:A:660:PRO:HD2	2.34	0.42
1:C:785:MET:HB3	1:C:785:MET:HE3	1.77	0.42
2:D:188:LYS:HA	2:D:191:VAL:HG12	2.00	0.42
1:C:195:LEU:HD11	1:C:211:ALA:HB2	2.02	0.42
2:D:557:VAL:HA	2:D:560:MET:HG3	2.01	0.42
2:D:740:GLY:HA3	2:D:798:GLY:HA3	2.01	0.42
1:A:79:CYS:SG	2:B:80:LYS:HB2	2.60	0.42
1:A:828:ILE:HA	1:A:831:ILE:HG22	2.02	0.42
2:B:244:ARG:HD2	2:B:396:PHE:CE1	2.55	0.42
2:B:394:LYS:NZ	2:B:399:CYS:O	2.51	0.42
2:B:514:ILE:HG12	2:B:524:PHE:CD2	2.54	0.42
2:D:610:GLY:HA2	2:D:613:PHE:CE1	2.55	0.42
2:D:702:HIS:HA	2:D:705:MET:HG3	2.02	0.42
2:D:343:TRP:CG	2:D:344:ASP:N	2.88	0.42
1:A:657:LEU:O	2:B:807:VAL:HG11	2.19	0.41
2:B:573:VAL:O	2:B:576:PHE:HB2	2.20	0.41
1:C:514:VAL:HG23	1:C:514:VAL:O	2.20	0.41
2:D:531:THR:HG22	2:D:733:ALA:HB2	2.02	0.41
1:A:570:VAL:HG22	1:A:636:TRP:CZ2	2.55	0.41
1:A:609:PHE:O	1:A:613:VAL:HG22	2.20	0.41
1:A:813:MET:SD	1:A:813:MET:N	2.93	0.41
1:C:146:HIS:CE1	1:C:179:ARG:HH12	2.38	0.41
2:D:196:VAL:HB	2:D:198:TRP:NE1	2.35	0.41
1:A:68:LYS:H	1:A:74:MET:HE1	1.85	0.41
1:A:102:PHE:HE1	1:A:125:MET:HG2	1.84	0.41
1:C:581:ASP:OD2	1:C:601:LEU:HB3	2.19	0.41
1:C:634:MET:HE1	2:D:610:GLY:N	2.36	0.41
2:D:301:THR:HG21	2:D:341:VAL:HG13	2.02	0.41
1:A:164:ILE:HG13	1:A:193:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:HG3	2:B:53:ASN:HD21	1.86	0.41
1:C:166:LEU:HD13	1:C:195:LEU:HB2	2.02	0.41
1:C:403:ILE:HG22	1:C:515:ALA:HB1	2.02	0.41
2:D:628:LYS:HA	2:D:631:VAL:HG22	2.01	0.41
1:A:67:HIS:HA	1:A:74:MET:HE1	2.02	0.41
1:A:398:LEU:HD21	1:A:768:TRP:NE1	2.36	0.41
1:A:790:LYS:HD3	1:A:790:LYS:HA	1.81	0.41
2:B:672:ARG:NH2	2:B:674:HIS:HB2	2.35	0.41
1:C:613:VAL:HG13	1:C:637:ALA:HA	2.03	0.41
2:B:486:GLY:HA2	2:B:494:ASN:O	2.21	0.41
2:B:636:PHE:HA	2:B:639:VAL:HG22	2.03	0.41
1:C:42:PHE:CE2	1:C:62:ALA:HB1	2.56	0.41
1:A:375:ASN:HD21	1:A:377:ARG:HG2	1.84	0.41
1:A:470:MET:HE2	1:A:470:MET:HB3	1.98	0.41
1:A:760:ILE:O	1:A:760:ILE:HG13	2.21	0.41
2:B:496:MET:HB3	2:B:508:ALA:HB1	2.03	0.41
2:B:536:MET:HA	2:B:749:THR:HA	2.02	0.41
2:B:684:THR:HG22	2:B:729:ILE:O	2.21	0.41
1:C:433:LYS:HG2	1:C:456:TYR:HB3	2.03	0.41
2:D:567:ILE:O	2:D:571:ILE:HG13	2.21	0.41
1:A:35:THR:OG1	1:A:36:ARG:N	2.53	0.41
1:A:113:PHE:HD2	2:B:79:PRO:HG3	1.84	0.41
1:A:429:ASP:OD1	1:A:429:ASP:N	2.53	0.41
2:B:294:ASP:O	2:B:298:ILE:HG12	2.20	0.41
2:B:608:LEU:HA	2:B:611:LEU:HD12	2.02	0.41
1:C:131:LYS:HA	1:C:131:LYS:HD3	1.89	0.41
1:C:232:TYR:OH	1:C:253:GLU:HB3	2.21	0.41
2:D:459:PHE:CE2	2:D:791:LEU:HB3	2.56	0.41
2:D:487:LYS:HG2	2:D:489:VAL:HG13	2.03	0.41
1:C:662:GLU:O	1:C:671:ARG:NH1	2.54	0.41
1:C:812:ASN:C	1:C:812:ASN:HD22	2.27	0.41
2:D:488:LYS:HD3	2:D:493:TRP:NE1	2.36	0.41
2:B:157:VAL:HG21	2:B:361:LEU:HD22	2.02	0.40
2:B:206:LEU:HD23	2:B:210:PHE:HD1	1.86	0.40
1:C:641:MET:SD	2:D:642:LEU:HD13	2.61	0.40
2:D:153:GLN:NE2	2:D:356:GLN:O	2.54	0.40
2:B:788:MET:N	2:B:788:MET:HE2	2.36	0.40
1:C:820:VAL:O	1:C:824:ILE:HG13	2.21	0.40
2:D:113:LEU:HD23	2:D:113:LEU:HA	1.93	0.40
1:A:615:LEU:HD21	2:D:635:ALA:HB3	2.03	0.40
2:B:751:GLY:HA3	2:B:754:TYR:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASN:ND2	3:N:1:NAG:O7	2.54	0.40
2:D:286:TYR:OH	2:D:294:ASP:OD2	2.29	0.40
2:D:437:ARG:HG3	2:D:478:TYR:HB2	2.03	0.40
1:A:32:VAL:HG12	1:A:65:VAL:HB	2.04	0.40
1:A:70:ASN:HD21	1:A:73:GLN:HG3	1.85	0.40
1:A:284:ALA:HA	1:A:287:VAL:HG12	2.04	0.40
2:B:172:LEU:HD11	2:B:183:PHE:HE2	1.86	0.40
1:C:490:VAL:HG12	1:C:495:LYS:O	2.22	0.40
2:D:531:THR:HG21	2:D:761:TYR:CE1	2.57	0.40
2:D:716:ALA:O	2:D:720:LEU:HD23	2.22	0.40
1:A:701:THR:O	1:A:704:ARG:HB2	2.22	0.40
2:B:793:THR:HA	2:B:797:THR:HB	2.04	0.40
1:C:458:PHE:CE2	1:C:788:LEU:HB3	2.56	0.40
1:C:790:LYS:HZ3	1:C:794:ARG:HH11	1.69	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	791/1108 (71%)	766 (97%)	25 (3%)	0	100	100
1	C	789/1108 (71%)	771 (98%)	18 (2%)	0	100	100
2	B	789/1127 (70%)	754 (96%)	35 (4%)	0	100	100
2	D	782/1127 (69%)	752 (96%)	30 (4%)	0	100	100
All	All	3151/4470 (70%)	3043 (97%)	108 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	686/956 (72%)	685 (100%)	1 (0%)	88	89
1	C	685/956 (72%)	685 (100%)	0	100	100
2	B	695/978 (71%)	695 (100%)	0	100	100
2	D	689/978 (70%)	689 (100%)	0	100	100
All	All	2755/3868 (71%)	2754 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	50	ASN
1	A	99	ASN
1	A	257	ASN
1	A	405	GLN
1	A	674	ASN
1	A	709	HIS
1	A	724	ASN
1	A	812	ASN
2	B	358	HIS
2	B	381	GLN
2	B	614	ASN
2	B	671	GLN
2	B	693	ASN
2	B	697	ASN
1	C	50	ASN
1	C	371	HIS
1	C	405	GLN

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Mol	Chain	Res	Type
1	C	521	ASN
1	C	742	GLN
2	D	323	GLN
2	D	335	HIS
2	D	702	HIS
2	D	710	GLN

### 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 ⓘ

40 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	$\# Z  > 2$
3	NAG	E	1	3,1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	G	1	3,1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	G	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	H	1	3,1	14,14,15	0.35	0	17,19,21	0.60	0
3	NAG	H	2	3	14,14,15	0.49	0	17,19,21	1.35	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.34	0	17,19,21	0.43	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.47	0
3	NAG	J	1	3,1	14,14,15	0.24	0	17,19,21	0.38	0
3	NAG	J	2	3	14,14,15	0.23	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	K	1	3,2	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	L	1	3,2	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	M	1	3,2	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	M	2	3	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	N	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	N	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	O	1	3,1	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	P	1	3,1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	Q	1	3,1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	R	1	3,1	14,14,15	0.25	0	17,19,21	0.36	0
3	NAG	R	2	3	14,14,15	0.26	0	17,19,21	0.57	0
3	NAG	S	1	3,1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	S	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	T	1	3,1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	T	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	U	1	3,1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	U	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	V	1	3,2	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	V	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	W	1	3,2	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	W	2	3	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	X	1	3,2	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	X	2	3	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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	2	3	-	6/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	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	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1
3	NAG	X	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C2-N2-C7	4.53	128.97	122.90
3	H	2	NAG	C1-C2-N2	2.16	113.84	110.43

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6

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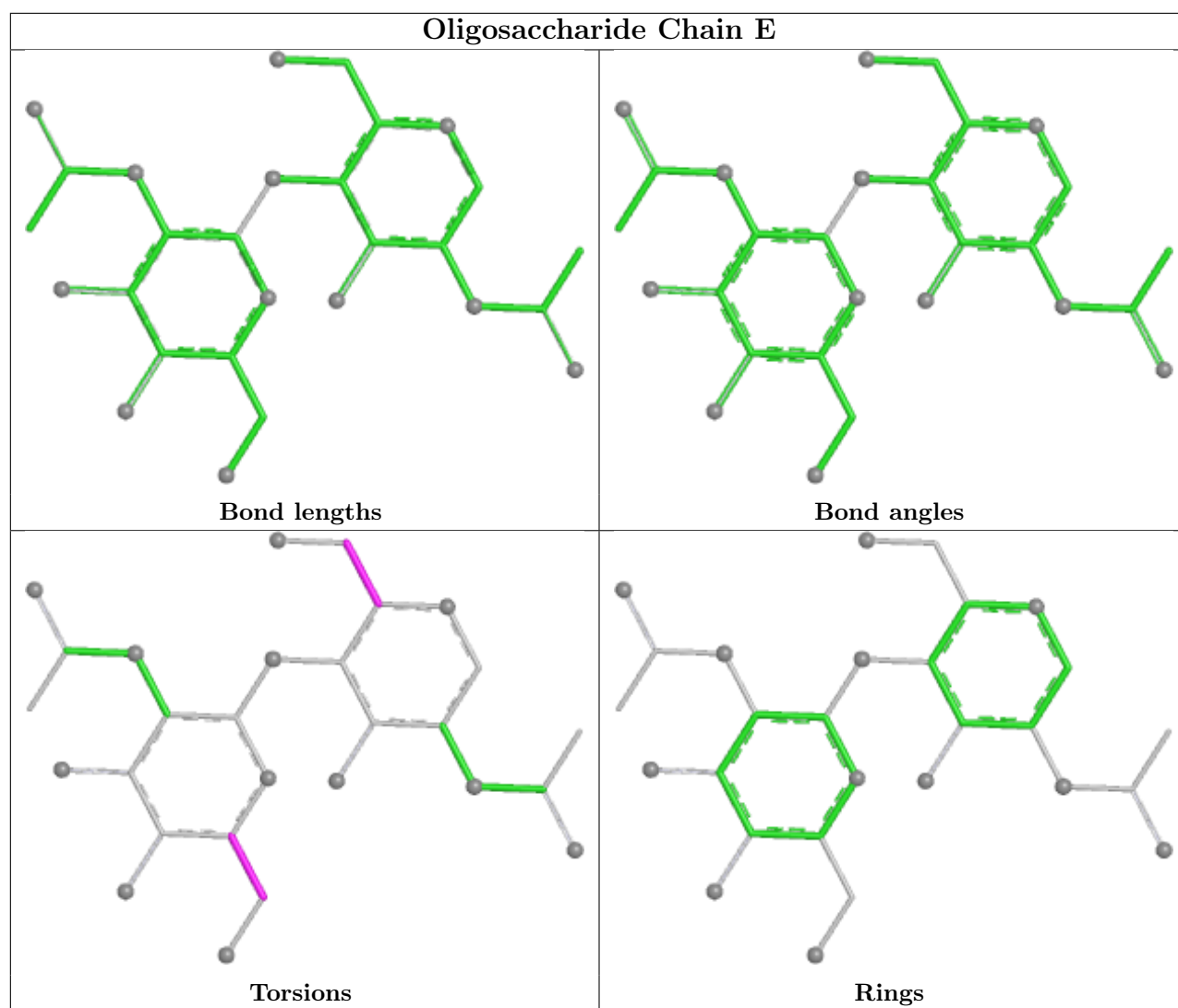
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C3-C2-N2-C7
3	U	2	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7
3	R	2	NAG	C1-C2-N2-C7
3	W	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	F	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6

There are no ring outliers.

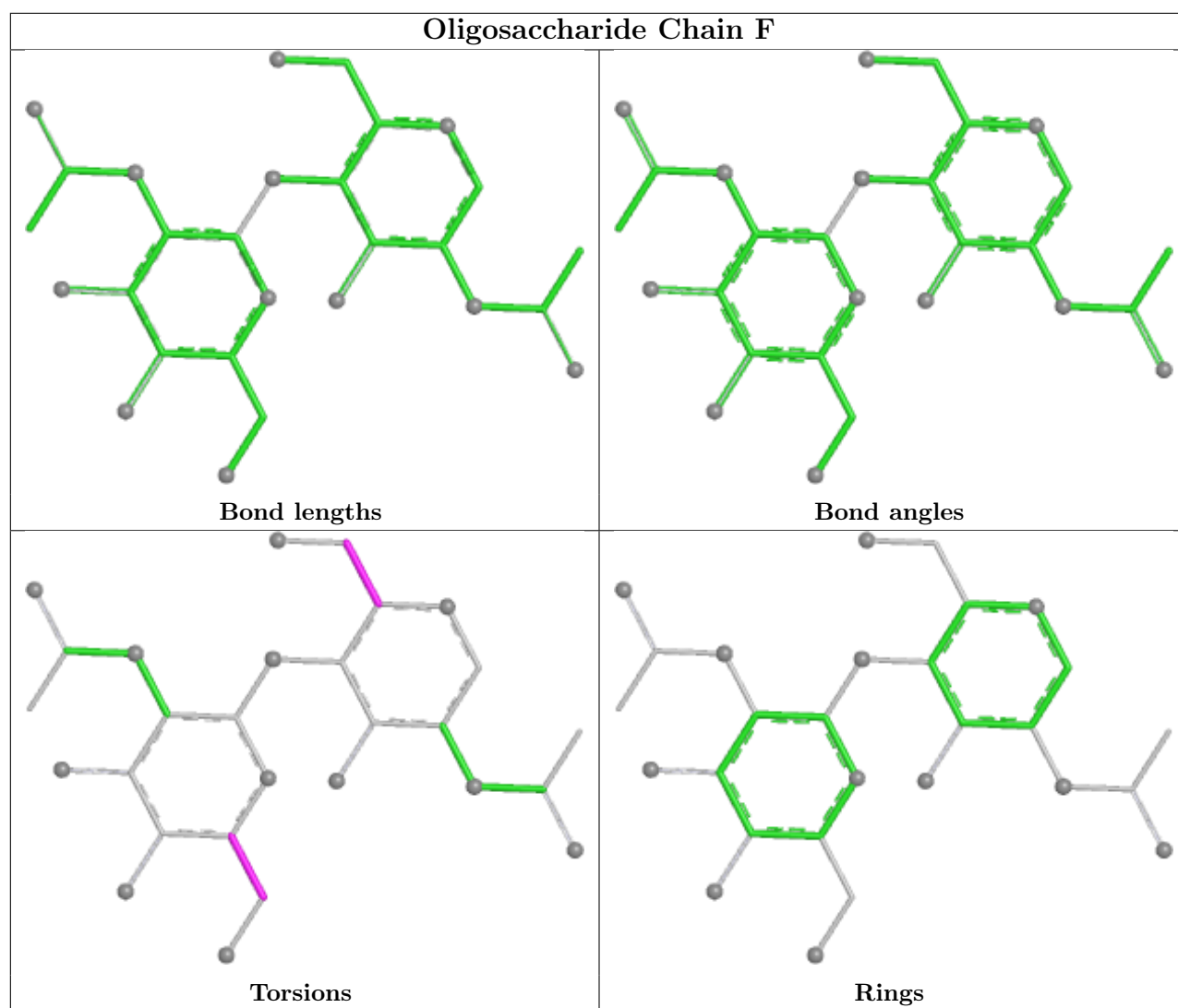
5 monomers are involved in 6 short contacts:

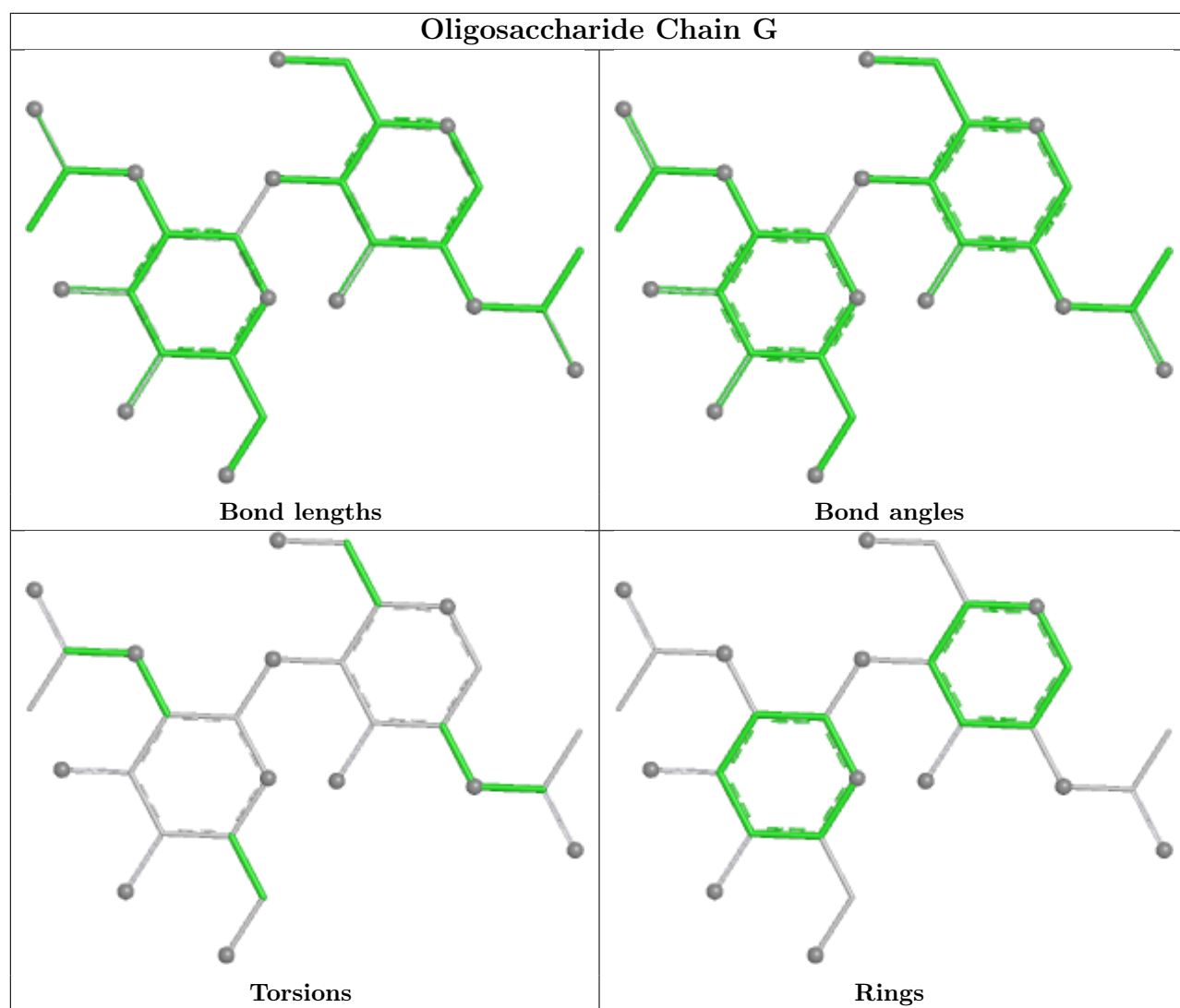
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1	NAG	1	0
3	H	2	NAG	1	0
3	R	1	NAG	1	0
3	N	1	NAG	1	0
3	M	1	NAG	2	0

