



## Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 04:35 am BST

PDB ID : 9EQ7  
EMDB ID : EMD-19905  
Title : Halobacterium salinarum archaeellum filament  
Authors : Grossman-Haham, I.; Shahar, A.  
Deposited on : 2024-03-21  
Resolution : 3.23 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

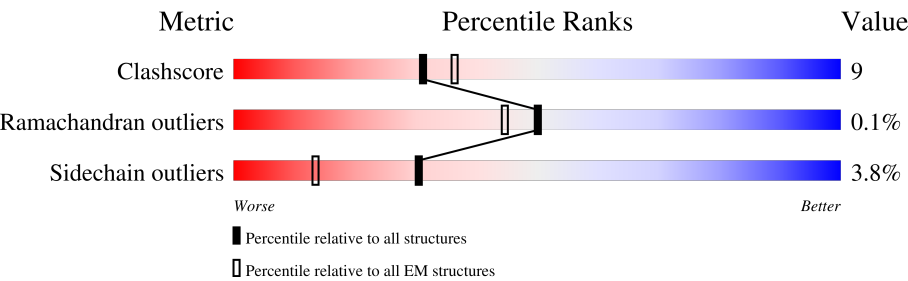
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.23 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.





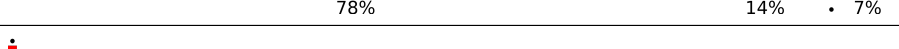
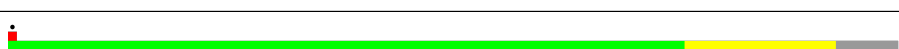



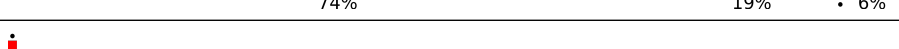



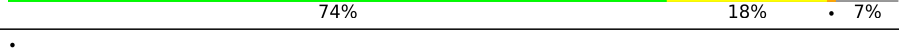

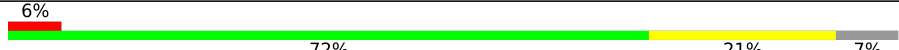










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>75%18%7%</div></div>
1	B	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>78%14%7%</div></div>
1	C	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>76%17%7%</div></div>
1	D	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>77%15%7%</div></div>
1	E	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>65%26%8%</div></div>
1	F	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>77%15%7%</div></div>
1	G	193	<div><div>6%</div><div></div><div><div></div><div></div><div></div><div></div></div><div>77%16%7%</div></div>
1	H	193	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>75%16%7%</div></div>

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Mol	Chain	Length	Quality of chain
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	
1	Z	193	
2	0	4	
2	1	4	
2	2	4	
2	3	4	
2	4	4	
2	5	4	
2	6	4	

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Mol	Chain	Length	Quality of chain
2	7	4	
2	8	4	
2	9	4	
2	AA	4	
2	BA	4	
2	CA	4	
2	DA	4	
2	EA	4	
2	FA	4	
2	GA	4	
2	HA	4	
2	IA	4	
2	JA	4	
2	KA	4	
2	LA	4	
2	MA	4	
2	NA	4	
2	OA	4	
2	PA	4	
2	a	4	
2	b	4	
2	c	4	
2	d	4	
2	e	4	
2	f	4	

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Mol	Chain	Length	Quality of chain
2	g	4	
2	h	4	
2	i	4	
2	j	4	
2	k	4	
2	l	4	
2	m	4	
2	n	4	
2	o	4	
2	p	4	
2	q	4	
2	r	4	
2	s	4	
2	t	4	
2	u	4	
2	v	4	
2	w	4	
2	x	4	
2	y	4	
2	z	4	

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	OA	1	X	-	-	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 36005 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	180	Total	C	N	O	S	0	0
			1278	807	216	253	2		
1	B	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	C	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	D	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	E	177	Total	C	N	O	S	0	0
			1263	798	213	250	2		
1	F	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	G	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	H	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	I	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	J	178	Total	C	N	O	S	0	0
			1268	801	214	251	2		
1	K	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	L	181	Total	C	N	O	S	0	0
			1283	810	217	254	2		
1	M	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	N	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	O	181	Total	C	N	O	S	0	0
			1283	810	217	254	2		
1	P	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	Q	181	Total	C	N	O	S	0	0
			1283	810	217	254	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	S	181	Total	C	N	O	S	0	0
			1283	810	217	254	2		
1	T	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	U	181	Total	C	N	O	S	0	0
			1283	810	217	254	2		
1	V	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	W	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	X	181	Total	C	N	O	S	0	0
			1283	810	217	254	2		
1	Y	179	Total	C	N	O	S	0	0
			1273	804	215	252	2		
1	Z	179	Total	C	N	O	S	0	0
			1270	801	215	252	2		

- Molecule 2 is an oligosaccharide called 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-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	a	4	Total	C	O	S	0	0
			55	24	29	2		
2	b	4	Total	C	O	S	0	0
			55	24	29	2		
2	c	4	Total	C	O	S	0	0
			55	24	29	2		
2	d	4	Total	C	O	S	0	0
			55	24	29	2		
2	e	4	Total	C	O	S	0	0
			55	24	29	2		
2	f	4	Total	C	O	S	0	0
			55	24	29	2		
2	g	4	Total	C	O	S	0	0
			55	24	29	2		
2	h	4	Total	C	O	S	0	0
			55	24	29	2		
2	i	4	Total	C	O	S	0	0
			55	24	29	2		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	j	4	Total 55	C 24	O 29	S 2	0	0
2	k	4	Total 55	C 24	O 29	S 2	0	0
2	l	4	Total 55	C 24	O 29	S 2	0	0
2	m	4	Total 55	C 24	O 29	S 2	0	0
2	n	4	Total 55	C 24	O 29	S 2	0	0
2	o	4	Total 55	C 24	O 29	S 2	0	0
2	p	4	Total 55	C 24	O 29	S 2	0	0
2	q	4	Total 55	C 24	O 29	S 2	0	0
2	r	4	Total 55	C 24	O 29	S 2	0	0
2	s	4	Total 55	C 24	O 29	S 2	0	0
2	t	4	Total 55	C 24	O 29	S 2	0	0
2	u	4	Total 55	C 24	O 29	S 2	0	0
2	v	4	Total 55	C 24	O 29	S 2	0	0
2	w	4	Total 55	C 24	O 29	S 2	0	0
2	x	4	Total 55	C 24	O 29	S 2	0	0
2	y	4	Total 55	C 24	O 29	S 2	0	0
2	z	4	Total 55	C 24	O 29	S 2	0	0
2	0	4	Total 55	C 24	O 29	S 2	0	0
2	1	4	Total 55	C 24	O 29	S 2	0	0
2	2	4	Total 55	C 24	O 29	S 2	0	0
2	3	4	Total 55	C 24	O 29	S 2	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	4	4	Total 55	C 24	O 29	S 2	0	0
2	5	4	Total 55	C 24	O 29	S 2	0	0
2	6	4	Total 55	C 24	O 29	S 2	0	0
2	7	4	Total 55	C 24	O 29	S 2	0	0
2	8	4	Total 55	C 24	O 29	S 2	0	0
2	9	4	Total 55	C 24	O 29	S 2	0	0
2	AA	4	Total 55	C 24	O 29	S 2	0	0
2	BA	4	Total 55	C 24	O 29	S 2	0	0
2	CA	4	Total 55	C 24	O 29	S 2	0	0
2	DA	4	Total 55	C 24	O 29	S 2	0	0
2	EA	4	Total 55	C 24	O 29	S 2	0	0
2	FA	4	Total 55	C 24	O 29	S 2	0	0
2	GA	4	Total 55	C 24	O 29	S 2	0	0
2	HA	4	Total 55	C 24	O 29	S 2	0	0
2	IA	4	Total 55	C 24	O 29	S 2	0	0
2	JA	4	Total 55	C 24	O 29	S 2	0	0
2	KA	4	Total 55	C 24	O 29	S 2	0	0
2	LA	4	Total 55	C 24	O 29	S 2	0	0
2	MA	4	Total 55	C 24	O 29	S 2	0	0
2	NA	4	Total 55	C 24	O 29	S 2	0	0
2	OA	4	Total 55	C 24	O 29	S 2	0	0

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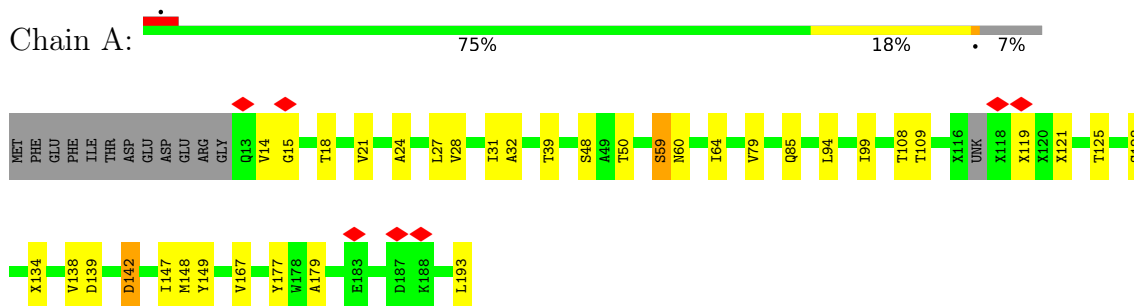
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	PA	4	Total	C	O	S	0	0
			55	24	29	2		

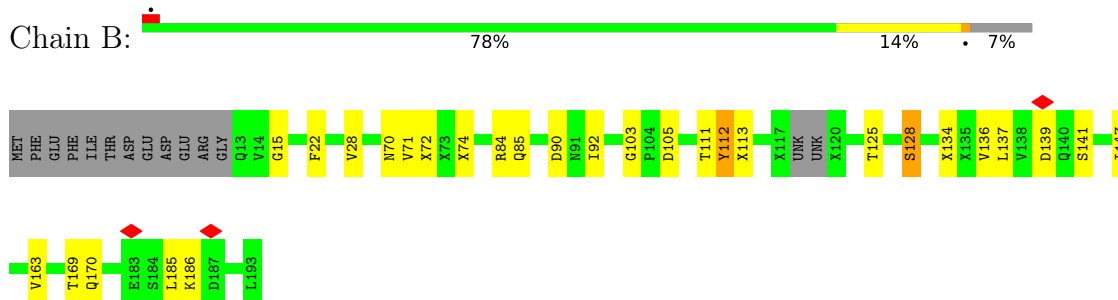
### 3 Residue-property plots

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.

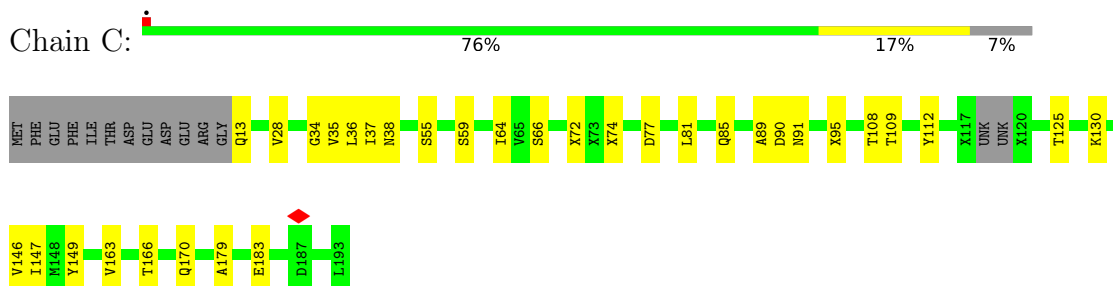
#### • Molecule 1: Archaeollin



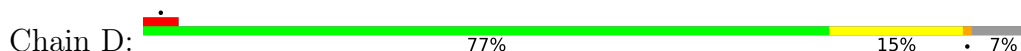
#### • Molecule 1: Archaeollin

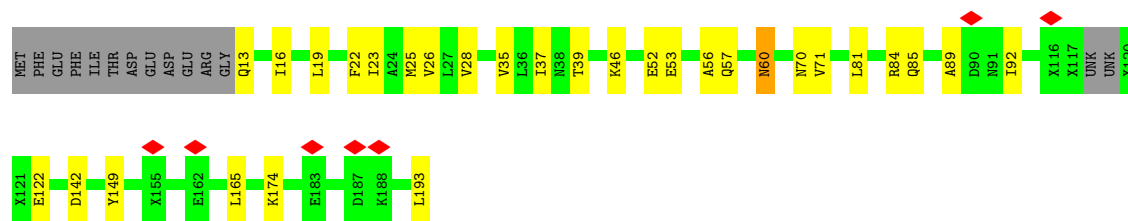


#### • Molecule 1: Archaeollin

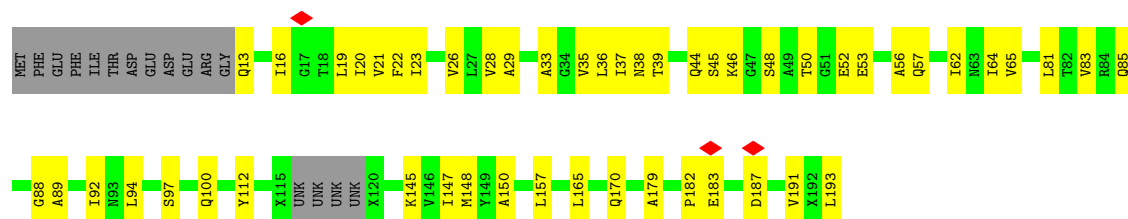


#### • Molecule 1: Archaeollin

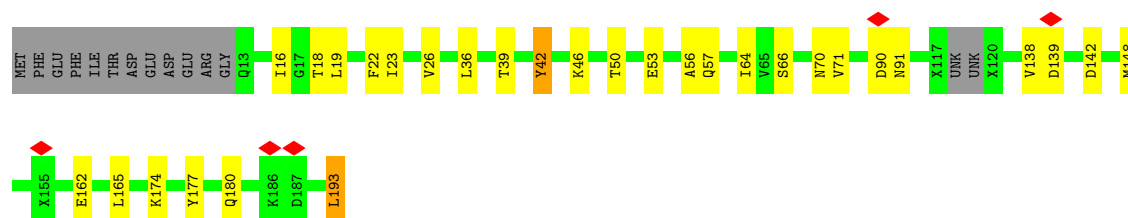
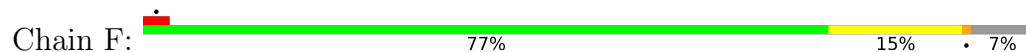




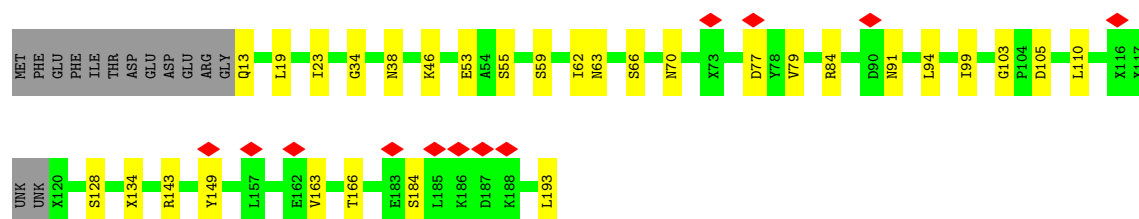
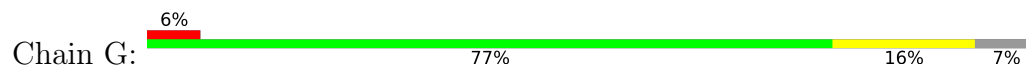
• Molecule 1: Archaeollin



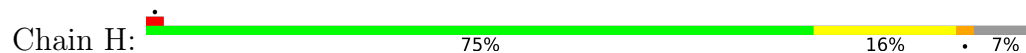
• Molecule 1: Archaeollin



• Molecule 1: Archaeollin

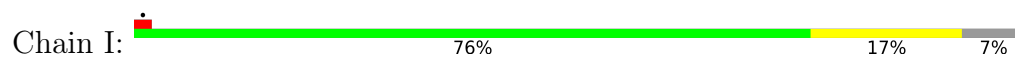


• Molecule 1: Archaeollin

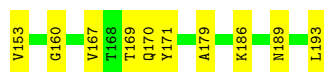
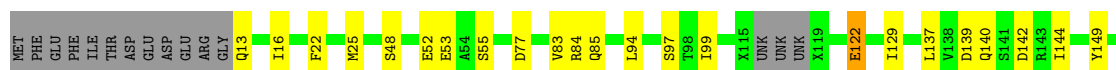




