



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:11 PM UTC

PDB ID : 9ETU / pdb_00009etu
EMDB ID : EMD-19962
Title : Archaeum filament from the Halobacterium salinarum deltaAgl27 strain
Authors : Grossman-Haham, I.; Shahar, A.
Deposited on : 2024-03-27
Resolution : 3.33 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

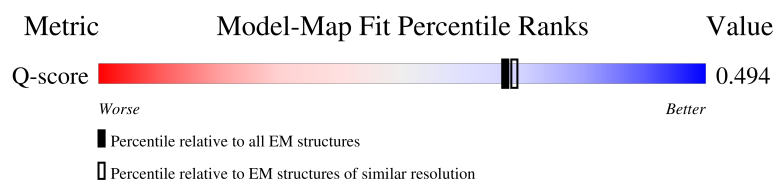
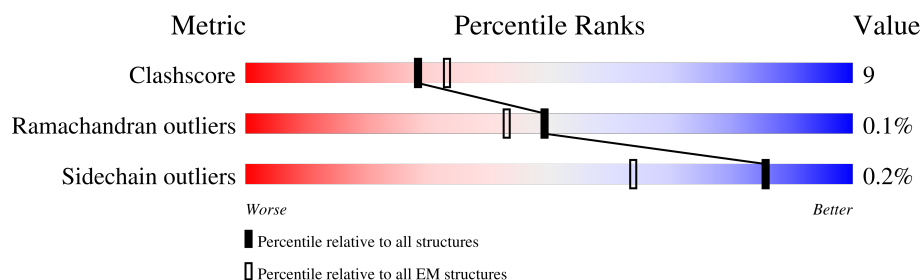
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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.



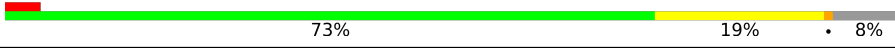
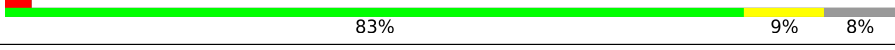
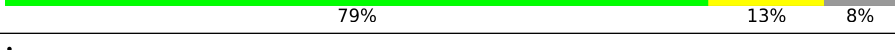
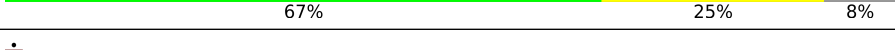
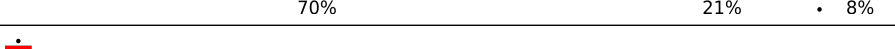
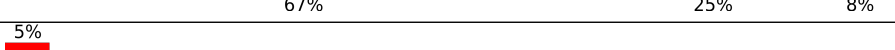
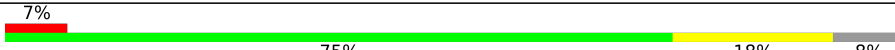
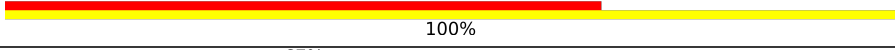
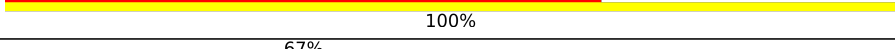
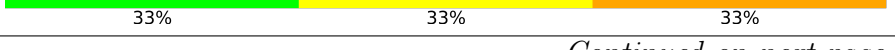
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14484 (2.83 - 3.83)

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	193	 6% 77% 15% 8%
1	B	193	 68% 24% 7%
1	C	193	 75% 17% 8%
1	D	193	 6% 66% 26% 7%

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Mol	Chain	Length	Quality of chain
1	E	193	
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	
1	O	193	
1	P	193	
1	Q	193	
1	R	193	
1	S	193	
1	T	193	
1	U	193	
1	V	193	
1	W	193	
1	X	193	
1	Y	193	
2	0	3	
2	1	3	
2	2	3	
2	3	3	

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Mol	Chain	Length	Quality of chain
2	4	3	67% 100%
2	5	3	67% 33% 33% 33%
2	6	3	67% 67% 33%
2	7	3	67% 33% 67%
2	8	3	67% 100%
2	9	3	67% 100%
2	AA	3	67% 33% 67%
2	BA	3	67% 100%
2	CA	3	67% 33% 67%
2	DA	3	67% 100%
2	EA	3	67% 33% 67%
2	FA	3	67% 33% 67%
2	GA	3	67% 33% 67%
2	HA	3	67% 33% 33% 33%
2	IA	3	67% 33% 67%
2	JA	3	67% 33% 67%
2	KA	3	67% 100%
2	LA	3	67% 100%
2	MA	3	67% 33% 67%
2	Z	3	67% 33% 67%
2	a	3	67% 33% 67%
2	b	3	67% 33% 67%
2	c	3	67% 100%
2	d	3	67% 100%
2	e	3	67% 100%

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Mol	Chain	Length	Quality of chain
2	f	3	
2	g	3	
2	h	3	
2	i	3	
2	j	3	
2	k	3	
2	l	3	
2	m	3	
2	n	3	
2	o	3	
2	p	3	
2	q	3	
2	r	3	
2	s	3	
2	t	3	
2	u	3	
2	v	3	
2	w	3	
2	x	3	
2	y	3	
2	z	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	LA	1	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 33665 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 Archaeollin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	B	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	C	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	D	180	Total	C	N	O	S	0	0
			1278	807	216	253	2		
1	E	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	F	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	G	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	H	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	I	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	J	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	K	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	L	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	M	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	N	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	O	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	P	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	Q	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	S	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	T	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	U	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	V	180	Total	C	N	O	S	0	0
			1278	807	216	253	2		
1	W	177	Total	C	N	O	S	0	0
			1263	798	213	250	2		
1	X	177	Total	C	N	O	S	0	0
			1263	798	213	250	2		
1	Y	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		

- Molecule 2 is an oligosaccharide called 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Z	3	Total	C	O	S	0	0
			39	18	20	1		
2	a	3	Total	C	O	S	0	0
			39	18	20	1		
2	b	3	Total	C	O	S	0	0
			39	18	20	1		
2	c	3	Total	C	O	S	0	0
			39	18	20	1		
2	d	3	Total	C	O	S	0	0
			39	18	20	1		
2	e	3	Total	C	O	S	0	0
			39	18	20	1		
2	f	3	Total	C	O	S	0	0
			39	18	20	1		
2	g	3	Total	C	O	S	0	0
			39	18	20	1		
2	h	3	Total	C	O	S	0	0
			39	18	20	1		
2	i	3	Total	C	O	S	0	0
			39	18	20	1		
2	j	3	Total	C	O	S	0	0
			39	18	20	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	k	3	Total	C	O	S	0	0
			39	18	20	1		
2	l	3	Total	C	O	S	0	0
			39	18	20	1		
2	m	3	Total	C	O	S	0	0
			39	18	20	1		
2	n	3	Total	C	O	S	0	0
			39	18	20	1		
2	o	3	Total	C	O	S	0	0
			39	18	20	1		
2	p	3	Total	C	O	S	0	0
			39	18	20	1		
2	q	3	Total	C	O	S	0	0
			39	18	20	1		
2	r	3	Total	C	O	S	0	0
			39	18	20	1		
2	s	3	Total	C	O	S	0	0
			39	18	20	1		
2	t	3	Total	C	O	S	0	0
			39	18	20	1		
2	u	3	Total	C	O	S	0	0
			39	18	20	1		
2	v	3	Total	C	O	S	0	0
			39	18	20	1		
2	w	3	Total	C	O	S	0	0
			39	18	20	1		
2	x	3	Total	C	O	S	0	0
			39	18	20	1		
2	y	3	Total	C	O	S	0	0
			39	18	20	1		
2	z	3	Total	C	O	S	0	0
			39	18	20	1		
2	0	3	Total	C	O	S	0	0
			39	18	20	1		
2	1	3	Total	C	O	S	0	0
			39	18	20	1		
2	2	3	Total	C	O	S	0	0
			39	18	20	1		
2	3	3	Total	C	O	S	0	0
			39	18	20	1		
2	4	3	Total	C	O	S	0	0
			39	18	20	1		

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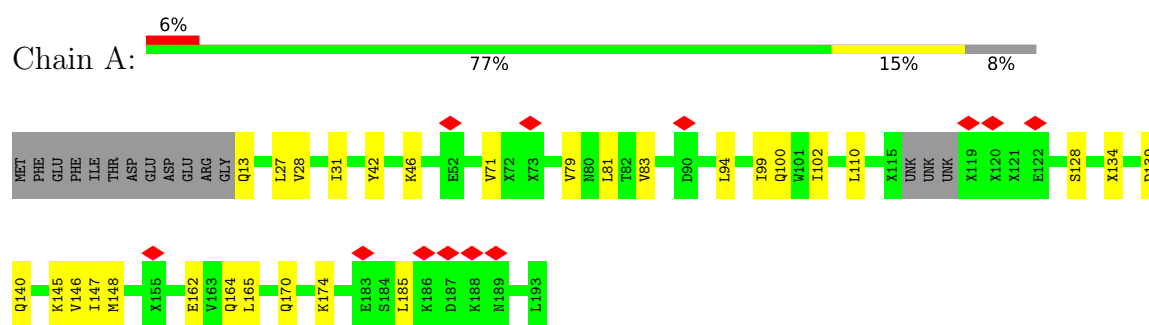
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	5	3	Total	C	O	S	0	0
			39	18	20	1		
2	6	3	Total	C	O	S	0	0
			39	18	20	1		
2	7	3	Total	C	O	S	0	0
			39	18	20	1		
2	8	3	Total	C	O	S	0	0
			39	18	20	1		
2	9	3	Total	C	O	S	0	0
			39	18	20	1		
2	AA	3	Total	C	O	S	0	0
			39	18	20	1		
2	BA	3	Total	C	O	S	0	0
			39	18	20	1		
2	CA	3	Total	C	O	S	0	0
			39	18	20	1		
2	DA	3	Total	C	O	S	0	0
			39	18	20	1		
2	EA	3	Total	C	O	S	0	0
			39	18	20	1		
2	FA	3	Total	C	O	S	0	0
			39	18	20	1		
2	GA	3	Total	C	O	S	0	0
			39	18	20	1		
2	HA	3	Total	C	O	S	0	0
			39	18	20	1		
2	IA	3	Total	C	O	S	0	0
			39	18	20	1		
2	JA	3	Total	C	O	S	0	0
			39	18	20	1		
2	KA	3	Total	C	O	S	0	0
			39	18	20	1		
2	LA	3	Total	C	O	S	0	0
			39	18	20	1		
2	MA	3	Total	C	O	S	0	0
			39	18	20	1		

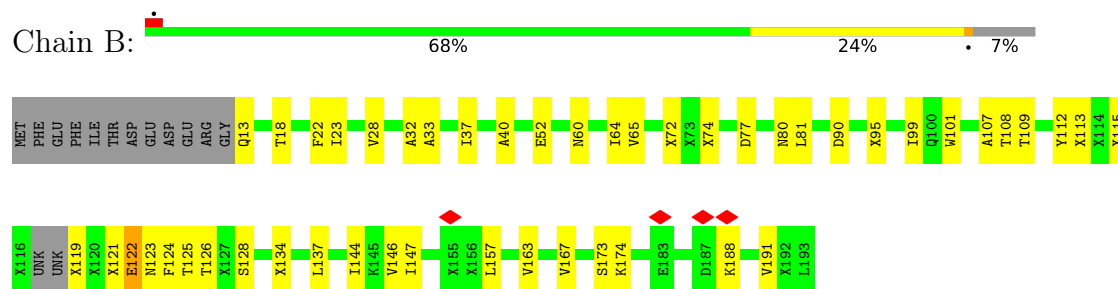
3 Residue-property plots

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.

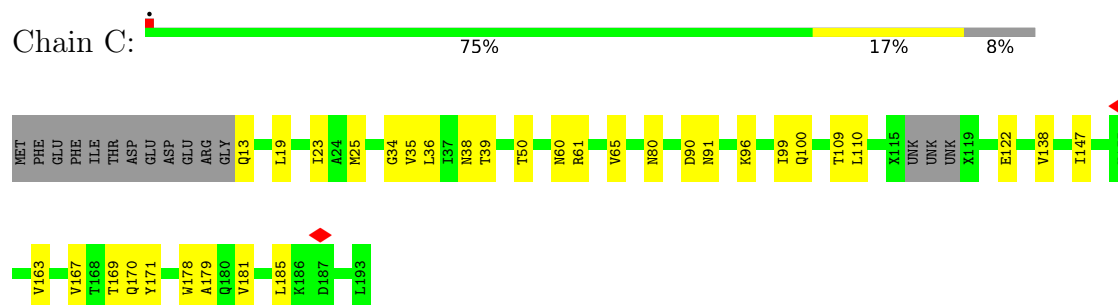
• Molecule 1: Archaeellin



• Molecule 1: Archaeellin

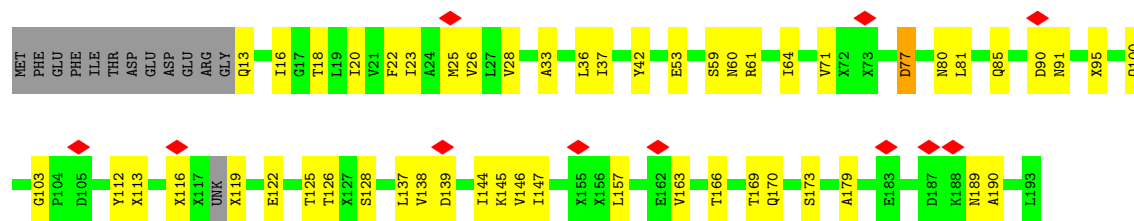


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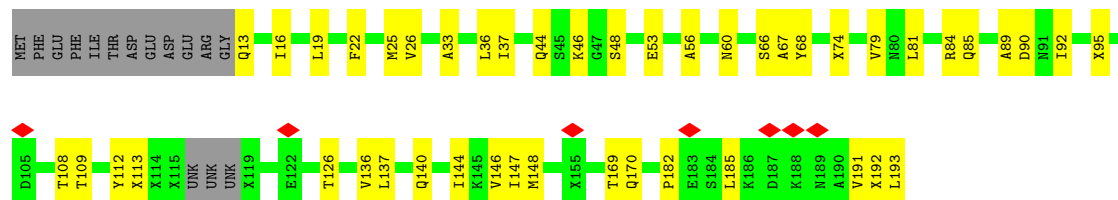


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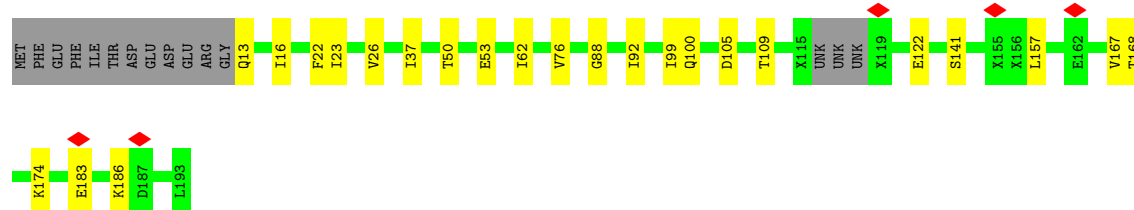
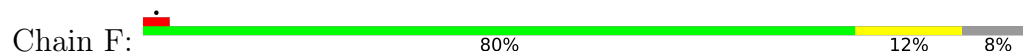




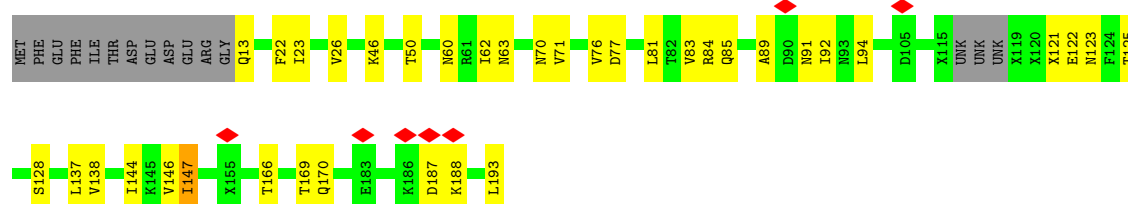
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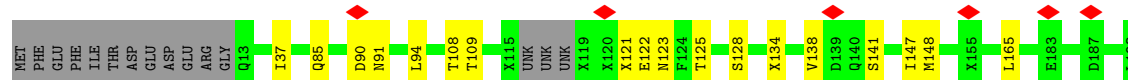
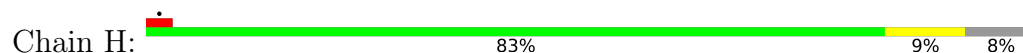
• Molecule 1: Archaeollin



• Molecule 1: Archaeollin

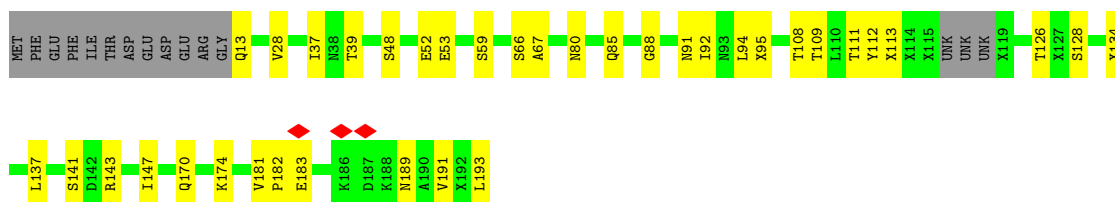


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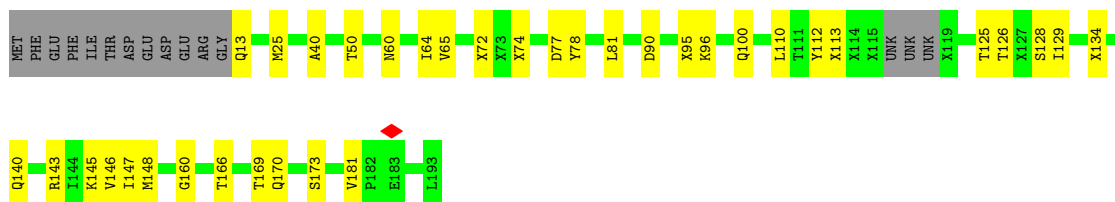


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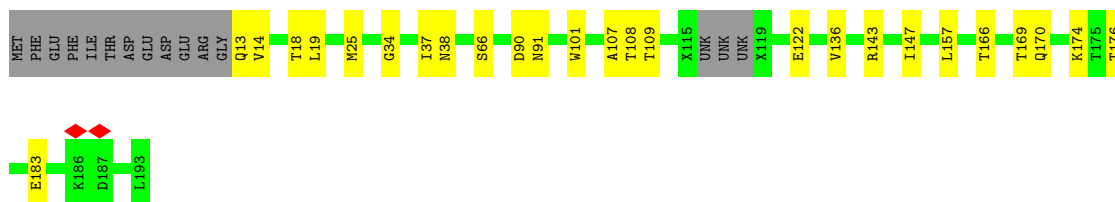
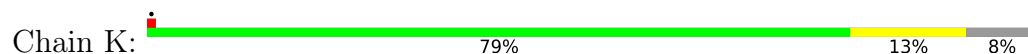




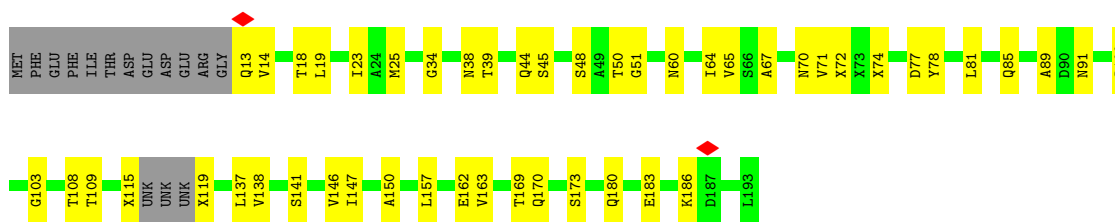
- Molecule 1: Archaeellin



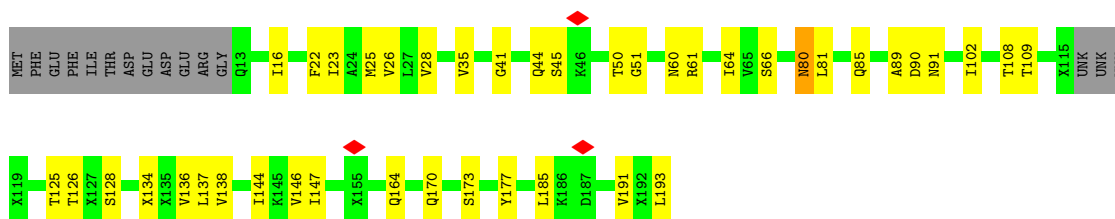
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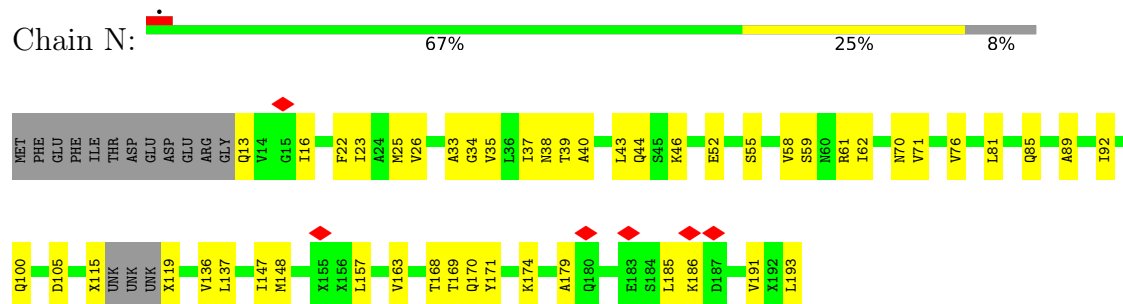
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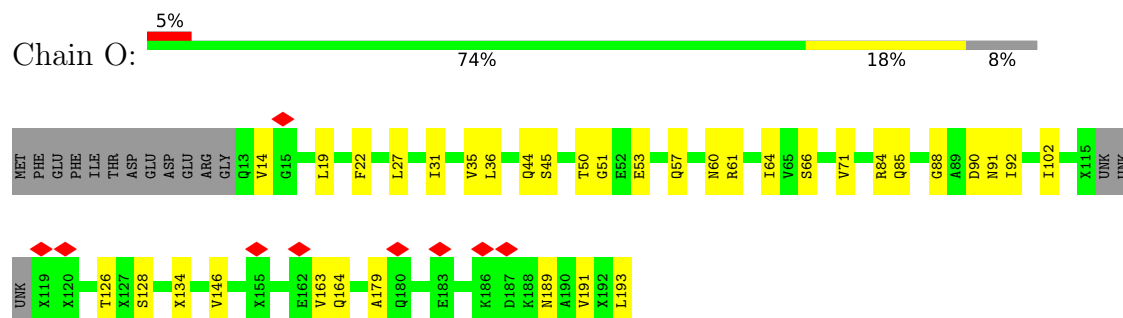
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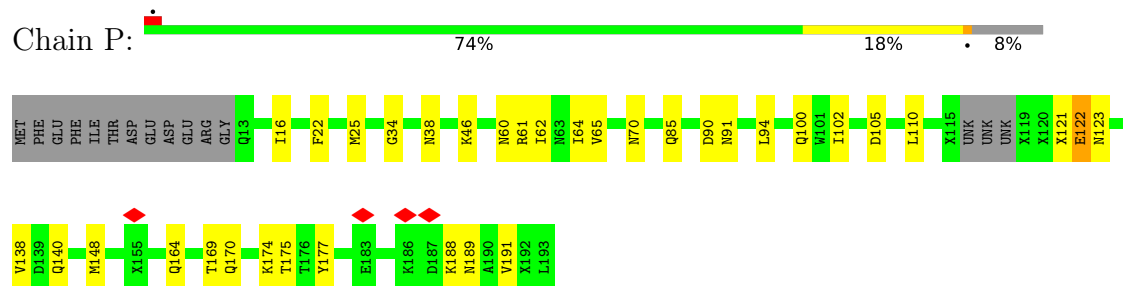
- Molecule 1: Archaeellin



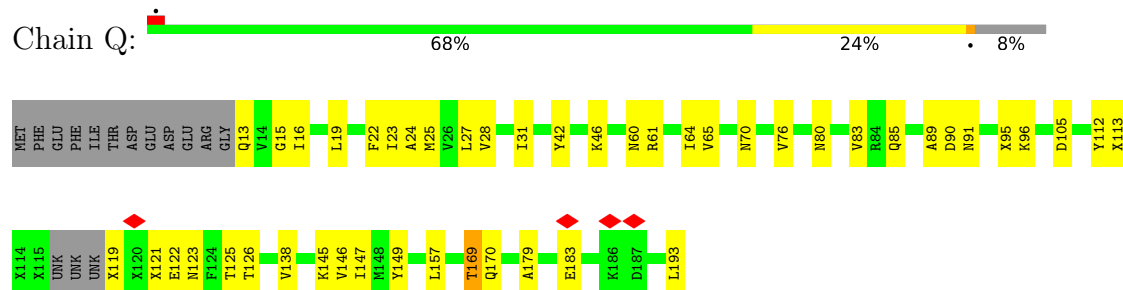
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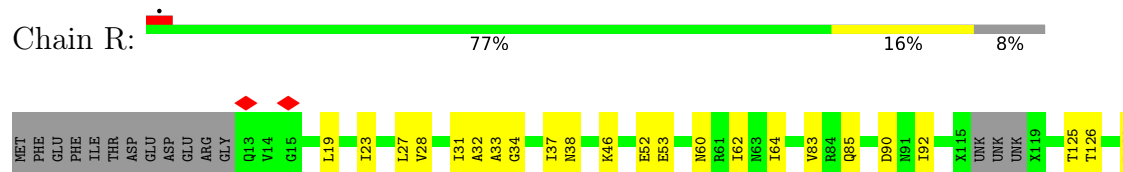
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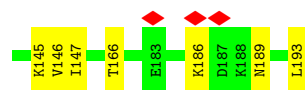


- Molecule 1: Archaeellin

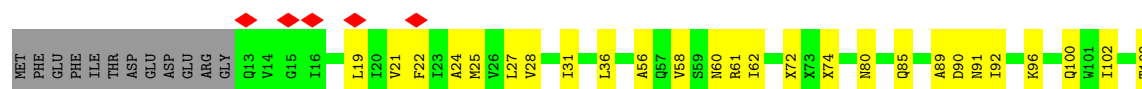
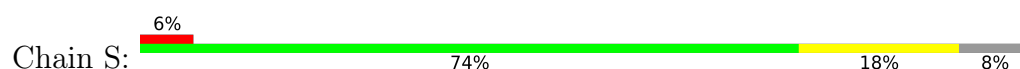


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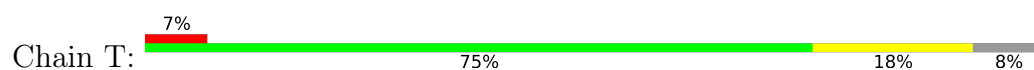




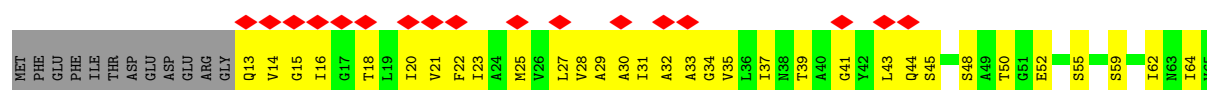
- Molecule 1: Archaeellin



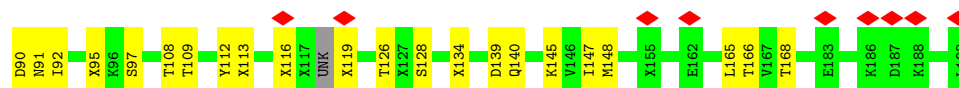
- Molecule 1: Archaeellin



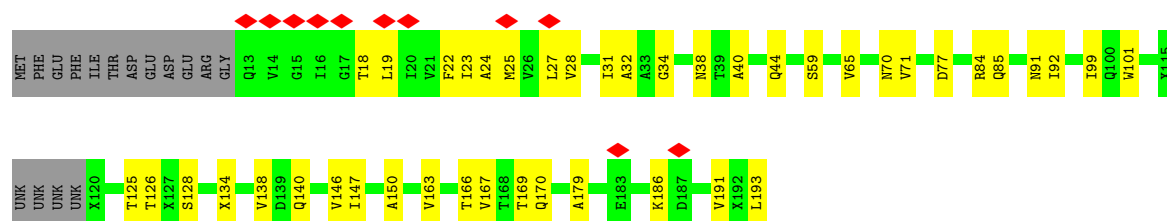
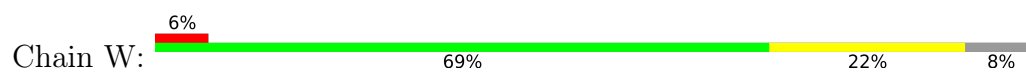
- Molecule 1: Archaeellin



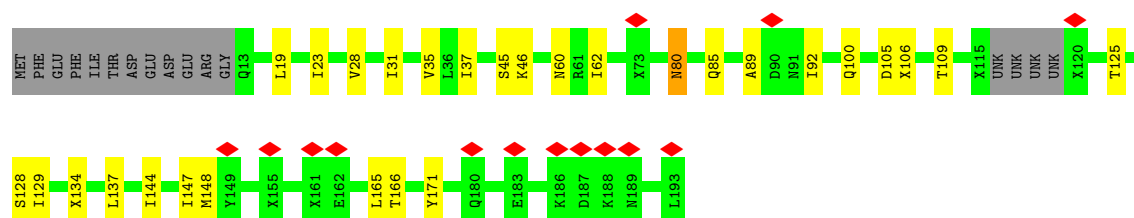
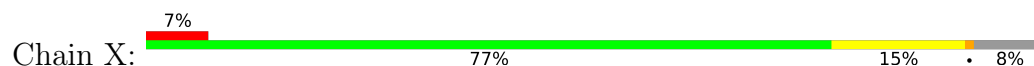
- Molecule 1: Archaeellin



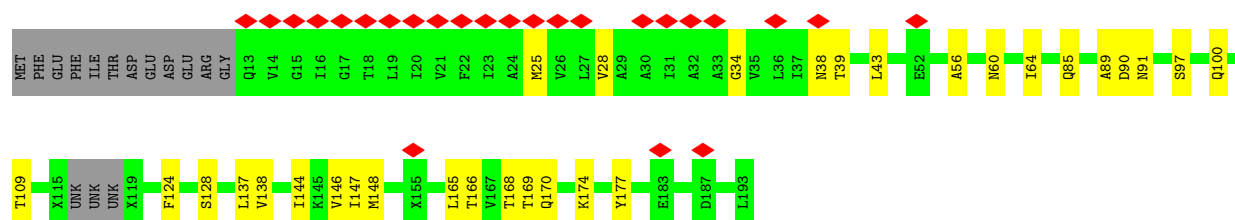
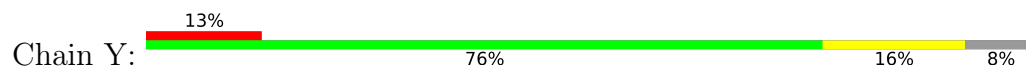
- Molecule 1: Archaeellin



- Molecule 1: Archaeollin



- Molecule 1: Archaeollin



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose





- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose





- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose





- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose





- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=107.91°, rise=5.46 Å, axial sym=C1	Depositor
Number of segments used	265906	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.546	Depositor
Minimum map value	-0.298	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	370.24, 370.24, 370.24	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89, 0.89, 0.89	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H1V, BDP, BGC

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	0/1141	0.31	0/1538
1	B	0.13	0/1141	0.31	0/1538
1	C	0.12	0/1141	0.30	0/1538
1	D	0.15	0/1141	0.36	0/1538
1	E	0.12	0/1141	0.32	0/1538
1	F	0.15	0/1141	0.31	0/1538
1	G	0.12	0/1141	0.30	0/1538
1	H	0.12	0/1141	0.31	0/1538
1	I	0.13	0/1141	0.31	0/1538
1	J	0.13	0/1141	0.31	0/1538
1	K	0.12	0/1141	0.33	0/1538
1	L	0.12	0/1141	0.34	0/1538
1	M	0.13	0/1141	0.34	0/1538
1	N	0.14	0/1141	0.36	0/1538
1	O	0.13	0/1141	0.35	0/1538
1	P	0.12	0/1141	0.32	0/1538
1	Q	0.12	0/1141	0.30	0/1538
1	R	0.12	0/1141	0.32	0/1538
1	S	0.11	0/1141	0.30	0/1538
1	T	0.14	0/1141	0.36	0/1538
1	U	0.13	0/1141	0.35	0/1538
1	V	0.14	0/1141	0.36	0/1538
1	W	0.12	0/1141	0.33	0/1538
1	X	0.13	0/1141	0.33	0/1538
1	Y	0.12	0/1141	0.30	0/1538
All	All	0.13	0/28525	0.33	0/38450