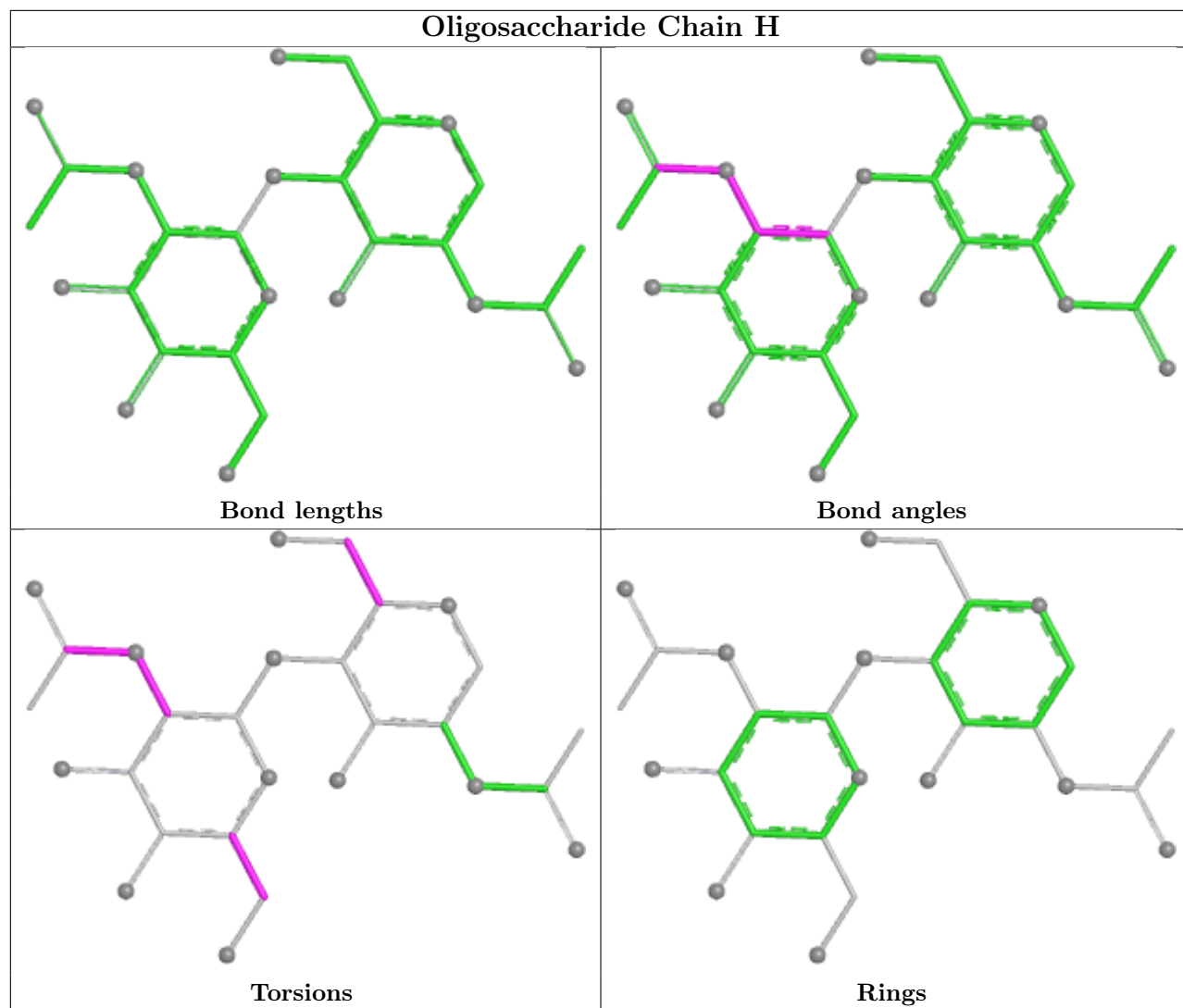
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