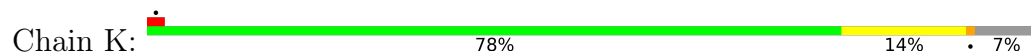
• Molecule 1: Archaeollin



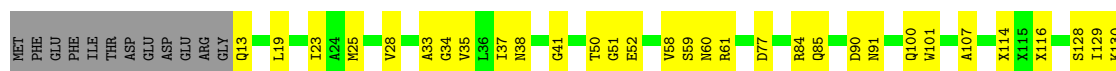
• Molecule 1: Archaeollin



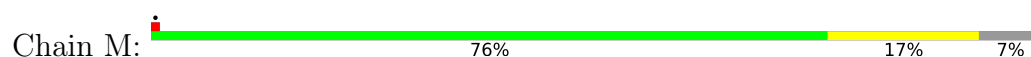
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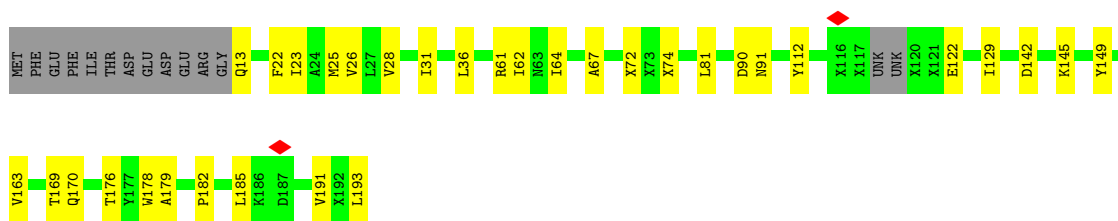


• Molecule 1: Archaeollin



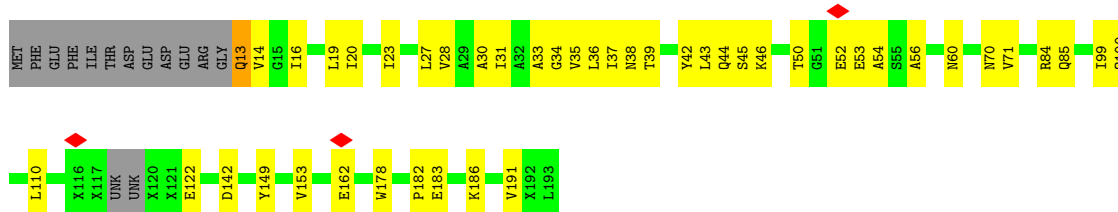
• Molecule 1: Archaeollin





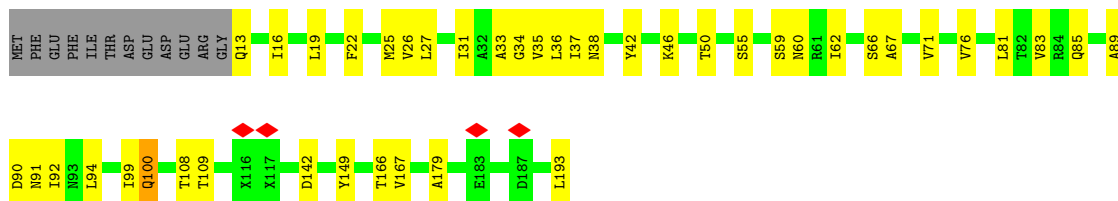
• Molecule 1: Archaeellin

Chain N: 69% 23% 7%



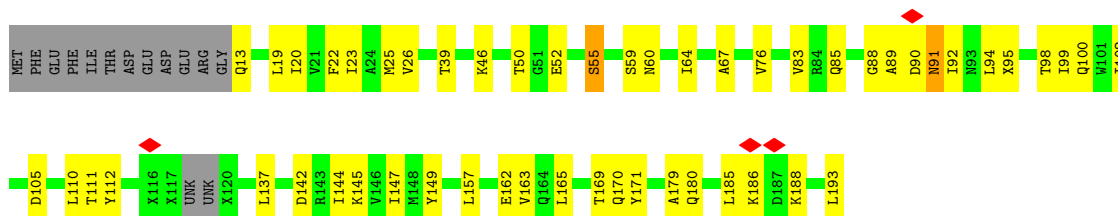
• Molecule 1: Archaeellin

Chain O: 72% 22% 6%



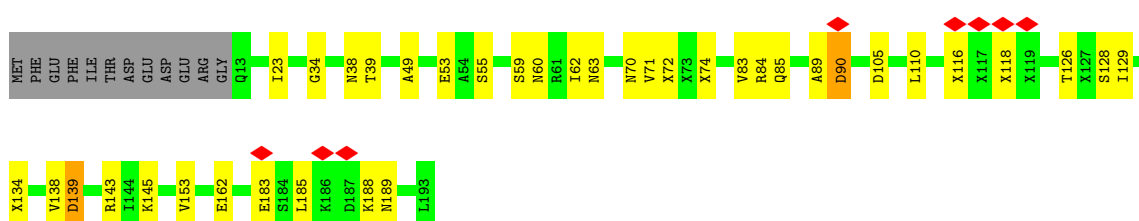
• Molecule 1: Archaeellin

Chain P: 65% 26% 7%




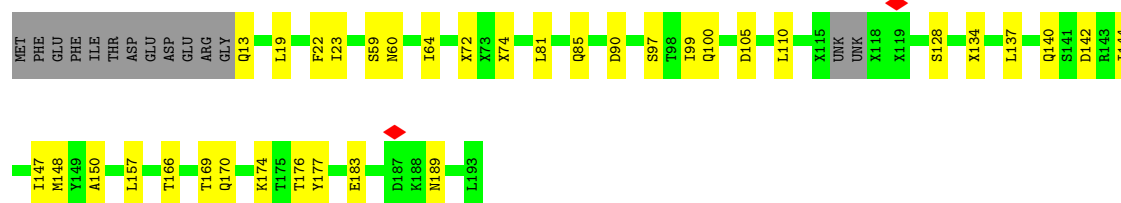
• Molecule 1: Archaeellin

Chain Q: 74% 19% 6%



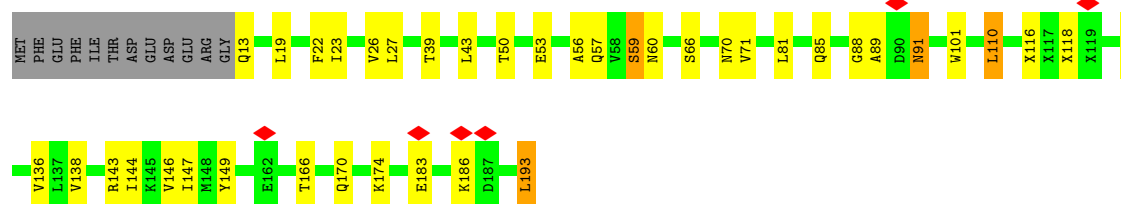
- Molecule 1: Archaeollin

Chain R: 




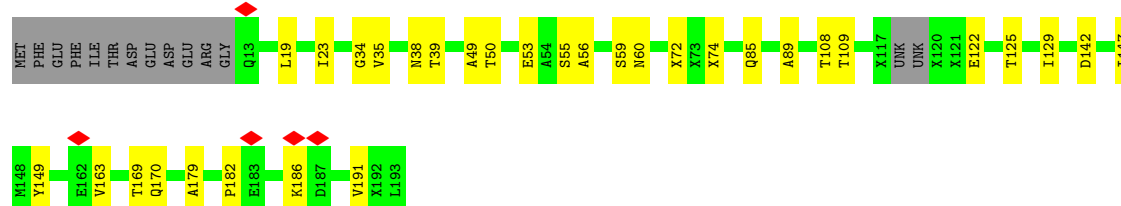
- Molecule 1: Archaeollin

Chain S: 



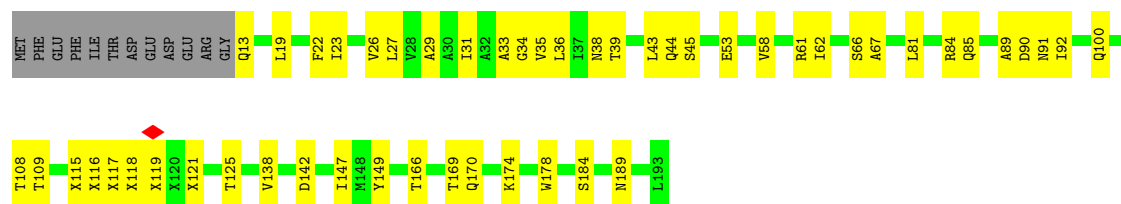
- Molecule 1: Archaeollin

Chain T: 



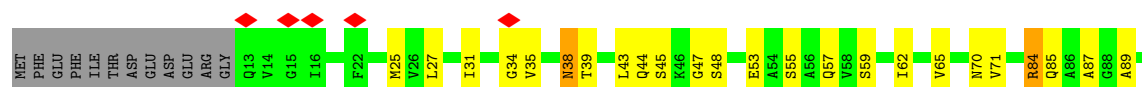
- Molecule 1: Archaeollin

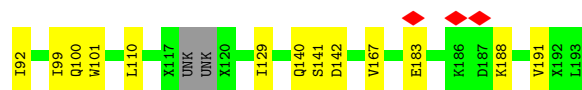
Chain U: 



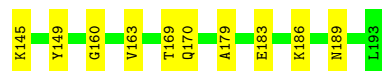
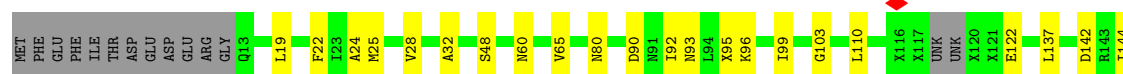
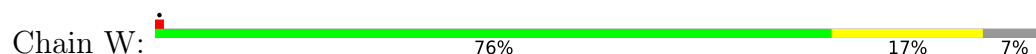
- Molecule 1: Archaeollin

Chain V: 

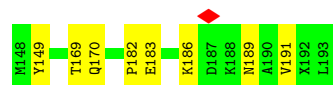
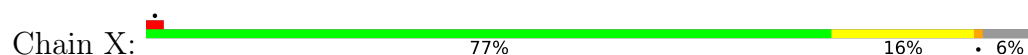




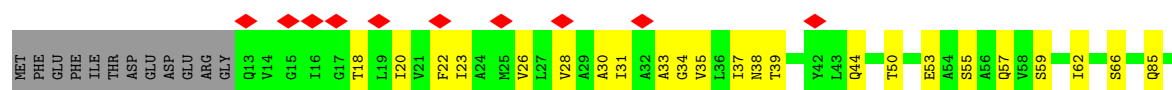
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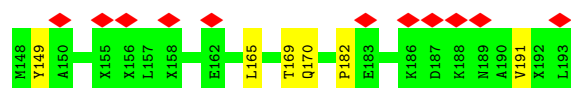
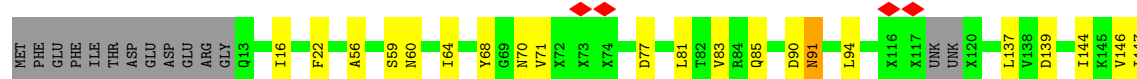
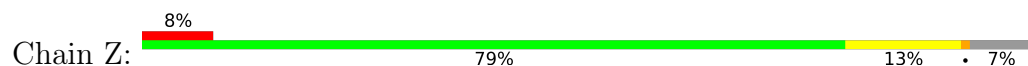
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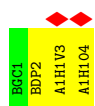
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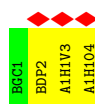
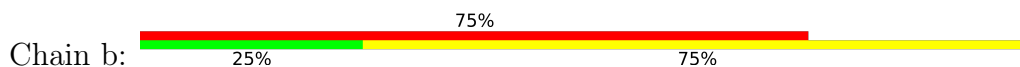
- Molecule 1: Archaeollin



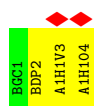
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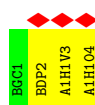
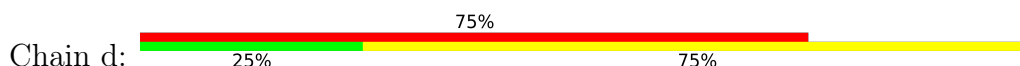
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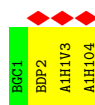
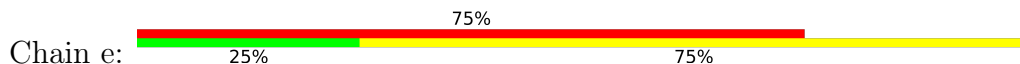
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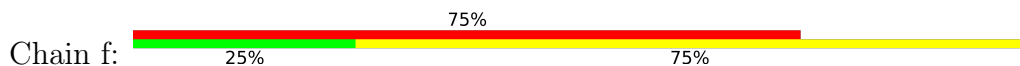
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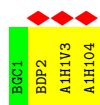


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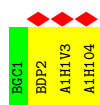
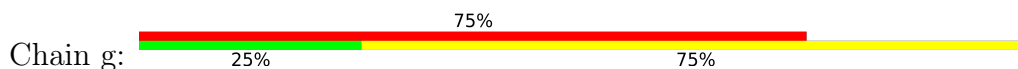


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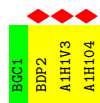
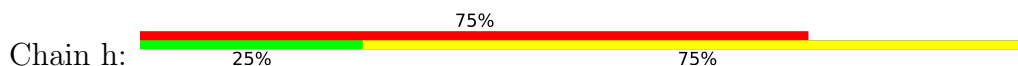




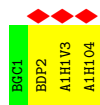
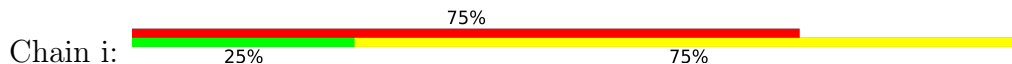
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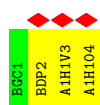
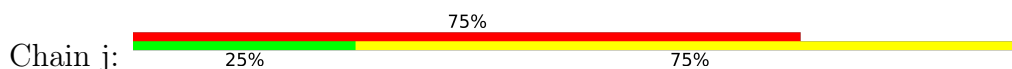
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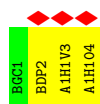
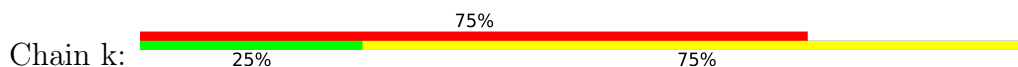
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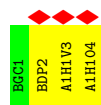
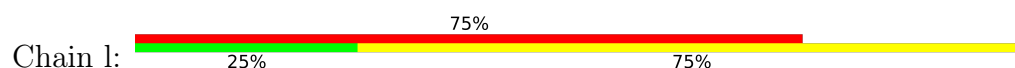
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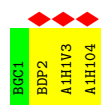
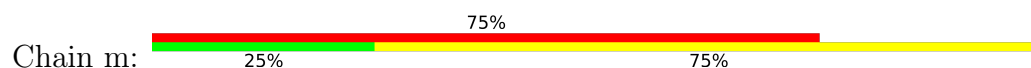
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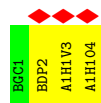
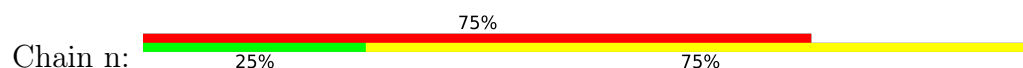
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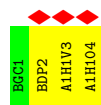
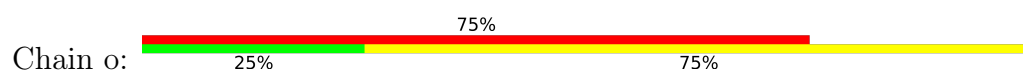
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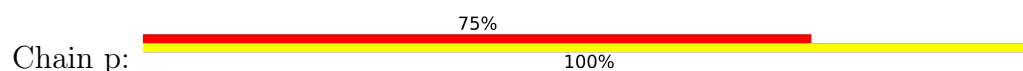
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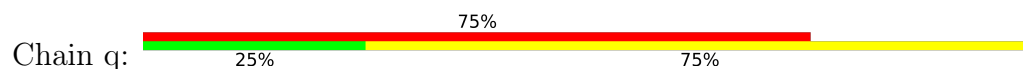
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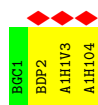