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

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	1268	0	1194	20	0
1	B	1273	0	1194	34	0
1	C	1268	0	1194	28	0
1	D	1278	0	1197	43	0
1	E	1268	0	1194	38	0
1	F	1268	0	1195	22	0
1	G	1268	0	1194	27	0
1	H	1268	0	1196	10	0
1	I	1268	0	1193	28	0
1	J	1268	0	1195	26	0
1	K	1268	0	1193	22	0
1	L	1268	0	1192	35	0
1	M	1268	0	1194	34	0
1	N	1268	0	1193	39	0
1	O	1268	0	1194	28	0
1	P	1268	0	1196	26	0
1	Q	1268	0	1193	37	0
1	R	1268	0	1194	26	0
1	S	1268	0	1195	25	0
1	T	1268	0	1192	22	0
1	U	1268	0	1193	41	0
1	V	1278	0	1195	25	0
1	W	1263	0	1193	31	0
1	X	1263	0	1193	23	0
1	Y	1268	0	1196	20	0
2	0	39	0	15	0	0
2	1	39	0	15	0	0
2	2	39	0	15	0	0
2	3	39	0	15	1	0
2	4	39	0	15	0	0
2	5	39	0	15	1	0
2	6	39	0	15	1	0
2	7	39	0	15	0	0
2	8	39	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	39	0	15	1	0
2	AA	39	0	15	1	0
2	BA	39	0	15	1	0
2	CA	39	0	15	0	0
2	DA	39	0	15	1	0
2	EA	39	0	15	0	0
2	FA	39	0	15	0	0
2	GA	39	0	15	1	0
2	HA	39	0	15	1	0
2	IA	39	0	15	0	0
2	JA	39	0	15	0	0
2	KA	39	0	15	0	0
2	LA	39	0	15	1	0
2	MA	39	0	15	0	0
2	Z	39	0	15	0	0
2	a	39	0	15	0	0
2	b	39	0	15	0	0
2	c	39	0	15	0	0
2	d	39	0	15	1	0
2	e	39	0	15	1	0
2	f	39	0	15	0	0
2	g	39	0	15	0	0
2	h	39	0	15	1	0
2	i	39	0	15	0	0
2	j	39	0	15	1	0
2	k	39	0	15	1	0
2	l	39	0	15	2	0
2	m	39	0	15	0	0
2	n	39	0	15	0	0
2	o	39	0	15	0	0
2	p	39	0	15	0	0
2	q	39	0	15	0	0
2	r	39	0	15	0	0
2	s	39	0	15	1	0
2	t	39	0	15	1	0
2	u	39	0	15	0	0
2	v	39	0	15	1	0
2	w	39	0	15	0	0
2	x	39	0	15	1	0
2	y	39	0	15	0	0
2	z	39	0	15	2	0
All	All	33665	0	30602	608	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 (608) 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:K:90:ASP:OD1	1:K:91:ASN:N	2.07	0.87
1:P:102:ILE:HB	1:P:164:GLN:HB2	1.60	0.82
1:J:13:GLN:HB2	1:K:25:MET:HG3	1.60	0.81
1:L:13:GLN:HB3	1:U:25:MET:HE1	1.62	0.80
1:G:137:LEU:HD12	1:G:144:ILE:HD12	1.64	0.79
1:J:13:GLN:HG2	1:Q:25:MET:HE1	1.66	0.78
1:L:13:GLN:HG3	1:W:25:MET:HE1	1.66	0.77
1:C:90:ASP:OD1	1:C:91:ASN:N	2.17	0.77
1:D:60:ASN:HD22	1:D:90:ASP:H	1.32	0.76
1:X:92:ILE:HB	1:X:137:LEU:HB2	1.66	0.75
1:T:25:MET:HA	1:T:28:VAL:HG12	1.70	0.73
1:A:102:ILE:HB	1:A:164:GLN:HB2	1.69	0.72
1:S:80:ASN:HD22	1:S:145:LYS:HD2	1.54	0.72
1:V:90:ASP:OD1	1:V:91:ASN:N	2.20	0.72
1:F:62:ILE:HD11	1:F:92:ILE:HG21	1.73	0.71
1:L:100:GLN:NE2	1:U:66:SER:OG	2.23	0.70
1:L:186:LYS:HG3	1:M:136:VAL:HG11	1.74	0.70
1:P:110:LEU:HD12	1:P:148:MET:HE2	1.72	0.70
1:R:34:GLY:O	1:R:38:ASN:ND2	2.25	0.70
1:Y:90:ASP:OD1	1:Y:91:ASN:N	2.22	0.70
1:K:170:GLN:HG3	1:L:141:SER:HB3	1.74	0.69
1:A:79:VAL:HG13	1:A:148:MET:HG3	1.74	0.69
1:D:61:ARG:HG2	1:D:173:SER:HB2	1.74	0.69
1:U:137:LEU:HG	1:U:144:ILE:HD12	1.74	0.69
1:G:60:ASN:HB3	1:G:92:ILE:HD11	1.74	0.69
1:T:85:GLN:HG2	1:T:89:ALA:HB3	1.74	0.68
1:K:13:GLN:HE22	1:O:14:VAL:HG11	1.58	0.68
1:Q:80:ASN:HD22	1:Q:145:LYS:HD2	1.59	0.68
1:U:25:MET:HA	1:U:28:VAL:HG22	1.76	0.67
1:A:139:ASP:OD2	1:A:140:GLN:N	2.28	0.66
1:A:46:LYS:NZ	1:B:90:ASP:OD2	2.27	0.66
1:E:95:UNK:HA	1:E:112:TYR:HD1	1.61	0.66
1:C:35:VAL:HG11	1:M:44:GLN:HB2	1.78	0.66
1:P:34:GLY:O	1:P:38:ASN:ND2	2.29	0.66
1:A:71:VAL:HG21	1:A:185:LEU:HD11	1.79	0.65
1:M:16:ILE:HG21	1:N:22:PHE:HE2	1.61	0.65
1:I:85:GLN:NE2	1:I:137:LEU:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:62:ILE:HD11	1:R:92:ILE:HG21	1.79	0.65
1:S:62:ILE:HD11	1:S:92:ILE:HG21	1.78	0.65
1:E:126:THR:HG22	1:E:146:VAL:HG12	1.79	0.65
1:F:122:GLU:N	1:F:122:GLU:OE1	2.29	0.65
1:Y:100:GLN:HG2	1:Y:109:THR:HG22	1.79	0.64
1:K:122:GLU:N	1:K:122:GLU:OE1	2.31	0.64
1:L:51:GLY:HA2	1:M:26:VAL:HG11	1.79	0.64
1:S:126:THR:HG22	1:S:146:VAL:HG12	1.79	0.64
1:D:23:ILE:HG23	1:M:50:THR:HG21	1.78	0.64
1:E:25:MET:HE1	1:G:13:GLN:HE21	1.61	0.64
1:O:126:THR:HG22	1:O:146:VAL:HG12	1.81	0.63
1:G:70:ASN:ND2	2:l:2:BDP:O6B	2.31	0.63
1:L:147:ILE:HD11	2:v:1:BGC:H6C1	1.81	0.63
1:L:34:GLY:O	1:L:38:ASN:ND2	2.31	0.63
1:R:85:GLN:HG2	1:R:92:ILE:HD12	1.80	0.63
1:W:128:SER:HB3	1:W:134:UNK:HA	1.80	0.63
1:C:122:GLU:OE2	1:C:122:GLU:N	2.31	0.63
1:O:44:GLN:NE2	1:O:45:SER:OG	2.32	0.63
1:O:102:ILE:HB	1:O:164:GLN:HB3	1.80	0.63
1:Q:85:GLN:HG2	1:Q:89:ALA:HB3	1.81	0.62
1:L:39:THR:HG21	1:N:22:PHE:HZ	1.63	0.62
1:I:13:GLN:NE2	1:P:25:MET:SD	2.72	0.62
1:E:44:GLN:O	1:E:48:SER:OG	2.17	0.62
1:T:99:ILE:HG21	1:T:148:MET:HE1	1.80	0.62
1:V:62:ILE:HD11	1:V:92:ILE:HG21	1.82	0.61
1:K:174:LYS:HD3	1:L:65:VAL:HG13	1.82	0.61
1:L:162:GLU:HG3	1:L:180:GLN:HE21	1.65	0.61
1:E:137:LEU:HG	1:E:144:ILE:HD12	1.83	0.61
1:M:81:LEU:HB2	1:M:146:VAL:HG22	1.82	0.61
1:S:58:VAL:O	1:S:61:ARG:NH1	2.33	0.61
1:G:62:ILE:HD11	1:G:92:ILE:HG21	1.83	0.61
1:Q:70:ASN:ND2	2:5:2:BDP:O6B	2.34	0.60
1:X:62:ILE:HD11	1:X:92:ILE:HG21	1.83	0.60
1:I:170:GLN:O	1:J:143:ARG:NH2	2.34	0.60
1:V:116:UNK:O	1:V:119:UNK:N	2.34	0.60
1:D:16:ILE:HG21	1:E:22:PHE:HE1	1.65	0.60
1:W:91:ASN:HD22	1:W:138:VAL:HG12	1.66	0.60
1:X:137:LEU:HD12	1:X:144:ILE:HD12	1.83	0.60
1:Q:85:GLN:NE2	1:Q:89:ALA:O	2.34	0.60
1:J:95:UNK:HA	1:J:112:TYR:HD2	1.66	0.60
1:R:46:LYS:NZ	1:W:59:SER:OG	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:21:VAL:HG12	1:U:25:MET:HE2	1.84	0.60
1:U:27:LEU:O	1:U:31:ILE:HD12	2.02	0.60
1:O:90:ASP:OD2	1:O:91:ASN:N	2.31	0.60
1:D:125:THR:O	1:D:147:ILE:N	2.26	0.59
1:E:46:LYS:NZ	1:F:88:GLY:O	2.28	0.59
1:J:60:ASN:O	1:J:173:SER:OG	2.16	0.59
1:N:46:LYS:NZ	1:O:88:GLY:O	2.33	0.59
1:B:99:ILE:HG12	1:B:167:VAL:HG22	1.83	0.59
1:X:105:ASP:OD2	1:X:106:UNK:N	2.35	0.59
1:N:147:ILE:HD11	2:z:1:BGC:H6C1	1.84	0.59
1:P:85:GLN:NE2	1:P:90:ASP:O	2.36	0.59
1:K:166:THR:HG22	1:K:176:THR:HG22	1.83	0.59
1:D:189:ASN:ND2	1:X:105:ASP:O	2.36	0.58
1:M:126:THR:HG22	1:M:146:VAL:HG12	1.86	0.58
1:B:28:VAL:HG21	1:C:36:LEU:HG	1.85	0.58
1:X:128:SER:HA	1:X:144:ILE:HG23	1.85	0.58
1:R:53:GLU:OE1	1:W:140:GLN:NE2	2.37	0.58
1:H:85:GLN:NE2	1:H:90:ASP:O	2.37	0.57
1:N:34:GLY:O	1:N:38:ASN:ND2	2.37	0.57
1:S:19:LEU:HA	1:S:22:PHE:HB3	1.86	0.57
1:U:126:THR:HG22	1:U:146:VAL:HG22	1.86	0.57
1:D:122:GLU:N	1:D:122:GLU:OE2	2.38	0.57
1:D:128:SER:HA	1:D:144:ILE:HG23	1.85	0.57
1:E:136:VAL:HG11	1:N:186:LYS:HG3	1.85	0.57
1:N:70:ASN:OD1	1:N:71:VAL:N	2.36	0.57
1:C:100:GLN:HG3	1:C:109:THR:HG22	1.86	0.57
1:D:119:UNK:N	1:D:125:THR:OG1	2.37	0.57
1:D:77:ASP:OD2	1:D:77:ASP:N	2.34	0.57
1:N:70:ASN:ND2	2:z:2:BDP:O6B	2.37	0.57
1:S:85:GLN:NE2	1:S:89:ALA:O	2.38	0.57
1:I:112:TYR:HD1	1:I:113:UNK:N	2.03	0.57
1:L:85:GLN:HG2	1:L:89:ALA:HB3	1.86	0.57
1:I:85:GLN:HG2	1:I:92:ILE:HD12	1.85	0.56
1:A:162:GLU:OE2	1:A:162:GLU:N	2.38	0.56
1:D:26:VAL:HG11	1:M:51:GLY:HA2	1.85	0.56
1:N:169:THR:HG22	1:N:170:GLN:H	1.70	0.56
1:U:85:GLN:HB3	1:U:89:ALA:HB3	1.87	0.56
1:C:171:TYR:OH	1:K:183:GLU:OE1	2.23	0.56
1:N:23:ILE:HG23	1:U:50:THR:HG21	1.88	0.56
1:O:53:GLU:OE2	1:S:140:GLN:NE2	2.39	0.56
1:R:60:ASN:HD22	1:R:90:ASP:H	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ALA:HB1	1:E:92:ILE:HD11	1.88	0.56
1:F:23:ILE:HG23	1:O:50:THR:HG21	1.87	0.56
1:M:85:GLN:HB3	1:M:89:ALA:HB3	1.88	0.56
1:Q:42:TYR:HE1	1:R:52:GLU:HA	1.71	0.56
1:Q:193:LEU:H	1:Q:193:LEU:HD23	1.70	0.56
1:D:116:UNK:O	1:D:119:UNK:N	2.39	0.56
1:K:34:GLY:O	1:K:38:ASN:ND2	2.39	0.56
1:O:19:LEU:HD12	1:V:43:LEU:HD12	1.86	0.56
1:L:14:VAL:O	1:L:18:THR:OG1	2.23	0.56
1:T:61:ARG:HB2	1:T:61:ARG:NH1	2.21	0.56
1:J:128:SER:HB3	1:J:134:UNK:HA	1.86	0.55
1:E:108:THR:OG1	1:E:109:THR:N	2.39	0.55
1:E:147:ILE:HD11	2:h:1:BGC:H6C1	1.88	0.55
1:G:128:SER:HA	1:G:144:ILE:HG23	1.88	0.55
1:P:174:LYS:HD2	1:Q:65:VAL:HG13	1.88	0.55
1:L:50:THR:HG21	1:M:23:ILE:HG23	1.88	0.55
1:U:27:LEU:O	1:U:30:ALA:N	2.40	0.55
1:D:126:THR:HG22	1:D:146:VAL:HG12	1.87	0.55
1:I:111:THR:OG1	1:I:112:TYR:N	2.40	0.55
1:M:108:THR:OG1	1:M:109:THR:N	2.38	0.55
1:U:30:ALA:O	1:U:34:GLY:N	2.39	0.55
1:D:80:ASN:HB3	1:D:145:LYS:HD2	1.88	0.55
1:J:125:THR:O	1:J:147:ILE:N	2.29	0.55
1:P:100:GLN:HE21	1:P:102:ILE:HD11	1.71	0.55
1:F:105:ASP:O	1:P:189:ASN:ND2	2.39	0.54
1:N:100:GLN:OE1	1:O:66:SER:OG	2.22	0.54
1:U:44:GLN:NE2	1:U:45:SER:OG	2.41	0.54
1:J:126:THR:HG22	1:J:146:VAL:HG12	1.88	0.54
1:Q:105:ASP:O	1:R:189:ASN:ND2	2.41	0.54
1:P:16:ILE:HD11	1:S:36:LEU:HB3	1.90	0.54
1:A:99:ILE:HG21	1:A:148:MET:HE1	1.90	0.54
1:M:22:PHE:O	1:M:26:VAL:HG23	2.08	0.54
1:B:64:ILE:HD13	1:B:81:LEU:HD13	1.89	0.54
1:O:193:LEU:HD12	1:O:193:LEU:H	1.72	0.54
1:N:105:ASP:O	1:O:189:ASN:ND2	2.41	0.54
1:R:60:ASN:ND2	1:R:90:ASP:H	2.06	0.53
1:C:147:ILE:HD11	2:d:1:BGC:H6C1	1.90	0.53
1:Q:126:THR:HG22	1:Q:146:VAL:HG12	1.90	0.53
1:V:54:ALA:O	1:V:58:VAL:HG22	2.08	0.53
1:N:115:UNK:O	1:N:119:UNK:N	2.40	0.53
1:Q:125:THR:O	1:Q:147:ILE:N	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:115:UNK:O	1:U:119:UNK:N	2.41	0.53
1:E:19:LEU:HD21	1:M:35:VAL:HG11	1.89	0.53
1:F:100:GLN:HG3	1:F:109:THR:HG22	1.91	0.53
1:N:76:VAL:HB	1:N:157:LEU:HB2	1.89	0.53
1:N:85:GLN:HB2	1:N:89:ALA:HB3	1.90	0.53
1:Y:128:SER:HA	1:Y:144:ILE:HG23	1.90	0.53
1:D:25:MET:HA	1:D:28:VAL:HG22	1.90	0.53
1:Q:179:ALA:HB1	1:Q:193:LEU:HD12	1.90	0.53
1:P:169:THR:HG22	1:P:170:GLN:H	1.74	0.53
1:B:60:ASN:O	1:B:173:SER:OG	2.25	0.53
1:O:163:VAL:HB	1:O:179:ALA:HB3	1.90	0.53
1:Q:13:GLN:HG3	1:S:25:MET:HE1	1.91	0.53
1:Q:15:GLY:HA3	1:S:28:VAL:HG22	1.90	0.53
1:E:74:UNK:HA	1:E:185:LEU:HD11	1.91	0.52
1:A:81:LEU:HD11	1:A:165:LEU:HD22	1.90	0.52
1:L:85:GLN:NE2	1:L:137:LEU:O	2.42	0.52
1:L:108:THR:OG1	1:L:109:THR:N	2.42	0.52
1:F:53:GLU:OE1	1:P:140:GLN:NE2	2.42	0.52
1:G:83:VAL:HG21	1:G:94:LEU:HD11	1.90	0.52
1:L:25:MET:SD	1:N:13:GLN:N	2.83	0.52
1:N:58:VAL:O	1:N:61:ARG:NH1	2.42	0.52
1:H:91:ASN:HD22	1:H:138:VAL:HA	1.75	0.52
1:I:108:THR:OG1	1:I:109:THR:N	2.43	0.52
1:L:150:ALA:HB1	1:L:157:LEU:HD13	1.91	0.52
1:V:95:UNK:HA	1:V:112:TYR:HD1	1.75	0.52
1:M:102:ILE:HB	1:M:164:GLN:HB3	1.91	0.52
1:S:21:VAL:O	1:S:25:MET:HG2	2.10	0.52
1:T:81:LEU:HB2	1:T:146:VAL:HG22	1.92	0.52
1:T:99:ILE:HG12	1:T:167:VAL:HG22	1.92	0.52
1:U:70:ASN:OD1	1:U:71:VAL:N	2.43	0.52
1:Y:85:GLN:HG2	1:Y:89:ALA:HB3	1.91	0.52
1:I:53:GLU:OE1	1:J:140:GLN:NE2	2.42	0.52
1:U:147:ILE:HG21	2:DA:1:BGC:H6C1	1.92	0.52
1:B:174:LYS:HD2	1:C:65:VAL:HG13	1.91	0.52
1:I:95:UNK:HA	1:I:112:TYR:HD2	1.75	0.52
1:D:103:GLY:HA2	1:D:163:VAL:HG12	1.92	0.52
1:O:128:SER:HB3	1:O:134:UNK:HA	1.92	0.52
1:Q:60:ASN:HD21	1:Q:90:ASP:HB2	1.75	0.52
1:T:25:MET:SD	1:T:25:MET:N	2.80	0.52
2:AA:2:BDP:O6A	2:AA:3:A1H1V:O23	2.27	0.52
1:C:99:ILE:HG12	1:C:167:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:LEU:HD12	1:K:157:LEU:H	1.75	0.51
1:P:64:ILE:HD12	1:P:177:TYR:HB2	1.93	0.51
1:S:100:GLN:HE21	1:S:102:ILE:HD11	1.74	0.51
1:T:77:ASP:OD1	1:T:78:TYR:N	2.44	0.51
1:V:128:SER:HB3	1:V:134:UNK:HA	1.91	0.51
1:S:24:ALA:O	1:S:28:VAL:HG12	2.10	0.51
1:D:36:LEU:HB3	1:X:28:VAL:HG21	1.92	0.51
1:E:170:GLN:HG3	1:F:141:SER:HB3	1.93	0.51
1:L:81:LEU:HB2	1:L:146:VAL:HB	1.93	0.51
1:W:70:ASN:ND2	2:HA:2:BDP:O6B	2.44	0.51
1:D:71:VAL:HG23	1:D:190:ALA:HA	1.92	0.51
1:M:193:LEU:HD12	1:M:193:LEU:H	1.76	0.51
1:I:59:SER:OG	1:I:88:GLY:O	2.28	0.51
1:V:42:TYR:HD2	1:V:43:LEU:HD23	1.76	0.51
1:J:112:TYR:HD1	1:J:113:UNK:N	2.08	0.51
1:X:100:GLN:HG3	1:X:109:THR:HG22	1.93	0.51
1:U:29:ALA:O	1:U:33:ALA:N	2.24	0.51
1:I:37:ILE:HG21	1:Q:61:ARG:CZ	2.41	0.50
1:Q:46:LYS:NZ	1:R:90:ASP:OD2	2.43	0.50
1:Y:25:MET:HA	1:Y:28:VAL:HG22	1.92	0.50
1:M:147:ILE:HD13	2:x:1:BGC:H6C1	1.93	0.50
1:W:18:THR:O	1:W:22:PHE:N	2.37	0.50
1:W:179:ALA:HB1	1:W:193:LEU:HD23	1.92	0.50
2:GA:2:BDP:O6A	2:GA:3:A1H1V:O23	2.28	0.50
1:E:19:LEU:HD13	1:N:43:LEU:HB3	1.92	0.50
1:N:55:SER:O	1:N:59:SER:OG	2.30	0.50
1:R:27:LEU:O	1:R:31:ILE:HD12	2.12	0.50
1:W:34:GLY:O	1:W:38:ASN:ND2	2.43	0.50
1:N:163:VAL:HB	1:N:179:ALA:HB3	1.92	0.50
1:P:60:ASN:OD1	1:P:90:ASP:N	2.39	0.50
1:X:60:ASN:HD22	1:X:171:TYR:HE1	1.59	0.50
1:B:32:ALA:HA	1:X:19:LEU:HD21	1.93	0.50
1:F:168:THR:HG22	1:F:174:LYS:HG2	1.92	0.50
1:L:44:GLN:O	1:L:48:SER:OG	2.21	0.50
1:F:16:ILE:HG21	1:P:22:PHE:HE1	1.75	0.50
1:J:160:GLY:H	1:J:181:VAL:HG13	1.77	0.50
1:W:169:THR:HG22	1:W:170:GLN:H	1.77	0.50
1:A:145:LYS:HZ3	1:A:147:ILE:HD11	1.76	0.50
1:I:182:PRO:HG2	1:I:191:VAL:HB	1.93	0.50
1:D:37:ILE:HG21	1:M:61:ARG:CZ	2.41	0.50
1:T:81:LEU:HD11	1:T:165:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HE2	1:B:191:VAL:HG12	1.94	0.50
1:D:22:PHE:O	1:D:26:VAL:HG23	2.12	0.50
1:P:121:UNK:C	1:P:123:ASN:H	2.25	0.50
1:Q:121:UNK:C	1:Q:123:ASN:H	2.25	0.50
1:U:37:ILE:O	1:U:41:GLY:N	2.42	0.50
1:C:34:GLY:O	1:C:38:ASN:ND2	2.45	0.49
1:L:19:LEU:O	1:L:23:ILE:HG13	2.12	0.49
1:D:20:ILE:HD11	1:E:26:VAL:HG12	1.94	0.49
1:P:16:ILE:HG21	1:Q:22:PHE:HE1	1.76	0.49
1:T:62:ILE:HG23	1:T:83:VAL:HB	1.95	0.49
1:C:13:GLN:HG3	1:J:25:MET:HE3	1.94	0.49
1:E:60:ASN:HD22	1:E:90:ASP:H	1.61	0.49
1:Q:22:PHE:HA	1:Q:25:MET:HB2	1.93	0.49
1:B:95:UNK:HA	1:B:112:TYR:HD1	1.77	0.49
1:F:76:VAL:HB	1:F:157:LEU:HB2	1.94	0.49
1:B:115:UNK:O	1:B:119:UNK:N	2.46	0.49
1:I:181:VAL:HA	1:I:193:LEU:HD22	1.93	0.49
1:M:61:ARG:HG3	1:M:173:SER:HB2	1.93	0.49
1:O:71:VAL:HG21	1:O:191:VAL:HG13	1.94	0.49
1:Q:95:UNK:HA	1:Q:112:TYR:HD1	1.77	0.49
1:Y:85:GLN:NE2	1:Y:90:ASP:O	2.46	0.49
1:I:66:SER:OG	1:I:67:ALA:N	2.46	0.49
1:B:137:LEU:HD21	1:B:144:ILE:HG22	1.95	0.49
1:H:148:MET:HE1	1:H:165:LEU:HD21	1.95	0.49
1:O:35:VAL:HG13	1:O:36:LEU:HD12	1.93	0.49
1:T:108:THR:OG1	1:T:109:THR:N	2.45	0.49
1:V:108:THR:OG1	1:V:109:THR:N	2.45	0.49
1:V:46:LYS:O	1:V:50:THR:HG23	2.12	0.49
1:D:53:GLU:OE2	1:E:140:GLN:NE2	2.45	0.49
1:O:27:LEU:O	1:O:31:ILE:HG13	2.13	0.49
1:W:99:ILE:HG12	1:W:167:VAL:HG22	1.95	0.49
1:C:60:ASN:HD21	1:C:90:ASP:HB3	1.78	0.48
1:V:97:SER:OG	1:V:168:THR:O	2.27	0.48
1:N:85:GLN:NE2	1:N:137:LEU:O	2.46	0.48
1:N:171:TYR:O	1:O:84:ARG:NH1	2.46	0.48
1:H:37:ILE:HG21	1:P:61:ARG:CZ	2.44	0.48
1:K:136:VAL:HG11	1:W:186:LYS:HG3	1.95	0.48
1:N:193:LEU:HD12	1:N:193:LEU:H	1.78	0.48
1:R:126:THR:HG22	1:R:146:VAL:HG12	1.95	0.48
1:V:112:TYR:HD2	1:V:113:UNK:N	2.10	0.48
1:B:126:THR:HB	1:B:144:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:96:LYS:NZ	2:6:1:BGC:O5	2.47	0.48
1:I:95:UNK:HA	1:I:112:TYR:CD2	2.49	0.48
1:T:64:ILE:HD13	1:T:81:LEU:HD13	1.95	0.48
1:V:148:MET:HE1	1:V:165:LEU:HD21	1.95	0.48
1:C:35:VAL:HA	1:C:38:ASN:HD22	1.79	0.48
1:D:64:ILE:HD13	1:D:81:LEU:HD23	1.96	0.48
1:W:27:LEU:O	1:W:31:ILE:HG13	2.13	0.48
1:F:13:GLN:N	1:N:25:MET:SD	2.87	0.48
1:H:125:THR:O	1:H:147:ILE:N	2.39	0.48
1:U:29:ALA:HA	1:U:32:ALA:HB3	1.96	0.48
1:B:125:THR:O	1:B:147:ILE:N	2.32	0.48
1:I:174:LYS:HD3	1:J:65:VAL:HG13	1.96	0.48
1:L:19:LEU:HD11	1:W:32:ALA:HA	1.96	0.48
1:B:13:GLN:HB2	1:C:25:MET:HE3	1.96	0.47
1:C:178:TRP:CG	1:X:45:SER:HG	2.32	0.47
1:F:22:PHE:O	1:F:26:VAL:HG23	2.14	0.47
1:F:99:ILE:HG12	1:F:167:VAL:HG22	1.96	0.47
1:W:125:THR:O	1:W:147:ILE:N	2.28	0.47
1:D:166:THR:O	1:D:166:THR:OG1	2.31	0.47
1:A:42:TYR:CE2	1:B:52:GLU:HG3	2.49	0.47
1:B:77:ASP:OD1	1:B:77:ASP:N	2.47	0.47
1:E:185:LEU:HD12	1:E:185:LEU:O	2.14	0.47
1:E:33:ALA:O	1:E:37:ILE:HG12	2.14	0.47
1:P:122:GLU:OE1	1:P:122:GLU:N	2.34	0.47
1:Q:169:THR:HG22	1:Q:170:GLN:H	1.79	0.47
1:T:27:LEU:O	1:T:31:ILE:HG12	2.14	0.47
1:Y:174:LYS:NZ	1:Y:174:LYS:HB3	2.28	0.47
1:A:99:ILE:O	1:A:110:LEU:N	2.48	0.47
1:J:166:THR:O	1:J:166:THR:OG1	2.31	0.47
1:N:136:VAL:HG21	1:U:186:LYS:HG3	1.97	0.47
1:S:61:ARG:NH1	1:S:61:ARG:HB2	2.29	0.47
1:U:55:SER:O	1:U:59:SER:OG	2.31	0.47
1:X:166:THR:O	1:X:166:THR:OG1	2.32	0.47
2:k:2:BDP:O6A	2:k:3:A1H1V:O23	2.32	0.47
1:B:121:UNK:O	1:B:123:ASN:N	2.47	0.47
1:L:183:GLU:OE1	1:M:170:GLN:NE2	2.46	0.47
1:Q:76:VAL:HB	1:Q:157:LEU:HB2	1.96	0.47
1:U:31:ILE:O	1:U:35:VAL:HG12	2.15	0.47
1:U:100:GLN:HE21	1:U:102:ILE:HD11	1.79	0.47
1:B:23:ILE:HG23	1:J:50:THR:HG21	1.97	0.47
1:G:76:VAL:HG11	1:G:193:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ASN:HD22	1:G:138:VAL:HA	1.80	0.47
1:N:33:ALA:O	1:N:37:ILE:HG13	2.15	0.47
1:U:14:VAL:O	1:U:18:THR:HG23	2.14	0.47
1:C:19:LEU:O	1:C:23:ILE:HG13	2.15	0.47
1:V:80:ASN:HD22	1:V:145:LYS:HD2	1.80	0.47
1:D:28:VAL:HG11	1:E:36:LEU:HB3	1.98	0.46
1:J:100:GLN:NE2	1:K:66:SER:OG	2.46	0.46
1:B:33:ALA:O	1:B:37:ILE:HD12	2.15	0.46
1:N:185:LEU:HD23	1:N:191:VAL:HG11	1.97	0.46
1:S:96:LYS:HB2	1:S:170:GLN:HB2	1.97	0.46
1:C:169:THR:HG22	1:C:170:GLN:H	1.80	0.46
1:M:25:MET:HA	1:M:28:VAL:HG12	1.96	0.46
1:R:19:LEU:HD21	1:T:32:ALA:HA	1.97	0.46
1:K:19:LEU:HD21	1:R:32:ALA:HA	1.97	0.46
1:V:85:GLN:NE2	1:V:139:ASP:O	2.48	0.46
1:W:70:ASN:OD1	1:W:71:VAL:N	2.49	0.46
1:X:148:MET:HE1	1:X:165:LEU:HD21	1.98	0.46
1:Y:64:ILE:HD12	1:Y:177:TYR:HB2	1.97	0.46
1:D:95:UNK:HA	1:D:112:TYR:HD1	1.80	0.46
1:F:186:LYS:HB3	1:F:186:LYS:HE2	1.53	0.46
1:R:166:THR:O	1:R:166:THR:OG1	2.32	0.46
1:L:60:ASN:N	1:L:60:ASN:OD1	2.49	0.46
1:Q:13:GLN:HA	1:Q:16:ILE:HD12	1.98	0.46
1:E:193:LEU:HD12	1:E:193:LEU:H	1.81	0.46
1:J:90:ASP:N	1:J:90:ASP:OD1	2.48	0.46
1:U:13:GLN:HA	1:U:16:ILE:HD12	1.98	0.46
1:C:96:LYS:HZ3	2:e:1:BGC:H6C2	1.80	0.46
1:E:112:TYR:HD2	1:E:113:UNK:N	2.14	0.46
1:I:80:ASN:HB3	1:I:147:ILE:HD13	1.98	0.46
1:U:15:GLY:O	1:U:18:THR:OG1	2.29	0.46
1:U:31:ILE:HD12	1:U:31:ILE:H	1.81	0.46
1:Y:56:ALA:HB1	1:Y:60:ASN:HD21	1.81	0.46
1:K:169:THR:HG22	1:K:170:GLN:H	1.81	0.45
1:M:85:GLN:NE2	1:M:89:ALA:O	2.49	0.45
1:B:112:TYR:HD2	1:B:113:UNK:N	2.14	0.45
1:V:39:THR:O	1:V:43:LEU:HG	2.16	0.45
1:Y:124:PHE:HD2	1:Y:146:VAL:HG13	1.80	0.45
1:T:163:VAL:HG23	1:T:179:ALA:HB3	1.98	0.45
1:W:24:ALA:O	1:W:28:VAL:HG12	2.17	0.45
1:A:81:LEU:HB2	1:A:146:VAL:HB	1.97	0.45
1:B:126:THR:HG22	1:B:146:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:28:VAL:HG23	1:W:40:ALA:HB2	1.99	0.45
1:U:64:ILE:HG21	1:U:177:TYR:HD1	1.81	0.45
1:X:19:LEU:O	1:X:23:ILE:HG13	2.16	0.45
1:H:108:THR:OG1	1:H:109:THR:N	2.49	0.45
1:O:64:ILE:HD12	1:O:64:ILE:H	1.81	0.45
1:Q:27:LEU:O	1:Q:31:ILE:HG12	2.17	0.45
1:B:80:ASN:OD1	1:B:80:ASN:N	2.50	0.45
1:B:122:GLU:OE2	1:B:122:GLU:N	2.30	0.45
1:L:70:ASN:OD1	1:L:71:VAL:N	2.50	0.45
1:Y:100:GLN:HB2	1:Y:166:THR:OG1	2.17	0.45
1:S:19:LEU:HD12	1:S:19:LEU:H	1.82	0.45
1:T:60:ASN:HD21	1:T:171:TYR:HD1	1.63	0.45
1:U:48:SER:O	1:U:52:GLU:HG3	2.17	0.45
1:V:25:MET:SD	1:V:25:MET:N	2.90	0.45
1:G:166:THR:O	1:G:166:THR:OG1	2.29	0.45
1:K:147:ILE:HD11	2:t:1:BGC:H6C1	1.98	0.45
1:S:91:ASN:HD21	1:S:138:VAL:HG23	1.81	0.45
1:T:147:ILE:HD13	2:BA:1:BGC:H6C1	1.98	0.45
1:B:108:THR:OG1	1:B:109:THR:N	2.50	0.45
1:I:128:SER:HB3	1:I:134:UNK:HA	1.97	0.45
1:I:141:SER:HA	1:I:143:ARG:HH12	1.82	0.45
1:N:16:ILE:HG21	1:O:22:PHE:CE1	2.52	0.45
1:P:46:LYS:NZ	1:Q:90:ASP:OD2	2.48	0.45
1:U:169:THR:HG22	1:U:170:GLN:H	1.80	0.45
1:X:80:ASN:OD1	1:X:80:ASN:N	2.50	0.45
2:j:1:BGC:O3	2:j:2:BDP:O5	2.33	0.45
1:D:85:GLN:NE2	1:D:139:ASP:O	2.50	0.44
1:U:185:LEU:HD23	1:U:191:VAL:HG11	1.99	0.44
1:W:65:VAL:HG23	1:W:84:ARG:HG2	1.97	0.44
1:L:44:GLN:HG3	1:L:45:SER:N	2.32	0.44
1:L:103:GLY:HA2	1:L:163:VAL:HG12	2.00	0.44
1:Q:19:LEU:O	1:Q:23:ILE:HG13	2.18	0.44
1:X:31:ILE:O	1:X:35:VAL:HG23	2.17	0.44
1:X:128:SER:HB2	1:X:134:UNK:HA	1.98	0.44
1:H:121:UNK:C	1:H:123:ASN:H	2.31	0.44
1:P:62:ILE:O	1:P:175:THR:OG1	2.28	0.44
1:S:27:LEU:O	1:S:31:ILE:HG13	2.16	0.44
1:V:43:LEU:O	1:V:47:GLY:N	2.32	0.44
1:W:19:LEU:O	1:W:23:ILE:HG12	2.17	0.44
1:S:91:ASN:HD22	1:S:138:VAL:HA	1.83	0.44
1:E:53:GLU:HA	1:E:56:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:THR:HG22	1:E:170:GLN:H	1.83	0.44
1:L:115:UNK:O	1:L:119:UNK:N	2.50	0.44
1:N:52:GLU:H	1:N:52:GLU:CD	2.25	0.44
1:Y:34:GLY:O	1:Y:38:ASN:ND2	2.50	0.44
1:B:22:PHE:HZ	1:I:39:THR:HG21	1.82	0.44
1:F:37:ILE:HG21	1:O:61:ARG:CZ	2.48	0.44
1:S:100:GLN:HA	1:S:109:THR:HA	2.00	0.44
1:C:99:ILE:O	1:C:110:LEU:N	2.49	0.44
1:F:174:LYS:HD2	1:P:65:VAL:HG13	2.00	0.44
1:H:128:SER:HB3	1:H:134:UNK:HA	2.00	0.44
1:J:64:ILE:HD13	1:J:81:LEU:HD23	1.99	0.44
1:J:96:LYS:NZ	2:s:1:BGC:O5	2.51	0.44
1:V:32:ALA:O	1:V:36:LEU:HG	2.18	0.44
1:X:85:GLN:HB3	1:X:89:ALA:HB3	2.00	0.44
1:G:121:UNK:O	1:G:123:ASN:N	2.51	0.44
1:B:128:SER:HB2	1:B:134:UNK:HA	1.99	0.43
1:G:187:ASP:O	1:G:188:LYS:HD2	2.18	0.43
1:M:90:ASP:OD1	1:M:90:ASP:N	2.51	0.43
1:Y:147:ILE:HD11	2:LA:1:BGC:H6C1	2.00	0.43
1:A:170:GLN:HE22	1:I:183:GLU:CD	2.25	0.43
1:E:182:PRO:HG2	1:E:191:VAL:HG21	2.00	0.43
1:Q:112:TYR:HD2	1:Q:113:UNK:N	2.17	0.43
1:D:16:ILE:HG21	1:E:22:PHE:CE1	2.48	0.43
1:E:16:ILE:HG21	1:F:22:PHE:HE1	1.82	0.43
1:I:126:THR:O	1:I:126:THR:OG1	2.32	0.43
1:W:85:GLN:HG2	1:W:92:ILE:HD12	2.00	0.43
1:G:46:LYS:O	1:G:50:THR:HG22	2.18	0.43
1:H:94:LEU:HD23	1:H:94:LEU:HA	1.87	0.43
1:J:77:ASP:OD2	1:J:78:TYR:N	2.51	0.43
1:G:125:THR:H	1:G:147:ILE:HG22	1.82	0.43
1:S:147:ILE:HG12	2:9:1:BGC:H6C1	2.00	0.43
1:V:88:GLY:H	1:V:140:GLN:HE21	1.65	0.43
1:D:91:ASN:ND2	1:D:138:VAL:HA	2.34	0.43
1:I:189:ASN:OD1	1:I:189:ASN:C	2.62	0.43
1:M:185:LEU:HD23	1:M:191:VAL:HG11	2.00	0.43
1:U:35:VAL:O	1:U:39:THR:HG23	2.19	0.43
1:K:101:TRP:O	1:K:107:ALA:HA	2.19	0.43
1:U:147:ILE:O	1:U:147:ILE:HG13	2.18	0.43
1:V:147:ILE:HD13	1:V:147:ILE:HA	1.83	0.43
1:J:110:LEU:HD12	1:J:148:MET:HE3	2.01	0.43
1:J:129:ILE:HD11	1:J:145:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:35:VAL:O	1:N:39:THR:OG1	2.21	0.43
1:Q:91:ASN:ND2	1:Q:138:VAL:HG12	2.34	0.43
1:S:150:ALA:HB1	1:S:157:LEU:HD13	2.00	0.43
1:D:112:TYR:HD2	1:D:113:UNK:N	2.17	0.43
1:E:25:MET:SD	1:G:13:GLN:N	2.92	0.43
1:Q:80:ASN:OD1	1:Q:80:ASN:N	2.51	0.43
1:Q:91:ASN:HD21	1:Q:138:VAL:HG12	1.84	0.43
1:R:31:ILE:HG23	1:W:44:GLN:NE2	2.33	0.43
1:U:64:ILE:HG13	1:U:83:VAL:HG12	2.01	0.43
1:S:72:UNK:O	1:S:74:UNK:N	2.52	0.43
1:U:20:ILE:HA	1:U:23:ILE:HD12	2.01	0.43
1:E:84:ARG:HG3	1:E:85:GLN:O	2.19	0.42
1:N:62:ILE:HD11	1:N:92:ILE:HG21	2.01	0.42
1:U:39:THR:O	1:U:43:LEU:HG	2.19	0.42
1:L:64:ILE:HD13	1:L:81:LEU:HD22	2.02	0.42
1:L:91:ASN:ND2	1:L:138:VAL:HG12	2.33	0.42
1:O:85:GLN:HG2	1:O:92:ILE:HD12	2.00	0.42
1:R:186:LYS:HD2	1:R:186:LYS:HA	1.84	0.42
1:U:62:ILE:O	1:U:175:THR:OG1	2.31	0.42
1:W:147:ILE:HD13	1:W:147:ILE:HA	1.78	0.42
1:U:71:VAL:HG22	1:U:76:VAL:HG22	2.01	0.42
1:W:126:THR:HG22	1:W:146:VAL:HG12	2.02	0.42
1:G:77:ASP:OD1	1:G:77:ASP:C	2.61	0.42
1:R:64:ILE:HG12	1:R:83:VAL:HG12	2.01	0.42
1:S:90:ASP:CG	1:S:91:ASN:H	2.27	0.42
1:A:27:LEU:O	1:A:31:ILE:HG13	2.20	0.42
1:L:60:ASN:O	1:L:173:SER:OG	2.21	0.42
1:T:26:VAL:HG23	1:T:27:LEU:HD12	2.01	0.42
1:U:31:ILE:O	1:U:35:VAL:N	2.45	0.42
1:W:22:PHE:C	1:W:22:PHE:CD2	2.97	0.42
1:A:100:GLN:HE21	1:A:102:ILE:HD11	1.84	0.42
1:C:91:ASN:OD1	1:C:138:VAL:HA	2.20	0.42
1:C:100:GLN:NE2	1:M:66:SER:OG	2.52	0.42
1:F:100:GLN:HA	1:F:109:THR:HA	2.01	0.42
1:M:44:GLN:NE2	1:M:45:SER:OG	2.52	0.42
1:O:60:ASN:ND2	1:O:90:ASP:H	2.17	0.42
1:P:62:ILE:HD11	1:P:94:LEU:HD21	2.01	0.42
1:T:48:SER:O	1:T:52:GLU:HG2	2.20	0.42
1:W:166:THR:O	1:W:166:THR:OG1	2.34	0.42
1:C:61:ARG:CZ	1:X:37:ILE:HG21	2.49	0.42
1:D:33:ALA:O	1:D:37:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:THR:HG22	1:D:170:GLN:H	1.85	0.42
1:G:169:THR:HG22	1:G:170:GLN:N	2.35	0.42
1:K:169:THR:HG22	1:K:170:GLN:N	2.34	0.42
1:M:41:GLY:O	1:M:44:GLN:HG3	2.20	0.42
1:D:163:VAL:HG23	1:D:179:ALA:HB3	2.02	0.42
1:D:112:TYR:C	1:D:112:TYR:CD2	2.98	0.42
1:N:81:LEU:HD13	1:N:148:MET:HE3	2.00	0.42
1:X:125:THR:O	1:X:147:ILE:HG22	2.19	0.42
1:D:13:GLN:N	1:D:13:GLN:OE1	2.53	0.42
1:E:148:MET:HE2	1:E:148:MET:HB3	1.85	0.42
1:F:26:VAL:HG11	1:O:51:GLY:HA2	2.01	0.42
1:F:183:GLU:CD	1:G:170:GLN:HE22	2.28	0.42
1:G:70:ASN:HB2	2:I:1:BGC:O2	2.20	0.42
1:M:128:SER:HB2	1:M:134:UNK:HA	2.02	0.42
1:P:70:ASN:ND2	2:3:2:BDP:O6B	2.53	0.42
1:V:84:ARG:NH1	1:V:85:GLN:O	2.52	0.42
1:C:50:THR:HG21	1:X:23:ILE:HG23	2.02	0.41
1:D:147:ILE:HD13	1:D:147:ILE:HA	1.88	0.41
1:Q:119:UNK:N	1:Q:149:TYR:HB2	2.35	0.41
1:A:13:GLN:NE2	1:B:18:THR:HG23	2.34	0.41
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.81	0.41
1:B:157:LEU:HD21	1:B:163:VAL:HG23	2.02	0.41
1:E:67:ALA:HB2	1:E:81:LEU:HD23	2.01	0.41
1:K:14:VAL:O	1:K:18:THR:OG1	2.37	0.41
1:N:168:THR:HG23	1:N:174:LYS:HG2	2.01	0.41
1:P:121:UNK:O	1:P:123:ASN:N	2.53	0.41
1:R:125:THR:O	1:R:147:ILE:N	2.51	0.41
1:S:56:ALA:O	1:S:60:ASN:HB2	2.20	0.41
1:V:166:THR:O	1:V:166:THR:OG1	2.33	0.41
1:A:174:LYS:HD3	1:B:65:VAL:HG13	2.01	0.41
1:C:181:VAL:HG12	1:C:185:LEU:HD21	2.02	0.41
1:M:80:ASN:OD1	1:M:80:ASN:N	2.52	0.41
1:M:125:THR:O	1:M:147:ILE:N	2.43	0.41
1:O:53:GLU:O	1:O:57:GLN:N	2.53	0.41
1:Q:112:TYR:CD2	1:Q:112:TYR:C	2.99	0.41
1:R:193:LEU:HD12	1:R:193:LEU:H	1.85	0.41
1:W:169:THR:HG22	1:W:170:GLN:N	2.35	0.41
1:Y:39:THR:O	1:Y:43:LEU:HG	2.20	0.41
1:A:83:VAL:HG21	1:A:94:LEU:HD11	2.01	0.41
1:C:39:THR:HG21	1:D:22:PHE:CZ	2.54	0.41
1:C:80:ASN:OD1	1:C:80:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:GLN:HE21	1:D:137:LEU:HB3	1.86	0.41
1:J:72:UNK:O	1:J:74:UNK:N	2.53	0.41
1:L:67:ALA:HB2	1:L:81:LEU:HD23	2.01	0.41
1:R:125:THR:HG22	1:R:147:ILE:HB	2.03	0.41
1:W:77:ASP:O	1:W:150:ALA:N	2.54	0.41
1:W:101:TRP:CZ3	1:W:163:VAL:HG11	2.56	0.41
1:G:63:ASN:HD22	1:G:84:ARG:HH21	1.68	0.41
1:I:170:GLN:HE22	1:Q:183:GLU:HG2	1.85	0.41
1:L:72:UNK:O	1:L:74:UNK:N	2.53	0.41
1:O:22:PHE:CD1	1:O:22:PHE:C	2.97	0.41
1:A:28:VAL:HG23	1:B:40:ALA:HB2	2.03	0.41
1:G:22:PHE:O	1:G:26:VAL:HG23	2.21	0.41
1:N:39:THR:HG22	1:N:43:LEU:HD23	2.03	0.41
1:N:170:GLN:NE2	1:U:183:GLU:OE2	2.46	0.41
1:R:23:ILE:O	1:R:27:LEU:HD23	2.20	0.41
1:T:145:LYS:HB3	1:T:145:LYS:HE2	1.66	0.41
1:V:126:THR:OG1	1:V:134:UNK:O	2.38	0.41
1:X:46:LYS:HD2	1:X:46:LYS:O	2.21	0.41
1:B:112:TYR:HA	1:B:124:PHE:O	2.21	0.41
1:G:85:GLN:HG2	1:G:89:ALA:HB3	2.02	0.41
1:I:48:SER:O	1:I:52:GLU:HG2	2.20	0.41
1:O:102:ILE:HD13	1:O:102:ILE:HA	1.99	0.41
1:P:188:LYS:HD2	1:P:191:VAL:HG12	2.03	0.41
1:R:33:ALA:O	1:R:37:ILE:HD12	2.21	0.41
1:D:59:SER:O	1:D:61:ARG:N	2.54	0.41
1:G:170:GLN:HG3	1:H:141:SER:HB3	2.03	0.41
1:N:46:LYS:HA	1:N:46:LYS:HD3	1.91	0.41
1:U:128:SER:HB3	1:U:134:UNK:HA	2.02	0.41
1:V:112:TYR:C	1:V:112:TYR:CD2	2.99	0.41
1:B:101:TRP:O	1:B:107:ALA:HA	2.21	0.41
1:E:13:GLN:HG2	1:M:25:MET:SD	2.60	0.41
1:E:85:GLN:HB3	1:E:89:ALA:HB3	2.03	0.41
1:G:70:ASN:OD1	1:G:71:VAL:N	2.53	0.41
1:G:81:LEU:HB2	1:G:146:VAL:HB	2.01	0.41
1:G:147:ILE:HD12	1:G:147:ILE:HA	1.92	0.41
1:J:169:THR:HG22	1:J:170:GLN:N	2.36	0.41
1:J:170:GLN:O	1:K:143:ARG:NH2	2.54	0.41
1:K:37:ILE:H	1:K:37:ILE:HG13	1.63	0.41
1:M:64:ILE:HD12	1:M:177:TYR:HB2	2.02	0.41
1:N:22:PHE:O	1:N:26:VAL:HG23	2.21	0.41
1:P:91:ASN:HD22	1:P:138:VAL:HG12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:24:ALA:O	1:Q:28:VAL:HG12	2.21	0.41
1:R:145:LYS:HE2	1:R:145:LYS:HB3	1.84	0.41
1:Y:85:GLN:N	1:Y:137:LEU:HD22	2.35	0.41
1:Y:91:ASN:ND2	1:Y:138:VAL:HA	2.36	0.41
1:Y:148:MET:HE1	1:Y:165:LEU:HD21	2.03	0.41
1:Y:169:THR:HG22	1:Y:170:GLN:H	1.86	0.41
1:B:72:UNK:O	1:B:74:UNK:N	2.50	0.41
1:D:100:GLN:NE2	1:E:66:SER:OG	2.53	0.41
1:W:71:VAL:HG21	1:W:191:VAL:HG13	2.03	0.41
1:Y:97:SER:OG	1:Y:168:THR:O	2.32	0.41
1:E:37:ILE:HG21	1:N:61:ARG:NH2	2.36	0.40
1:F:50:THR:HG21	1:G:23:ILE:HG23	2.04	0.40
1:Q:64:ILE:HG12	1:Q:83:VAL:HG12	2.02	0.40
1:Y:144:ILE:HD12	1:Y:144:ILE:H	1.86	0.40
1:A:128:SER:HB2	1:A:134:UNK:HA	2.02	0.40
1:E:68:TYR:HA	1:E:192:UNK:HA	2.04	0.40
1:I:91:ASN:OD1	1:I:91:ASN:N	2.54	0.40
1:L:77:ASP:OD1	1:L:78:TYR:N	2.55	0.40
1:M:91:ASN:ND2	1:M:138:VAL:HG12	2.36	0.40
1:M:137:LEU:HD12	1:M:144:ILE:HD12	2.02	0.40
1:T:16:ILE:O	1:T:20:ILE:HG12	2.21	0.40
1:U:22:PHE:HA	1:U:25:MET:HE3	2.03	0.40
1:C:36:LEU:HD22	1:D:18:THR:HG21	2.03	0.40
1:C:163:VAL:HG22	1:C:179:ALA:HB3	2.04	0.40
1:D:42:TYR:C	1:D:42:TYR:CD1	2.99	0.40
1:I:28:VAL:HG23	1:J:40:ALA:HB2	2.03	0.40
1:I:94:LEU:HD23	1:I:94:LEU:HA	1.86	0.40
1:K:108:THR:OG1	1:K:109:THR:N	2.53	0.40
1:M:60:ASN:OD1	1:M:60:ASN:C	2.63	0.40
1:N:40:ALA:O	1:N:44:GLN:HG2	2.20	0.40
1:R:85:GLN:NE2	1:R:139:ASP:O	2.54	0.40
1:W:70:ASN:OD1	1:W:70:ASN:C	2.65	0.40
1:D:157:LEU:HD23	1:D:157:LEU:HA	1.89	0.40
1:E:79:VAL:O	1:E:148:MET:HB2	2.21	0.40
1:L:169:THR:HG22	1:L:170:GLN:H	1.86	0.40
1:K:13:GLN:NE2	1:O:14:VAL:HG11	2.32	0.40
1:T:72:UNK:O	1:T:74:UNK:N	2.54	0.40
1:X:129:ILE:HD13	1:X:129:ILE:HA	1.90	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	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	B	150/193 (78%)	146 (97%)	3 (2%)	1 (1%)	18	49
1	C	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	D	150/193 (78%)	142 (95%)	8 (5%)	0	100	100
1	E	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	F	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	G	150/193 (78%)	144 (96%)	5 (3%)	1 (1%)	18	49
1	H	150/193 (78%)	146 (97%)	3 (2%)	1 (1%)	18	49
1	I	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	J	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	K	150/193 (78%)	147 (98%)	3 (2%)	0	100	100
1	L	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	M	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	N	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	O	150/193 (78%)	142 (95%)	8 (5%)	0	100	100
1	P	150/193 (78%)	146 (97%)	3 (2%)	1 (1%)	18	49
1	Q	150/193 (78%)	143 (95%)	6 (4%)	1 (1%)	18	49
1	R	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
1	S	150/193 (78%)	142 (95%)	8 (5%)	0	100	100
1	T	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	U	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	V	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	W	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
1	X	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	Y	150/193 (78%)	146 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3750/4825 (78%)	3615 (96%)	130 (4%)	5 (0%)	49 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	GLU
1	G	122	GLU
1	Q	122	GLU
1	P	122	GLU
1	H	122	GLU