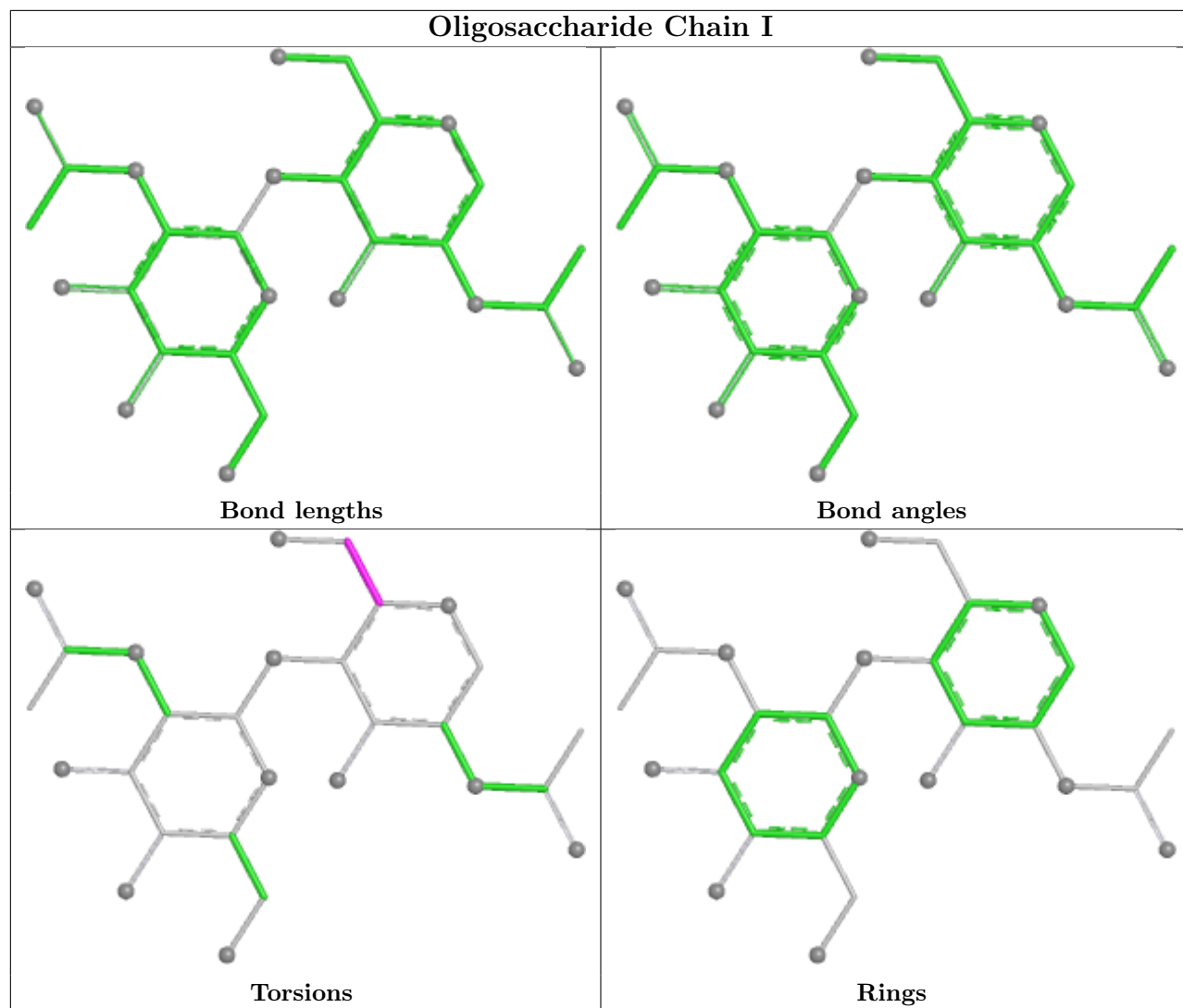


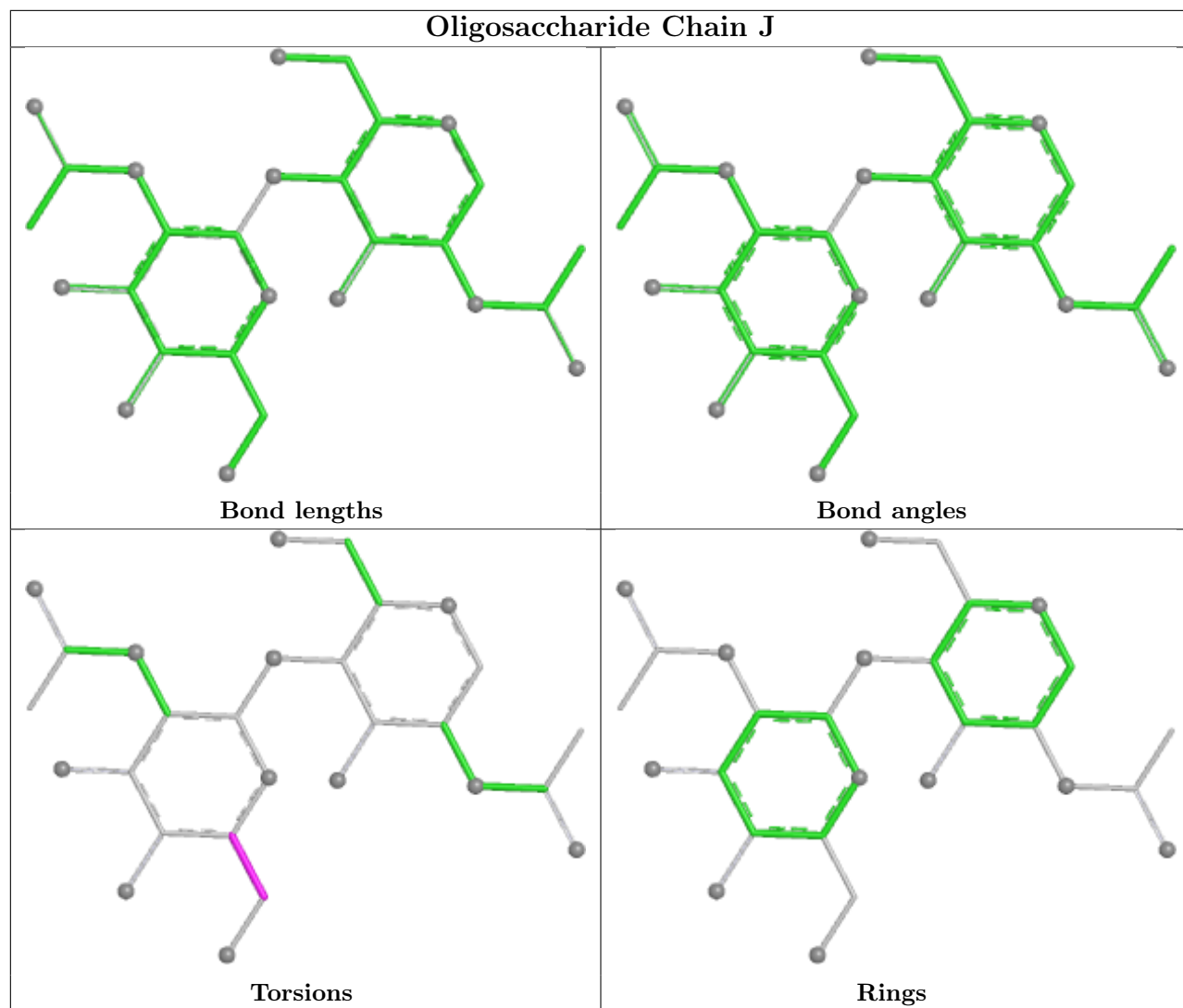


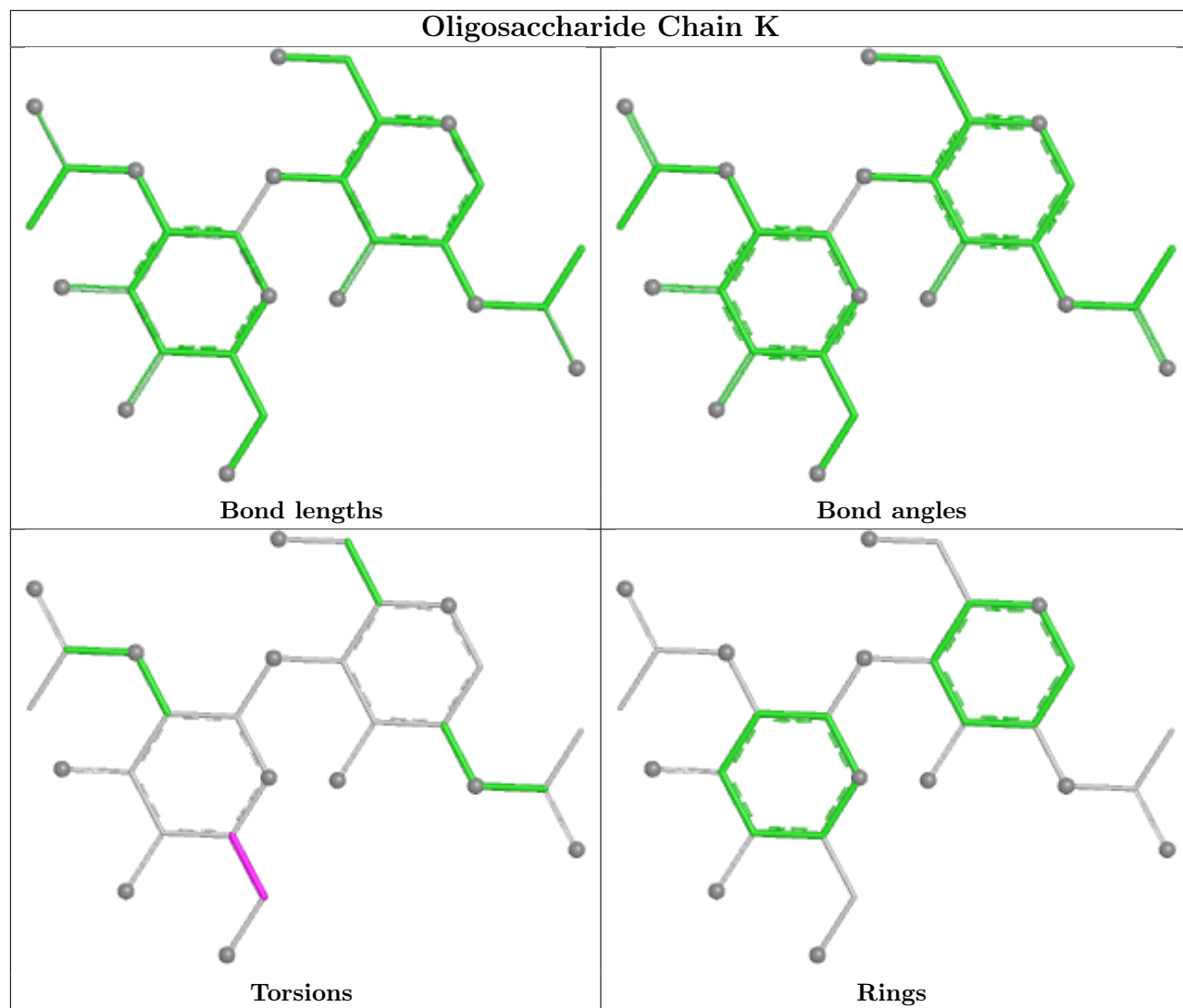


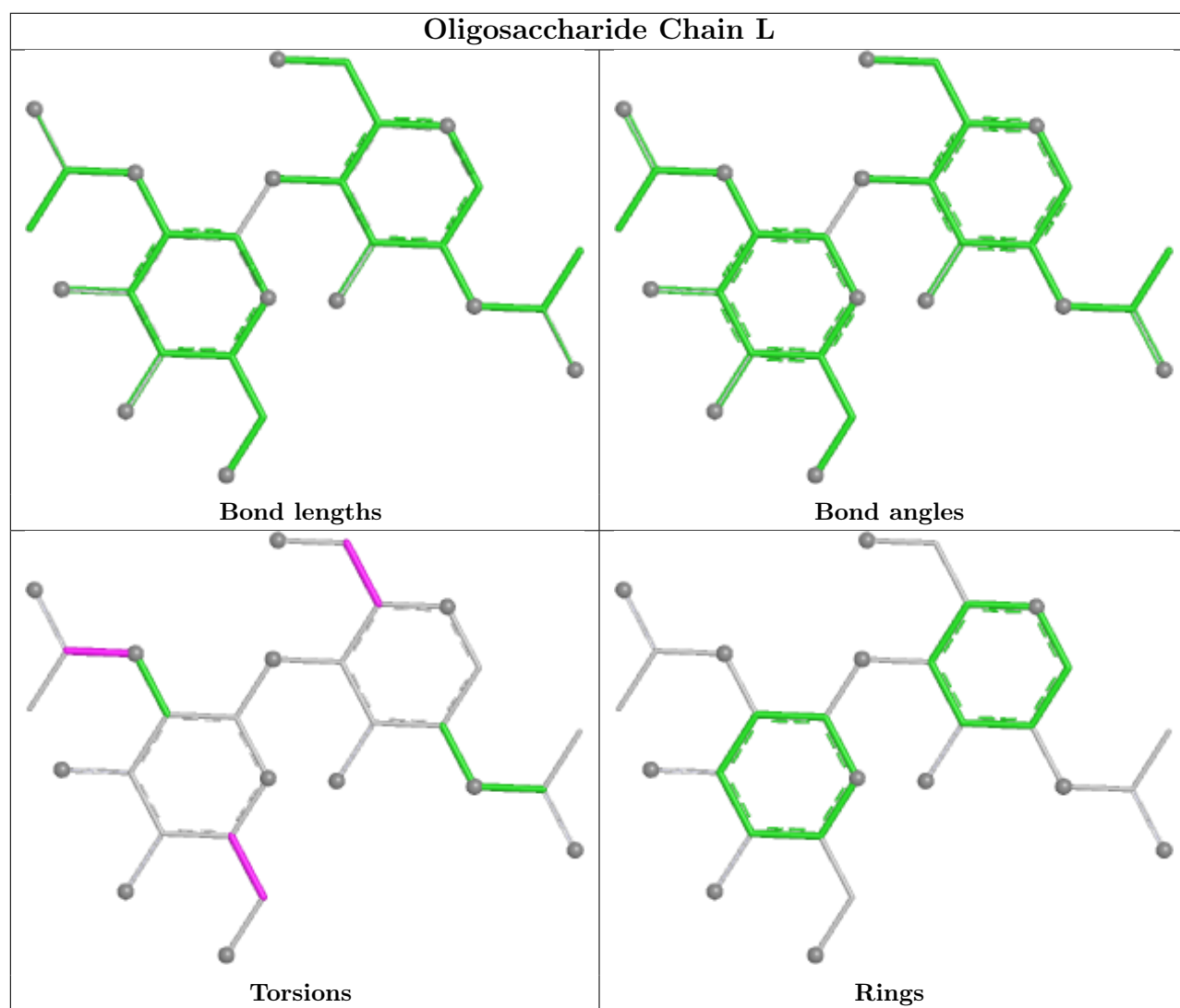


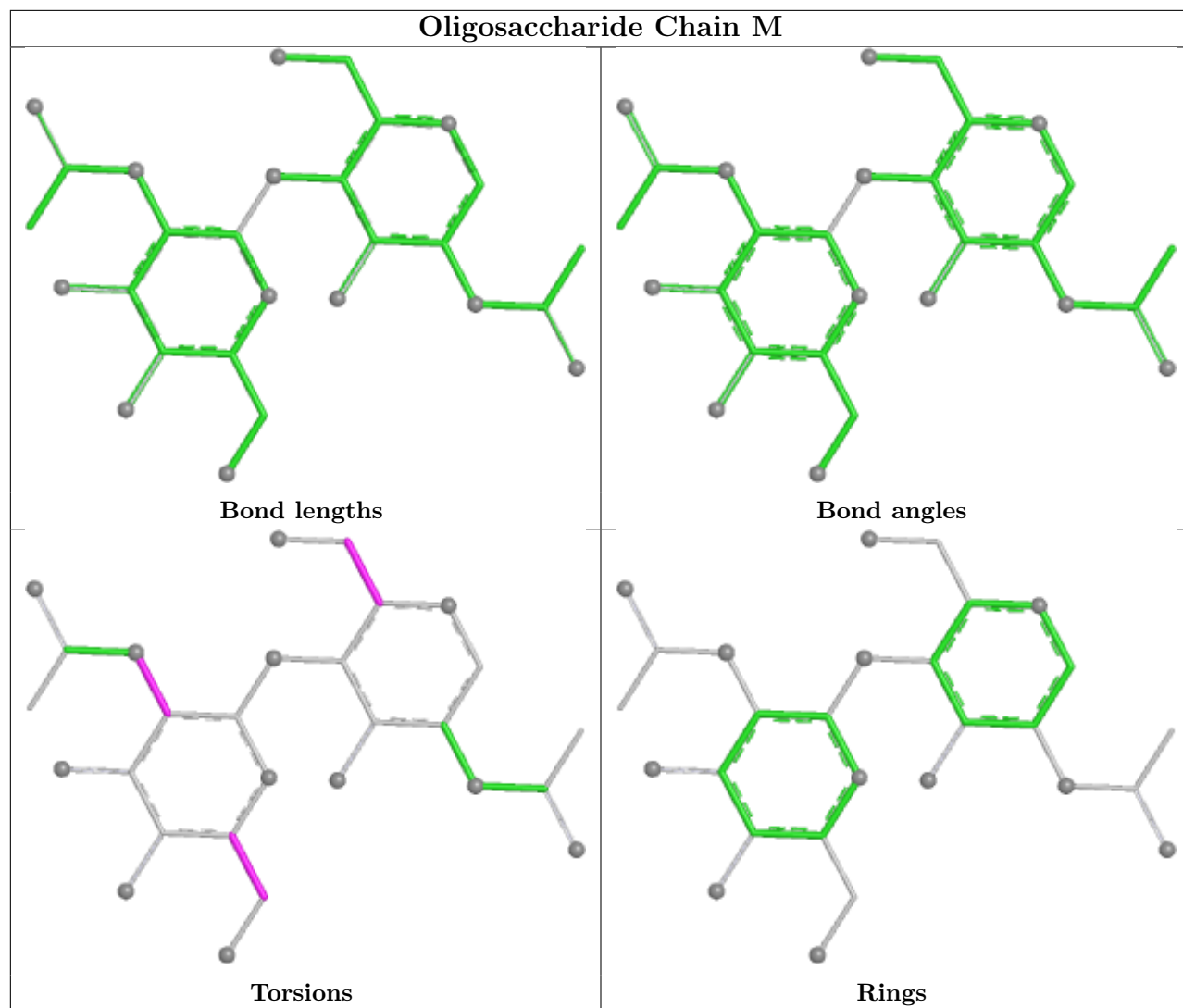




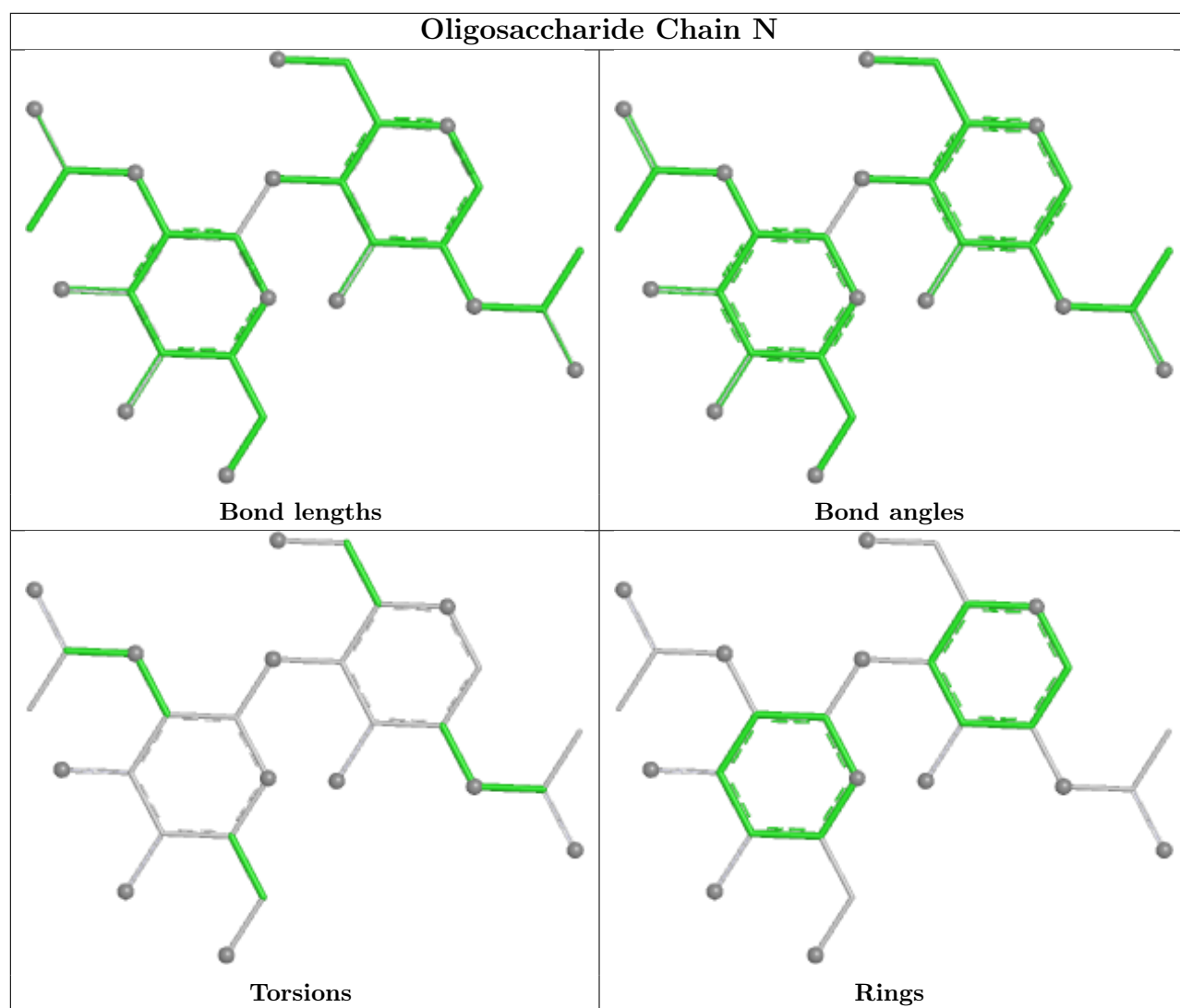


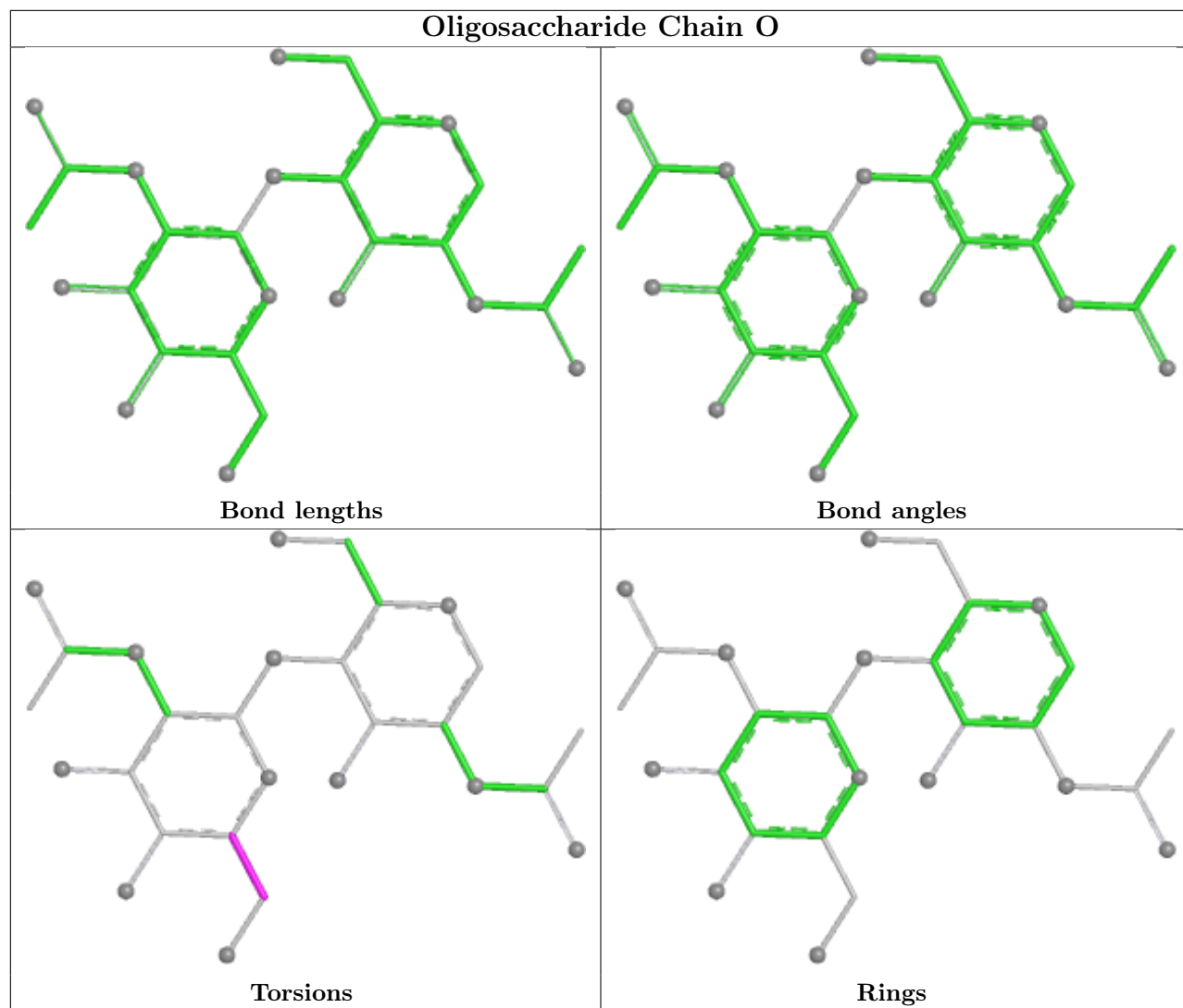


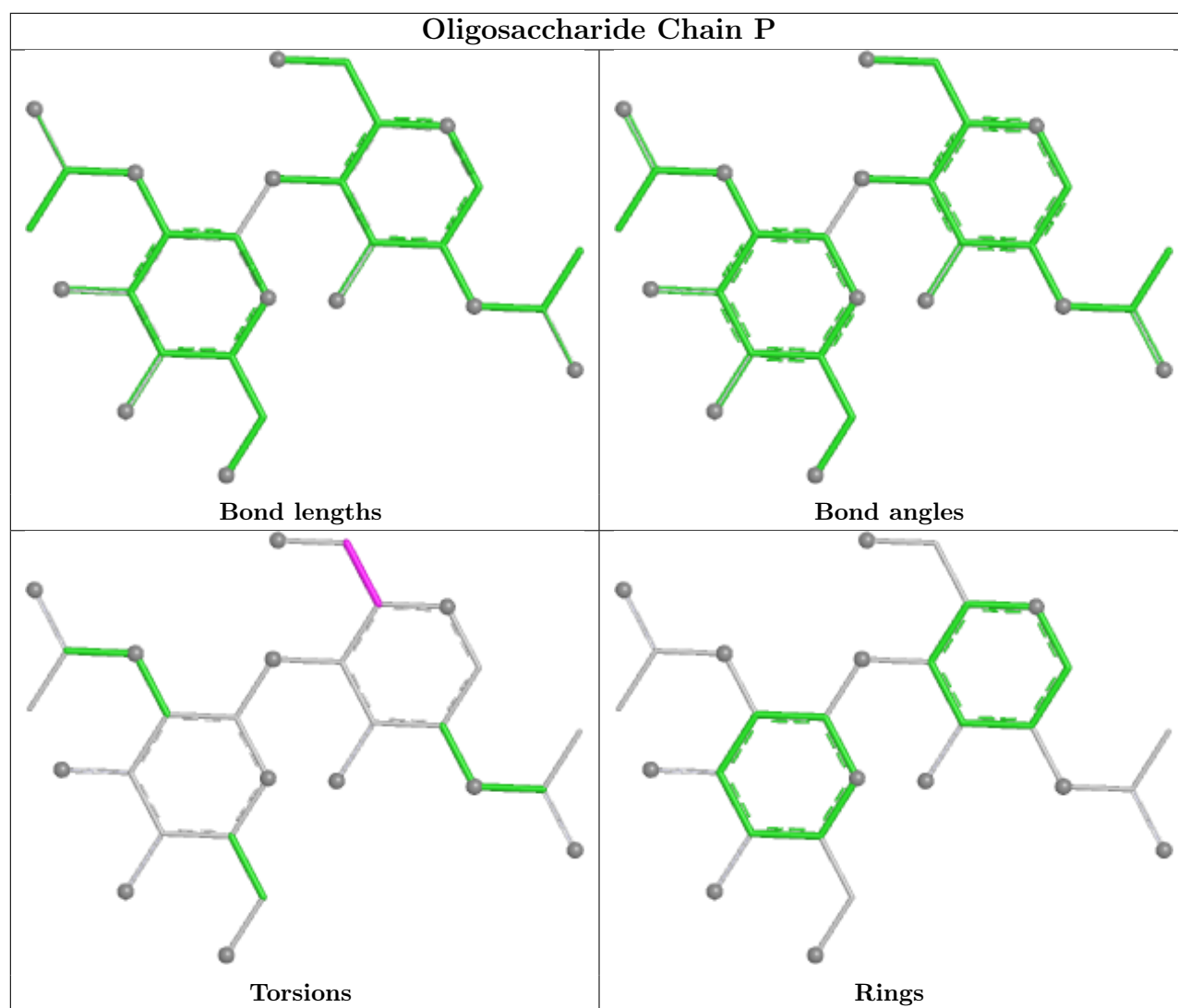


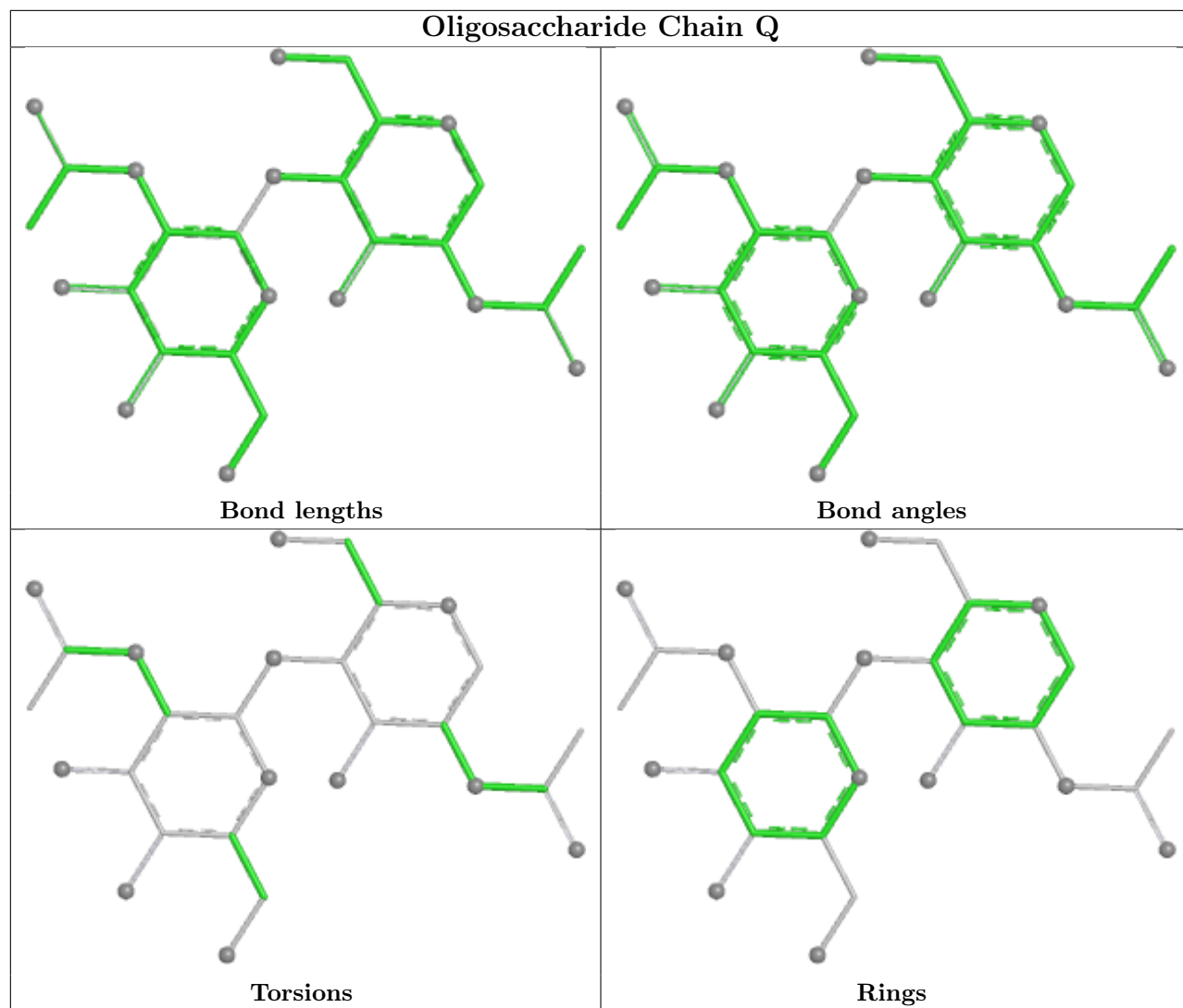


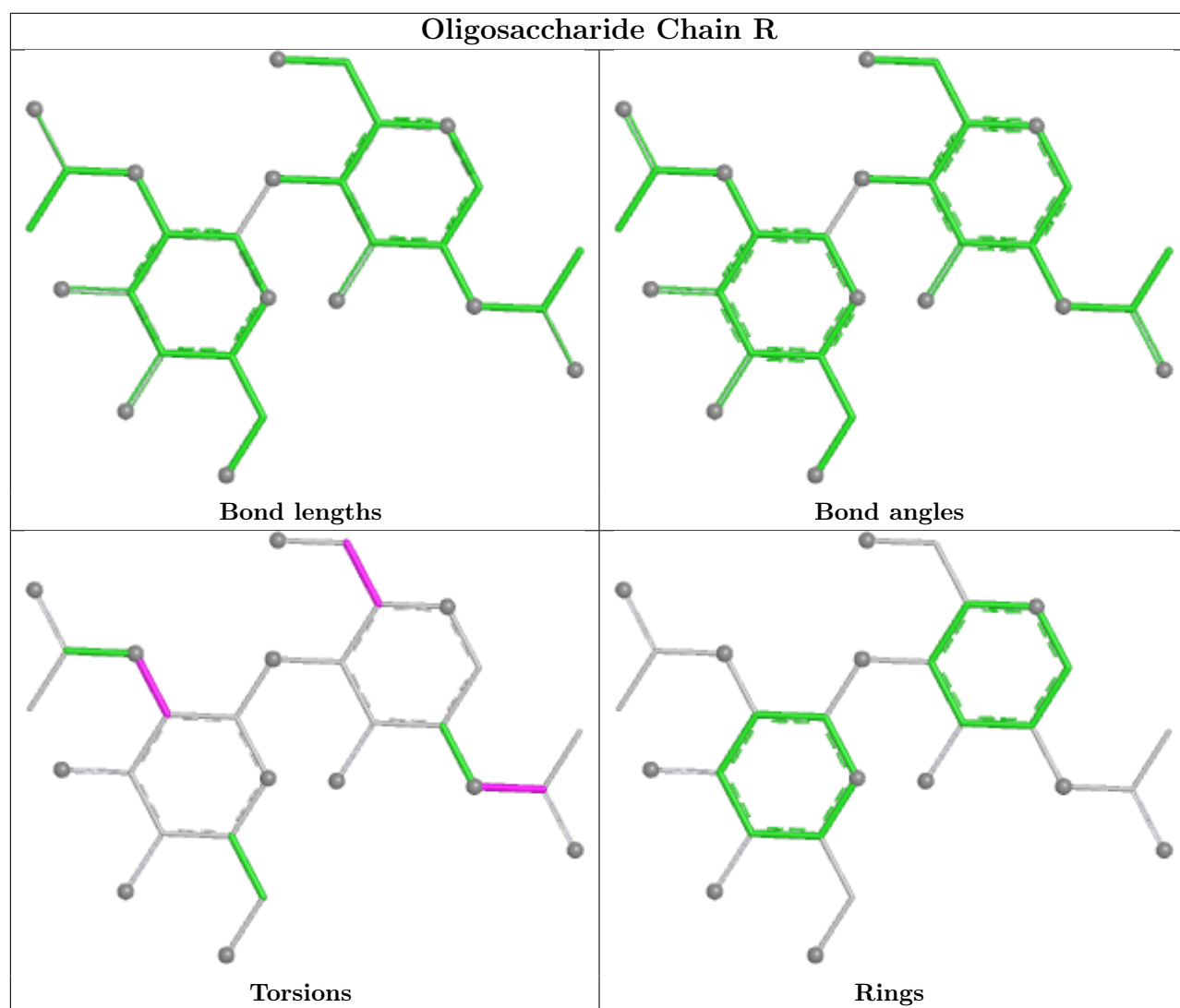


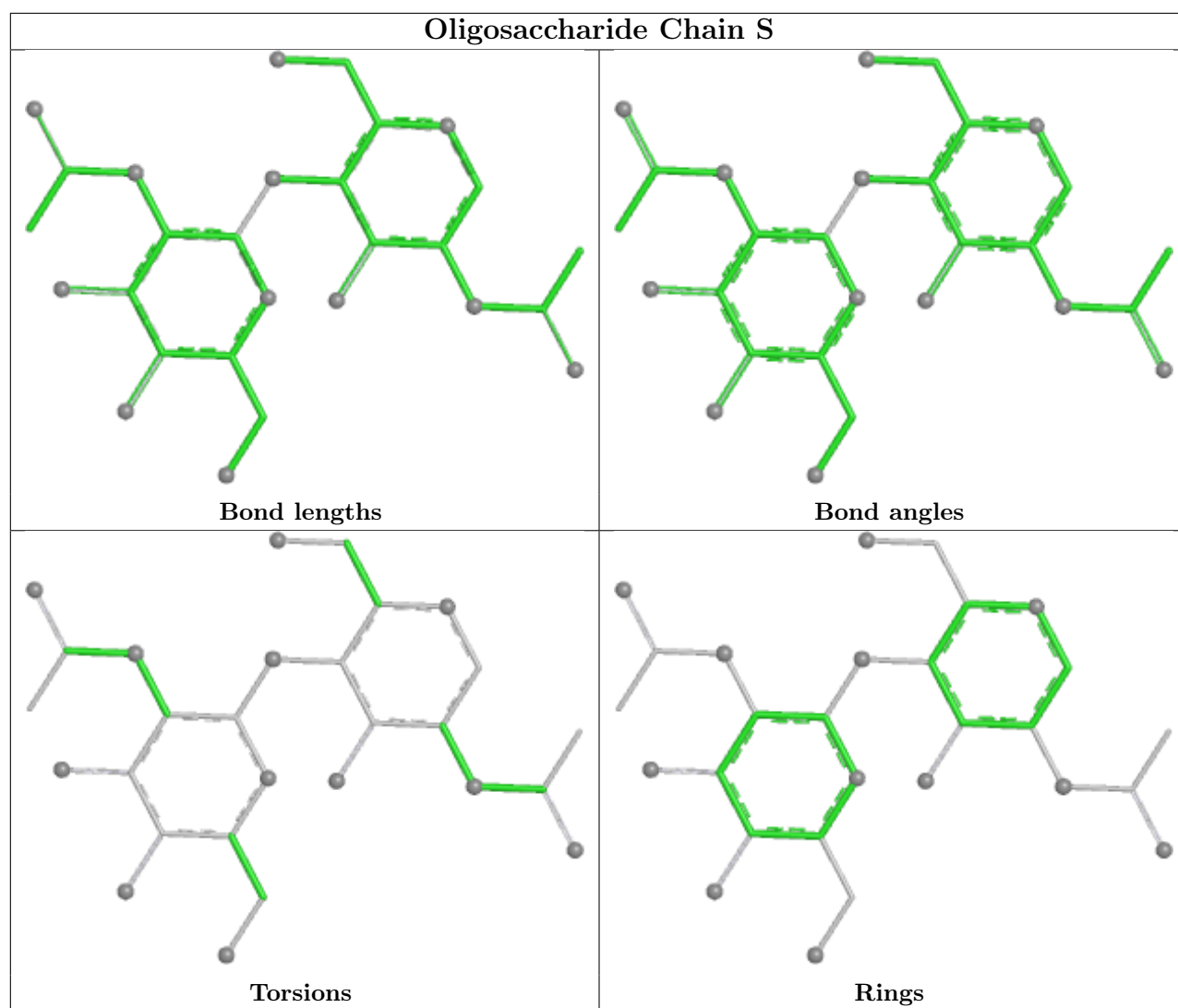


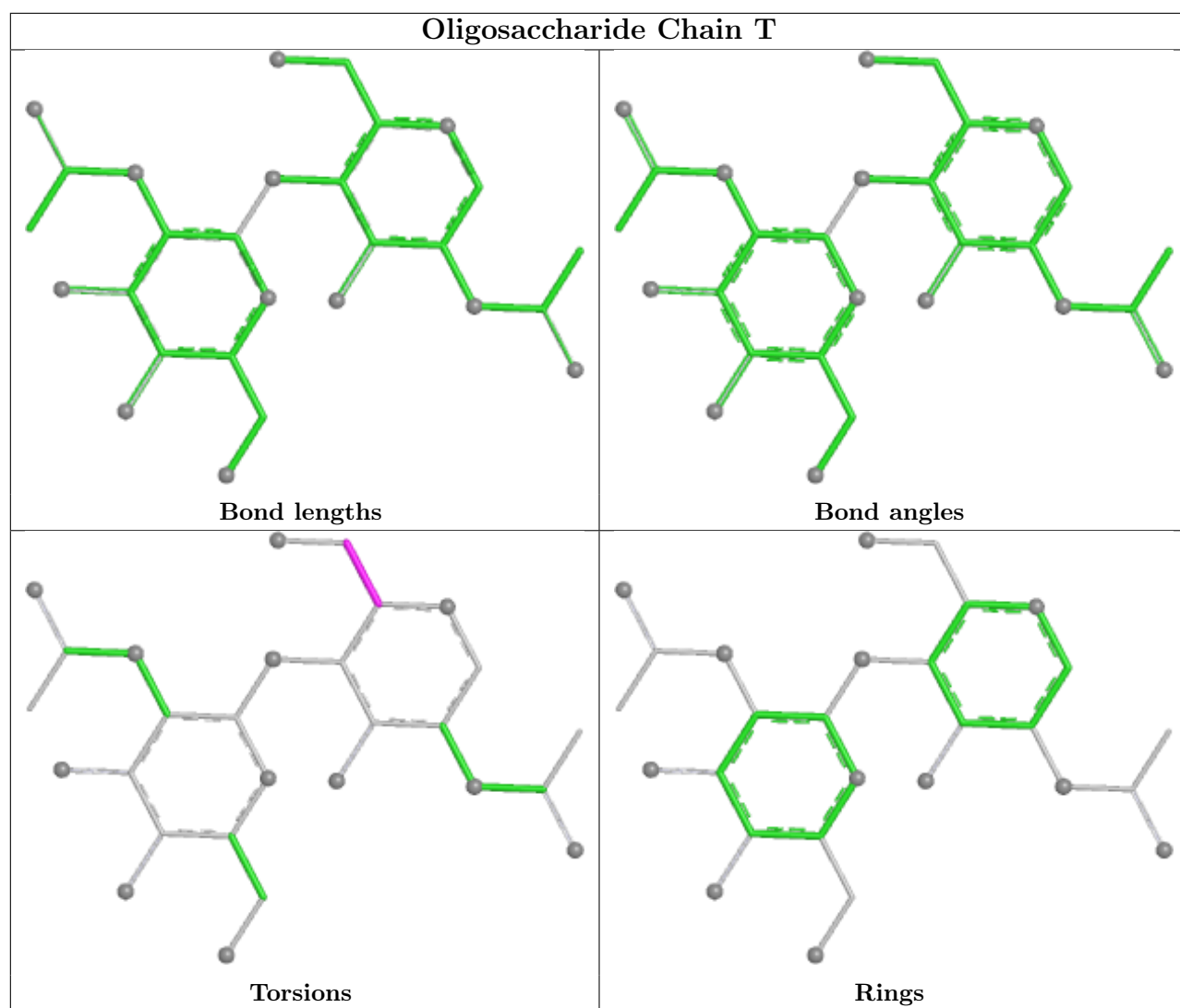


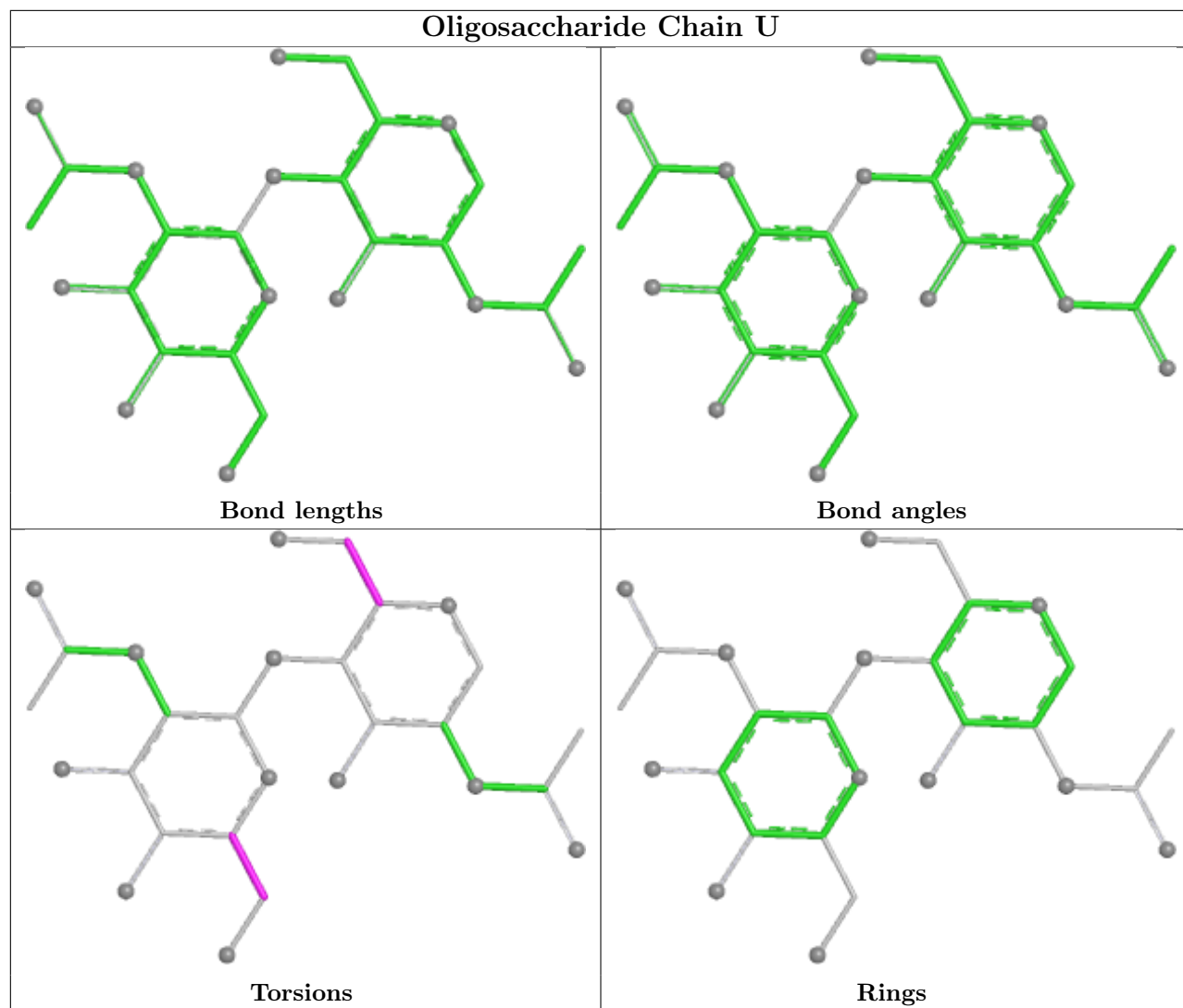




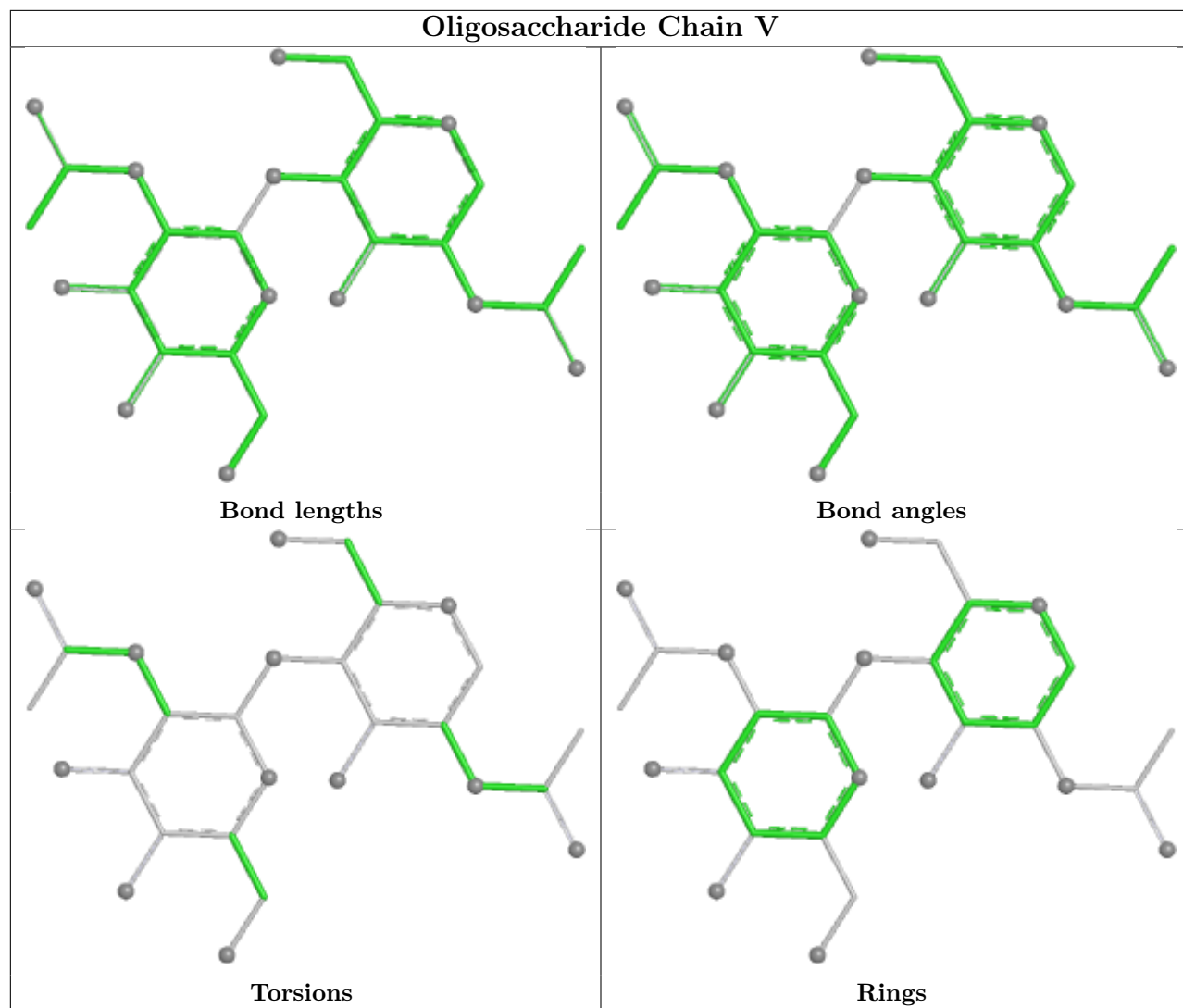


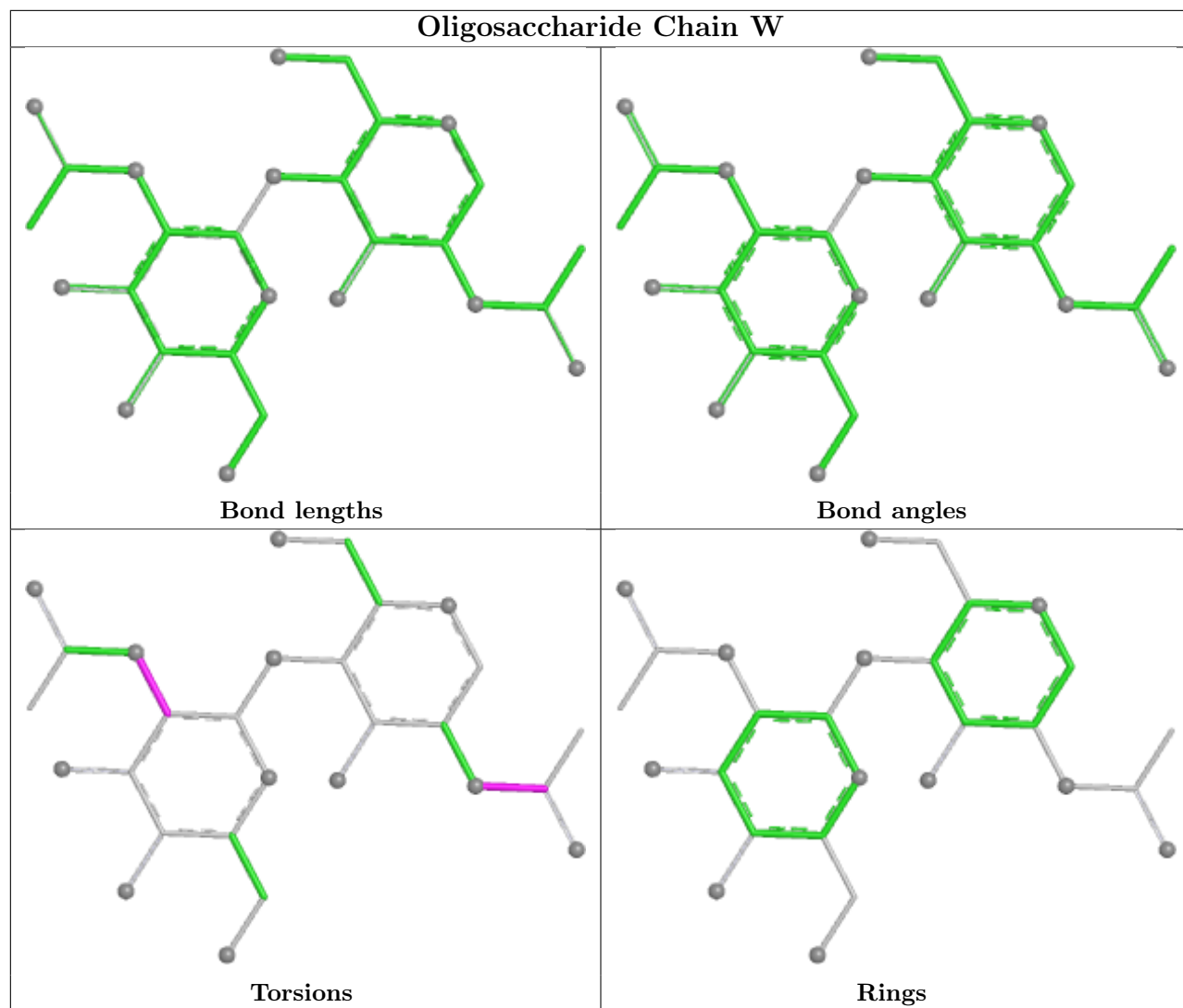


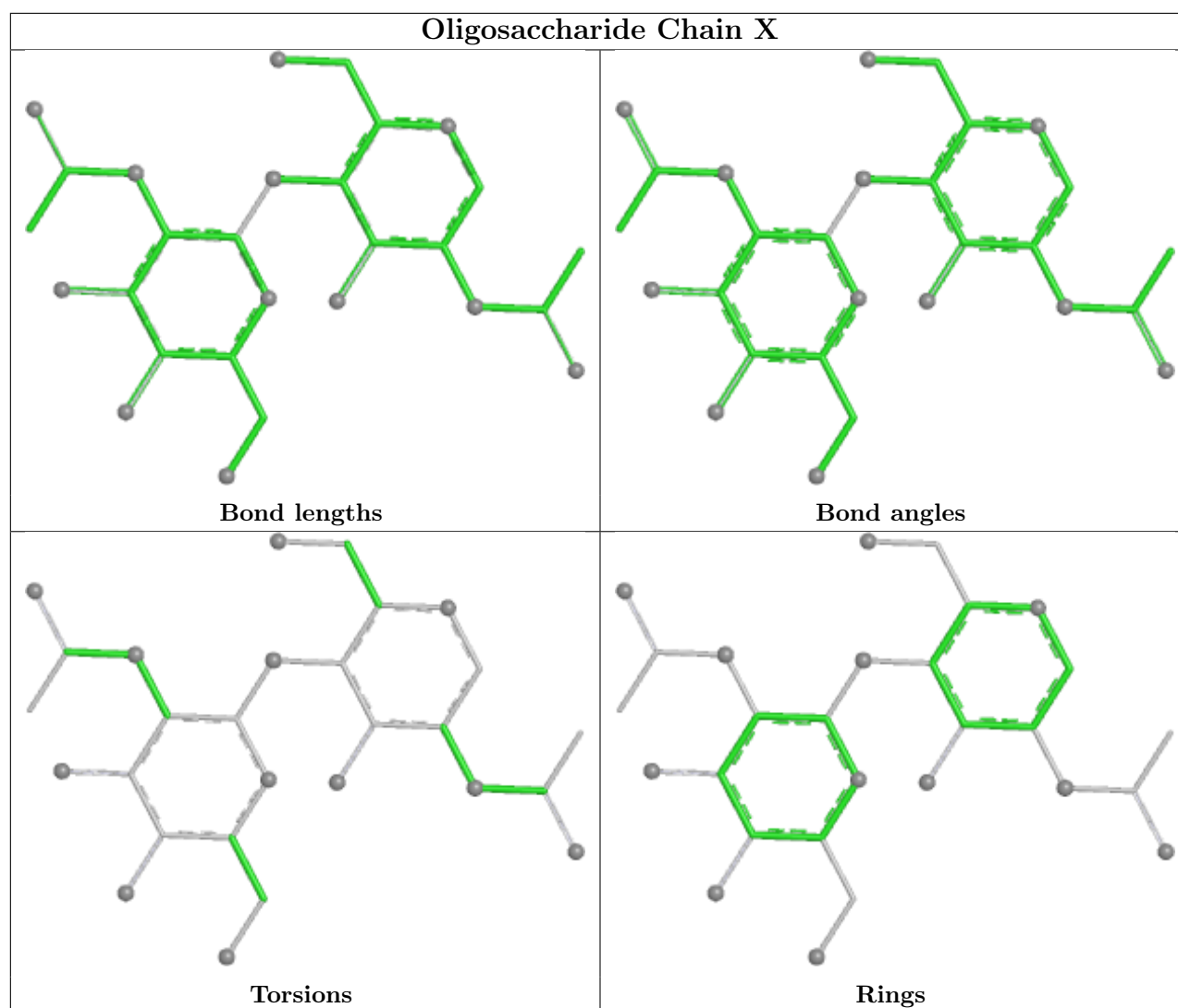












## 5.6 Ligand geometry [i](#)

15 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	A	1204	1	14,14,15	0.52	0	17,19,21	1.34	2 (11%)
4	NAG	A	1203	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	C	1201	1	14,14,15	0.24	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1202	2	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	B	1201	2	14,14,15	0.53	0	17,19,21	0.58	0
4	NAG	B	1202	2	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	C	1203	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	C	1202	1	14,14,15	0.32	0	17,19,21	0.55	0
4	NAG	B	1204	2	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	A	1201	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	D	1204	2	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	D	1203	2	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	A	1202	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	B	1203	2	14,14,15	0.43	0	17,19,21	1.33	2 (11%)