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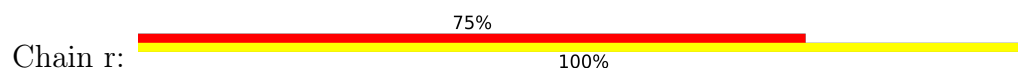


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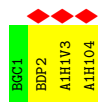
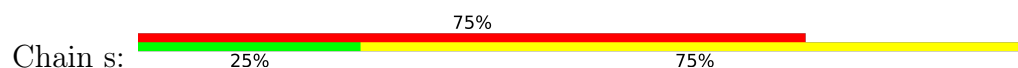




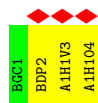
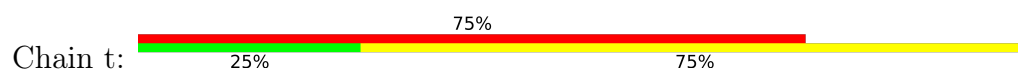
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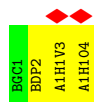
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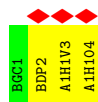
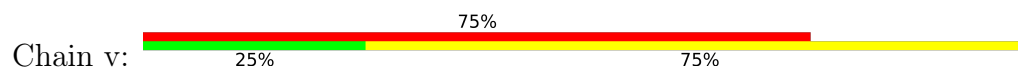
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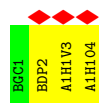
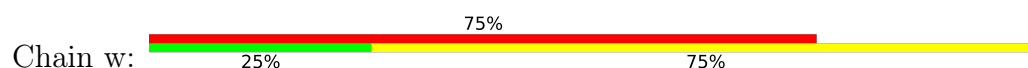
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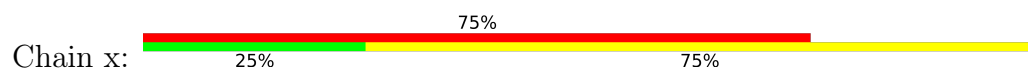
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- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



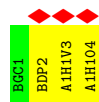
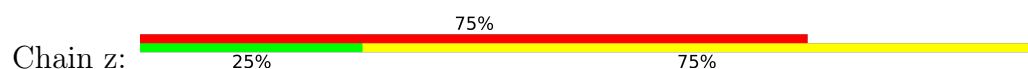
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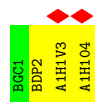
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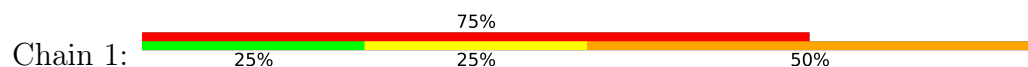
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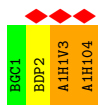


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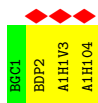
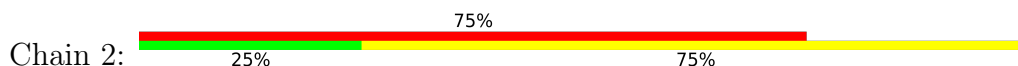


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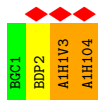
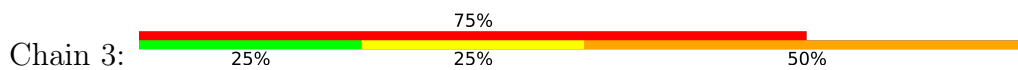




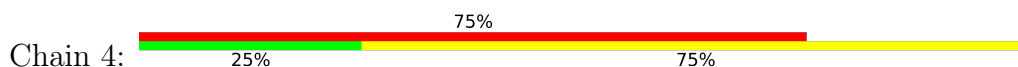
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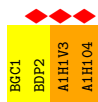
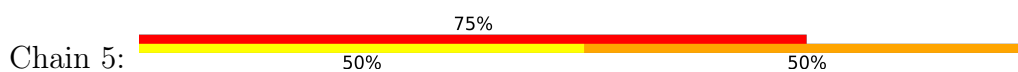
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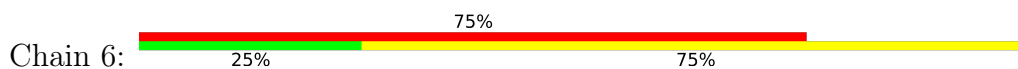
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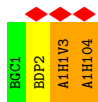
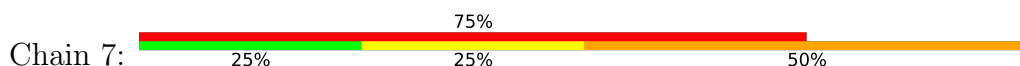
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- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



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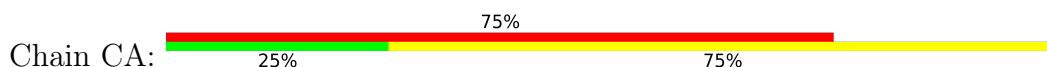
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose

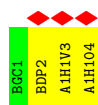


- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose

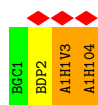
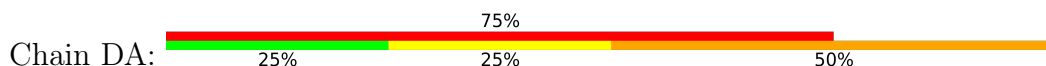


- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose

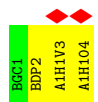




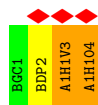
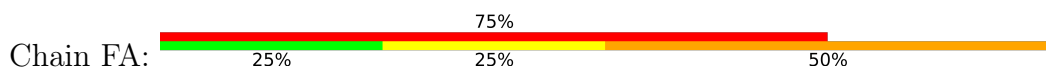
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



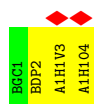
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



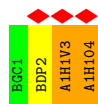
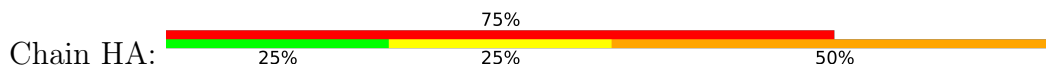
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



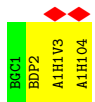
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



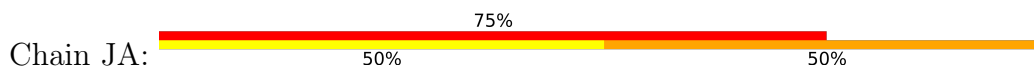
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



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



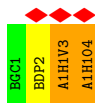
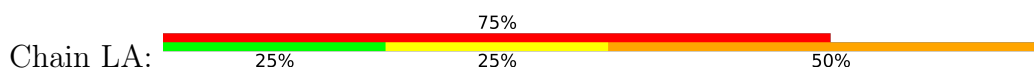
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



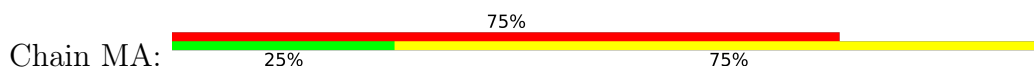
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



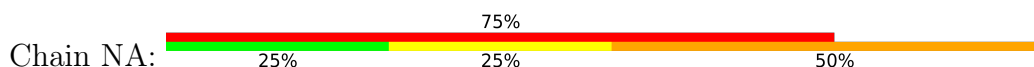
- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose

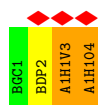


- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose

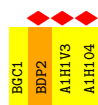
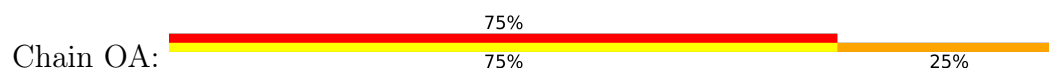


- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose

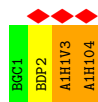
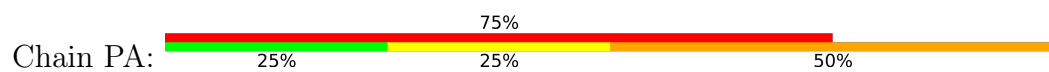




- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-beta-D-glucopyranuronic acid-(1-4)-beta-D-glucopyranose



- Molecule 2: 2-O-sulfo-beta-D-glucopyranuronic acid-(1-4)-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=107.95°, rise=5.49 Å, axial sym=C1	Depositor
Number of segments used	334202	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	0.544	Depositor
Minimum map value	-0.346	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BDP, A1H10, BGC, A1H1V