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	123/134 (92%)	123 (100%)	0	100 100
1	B	123/134 (92%)	123 (100%)	0	100 100
1	C	123/134 (92%)	123 (100%)	0	100 100
1	D	123/134 (92%)	122 (99%)	1 (1%)	73 78
1	E	123/134 (92%)	123 (100%)	0	100 100
1	F	123/134 (92%)	123 (100%)	0	100 100
1	G	123/134 (92%)	122 (99%)	1 (1%)	73 78
1	H	123/134 (92%)	123 (100%)	0	100 100
1	I	123/134 (92%)	123 (100%)	0	100 100
1	J	123/134 (92%)	123 (100%)	0	100 100
1	K	123/134 (92%)	123 (100%)	0	100 100
1	L	123/134 (92%)	123 (100%)	0	100 100
1	M	123/134 (92%)	122 (99%)	1 (1%)	73 78
1	N	123/134 (92%)	123 (100%)	0	100 100
1	O	123/134 (92%)	123 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	123/134 (92%)	122 (99%)	1 (1%)	73	78
1	Q	123/134 (92%)	122 (99%)	1 (1%)	73	78
1	R	123/134 (92%)	123 (100%)	0	100	100
1	S	123/134 (92%)	123 (100%)	0	100	100
1	T	123/134 (92%)	123 (100%)	0	100	100
1	U	123/134 (92%)	123 (100%)	0	100	100
1	V	123/134 (92%)	122 (99%)	1 (1%)	73	78
1	W	123/134 (92%)	123 (100%)	0	100	100
1	X	123/134 (92%)	122 (99%)	1 (1%)	73	78
1	Y	123/134 (92%)	123 (100%)	0	100	100
All	All	3075/3350 (92%)	3068 (100%)	7 (0%)	85	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	77	ASP
1	G	147	ILE
1	M	80	ASN
1	P	105	ASP
1	Q	169	THR
1	V	38	ASN
1	X	80	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	100	GLN
1	B	63	ASN
1	B	170	GLN
1	C	13	GLN
1	C	38	ASN
1	C	85	GLN
1	D	60	ASN
1	D	85	GLN
1	D	91	ASN
1	D	100	GLN

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Mol	Chain	Res	Type
1	E	13	GLN
1	E	44	GLN
1	G	13	GLN
1	G	85	GLN
1	G	91	ASN
1	H	13	GLN
1	H	85	GLN
1	H	91	ASN
1	H	100	GLN
1	H	170	GLN
1	I	13	GLN
1	I	63	ASN
1	J	85	GLN
1	J	100	GLN
1	K	13	GLN
1	K	38	ASN
1	K	85	GLN
1	L	13	GLN
1	L	38	ASN
1	L	85	GLN
1	L	100	GLN
1	L	123	ASN
1	L	180	GLN
1	M	44	GLN
1	M	63	ASN
1	M	85	GLN
1	N	38	ASN
1	N	57	GLN
1	N	85	GLN
1	N	180	GLN
1	O	44	GLN
1	O	60	ASN
1	O	85	GLN
1	P	13	GLN
1	P	38	ASN
1	P	85	GLN
1	P	164	GLN
1	Q	13	GLN
1	Q	60	ASN
1	Q	85	GLN
1	Q	91	ASN
1	R	13	GLN

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Mol	Chain	Res	Type
1	R	60	ASN
1	R	63	ASN
1	R	85	GLN
1	S	13	GLN
1	S	85	GLN
1	S	91	ASN
1	S	100	GLN
1	T	60	ASN
1	U	13	GLN
1	U	44	GLN
1	U	85	GLN
1	U	100	GLN
1	U	180	GLN
1	V	100	GLN
1	V	140	GLN
1	V	180	GLN
1	W	13	GLN
1	W	38	ASN
1	W	44	GLN
1	W	63	ASN
1	X	170	GLN
1	Y	38	ASN
1	Y	60	ASN
1	Y	63	ASN
1	Y	85	GLN
1	Y	91	ASN
1	Y	189	ASN

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 ⓘ

150 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	BGC	0	1	1,2	11,11,12	0.25	0	15,15,17	1.22	2 (13%)
2	BDP	0	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	0	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	5 (29%)
2	BGC	1	1	1,2	11,11,12	0.22	0	15,15,17	0.70	0
2	BDP	1	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.60	3 (21%)
2	A1H1V	1	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.58	4 (23%)
2	BGC	2	1	1,2	11,11,12	0.28	0	15,15,17	1.52	2 (13%)
2	BDP	2	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.48	2 (14%)
2	A1H1V	2	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.63	4 (23%)
2	BGC	3	1	1,2	11,11,12	0.19	0	15,15,17	0.57	0
2	BDP	3	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.59	4 (28%)
2	A1H1V	3	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	4 (23%)
2	BGC	4	1	1,2	11,11,12	0.24	0	15,15,17	1.11	2 (13%)
2	BDP	4	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	4	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.63	4 (23%)
2	BGC	5	1	1,2	11,11,12	0.24	0	15,15,17	0.71	0
2	BDP	5	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.62	4 (28%)
2	A1H1V	5	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	4 (23%)
2	BGC	6	1	1,2	11,11,12	0.21	0	15,15,17	0.88	1 (6%)
2	BDP	6	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	6	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	6 (35%)
2	BGC	7	1	1,2	11,11,12	0.20	0	15,15,17	0.65	0
2	BDP	7	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.49	2 (14%)
2	A1H1V	7	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	8	1	1,2	11,11,12	0.25	0	15,15,17	1.34	2 (13%)
2	BDP	8	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.51	2 (14%)
2	A1H1V	8	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.62	4 (23%)
2	BGC	9	1	1,2	11,11,12	0.22	0	15,15,17	0.57	0
2	BDP	9	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.47	2 (14%)
2	A1H1V	9	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	AA	1	1,2	11,11,12	0.21	0	15,15,17	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BDP	AA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	AA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	BA	1	1,2	11,11,12	0.20	0	15,15,17	0.55	0
2	BDP	BA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.54	2 (14%)
2	A1H1V	BA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	CA	1	1,2	11,11,12	0.17	0	15,15,17	0.52	0
2	BDP	CA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.61	2 (14%)
2	A1H1V	CA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	DA	1	1,2	11,11,12	0.23	0	15,15,17	0.68	0
2	BDP	DA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.57	3 (21%)
2	A1H1V	DA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	5 (29%)
2	BGC	EA	1	1,2	11,11,12	0.20	0	15,15,17	0.71	0
2	BDP	EA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	EA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.63	5 (29%)
2	BGC	FA	1	1,2	11,11,12	0.20	0	15,15,17	0.63	0
2	BDP	FA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.63	4 (28%)
2	A1H1V	FA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	4 (23%)
2	BGC	GA	1	1,2	11,11,12	0.18	0	15,15,17	0.50	0
2	BDP	GA	2	2	12,12,13	1.99	1 (8%)	14,17,19	1.54	3 (21%)
2	A1H1V	GA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.63	4 (23%)
2	BGC	HA	1	1,2	11,11,12	0.22	0	15,15,17	0.74	0
2	BDP	HA	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	HA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	IA	1	1,2	11,11,12	0.19	0	15,15,17	0.52	0
2	BDP	IA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	IA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.62	4 (23%)
2	BGC	JA	1	1,2	11,11,12	0.20	0	15,15,17	0.63	0
2	BDP	JA	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.64	3 (21%)
2	A1H1V	JA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	KA	1	1,2	11,11,12	0.25	0	15,15,17	1.22	2 (13%)
2	BDP	KA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.42	2 (14%)
2	A1H1V	KA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.62	6 (35%)
2	BGC	LA	1	1,2	11,11,12	0.20	0	15,15,17	0.52	0
2	BDP	LA	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.65	4 (28%)
2	A1H1V	LA	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	4 (23%)
2	BGC	MA	1	1,2	11,11,12	0.18	0	15,15,17	0.62	0
2	BDP	MA	2	2	12,12,13	1.99	1 (8%)	14,17,19	1.57	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H1V	MA	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.62	4 (23%)
2	BGC	Z	1	1,2	11,11,12	0.20	0	15,15,17	0.63	0
2	BDP	Z	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.55	2 (14%)
2	A1H1V	Z	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.58	4 (23%)
2	BGC	a	1	1,2	11,11,12	0.20	0	15,15,17	0.55	0
2	BDP	a	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.47	2 (14%)
2	A1H1V	a	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.56	4 (23%)
2	BGC	b	1	1,2	11,11,12	0.20	0	15,15,17	0.63	0
2	BDP	b	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.49	2 (14%)
2	A1H1V	b	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	5 (29%)
2	BGC	c	1	1,2	11,11,12	0.25	0	15,15,17	1.20	2 (13%)
2	BDP	c	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.58	2 (14%)
2	A1H1V	c	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	d	1	1,2	11,11,12	0.18	0	15,15,17	0.61	0
2	BDP	d	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.60	4 (28%)
2	A1H1V	d	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	4 (23%)
2	BGC	e	1	1,2	11,11,12	0.18	0	15,15,17	0.50	0
2	BDP	e	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.72	4 (28%)
2	A1H1V	e	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	f	1	1,2	11,11,12	0.18	0	15,15,17	0.51	0
2	BDP	f	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.60	4 (28%)
2	A1H1V	f	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.53	5 (29%)
2	BGC	g	1	1,2	11,11,12	0.22	0	15,15,17	0.97	2 (13%)
2	BDP	g	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.45	2 (14%)
2	A1H1V	g	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.61	6 (35%)
2	BGC	h	1	1,2	11,11,12	0.22	0	15,15,17	0.70	0
2	BDP	h	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.59	3 (21%)
2	A1H1V	h	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	4 (23%)
2	BGC	i	1	1,2	11,11,12	0.22	0	15,15,17	1.05	2 (13%)
2	BDP	i	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.48	2 (14%)
2	A1H1V	i	3	2	16,16,17	1.20	2 (12%)	17,24,26	1.44	4 (23%)
2	BGC	j	1	1,2	11,11,12	0.20	0	15,15,17	0.54	0
2	BDP	j	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.58	2 (14%)
2	A1H1V	j	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.56	4 (23%)
2	BGC	k	1	1,2	11,11,12	0.26	0	15,15,17	1.41	2 (13%)
2	BDP	k	2	2	12,12,13	1.99	1 (8%)	14,17,19	1.51	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H1V	k	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.62	4 (23%)
2	BGC	l	1	1,2	11,11,12	0.21	0	15,15,17	0.67	0
2	BDP	l	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.68	4 (28%)
2	A1H1V	l	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.59	4 (23%)
2	BGC	m	1	1,2	11,11,12	0.22	0	15,15,17	0.88	0
2	BDP	m	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.55	2 (14%)
2	A1H1V	m	3	2	16,16,17	1.20	2 (12%)	17,24,26	1.43	4 (23%)
2	BGC	n	1	1,2	11,11,12	0.23	0	15,15,17	0.92	1 (6%)
2	BDP	n	2	2	12,12,13	1.99	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	n	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.61	5 (29%)
2	BGC	o	1	1,2	11,11,12	0.21	0	15,15,17	0.83	1 (6%)
2	BDP	o	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.50	2 (14%)
2	A1H1V	o	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	p	1	1,2	11,11,12	0.17	0	15,15,17	0.70	0
2	BDP	p	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.43	2 (14%)
2	A1H1V	p	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.62	4 (23%)
2	BGC	q	1	1,2	11,11,12	0.23	0	15,15,17	1.00	1 (6%)
2	BDP	q	2	2	12,12,13	1.99	1 (8%)	14,17,19	1.55	2 (14%)
2	A1H1V	q	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	r	1	1,2	11,11,12	0.21	0	15,15,17	0.53	0
2	BDP	r	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	r	3	2	16,16,17	1.33	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	s	1	1,2	11,11,12	0.21	0	15,15,17	0.96	2 (13%)
2	BDP	s	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	s	3	2	16,16,17	1.21	2 (12%)	17,24,26	1.44	4 (23%)
2	BGC	t	1	1,2	11,11,12	0.20	0	15,15,17	0.52	0
2	BDP	t	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.50	2 (14%)
2	A1H1V	t	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	u	1	1,2	11,11,12	0.18	0	15,15,17	0.59	0
2	BDP	u	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.56	2 (14%)
2	A1H1V	u	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.60	5 (29%)
2	BGC	v	1	1,2	11,11,12	0.19	0	15,15,17	0.58	0
2	BDP	v	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.54	2 (14%)
2	A1H1V	v	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.59	4 (23%)
2	BGC	w	1	1,2	11,11,12	0.16	0	15,15,17	0.55	0
2	BDP	w	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.62	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H1V	w	3	2	16,16,17	1.34	3 (18%)	17,24,26	1.60	4 (23%)
2	BGC	x	1	1,2	11,11,12	0.20	0	15,15,17	0.58	0
2	BDP	x	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.53	2 (14%)
2	A1H1V	x	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.61	4 (23%)
2	BGC	y	1	1,2	11,11,12	0.24	0	15,15,17	1.17	2 (13%)
2	BDP	y	2	2	12,12,13	2.01	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	y	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.60	6 (35%)
2	BGC	z	1	1,2	11,11,12	0.20	0	15,15,17	0.70	0
2	BDP	z	2	2	12,12,13	2.00	1 (8%)	14,17,19	1.70	4 (28%)
2	A1H1V	z	3	2	16,16,17	1.35	3 (18%)	17,24,26	1.61	4 (23%)

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	BGC	0	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	0	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	0	3	2	-	3/9/26/29	0/1/1/1
2	BGC	1	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	1	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	1	3	2	-	3/9/26/29	0/1/1/1
2	BGC	2	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	2	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	2	3	2	-	3/9/26/29	0/1/1/1
2	BGC	3	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	3	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	3	3	2	-	3/9/26/29	0/1/1/1
2	BGC	4	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	4	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	4	3	2	-	3/9/26/29	0/1/1/1
2	BGC	5	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	5	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	5	3	2	-	3/9/26/29	0/1/1/1
2	BGC	6	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	6	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	6	3	2	-	3/9/26/29	0/1/1/1
2	BGC	7	1	1,2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	7	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	7	3	2	-	3/9/26/29	0/1/1/1
2	BGC	8	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	8	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	8	3	2	-	3/9/26/29	0/1/1/1
2	BGC	9	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	9	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	9	3	2	-	3/9/26/29	0/1/1/1
2	BGC	AA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	AA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	AA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	BA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	BA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	BA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	CA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	CA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	CA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	DA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	DA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	DA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	EA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	EA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	EA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	FA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	FA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	FA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	GA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	GA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	GA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	HA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	HA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	HA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	IA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	IA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	IA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	JA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	JA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	JA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	KA	1	1,2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	KA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	KA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	LA	1	1,2	1/1/4/5	1/2/19/22	0/1/1/1
2	BDP	LA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	LA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	MA	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	MA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	MA	3	2	-	3/9/26/29	0/1/1/1
2	BGC	Z	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	Z	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	Z	3	2	-	3/9/26/29	0/1/1/1
2	BGC	a	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	a	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	a	3	2	-	3/9/26/29	0/1/1/1
2	BGC	b	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	b	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	b	3	2	-	3/9/26/29	0/1/1/1
2	BGC	c	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	c	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	c	3	2	-	3/9/26/29	0/1/1/1
2	BGC	d	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	d	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	d	3	2	-	3/9/26/29	0/1/1/1
2	BGC	e	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	e	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	e	3	2	-	3/9/26/29	0/1/1/1
2	BGC	f	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	f	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	f	3	2	-	3/9/26/29	0/1/1/1
2	BGC	g	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	g	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	g	3	2	-	3/9/26/29	0/1/1/1
2	BGC	h	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	h	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	h	3	2	-	3/9/26/29	0/1/1/1
2	BGC	i	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	i	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	i	3	2	-	3/9/26/29	0/1/1/1
2	BGC	j	1	1,2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	j	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	j	3	2	-	3/9/26/29	0/1/1/1
2	BGC	k	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	k	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	k	3	2	-	3/9/26/29	0/1/1/1
2	BGC	l	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	l	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	l	3	2	-	3/9/26/29	0/1/1/1
2	BGC	m	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	m	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	m	3	2	-	3/9/26/29	0/1/1/1
2	BGC	n	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	n	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	n	3	2	-	3/9/26/29	0/1/1/1
2	BGC	o	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	o	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	o	3	2	-	3/9/26/29	0/1/1/1
2	BGC	p	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	p	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	p	3	2	-	3/9/26/29	0/1/1/1
2	BGC	q	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	q	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	q	3	2	-	3/9/26/29	0/1/1/1
2	BGC	r	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	r	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	r	3	2	-	3/9/26/29	0/1/1/1
2	BGC	s	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	s	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	s	3	2	-	3/9/26/29	0/1/1/1
2	BGC	t	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	t	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	t	3	2	-	3/9/26/29	0/1/1/1
2	BGC	u	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	u	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	u	3	2	-	3/9/26/29	0/1/1/1
2	BGC	v	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	v	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	v	3	2	-	3/9/26/29	0/1/1/1
2	BGC	w	1	1,2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	w	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	w	3	2	-	3/9/26/29	0/1/1/1
2	BGC	x	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	x	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	x	3	2	-	3/9/26/29	0/1/1/1
2	BGC	y	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	y	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	y	3	2	-	3/9/26/29	0/1/1/1
2	BGC	z	1	1,2	-	1/2/19/22	0/1/1/1
2	BDP	z	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	z	3	2	-	3/9/26/29	0/1/1/1

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	2	BDP	O6A-C6	6.84	1.42	1.22
2	c	2	BDP	O6A-C6	6.84	1.42	1.22
2	6	2	BDP	O6A-C6	6.83	1.42	1.22
2	o	2	BDP	O6A-C6	6.83	1.42	1.22
2	s	2	BDP	O6A-C6	6.83	1.42	1.22
2	2	2	BDP	O6A-C6	6.83	1.42	1.22
2	y	2	BDP	O6A-C6	6.82	1.42	1.22
2	b	2	BDP	O6A-C6	6.82	1.42	1.22
2	7	2	BDP	O6A-C6	6.82	1.42	1.22
2	j	2	BDP	O6A-C6	6.82	1.42	1.22
2	LA	2	BDP	O6A-C6	6.82	1.42	1.22
2	1	2	BDP	O6A-C6	6.82	1.42	1.22
2	HA	2	BDP	O6A-C6	6.81	1.42	1.22
2	5	2	BDP	O6A-C6	6.81	1.42	1.22
2	FA	2	BDP	O6A-C6	6.81	1.42	1.22
2	d	2	BDP	O6A-C6	6.81	1.42	1.22
2	JA	2	BDP	O6A-C6	6.81	1.42	1.22
2	9	2	BDP	O6A-C6	6.81	1.42	1.22
2	IA	2	BDP	O6A-C6	6.81	1.42	1.22
2	l	2	BDP	O6A-C6	6.81	1.42	1.22
2	4	2	BDP	O6A-C6	6.81	1.42	1.22
2	v	2	BDP	O6A-C6	6.81	1.42	1.22
2	h	2	BDP	O6A-C6	6.81	1.42	1.22
2	z	2	BDP	O6A-C6	6.81	1.42	1.22
2	p	2	BDP	O6A-C6	6.80	1.42	1.22
2	m	2	BDP	O6A-C6	6.80	1.42	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EA	2	BDP	O6A-C6	6.80	1.42	1.22
2	w	2	BDP	O6A-C6	6.80	1.42	1.22
2	a	2	BDP	O6A-C6	6.80	1.42	1.22
2	Z	2	BDP	O6A-C6	6.80	1.42	1.22
2	u	2	BDP	O6A-C6	6.80	1.42	1.22
2	3	2	BDP	O6A-C6	6.80	1.42	1.22
2	KA	2	BDP	O6A-C6	6.80	1.42	1.22
2	8	2	BDP	O6A-C6	6.80	1.42	1.22
2	r	2	BDP	O6A-C6	6.80	1.42	1.22
2	CA	2	BDP	O6A-C6	6.80	1.42	1.22
2	x	2	BDP	O6A-C6	6.79	1.42	1.22
2	t	2	BDP	O6A-C6	6.79	1.42	1.22
2	BA	2	BDP	O6A-C6	6.79	1.42	1.22
2	i	2	BDP	O6A-C6	6.79	1.42	1.22
2	f	2	BDP	O6A-C6	6.79	1.42	1.22
2	DA	2	BDP	O6A-C6	6.79	1.42	1.22
2	g	2	BDP	O6A-C6	6.79	1.42	1.22
2	AA	2	BDP	O6A-C6	6.79	1.42	1.22
2	k	2	BDP	O6A-C6	6.79	1.42	1.22
2	q	2	BDP	O6A-C6	6.78	1.42	1.22
2	e	2	BDP	O6A-C6	6.78	1.42	1.22
2	GA	2	BDP	O6A-C6	6.77	1.42	1.22
2	MA	2	BDP	O6A-C6	6.77	1.42	1.22
2	n	2	BDP	O6A-C6	6.77	1.42	1.22
2	MA	3	A1H1V	O6B-C6	3.67	1.42	1.30
2	w	3	A1H1V	O6B-C6	3.67	1.42	1.30
2	s	3	A1H1V	O6B-C6	3.66	1.42	1.30
2	n	3	A1H1V	O6B-C6	3.66	1.42	1.30
2	k	3	A1H1V	O6B-C6	3.66	1.42	1.30
2	6	3	A1H1V	O6B-C6	3.66	1.42	1.30
2	b	3	A1H1V	O6B-C6	3.66	1.42	1.30
2	g	3	A1H1V	O6B-C6	3.66	1.42	1.30
2	z	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	d	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	x	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	p	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	l	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	FA	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	LA	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	2	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	y	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	DA	3	A1H1V	O6B-C6	3.65	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	u	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	9	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	AA	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	3	3	A1H1V	O6B-C6	3.65	1.42	1.30
2	t	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	v	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	BA	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	CA	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	EA	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	q	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	f	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	e	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	5	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	GA	3	A1H1V	O6B-C6	3.64	1.42	1.30
2	JA	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	0	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	HA	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	1	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	4	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	Z	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	a	3	A1H1V	O6B-C6	3.63	1.42	1.30
2	h	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	r	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	o	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	8	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	i	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	c	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	KA	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	IA	3	A1H1V	O6B-C6	3.62	1.42	1.30
2	j	3	A1H1V	O6B-C6	3.61	1.42	1.30
2	m	3	A1H1V	O6B-C6	3.61	1.42	1.30
2	i	3	A1H1V	O6A-C6	2.65	1.29	1.22
2	IA	3	A1H1V	O6A-C6	2.64	1.29	1.22
2	m	3	A1H1V	O6A-C6	2.64	1.29	1.22
2	t	3	A1H1V	O6A-C6	2.64	1.29	1.22
2	o	3	A1H1V	O6A-C6	2.64	1.29	1.22
2	l	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	GA	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	a	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	q	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	2	3	A1H1V	O6A-C6	2.63	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	z	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	v	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	LA	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	EA	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	g	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	0	3	A1H1V	O6A-C6	2.63	1.29	1.22
2	s	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	HA	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	CA	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	7	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	8	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	JA	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	y	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	AA	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	n	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	9	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	KA	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	MA	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	j	3	A1H1V	O6A-C6	2.62	1.29	1.22
2	f	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	x	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	4	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	Z	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	d	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	FA	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	k	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	p	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	1	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	3	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	6	3	A1H1V	O6A-C6	2.61	1.29	1.22
2	w	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	c	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	DA	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	BA	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	e	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	u	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	r	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	h	3	A1H1V	O6A-C6	2.60	1.29	1.22
2	b	3	A1H1V	O6A-C6	2.59	1.29	1.22
2	5	3	A1H1V	O6A-C6	2.59	1.29	1.22
2	JA	3	A1H1V	O24-S1	2.30	1.55	1.45
2	k	3	A1H1V	O24-S1	2.30	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	c	3	A1H1V	O24-S1	2.29	1.55	1.45
2	l	3	A1H1V	O24-S1	2.29	1.55	1.45
2	o	3	A1H1V	O24-S1	2.29	1.55	1.45
2	a	3	A1H1V	O24-S1	2.29	1.55	1.45
2	f	3	A1H1V	O24-S1	2.29	1.55	1.45
2	KA	3	A1H1V	O24-S1	2.29	1.55	1.45
2	AA	3	A1H1V	O24-S1	2.29	1.55	1.45
2	DA	3	A1H1V	O24-S1	2.29	1.55	1.45
2	x	3	A1H1V	O24-S1	2.29	1.55	1.45
2	u	3	A1H1V	O24-S1	2.28	1.55	1.45
2	y	3	A1H1V	O24-S1	2.28	1.55	1.45
2	w	3	A1H1V	O24-S1	2.28	1.55	1.45
2	8	3	A1H1V	O24-S1	2.28	1.55	1.45
2	MA	3	A1H1V	O24-S1	2.28	1.55	1.45
2	e	3	A1H1V	O24-S1	2.27	1.55	1.45
2	j	3	A1H1V	O24-S1	2.27	1.55	1.45
2	LA	3	A1H1V	O24-S1	2.27	1.55	1.45
2	Z	3	A1H1V	O24-S1	2.27	1.55	1.45
2	IA	3	A1H1V	O24-S1	2.27	1.55	1.45
2	0	3	A1H1V	O24-S1	2.27	1.55	1.45
2	2	3	A1H1V	O24-S1	2.27	1.55	1.45
2	6	3	A1H1V	O24-S1	2.27	1.55	1.45
2	9	3	A1H1V	O24-S1	2.27	1.55	1.45
2	5	3	A1H1V	O24-S1	2.27	1.55	1.45
2	g	3	A1H1V	O24-S1	2.27	1.55	1.45
2	3	3	A1H1V	O24-S1	2.27	1.55	1.45
2	n	3	A1H1V	O24-S1	2.27	1.55	1.45
2	q	3	A1H1V	O24-S1	2.27	1.55	1.45
2	CA	3	A1H1V	O24-S1	2.27	1.55	1.45
2	d	3	A1H1V	O24-S1	2.27	1.55	1.45
2	b	3	A1H1V	O24-S1	2.27	1.55	1.45
2	FA	3	A1H1V	O24-S1	2.27	1.55	1.45
2	p	3	A1H1V	O24-S1	2.26	1.55	1.45
2	7	3	A1H1V	O24-S1	2.26	1.55	1.45
2	4	3	A1H1V	O24-S1	2.26	1.55	1.45
2	h	3	A1H1V	O24-S1	2.26	1.55	1.45
2	r	3	A1H1V	O24-S1	2.26	1.55	1.45
2	GA	3	A1H1V	O24-S1	2.26	1.55	1.45
2	EA	3	A1H1V	O24-S1	2.26	1.55	1.45
2	v	3	A1H1V	O24-S1	2.26	1.55	1.45
2	BA	3	A1H1V	O24-S1	2.26	1.55	1.45
2	z	3	A1H1V	O24-S1	2.26	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	3	A1H1V	O24-S1	2.26	1.55	1.45
2	t	3	A1H1V	O24-S1	2.26	1.55	1.45
2	HA	3	A1H1V	O24-S1	2.25	1.55	1.45