4	NAG	D	1201	2	14,14,15	0.21	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	A	1204	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1202	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1201	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1202	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1203	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1202	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1204	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1204	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1203	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1203	2	-	6/6/23/26	0/1/1/1
4	NAG	D	1201	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1203	NAG	C2-N2-C7	4.58	129.03	122.90
4	A	1204	NAG	C2-N2-C7	4.57	129.02	122.90
4	A	1204	NAG	C1-C2-N2	2.29	114.04	110.43
4	B	1203	NAG	C1-C2-N2	2.20	113.89	110.43

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1203	NAG	O5-C5-C6-O6
4	B	1201	NAG	O5-C5-C6-O6
4	A	1203	NAG	C4-C5-C6-O6
4	B	1202	NAG	C4-C5-C6-O6
4	B	1201	NAG	C4-C5-C6-O6
4	B	1202	NAG	O5-C5-C6-O6
4	A	1204	NAG	C8-C7-N2-C2
4	A	1204	NAG	O7-C7-N2-C2
4	B	1202	NAG	C8-C7-N2-C2
4	B	1202	NAG	O7-C7-N2-C2
4	B	1203	NAG	C8-C7-N2-C2
4	B	1203	NAG	O7-C7-N2-C2
4	B	1204	NAG	C8-C7-N2-C2
4	B	1204	NAG	O7-C7-N2-C2
4	D	1202	NAG	C8-C7-N2-C2
4	D	1202	NAG	O7-C7-N2-C2
4	D	1203	NAG	C8-C7-N2-C2
4	D	1203	NAG	O7-C7-N2-C2
4	C	1202	NAG	O5-C5-C6-O6
4	C	1202	NAG	C4-C5-C6-O6
4	A	1204	NAG	O5-C5-C6-O6
4	D	1204	NAG	C1-C2-N2-C7
4	D	1201	NAG	C4-C5-C6-O6
4	B	1201	NAG	C3-C2-N2-C7
4	C	1202	NAG	C3-C2-N2-C7
4	D	1204	NAG	C3-C2-N2-C7
4	A	1201	NAG	C1-C2-N2-C7
4	A	1204	NAG	C1-C2-N2-C7
4	B	1201	NAG	C1-C2-N2-C7
4	B	1203	NAG	C1-C2-N2-C7
4	C	1202	NAG	C1-C2-N2-C7
4	C	1203	NAG	C1-C2-N2-C7
4	B	1203	NAG	C4-C5-C6-O6
4	A	1204	NAG	C3-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