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	0.25	0/1141	0.45	0/1538
1	B	0.25	0/1141	0.45	0/1538
1	C	0.25	0/1141	0.45	0/1538
1	D	0.26	0/1141	0.46	0/1538
1	E	0.25	0/1141	0.46	0/1538
1	F	0.26	0/1141	0.49	0/1538
1	G	0.25	0/1141	0.44	0/1538
1	H	0.25	0/1141	0.49	1/1538 (0.1%)
1	I	0.25	0/1141	0.45	0/1538
1	J	0.26	0/1141	0.47	0/1538
1	K	0.26	0/1141	0.46	0/1538
1	L	0.26	0/1141	0.47	0/1538
1	M	0.25	0/1141	0.47	0/1538
1	N	0.26	0/1141	0.48	0/1538
1	O	0.25	0/1141	0.47	0/1538
1	P	0.25	0/1141	0.45	0/1538
1	Q	0.25	0/1141	0.46	0/1538
1	R	0.25	0/1141	0.46	0/1538
1	S	0.25	0/1141	0.47	0/1538
1	T	0.26	0/1141	0.45	0/1538
1	U	0.25	0/1141	0.47	0/1538
1	V	0.26	0/1141	0.45	0/1538
1	W	0.26	0/1141	0.47	0/1538
1	X	0.25	0/1141	0.47	0/1538
1	Y	0.25	0/1141	0.47	0/1538
1	Z	0.24	0/1138	0.45	0/1534
All	All	0.25	0/29663	0.46	1/39984 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	185	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1278	0	1197	21	0
1	B	1273	0	1197	17	0
1	C	1273	0	1197	19	0
1	D	1273	0	1196	22	0
1	E	1263	0	1194	37	0
1	F	1273	0	1195	23	0
1	G	1273	0	1195	16	0
1	H	1273	0	1194	25	0
1	I	1273	0	1198	25	0
1	J	1268	0	1195	20	0
1	K	1273	0	1198	20	0
1	L	1283	0	1193	28	0
1	M	1273	0	1197	19	0
1	N	1273	0	1195	34	0
1	O	1283	0	1195	30	0
1	P	1273	0	1197	38	0
1	Q	1283	0	1197	27	0
1	R	1273	0	1196	26	0
1	S	1283	0	1193	28	0
1	T	1273	0	1196	19	0
1	U	1283	0	1194	32	0
1	V	1273	0	1197	27	0
1	W	1273	0	1194	24	0
1	X	1283	0	1198	18	0
1	Y	1273	0	1192	26	0
1	Z	1270	0	1185	17	0
2	0	55	0	15	0	0
2	1	55	0	15	1	0
2	2	55	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	55	0	15	3	0
2	4	55	0	15	0	0
2	5	55	0	15	5	0
2	6	55	0	15	0	0
2	7	55	0	15	2	0
2	8	55	0	15	1	0
2	9	55	0	15	2	0
2	AA	55	0	15	1	0
2	BA	55	0	15	1	0
2	CA	55	0	15	0	0
2	DA	55	0	15	1	0
2	EA	55	0	15	0	0
2	FA	55	0	15	2	0
2	GA	55	0	15	0	0
2	HA	55	0	15	2	0
2	IA	55	0	15	0	0
2	JA	55	0	15	5	0
2	KA	55	0	15	1	0
2	LA	55	0	15	1	0
2	MA	55	0	15	0	0
2	NA	55	0	15	3	0
2	OA	55	0	15	2	0
2	PA	55	0	15	3	0
2	a	55	0	15	0	0
2	b	55	0	15	0	0
2	c	55	0	15	0	0
2	d	55	0	15	0	0
2	e	55	0	15	0	0
2	f	55	0	15	0	0
2	g	55	0	15	0	0
2	h	55	0	15	0	0
2	i	55	0	15	0	0
2	j	55	0	15	0	0
2	k	55	0	15	0	0
2	l	55	0	15	0	0
2	m	55	0	15	0	0
2	n	55	0	15	0	0
2	o	55	0	15	0	0
2	p	55	0	15	0	0
2	q	55	0	15	0	0
2	r	55	0	15	0	0
2	s	55	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	t	55	0	15	0	0
2	u	55	0	15	0	0
2	v	55	0	15	0	0
2	w	55	0	15	0	0
2	x	55	0	15	0	0
2	y	55	0	15	0	0
2	z	55	0	15	0	0
All	All	36005	0	31855	549	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 (549) 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:U:90:ASP:OD1	1:U:91:ASN:N	2.05	0.90
1:O:90:ASP:OD2	1:O:91:ASN:N	2.08	0.86
1:H:90:ASP:OD2	1:H:91:ASN:N	2.10	0.83
1:L:90:ASP:OD1	1:L:91:ASN:N	2.12	0.82
1:N:16:ILE:HG21	1:O:22:PHE:HE2	1.49	0.75
1:Z:182:PRO:HG3	1:Z:191:VAL:HG21	1.68	0.73
1:F:90:ASP:OD2	1:F:91:ASN:N	2.19	0.73
1:N:14:VAL:HG22	1:P:13:GLN:HE22	1.53	0.73
1:U:44:GLN:NE2	1:U:45:SER:OG	2.21	0.73
1:X:90:ASP:OD1	1:X:91:ASN:N	2.23	0.71
1:M:90:ASP:OD1	1:M:91:ASN:N	2.22	0.71
1:C:28:VAL:HG21	1:M:36:LEU:HD22	1.72	0.70
1:N:122:GLU:OE1	1:N:122:GLU:N	2.24	0.70
1:D:16:ILE:HG21	1:E:22:PHE:HE1	1.55	0.70
1:B:85:GLN:NE2	1:B:139:ASP:O	2.25	0.69
1:D:52:GLU:OE2	1:D:52:GLU:N	2.24	0.69
1:D:16:ILE:HA	1:D:19:LEU:HD12	1.76	0.68
1:U:53:GLU:OE2	1:V:140:GLN:NE2	2.27	0.68
1:H:105:ASP:O	1:I:189:ASN:ND2	2.27	0.68
1:C:13:GLN:N	1:J:25:MET:SD	2.68	0.67
1:B:128:SER:HB2	1:B:134:UNK:HA	1.75	0.67
1:V:53:GLU:OE1	1:Y:140:GLN:NE2	2.23	0.67
1:E:20:ILE:HD11	1:F:26:VAL:HG12	1.77	0.67
1:O:71:VAL:HG12	1:O:76:VAL:HG12	1.77	0.67
1:S:13:GLN:N	1:V:25:MET:SD	2.67	0.66
1:W:103:GLY:HA2	1:W:163:VAL:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:183:GLU:N	1:W:183:GLU:OE2	2.29	0.66
1:O:100:GLN:NE2	1:S:66:SER:OG	2.26	0.66
1:X:85:GLN:NE2	1:X:137:LEU:O	2.28	0.66
1:P:169:THR:O	1:Q:143:ARG:NH2	2.28	0.66
1:P:85:GLN:HB3	1:P:89:ALA:HB3	1.78	0.66
1:I:105:ASP:O	1:J:189:ASN:ND2	2.28	0.65
1:T:163:VAL:HG23	1:T:179:ALA:HB3	1.78	0.65
1:U:170:GLN:HG3	1:V:141:SER:HB3	1.77	0.65
1:Z:147:ILE:HD11	2:OA:1:BGC:H5	1.78	0.65
1:R:183:GLU:OE1	1:R:183:GLU:N	2.26	0.64
1:E:35:VAL:HG11	1:G:19:LEU:HD21	1.79	0.63
1:E:13:GLN:HE21	1:F:18:THR:HG23	1.62	0.63
1:P:100:GLN:HE21	1:P:102:ILE:HD11	1.62	0.63
1:E:53:GLU:O	1:E:57:GLN:N	2.31	0.63
1:D:28:VAL:HG21	1:E:36:LEU:HB3	1.80	0.63
1:V:183:GLU:OE2	1:V:183:GLU:N	2.32	0.63
1:N:35:VAL:O	1:N:39:THR:OG1	2.16	0.62
1:B:28:VAL:HG21	1:C:36:LEU:HG	1.82	0.62
1:E:28:VAL:HG21	1:F:36:LEU:HB3	1.80	0.62
1:K:137:LEU:HG	1:K:144:ILE:HD12	1.81	0.62
1:O:179:ALA:HB1	1:O:193:LEU:HD23	1.82	0.62
1:W:96:LYS:HZ3	2:JA:1:BGC:H6C2	1.65	0.61
1:E:100:GLN:NE2	1:F:66:SER:OG	2.30	0.61
1:F:53:GLU:O	1:F:57:GLN:N	2.32	0.61
1:P:105:ASP:O	1:Q:189:ASN:ND2	2.33	0.61
1:B:141:SER:HB3	1:Z:170:GLN:HG3	1.83	0.61
1:P:162:GLU:HG2	1:P:180:GLN:HG3	1.82	0.60
1:U:85:GLN:HB3	1:U:89:ALA:HB3	1.83	0.60
1:W:122:GLU:OE1	1:W:122:GLU:N	2.29	0.60
1:F:50:THR:HG21	1:G:23:ILE:HG23	1.83	0.60
1:M:28:VAL:HG21	1:N:36:LEU:HG	1.83	0.60
1:H:95:UNK:HA	1:H:112:TYR:HD1	1.65	0.60
1:P:23:ILE:HG23	1:S:50:THR:HG21	1.83	0.60
1:O:16:ILE:HG21	1:S:22:PHE:HE1	1.66	0.60
1:V:34:GLY:O	1:V:38:ASN:ND2	2.34	0.60
1:G:13:GLN:NE2	1:H:18:THR:OG1	2.35	0.59
1:J:137:LEU:HD12	1:J:144:ILE:HD12	1.83	0.59
1:E:150:ALA:HB1	1:E:157:LEU:HD23	1.84	0.59
1:Z:81:LEU:HB2	1:Z:146:VAL:HB	1.84	0.59
1:M:193:LEU:HD12	1:M:193:LEU:H	1.68	0.59
1:E:145:LYS:HD2	1:E:147:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:3:A1H1V:O22	2:1:4:A1H10:O2S	2.21	0.59
1:A:119:UNK:O	1:A:121:UNK:N	2.36	0.58
1:D:13:GLN:HE22	1:E:21:VAL:HG12	1.67	0.58
1:G:34:GLY:O	1:G:38:ASN:ND2	2.36	0.58
1:A:85:GLN:NE2	1:A:139:ASP:O	2.36	0.58
1:I:139:ASP:N	1:I:142:ASP:OD1	2.36	0.58
1:O:85:GLN:NE2	1:O:89:ALA:O	2.36	0.58
1:Q:23:ILE:HG23	1:T:50:THR:HG21	1.86	0.58
2:3:3:A1H1V:O22	2:3:4:A1H10:O2S	2.22	0.58
2:9:3:A1H1V:O22	2:9:4:A1H10:O2S	2.21	0.58
1:H:23:ILE:HG23	1:P:50:THR:HG21	1.85	0.58
1:W:169:THR:O	1:X:143:ARG:NH2	2.36	0.58
1:J:52:GLU:OE1	1:J:52:GLU:N	2.37	0.57
1:R:150:ALA:HB1	1:R:157:LEU:HD13	1.85	0.57
1:H:46:LYS:NZ	1:I:90:ASP:OD1	2.37	0.57
1:L:19:LEU:HD21	1:W:32:ALA:HA	1.86	0.57
1:P:185:LEU:HA	1:P:188:LYS:HD3	1.85	0.57
2:NA:3:A1H1V:O22	2:NA:4:A1H10:O2S	2.22	0.57
1:O:34:GLY:O	1:O:38:ASN:ND2	2.38	0.57
1:R:64:ILE:HD13	1:R:81:LEU:HD23	1.87	0.57
1:D:35:VAL:O	1:D:39:THR:OG1	2.18	0.57
1:P:170:GLN:HE22	1:S:183:GLU:HG2	1.67	0.57
1:Z:169:THR:HG22	1:Z:170:GLN:H	1.69	0.57
1:V:62:ILE:HD11	1:V:92:ILE:HG21	1.86	0.56
1:V:70:ASN:OD1	1:V:71:VAL:N	2.37	0.56
1:L:34:GLY:O	1:L:38:ASN:ND2	2.37	0.56
1:L:128:SER:HB3	1:L:134:UNK:HA	1.88	0.56
1:U:19:LEU:HD21	1:X:32:ALA:HA	1.86	0.56
1:L:28:VAL:HG21	1:U:36:LEU:HB3	1.88	0.56
1:R:13:GLN:HB3	1:W:25:MET:HG3	1.87	0.56
2:7:3:A1H1V:O24	2:7:4:A1H10:O1S	2.23	0.56
2:JA:3:A1H1V:O22	2:JA:4:A1H10:O2S	2.23	0.56
1:Q:53:GLU:OE1	1:R:140:GLN:NE2	2.39	0.56
1:Q:128:SER:HB2	1:Q:134:UNK:HA	1.88	0.56
1:E:53:GLU:HA	1:E:56:ALA:HB3	1.86	0.56
1:H:122:GLU:HA	1:H:153:VAL:HG12	1.88	0.56
2:PA:3:A1H1V:O22	2:PA:4:A1H10:O2S	2.24	0.56
1:G:79:VAL:HG23	1:G:193:LEU:HD13	1.87	0.56
1:H:62:ILE:HD11	1:H:92:ILE:HG21	1.86	0.56
1:U:119:UNK:O	1:U:121:UNK:N	2.39	0.56
1:S:85:GLN:HB3	1:S:89:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:20:ILE:HA	1:Y:23:ILE:HD12	1.87	0.55
1:Y:100:GLN:HB3	1:Y:166:THR:HG22	1.87	0.55
1:E:45:SER:HB3	1:N:178:TRP:HB2	1.87	0.55
1:T:34:GLY:O	1:T:38:ASN:ND2	2.39	0.55
1:T:108:THR:OG1	1:T:109:THR:N	2.39	0.55
1:F:193:LEU:HD12	1:F:193:LEU:H	1.72	0.55
1:H:83:VAL:HG21	1:H:94:LEU:HD21	1.89	0.55
1:J:122:GLU:HA	1:J:153:VAL:HG12	1.87	0.55
2:5:3:A1H1V:O24	2:5:4:A1H10:O2S	2.25	0.55
1:A:179:ALA:HB1	1:A:193:LEU:HD23	1.88	0.55
1:O:108:THR:OG1	1:O:109:THR:N	2.40	0.55
2:5:3:A1H1V:O22	2:5:4:A1H10:O2S	2.25	0.55
1:V:43:LEU:O	1:V:47:GLY:N	2.34	0.55
1:G:84:ARG:HD3	1:G:143:ARG:HH12	1.71	0.55
1:O:19:LEU:HD21	1:U:35:VAL:HG11	1.88	0.55
1:Q:85:GLN:NE2	1:Q:89:ALA:O	2.40	0.55
1:N:27:LEU:O	1:N:31:ILE:HG13	2.07	0.54
1:P:90:ASP:OD2	1:P:91:ASN:N	2.40	0.54
1:Z:56:ALA:O	1:Z:60:ASN:ND2	2.40	0.54
1:H:13:GLN:HE21	1:I:18:THR:HG23	1.72	0.54
1:Q:60:ASN:ND2	1:Q:90:ASP:H	2.05	0.54
1:Z:70:ASN:ND2	2:OA:2:BDP:O6B	2.40	0.54
2:LA:3:A1H1V:O22	2:LA:4:A1H10:O2S	2.26	0.54
1:E:170:GLN:HE22	1:N:183:GLU:CD	2.11	0.54
1:E:179:ALA:HB1	1:E:193:LEU:HD12	1.89	0.54
1:P:95:UNK:HA	1:P:112:TYR:HD2	1.73	0.54
1:Y:55:SER:O	1:Y:59:SER:OG	2.21	0.54
1:H:128:SER:HB2	1:H:134:UNK:HA	1.88	0.54
1:T:169:THR:HG22	1:T:170:GLN:H	1.73	0.54
1:I:166:THR:HG22	1:I:176:THR:HG23	1.89	0.54
1:O:46:LYS:NZ	1:S:88:GLY:O	2.40	0.54
1:L:37:ILE:O	1:L:41:GLY:N	2.39	0.54
1:J:16:ILE:HG12	1:K:22:PHE:HE1	1.71	0.54
1:V:35:VAL:HG11	1:Y:44:GLN:HB2	1.90	0.54
1:M:22:PHE:O	1:M:26:VAL:HG23	2.08	0.53
2:DA:3:A1H1V:O22	2:DA:4:A1H10:O2S	2.26	0.53
1:G:46:LYS:NZ	1:H:88:GLY:O	2.41	0.53
1:P:145:LYS:HE3	1:P:147:ILE:HD11	1.91	0.53
1:V:35:VAL:O	1:V:39:THR:HG23	2.08	0.53
1:V:100:GLN:NE2	1:Y:66:SER:OG	2.41	0.53
1:I:174:LYS:NZ	1:I:174:LYS:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:34:GLY:O	1:Y:38:ASN:ND2	2.42	0.53
1:Y:137:LEU:HD12	1:Y:144:ILE:HD12	1.91	0.53
1:E:85:GLN:HB3	1:E:89:ALA:HB3	1.90	0.53
1:E:148:MET:HE1	1:E:165:LEU:HD21	1.89	0.53
1:W:163:VAL:HG23	1:W:179:ALA:HB3	1.90	0.53
1:D:85:GLN:HB3	1:D:89:ALA:HB3	1.90	0.53
1:E:23:ILE:HG23	1:N:50:THR:HG21	1.89	0.53
1:G:103:GLY:HA2	1:G:163:VAL:HG12	1.91	0.53
1:I:122:GLU:N	1:I:122:GLU:OE2	2.42	0.53
1:M:31:ILE:O	1:N:44:GLN:NE2	2.41	0.53
1:W:24:ALA:O	1:W:28:VAL:HG23	2.09	0.53
1:C:34:GLY:O	1:C:38:ASN:ND2	2.42	0.53
1:N:100:GLN:NE2	1:O:66:SER:OG	2.42	0.53
1:M:163:VAL:HG22	1:M:179:ALA:HB3	1.90	0.53
1:X:128:SER:HB2	1:X:134:UNK:HA	1.91	0.53
1:S:19:LEU:O	1:S:23:ILE:HG13	2.09	0.53
1:T:55:SER:O	1:T:59:SER:OG	2.23	0.53
2:7:3:A1H1V:O22	2:7:4:A1H10:O2S	2.26	0.53
1:P:163:VAL:HG22	1:P:179:ALA:HB3	1.92	0.52
2:NA:3:A1H1V:O24	2:NA:4:A1H10:O2S	2.28	0.52
1:J:179:ALA:HB1	1:J:193:LEU:HD23	1.89	0.52
1:L:185:LEU:HD23	1:L:191:VAL:HG21	1.91	0.52
1:Q:34:GLY:O	1:Q:38:ASN:ND2	2.42	0.52
1:N:28:VAL:HG21	1:O:36:LEU:HB3	1.91	0.52
1:A:15:GLY:O	1:A:18:THR:OG1	2.25	0.52
1:C:90:ASP:OD2	1:C:91:ASN:N	2.36	0.52
1:D:70:ASN:OD1	1:D:71:VAL:N	2.42	0.52
1:S:53:GLU:O	1:S:57:GLN:N	2.36	0.52
1:H:60:ASN:ND2	1:H:90:ASP:H	2.07	0.52
1:L:84:ARG:NH1	1:L:85:GLN:O	2.43	0.52
1:Q:162:GLU:N	1:Q:162:GLU:OE2	2.43	0.52
1:S:91:ASN:HD22	1:S:138:VAL:HG12	1.75	0.52
2:HA:3:A1H1V:O24	2:HA:4:A1H10:O2S	2.27	0.52
1:G:128:SER:HB2	1:G:134:UNK:HA	1.91	0.52
1:O:13:GLN:OE1	1:O:13:GLN:N	2.43	0.52
1:F:42:TYR:HE2	1:P:52:GLU:HG2	1.75	0.52
1:N:45:SER:HB3	1:U:178:TRP:HB2	1.91	0.52
1:D:53:GLU:O	1:D:57:GLN:N	2.39	0.52
1:G:105:ASP:OD2	1:G:105:ASP:N	2.37	0.52
1:A:108:THR:OG1	1:A:109:THR:N	2.43	0.51
1:C:108:THR:OG1	1:C:109:THR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:128:SER:HB3	1:K:134:UNK:HA	1.91	0.51
1:Q:55:SER:O	1:Q:59:SER:OG	2.24	0.51
1:R:105:ASP:O	1:W:189:ASN:ND2	2.44	0.51
1:S:122:GLU:OE1	1:S:122:GLU:N	2.43	0.51
1:Y:28:VAL:HA	1:Y:31:ILE:HD12	1.92	0.51
1:Y:35:VAL:O	1:Y:39:THR:OG1	2.15	0.51
1:T:182:PRO:HG2	1:T:191:VAL:HB	1.90	0.51
1:I:22:PHE:HZ	1:P:39:THR:HG21	1.75	0.51
1:T:19:LEU:O	1:T:23:ILE:HG13	2.10	0.51
1:A:27:LEU:O	1:A:31:ILE:HG12	2.11	0.51
1:H:95:UNK:HA	1:H:112:TYR:CD1	2.44	0.51
2:BA:3:A1H1V:O24	2:BA:4:A1H10:O2S	2.28	0.51
2:FA:3:A1H1V:O22	2:FA:4:A1H10:O2S	2.29	0.51
1:E:22:PHE:O	1:E:26:VAL:HG23	2.10	0.51
1:T:85:GLN:HB3	1:T:89:ALA:HB3	1.93	0.51
1:E:193:LEU:HD23	1:E:193:LEU:H	1.75	0.51
1:W:80:ASN:HB3	1:W:145:LYS:HD2	1.93	0.51
1:X:147:ILE:HD13	2:KA:1:BGC:H6C1	1.92	0.51
1:Z:85:GLN:NE2	1:Z:90:ASP:O	2.42	0.51
1:B:111:THR:HG22	1:B:112:TYR:H	1.76	0.50
1:U:53:GLU:HG2	1:V:87:ALA:HA	1.94	0.50
1:J:171:TYR:OH	1:R:183:GLU:OE2	2.22	0.50
1:M:25:MET:HA	1:M:28:VAL:HB	1.92	0.50
1:O:59:SER:OG	1:O:60:ASN:OD1	2.30	0.50
1:L:114:UNK:O	1:L:116:UNK:N	2.45	0.50
1:H:49:ALA:O	1:H:53:GLU:HG2	2.12	0.50
1:O:99:ILE:HG12	1:O:167:VAL:HG22	1.92	0.50
1:B:136:VAL:HG21	1:J:186:LYS:HG3	1.92	0.50
1:H:185:LEU:HD23	1:H:185:LEU:O	2.11	0.50
1:D:19:LEU:O	1:D:23:ILE:HG13	2.12	0.50
1:E:170:GLN:NE2	1:N:183:GLU:OE2	2.45	0.50
1:Y:108:THR:OG1	1:Y:109:THR:N	2.44	0.50
1:I:81:LEU:HD11	1:I:165:LEU:HD13	1.93	0.50
1:U:67:ALA:HB2	1:U:81:LEU:HD23	1.94	0.50
1:R:99:ILE:O	1:R:110:LEU:N	2.45	0.49
1:V:99:ILE:HG12	1:V:167:VAL:HA	1.93	0.49
1:F:162:GLU:OE1	1:F:180:GLN:NE2	2.45	0.49
1:A:32:ALA:HA	1:W:19:LEU:HD21	1.95	0.49
1:D:46:LYS:NZ	1:E:88:GLY:O	2.43	0.49
1:U:108:THR:OG1	1:U:109:THR:N	2.45	0.49
1:K:193:LEU:HD12	1:K:193:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:185:LEU:HA	1:Q:188:LYS:HD2	1.95	0.49
1:V:55:SER:O	1:V:59:SER:OG	2.24	0.49
1:C:64:ILE:HD12	1:C:81:LEU:HD23	1.94	0.49
1:H:114:UNK:O	1:H:116:UNK:N	2.45	0.49
1:I:58:VAL:O	1:I:61:ARG:NH1	2.45	0.49
1:L:35:VAL:HG21	1:N:19:LEU:HD21	1.94	0.49
1:E:62:ILE:HD11	1:E:92:ILE:HG21	1.94	0.49
1:M:129:ILE:HD11	1:M:145:LYS:HE3	1.95	0.49
1:Q:70:ASN:OD1	1:Q:71:VAL:N	2.46	0.49
1:U:100:GLN:HB2	1:U:166:THR:HB	1.95	0.49
1:Y:30:ALA:O	1:Y:34:GLY:N	2.42	0.49
1:Y:53:GLU:O	1:Y:57:GLN:N	2.43	0.49
1:D:60:ASN:HB3	1:D:92:ILE:HD11	1.95	0.48
1:E:35:VAL:O	1:E:39:THR:HG23	2.13	0.48
1:I:60:ASN:O	1:I:173:SER:OG	2.20	0.48
1:Q:63:ASN:HD22	1:Q:84:ARG:HH12	1.61	0.48
1:B:15:GLY:HA3	1:I:28:VAL:HG12	1.95	0.48
1:C:166:THR:O	1:C:166:THR:OG1	2.27	0.48
1:S:193:LEU:HD12	1:S:193:LEU:H	1.78	0.48
1:T:125:THR:HB	1:T:147:ILE:HB	1.94	0.48
1:U:174:LYS:HD2	1:V:65:VAL:HG13	1.95	0.48
1:Z:77:ASP:HB3	1:Z:149:TYR:HE1	1.77	0.48
1:K:85:GLN:HE21	1:K:140:GLN:HA	1.78	0.48
1:P:85:GLN:NE2	1:P:89:ALA:O	2.46	0.48
1:R:128:SER:HA	1:R:144:ILE:HG23	1.95	0.48
1:V:27:LEU:O	1:V:31:ILE:HG12	2.14	0.48
1:D:84:ARG:NH1	1:D:85:GLN:O	2.47	0.48
1:G:99:ILE:HG23	1:G:110:LEU:HB2	1.95	0.48
1:P:76:VAL:HB	1:P:157:LEU:HB2	1.95	0.48
1:B:70:ASN:OD1	1:B:71:VAL:N	2.46	0.48
1:J:83:VAL:HG21	1:J:94:LEU:HD11	1.94	0.48
1:N:52:GLU:H	1:N:52:GLU:CD	2.16	0.48
1:E:182:PRO:HG3	1:E:191:VAL:HG21	1.96	0.48
1:F:70:ASN:OD1	1:F:71:VAL:N	2.47	0.48
1:J:13:GLN:HB3	1:K:25:MET:SD	2.54	0.48
1:R:85:GLN:HG3	1:R:137:LEU:HD23	1.94	0.48
1:X:113:UNK:O	1:X:115:UNK:N	2.47	0.48
1:P:99:ILE:HD11	1:P:165:LEU:HD22	1.96	0.47
1:S:53:GLU:HA	1:S:56:ALA:HB3	1.96	0.47
1:U:29:ALA:O	1:U:33:ALA:N	2.42	0.47
1:Z:64:ILE:HD13	1:Z:81:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:GLU:HA	1:F:56:ALA:HB3	1.96	0.47
1:U:27:LEU:O	1:U:31:ILE:HG13	2.14	0.47
2:JA:3:A1H1V:O24	2:JA:4:A1H10:O2S	2.33	0.47
1:I:72:UNK:O	1:I:74:UNK:N	2.47	0.47