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1	BGC	O4-C4-C3	-4.24	100.38	110.38
2	n	2	BDP	O6B-C6-O6A	-3.81	115.44	124.08
2	k	1	BGC	O4-C4-C3	-3.80	101.41	110.38
2	y	2	BDP	O6B-C6-O6A	-3.78	115.50	124.08
2	0	2	BDP	O6B-C6-O6A	-3.76	115.55	124.08
2	i	2	BDP	O6B-C6-O6A	-3.75	115.57	124.08
2	z	2	BDP	O6B-C6-O6A	-3.75	115.57	124.08
2	8	2	BDP	O6B-C6-O6A	-3.75	115.58	124.08
2	3	3	A1H1V	O6B-C6-O6A	-3.75	115.58	124.08
2	q	2	BDP	O6B-C6-O6A	-3.74	115.59	124.08
2	o	2	BDP	O6B-C6-O6A	-3.74	115.60	124.08
2	IA	3	A1H1V	O6B-C6-O6A	-3.74	115.60	124.08
2	g	3	A1H1V	O6B-C6-O6A	-3.74	115.60	124.08
2	p	3	A1H1V	O6B-C6-O6A	-3.73	115.61	124.08
2	6	2	BDP	O6B-C6-O6A	-3.73	115.61	124.08
2	CA	3	A1H1V	O6B-C6-O6A	-3.73	115.61	124.08
2	s	2	BDP	O6B-C6-O6A	-3.73	115.61	124.08
2	0	3	A1H1V	O6B-C6-O6A	-3.73	115.62	124.08
2	4	2	BDP	O6B-C6-O6A	-3.73	115.62	124.08
2	EA	2	BDP	O6B-C6-O6A	-3.73	115.62	124.08
2	c	2	BDP	O6B-C6-O6A	-3.73	115.62	124.08
2	e	3	A1H1V	O6B-C6-O6A	-3.73	115.62	124.08
2	MA	3	A1H1V	O6B-C6-O6A	-3.72	115.63	124.08
2	d	2	BDP	O6B-C6-O6A	-3.72	115.64	124.08
2	m	2	BDP	O6B-C6-O6A	-3.72	115.64	124.08
2	x	2	BDP	O6B-C6-O6A	-3.72	115.64	124.08
2	z	3	A1H1V	O6B-C6-O6A	-3.72	115.64	124.08
2	k	2	BDP	O6B-C6-O6A	-3.71	115.65	124.08
2	8	3	A1H1V	O6B-C6-O6A	-3.71	115.65	124.08
2	a	3	A1H1V	O6B-C6-O6A	-3.71	115.66	124.08
2	m	3	A1H1V	O6B-C6-O6A	-3.71	115.66	124.08
2	u	2	BDP	O6B-C6-O6A	-3.71	115.66	124.08
2	MA	2	BDP	O6B-C6-O6A	-3.71	115.66	124.08
2	a	2	BDP	O6B-C6-O6A	-3.71	115.66	124.08
2	2	3	A1H1V	O6B-C6-O6A	-3.71	115.66	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KA	2	BDP	O6B-C6-O6A	-3.71	115.66	124.08
2	GA	3	A1H1V	O6B-C6-O6A	-3.71	115.67	124.08
2	c	3	A1H1V	O6B-C6-O6A	-3.71	115.67	124.08
2	w	2	BDP	O6B-C6-O6A	-3.71	115.67	124.08
2	t	3	A1H1V	O6B-C6-O6A	-3.71	115.67	124.08
2	x	3	A1H1V	O6B-C6-O6A	-3.71	115.67	124.08
2	9	2	BDP	O6B-C6-O6A	-3.71	115.67	124.08
2	HA	2	BDP	O6B-C6-O6A	-3.71	115.67	124.08
2	e	2	BDP	O6B-C6-O6A	-3.70	115.68	124.08
2	AA	2	BDP	O6B-C6-O6A	-3.70	115.68	124.08
2	4	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.08
2	BA	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.08
2	s	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.08
2	1	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.08
2	k	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.08
2	IA	2	BDP	O6B-C6-O6A	-3.70	115.69	124.08
2	j	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.08
2	f	2	BDP	O6B-C6-O6A	-3.70	115.69	124.08
2	g	2	BDP	O6B-C6-O6A	-3.70	115.69	124.08
2	j	2	BDP	O6B-C6-O6A	-3.70	115.69	124.08
2	BA	2	BDP	O6B-C6-O6A	-3.70	115.70	124.08
2	l	3	A1H1V	O6B-C6-O6A	-3.69	115.70	124.08
2	9	3	A1H1V	O6B-C6-O6A	-3.69	115.70	124.08
2	KA	3	A1H1V	O6B-C6-O6A	-3.69	115.70	124.08
2	i	3	A1H1V	O6B-C6-O6A	-3.69	115.71	124.08
2	q	3	A1H1V	O6B-C6-O6A	-3.69	115.71	124.08
2	y	3	A1H1V	O6B-C6-O6A	-3.69	115.71	124.08
2	AA	3	A1H1V	O6B-C6-O6A	-3.69	115.71	124.08
2	r	2	BDP	O6B-C6-O6A	-3.69	115.71	124.08
2	v	2	BDP	O6B-C6-O6A	-3.69	115.71	124.08
2	Z	3	A1H1V	O6B-C6-O6A	-3.69	115.72	124.08
2	o	3	A1H1V	O6B-C6-O6A	-3.69	115.72	124.08
2	EA	3	A1H1V	O6B-C6-O6A	-3.69	115.72	124.08
2	LA	3	A1H1V	O6B-C6-O6A	-3.69	115.72	124.08
2	2	2	BDP	O6B-C6-O6A	-3.68	115.72	124.08
2	w	3	A1H1V	O6B-C6-O6A	-3.68	115.72	124.08
2	CA	2	BDP	O6B-C6-O6A	-3.68	115.72	124.08
2	d	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.08
2	u	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.08
2	JA	2	BDP	O6B-C6-O6A	-3.68	115.73	124.08
2	FA	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.08
2	LA	2	BDP	O6B-C6-O6A	-3.68	115.73	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FA	2	BDP	O6B-C6-O6A	-3.68	115.73	124.08
2	Z	2	BDP	O6B-C6-O6A	-3.68	115.74	124.08
2	HA	3	A1H1V	O6B-C6-O6A	-3.68	115.74	124.08
2	r	3	A1H1V	O6B-C6-O6A	-3.68	115.74	124.08
2	5	3	A1H1V	O6B-C6-O6A	-3.68	115.74	124.08
2	1	2	BDP	O6B-C6-O6A	-3.67	115.74	124.08
2	b	3	A1H1V	O6B-C6-O6A	-3.67	115.75	124.08
2	3	2	BDP	O6B-C6-O6A	-3.67	115.75	124.08
2	h	3	A1H1V	O6B-C6-O6A	-3.67	115.75	124.08
2	7	2	BDP	O6B-C6-O6A	-3.67	115.75	124.08
2	7	3	A1H1V	O6B-C6-O6A	-3.67	115.75	124.08
2	p	2	BDP	O6B-C6-O6A	-3.67	115.76	124.08
2	f	3	A1H1V	O6B-C6-O6A	-3.67	115.76	124.08
2	v	3	A1H1V	O6B-C6-O6A	-3.67	115.76	124.08
2	6	3	A1H1V	O6B-C6-O6A	-3.67	115.76	124.08
2	DA	2	BDP	O6B-C6-O6A	-3.66	115.77	124.08
2	JA	3	A1H1V	O6B-C6-O6A	-3.66	115.77	124.08
2	l	2	BDP	O6B-C6-O6A	-3.66	115.78	124.08
2	GA	2	BDP	O6B-C6-O6A	-3.65	115.79	124.08
2	n	3	A1H1V	O6B-C6-O6A	-3.65	115.79	124.08
2	DA	3	A1H1V	O6B-C6-O6A	-3.65	115.80	124.08
2	h	2	BDP	O6B-C6-O6A	-3.65	115.80	124.08
2	8	1	BGC	O4-C4-C3	-3.64	101.80	110.38
2	t	2	BDP	O6B-C6-O6A	-3.62	115.86	124.08
2	b	2	BDP	O6B-C6-O6A	-3.54	116.06	124.08
2	5	2	BDP	O6B-C6-O6A	-3.48	116.19	124.08
2	0	1	BGC	O4-C4-C3	-3.15	102.96	110.38
2	c	1	BGC	O4-C4-C3	-3.09	103.10	110.38
2	KA	1	BGC	O4-C4-C5	3.06	116.85	109.32
2	n	3	A1H1V	O6A-C6-C5	-3.03	109.88	120.81
2	4	1	BGC	O4-C4-C3	-3.02	103.25	110.38
2	5	3	A1H1V	O6A-C6-C5	-3.00	109.97	120.81
2	HA	3	A1H1V	O6A-C6-C5	-3.00	110.00	120.81
2	4	3	A1H1V	O6A-C6-C5	-2.99	110.01	120.81
2	l	3	A1H1V	O6A-C6-C5	-2.99	110.01	120.81
2	v	3	A1H1V	O6A-C6-C5	-2.99	110.01	120.81
2	JA	3	A1H1V	O6A-C6-C5	-2.99	110.02	120.81
2	h	3	A1H1V	O6A-C6-C5	-2.99	110.02	120.81
2	2	3	A1H1V	O6A-C6-C5	-2.99	110.02	120.81
2	EA	3	A1H1V	O6A-C6-C5	-2.98	110.04	120.81
2	y	3	A1H1V	O6A-C6-C5	-2.98	110.05	120.81
2	MA	3	A1H1V	O6A-C6-C5	-2.98	110.05	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3	A1H1V	O6A-C6-C5	-2.98	110.05	120.81
2	u	3	A1H1V	O6A-C6-C5	-2.98	110.06	120.81
2	DA	3	A1H1V	O6A-C6-C5	-2.98	110.06	120.81
2	t	3	A1H1V	O6A-C6-C5	-2.97	110.07	120.81
2	o	3	A1H1V	O6A-C6-C5	-2.97	110.08	120.81
2	z	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	i	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	8	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	BA	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	KA	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	e	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	GA	3	A1H1V	O6A-C6-C5	-2.97	110.09	120.81
2	r	3	A1H1V	O6A-C6-C5	-2.97	110.10	120.81
2	g	3	A1H1V	O6A-C6-C5	-2.97	110.11	120.81
2	b	3	A1H1V	O6A-C6-C5	-2.96	110.11	120.81
2	c	3	A1H1V	O6A-C6-C5	-2.96	110.11	120.81
2	q	3	A1H1V	O6A-C6-C5	-2.96	110.11	120.81
2	x	3	A1H1V	O6A-C6-C5	-2.96	110.12	120.81
2	CA	3	A1H1V	O6A-C6-C5	-2.96	110.12	120.81
2	m	3	A1H1V	O6A-C6-C5	-2.96	110.13	120.81
2	1	3	A1H1V	O6A-C6-C5	-2.96	110.13	120.81
2	IA	3	A1H1V	O6A-C6-C5	-2.96	110.13	120.81
2	j	3	A1H1V	O6A-C6-C5	-2.96	110.13	120.81
2	f	3	A1H1V	O6A-C6-C5	-2.96	110.14	120.81
2	Z	3	A1H1V	O6A-C6-C5	-2.96	110.14	120.81
2	w	3	A1H1V	O6A-C6-C5	-2.96	110.14	120.81
2	7	3	A1H1V	O6A-C6-C5	-2.96	110.14	120.81
2	d	3	A1H1V	O6A-C6-C5	-2.96	110.14	120.81
2	a	3	A1H1V	O6A-C6-C5	-2.95	110.15	120.81
2	s	3	A1H1V	O6A-C6-C5	-2.95	110.15	120.81
2	3	3	A1H1V	O6A-C6-C5	-2.95	110.15	120.81
2	AA	3	A1H1V	O6A-C6-C5	-2.95	110.15	120.81
2	6	3	A1H1V	O6A-C6-C5	-2.95	110.16	120.81
2	FA	3	A1H1V	O6A-C6-C5	-2.95	110.16	120.81
2	k	3	A1H1V	O6A-C6-C5	-2.95	110.16	120.81
2	0	3	A1H1V	O6A-C6-C5	-2.95	110.17	120.81
2	LA	3	A1H1V	O6A-C6-C5	-2.93	110.22	120.81
2	p	3	A1H1V	O6A-C6-C5	-2.92	110.28	120.81
2	5	2	BDP	O6A-C6-C5	-2.89	110.37	120.81
2	n	2	BDP	O6A-C6-C5	-2.88	110.40	120.81
2	2	1	BGC	O4-C4-C5	2.87	116.40	109.32
2	s	2	BDP	O6A-C6-C5	-2.86	110.50	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KA	2	BDP	O6A-C6-C5	-2.84	110.55	120.81
2	m	2	BDP	O6A-C6-C5	-2.83	110.58	120.81
2	o	2	BDP	O6A-C6-C5	-2.83	110.59	120.81
2	g	2	BDP	O6A-C6-C5	-2.83	110.60	120.81
2	GA	2	BDP	O6A-C6-C5	-2.82	110.62	120.81
2	i	2	BDP	O6A-C6-C5	-2.82	110.63	120.81
2	6	2	BDP	O6A-C6-C5	-2.82	110.64	120.81
2	y	2	BDP	O6A-C6-C5	-2.82	110.64	120.81
2	j	2	BDP	O6A-C6-C5	-2.82	110.64	120.81
2	y	1	BGC	O4-C4-C3	-2.81	103.75	110.38
2	0	2	BDP	O6A-C6-C5	-2.81	110.66	120.81
2	4	2	BDP	O6A-C6-C5	-2.80	110.69	120.81
2	EA	2	BDP	O6A-C6-C5	-2.80	110.69	120.81
2	AA	2	BDP	O6A-C6-C5	-2.80	110.70	120.81
2	JA	2	BDP	O6A-C6-C5	-2.79	110.72	120.81
2	c	2	BDP	O6A-C6-C5	-2.79	110.73	120.81
2	2	2	BDP	O6A-C6-C5	-2.79	110.74	120.81
2	e	2	BDP	O6A-C6-C5	-2.78	110.76	120.81
2	k	2	BDP	O6A-C6-C5	-2.78	110.79	120.81
2	f	2	BDP	O6A-C6-C5	-2.78	110.79	120.81
2	CA	2	BDP	O6A-C6-C5	-2.77	110.81	120.81
2	u	2	BDP	O6A-C6-C5	-2.77	110.82	120.81
2	h	2	BDP	O6A-C6-C5	-2.76	110.84	120.81
2	w	2	BDP	O6A-C6-C5	-2.76	110.84	120.81
2	DA	2	BDP	O6A-C6-C5	-2.76	110.84	120.81
2	8	2	BDP	O6A-C6-C5	-2.76	110.84	120.81
2	IA	2	BDP	O6A-C6-C5	-2.76	110.85	120.81
2	q	2	BDP	O6A-C6-C5	-2.76	110.86	120.81
2	3	2	BDP	O6A-C6-C5	-2.76	110.86	120.81
2	d	2	BDP	O6A-C6-C5	-2.75	110.87	120.81
2	BA	2	BDP	O6A-C6-C5	-2.75	110.87	120.81
2	9	2	BDP	O6A-C6-C5	-2.75	110.87	120.81
2	a	2	BDP	O6A-C6-C5	-2.75	110.89	120.81
2	l	2	BDP	O6A-C6-C5	-2.75	110.90	120.81
2	LA	2	BDP	O6A-C6-C5	-2.75	110.90	120.81
2	MA	2	BDP	O6A-C6-C5	-2.74	110.92	120.81
2	t	2	BDP	O6A-C6-C5	-2.74	110.94	120.81
2	FA	2	BDP	O6A-C6-C5	-2.74	110.94	120.81
2	b	2	BDP	O6A-C6-C5	-2.73	110.94	120.81
2	1	2	BDP	O6A-C6-C5	-2.73	110.94	120.81
2	HA	2	BDP	O6A-C6-C5	-2.73	110.94	120.81
2	z	2	BDP	O6A-C6-C5	-2.73	110.96	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	2	BDP	O6A-C6-C5	-2.73	110.96	120.81
2	x	2	BDP	O6A-C6-C5	-2.73	110.97	120.81
2	Z	2	BDP	O6A-C6-C5	-2.72	110.98	120.81
2	q	1	BGC	O4-C4-C3	-2.72	103.96	110.38
2	y	1	BGC	O4-C4-C5	2.72	116.03	109.32
2	p	2	BDP	O6A-C6-C5	-2.72	110.99	120.81
2	v	2	BDP	O6A-C6-C5	-2.72	110.99	120.81
2	j	3	A1H1V	C1-C2-C3	2.71	113.01	109.29
2	r	2	BDP	O6A-C6-C5	-2.71	111.02	120.81
2	k	1	BGC	O4-C4-C5	2.68	115.93	109.32
2	2	3	A1H1V	C1-C2-C3	2.68	112.97	109.29
2	k	3	A1H1V	C1-C2-C3	2.68	112.96	109.29
2	z	2	BDP	C1-C2-C3	-2.67	105.76	109.64
2	EA	3	A1H1V	C1-C2-C3	2.65	112.92	109.29
2	4	3	A1H1V	C1-C2-C3	2.65	112.92	109.29
2	8	3	A1H1V	C1-C2-C3	2.64	112.90	109.29
2	i	1	BGC	O4-C4-C3	-2.61	104.23	110.38
2	a	3	A1H1V	C1-C2-C3	2.60	112.85	109.29
2	KA	1	BGC	O4-C4-C3	-2.59	104.27	110.38
2	8	1	BGC	O4-C4-C5	2.58	115.69	109.32
2	LA	3	A1H1V	C3-O3-S1	2.58	125.22	119.04
2	IA	3	A1H1V	C1-C2-C3	2.58	112.82	109.29
2	q	3	A1H1V	C1-C2-C3	2.58	112.82	109.29
2	AA	3	A1H1V	C1-C2-C3	2.57	112.81	109.29
2	z	3	A1H1V	C3-O3-S1	2.55	125.16	119.04
2	GA	3	A1H1V	C1-C2-C3	2.55	112.78	109.29
2	KA	3	A1H1V	C1-C2-C3	2.54	112.77	109.29
2	MA	3	A1H1V	C1-C2-C3	2.54	112.77	109.29
2	c	3	A1H1V	C1-C2-C3	2.53	112.76	109.29
2	FA	3	A1H1V	C3-O3-S1	2.51	125.07	119.04
2	x	3	A1H1V	C1-C2-C3	2.51	112.73	109.29
2	HA	3	A1H1V	C1-C2-C3	2.50	112.72	109.29
2	0	1	BGC	O4-C4-C5	2.50	115.48	109.32
2	l	2	BDP	C1-C2-C3	-2.50	106.00	109.64
2	l	2	BDP	O4-C4-C5	-2.48	104.09	109.76
2	LA	2	BDP	O4-C4-C5	-2.47	104.11	109.76
2	p	3	A1H1V	C3-O3-S1	2.47	124.96	119.04
2	CA	3	A1H1V	C1-C2-C3	2.47	112.67	109.29
2	3	3	A1H1V	C3-O3-S1	2.47	124.95	119.04
2	s	3	A1H1V	C3-O3-S1	2.46	124.95	119.04
2	5	3	A1H1V	C3-O3-S1	2.46	124.94	119.04
2	e	3	A1H1V	C1-C2-C3	2.46	112.66	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	3	A1H1V	C3-O3-S1	2.46	124.94	119.04
2	w	3	A1H1V	C1-C2-C3	2.46	112.65	109.29
2	u	3	A1H1V	C3-O3-S1	2.45	124.91	119.04
2	6	3	A1H1V	C1-C2-C3	2.44	112.63	109.29
2	f	3	A1H1V	O22-S1-O23	2.43	117.07	108.56
2	d	3	A1H1V	C3-O3-S1	2.42	124.86	119.04
2	a	3	A1H1V	O22-S1-O23	2.42	117.04	108.56
2	h	3	A1H1V	C3-O3-S1	2.41	124.83	119.04
2	l	3	A1H1V	C3-O3-S1	2.41	124.82	119.04
2	c	1	BGC	O4-C4-C5	2.41	115.26	109.32
2	z	2	BDP	O4-C4-C5	-2.40	104.28	109.76
2	g	1	BGC	O4-C4-C3	-2.37	104.78	110.38
2	i	3	A1H1V	C1-C2-C3	2.37	112.54	109.29
2	FA	2	BDP	C1-C2-C3	-2.37	106.19	109.64
2	g	3	A1H1V	C1-C2-C3	2.35	112.52	109.29
2	JA	2	BDP	C1-C2-C3	-2.35	106.22	109.64
2	n	3	A1H1V	C1-C2-C3	2.35	112.51	109.29
2	5	2	BDP	C1-C2-C3	-2.34	106.23	109.64
2	AA	1	BGC	O4-C4-C3	-2.34	104.85	110.38
2	e	2	BDP	O4-C4-C5	-2.33	104.44	109.76
2	FA	2	BDP	O4-C4-C5	-2.32	104.46	109.76
2	l	3	A1H1V	C3-O3-S1	2.32	124.61	119.04
2	9	3	A1H1V	C3-O3-S1	2.32	124.60	119.04
2	m	3	A1H1V	C3-O3-S1	2.32	124.60	119.04
2	r	3	A1H1V	C3-O3-S1	2.32	124.60	119.04
2	v	3	A1H1V	C3-O3-S1	2.31	124.59	119.04
2	l	2	BDP	O4-C4-C5	-2.31	104.47	109.76
2	LA	2	BDP	C1-C2-C3	-2.31	106.28	109.64
2	i	1	BGC	O4-C4-C5	2.30	114.98	109.32
2	0	3	A1H1V	C1-C2-C3	2.30	112.44	109.29
2	BA	3	A1H1V	C3-O3-S1	2.29	124.53	119.04
2	b	3	A1H1V	C3-O3-S1	2.28	124.51	119.04
2	y	3	A1H1V	C1-C2-C3	2.27	112.40	109.29
2	DA	3	A1H1V	C3-O3-S1	2.27	124.48	119.04
2	h	3	A1H1V	O22-S1-O23	2.26	116.45	108.56
2	7	3	A1H1V	C1-C2-C3	2.25	112.38	109.29
2	JA	3	A1H1V	C1-C2-C3	2.25	112.38	109.29
2	JA	3	A1H1V	O22-S1-O23	2.25	116.44	108.56
2	Z	3	A1H1V	O22-S1-O23	2.25	116.44	108.56
2	o	1	BGC	O4-C4-C3	-2.25	105.08	110.38
2	HA	3	A1H1V	O22-S1-O23	2.24	116.41	108.56
2	Z	3	A1H1V	C3-O3-S1	2.24	124.42	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	v	3	A1H1V	O22-S1-O23	2.24	116.39	108.56
2	x	3	A1H1V	O22-S1-O23	2.24	116.38	108.56
2	DA	3	A1H1V	O22-S1-O23	2.24	116.38	108.56
2	1	3	A1H1V	O22-S1-O23	2.23	116.36	108.56
2	f	3	A1H1V	C3-O3-S1	2.23	124.38	119.04
2	g	3	A1H1V	C3-O3-S1	2.22	124.38	119.04
2	t	3	A1H1V	O22-S1-O23	2.22	116.32	108.56
2	AA	1	BGC	O4-C4-C5	2.22	114.78	109.32
2	l	3	A1H1V	O22-S1-O23	2.22	116.31	108.56
2	y	3	A1H1V	C3-O3-S1	2.21	124.35	119.04
2	n	3	A1H1V	O22-S1-O23	2.21	116.29	108.56
2	t	3	A1H1V	C1-C2-C3	2.21	112.32	109.29
2	s	1	BGC	O4-C4-C5	2.21	114.77	109.32
2	3	3	A1H1V	O22-S1-O23	2.21	116.29	108.56
2	LA	3	A1H1V	O22-S1-O23	2.21	116.28	108.56
2	i	3	A1H1V	C3-O3-S1	2.20	124.32	119.04
2	AA	3	A1H1V	O22-S1-O23	2.20	116.26	108.56
2	r	3	A1H1V	O22-S1-O23	2.20	116.26	108.56
2	b	3	A1H1V	O22-S1-O23	2.20	116.25	108.56
2	7	3	A1H1V	C3-O3-S1	2.20	124.31	119.04
2	7	3	A1H1V	O22-S1-O23	2.19	116.23	108.56
2	d	2	BDP	C1-C2-C3	-2.19	106.45	109.64
2	q	3	A1H1V	O22-S1-O23	2.19	116.23	108.56
2	5	3	A1H1V	O22-S1-O23	2.19	116.22	108.56
2	BA	3	A1H1V	O22-S1-O23	2.19	116.22	108.56
2	t	3	A1H1V	C3-O3-S1	2.19	124.28	119.04
2	n	3	A1H1V	C3-O3-S1	2.19	124.28	119.04
2	9	3	A1H1V	O22-S1-O23	2.19	116.21	108.56
2	d	3	A1H1V	O22-S1-O23	2.19	116.21	108.56
2	KA	3	A1H1V	C3-O3-S1	2.18	124.28	119.04
2	GA	3	A1H1V	O22-S1-O23	2.18	116.20	108.56
2	MA	3	A1H1V	O22-S1-O23	2.18	116.19	108.56
2	p	3	A1H1V	O22-S1-O23	2.18	116.18	108.56
2	e	3	A1H1V	O22-S1-O23	2.18	116.17	108.56
2	c	3	A1H1V	O22-S1-O23	2.18	116.17	108.56
2	FA	3	A1H1V	O22-S1-O23	2.18	116.17	108.56
2	n	1	BGC	C1-C2-C3	2.18	112.81	109.64
2	BA	3	A1H1V	C1-C2-C3	2.17	112.27	109.29
2	z	3	A1H1V	O22-S1-O23	2.17	116.16	108.56
2	m	3	A1H1V	C1-C2-C3	2.17	112.27	109.29
2	8	3	A1H1V	O22-S1-O23	2.17	116.16	108.56
2	4	3	A1H1V	O22-S1-O23	2.17	116.16	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	3	A1H1V	O22-S1-O23	2.17	116.16	108.56
2	IA	3	A1H1V	O22-S1-O23	2.17	116.15	108.56
2	2	3	A1H1V	O22-S1-O23	2.17	116.14	108.56
2	f	2	BDP	C1-C2-C3	-2.16	106.50	109.64
2	0	3	A1H1V	C3-O3-S1	2.15	124.20	119.04
2	w	3	A1H1V	O22-S1-O23	2.15	116.07	108.56
2	CA	3	A1H1V	O22-S1-O23	2.15	116.06	108.56
2	s	3	A1H1V	C1-C2-C3	2.14	112.22	109.29
2	5	2	BDP	O4-C4-C5	-2.14	104.88	109.76
2	s	1	BGC	O4-C4-C3	-2.13	105.35	110.38
2	j	3	A1H1V	O22-S1-O23	2.13	116.00	108.56
2	3	2	BDP	C1-C2-C3	-2.13	106.55	109.64
2	b	3	A1H1V	C1-C2-C3	2.13	112.20	109.29
2	e	2	BDP	C1-C2-C3	-2.12	106.56	109.64
2	JA	3	A1H1V	C3-O3-S1	2.12	124.12	119.04
2	6	3	A1H1V	C3-O3-S1	2.12	124.11	119.04
2	u	3	A1H1V	O22-S1-O3	2.11	111.23	106.37
2	EA	3	A1H1V	O22-S1-O23	2.11	115.95	108.56
2	6	3	A1H1V	O22-S1-O3	2.11	111.22	106.37
2	f	3	A1H1V	C1-C2-C3	2.09	112.15	109.29
2	DA	3	A1H1V	C1-C2-C3	2.09	112.15	109.29
2	r	3	A1H1V	C1-C2-C3	2.08	112.14	109.29
2	9	3	A1H1V	C1-C2-C3	2.07	112.13	109.29
2	h	2	BDP	O4-C4-C5	-2.07	105.03	109.76
2	6	3	A1H1V	O22-S1-O23	2.07	115.81	108.56
2	MA	2	BDP	O3-C3-C2	-2.07	105.84	110.05
2	KA	3	A1H1V	O22-S1-O3	2.06	111.12	106.37
2	DA	2	BDP	O4-C4-C5	-2.06	105.05	109.76
2	f	2	BDP	O4-C4-C5	-2.05	105.07	109.76
2	g	3	A1H1V	O22-S1-O23	2.04	115.70	108.56
2	y	3	A1H1V	O22-S1-O23	2.04	115.70	108.56
2	o	3	A1H1V	O22-S1-O23	2.03	115.67	108.56
2	u	3	A1H1V	O22-S1-O23	2.03	115.67	108.56
2	KA	3	A1H1V	O22-S1-O23	2.03	115.66	108.56
2	0	3	A1H1V	O22-S1-O23	2.02	115.63	108.56
2	3	2	BDP	O4-C4-C5	-2.02	105.14	109.76
2	o	3	A1H1V	O22-S1-O3	2.02	111.02	106.37
2	6	1	BGC	O4-C4-C3	-2.02	105.61	110.38
2	g	1	BGC	O4-C4-C5	2.02	114.30	109.32
2	w	2	BDP	O3-C3-C2	-2.02	105.94	110.05
2	d	2	BDP	O4-C4-C5	-2.01	105.17	109.76
2	EA	3	A1H1V	C3-O3-S1	2.01	123.86	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	1	BGC	O4-C4-C5	2.01	114.27	109.32
2	y	3	A1H1V	O22-S1-O3	2.01	110.99	106.37
2	g	3	A1H1V	O22-S1-O3	2.01	110.98	106.37
2	GA	2	BDP	O4-C4-C5	-2.00	105.19	109.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	LA	1	BGC	C1

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	2	BDP	C4-C5-C6-O6B
2	Z	3	A1H1V	C4-C5-C6-O6A
2	Z	3	A1H1V	C4-C3-O3-S1
2	Z	3	A1H1V	C2-C3-O3-S1
2	a	2	BDP	C4-C5-C6-O6B
2	a	3	A1H1V	C4-C5-C6-O6A
2	a	3	A1H1V	C4-C3-O3-S1
2	a	3	A1H1V	C2-C3-O3-S1
2	b	2	BDP	C4-C5-C6-O6B
2	b	3	A1H1V	C4-C5-C6-O6A
2	b	3	A1H1V	C4-C3-O3-S1
2	b	3	A1H1V	C2-C3-O3-S1
2	c	2	BDP	C4-C5-C6-O6B
2	c	3	A1H1V	C4-C5-C6-O6A
2	c	3	A1H1V	C4-C3-O3-S1
2	c	3	A1H1V	C2-C3-O3-S1
2	d	2	BDP	C4-C5-C6-O6B
2	d	3	A1H1V	C4-C5-C6-O6A
2	d	3	A1H1V	C4-C3-O3-S1
2	d	3	A1H1V	C2-C3-O3-S1
2	e	2	BDP	C4-C5-C6-O6B
2	e	3	A1H1V	C4-C5-C6-O6A
2	e	3	A1H1V	C4-C3-O3-S1
2	e	3	A1H1V	C2-C3-O3-S1
2	f	2	BDP	C4-C5-C6-O6B
2	f	3	A1H1V	C4-C5-C6-O6A
2	f	3	A1H1V	C4-C3-O3-S1
2	f	3	A1H1V	C2-C3-O3-S1
2	g	2	BDP	C4-C5-C6-O6B

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Mol	Chain	Res	Type	Atoms
2	g	3	A1H1V	C4-C5-C6-O6A
2	g	3	A1H1V	C4-C3-O3-S1
2	g	3	A1H1V	C2-C3-O3-S1
2	h	2	BDP	C4-C5-C6-O6B
2	h	3	A1H1V	C4-C5-C6-O6A
2	h	3	A1H1V	C4-C3-O3-S1
2	h	3	A1H1V	C2-C3-O3-S1
2	i	2	BDP	C4-C5-C6-O6B
2	i	3	A1H1V	C4-C5-C6-O6A
2	i	3	A1H1V	C4-C3-O3-S1
2	i	3	A1H1V	C2-C3-O3-S1
2	j	2	BDP	C4-C5-C6-O6B
2	j	3	A1H1V	C4-C5-C6-O6A
2	j	3	A1H1V	C4-C3-O3-S1
2	j	3	A1H1V	C2-C3-O3-S1
2	k	2	BDP	C4-C5-C6-O6B
2	k	3	A1H1V	C4-C5-C6-O6A
2	k	3	A1H1V	C4-C3-O3-S1
2	k	3	A1H1V	C2-C3-O3-S1
2	l	2	BDP	C4-C5-C6-O6B
2	l	3	A1H1V	C4-C5-C6-O6A
2	l	3	A1H1V	C4-C3-O3-S1
2	l	3	A1H1V	C2-C3-O3-S1
2	m	2	BDP	C4-C5-C6-O6B
2	m	3	A1H1V	C4-C5-C6-O6A
2	m	3	A1H1V	C4-C3-O3-S1
2	m	3	A1H1V	C2-C3-O3-S1
2	n	2	BDP	C4-C5-C6-O6B
2	n	3	A1H1V	C4-C5-C6-O6A
2	n	3	A1H1V	C4-C3-O3-S1
2	n	3	A1H1V	C2-C3-O3-S1
2	o	2	BDP	C4-C5-C6-O6B
2	o	3	A1H1V	C4-C5-C6-O6A
2	o	3	A1H1V	C4-C3-O3-S1
2	o	3	A1H1V	C2-C3-O3-S1
2	p	2	BDP	C4-C5-C6-O6B
2	p	3	A1H1V	C4-C5-C6-O6A
2	p	3	A1H1V	C4-C3-O3-S1
2	p	3	A1H1V	C2-C3-O3-S1
2	q	2	BDP	C4-C5-C6-O6B
2	q	3	A1H1V	C4-C5-C6-O6A
2	q	3	A1H1V	C4-C3-O3-S1

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Mol	Chain	Res	Type	Atoms
2	q	3	A1H1V	C2-C3-O3-S1
2	r	2	BDP	C4-C5-C6-O6B
2	r	3	A1H1V	C4-C5-C6-O6A
2	r	3	A1H1V	C4-C3-O3-S1
2	r	3	A1H1V	C2-C3-O3-S1
2	s	2	BDP	C4-C5-C6-O6B
2	s	3	A1H1V	C4-C5-C6-O6A
2	s	3	A1H1V	C4-C3-O3-S1
2	s	3	A1H1V	C2-C3-O3-S1
2	t	2	BDP	C4-C5-C6-O6B
2	t	3	A1H1V	C4-C5-C6-O6A
2	t	3	A1H1V	C4-C3-O3-S1
2	t	3	A1H1V	C2-C3-O3-S1
2	u	2	BDP	C4-C5-C6-O6B
2	u	3	A1H1V	C4-C5-C6-O6A
2	u	3	A1H1V	C4-C3-O3-S1
2	u	3	A1H1V	C2-C3-O3-S1
2	v	2	BDP	C4-C5-C6-O6B
2	v	3	A1H1V	C4-C5-C6-O6A
2	v	3	A1H1V	C4-C3-O3-S1
2	v	3	A1H1V	C2-C3-O3-S1
2	w	2	BDP	C4-C5-C6-O6B
2	w	3	A1H1V	C4-C5-C6-O6A
2	w	3	A1H1V	C4-C3-O3-S1
2	w	3	A1H1V	C2-C3-O3-S1
2	x	2	BDP	C4-C5-C6-O6B
2	x	3	A1H1V	C4-C5-C6-O6A
2	x	3	A1H1V	C4-C3-O3-S1
2	x	3	A1H1V	C2-C3-O3-S1
2	y	2	BDP	C4-C5-C6-O6B
2	y	3	A1H1V	C4-C5-C6-O6A
2	y	3	A1H1V	C4-C3-O3-S1
2	y	3	A1H1V	C2-C3-O3-S1
2	z	2	BDP	C4-C5-C6-O6B
2	z	3	A1H1V	C4-C5-C6-O6A
2	z	3	A1H1V	C4-C3-O3-S1
2	z	3	A1H1V	C2-C3-O3-S1
2	0	2	BDP	C4-C5-C6-O6B
2	0	3	A1H1V	C4-C5-C6-O6A
2	0	3	A1H1V	C4-C3-O3-S1
2	0	3	A1H1V	C2-C3-O3-S1
2	1	2	BDP	C4-C5-C6-O6B

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Mol	Chain	Res	Type	Atoms
2	1	3	A1H1V	C4-C5-C6-O6A
2	1	3	A1H1V	C4-C3-O3-S1
2	1	3	A1H1V	C2-C3-O3-S1
2	2	2	BDP	C4-C5-C6-O6B
2	2	3	A1H1V	C4-C5-C6-O6A
2	2	3	A1H1V	C4-C3-O3-S1
2	2	3	A1H1V	C2-C3-O3-S1
2	3	2	BDP	C4-C5-C6-O6B
2	3	3	A1H1V	C4-C5-C6-O6A
2	3	3	A1H1V	C4-C3-O3-S1
2	3	3	A1H1V	C2-C3-O3-S1
2	4	2	BDP	C4-C5-C6-O6B
2	4	3	A1H1V	C4-C5-C6-O6A
2	4	3	A1H1V	C4-C3-O3-S1
2	4	3	A1H1V	C2-C3-O3-S1
2	5	2	BDP	C4-C5-C6-O6B
2	5	3	A1H1V	C4-C5-C6-O6A
2	5	3	A1H1V	C4-C3-O3-S1
2	5	3	A1H1V	C2-C3-O3-S1
2	6	2	BDP	C4-C5-C6-O6B
2	6	3	A1H1V	C4-C5-C6-O6A
2	6	3	A1H1V	C4-C3-O3-S1
2	6	3	A1H1V	C2-C3-O3-S1
2	7	2	BDP	C4-C5-C6-O6B
2	7	3	A1H1V	C4-C5-C6-O6A
2	7	3	A1H1V	C4-C3-O3-S1
2	7	3	A1H1V	C2-C3-O3-S1
2	8	2	BDP	C4-C5-C6-O6B
2	8	3	A1H1V	C4-C5-C6-O6A
2	8	3	A1H1V	C4-C3-O3-S1
2	8	3	A1H1V	C2-C3-O3-S1
2	9	2	BDP	C4-C5-C6-O6B
2	9	3	A1H1V	C4-C5-C6-O6A
2	9	3	A1H1V	C4-C3-O3-S1
2	9	3	A1H1V	C2-C3-O3-S1
2	AA	2	BDP	C4-C5-C6-O6B
2	AA	3	A1H1V	C4-C5-C6-O6A
2	AA	3	A1H1V	C4-C3-O3-S1
2	AA	3	A1H1V	C2-C3-O3-S1
2	BA	2	BDP	C4-C5-C6-O6B
2	BA	3	A1H1V	C4-C5-C6-O6A
2	BA	3	A1H1V	C4-C3-O3-S1

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Mol	Chain	Res	Type	Atoms
2	BA	3	A1H1V	C2-C3-O3-S1
2	CA	2	BDP	C4-C5-C6-O6B
2	CA	3	A1H1V	C4-C5-C6-O6A
2	CA	3	A1H1V	C4-C3-O3-S1
2	CA	3	A1H1V	C2-C3-O3-S1
2	DA	2	BDP	C4-C5-C6-O6B
2	DA	3	A1H1V	C4-C5-C6-O6A
2	DA	3	A1H1V	C4-C3-O3-S1
2	DA	3	A1H1V	C2-C3-O3-S1
2	EA	2	BDP	C4-C5-C6-O6B
2	EA	3	A1H1V	C4-C5-C6-O6A
2	EA	3	A1H1V	C4-C3-O3-S1
2	EA	3	A1H1V	C2-C3-O3-S1
2	FA	2	BDP	C4-C5-C6-O6B
2	FA	3	A1H1V	C4-C5-C6-O6A
2	FA	3	A1H1V	C4-C3-O3-S1
2	FA	3	A1H1V	C2-C3-O3-S1
2	GA	2	BDP	C4-C5-C6-O6B
2	GA	3	A1H1V	C4-C5-C6-O6A
2	GA	3	A1H1V	C4-C3-O3-S1
2	GA	3	A1H1V	C2-C3-O3-S1
2	HA	2	BDP	C4-C5-C6-O6B
2	HA	3	A1H1V	C4-C5-C6-O6A
2	HA	3	A1H1V	C4-C3-O3-S1
2	HA	3	A1H1V	C2-C3-O3-S1
2	IA	2	BDP	C4-C5-C6-O6B
2	IA	3	A1H1V	C4-C5-C6-O6A
2	IA	3	A1H1V	C4-C3-O3-S1
2	IA	3	A1H1V	C2-C3-O3-S1
2	JA	2	BDP	C4-C5-C6-O6B
2	JA	3	A1H1V	C4-C5-C6-O6A
2	JA	3	A1H1V	C4-C3-O3-S1
2	JA	3	A1H1V	C2-C3-O3-S1
2	KA	2	BDP	C4-C5-C6-O6B
2	KA	3	A1H1V	C4-C5-C6-O6A
2	KA	3	A1H1V	C4-C3-O3-S1
2	KA	3	A1H1V	C2-C3-O3-S1
2	LA	2	BDP	C4-C5-C6-O6B
2	LA	3	A1H1V	C4-C5-C6-O6A
2	LA	3	A1H1V	C4-C3-O3-S1
2	LA	3	A1H1V	C2-C3-O3-S1
2	MA	2	BDP	C4-C5-C6-O6B

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Mol	Chain	Res	Type	Atoms
2	MA	3	A1H1V	C4-C5-C6-O6A
2	MA	3	A1H1V	C4-C3-O3-S1
2	MA	3	A1H1V	C2-C3-O3-S1
2	k	1	BGC	O5-C5-C6-O6
2	c	1	BGC	O5-C5-C6-O6
2	2	1	BGC	O5-C5-C6-O6
2	8	1	BGC	O5-C5-C6-O6
2	AA	1	BGC	O5-C5-C6-O6
2	0	1	BGC	O5-C5-C6-O6
2	4	1	BGC	O5-C5-C6-O6
2	a	1	BGC	O5-C5-C6-O6
2	d	1	BGC	O5-C5-C6-O6
2	e	1	BGC	O5-C5-C6-O6
2	f	1	BGC	O5-C5-C6-O6
2	t	1	BGC	O5-C5-C6-O6
2	u	1	BGC	O5-C5-C6-O6
2	x	1	BGC	O5-C5-C6-O6
2	z	1	BGC	O5-C5-C6-O6
2	3	1	BGC	O5-C5-C6-O6
2	DA	1	BGC	O5-C5-C6-O6
2	IA	1	BGC	O5-C5-C6-O6
2	MA	1	BGC	O5-C5-C6-O6
2	Z	1	BGC	O5-C5-C6-O6
2	j	1	BGC	O5-C5-C6-O6
2	r	1	BGC	O5-C5-C6-O6
2	v	1	BGC	O5-C5-C6-O6
2	w	1	BGC	O5-C5-C6-O6
2	1	1	BGC	O5-C5-C6-O6
2	7	1	BGC	O5-C5-C6-O6
2	9	1	BGC	O5-C5-C6-O6
2	BA	1	BGC	O5-C5-C6-O6
2	CA	1	BGC	O5-C5-C6-O6
2	FA	1	BGC	O5-C5-C6-O6
2	JA	1	BGC	O5-C5-C6-O6
2	LA	1	BGC	O5-C5-C6-O6
2	h	1	BGC	O5-C5-C6-O6
2	l	1	BGC	O5-C5-C6-O6
2	n	1	BGC	O5-C5-C6-O6
2	p	1	BGC	O5-C5-C6-O6
2	GA	1	BGC	O5-C5-C6-O6
2	HA	1	BGC	O5-C5-C6-O6
2	y	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	b	1	BGC	O5-C5-C6-O6
2	5	1	BGC	O5-C5-C6-O6
2	6	1	BGC	O5-C5-C6-O6
2	q	1	BGC	O5-C5-C6-O6
2	i	1	BGC	O5-C5-C6-O6
2	g	1	BGC	O5-C5-C6-O6
2	s	1	BGC	O5-C5-C6-O6
2	EA	1	BGC	O5-C5-C6-O6
2	KA	1	BGC	O5-C5-C6-O6
2	m	1	BGC	O5-C5-C6-O6
2	o	1	BGC	O5-C5-C6-O6

There are no ring outliers.