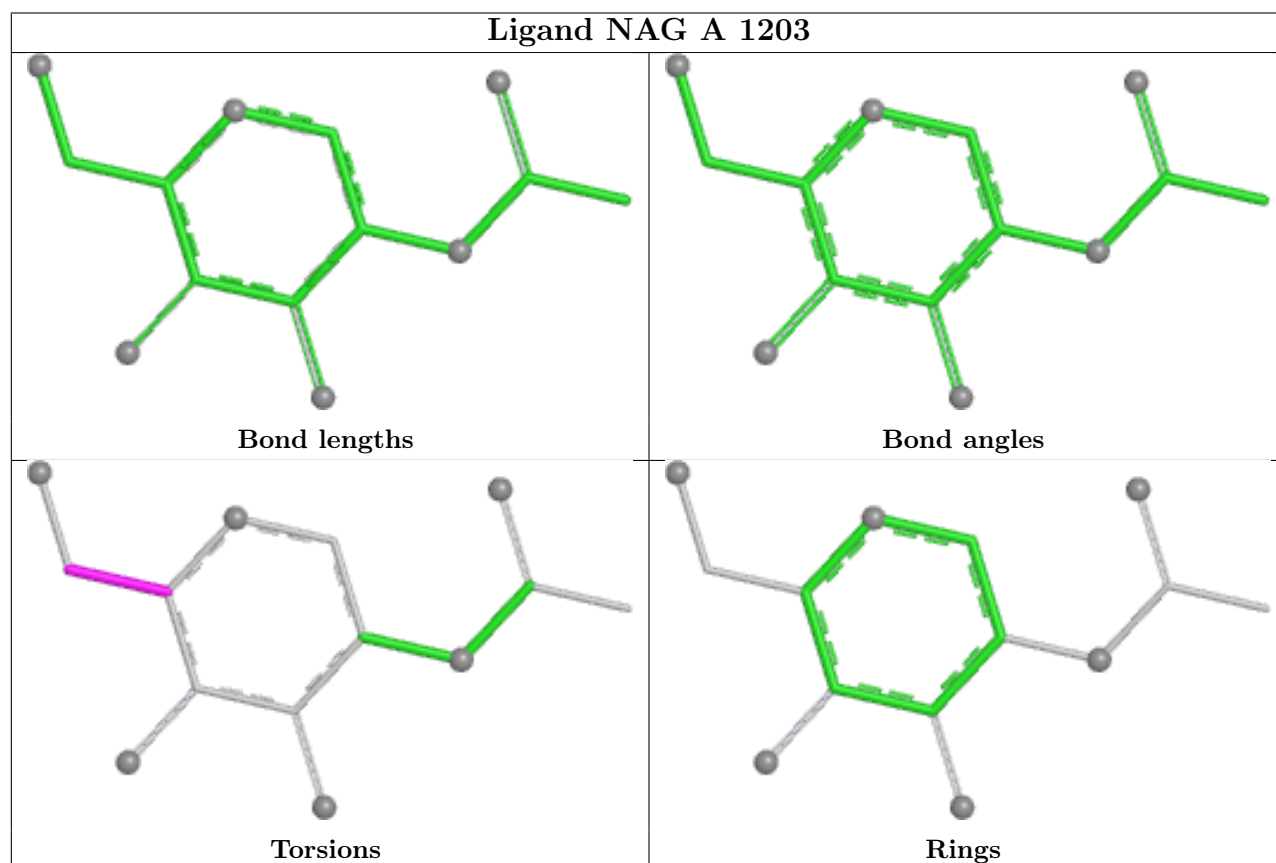
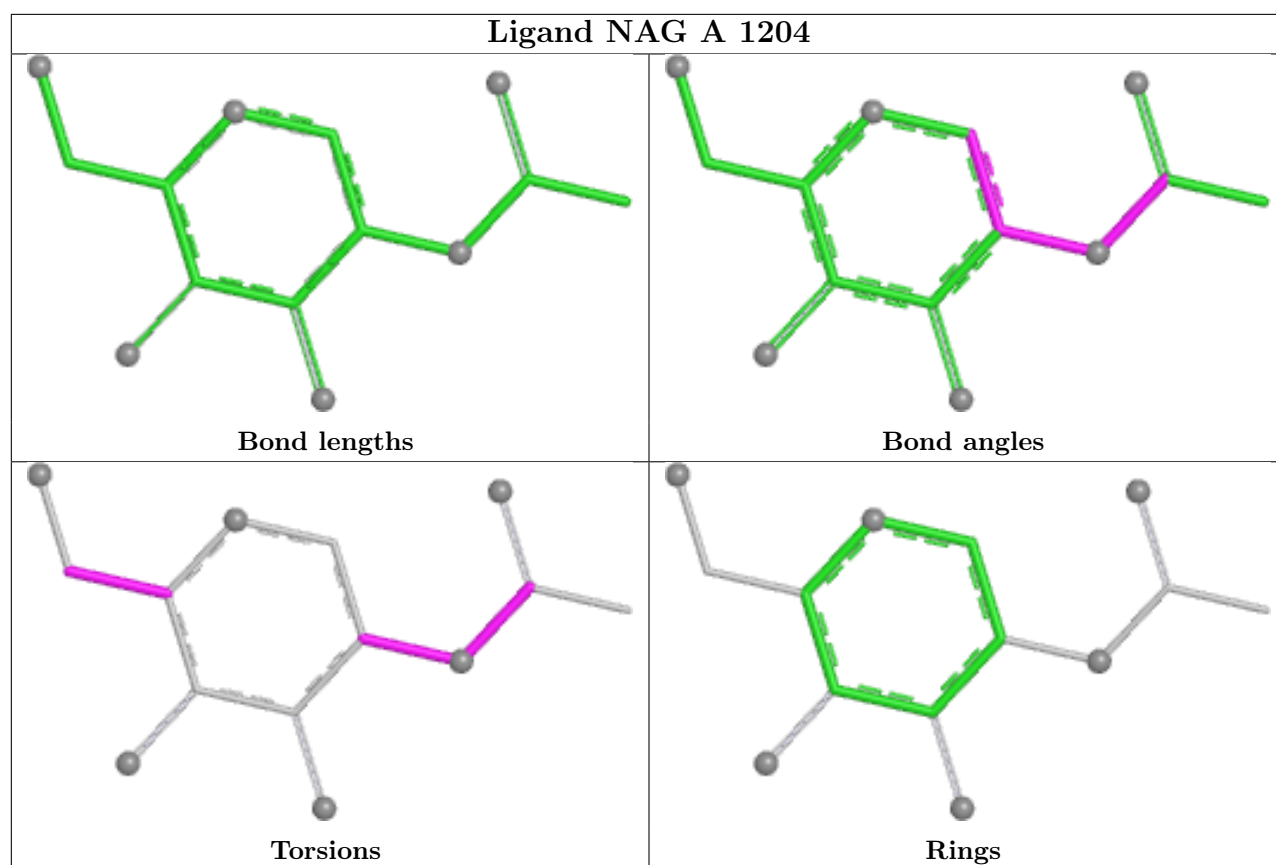
Mol	Chain	Res	Type	Atoms
4	B	1203	NAG	C3-C2-N2-C7
4	B	1203	NAG	O5-C5-C6-O6

There are no ring outliers.

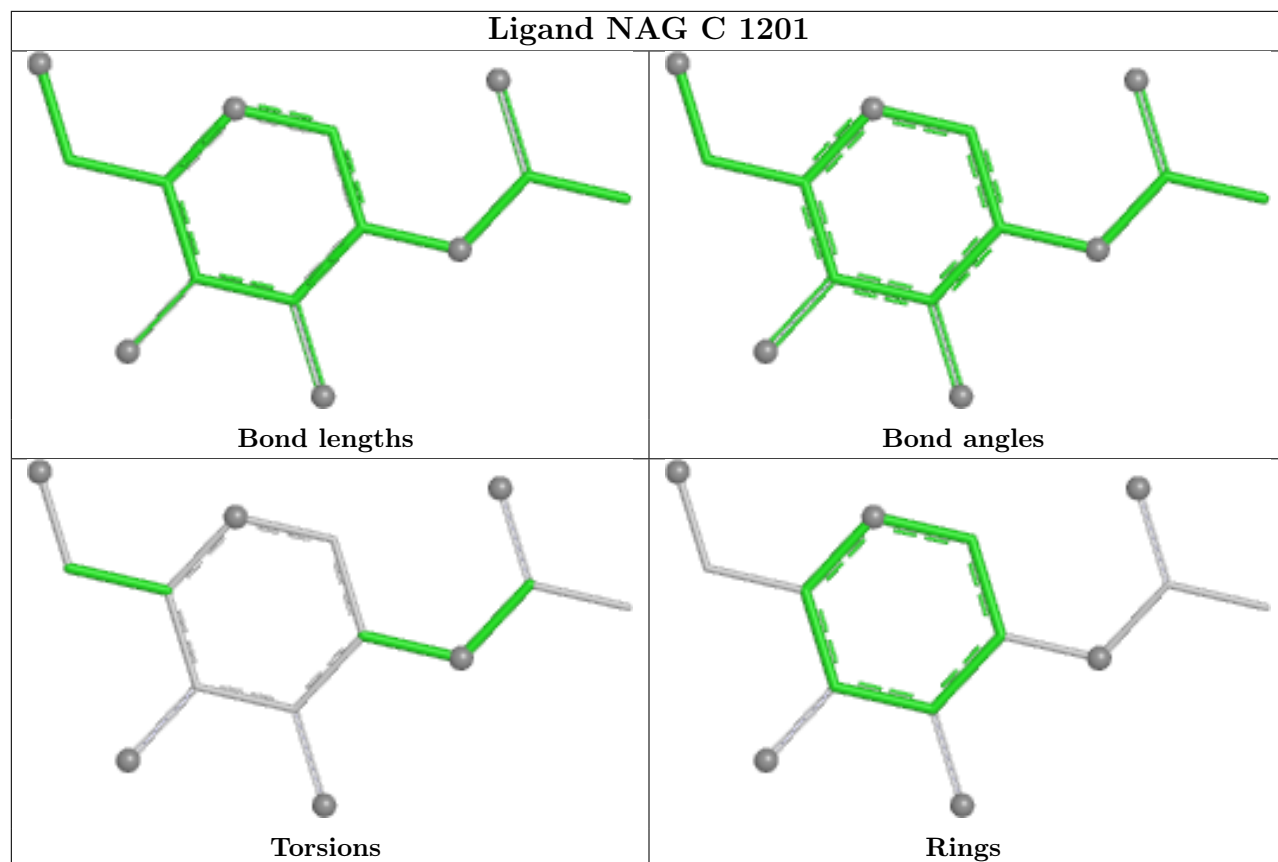
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1204	NAG	1	0
4	A	1203	NAG	1	0
4	C	1202	NAG	1	0
4	B	1203	NAG	1	0

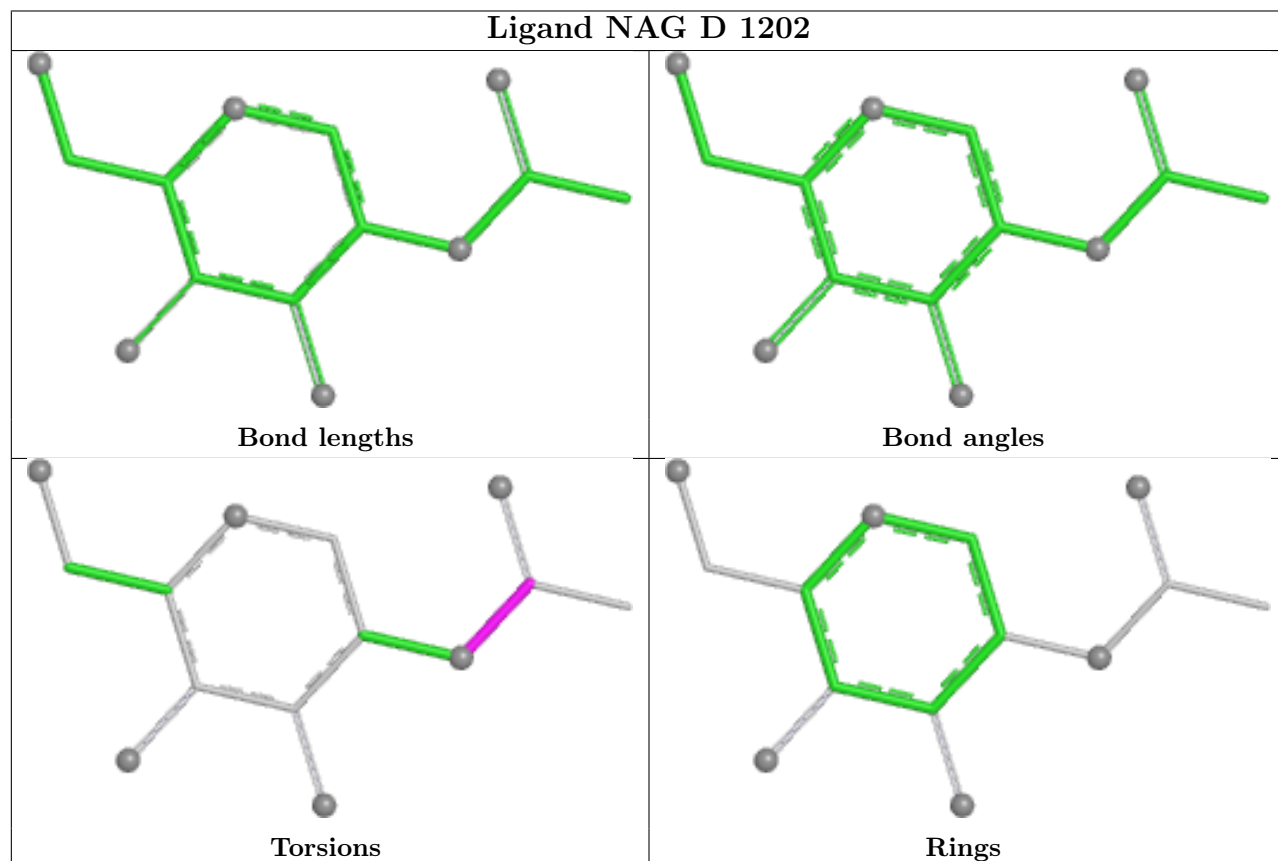
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand NAG C 1201