1:U:34:GLY:O	1:U:38:ASN:ND2	2.46	0.47
1:C:170:GLN:HG3	1:K:183:GLU:OE2	2.13	0.47
1:Q:126:THR:O	1:Q:126:THR:OG1	2.32	0.47
1:R:100:GLN:HB3	1:R:166:THR:OG1	2.14	0.47
1:F:22:PHE:O	1:F:26:VAL:HG22	2.14	0.47
1:H:39:THR:HG21	1:Z:22:PHE:HZ	1.80	0.47
1:N:19:LEU:O	1:N:23:ILE:HG13	2.15	0.47
1:Q:49:ALA:O	1:Q:53:GLU:HG3	2.15	0.47
1:S:81:LEU:HB2	1:S:146:VAL:HB	1.97	0.47
1:O:83:VAL:HG21	1:O:94:LEU:HD11	1.97	0.47
1:O:85:GLN:HB3	1:O:89:ALA:HB3	1.97	0.47
1:W:93:ASN:OD1	1:W:95:UNK:N	2.48	0.47
2:3:3:A1H1V:O24	2:3:4:A1H10:O2S	2.32	0.47
1:R:72:UNK:O	1:R:74:UNK:N	2.46	0.47
1:U:115:UNK:O	1:U:117:UNK:N	2.48	0.47
1:P:186:LYS:HB3	1:P:186:LYS:HE3	1.69	0.47
1:R:64:ILE:HD12	1:R:177:TYR:HB2	1.96	0.47
1:S:70:ASN:OD1	1:S:71:VAL:N	2.47	0.47
2:HA:3:A1H1V:O22	2:HA:4:A1H10:O2S	2.32	0.47
1:Z:70:ASN:OD1	1:Z:71:VAL:N	2.48	0.46
1:A:24:ALA:O	1:A:28:VAL:HG23	2.15	0.46
1:D:22:PHE:O	1:D:26:VAL:HG22	2.15	0.46
1:D:35:VAL:HG21	1:E:44:GLN:HA	1.96	0.46
1:L:163:VAL:HG22	1:L:179:ALA:HB3	1.97	0.46
1:O:19:LEU:HD13	1:V:43:LEU:HB2	1.97	0.46
1:O:166:THR:O	1:O:166:THR:OG1	2.31	0.46
1:S:116:UNK:O	1:S:118:UNK:N	2.48	0.46
1:J:53:GLU:HB2	1:K:87:ALA:HB1	1.98	0.46
1:S:23:ILE:HG23	1:Y:50:THR:HG21	1.98	0.46
1:I:13:GLN:N	1:P:25:MET:SD	2.88	0.46
1:U:58:VAL:O	1:U:61:ARG:NH1	2.47	0.46
1:W:92:ILE:HD11	1:W:169:THR:HG21	1.97	0.46
1:A:14:VAL:HG11	1:Y:18:THR:HG22	1.96	0.46
1:M:67:ALA:HB2	1:M:81:LEU:HD23	1.97	0.46
1:N:19:LEU:HD13	1:U:43:LEU:HB3	1.97	0.46
1:F:23:ILE:HG23	1:O:50:THR:HG21	1.98	0.46
1:F:148:MET:HE1	1:F:165:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:ASP:OD1	1:L:77:ASP:N	2.46	0.46
1:U:84:ARG:NH1	1:U:85:GLN:O	2.49	0.46
1:U:125:THR:O	1:U:147:ILE:N	2.36	0.46
1:Q:143:ARG:HG2	1:Q:143:ARG:HH11	1.81	0.46
1:S:110:LEU:HD12	1:S:110:LEU:H	1.80	0.46
1:B:103:GLY:HA2	1:B:163:VAL:HG13	1.98	0.46
1:D:53:GLU:HA	1:D:56:ALA:HB3	1.97	0.46
1:A:64:ILE:HD12	1:A:177:TYR:HB2	1.99	0.45
1:N:31:ILE:O	1:N:35:VAL:HG12	2.16	0.45
1:V:44:GLN:O	1:V:48:SER:OG	2.25	0.45
1:W:137:LEU:CD2	1:W:144:ILE:HG12	2.47	0.45
1:Z:169:THR:HG22	1:Z:170:GLN:N	2.30	0.45
1:I:64:ILE:HD12	1:I:177:TYR:HB2	1.98	0.45
1:N:52:GLU:O	1:N:56:ALA:N	2.39	0.45
1:V:39:THR:O	1:V:43:LEU:HD12	2.16	0.45
1:Y:33:ALA:O	1:Y:37:ILE:HG13	2.16	0.45
1:L:100:GLN:NE2	1:U:66:SER:OG	2.46	0.45
1:Q:105:ASP:O	1:R:189:ASN:ND2	2.50	0.45
1:S:23:ILE:O	1:S:27:LEU:HD12	2.16	0.45
1:Y:102:ILE:HB	1:Y:164:GLN:HB3	1.98	0.45
1:R:85:GLN:HG3	1:R:137:LEU:HB3	1.98	0.45
1:X:186:LYS:HA	1:X:186:LYS:HD2	1.76	0.45
1:O:33:ALA:O	1:O:37:ILE:HG13	2.17	0.45
1:P:60:ASN:HB3	1:P:92:ILE:HD11	1.99	0.45
1:T:85:GLN:NE2	1:T:89:ALA:O	2.49	0.45
1:A:128:SER:HB2	1:A:134:UNK:HA	1.99	0.45
1:L:130:LYS:HE3	1:L:130:LYS:HB3	1.67	0.45
1:P:99:ILE:HG23	1:P:110:LEU:HB2	1.99	0.45
1:Z:83:VAL:HG21	1:Z:94:LEU:HD11	1.97	0.45
1:C:81:LEU:HB2	1:C:146:VAL:HG22	1.98	0.45
1:F:46:LYS:NZ	1:P:88:GLY:O	2.36	0.45
1:I:122:GLU:O	1:I:123:ASN:ND2	2.50	0.45
1:M:64:ILE:HD13	1:M:81:LEU:HD22	1.98	0.45
1:J:97:SER:HB2	1:J:169:THR:HA	1.99	0.45
1:O:62:ILE:HD11	1:O:92:ILE:HG21	1.98	0.45
1:U:35:VAL:O	1:U:39:THR:HG23	2.17	0.45
1:V:188:LYS:HE2	1:V:191:VAL:HG12	1.98	0.45
2:9:3:A1H1V:O24	2:9:4:A1H10:O2S	2.35	0.45
1:K:64:ILE:HD12	1:K:177:TYR:HB2	1.99	0.44
1:P:55:SER:O	1:P:59:SER:OG	2.32	0.44
1:S:186:LYS:HD3	1:S:186:LYS:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:91:ASN:ND2	1:U:138:VAL:HA	2.32	0.44
1:U:169:THR:HG22	1:U:170:GLN:H	1.81	0.44
1:A:138:VAL:HG23	1:A:139:ASP:H	1.83	0.44
1:M:182:PRO:HG2	1:M:191:VAL:HB	1.99	0.44
1:S:101:TRP:HB2	1:S:110:LEU:HD11	1.99	0.44
1:B:92:ILE:HB	1:B:137:LEU:HB2	2.00	0.44
1:E:26:VAL:HG12	1:N:54:ALA:HB3	1.98	0.44
1:J:22:PHE:HZ	1:Q:39:THR:HG21	1.82	0.44
1:K:112:TYR:HD1	1:K:113:UNK:N	2.15	0.44
1:M:62:ILE:HD12	1:M:169:THR:HG22	2.00	0.44
1:N:182:PRO:HG2	1:N:191:VAL:HB	1.99	0.44
1:O:27:LEU:O	1:O:31:ILE:HG13	2.18	0.44
1:P:98:THR:HG22	1:P:111:THR:HG22	1.98	0.44
1:R:19:LEU:O	1:R:23:ILE:HG13	2.18	0.44
1:R:19:LEU:HD21	1:T:35:VAL:HG11	1.99	0.44
1:S:166:THR:O	1:S:166:THR:OG1	2.31	0.44
1:V:85:GLN:HB3	1:V:89:ALA:HB3	1.98	0.44
1:X:60:ASN:HD21	1:X:90:ASP:HB3	1.81	0.44
1:E:16:ILE:HG23	1:N:43:LEU:HD22	1.99	0.44
1:H:180:GLN:HA	1:H:180:GLN:OE1	2.17	0.44
1:M:72:UNK:O	1:M:74:UNK:N	2.50	0.44
1:W:170:GLN:H	1:W:170:GLN:HG2	1.61	0.44
2:NA:3:A1H1V:S1	2:NA:4:A1H10:O2S	2.75	0.44
1:I:85:GLN:HG3	1:I:137:LEU:HB3	1.99	0.44
1:L:50:THR:HG21	1:M:23:ILE:HG23	2.00	0.44
1:X:182:PRO:HG2	1:X:191:VAL:HB	2.00	0.44
1:B:72:UNK:O	1:B:74:UNK:N	2.50	0.44
1:F:64:ILE:HD12	1:F:177:TYR:HB2	1.99	0.44
1:M:176:THR:HB	1:M:178:TRP:HZ3	1.83	0.44
1:S:59:SER:OG	1:S:60:ASN:N	2.51	0.44
1:S:147:ILE:HD11	2:AA:1:BGC:H6C1	2.00	0.44
1:E:64:ILE:HG12	1:E:81:LEU:HD23	2.00	0.44
1:G:166:THR:O	1:G:166:THR:OG1	2.31	0.44
2:PA:3:A1H1V:O24	2:PA:4:A1H10:O2S	2.36	0.44
1:D:81:LEU:HD11	1:D:165:LEU:HD13	2.00	0.44
1:N:70:ASN:OD1	1:N:71:VAL:N	2.51	0.44
2:FA:3:A1H1V:O24	2:FA:4:A1H10:O2S	2.36	0.44
1:A:21:VAL:HG11	1:X:18:THR:HG21	1.99	0.44
1:J:99:ILE:HG12	1:J:167:VAL:HG22	1.99	0.44
1:O:25:MET:SD	1:P:13:GLN:N	2.91	0.44
1:R:169:THR:HG22	1:R:170:GLN:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:72:UNK:O	1:X:74:UNK:N	2.49	0.44
1:Y:85:GLN:HB3	1:Y:89:ALA:HB3	2.00	0.44
2:5:3:A1H1V:S1	2:5:4:A1H10:O2S	2.76	0.44
1:A:59:SER:OG	1:A:60:ASN:N	2.51	0.43
1:B:22:PHE:HE1	1:Z:16:ILE:HG21	1.83	0.43
1:D:16:ILE:HG21	1:E:22:PHE:CE1	2.43	0.43
1:E:46:LYS:O	1:E:50:THR:HG23	2.18	0.43
1:G:53:GLU:OE1	1:H:140:GLN:NE2	2.51	0.43
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.87	0.43
1:N:99:ILE:O	1:N:110:LEU:N	2.47	0.43
1:W:96:LYS:NZ	2:JA:1:BGC:H6C2	2.33	0.43
1:V:44:GLN:HG3	1:V:45:SER:N	2.33	0.43
1:Y:23:ILE:O	1:Y:26:VAL:HG22	2.18	0.43
1:L:58:VAL:O	1:L:61:ARG:NH1	2.46	0.43
1:P:67:ALA:O	1:P:193:LEU:HB2	2.19	0.43
1:R:128:SER:HB3	1:R:134:UNK:HA	1.98	0.43
1:S:22:PHE:O	1:S:26:VAL:HG23	2.18	0.43
1:W:28:VAL:HG13	1:X:40:ALA:HB2	1.99	0.43
1:U:22:PHE:O	1:U:26:VAL:HG23	2.18	0.43
1:X:95:UNK:HA	1:X:112:TYR:HD1	1.83	0.43
1:K:72:UNK:O	1:K:74:UNK:N	2.49	0.43
1:K:99:ILE:HG12	1:K:167:VAL:HG13	2.01	0.43
1:L:51:GLY:HA2	1:M:26:VAL:HG11	2.00	0.43
1:Z:137:LEU:HD12	1:Z:144:ILE:HD12	2.00	0.43
1:B:125:THR:O	1:B:147:ILE:N	2.33	0.43
1:Q:116:UNK:O	1:Q:118:UNK:N	2.52	0.43
1:R:147:ILE:HG12	2:8:1:BGC:H6C1	2.01	0.43
1:I:100:GLN:HB3	1:I:166:THR:OG1	2.19	0.43
1:J:170:GLN:HB2	1:K:141:SER:HB3	2.01	0.43
1:L:85:GLN:HG3	1:L:137:LEU:HD23	2.00	0.43
1:U:116:UNK:O	1:U:118:UNK:N	2.51	0.43
1:Z:91:ASN:OD1	1:Z:91:ASN:N	2.51	0.43
1:J:16:ILE:HG21	1:K:26:VAL:HG22	2.01	0.43
1:L:19:LEU:O	1:L:23:ILE:HG13	2.19	0.43
1:A:39:THR:HG21	1:W:22:PHE:HZ	1.84	0.42
1:C:125:THR:O	1:C:147:ILE:N	2.34	0.42
1:I:60:ASN:HD21	1:I:90:ASP:HB2	1.84	0.42
1:L:129:ILE:HD13	1:L:129:ILE:HA	1.91	0.42
1:O:19:LEU:O	1:O:22:PHE:HB3	2.18	0.42
1:T:49:ALA:O	1:T:53:GLU:HG2	2.19	0.42
1:I:183:GLU:CD	1:I:183:GLU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:ARG:NH1	1:N:85:GLN:O	2.52	0.42
1:R:174:LYS:HD2	1:W:65:VAL:HG13	2.00	0.42
1:T:56:ALA:O	1:T:60:ASN:HB3	2.18	0.42
1:W:96:LYS:HA	1:X:130:LYS:HE2	1.99	0.42
1:X:169:THR:HG22	1:X:170:GLN:H	1.83	0.42
1:A:125:THR:HB	1:A:147:ILE:HB	2.00	0.42
1:P:94:LEU:HD23	1:P:94:LEU:HA	1.78	0.42
1:B:84:ARG:NH1	1:B:85:GLN:O	2.52	0.42
1:F:42:TYR:CE2	1:P:52:GLU:HG2	2.52	0.42
1:T:129:ILE:HD13	1:T:129:ILE:HA	1.89	0.42
1:E:48:SER:O	1:E:52:GLU:HG2	2.19	0.42
1:N:30:ALA:O	1:N:34:GLY:N	2.43	0.42
1:T:186:LYS:HA	1:T:186:LYS:HD3	1.83	0.42
1:C:35:VAL:HG21	1:D:19:LEU:HD21	2.02	0.42
1:F:19:LEU:O	1:F:23:ILE:HG13	2.20	0.42
1:U:13:GLN:N	1:U:13:GLN:OE1	2.52	0.42
2:5:3:A1H1V:O22	2:5:4:A1H10:O1S	2.37	0.42
1:D:37:ILE:HG21	1:M:61:ARG:CZ	2.49	0.42
1:I:170:GLN:HE22	1:Q:183:GLU:HG2	1.84	0.42
1:N:46:LYS:NZ	1:N:50:THR:OG1	2.53	0.42
1:P:171:TYR:O	1:Q:84:ARG:NH2	2.53	0.42
1:Q:138:VAL:HG23	1:Q:139:ASP:H	1.85	0.42
1:V:65:VAL:HG23	1:V:84:ARG:HG2	2.01	0.42
1:V:101:TRP:HB2	1:V:110:LEU:HD11	2.02	0.42
1:C:37:ILE:HG21	1:K:61:ARG:NH1	2.34	0.42
1:L:25:MET:SD	1:N:13:GLN:N	2.93	0.42
1:Y:62:ILE:HD13	1:Y:62:ILE:HA	1.90	0.42
2:3:3:A1H1V:S1	2:3:4:A1H10:O2S	2.78	0.42
1:D:174:LYS:HD3	1:E:65:VAL:HG13	2.01	0.42
1:O:35:VAL:HG11	1:P:19:LEU:HD21	2.01	0.42
1:Q:105:ASP:HA	1:R:189:ASN:HD22	1.85	0.42
1:V:129:ILE:HD13	1:V:129:ILE:HA	1.86	0.42
2:5:3:A1H1V:O22	2:5:4:A1H10:S	2.78	0.42
1:P:64:ILE:HG13	1:P:83:VAL:HG12	2.02	0.42
1:R:169:THR:HG22	1:R:170:GLN:N	2.35	0.42
1:T:72:UNK:O	1:T:74:UNK:N	2.51	0.42
1:U:62:ILE:HD11	1:U:92:ILE:HG21	2.02	0.42
1:J:94:LEU:HD23	1:J:94:LEU:HA	1.93	0.41
1:Q:129:ILE:HD11	1:Q:145:LYS:HB2	2.02	0.41
1:A:99:ILE:HG12	1:A:167:VAL:HG22	2.01	0.41
1:A:142:ASP:OD2	1:A:142:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:LEU:O	1:E:23:ILE:HG13	2.20	0.41
1:E:83:VAL:HG21	1:E:94:LEU:HD11	2.01	0.41
1:E:29:ALA:O	1:E:33:ALA:N	2.48	0.41
1:E:33:ALA:O	1:E:37:ILE:HG13	2.20	0.41
1:Q:62:ILE:HG23	1:Q:83:VAL:HB	2.03	0.41
1:T:169:THR:HG22	1:T:170:GLN:N	2.34	0.41
1:A:50:THR:HG21	1:R:23:ILE:HG23	2.01	0.41
1:F:174:LYS:HB2	1:F:174:LYS:HE2	1.79	0.41
1:J:129:ILE:HD13	1:J:129:ILE:HA	1.86	0.41
1:N:162:GLU:OE1	1:N:178:TRP:HD1	2.03	0.41
1:P:22:PHE:O	1:P:26:VAL:HG23	2.20	0.41
1:L:13:GLN:N	1:W:25:MET:SD	2.94	0.41
1:L:101:TRP:O	1:L:107:ALA:HA	2.21	0.41
1:G:62:ILE:HD12	1:G:94:LEU:HD21	2.03	0.41
1:H:112:TYR:HD2	1:H:113:UNK:N	2.17	0.41
1:K:91:ASN:OD1	1:K:91:ASN:N	2.53	0.41
1:Y:174:LYS:HB2	1:Y:174:LYS:HE2	1.84	0.41
1:G:55:SER:O	1:G:59:SER:OG	2.28	0.41
1:K:136:VAL:HG21	1:W:186:LYS:HG3	2.02	0.41
1:L:183:GLU:OE1	1:M:170:GLN:NE2	2.53	0.41
1:N:20:ILE:HD11	1:O:26:VAL:HG12	2.02	0.41
1:Q:72:UNK:O	1:Q:74:UNK:N	2.53	0.41
1:U:19:LEU:O	1:U:23:ILE:HG13	2.20	0.41
1:Y:103:GLY:HA2	1:Y:163:VAL:HG22	2.03	0.41
1:Y:179:ALA:HB1	1:Y:193:LEU:HD23	2.03	0.41
1:F:39:THR:HG21	1:H:22:PHE:HZ	1.85	0.41
1:G:84:ARG:HD3	1:G:143:ARG:NH1	2.35	0.41
1:H:91:ASN:N	1:H:91:ASN:OD1	2.54	0.41
1:I:128:SER:HB3	1:I:134:UNK:HA	2.02	0.41
1:K:94:LEU:HD23	1:K:94:LEU:HA	1.88	0.41
1:L:170:GLN:HG3	1:X:183:GLU:OE1	2.21	0.41
1:O:85:GLN:HE21	1:O:89:ALA:HB3	1.85	0.41
1:P:20:ILE:HA	1:P:23:ILE:HD12	2.03	0.41
1:S:136:VAL:HG21	1:Y:186:LYS:HG3	2.02	0.41
2:JA:3:A1H1V:S1	2:JA:4:A1H10:O2S	2.78	0.41
1:C:37:ILE:HG21	1:K:61:ARG:CZ	2.51	0.41
1:C:77:ASP:OD1	1:C:77:ASP:N	2.46	0.41
1:C:95:UNK:HA	1:C:112:TYR:HD2	1.86	0.41
1:N:46:LYS:O	1:N:50:THR:OG1	2.35	0.41
1:R:166:THR:HG22	1:R:176:THR:HG23	2.03	0.41
1:V:53:GLU:O	1:V:57:GLN:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:TYR:HD1	1:B:113:UNK:N	2.19	0.40
1:C:163:VAL:HG22	1:C:179:ALA:HB3	2.03	0.40
1:F:16:ILE:HG21	1:P:22:PHE:HE1	1.86	0.40
1:I:60:ASN:ND2	1:I:90:ASP:H	2.20	0.40
1:O:67:ALA:HB2	1:O:81:LEU:HD23	2.03	0.40
1:Q:110:LEU:HD21	1:Q:153:VAL:HG11	2.03	0.40
1:R:22:PHE:HZ	1:T:39:THR:HG21	1.87	0.40
1:S:39:THR:HG22	1:S:43:LEU:HD13	2.03	0.40
1:S:143:ARG:C	1:S:144:ILE:HD13	2.41	0.40
1:H:166:THR:O	1:H:166:THR:OG1	2.36	0.40
1:L:33:ALA:O	1:L:37:ILE:HG13	2.21	0.40
1:W:99:ILE:O	1:W:110:LEU:N	2.51	0.40
1:F:138:VAL:HG23	1:F:139:ASP:OD1	2.21	0.40
1:Y:62:ILE:HD11	1:Y:92:ILE:HG21	2.03	0.40
1:Y:163:VAL:HG12	1:Y:165:LEU:HD12	2.04	0.40
1:B:169:THR:HG22	1:B:170:GLN:N	2.36	0.40
1:C:72:UNK:O	1:C:74:UNK:N	2.53	0.40
1:D:122:GLU:OE2	1:D:122:GLU:N	2.44	0.40
1:H:137:LEU:HD21	1:H:144:ILE:HG13	2.03	0.40
1:N:33:ALA:O	1:N:37:ILE:HG13	2.22	0.40
1:N:186:LYS:HE2	1:N:186:LYS:HB3	1.80	0.40
1:X:20:ILE:HA	1:X:23:ILE:HD12	2.02	0.40
1:A:79:VAL:O	1:A:148:MET:HB2	2.22	0.40
1:B:169:THR:HG22	1:B:170:GLN:H	1.87	0.40
1:C:85:GLN:NE2	1:C:89:ALA:O	2.55	0.40
1:I:57:GLN:NE2	1:J:84:ARG:HH22	2.20	0.40
1:K:42:TYR:HE2	1:L:52:GLU:HA	1.86	0.40
1:L:60:ASN:HD21	1:L:90:ASP:HB3	1.87	0.40
1:P:46:LYS:HD3	1:P:46:LYS:HA	1.91	0.40
1:P:137:LEU:HG	1:P:144:ILE:HD12	2.03	0.40
2:PA:3:A1H1V:S1	2:PA:4:A1H10:O2S	2.80	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%)	144 (96%)	5 (3%)	1 (1%)	19	51
1	C	150/193 (78%)	147 (98%)	3 (2%)	0	100	100
1	D	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	E	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	F	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
1	G	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	H	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	I	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	J	150/193 (78%)	144 (96%)	5 (3%)	1 (1%)	19	51
1	K	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	L	150/193 (78%)	147 (98%)	3 (2%)	0	100	100
1	M	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	N	150/193 (78%)	139 (93%)	10 (7%)	1 (1%)	19	51
1	O	150/193 (78%)	147 (98%)	3 (2%)	0	100	100
1	P	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
1	Q	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
1	R	150/193 (78%)	140 (93%)	10 (7%)	0	100	100
1	S	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	T	150/193 (78%)	144 (96%)	6 (4%)	0	100	100
1	U	150/193 (78%)	147 (98%)	3 (2%)	0	100	100
1	V	150/193 (78%)	145 (97%)	5 (3%)	0	100	100
1	W	150/193 (78%)	144 (96%)	5 (3%)	1 (1%)	19	51
1	X	150/193 (78%)	146 (97%)	4 (3%)	0	100	100
1	Y	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
1	Z	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
All	All	3900/5018 (78%)	3752 (96%)	144 (4%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	160	GLY
1	J	160	GLY
1	B	128	SER
1	N	153	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/134 (92%)	119 (97%)	4 (3%)	33	61
1	B	123/134 (92%)	118 (96%)	5 (4%)	26	56
1	C	123/134 (92%)	117 (95%)	6 (5%)	21	51
1	D	123/134 (92%)	118 (96%)	5 (4%)	26	56
1	E	123/134 (92%)	118 (96%)	5 (4%)	26	56
1	F	123/134 (92%)	120 (98%)	3 (2%)	44	68
1	G	123/134 (92%)	116 (94%)	7 (6%)	17	47
1	H	123/134 (92%)	119 (97%)	4 (3%)	33	61
1	I	123/134 (92%)	122 (99%)	1 (1%)	79	88
1	J	123/134 (92%)	114 (93%)	9 (7%)	11	38
1	K	123/134 (92%)	118 (96%)	5 (4%)	26	56
1	L	123/134 (92%)	119 (97%)	4 (3%)	33	61
1	M	123/134 (92%)	117 (95%)	6 (5%)	21	51
1	N	123/134 (92%)	116 (94%)	7 (6%)	17	47
1	O	123/134 (92%)	118 (96%)	5 (4%)	26	56
1	P	123/134 (92%)	119 (97%)	4 (3%)	33	61
1	Q	123/134 (92%)	121 (98%)	2 (2%)	58	77
1	R	123/134 (92%)	117 (95%)	6 (5%)	21	51
1	S	123/134 (92%)	116 (94%)	7 (6%)	17	47
1	T	123/134 (92%)	120 (98%)	3 (2%)	44	68
1	U	123/134 (92%)	119 (97%)	4 (3%)	33	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	123/134 (92%)	120 (98%)	3 (2%)	44	68
1	W	123/134 (92%)	118 (96%)	5 (4%)	26	56
1	X	123/134 (92%)	117 (95%)	6 (5%)	21	51
1	Y	123/134 (92%)	122 (99%)	1 (1%)	79	88
1	Z	122/134 (91%)	117 (96%)	5 (4%)	26	56
All	All	3197/3484 (92%)	3075 (96%)	122 (4%)	30	58