27 monomers are involved in 23 short contacts:

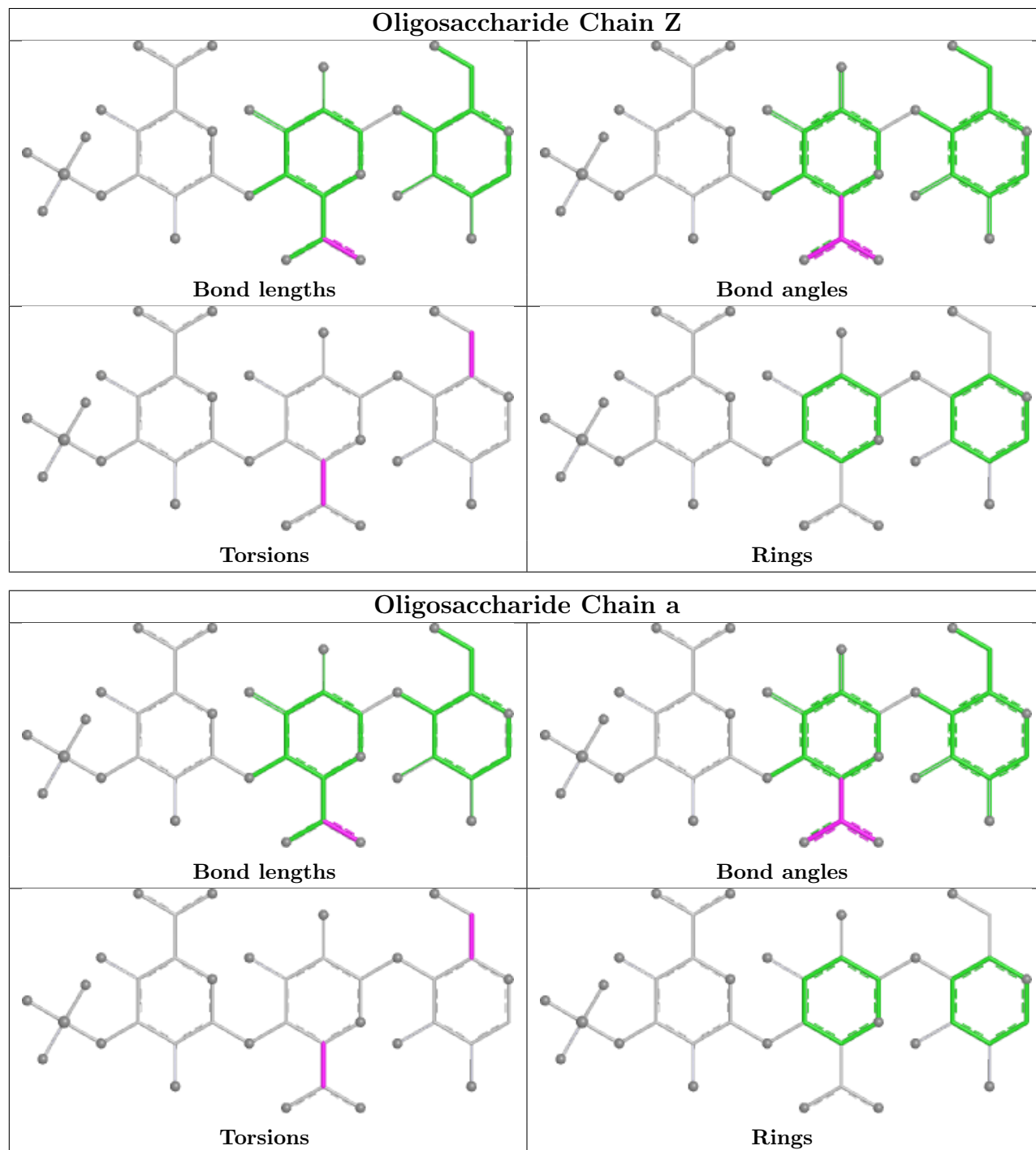
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	d	1	BGC	1	0
2	LA	1	BGC	1	0
2	l	1	BGC	1	0
2	j	2	BDP	1	0
2	GA	3	A1H1V	1	0
2	e	1	BGC	1	0
2	k	2	BDP	1	0
2	6	1	BGC	1	0
2	v	1	BGC	1	0
2	s	1	BGC	1	0
2	HA	2	BDP	1	0
2	DA	1	BGC	1	0
2	x	1	BGC	1	0
2	l	2	BDP	1	0
2	GA	2	BDP	1	0
2	AA	3	A1H1V	1	0
2	9	1	BGC	1	0
2	5	2	BDP	1	0
2	AA	2	BDP	1	0
2	z	2	BDP	1	0
2	BA	1	BGC	1	0
2	z	1	BGC	1	0
2	3	2	BDP	1	0
2	k	3	A1H1V	1	0
2	h	1	BGC	1	0
2	t	1	BGC	1	0

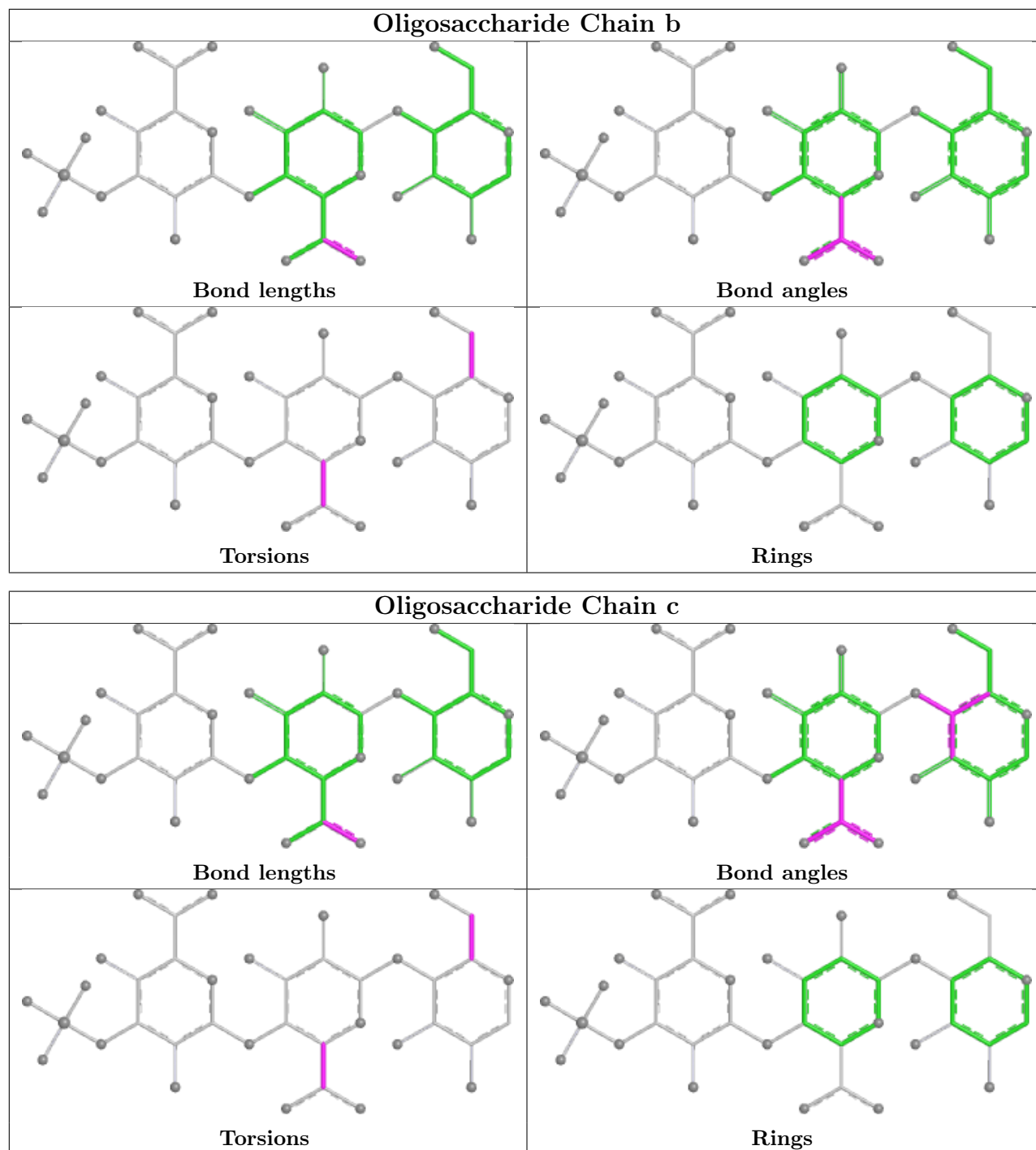
Continued on next page...

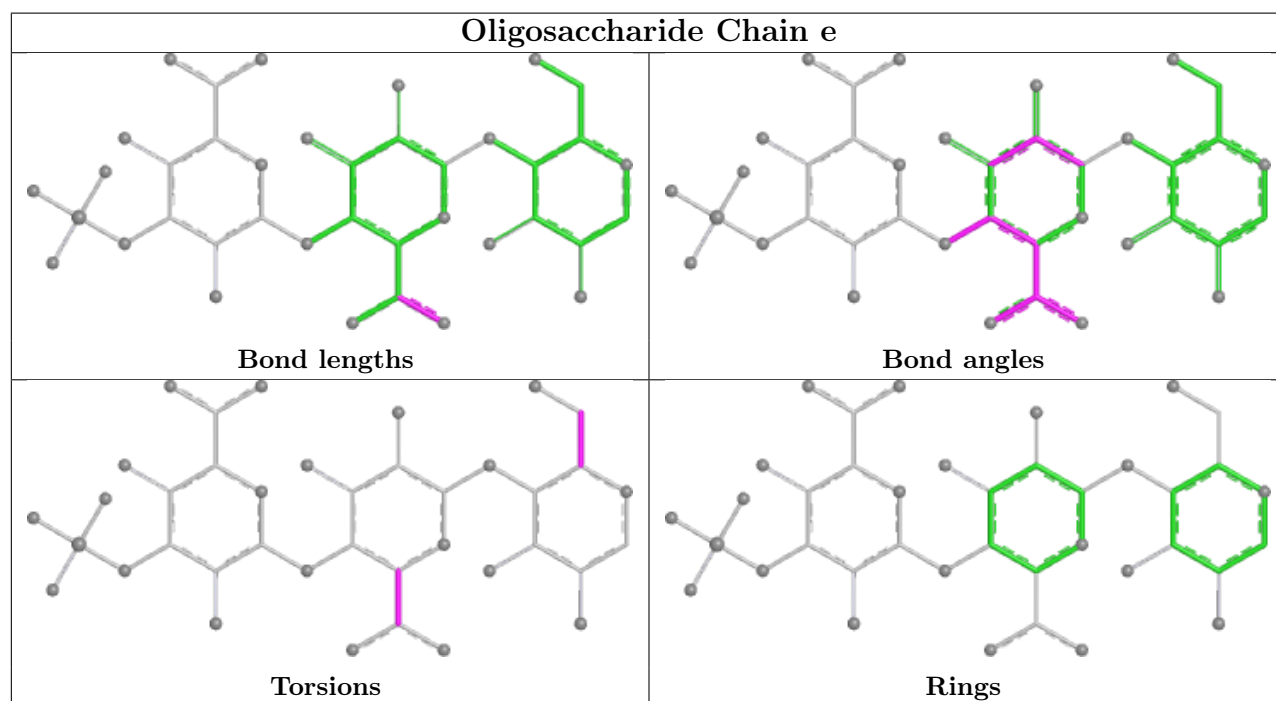
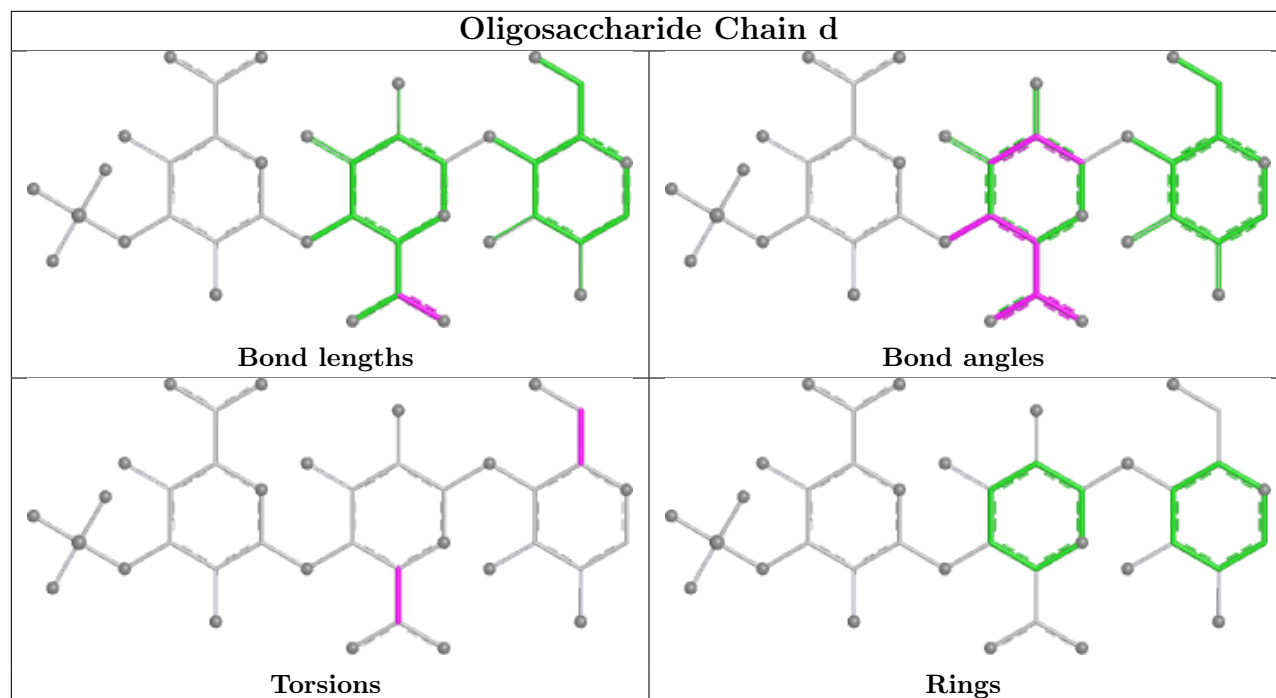
Continued from previous page...

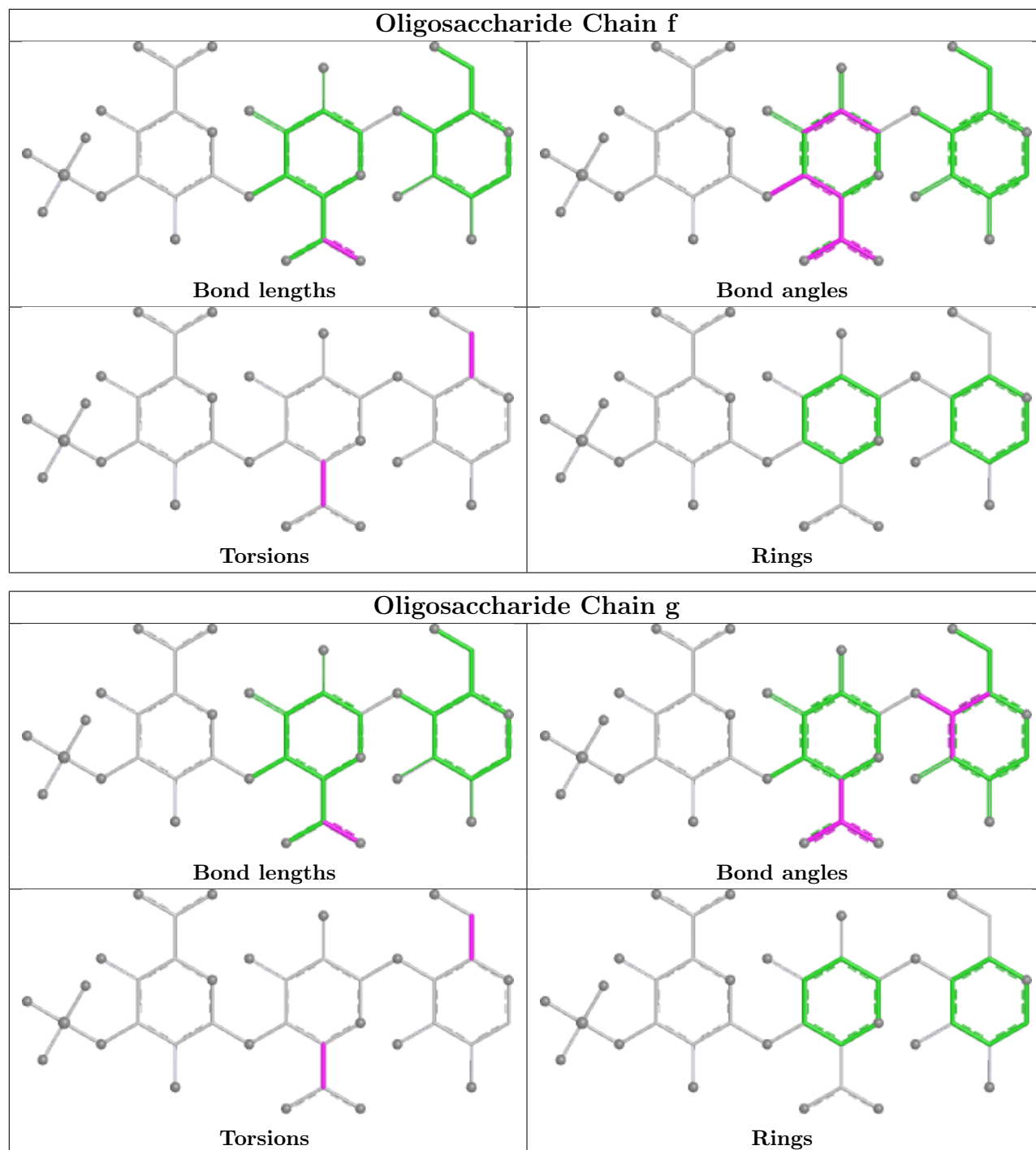
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	j	1	BGC	1	0

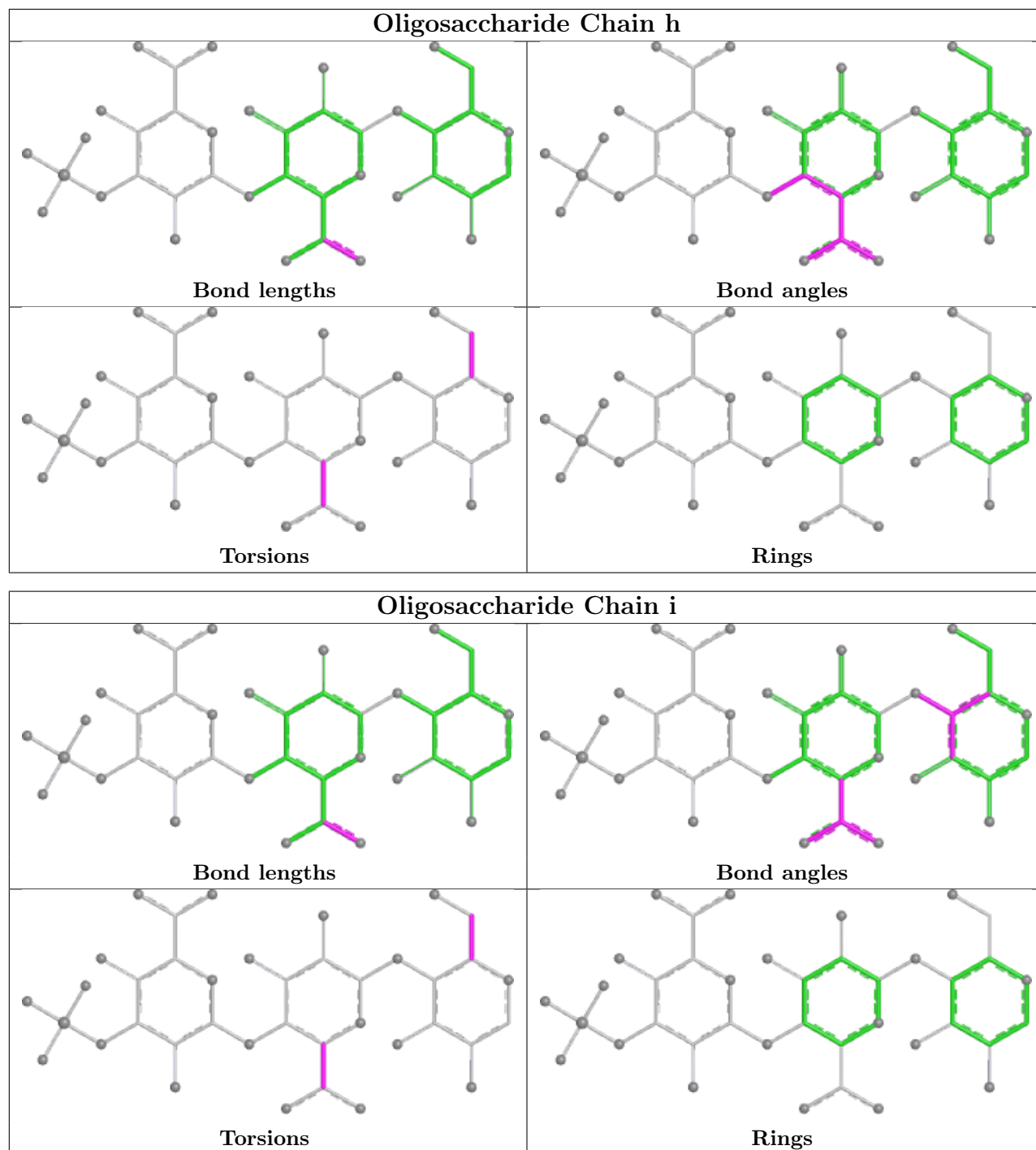
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