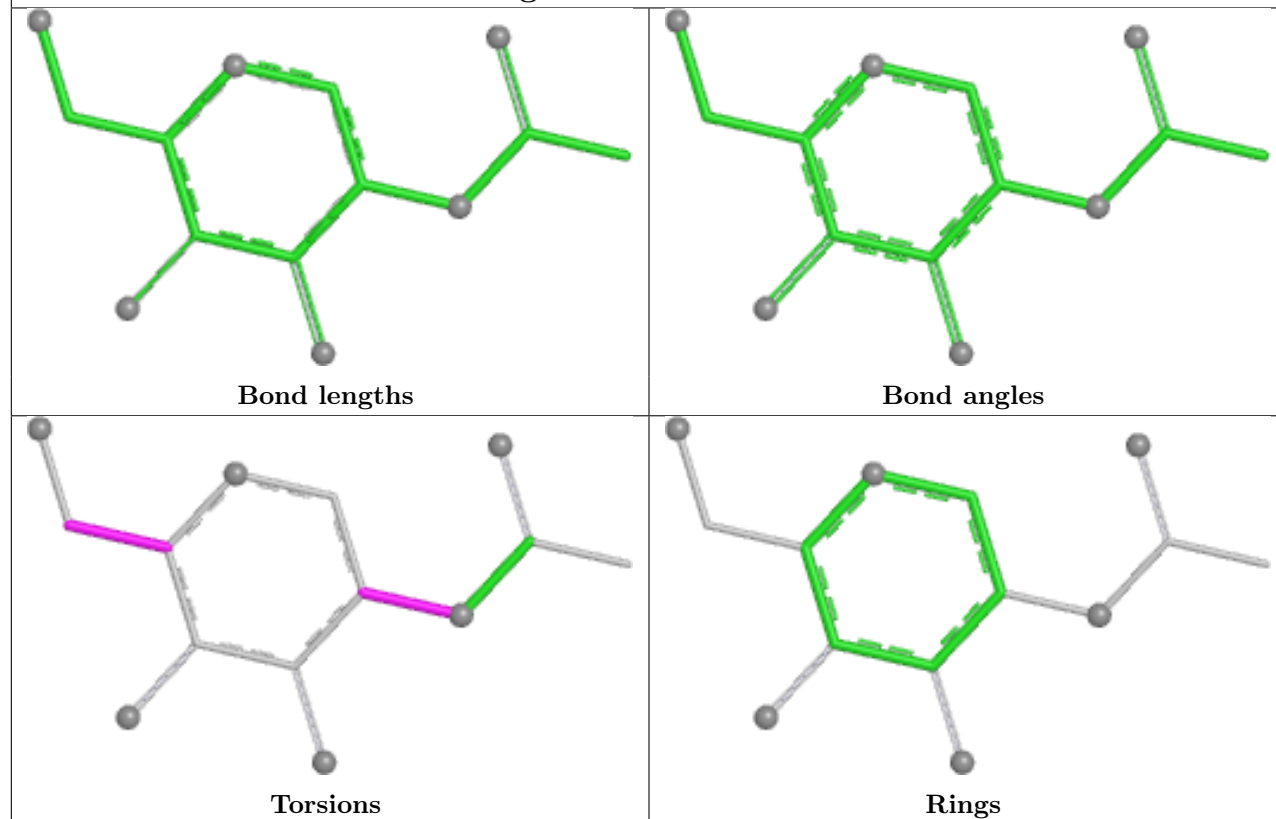


## Ligand NAG D 1202

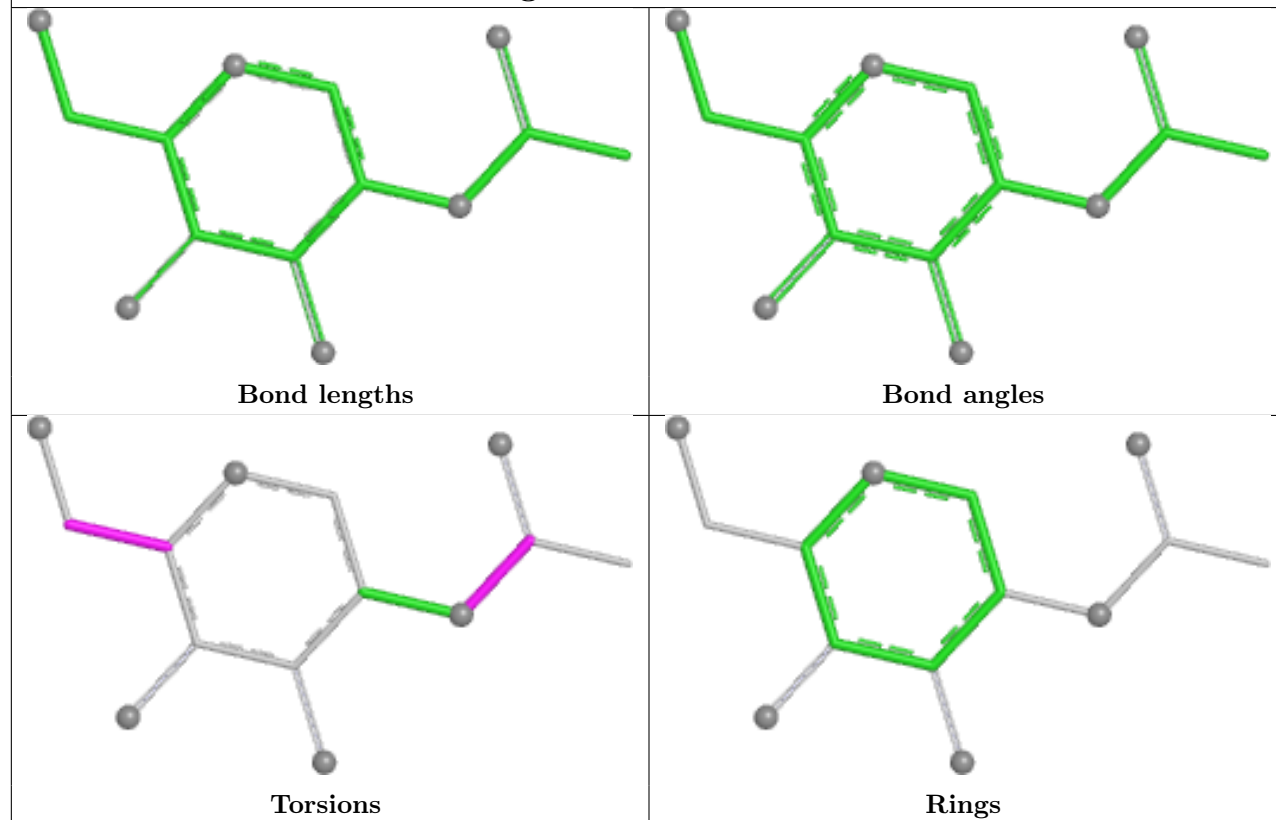




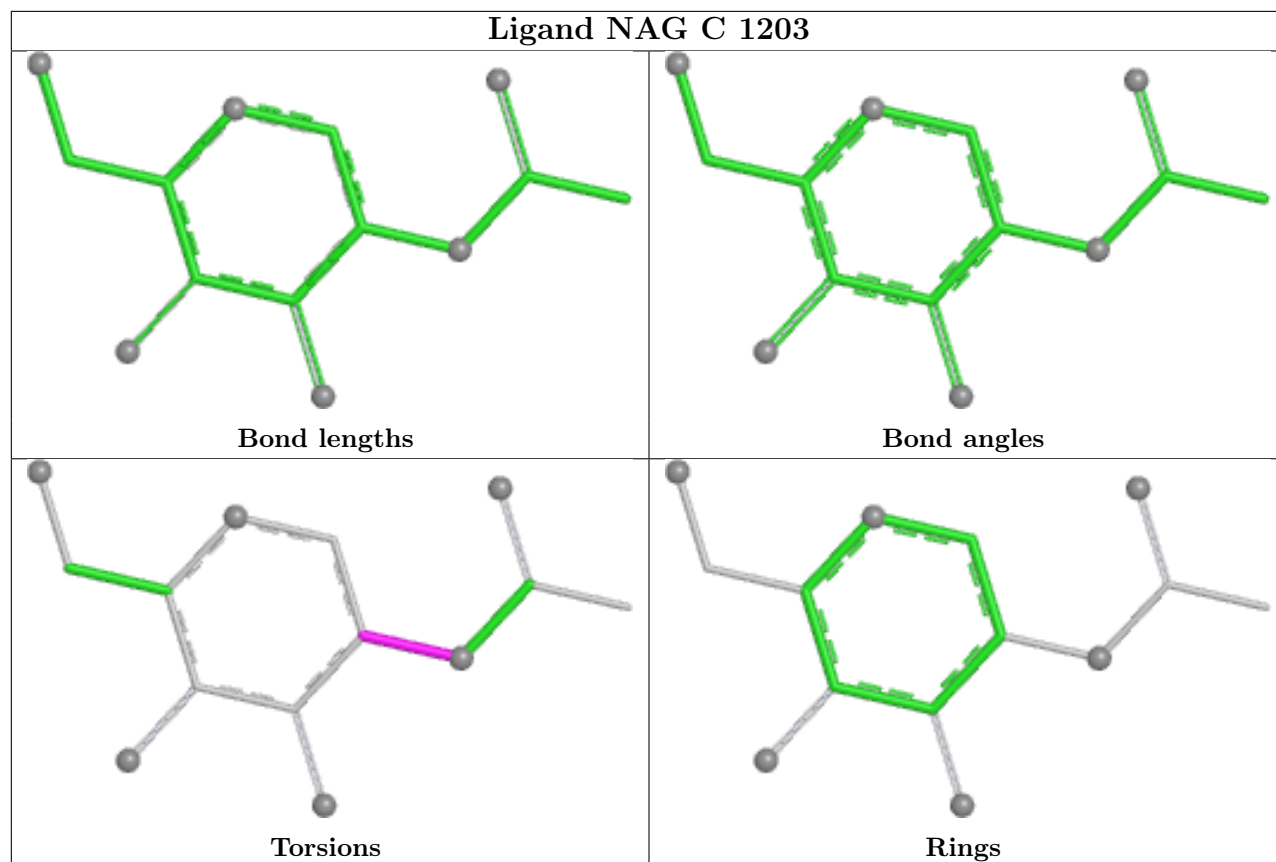
## Ligand NAG B 1201



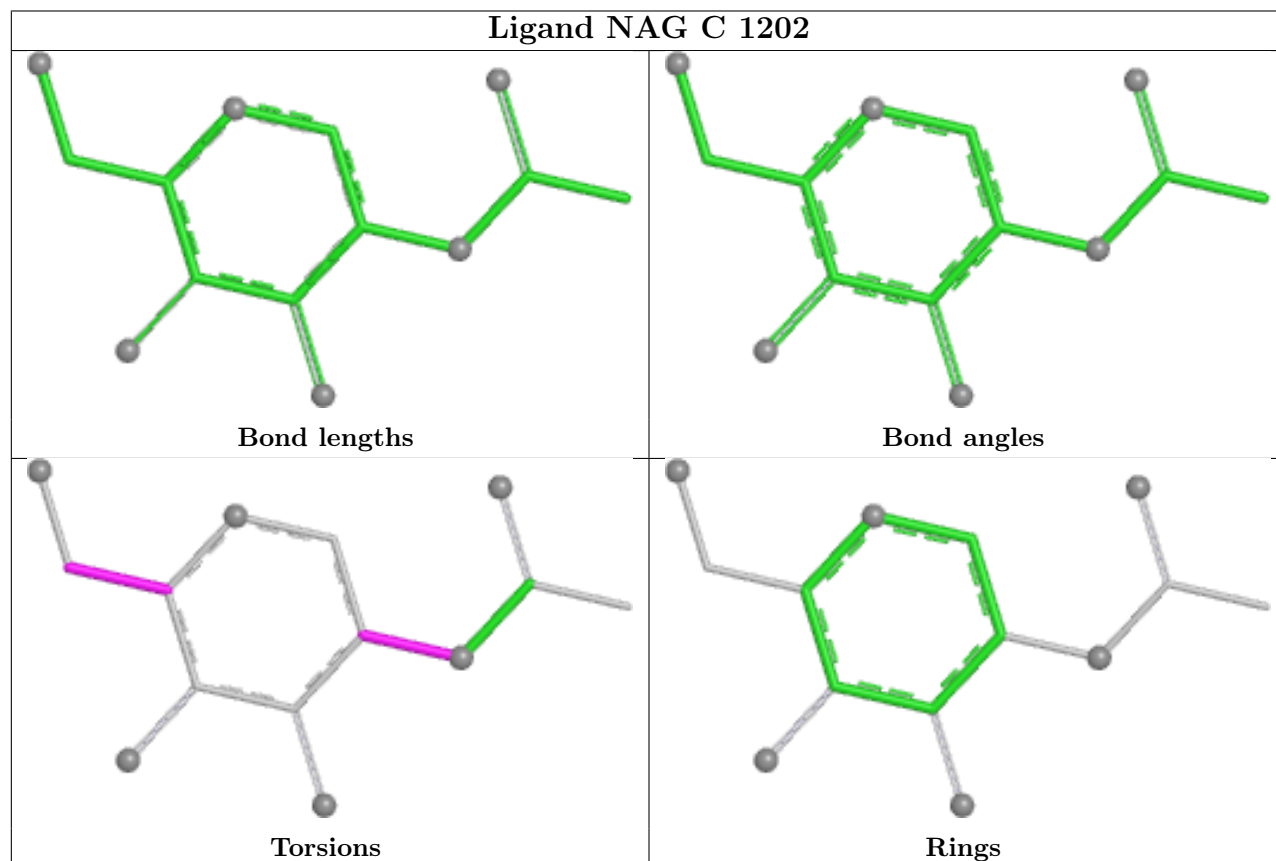
## Ligand NAG B 1202



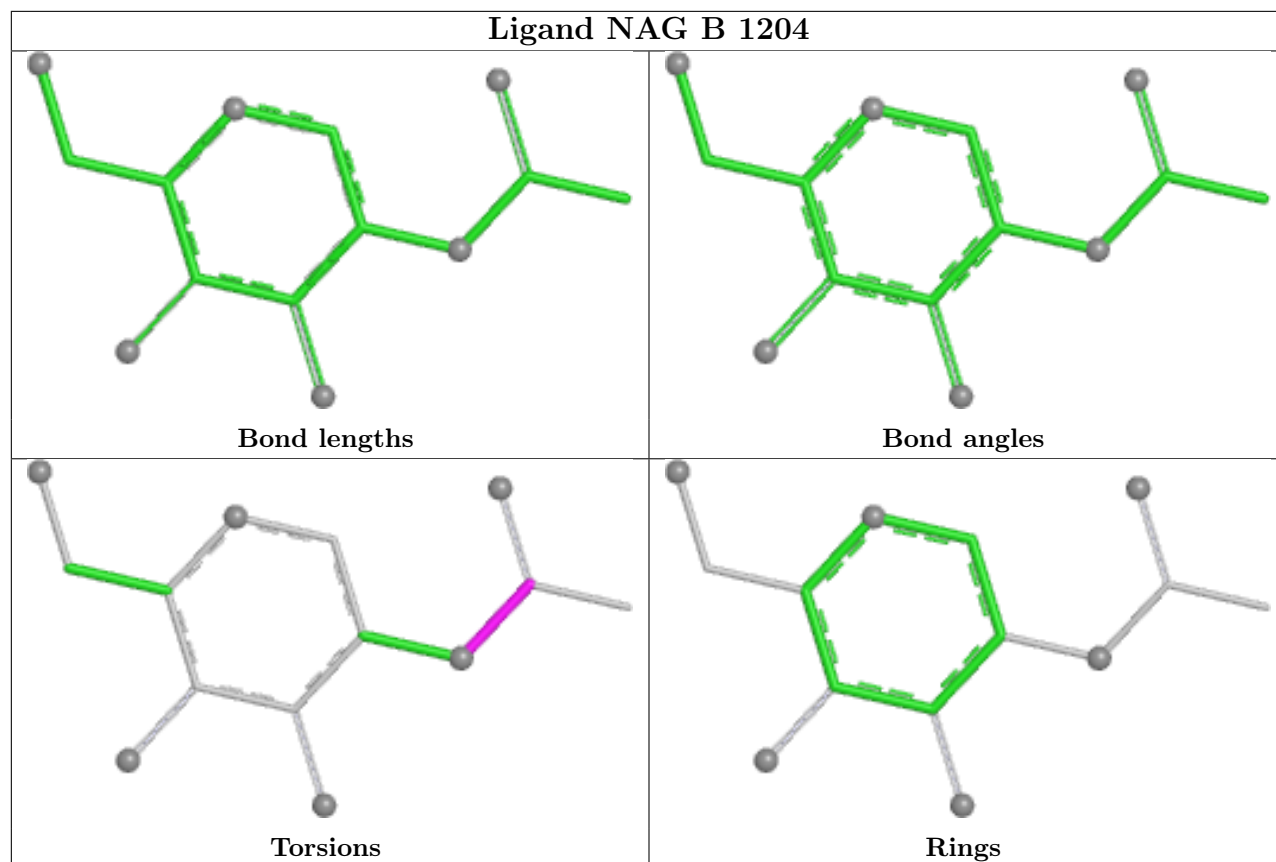
## Ligand NAG C 1203



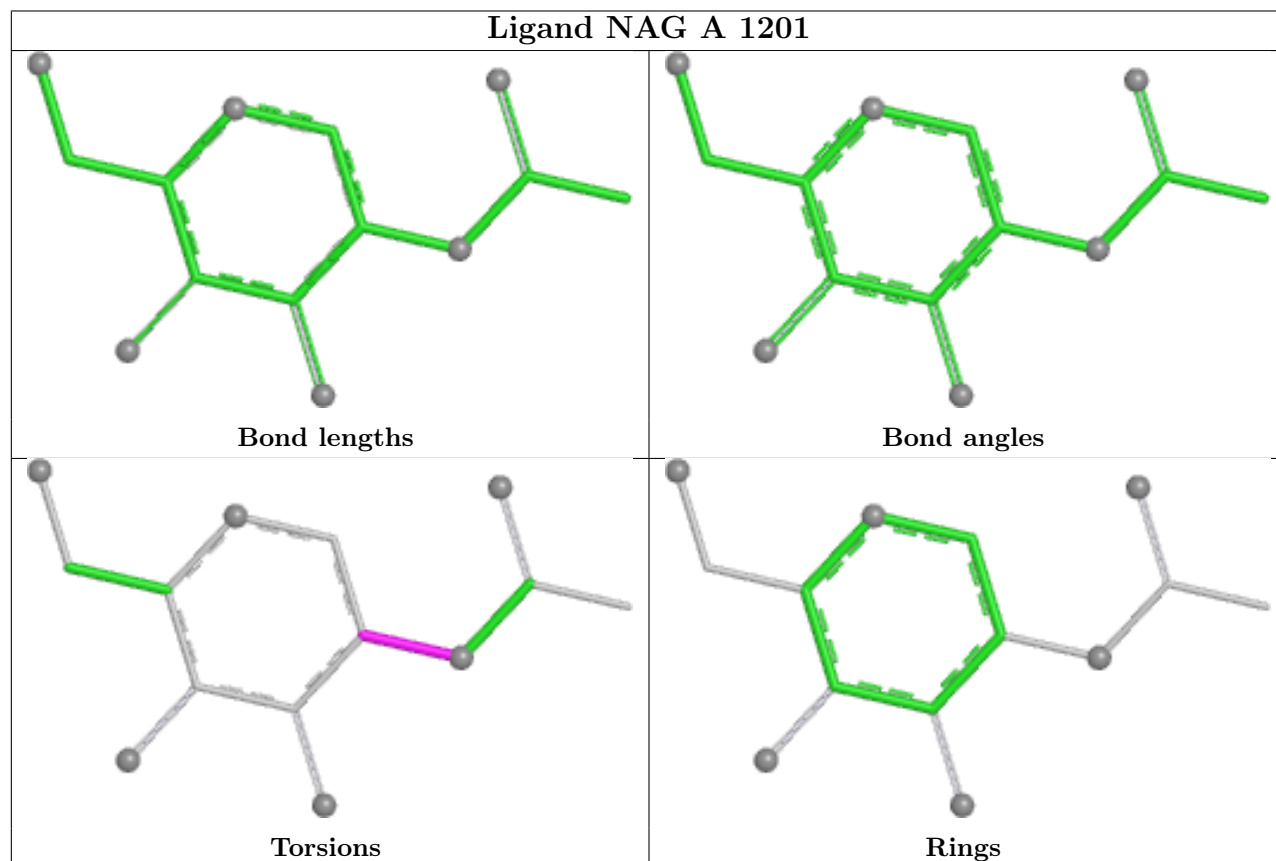
## Ligand NAG C 1202

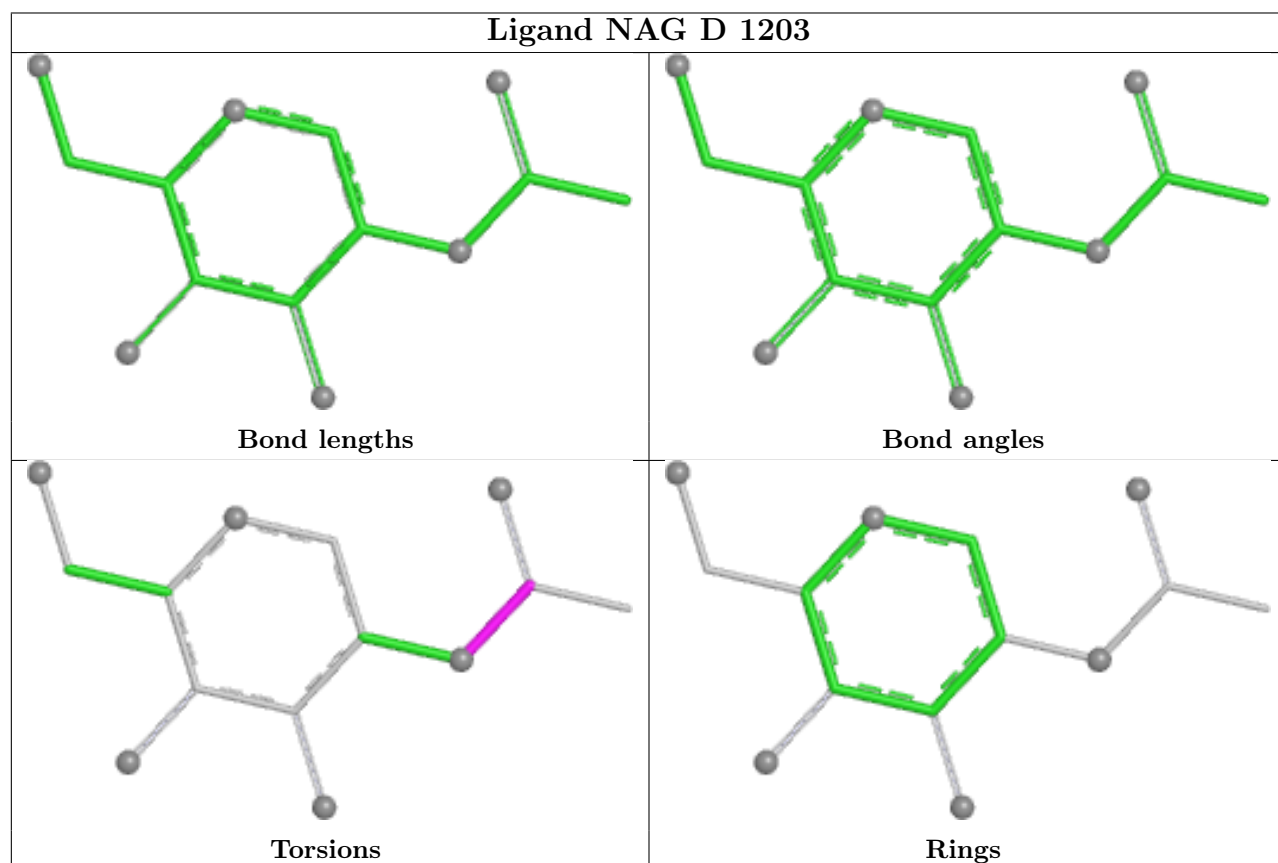
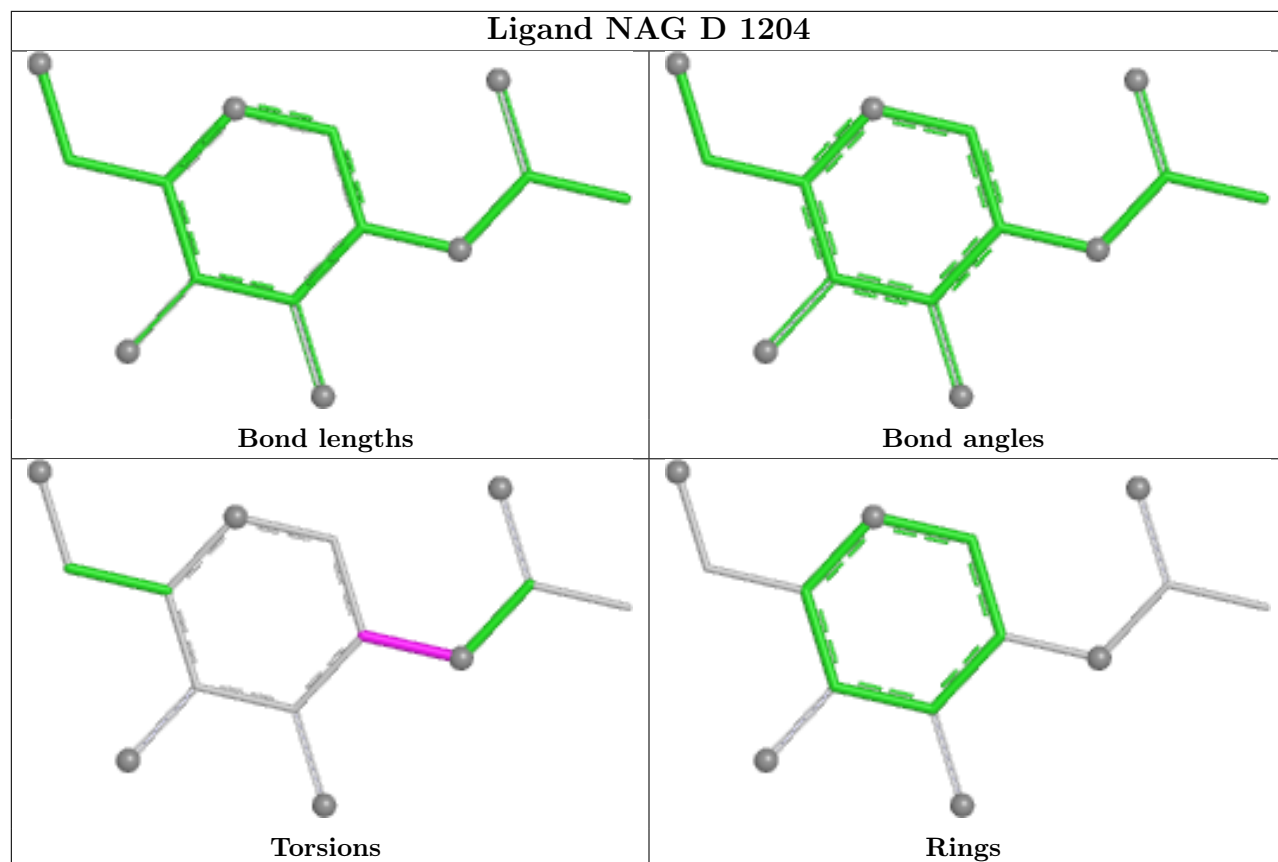