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	59	SER
1	A	142	ASP
1	A	149	TYR
1	B	90	ASP
1	B	105	ASP
1	B	112	TYR
1	B	185	LEU
1	B	186	LYS
1	C	55	SER
1	C	59	SER
1	C	66	SER
1	C	130	LYS
1	C	149	TYR
1	C	183	GLU
1	D	25	MET
1	D	60	ASN
1	D	142	ASP
1	D	149	TYR
1	D	193	LEU
1	E	38	ASN
1	E	97	SER
1	E	112	TYR
1	E	183	GLU
1	E	187	ASP
1	F	42	TYR
1	F	142	ASP
1	F	193	LEU
1	G	63	ASN
1	G	66	SER

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Mol	Chain	Res	Type
1	G	70	ASN
1	G	77	ASP
1	G	91	ASN
1	G	149	TYR
1	G	184	SER
1	H	66	SER
1	H	91	ASN
1	H	112	TYR
1	H	142	ASP
1	I	130	LYS
1	J	48	SER
1	J	55	SER
1	J	77	ASP
1	J	85	GLN
1	J	122	GLU
1	J	139	ASP
1	J	140	GLN
1	J	142	ASP
1	J	149	TYR
1	K	46	LYS
1	K	91	ASN
1	K	112	TYR
1	K	149	TYR
1	K	187	ASP
1	L	59	SER
1	L	149	TYR
1	L	184	SER
1	L	186	LYS
1	M	13	GLN
1	M	112	TYR
1	M	122	GLU
1	M	142	ASP
1	M	149	TYR
1	M	185	LEU
1	N	13	GLN
1	N	38	ASN
1	N	42	TYR
1	N	53	GLU
1	N	60	ASN
1	N	142	ASP
1	N	149	TYR
1	O	42	TYR