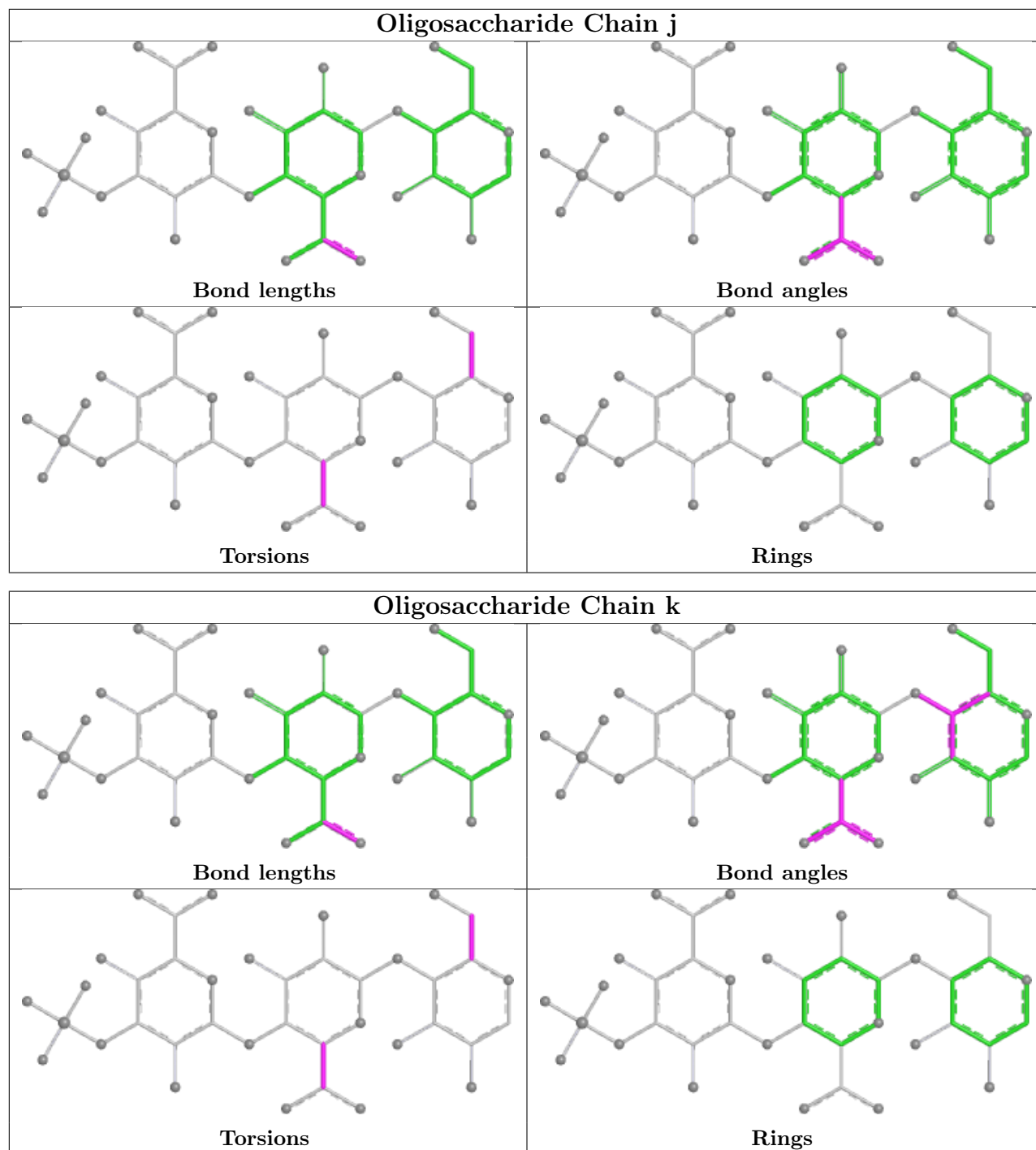


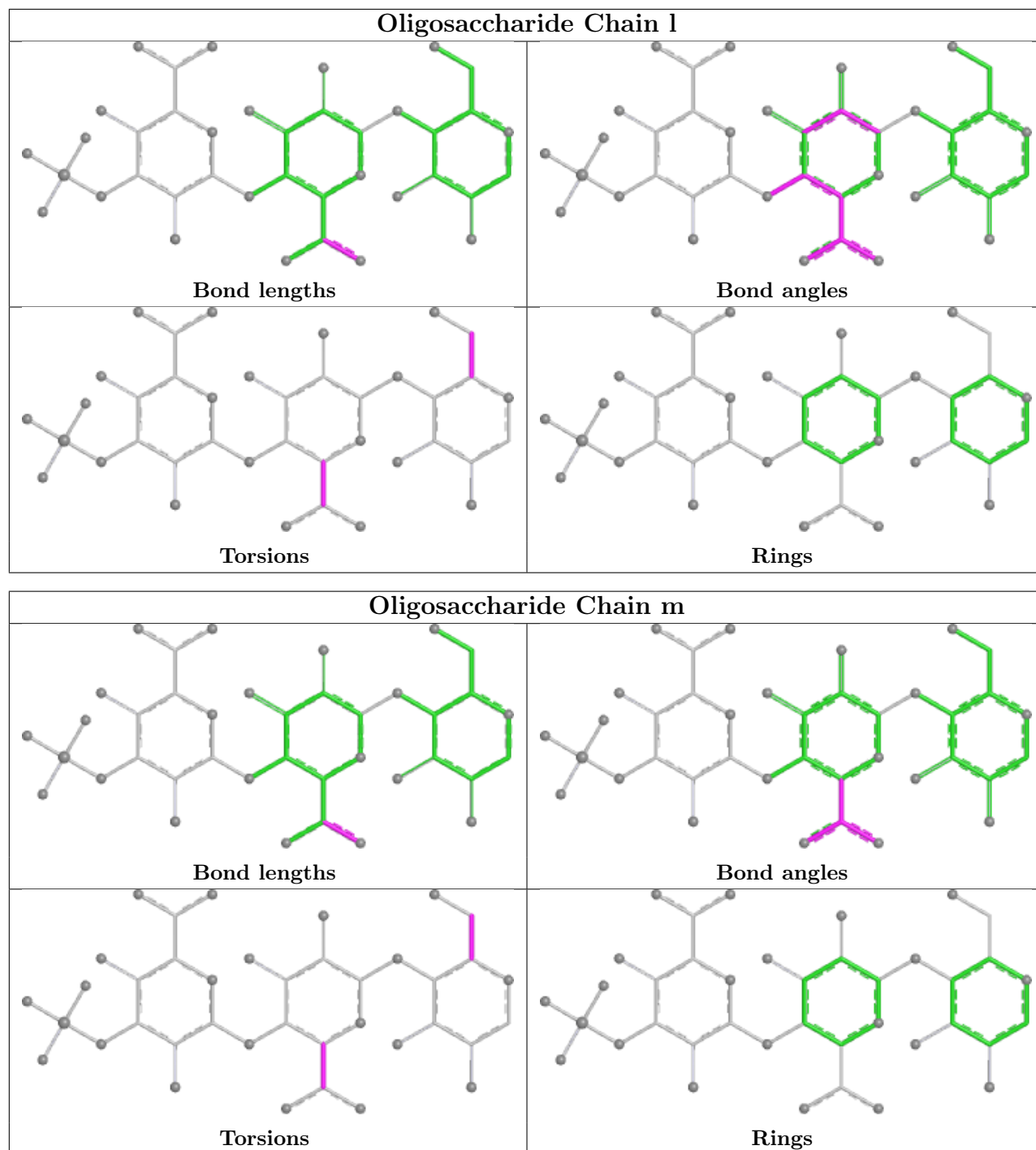


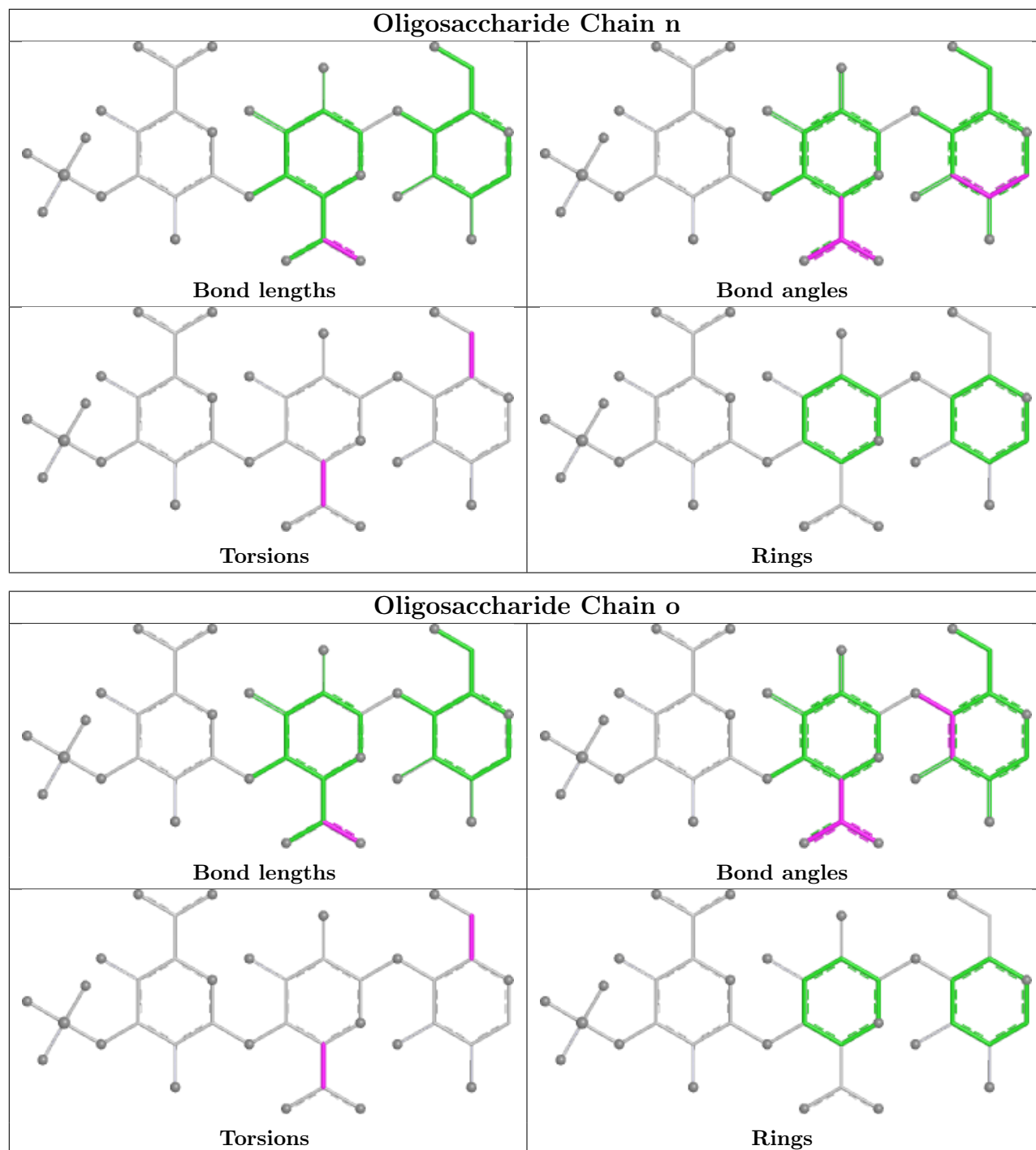


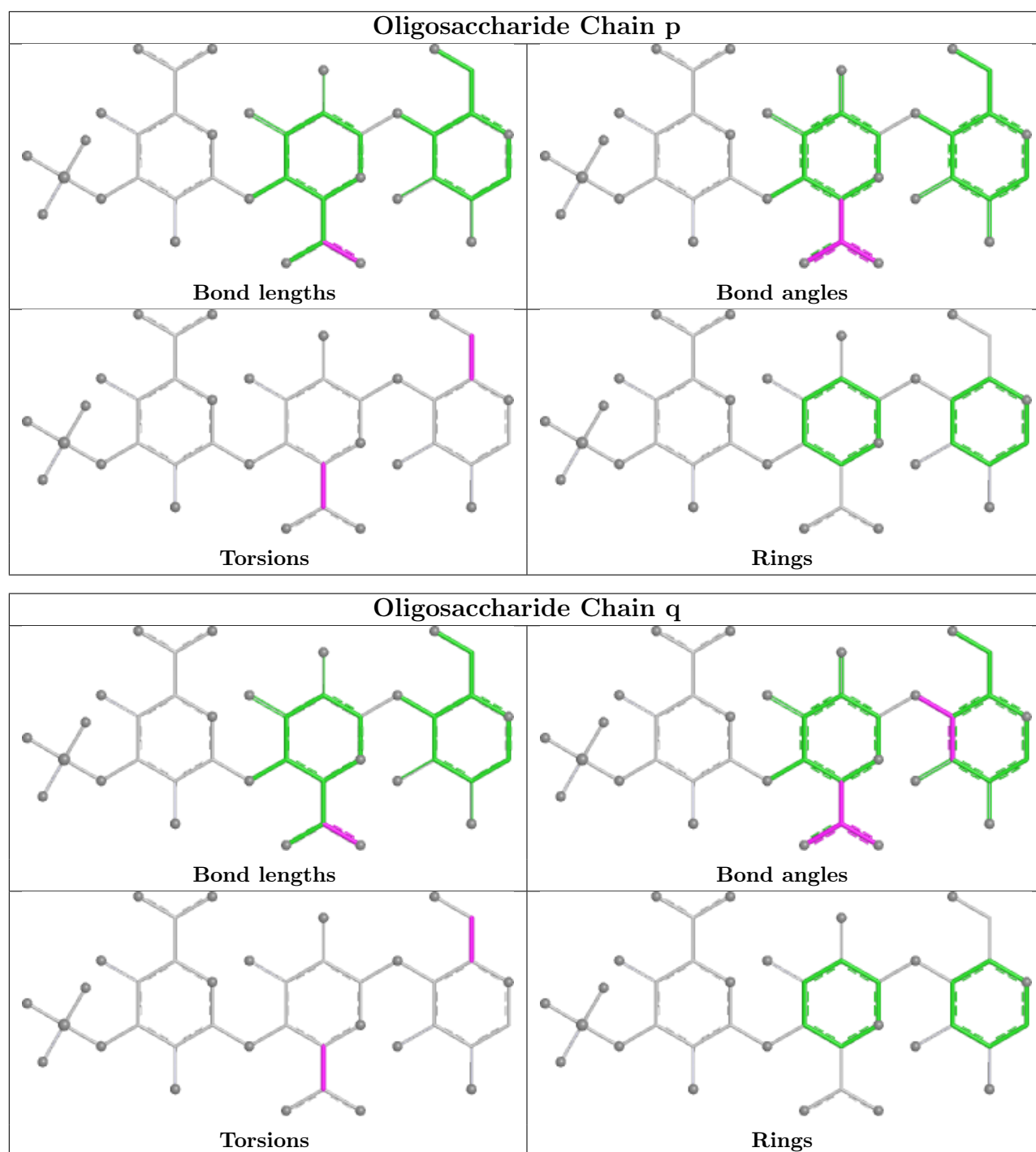


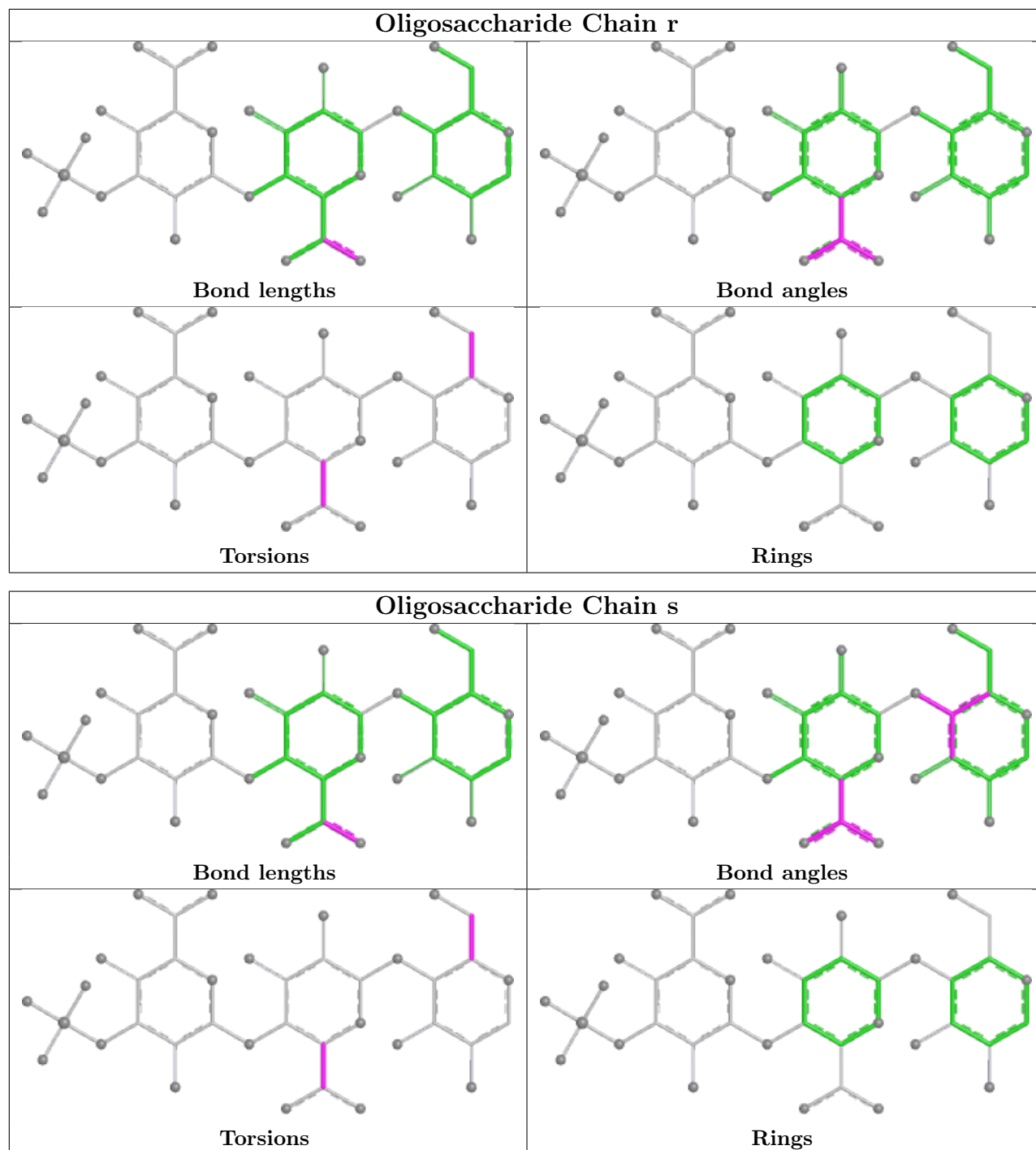


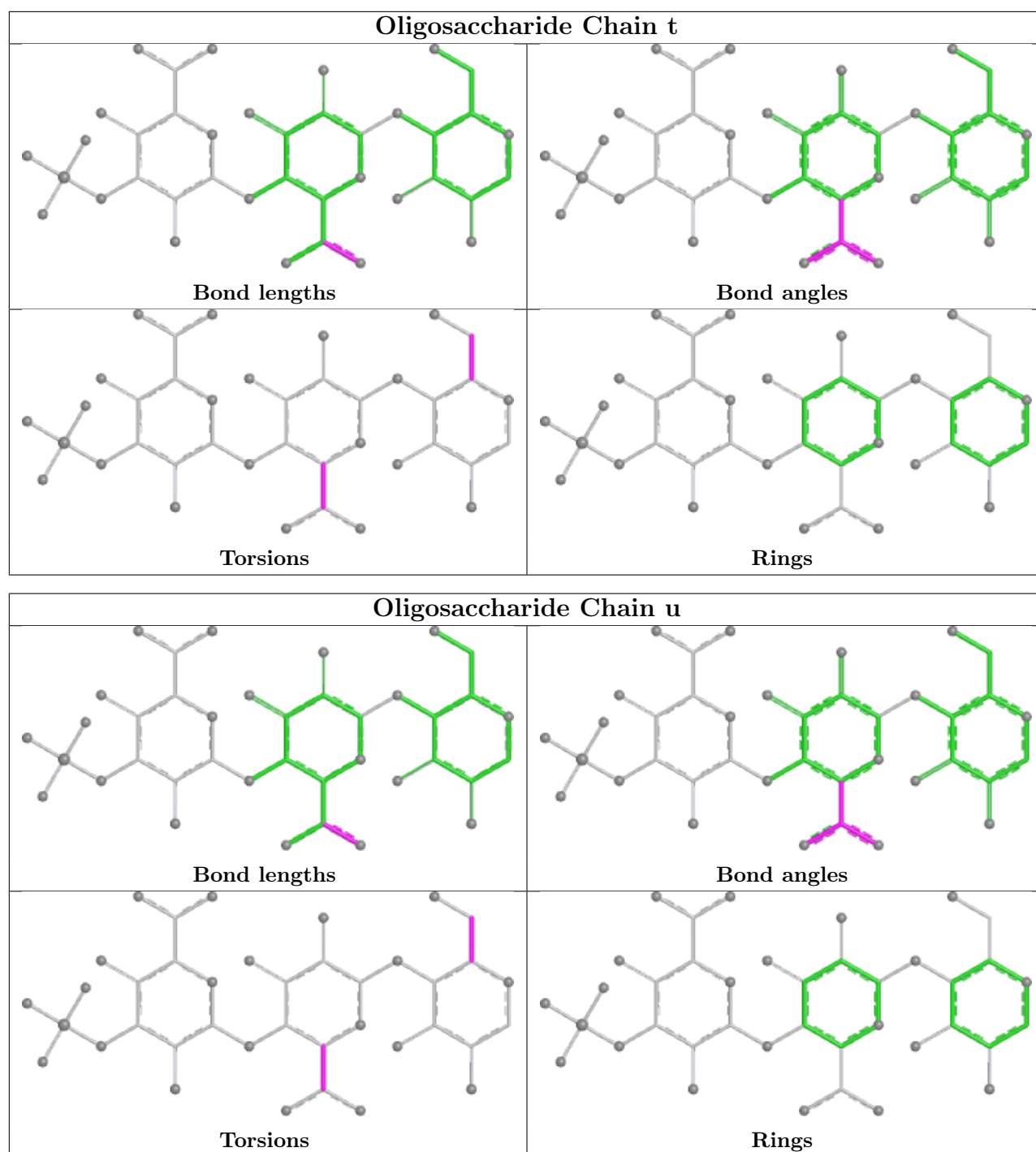


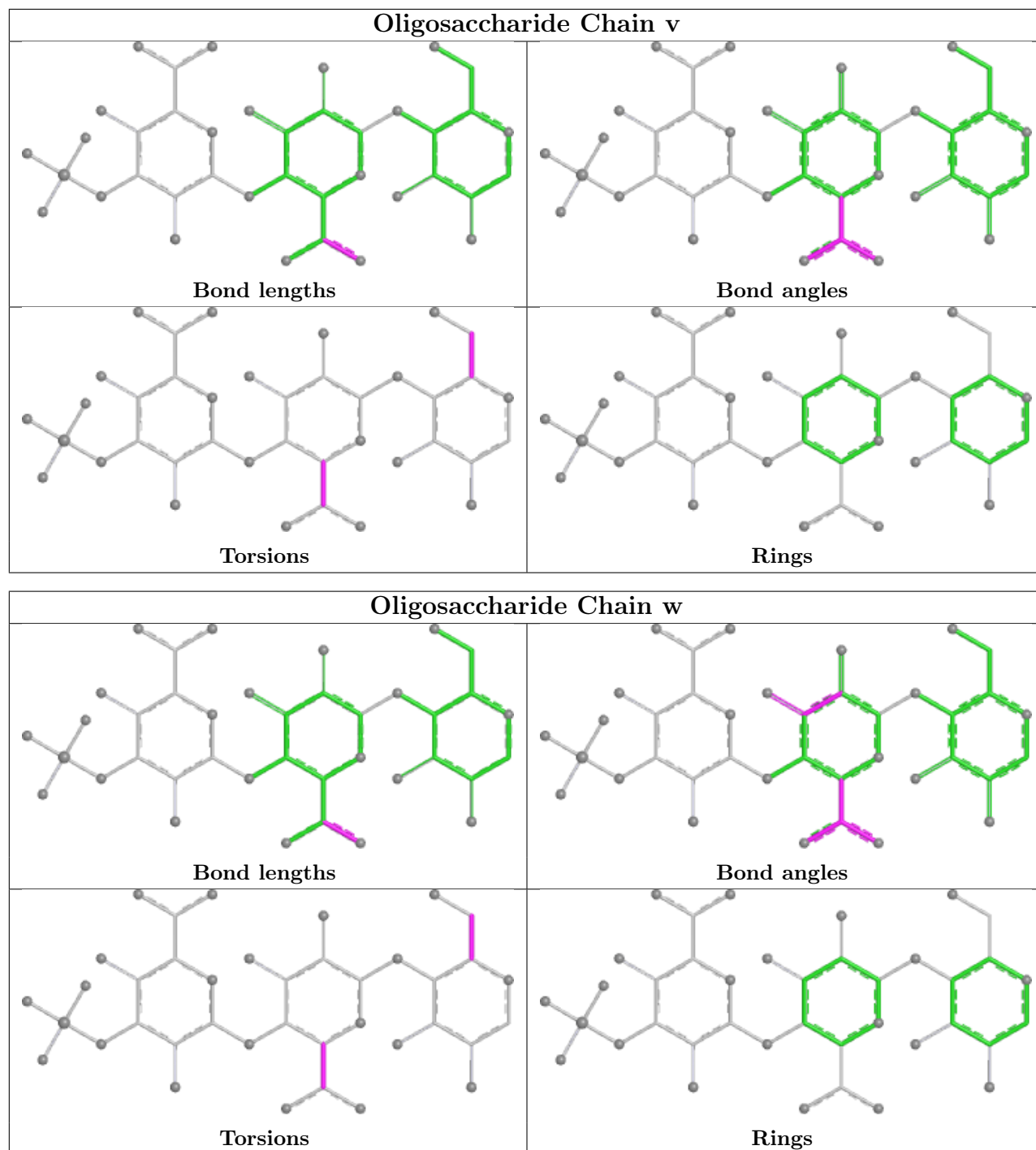


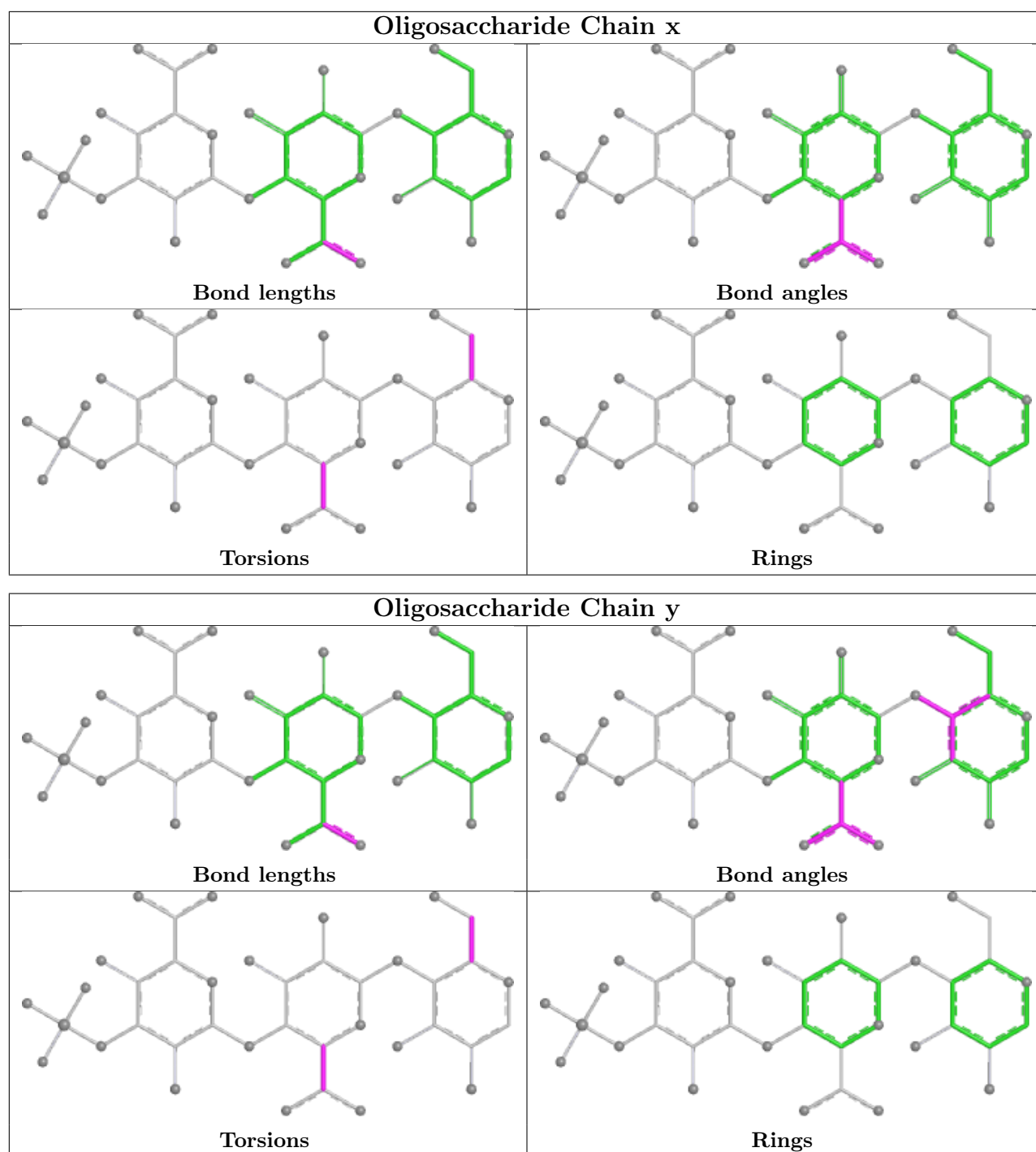


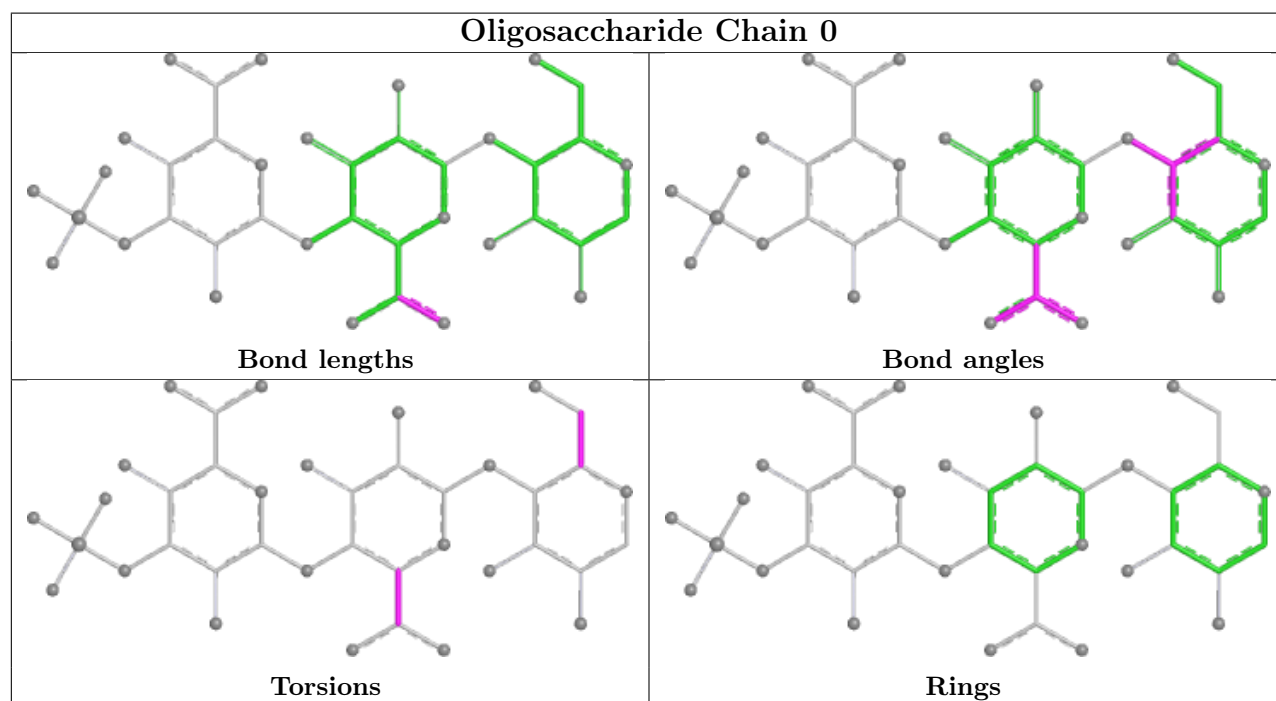
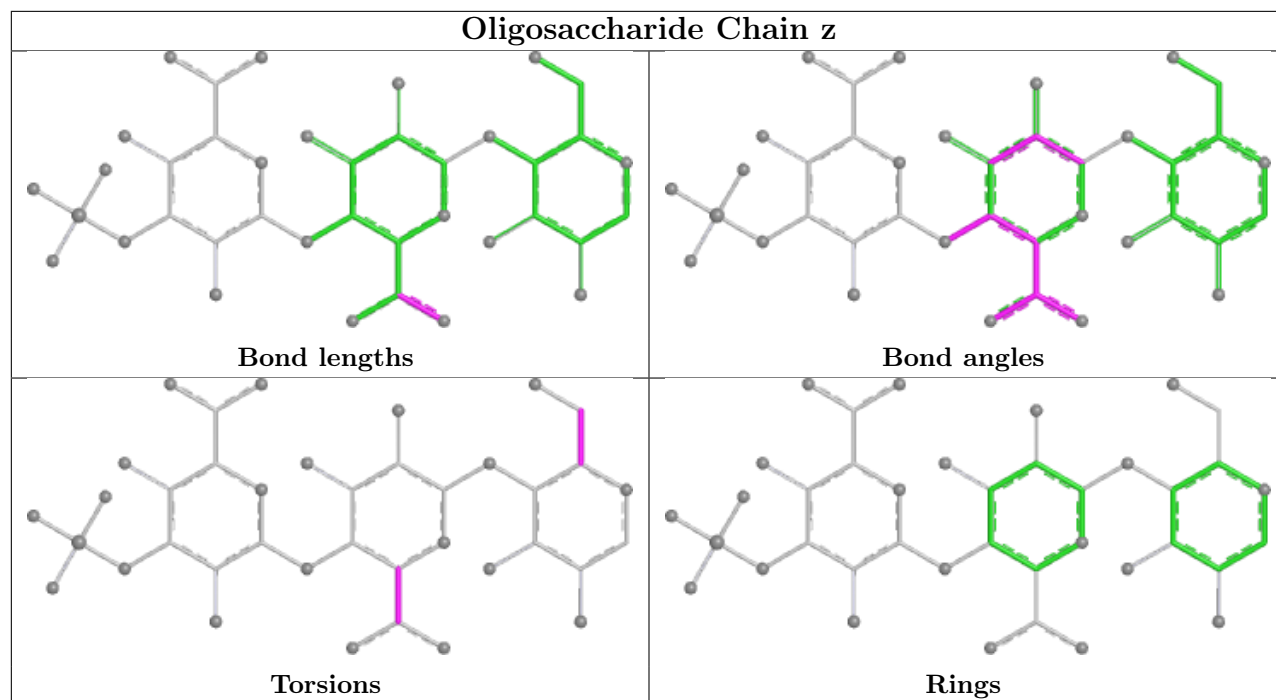


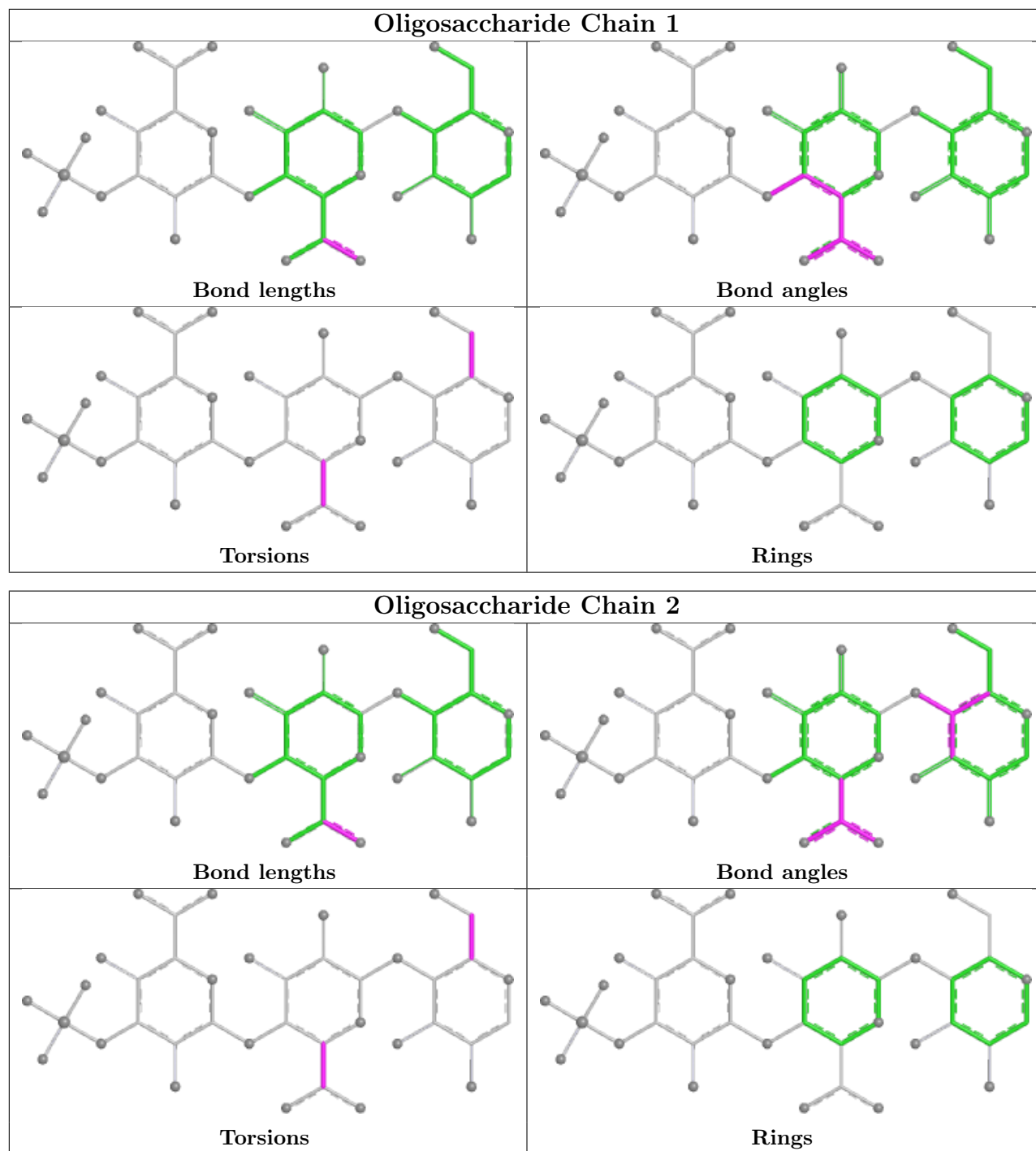


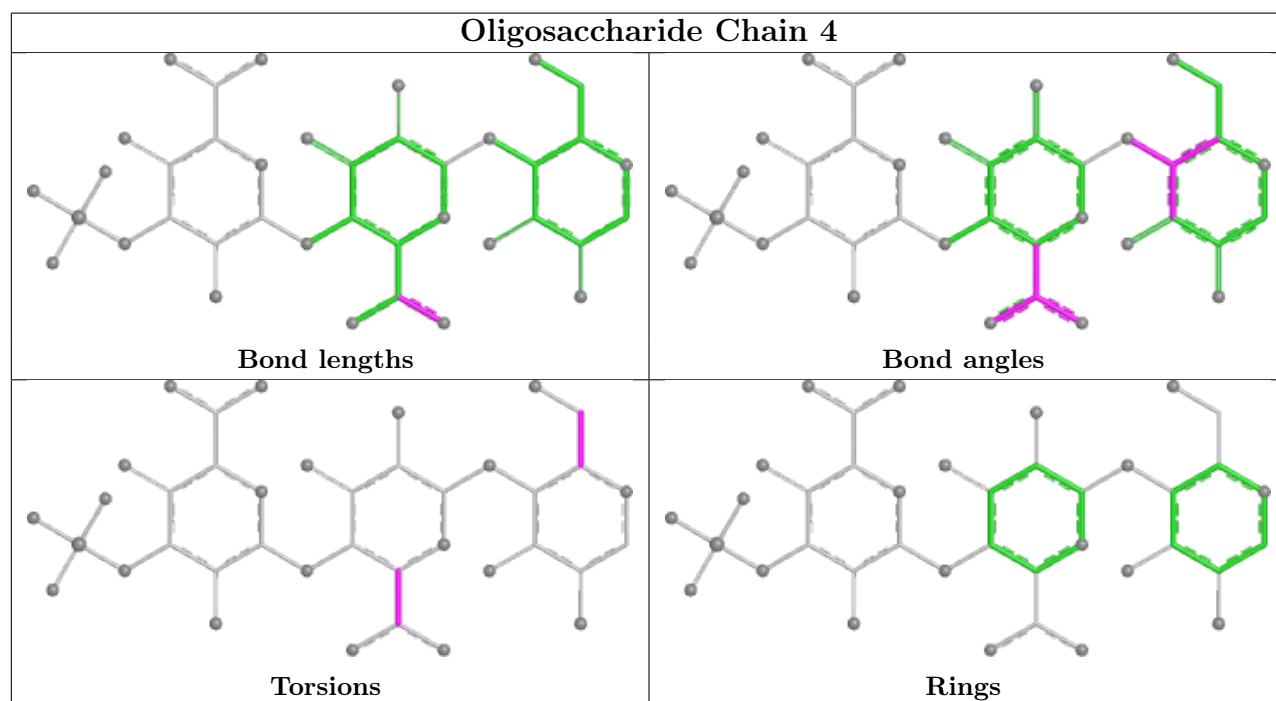
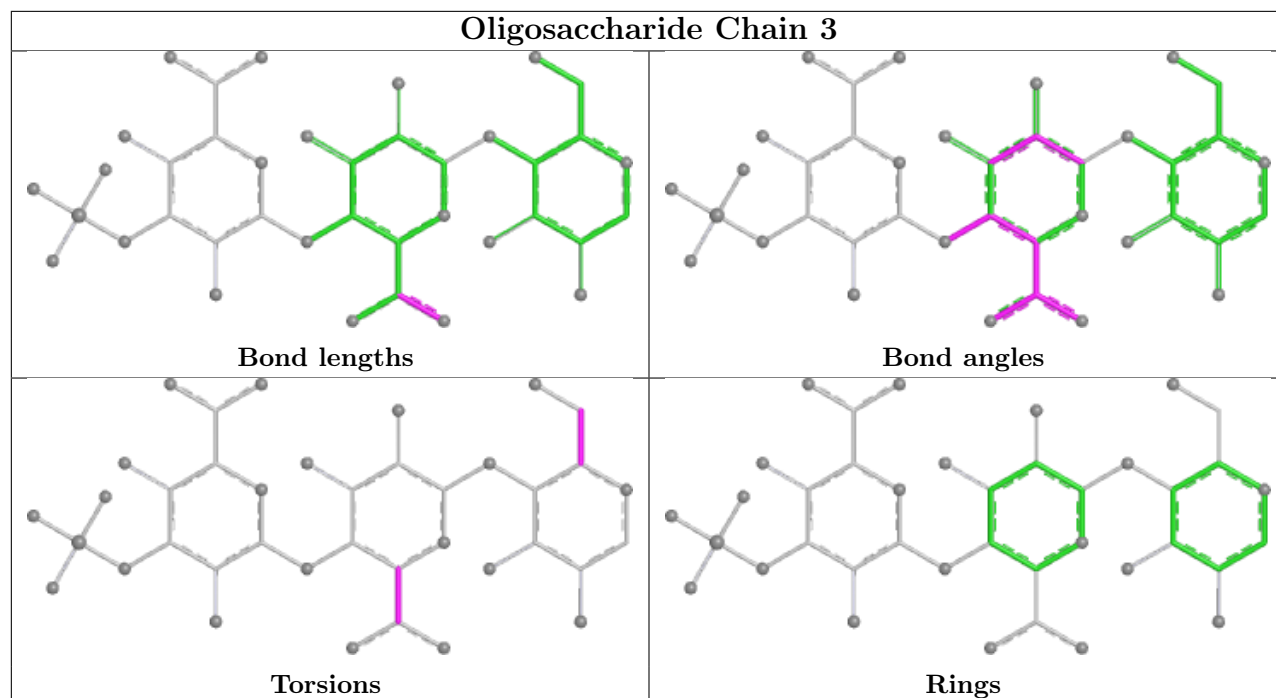


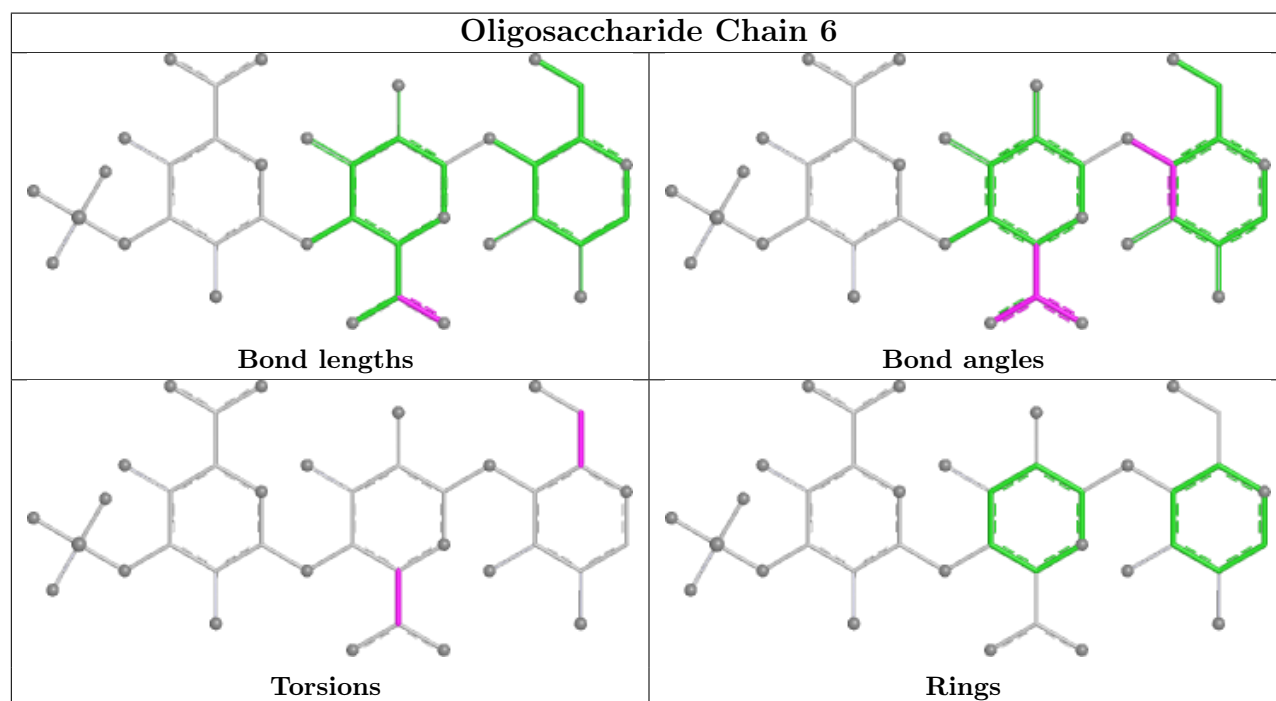
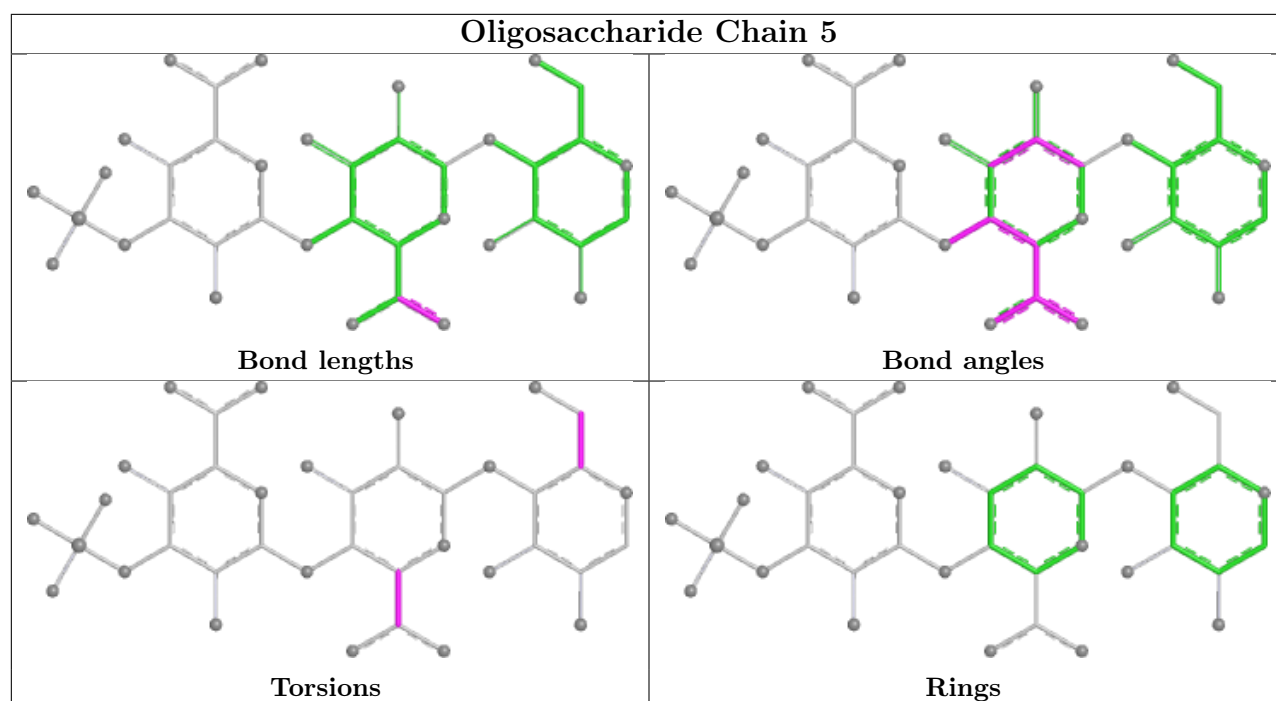