## Ligand NAG B 1204

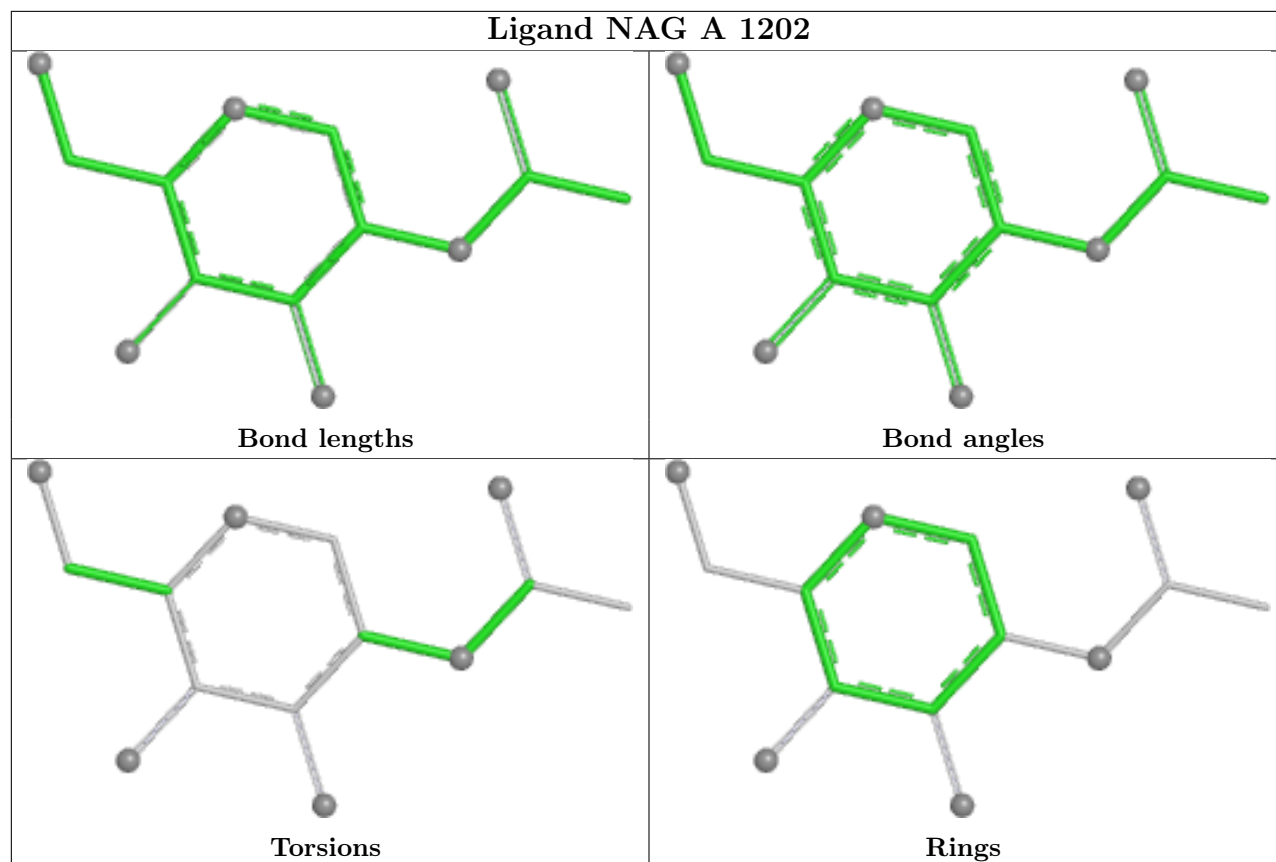


## Ligand NAG A 1201

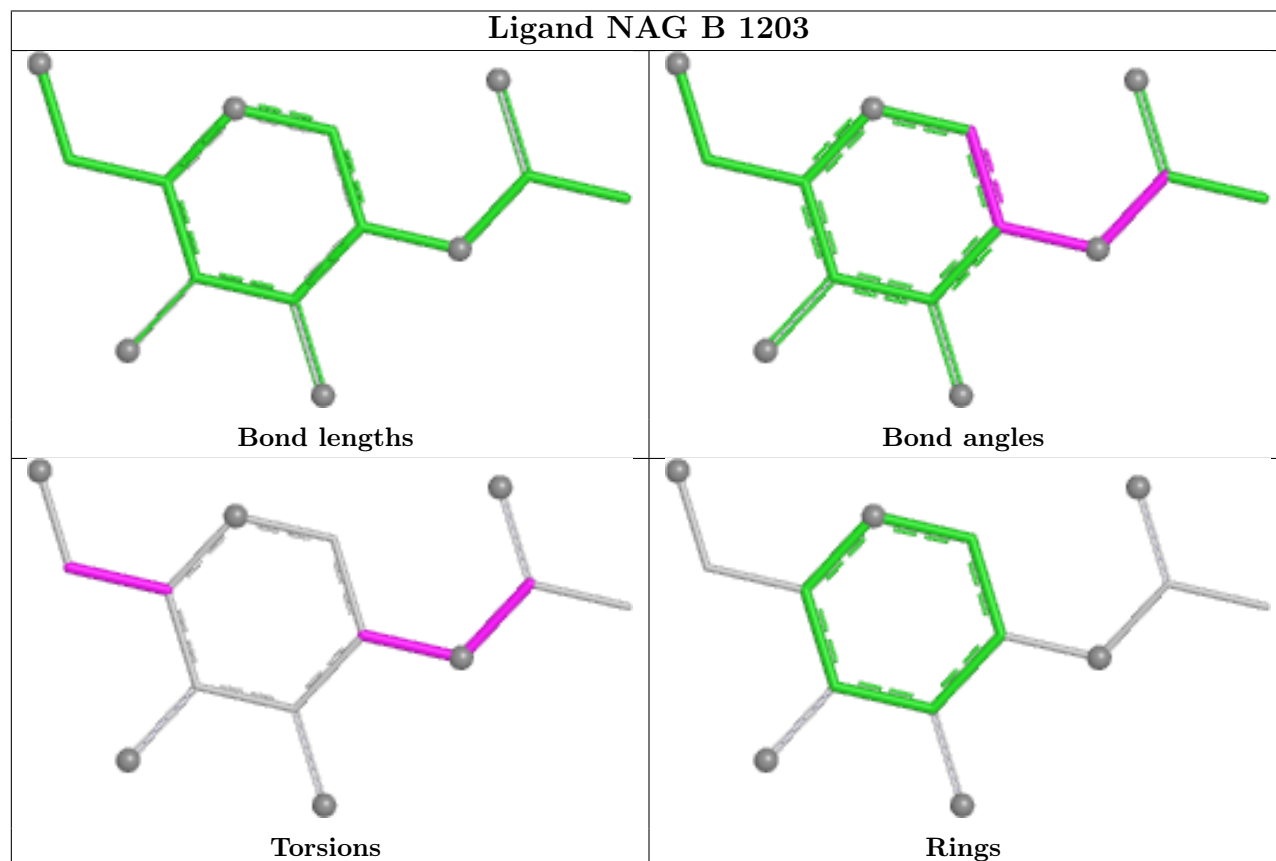


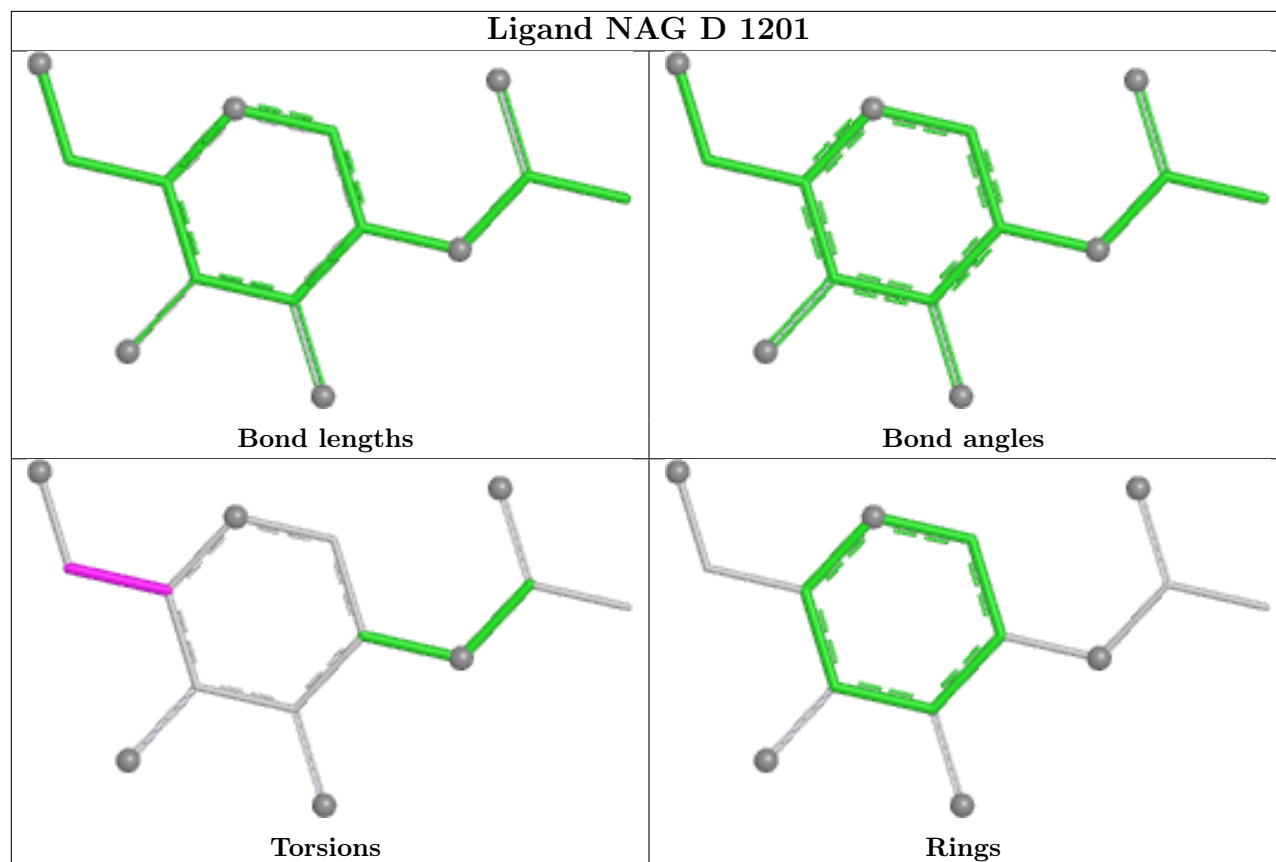


## Ligand NAG A 1202



## Ligand NAG B 1203





## 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.

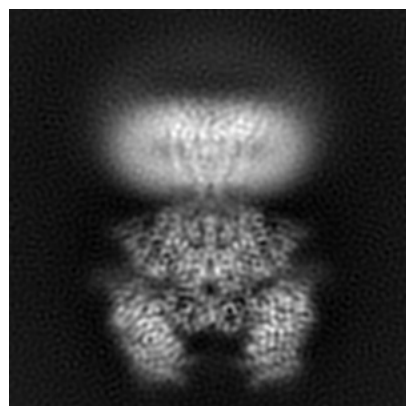
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45285. These allow visual inspection of the internal detail of the map and identification of artifacts.

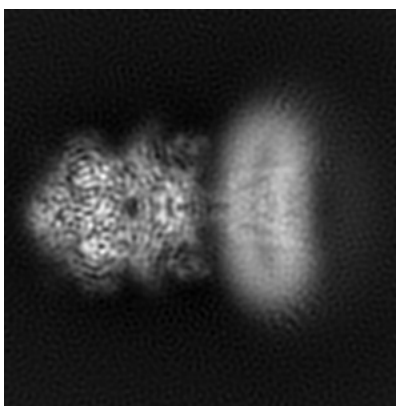
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

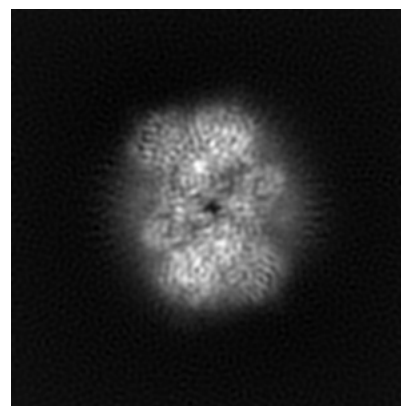
#### 6.1.1 Primary map



X

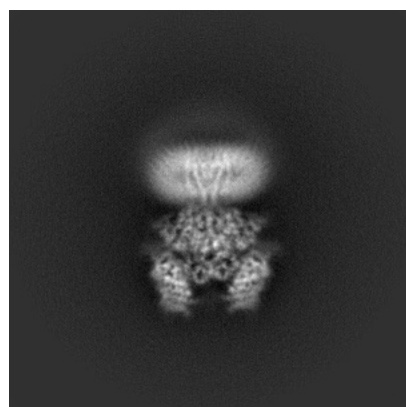


Y

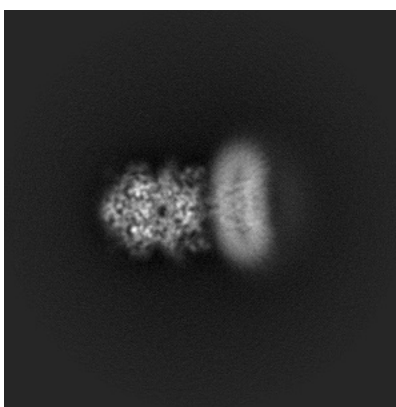


Z

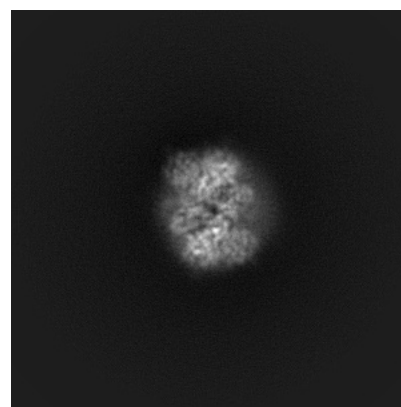
#### 6.1.2 Raw map



X



Y

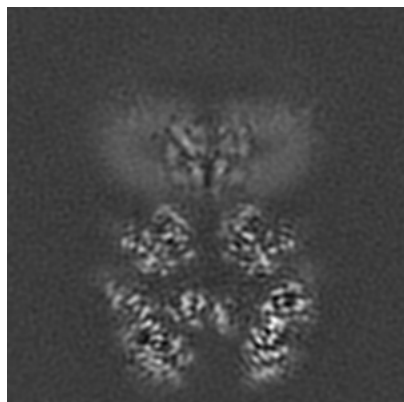


Z

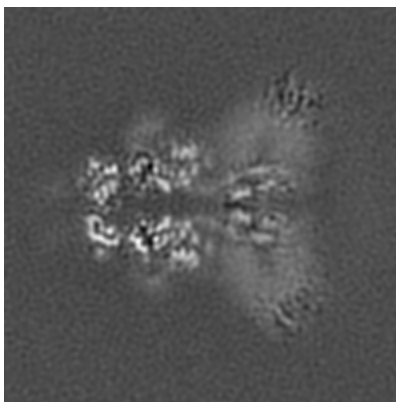
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

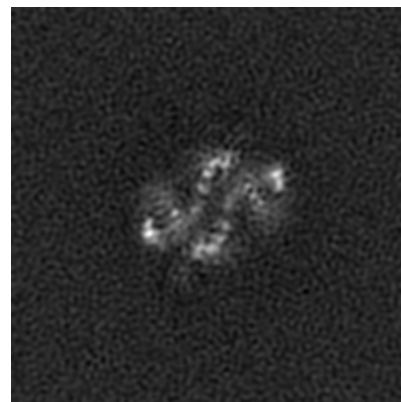
### 6.2.1 Primary map



X Index: 150

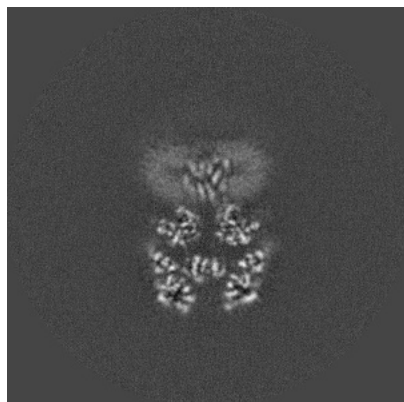


Y Index: 150

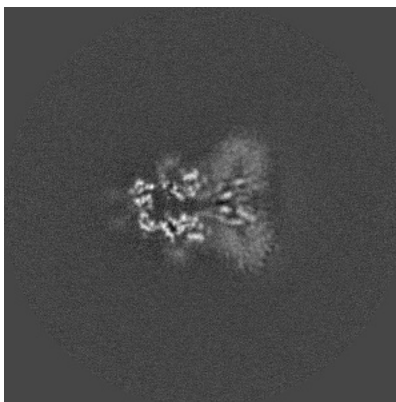


Z Index: 150

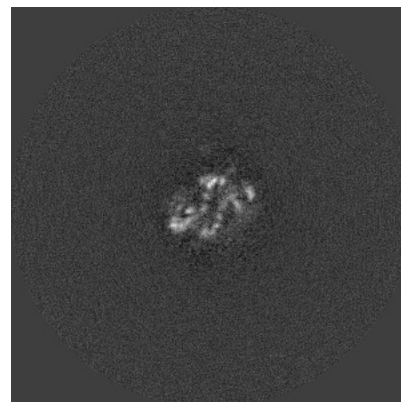
### 6.2.2 Raw map



X Index: 256



Y Index: 256



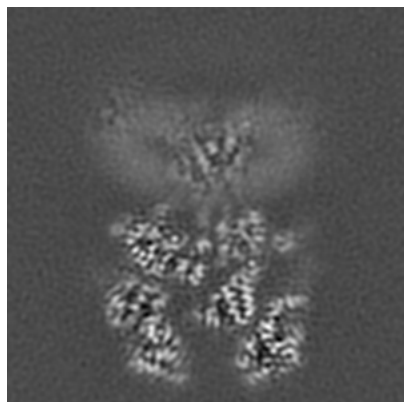
Z Index: 256

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

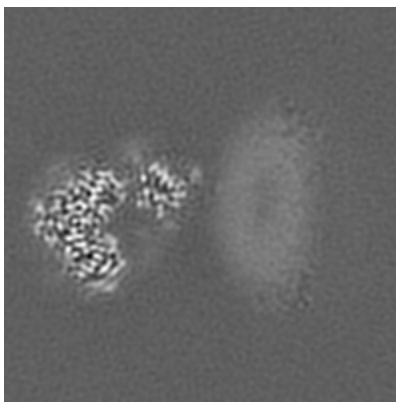


## 6.3 Largest variance slices [i](#)

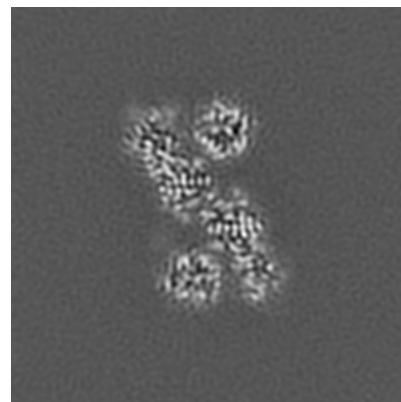
### 6.3.1 Primary map



X Index: 140

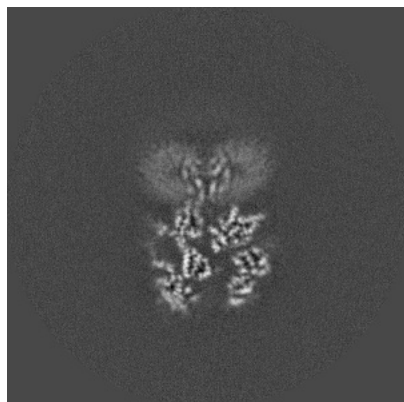


Y Index: 197

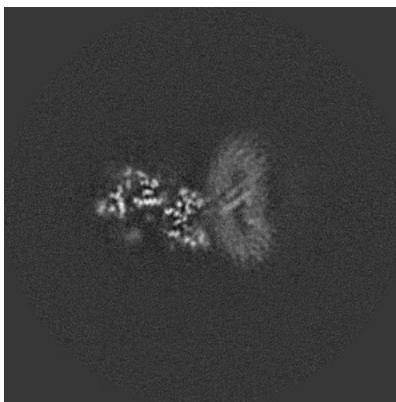


Z Index: 74

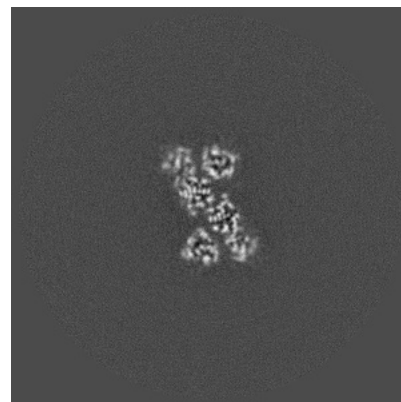
### 6.3.2 Raw map



X Index: 263



Y Index: 229

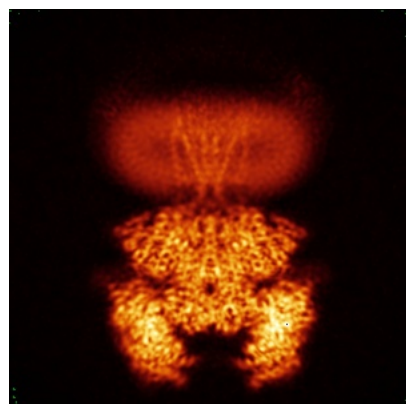


Z Index: 183

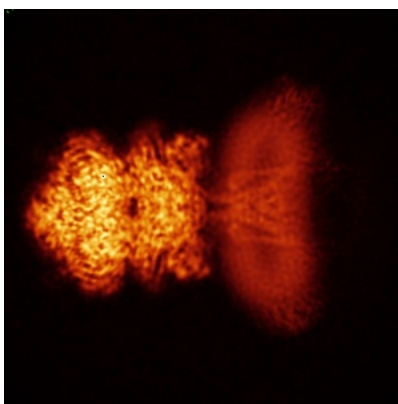
The images above show the largest variance slices of the map in three orthogonal directions.

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

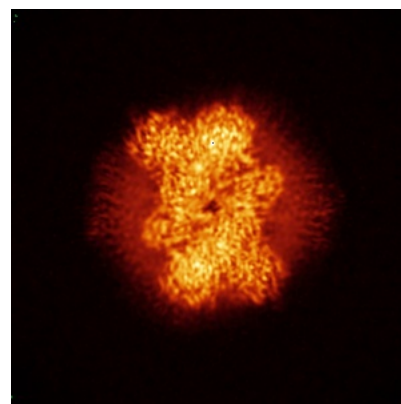
### 6.4.1 Primary map



X

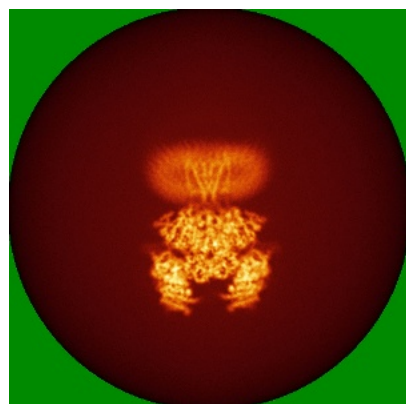


Y

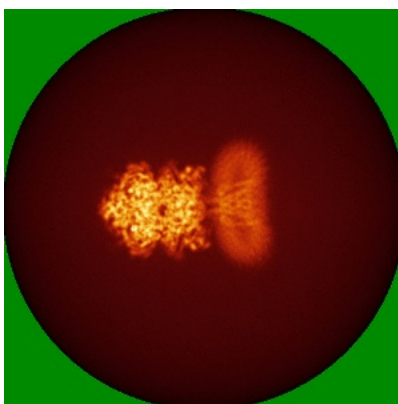


Z

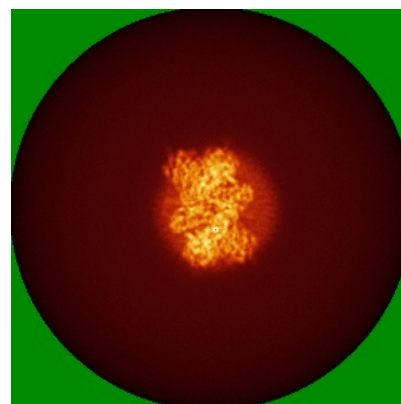
### 6.4.2 Raw map



X



Y

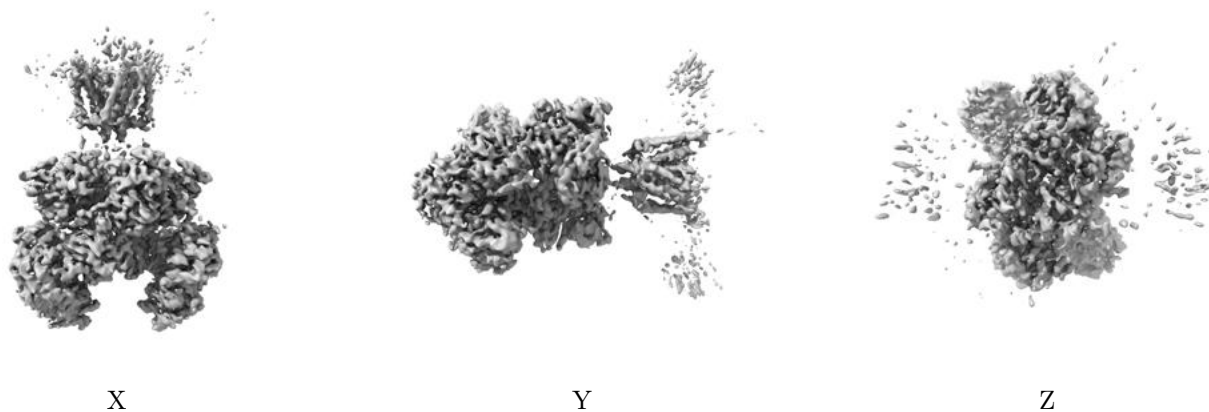


Z

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.