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Mol	Chain	Res	Type
1	O	55	SER
1	O	100	GLN
1	O	142	ASP
1	O	149	TYR
1	P	55	SER
1	P	91	ASN
1	P	142	ASP
1	P	149	TYR
1	Q	90	ASP
1	Q	139	ASP
1	R	59	SER
1	R	60	ASN
1	R	90	ASP
1	R	97	SER
1	R	142	ASP
1	R	148	MET
1	S	59	SER
1	S	91	ASN
1	S	110	LEU
1	S	149	TYR
1	S	170	GLN
1	S	174	LYS
1	S	193	LEU
1	T	122	GLU
1	T	142	ASP
1	T	149	TYR
1	U	142	ASP
1	U	149	TYR
1	U	184	SER
1	U	189	ASN
1	V	38	ASN
1	V	84	ARG
1	V	142	ASP
1	W	48	SER
1	W	60	ASN
1	W	90	ASP
1	W	142	ASP
1	W	149	TYR
1	X	22	PHE
1	X	42	TYR
1	X	55	SER
1	X	112	TYR

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Mol	Chain	Res	Type
1	X	149	TYR
1	X	189	ASN
1	Y	22	PHE
1	Z	59	SER
1	Z	68	TYR
1	Z	91	ASN
1	Z	139	ASP
1	Z	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	B	44	GLN
1	B	85	GLN
1	C	38	ASN
1	C	85	GLN
1	C	91	ASN
1	D	13	GLN
1	E	13	GLN
1	E	38	ASN
1	E	44	GLN
1	E	85	GLN
1	E	100	GLN
1	F	180	GLN
1	G	13	GLN
1	G	38	ASN
1	G	180	GLN
1	H	38	ASN
1	H	60	ASN
1	I	13	GLN
1	I	57	GLN
1	I	60	ASN
1	I	85	GLN
1	I	123	ASN
1	J	140	GLN
1	J	164	GLN
1	K	44	GLN
1	K	85	GLN
1	L	38	ASN
1	L	57	GLN
1	L	85	GLN

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Mol	Chain	Res	Type
1	L	100	GLN
1	L	164	GLN
1	M	13	GLN
1	M	38	ASN
1	N	13	GLN
1	N	100	GLN
1	O	13	GLN
1	O	38	ASN
1	O	63	ASN
1	O	85	GLN
1	O	100	GLN
1	P	13	GLN
1	P	85	GLN
1	P	100	GLN
1	P	164	GLN
1	P	170	GLN
1	Q	38	ASN
1	Q	60	ASN
1	Q	63	ASN
1	Q	85	GLN
1	Q	140	GLN
1	Q	170	GLN
1	R	60	ASN
1	R	180	GLN
1	R	189	ASN
1	S	170	GLN
1	T	38	ASN
1	T	85	GLN
1	T	180	GLN
1	U	13	GLN
1	U	38	ASN
1	U	44	GLN
1	U	91	ASN
1	U	100	GLN
1	V	13	GLN
1	V	38	ASN
1	V	85	GLN
1	V	100	GLN
1	W	91	ASN
1	X	63	ASN
1	X	91	ASN
1	Y	38	ASN

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Mol	Chain	Res	Type
1	Y	85	GLN
1	Z	38	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 ⓘ

208 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	2,1	11,11,12	0.24	0	15,15,17	0.70	0
2	BDP	0	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.59	2 (14%)
2	A1H1V	0	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.68	5 (33%)
2	A1H10	0	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.59	3 (17%)
2	BGC	1	1	2,1	11,11,12	0.20	0	15,15,17	0.79	0
2	BDP	1	2	2	12,12,13	1.94	1 (8%)	14,17,19	2.06	5 (35%)
2	A1H1V	1	3	2	16,16,17	1.19	2 (12%)	15,24,26	1.69	4 (26%)
2	A1H10	1	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.67	3 (17%)
2	BGC	2	1	2,1	11,11,12	0.19	0	15,15,17	0.74	0
2	BDP	2	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.60	2 (14%)
2	A1H1V	2	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.72	5 (33%)
2	A1H10	2	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.59	3 (17%)
2	BGC	3	1	2,1	11,11,12	0.21	0	15,15,17	0.76	0
2	BDP	3	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.97	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1H1V	3	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.65	4 (26%)
2	A1H10	3	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.66	3 (17%)
2	BGC	4	1	2,1	11,11,12	0.18	0	15,15,17	0.64	0
2	BDP	4	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.64	4 (28%)
2	A1H1V	4	3	2	16,16,17	1.34	3 (18%)	15,24,26	1.69	5 (33%)
2	A1H10	4	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.65	3 (17%)
2	BGC	5	1	2,1	11,11,12	0.24	0	15,15,17	1.12	1 (6%)
2	BDP	5	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.83	4 (28%)
2	A1H1V	5	3	2	16,16,17	1.19	2 (12%)	15,24,26	1.66	4 (26%)
2	A1H10	5	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.64	3 (17%)
2	BGC	6	1	2,1	11,11,12	0.19	0	15,15,17	0.75	0
2	BDP	6	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.62	3 (21%)
2	A1H1V	6	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.69	5 (33%)
2	A1H10	6	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.64	3 (17%)
2	BGC	7	1	2,1	11,11,12	0.18	0	15,15,17	0.58	0
2	BDP	7	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.58	2 (14%)
2	A1H1V	7	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.78	5 (33%)
2	A1H10	7	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.64	3 (17%)
2	BGC	8	1	2,1	11,11,12	0.21	0	15,15,17	0.59	0
2	BDP	8	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	8	3	2	16,16,17	1.34	3 (18%)	15,24,26	1.72	5 (33%)
2	A1H10	8	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.65	3 (17%)
2	BGC	9	1	2,1	11,11,12	0.22	0	15,15,17	0.87	1 (6%)
2	BDP	9	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.95	5 (35%)
2	A1H1V	9	3	2	16,16,17	1.19	2 (12%)	15,24,26	1.66	4 (26%)
2	A1H10	9	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.66	3 (17%)
2	BGC	AA	1	2,1	11,11,12	0.19	0	15,15,17	0.57	0
2	BDP	AA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.49	2 (14%)
2	A1H1V	AA	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.74	5 (33%)
2	A1H10	AA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.73	3 (17%)
2	BGC	BA	1	2,1	11,11,12	0.28	0	15,15,17	1.43	3 (20%)
2	BDP	BA	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.53	2 (14%)
2	A1H1V	BA	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.77	5 (33%)
2	A1H10	BA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.67	3 (17%)
2	BGC	CA	1	2,1	11,11,12	0.18	0	15,15,17	0.75	0
2	BDP	CA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.69	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1H1V	CA	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.71	5 (33%)
2	A1H10	CA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.64	3 (17%)
2	BGC	DA	1	2,1	11,11,12	0.21	0	15,15,17	0.63	0
2	BDP	DA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.55	2 (14%)
2	A1H1V	DA	3	2	16,16,17	1.19	2 (12%)	15,24,26	1.68	4 (26%)
2	A1H10	DA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	EA	1	2,1	11,11,12	0.20	0	15,15,17	0.66	0
2	BDP	EA	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	EA	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.71	5 (33%)
2	A1H10	EA	4	2	16,16,17	1.40	4 (25%)	17,24,26	1.69	3 (17%)
2	BGC	FA	1	2,1	11,11,12	0.22	0	15,15,17	0.69	0
2	BDP	FA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.55	2 (14%)
2	A1H1V	FA	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.63	4 (26%)
2	A1H10	FA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	GA	1	2,1	11,11,12	0.23	0	15,15,17	0.79	0
2	BDP	GA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.61	2 (14%)
2	A1H1V	GA	3	2	16,16,17	1.32	3 (18%)	15,24,26	1.68	5 (33%)
2	A1H10	GA	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.63	3 (17%)
2	BGC	HA	1	2,1	11,11,12	0.21	0	15,15,17	0.71	0
2	BDP	HA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.51	2 (14%)
2	A1H1V	HA	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.63	4 (26%)
2	A1H10	HA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	IA	1	2,1	11,11,12	0.28	0	15,15,17	0.62	0
2	BDP	IA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.58	2 (14%)
2	A1H1V	IA	3	2	16,16,17	1.32	3 (18%)	15,24,26	1.70	5 (33%)
2	A1H10	IA	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.66	3 (17%)
2	BGC	JA	1	2,1	11,11,12	0.20	0	15,15,17	0.74	0
2	BDP	JA	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.59	2 (14%)
2	A1H1V	JA	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.60	4 (26%)
2	A1H10	JA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.69	3 (17%)
2	BGC	KA	1	2,1	11,11,12	0.19	0	15,15,17	0.60	0
2	BDP	KA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.62	3 (21%)
2	A1H1V	KA	3	2	16,16,17	1.34	3 (18%)	15,24,26	1.77	5 (33%)
2	A1H10	KA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.67	3 (17%)
2	BGC	LA	1	2,1	11,11,12	0.20	0	15,15,17	0.56	0
2	BDP	LA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.56	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1H1V	LA	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.65	4 (26%)
2	A1H10	LA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	MA	1	2,1	11,11,12	0.21	0	15,15,17	0.72	0
2	BDP	MA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.58	3 (21%)
2	A1H1V	MA	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.70	5 (33%)
2	A1H10	MA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	NA	1	2,1	11,11,12	0.22	0	15,15,17	0.75	0
2	BDP	NA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	NA	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.59	4 (26%)
2	A1H10	NA	4	2	16,16,17	1.40	4 (25%)	17,24,26	1.71	3 (17%)
2	BGC	OA	1	2,1	11,11,12	0.19	0	15,15,17	0.71	0
2	BDP	OA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.78	4 (28%)
2	A1H1V	OA	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.71	5 (33%)
2	A1H10	OA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.62	3 (17%)
2	BGC	PA	1	2,1	11,11,12	0.20	0	15,15,17	0.83	0
2	BDP	PA	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.60	2 (14%)
2	A1H1V	PA	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.63	4 (26%)
2	A1H10	PA	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.70	3 (17%)
2	BGC	a	1	2,1	11,11,12	0.20	0	15,15,17	0.76	0
2	BDP	a	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.63	3 (21%)
2	A1H1V	a	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.70	5 (33%)
2	A1H10	a	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.62	3 (17%)
2	BGC	b	1	2,1	11,11,12	0.21	0	15,15,17	0.61	0
2	BDP	b	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.50	2 (14%)
2	A1H1V	b	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.63	4 (26%)
2	A1H10	b	4	2	16,16,17	1.40	4 (25%)	17,24,26	1.69	3 (17%)
2	BGC	c	1	2,1	11,11,12	0.18	0	15,15,17	0.61	0
2	BDP	c	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.56	3 (21%)
2	A1H1V	c	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.69	4 (26%)
2	A1H10	c	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.64	3 (17%)
2	BGC	d	1	2,1	11,11,12	0.24	0	15,15,17	0.76	0
2	BDP	d	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.61	2 (14%)
2	A1H1V	d	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.64	4 (26%)
2	A1H10	d	4	2	16,16,17	1.40	4 (25%)	17,24,26	1.74	3 (17%)
2	BGC	e	1	2,1	11,11,12	0.21	0	15,15,17	0.65	0
2	BDP	e	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.56	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1H1V	e	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.74	5 (33%)
2	A1H10	e	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.62	3 (17%)
2	BGC	f	1	2,1	11,11,12	0.20	0	15,15,17	0.68	0
2	BDP	f	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	f	3	2	16,16,17	1.19	2 (12%)	15,24,26	1.59	4 (26%)
2	A1H10	f	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	g	1	2,1	11,11,12	0.22	0	15,15,17	0.90	0
2	BDP	g	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.62	2 (14%)
2	A1H1V	g	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.68	5 (33%)
2	A1H10	g	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.66	3 (17%)
2	BGC	h	1	2,1	11,11,12	0.22	0	15,15,17	0.75	0
2	BDP	h	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.57	2 (14%)
2	A1H1V	h	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.64	4 (26%)
2	A1H10	h	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.72	3 (17%)
2	BGC	i	1	2,1	11,11,12	0.21	0	15,15,17	0.75	0
2	BDP	i	2	2	12,12,13	1.95	1 (8%)	14,17,19	1.59	2 (14%)
2	A1H1V	i	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.73	5 (33%)
2	A1H10	i	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.61	3 (17%)
2	BGC	j	1	2,1	11,11,12	0.20	0	15,15,17	0.70	0
2	BDP	j	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.51	2 (14%)
2	A1H1V	j	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.71	4 (26%)
2	A1H10	j	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.67	3 (17%)
2	BGC	k	1	2,1	11,11,12	0.21	0	15,15,17	0.80	0
2	BDP	k	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.74	4 (28%)
2	A1H1V	k	3	2	16,16,17	1.34	3 (18%)	15,24,26	1.67	5 (33%)
2	A1H10	k	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.62	3 (17%)
2	BGC	l	1	2,1	11,11,12	0.21	0	15,15,17	0.60	0
2	BDP	l	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.49	2 (14%)
2	A1H1V	l	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.63	4 (26%)
2	A1H10	l	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.69	3 (17%)
2	BGC	m	1	2,1	11,11,12	0.23	0	15,15,17	0.83	0
2	BDP	m	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.59	2 (14%)
2	A1H1V	m	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.68	5 (33%)
2	A1H10	m	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.64	3 (17%)
2	BGC	n	1	2,1	11,11,12	0.21	0	15,15,17	0.69	0
2	BDP	n	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.55	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1H1V	n	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.63	4 (26%)
2	A1H10	n	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	o	1	2,1	11,11,12	0.18	0	15,15,17	0.67	0
2	BDP	o	2	2	12,12,13	1.95	1 (8%)	14,17,19	1.60	3 (21%)
2	A1H1V	o	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.73	5 (33%)
2	A1H10	o	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.62	3 (17%)
2	BGC	p	1	2,1	11,11,12	0.27	0	15,15,17	1.17	2 (13%)
2	BDP	p	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.87	6 (42%)
2	A1H1V	p	3	2	16,16,17	1.19	2 (12%)	15,24,26	1.61	4 (26%)
2	A1H10	p	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.66	3 (17%)
2	BGC	q	1	2,1	11,11,12	0.24	0	15,15,17	0.83	0
2	BDP	q	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.61	3 (21%)
2	A1H1V	q	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.67	5 (33%)
2	A1H10	q	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.58	3 (17%)
2	BGC	r	1	2,1	11,11,12	0.28	0	15,15,17	1.66	3 (20%)
2	BDP	r	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.53	2 (14%)
2	A1H1V	r	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.66	4 (26%)
2	A1H10	r	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.68	3 (17%)
2	BGC	s	1	2,1	11,11,12	0.20	0	15,15,17	0.68	0
2	BDP	s	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.59	2 (14%)
2	A1H1V	s	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.71	5 (33%)
2	A1H10	s	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.67	3 (17%)
2	BGC	t	1	2,1	11,11,12	0.19	0	15,15,17	0.63	0
2	BDP	t	2	2	12,12,13	1.95	1 (8%)	14,17,19	1.50	2 (14%)
2	A1H1V	t	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.70	4 (26%)
2	A1H10	t	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.71	3 (17%)
2	BGC	u	1	2,1	11,11,12	0.17	0	15,15,17	0.68	0
2	BDP	u	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.60	3 (21%)
2	A1H1V	u	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.72	5 (33%)
2	A1H10	u	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.65	3 (17%)
2	BGC	v	1	2,1	11,11,12	0.19	0	15,15,17	0.61	0
2	BDP	v	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.59	2 (14%)
2	A1H1V	v	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.65	4 (26%)
2	A1H10	v	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.70	3 (17%)
2	BGC	w	1	2,1	11,11,12	0.21	0	15,15,17	0.80	0
2	BDP	w	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.61	2 (14%)

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	1.33	3 (18%)	15,24,26	1.70	5 (33%)
2	A1H10	w	4	2	16,16,17	1.42	4 (25%)	17,24,26	1.60	3 (17%)
2	BGC	x	1	2,1	11,11,12	0.22	0	15,15,17	0.63	0
2	BDP	x	2	2	12,12,13	1.94	1 (8%)	14,17,19	1.54	2 (14%)
2	A1H1V	x	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.62	4 (26%)
2	A1H10	x	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.69	3 (17%)
2	BGC	y	1	2,1	11,11,12	0.23	0	15,15,17	0.69	0
2	BDP	y	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.61	3 (21%)
2	A1H1V	y	3	2	16,16,17	1.33	3 (18%)	15,24,26	1.64	5 (33%)
2	A1H10	y	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.59	3 (17%)
2	BGC	z	1	2,1	11,11,12	0.20	0	15,15,17	0.66	0
2	BDP	z	2	2	12,12,13	1.93	1 (8%)	14,17,19	1.52	2 (14%)
2	A1H1V	z	3	2	16,16,17	1.18	2 (12%)	15,24,26	1.61	4 (26%)
2	A1H10	z	4	2	16,16,17	1.41	4 (25%)	17,24,26	1.71	3 (17%)