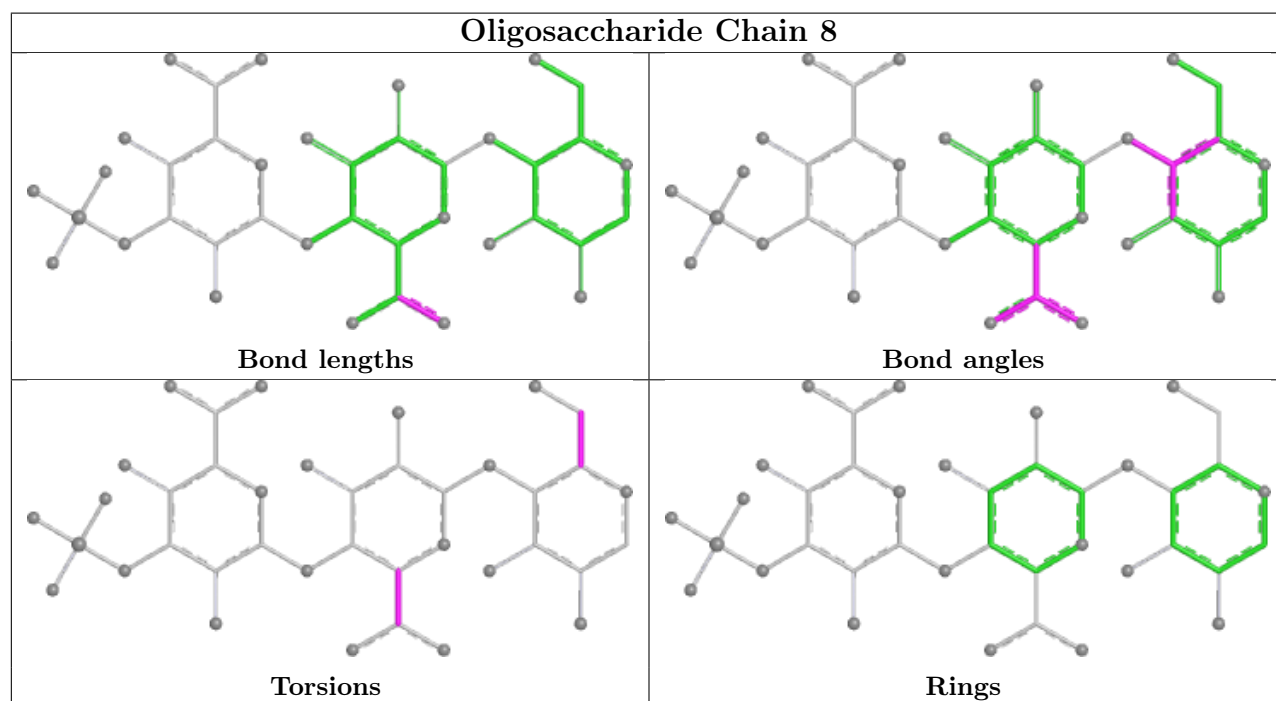
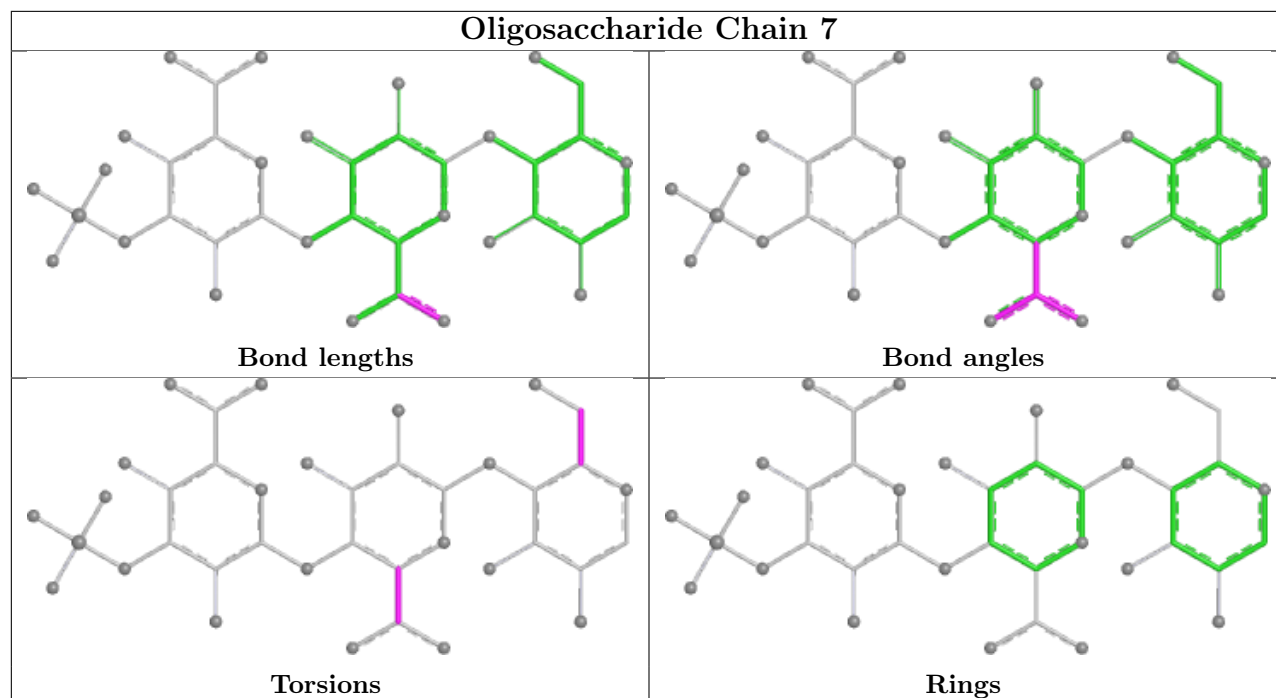


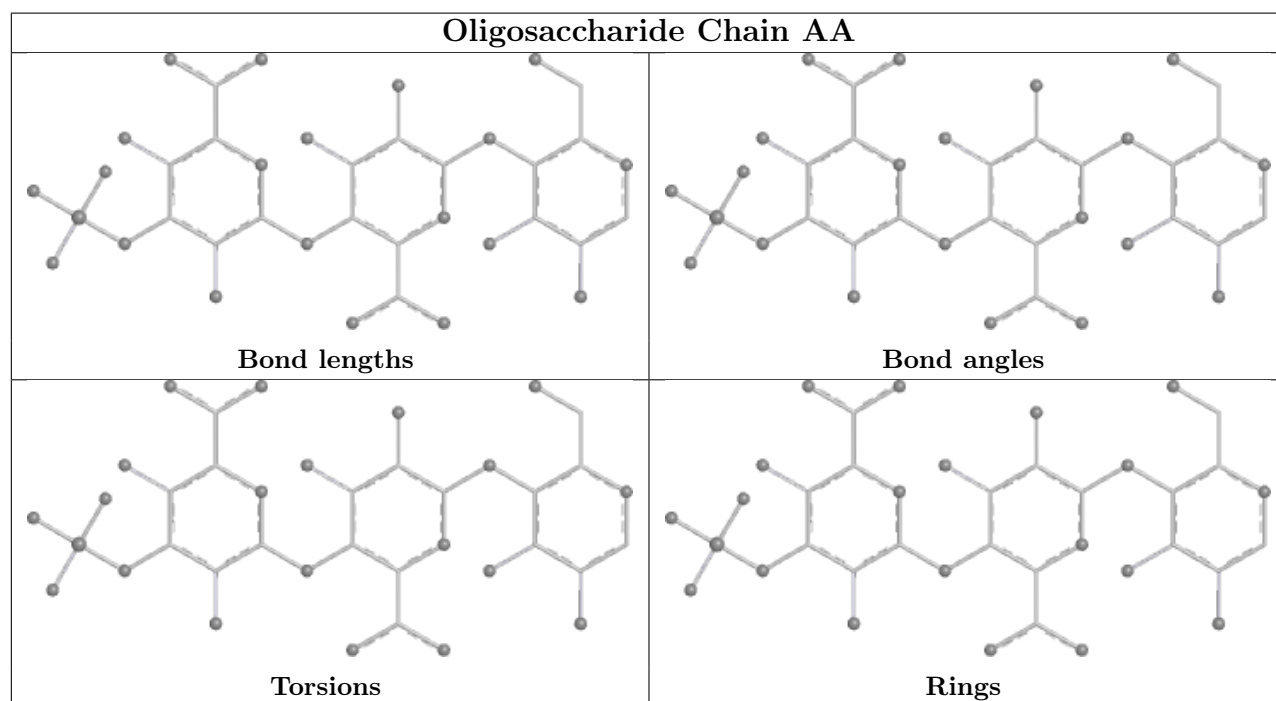
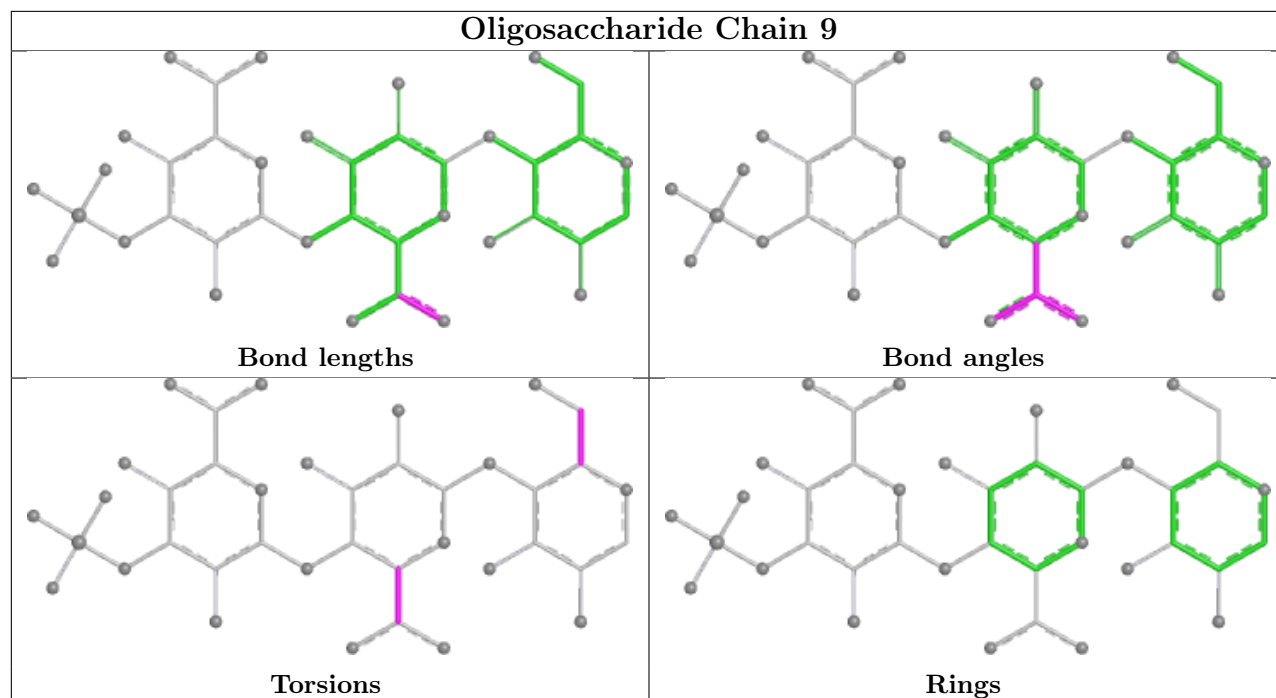


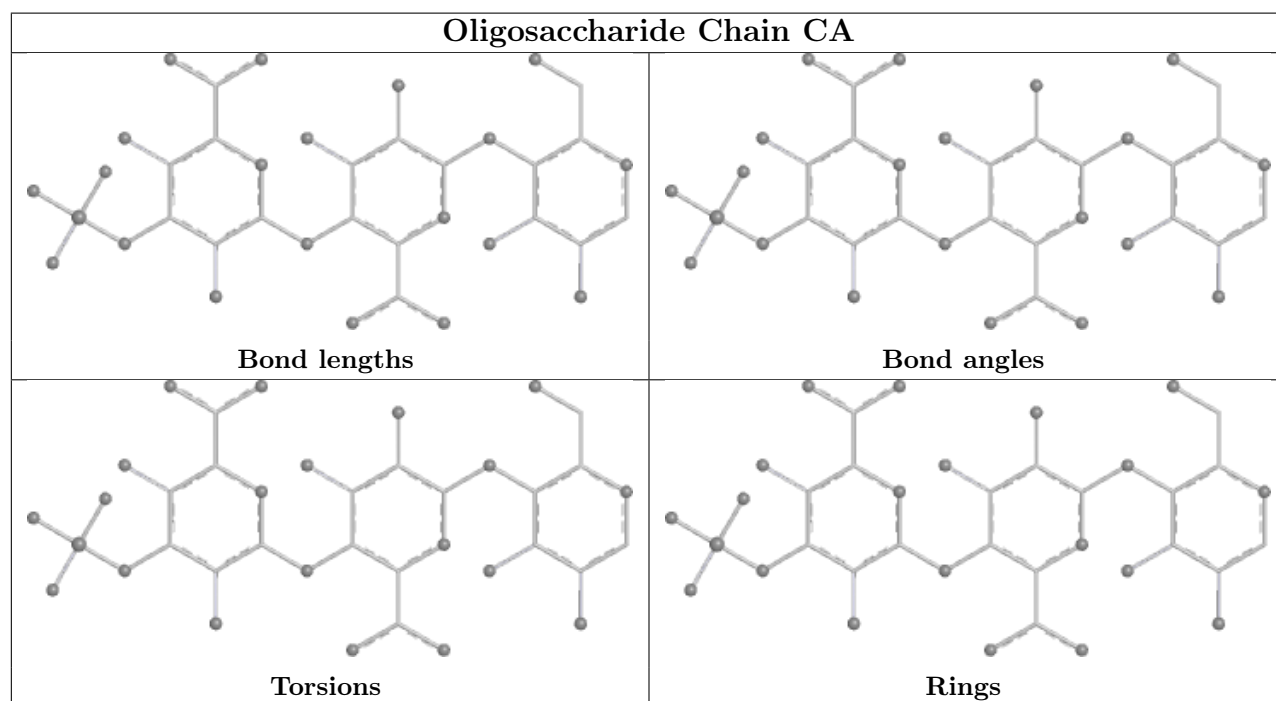
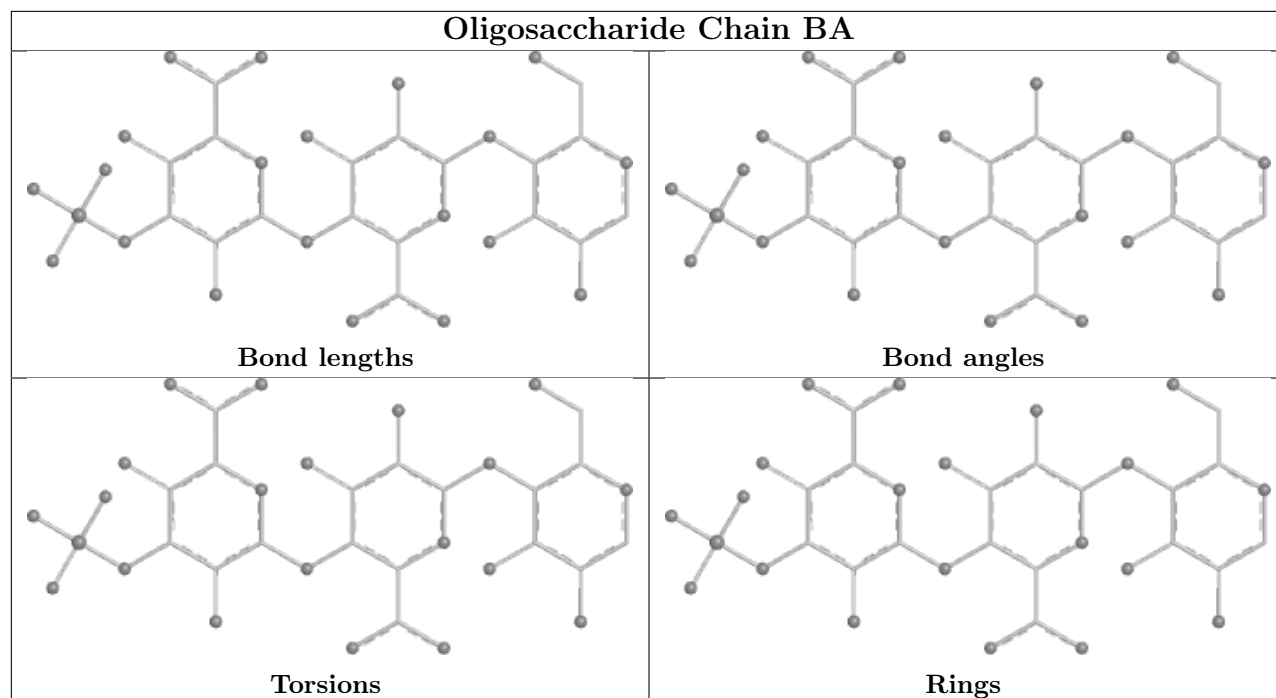


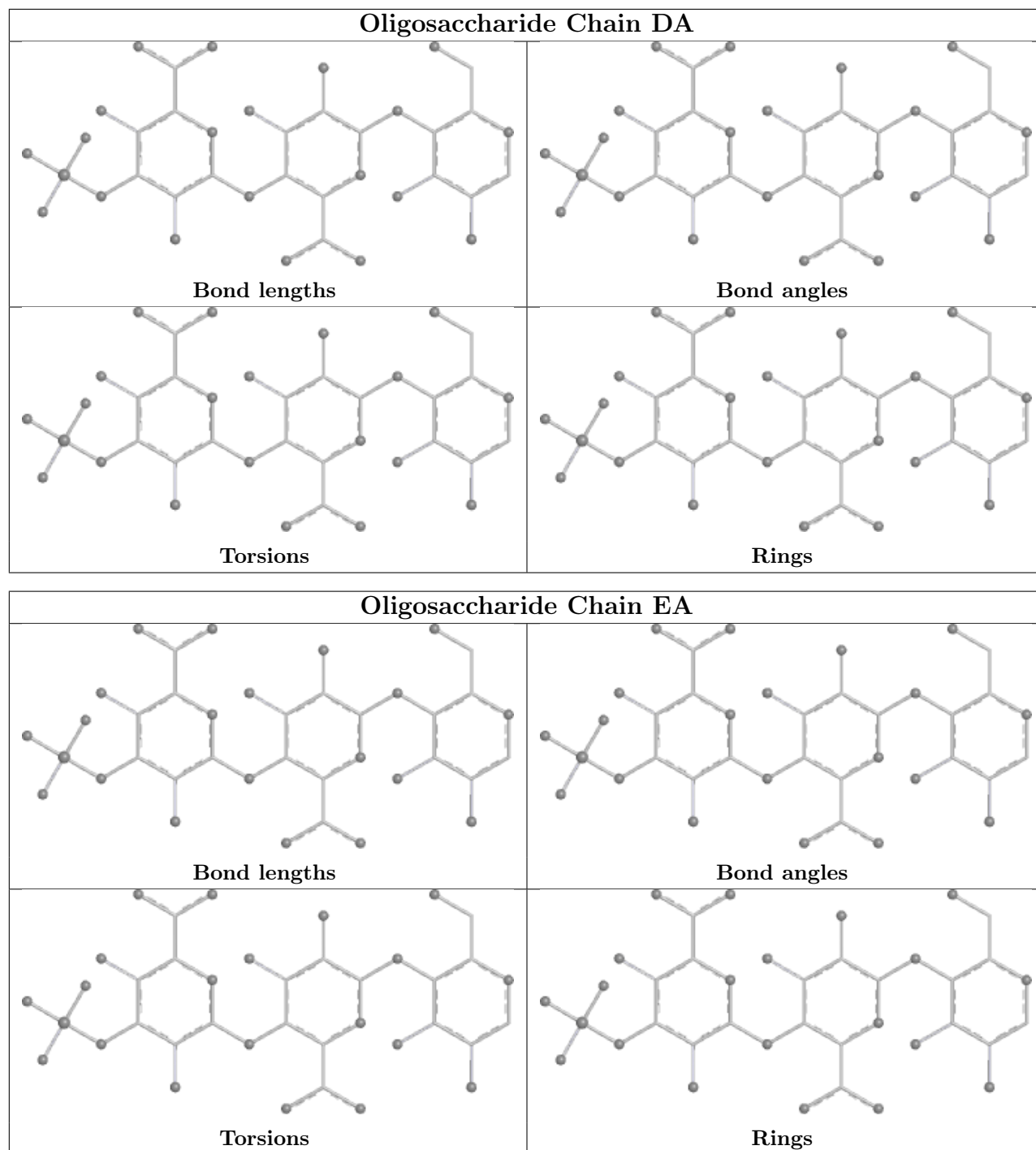


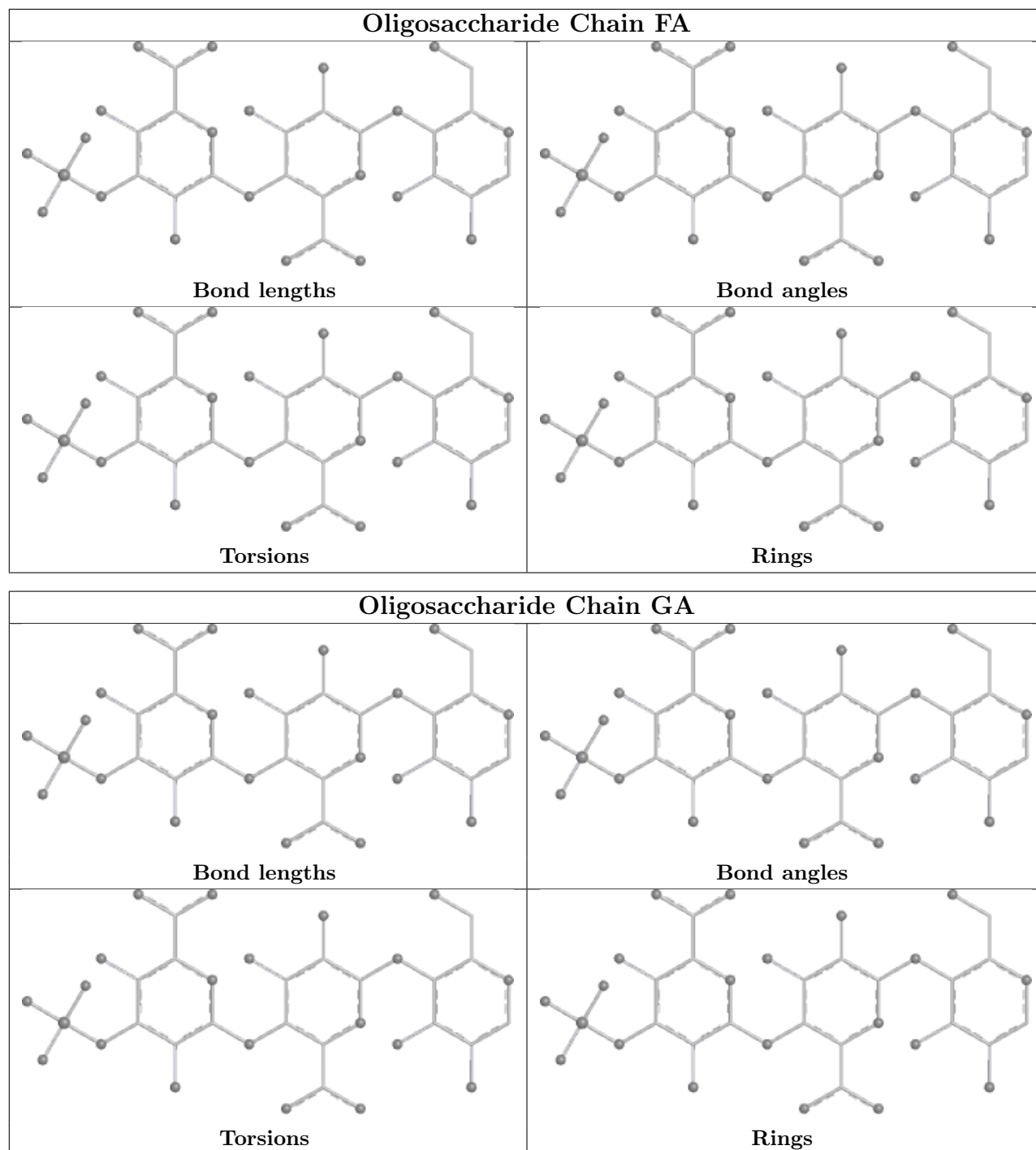


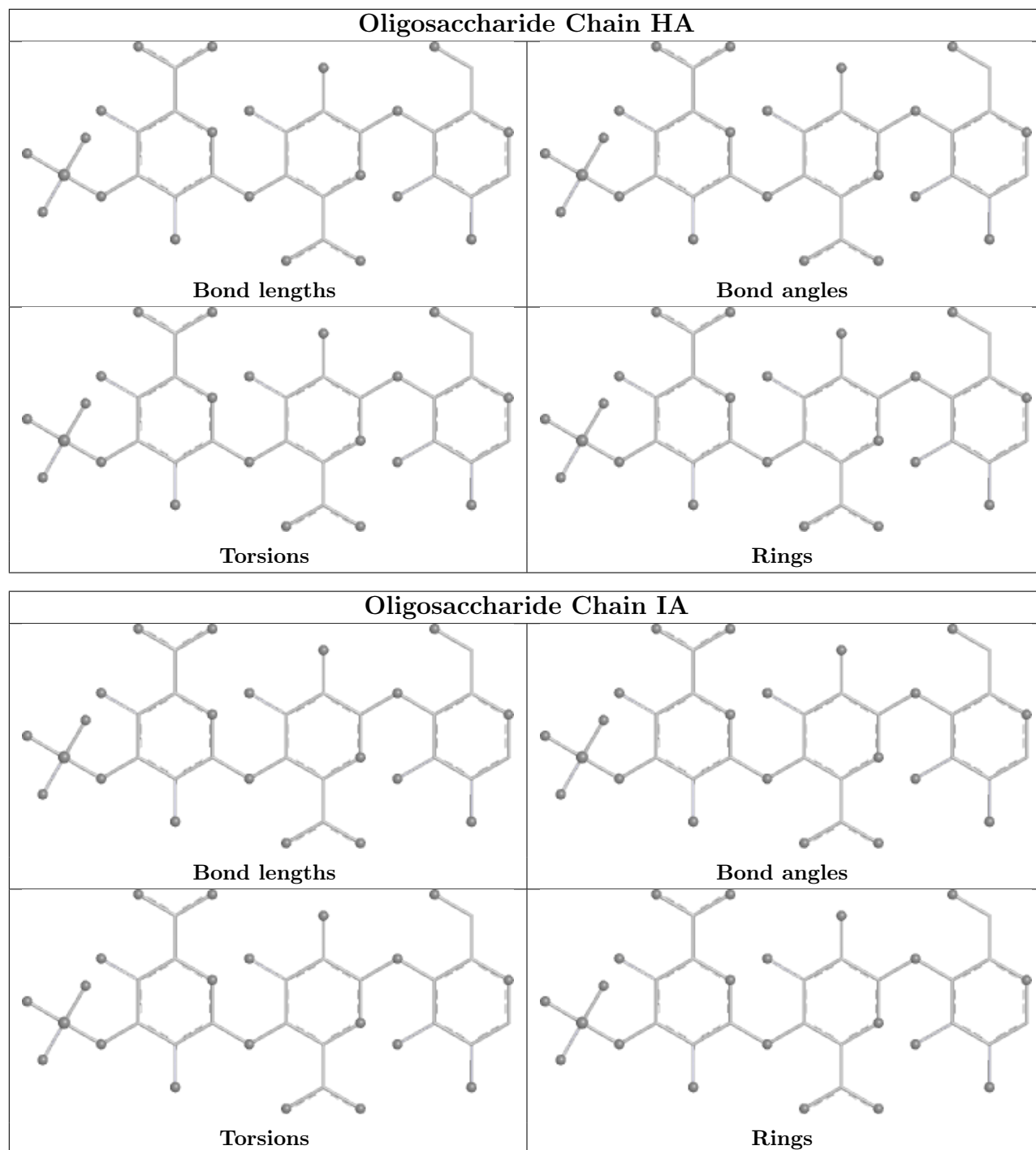


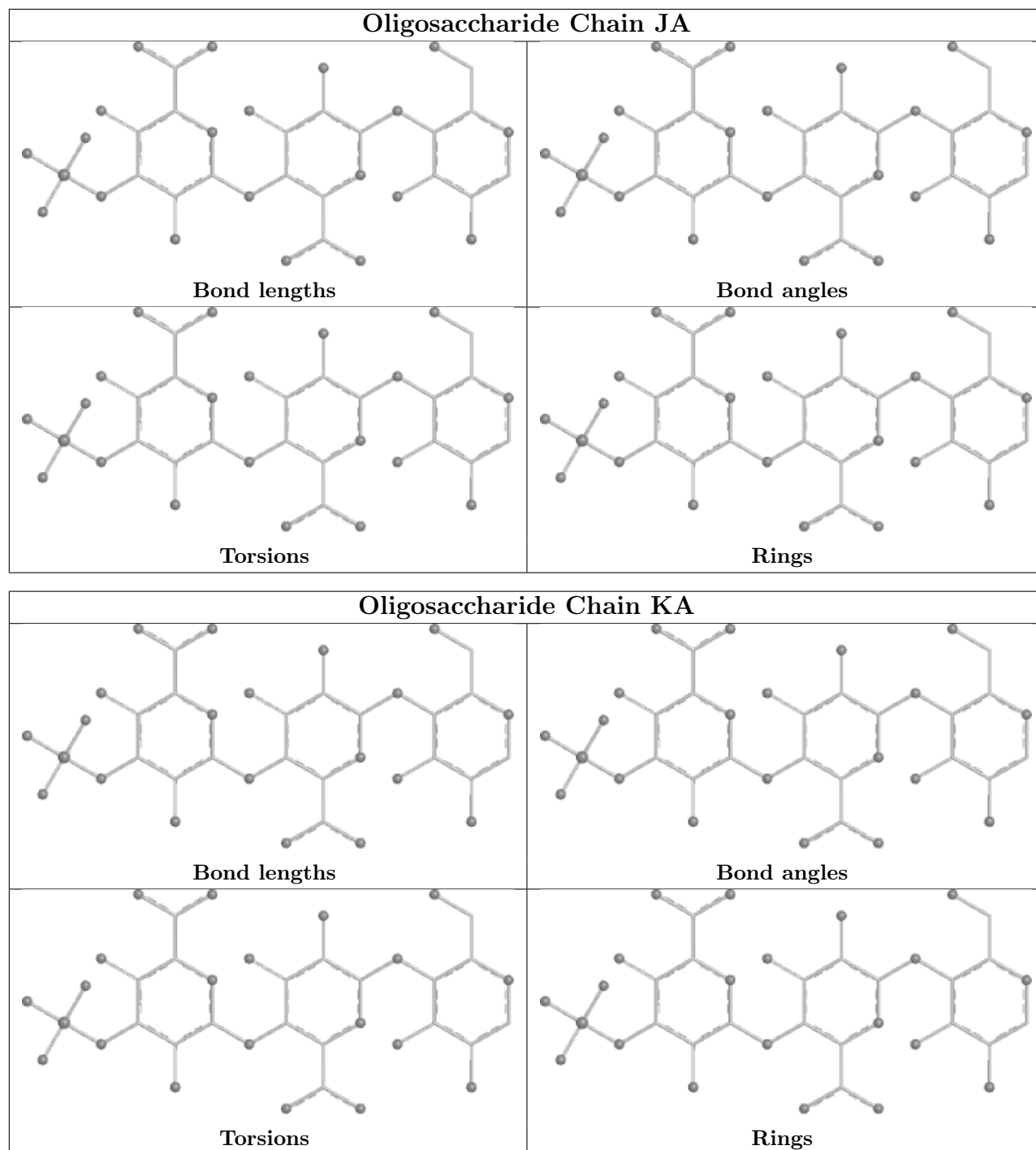


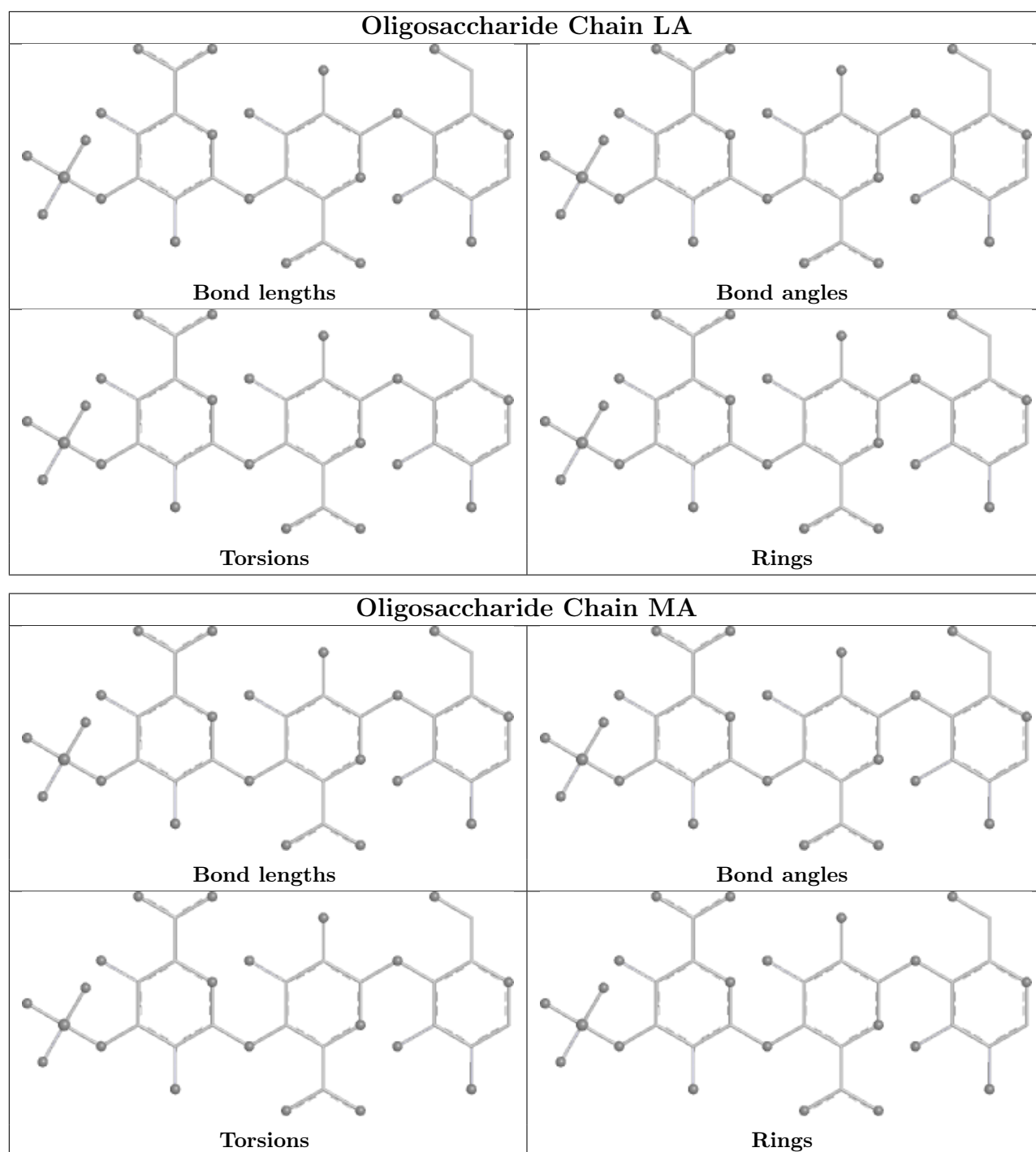












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

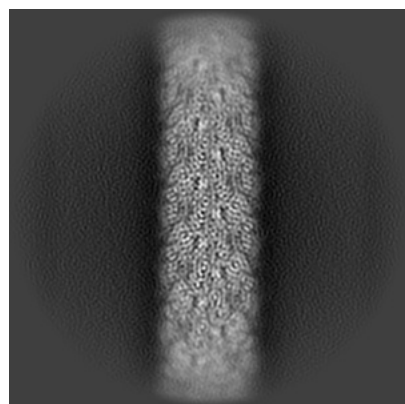
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19962. These allow visual inspection of the internal detail of the map and identification of artifacts.