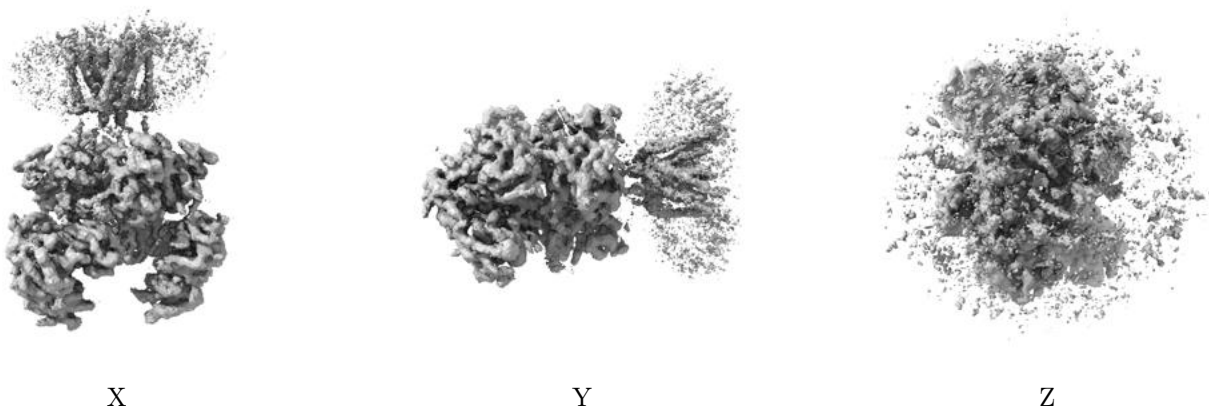
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

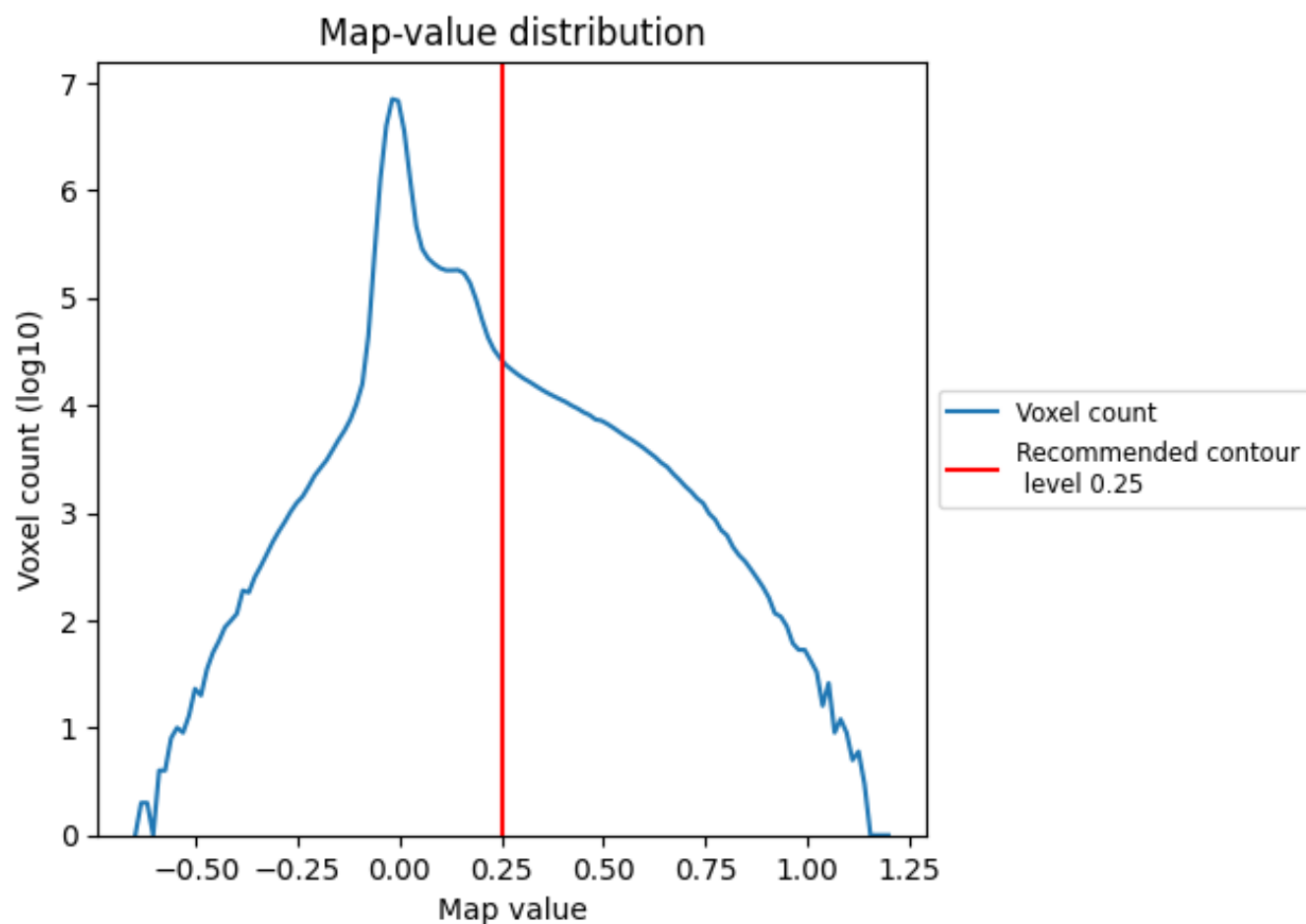
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

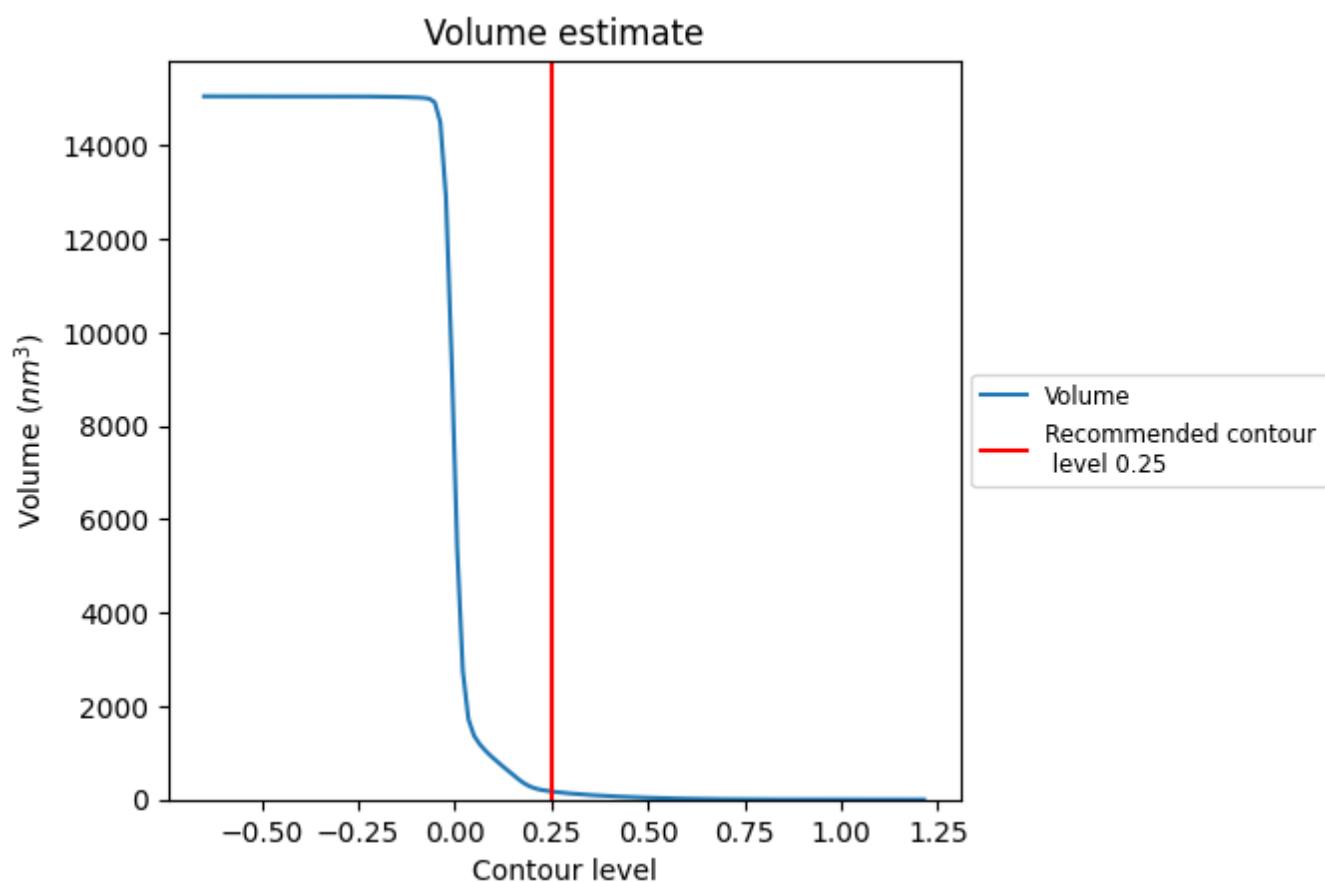
This section contains the results of statistical analysis of the map.

### 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.

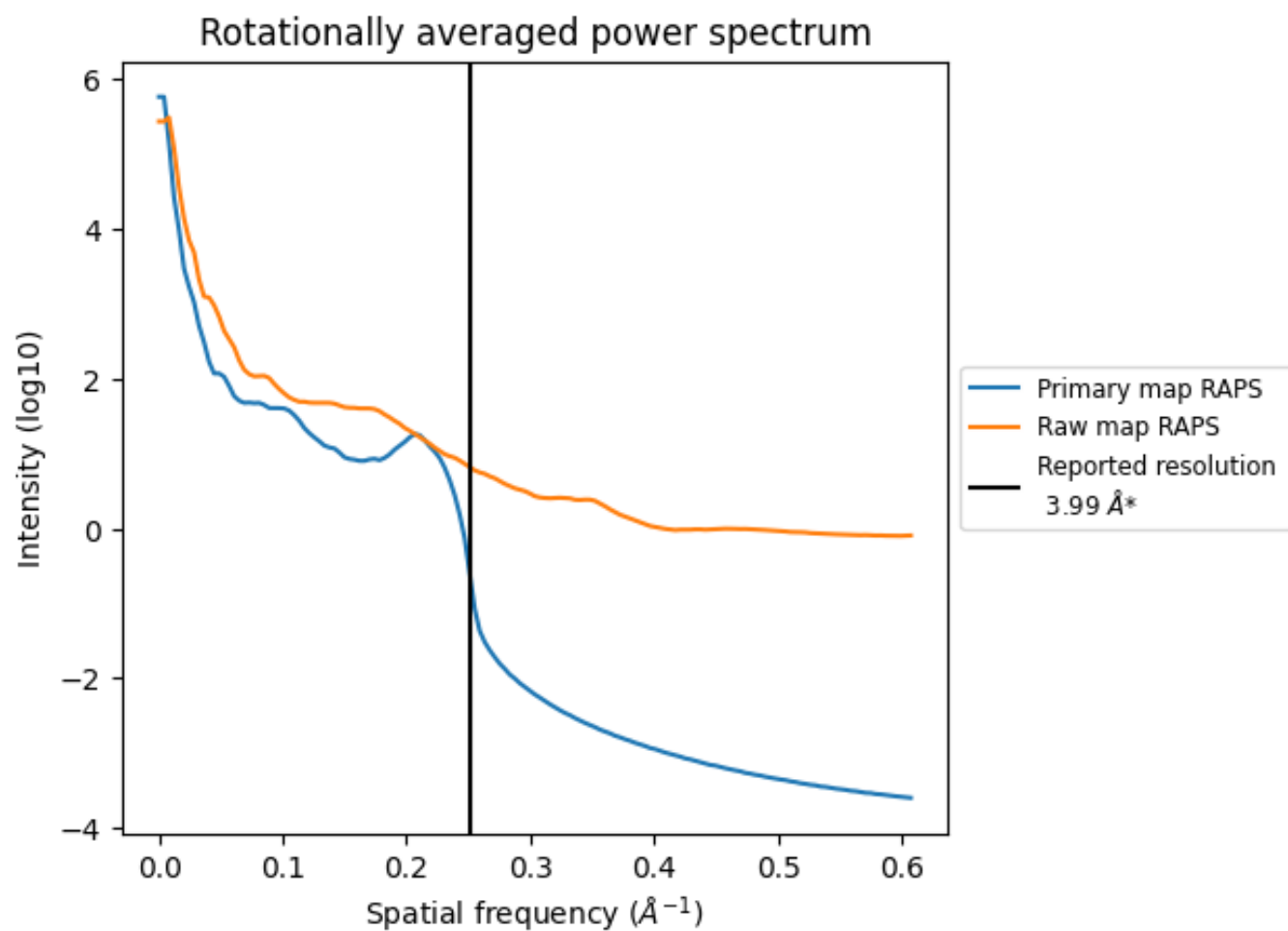
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174  $\text{nm}^3$ ; this corresponds to an approximate mass of 157 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 ⓘ

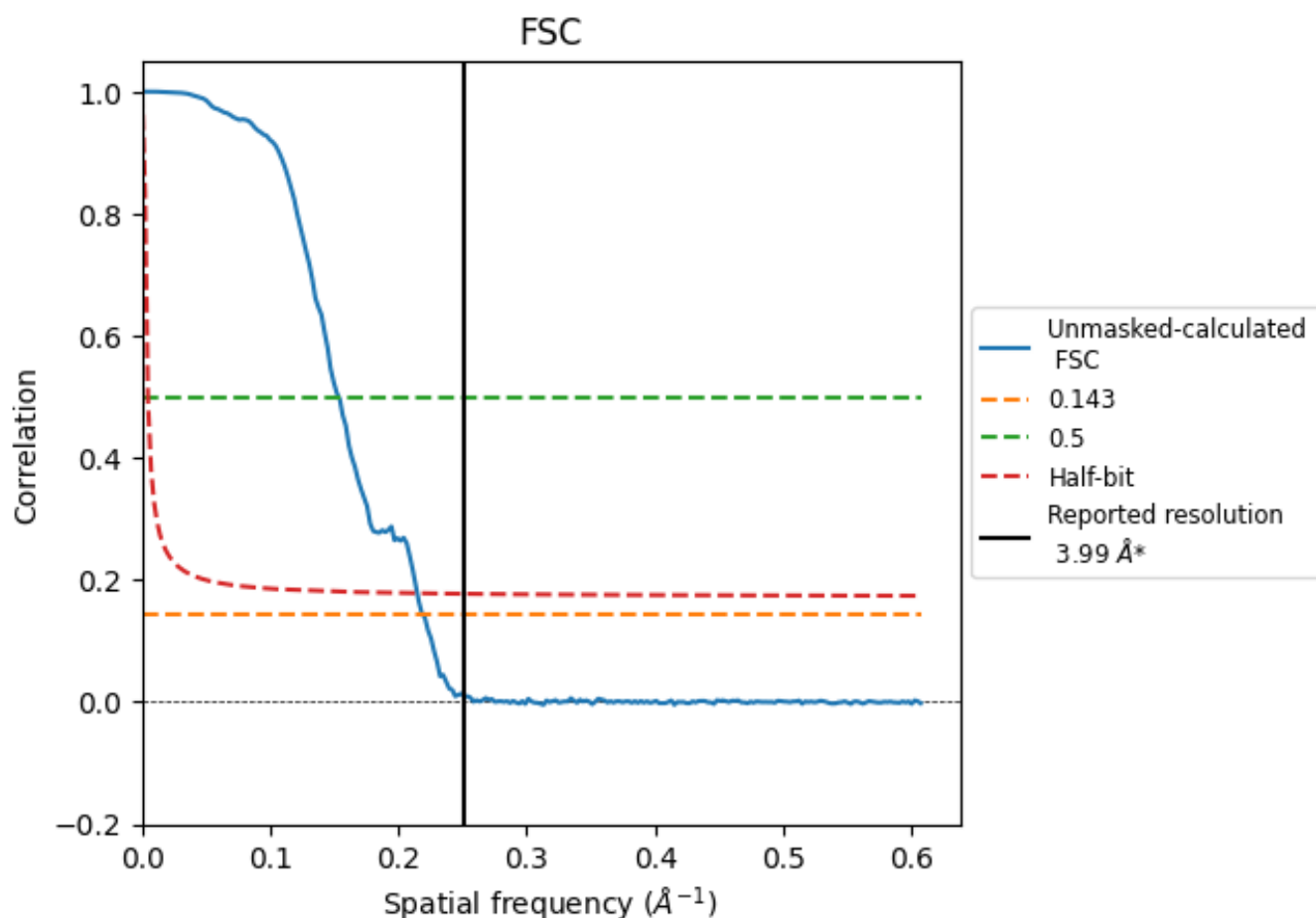


\*Reported resolution corresponds to spatial frequency of 0.251  $\text{\AA}^{-1}$

## 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 0.251  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.56	6.52	4.66

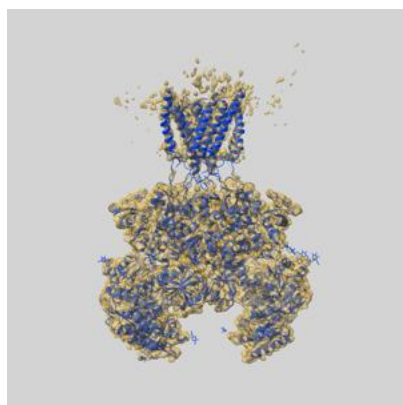
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.56 differs from the reported value 3.99 by more than 10 %



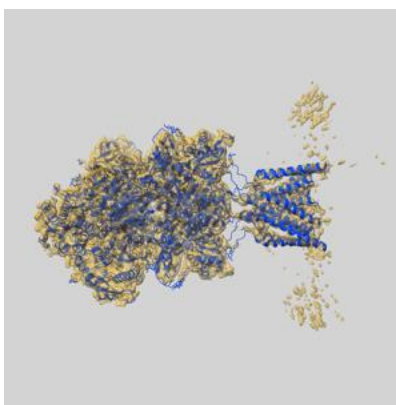
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45285 and PDB model 9C7R. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

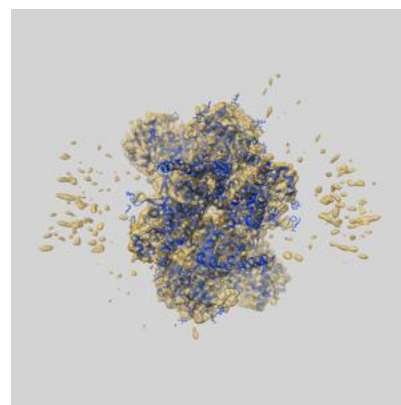
### 9.1 Map-model overlay [i](#)



X



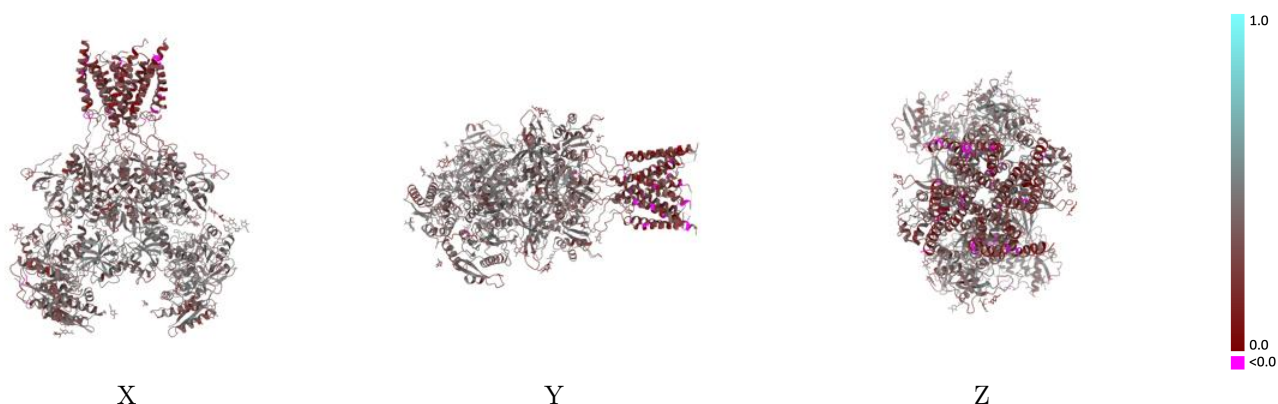
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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](#)

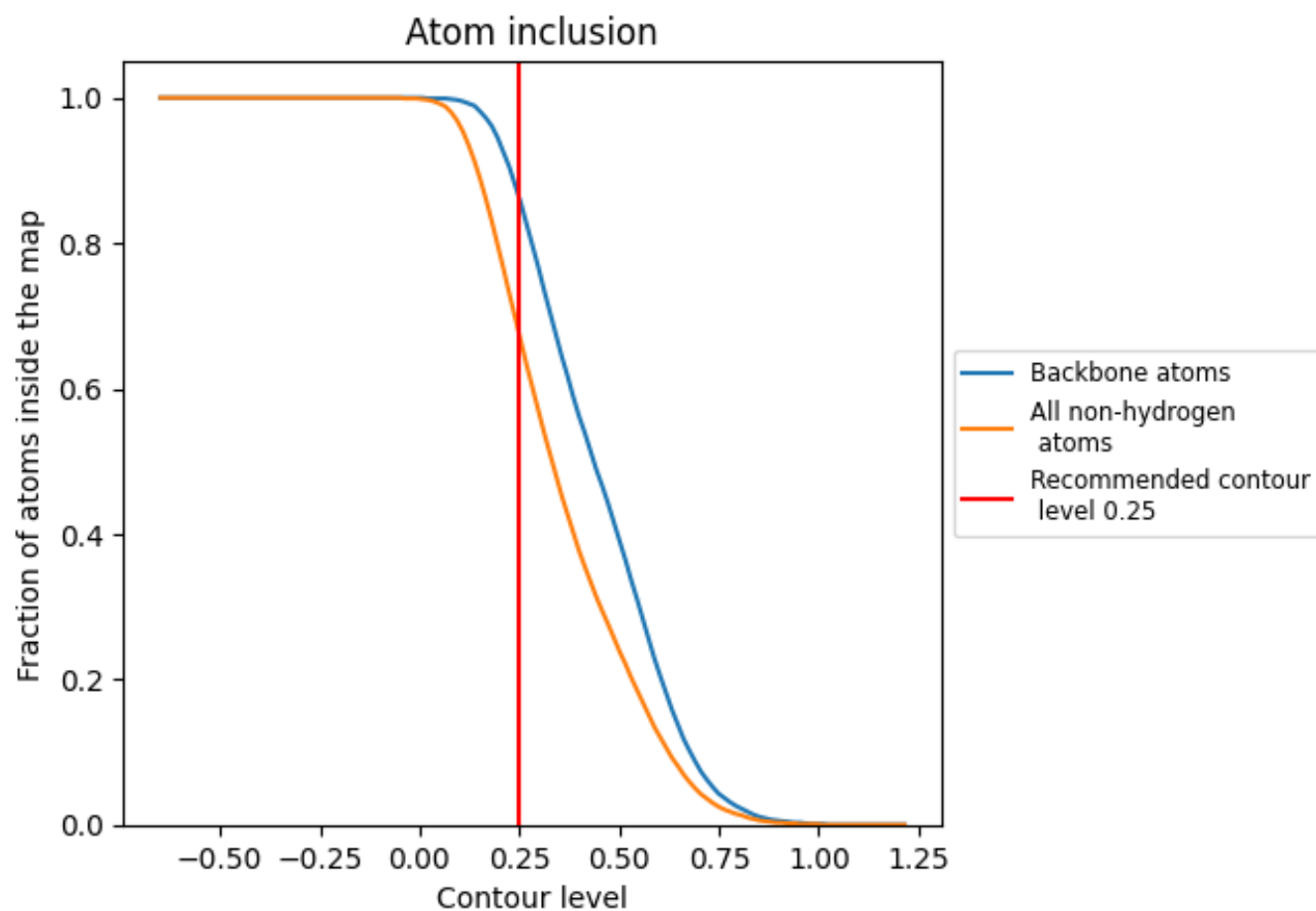


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 67% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6740	 0.3670
A	 0.6810	 0.3620
B	 0.6670	 0.3640
C	 0.6970	 0.3760
D	 0.6750	 0.3670
E	 0.6070	 0.3740
F	 0.3570	 0.2860
G	 0.5000	 0.3550
H	 0.3210	 0.3610
I	 0.5710	 0.4050
J	 0.5000	 0.3550
K	 0.0360	 0.3150
L	 0.1790	 0.2860
M	 0.5000	 0.4040
N	 0.7140	 0.4430
O	 0.3930	 0.3970
P	 0.3570	 0.4310
Q	 0.5710	 0.3970
R	 0.2500	 0.2100
S	 0.6070	 0.3860
T	 0.2140	 0.2120
U	 0.5360	 0.3450
V	 0.1790	 0.3010
W	 0.1430	 0.3280
X	 0.6070	 0.4300