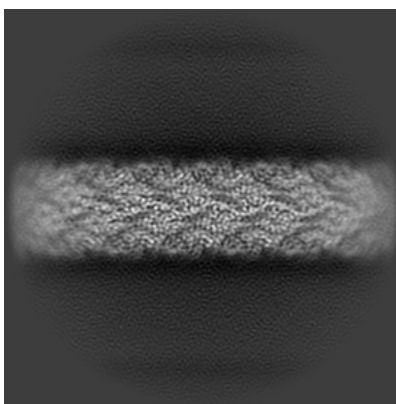
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

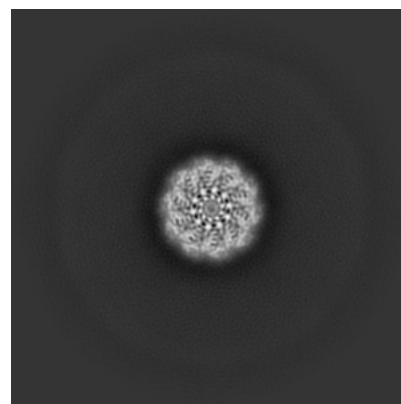
6.1.1 Primary map



X

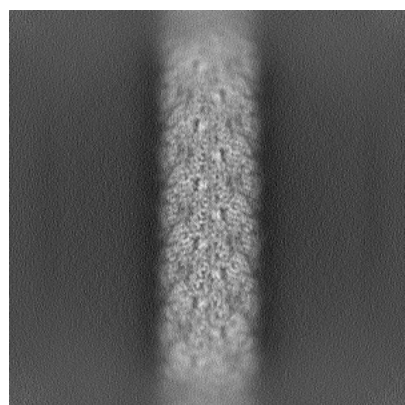


Y

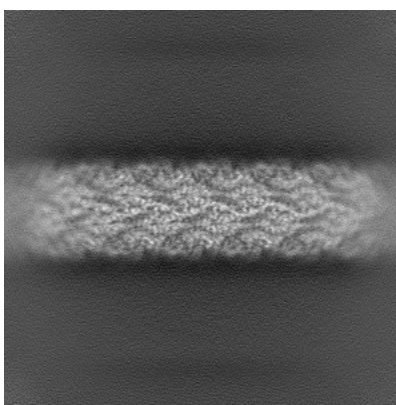


Z

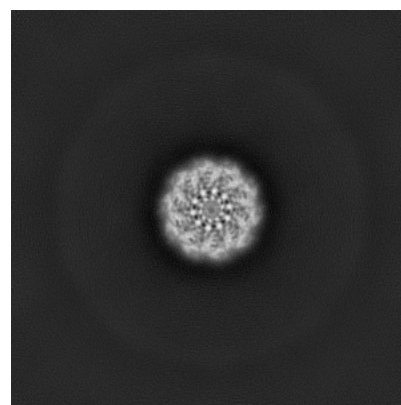
6.1.2 Raw map



X



Y

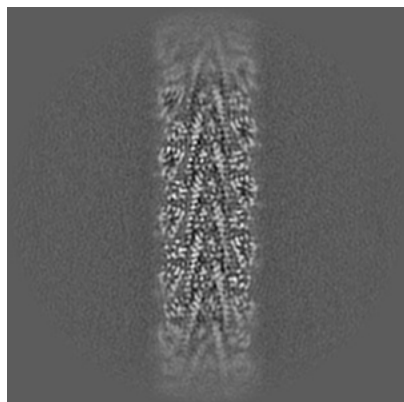


Z

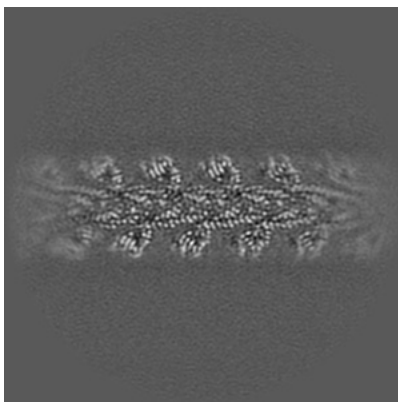
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

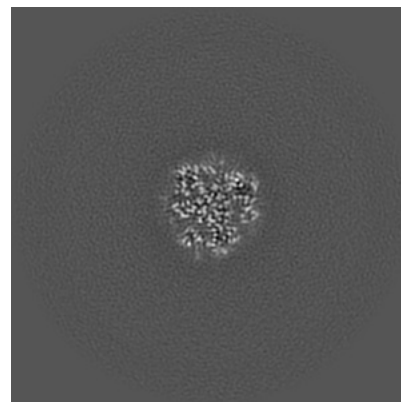
6.2.1 Primary map



X Index: 208

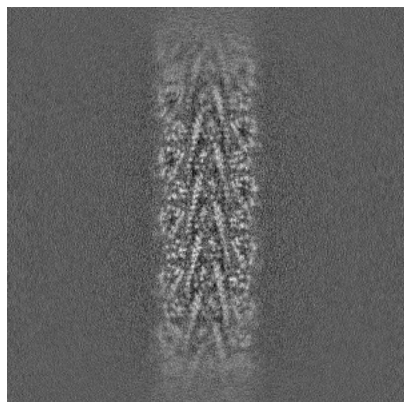


Y Index: 208

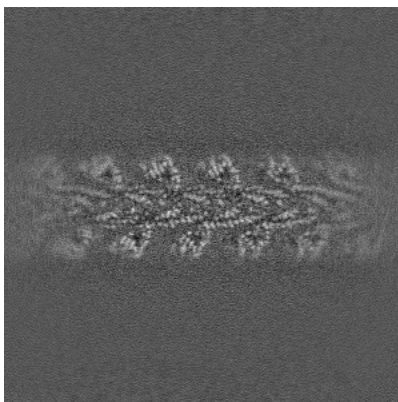


Z Index: 208

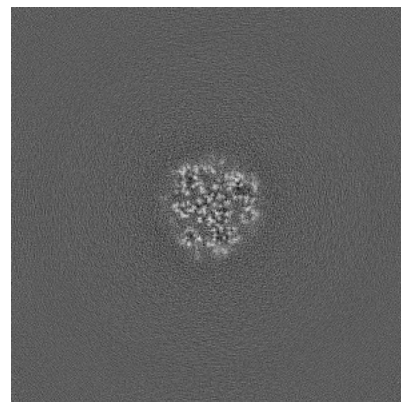
6.2.2 Raw map



X Index: 208



Y Index: 208

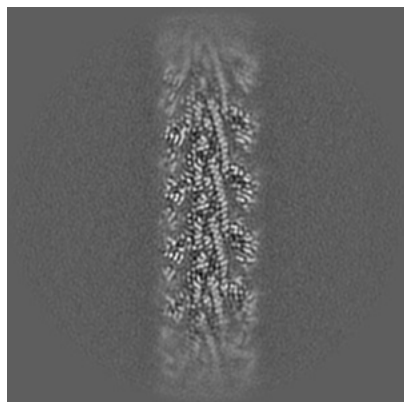


Z Index: 208

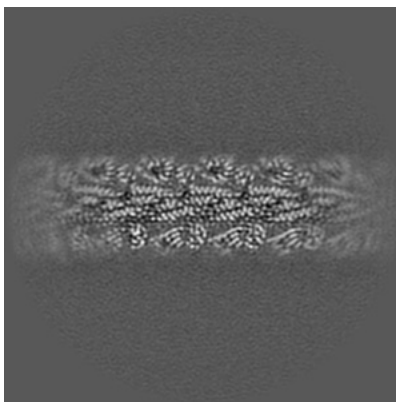
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

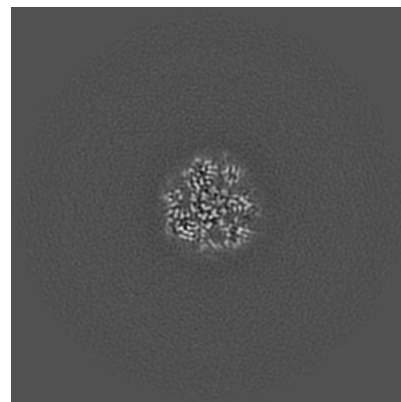
6.3.1 Primary map



X Index: 201

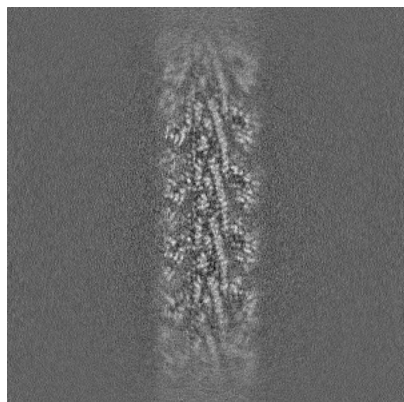


Y Index: 199

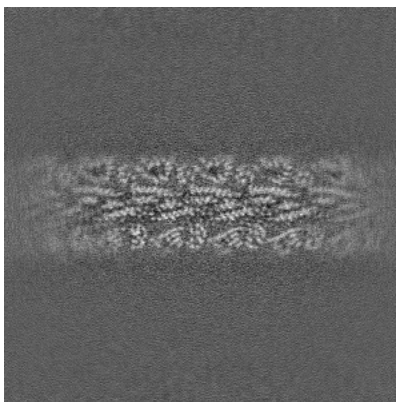


Z Index: 176

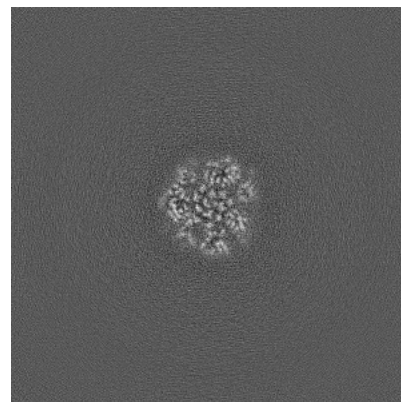
6.3.2 Raw map



X Index: 201



Y Index: 199

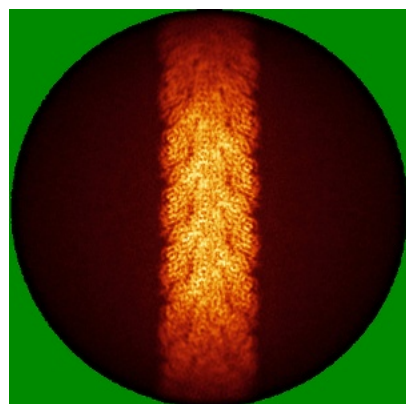


Z Index: 194

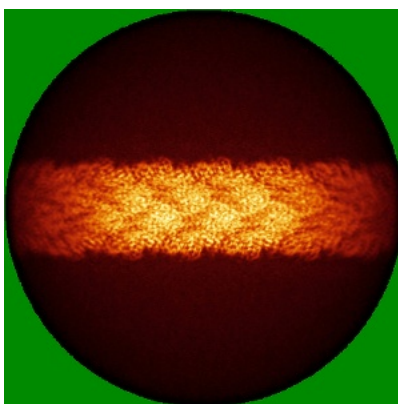
The images above show the largest variance slices of the map in three orthogonal directions.

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

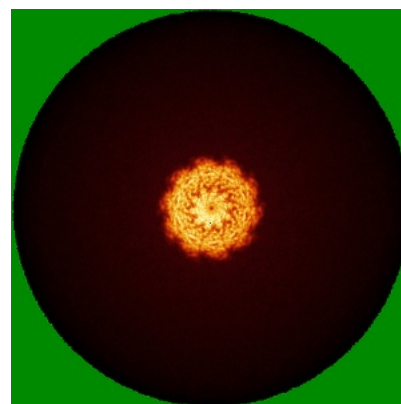
6.4.1 Primary map



X

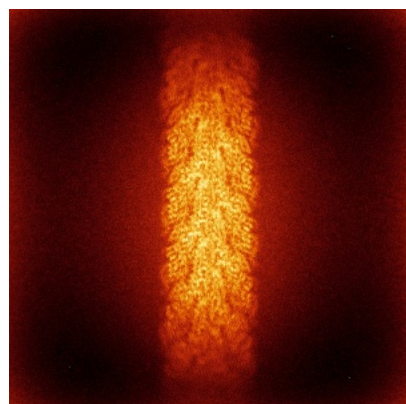


Y

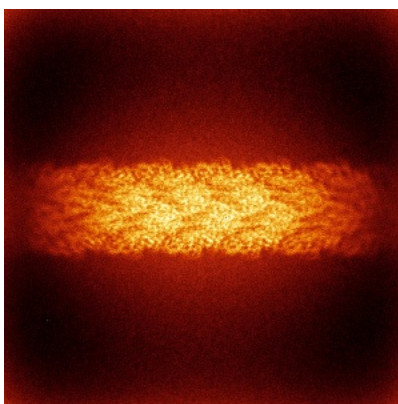


Z

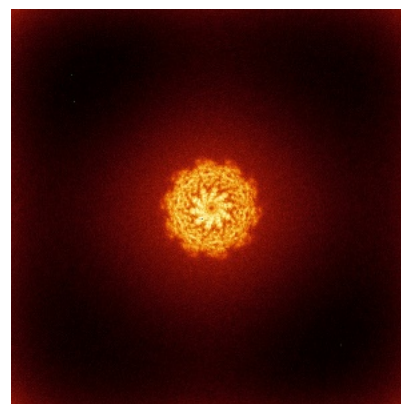
6.4.2 Raw map



X



Y

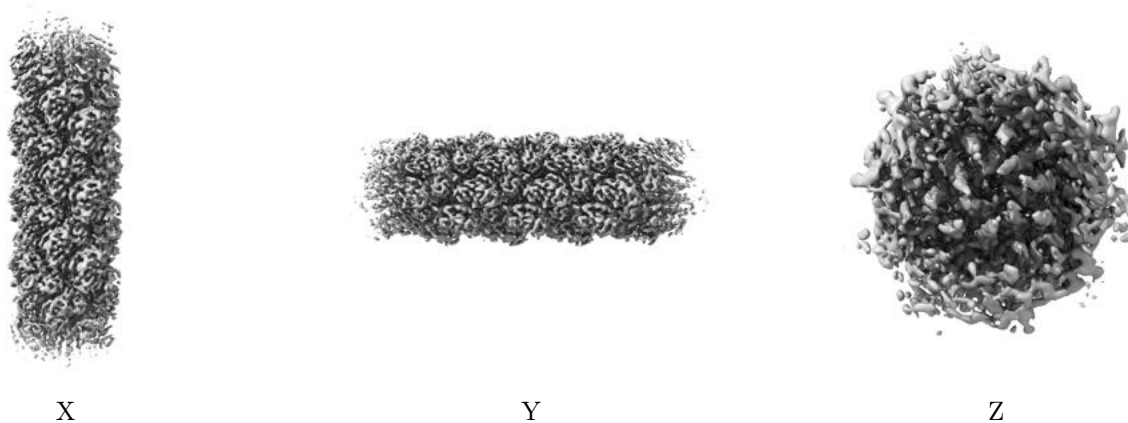


Z

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.

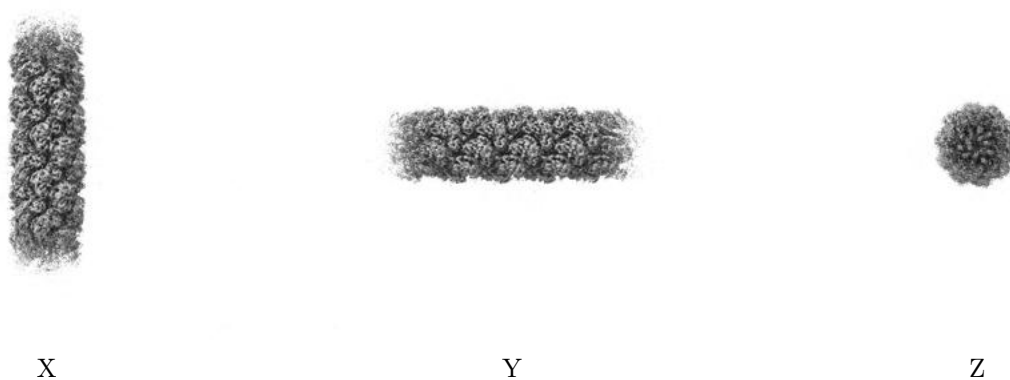
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

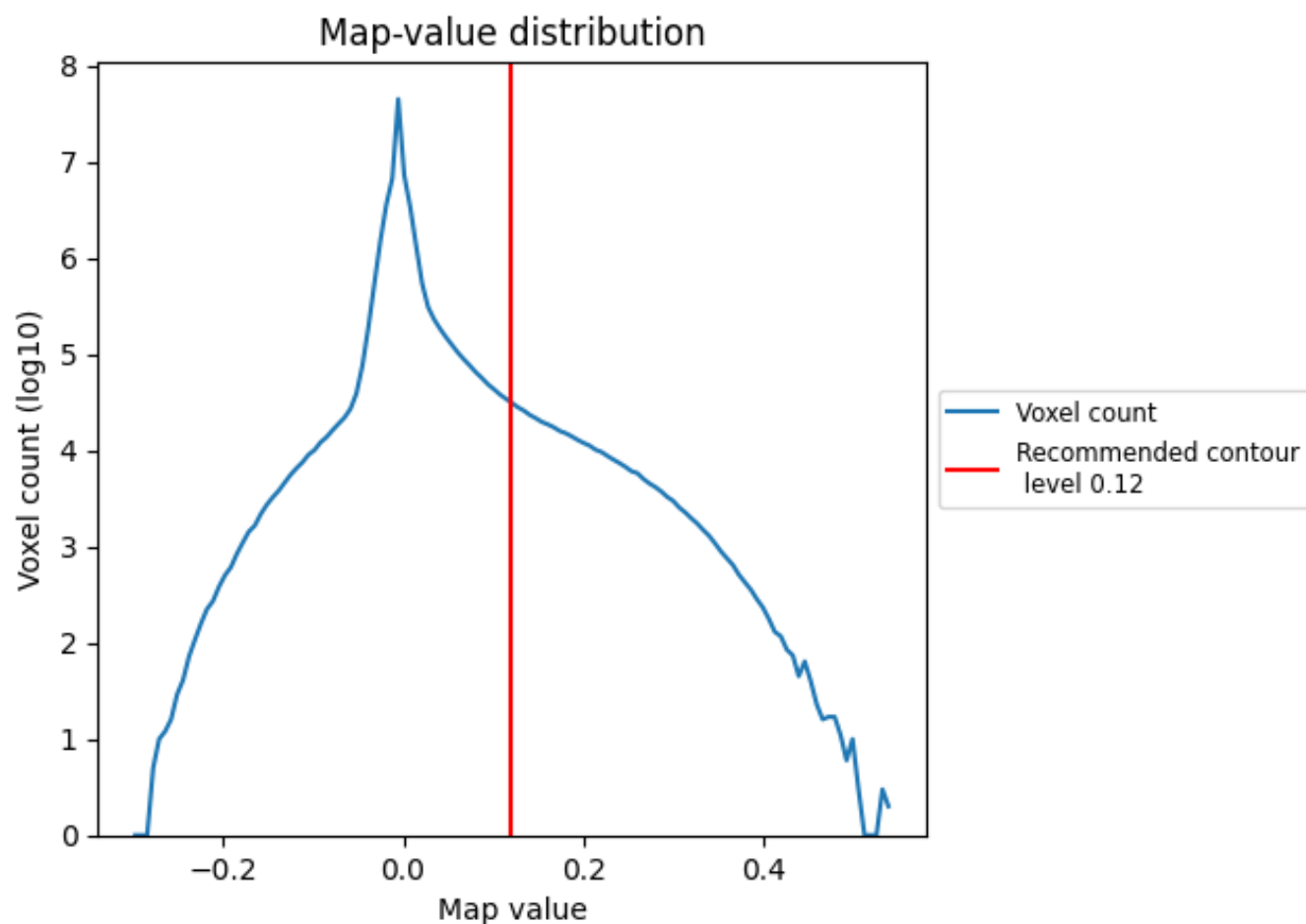
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

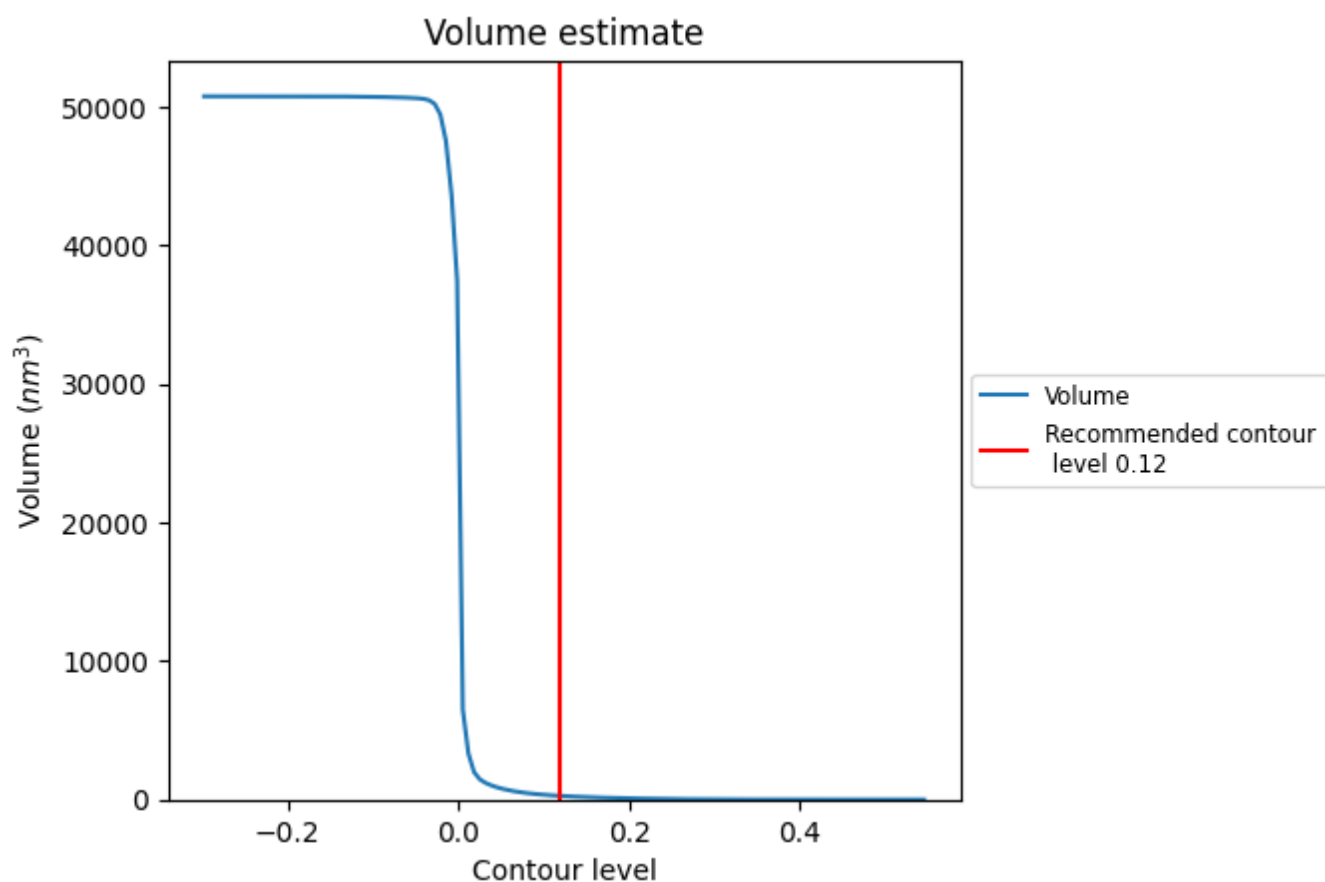
This section contains the results of statistical analysis of the map.

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.

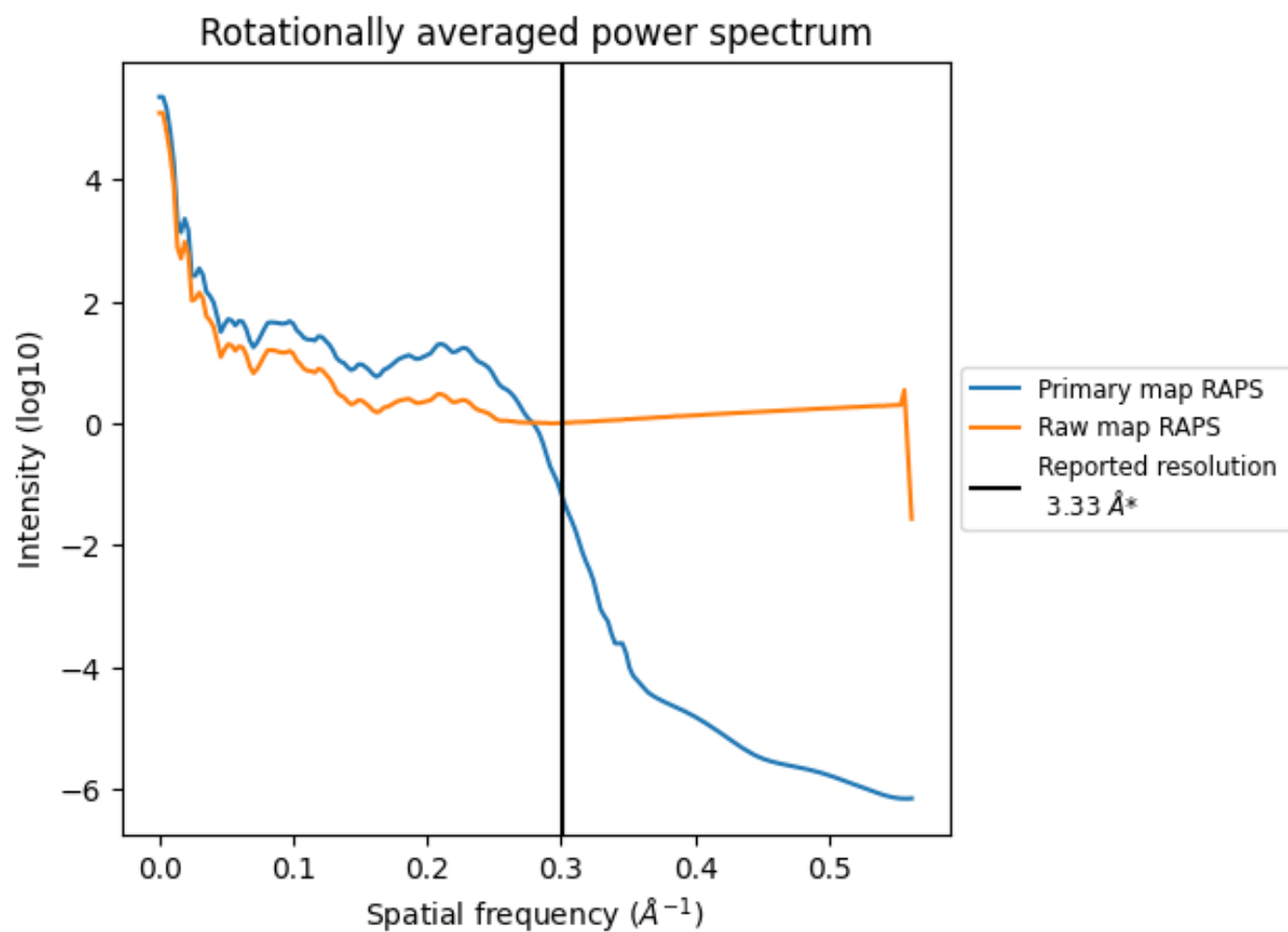
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 264 nm³; this corresponds to an approximate mass of 238 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 ⓘ

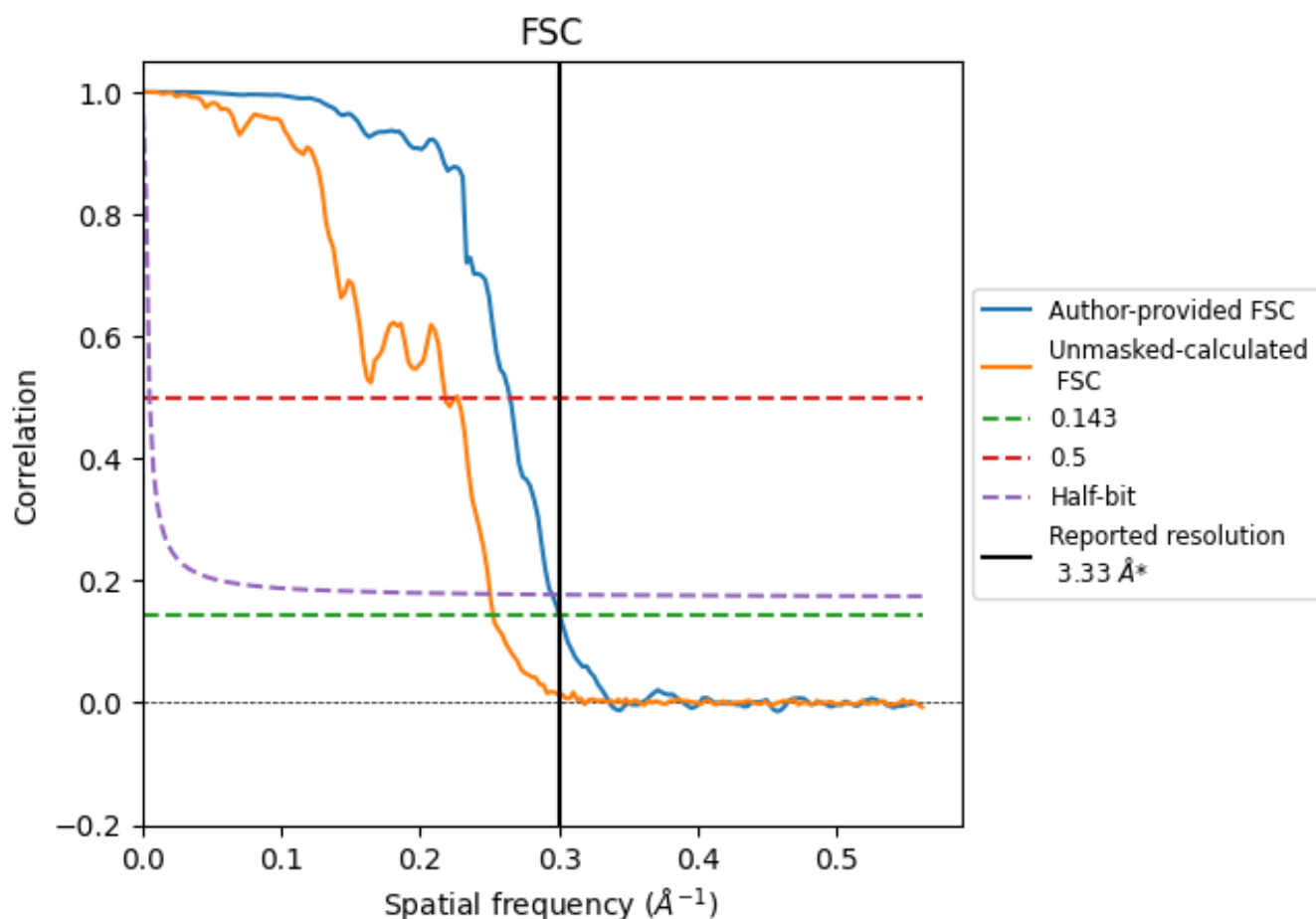


*Reported resolution corresponds to spatial frequency of 0.300 $\text{\AA}^{-1}$

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 0.300 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

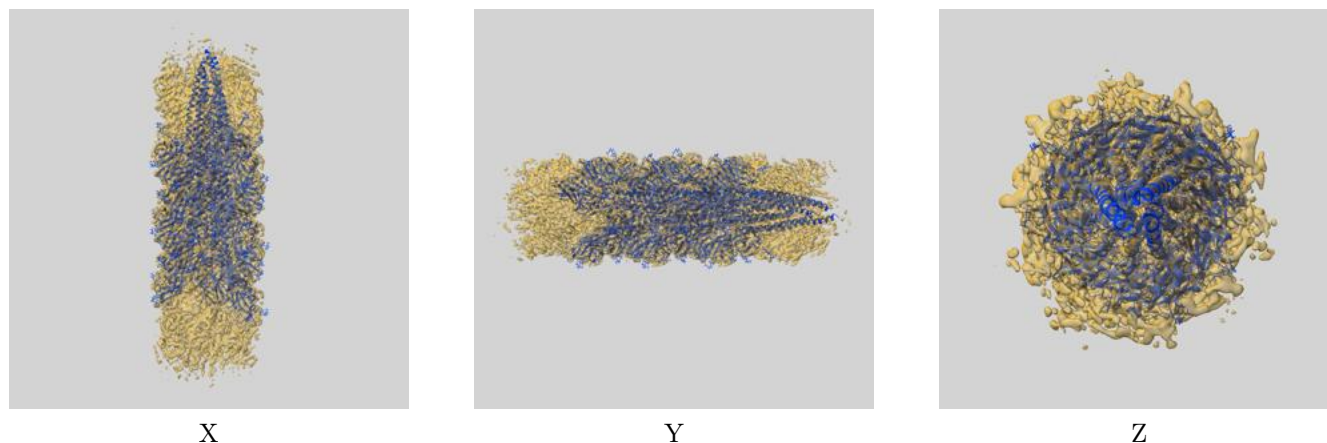
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.78	3.39
Unmasked-calculated*	3.95	4.58	3.99

*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 3.95 differs from the reported value 3.33 by more than 10 %

9 Map-model fit [i](#)

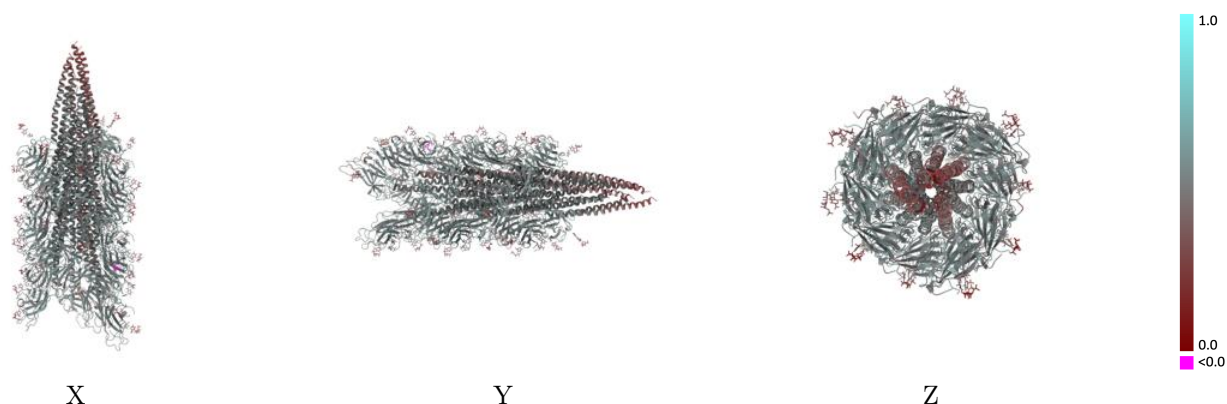
This section contains information regarding the fit between EMDB map EMD-19962 and PDB model 9ETU. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



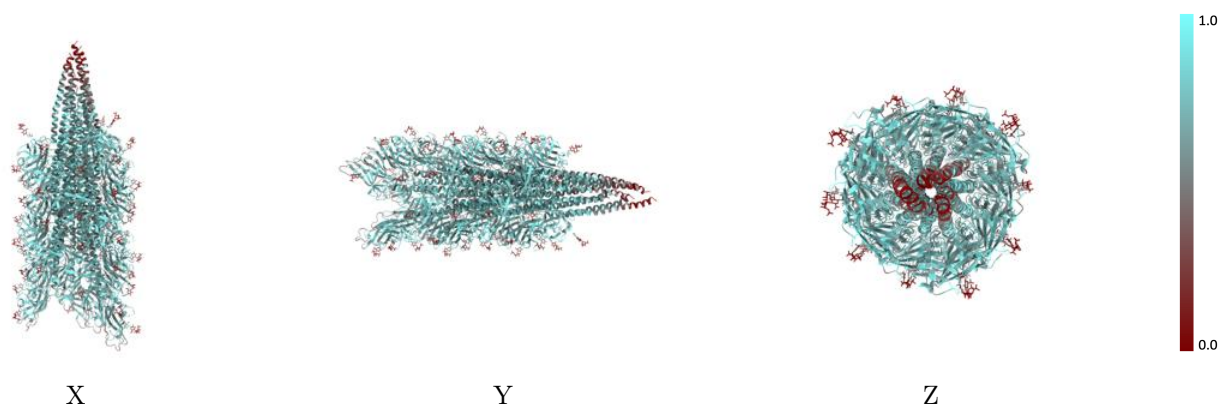
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



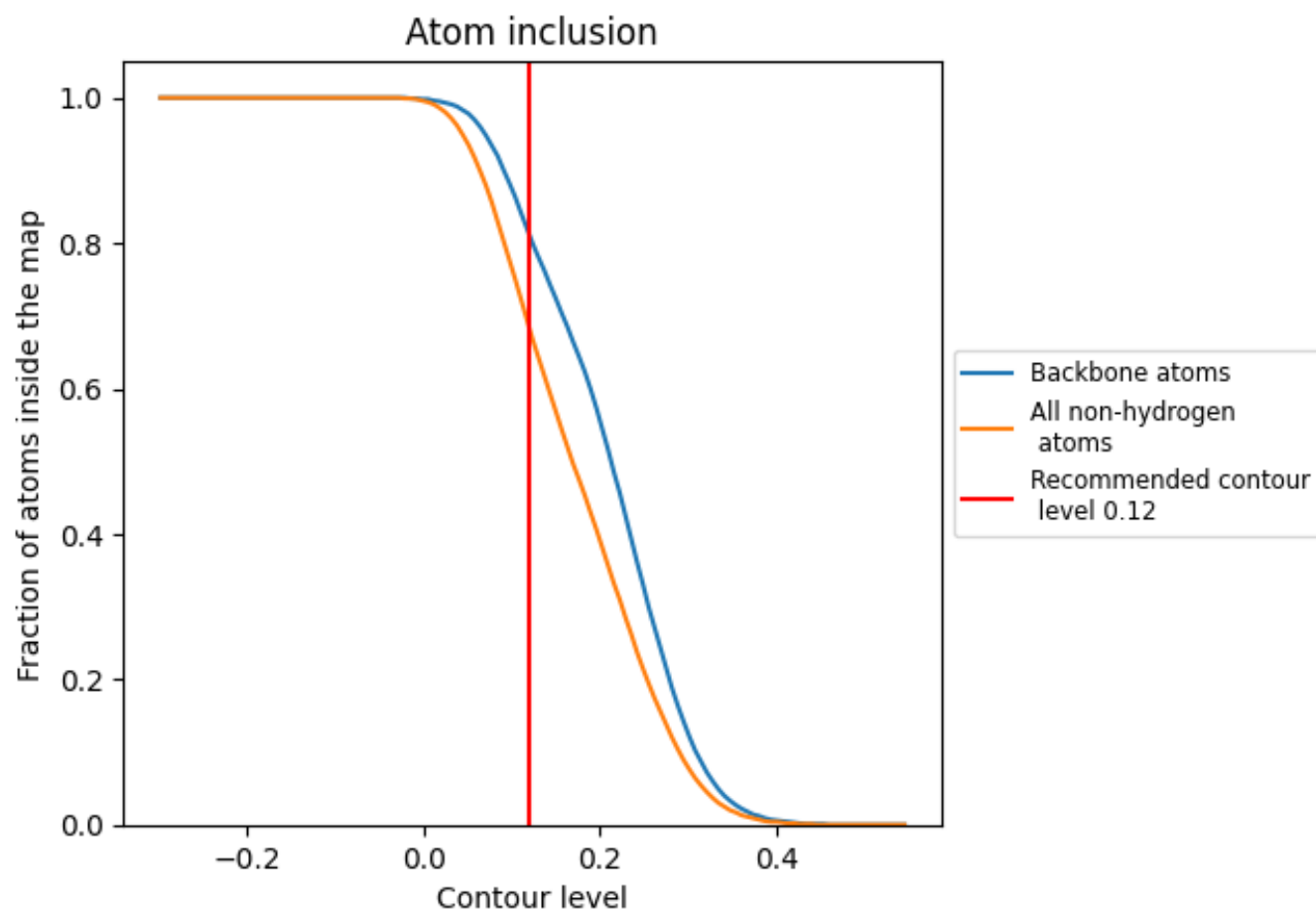
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.4940
0	 0.2560	 0.4030
1	 0.3080	 0.3540
2	 0.3080	 0.3010
3	 0.3080	 0.3500
4	 0.2560	 0.2870
5	 0.3080	 0.2640
6	 0.2050	 0.3670
7	 0.3330	 0.3050
8	 0.2820	 0.2730
9	 0.2820	 0.4060
A	 0.7020	 0.5100
AA	 0.2310	 0.2480
B	 0.7370	 0.5170
BA	 0.3330	 0.3610
C	 0.7450	 0.5190
CA	 0.2310	 0.2590
D	 0.6820	 0.4840
DA	 0.3330	 0.3580
E	 0.6840	 0.4980
EA	 0.2560	 0.4000
F	 0.7220	 0.5080
FA	 0.3080	 0.3250
G	 0.6950	 0.5040
GA	 0.1790	 0.2980
H	 0.7310	 0.5150
HA	 0.3330	 0.3960
I	 0.7440	 0.5240
IA	 0.2310	 0.3460
J	 0.7530	 0.5210
JA	 0.2560	 0.2890
K	 0.7520	 0.5200
KA	 0.2310	 0.3740
L	 0.7400	 0.5170
LA	 0.3330	 0.3240



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Chain	Atom inclusion	Q-score
M	 0.7140	 0.5070
MA	 0.1790	 0.3310
N	 0.7260	 0.4970
O	 0.7000	 0.4980
P	 0.7310	 0.5160
Q	 0.7560	 0.5170
R	 0.7310	 0.5170
S	 0.6960	 0.4990
T	 0.6760	 0.4890
U	 0.6680	 0.4820
V	 0.6260	 0.4650
W	 0.7030	 0.5040
X	 0.6610	 0.4940
Y	 0.6500	 0.4780
Z	 0.2560	 0.3240
a	 0.2560	 0.3520
b	 0.3080	 0.3880
c	 0.2560	 0.3680
d	 0.2820	 0.3120
e	 0.2310	 0.3870
f	 0.2560	 0.3410
g	 0.3080	 0.2790
h	 0.2560	 0.3190
i	 0.2820	 0.3040
j	 0.3330	 0.4160
k	 0.2560	 0.3700
l	 0.3330	 0.3450
m	 0.2310	 0.3030
n	 0.3850	 0.3050
o	 0.2050	 0.2990
p	 0.3080	 0.3990
q	 0.2050	 0.3800
r	 0.3080	 0.3680
s	 0.2560	 0.2730
t	 0.3330	 0.3930
u	 0.2820	 0.2890
v	 0.3590	 0.2950
w	 0.2560	 0.3800
x	 0.3330	 0.3570
y	 0.2560	 0.3360
z	 0.3080	 0.4340