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	2,1	-	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	A1H10	0	4	2	-	2/9/26/29	0/1/1/1
2	BGC	1	1	2,1	-	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	A1H10	1	4	2	-	2/9/26/29	0/1/1/1
2	BGC	2	1	2,1	-	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	A1H10	2	4	2	-	2/9/26/29	0/1/1/1
2	BGC	3	1	2,1	-	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	A1H10	3	4	2	-	2/9/26/29	0/1/1/1
2	BGC	4	1	2,1	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	A1H10	4	4	2	-	2/9/26/29	0/1/1/1
2	BGC	5	1	2,1	-	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	A1H10	5	4	2	-	2/9/26/29	0/1/1/1
2	BGC	6	1	2,1	-	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	A1H10	6	4	2	-	2/9/26/29	0/1/1/1
2	BGC	7	1	2,1	-	1/2/19/22	0/1/1/1
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	A1H10	7	4	2	-	2/9/26/29	0/1/1/1
2	BGC	8	1	2,1	-	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	A1H10	8	4	2	-	2/9/26/29	0/1/1/1
2	BGC	9	1	2,1	-	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	A1H10	9	4	2	-	2/9/26/29	0/1/1/1
2	BGC	AA	1	2,1	-	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	A1H10	AA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	BA	1	2,1	-	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	A1H10	BA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	CA	1	2,1	-	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	A1H10	CA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	DA	1	2,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H10	DA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	EA	1	2,1	-	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	A1H10	EA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	FA	1	2,1	-	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	A1H10	FA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	GA	1	2,1	-	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	A1H10	GA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	HA	1	2,1	-	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	A1H10	HA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	IA	1	2,1	-	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	A1H10	IA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	JA	1	2,1	-	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	A1H10	JA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	KA	1	2,1	-	1/2/19/22	0/1/1/1
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	A1H10	KA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	LA	1	2,1	-	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	A1H10	LA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	MA	1	2,1	-	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	A1H10	MA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	NA	1	2,1	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	NA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	NA	3	2	-	3/9/26/29	0/1/1/1
2	A1H10	NA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	OA	1	2,1	1/1/4/5	1/2/19/22	0/1/1/1
2	BDP	OA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	OA	3	2	-	3/9/26/29	0/1/1/1
2	A1H10	OA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	PA	1	2,1	-	1/2/19/22	0/1/1/1
2	BDP	PA	2	2	-	1/4/21/24	0/1/1/1
2	A1H1V	PA	3	2	-	3/9/26/29	0/1/1/1
2	A1H10	PA	4	2	-	2/9/26/29	0/1/1/1
2	BGC	a	1	2,1	-	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	A1H10	a	4	2	-	2/9/26/29	0/1/1/1
2	BGC	b	1	2,1	-	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	A1H10	b	4	2	-	2/9/26/29	0/1/1/1
2	BGC	c	1	2,1	-	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	A1H10	c	4	2	-	2/9/26/29	0/1/1/1
2	BGC	d	1	2,1	-	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	A1H10	d	4	2	-	2/9/26/29	0/1/1/1
2	BGC	e	1	2,1	-	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	A1H10	e	4	2	-	2/9/26/29	0/1/1/1
2	BGC	f	1	2,1	-	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	A1H10	f	4	2	-	2/9/26/29	0/1/1/1
2	BGC	g	1	2,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H10	g	4	2	-	2/9/26/29	0/1/1/1
2	BGC	h	1	2,1	-	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	A1H10	h	4	2	-	2/9/26/29	0/1/1/1
2	BGC	i	1	2,1	-	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	A1H10	i	4	2	-	2/9/26/29	0/1/1/1
2	BGC	j	1	2,1	-	1/2/19/22	0/1/1/1
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	A1H10	j	4	2	-	2/9/26/29	0/1/1/1
2	BGC	k	1	2,1	-	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	A1H10	k	4	2	-	2/9/26/29	0/1/1/1
2	BGC	l	1	2,1	-	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	A1H10	l	4	2	-	2/9/26/29	0/1/1/1
2	BGC	m	1	2,1	-	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	A1H10	m	4	2	-	2/9/26/29	0/1/1/1
2	BGC	n	1	2,1	-	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	A1H10	n	4	2	-	2/9/26/29	0/1/1/1
2	BGC	o	1	2,1	-	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	A1H10	o	4	2	-	2/9/26/29	0/1/1/1
2	BGC	p	1	2,1	-	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	A1H10	p	4	2	-	2/9/26/29	0/1/1/1
2	BGC	q	1	2,1	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	A1H10	q	4	2	-	2/9/26/29	0/1/1/1
2	BGC	r	1	2,1	-	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	A1H10	r	4	2	-	2/9/26/29	0/1/1/1
2	BGC	s	1	2,1	-	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	A1H10	s	4	2	-	2/9/26/29	0/1/1/1
2	BGC	t	1	2,1	-	0/2/19/22	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	A1H10	t	4	2	-	2/9/26/29	0/1/1/1
2	BGC	u	1	2,1	-	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	A1H10	u	4	2	-	2/9/26/29	0/1/1/1
2	BGC	v	1	2,1	-	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	A1H10	v	4	2	-	2/9/26/29	0/1/1/1
2	BGC	w	1	2,1	-	1/2/19/22	0/1/1/1
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	A1H10	w	4	2	-	2/9/26/29	0/1/1/1
2	BGC	x	1	2,1	-	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	A1H10	x	4	2	-	2/9/26/29	0/1/1/1
2	BGC	y	1	2,1	-	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	A1H10	y	4	2	-	2/9/26/29	0/1/1/1
2	BGC	z	1	2,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H10	z	4	2	-	2/9/26/29	0/1/1/1

All (392) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	c	2	BDP	O6A-C6	6.61	1.42	1.22
2	t	2	BDP	O6A-C6	6.61	1.42	1.22
2	i	2	BDP	O6A-C6	6.61	1.42	1.22
2	o	2	BDP	O6A-C6	6.61	1.42	1.22
2	d	2	BDP	O6A-C6	6.60	1.42	1.22
2	l	2	BDP	O6A-C6	6.60	1.42	1.22
2	IA	2	BDP	O6A-C6	6.60	1.42	1.22
2	a	2	BDP	O6A-C6	6.60	1.42	1.22
2	FA	2	BDP	O6A-C6	6.60	1.42	1.22
2	q	2	BDP	O6A-C6	6.59	1.42	1.22
2	m	2	BDP	O6A-C6	6.59	1.42	1.22
2	1	2	BDP	O6A-C6	6.59	1.42	1.22
2	AA	2	BDP	O6A-C6	6.59	1.42	1.22
2	g	2	BDP	O6A-C6	6.59	1.42	1.22
2	4	2	BDP	O6A-C6	6.59	1.42	1.22
2	9	2	BDP	O6A-C6	6.59	1.42	1.22
2	PA	2	BDP	O6A-C6	6.59	1.42	1.22
2	x	2	BDP	O6A-C6	6.59	1.42	1.22
2	n	2	BDP	O6A-C6	6.59	1.42	1.22
2	HA	2	BDP	O6A-C6	6.59	1.42	1.22
2	j	2	BDP	O6A-C6	6.59	1.42	1.22
2	0	2	BDP	O6A-C6	6.59	1.42	1.22
2	r	2	BDP	O6A-C6	6.59	1.42	1.22
2	v	2	BDP	O6A-C6	6.59	1.42	1.22
2	DA	2	BDP	O6A-C6	6.59	1.42	1.22
2	p	2	BDP	O6A-C6	6.59	1.42	1.22
2	NA	2	BDP	O6A-C6	6.58	1.42	1.22
2	b	2	BDP	O6A-C6	6.58	1.42	1.22
2	e	2	BDP	O6A-C6	6.58	1.42	1.22
2	GA	2	BDP	O6A-C6	6.58	1.42	1.22
2	k	2	BDP	O6A-C6	6.58	1.42	1.22
2	5	2	BDP	O6A-C6	6.58	1.42	1.22
2	CA	2	BDP	O6A-C6	6.58	1.42	1.22
2	f	2	BDP	O6A-C6	6.58	1.42	1.22
2	s	2	BDP	O6A-C6	6.58	1.42	1.22
2	OA	2	BDP	O6A-C6	6.58	1.42	1.22
2	8	2	BDP	O6A-C6	6.57	1.42	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	KA	2	BDP	O6A-C6	6.57	1.42	1.22
2	u	2	BDP	O6A-C6	6.57	1.42	1.22
2	7	2	BDP	O6A-C6	6.57	1.42	1.22
2	LA	2	BDP	O6A-C6	6.57	1.42	1.22
2	z	2	BDP	O6A-C6	6.57	1.42	1.22
2	h	2	BDP	O6A-C6	6.57	1.42	1.22
2	w	2	BDP	O6A-C6	6.57	1.42	1.22
2	MA	2	BDP	O6A-C6	6.57	1.42	1.22
2	EA	2	BDP	O6A-C6	6.57	1.42	1.22
2	2	2	BDP	O6A-C6	6.57	1.42	1.22
2	JA	2	BDP	O6A-C6	6.57	1.42	1.22
2	BA	2	BDP	O6A-C6	6.56	1.42	1.22
2	6	2	BDP	O6A-C6	6.56	1.42	1.22
2	3	2	BDP	O6A-C6	6.55	1.42	1.22
2	y	2	BDP	O6A-C6	6.55	1.42	1.22
2	t	4	A1H10	O6B-C6	3.60	1.42	1.30
2	c	4	A1H10	O6B-C6	3.60	1.42	1.30
2	5	4	A1H10	O6B-C6	3.59	1.42	1.30
2	f	3	A1H1V	O6B-C6	3.58	1.42	1.30
2	h	4	A1H10	O6B-C6	3.58	1.42	1.30
2	PA	4	A1H10	O6B-C6	3.58	1.42	1.30
2	p	3	A1H1V	O6B-C6	3.58	1.42	1.30
2	r	4	A1H10	O6B-C6	3.58	1.42	1.30
2	k	3	A1H1V	O6B-C6	3.58	1.42	1.30
2	LA	4	A1H10	O6B-C6	3.58	1.42	1.30
2	d	4	A1H10	O6B-C6	3.58	1.42	1.30
2	1	3	A1H1V	O6B-C6	3.58	1.42	1.30
2	FA	4	A1H10	O6B-C6	3.58	1.42	1.30
2	3	4	A1H10	O6B-C6	3.58	1.42	1.30
2	HA	4	A1H10	O6B-C6	3.58	1.42	1.30
2	DA	3	A1H1V	O6B-C6	3.58	1.42	1.30
2	9	4	A1H10	O6B-C6	3.58	1.42	1.30
2	y	3	A1H1V	O6B-C6	3.58	1.42	1.30
2	m	4	A1H10	O6B-C6	3.57	1.42	1.30
2	GA	4	A1H10	O6B-C6	3.57	1.42	1.30
2	d	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	JA	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	o	4	A1H10	O6B-C6	3.57	1.42	1.30
2	z	4	A1H10	O6B-C6	3.57	1.42	1.30
2	g	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	BA	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	LA	3	A1H1V	O6B-C6	3.57	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	6	4	A1H10	O6B-C6	3.57	1.42	1.30
2	q	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	2	4	A1H10	O6B-C6	3.57	1.42	1.30
2	9	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	z	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	0	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	5	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	8	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	EA	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	r	3	A1H1V	O6B-C6	3.57	1.42	1.30
2	i	4	A1H10	O6B-C6	3.57	1.42	1.30
2	l	4	A1H10	O6B-C6	3.57	1.42	1.30
2	v	4	A1H10	O6B-C6	3.57	1.42	1.30
2	7	4	A1H10	O6B-C6	3.57	1.42	1.30
2	IA	4	A1H10	O6B-C6	3.56	1.42	1.30
2	BA	4	A1H10	O6B-C6	3.56	1.42	1.30
2	g	4	A1H10	O6B-C6	3.56	1.42	1.30
2	y	4	A1H10	O6B-C6	3.56	1.42	1.30
2	q	4	A1H10	O6B-C6	3.56	1.42	1.30
2	CA	4	A1H10	O6B-C6	3.56	1.42	1.30
2	j	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	f	4	A1H10	O6B-C6	3.56	1.42	1.30
2	FA	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	u	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	DA	4	A1H10	O6B-C6	3.56	1.42	1.30
2	OA	4	A1H10	O6B-C6	3.56	1.42	1.30
2	o	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	w	4	A1H10	O6B-C6	3.56	1.42	1.30
2	x	4	A1H10	O6B-C6	3.56	1.42	1.30
2	HA	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	t	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	w	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	i	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	j	4	A1H10	O6B-C6	3.56	1.42	1.30
2	n	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	4	4	A1H10	O6B-C6	3.56	1.42	1.30
2	2	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	CA	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	a	4	A1H10	O6B-C6	3.56	1.42	1.30
2	6	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	JA	4	A1H10	O6B-C6	3.56	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	4	A1H10	O6B-C6	3.56	1.42	1.30
2	u	4	A1H10	O6B-C6	3.56	1.42	1.30
2	s	4	A1H10	O6B-C6	3.56	1.42	1.30
2	AA	3	A1H1V	O6B-C6	3.56	1.42	1.30
2	EA	4	A1H10	O6B-C6	3.56	1.42	1.30
2	c	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	NA	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	m	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	3	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	MA	4	A1H10	O6B-C6	3.55	1.42	1.30
2	8	4	A1H10	O6B-C6	3.55	1.42	1.30
2	e	4	A1H10	O6B-C6	3.55	1.42	1.30
2	n	4	A1H10	O6B-C6	3.55	1.42	1.30
2	s	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	p	4	A1H10	O6B-C6	3.55	1.42	1.30
2	b	4	A1H10	O6B-C6	3.55	1.42	1.30
2	KA	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	KA	4	A1H10	O6B-C6	3.55	1.42	1.30
2	k	4	A1H10	O6B-C6	3.55	1.42	1.30
2	PA	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	GA	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	l	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	OA	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	MA	3	A1H1V	O6B-C6	3.55	1.42	1.30
2	NA	4	A1H10	O6B-C6	3.55	1.42	1.30
2	1	4	A1H10	O6B-C6	3.54	1.42	1.30
2	e	3	A1H1V	O6B-C6	3.54	1.42	1.30
2	h	3	A1H1V	O6B-C6	3.54	1.42	1.30
2	7	3	A1H1V	O6B-C6	3.54	1.42	1.30
2	a	3	A1H1V	O6B-C6	3.54	1.42	1.30
2	AA	4	A1H10	O6B-C6	3.54	1.42	1.30
2	v	3	A1H1V	O6B-C6	3.54	1.42	1.30
2	IA	3	A1H1V	O6B-C6	3.54	1.42	1.30
2	x	3	A1H1V	O6B-C6	3.53	1.42	1.30
2	b	3	A1H1V	O6B-C6	3.52	1.42	1.30
2	q	4	A1H10	O6A-C6	2.56	1.29	1.22
2	KA	4	A1H10	O6A-C6	2.56	1.29	1.22
2	IA	4	A1H10	O6A-C6	2.56	1.29	1.22
2	v	4	A1H10	O6A-C6	2.56	1.29	1.22
2	KA	3	A1H1V	O6A-C6	2.56	1.29	1.22
2	b	3	A1H1V	O6A-C6	2.55	1.29	1.22
2	BA	4	A1H10	O6A-C6	2.55	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8	3	A1H1V	O6A-C6	2.55	1.29	1.22
2	MA	4	A1H10	O6A-C6	2.55	1.29	1.22
2	5	3	A1H1V	O6A-C6	2.55	1.29	1.22
2	7	4	A1H10	O6A-C6	2.55	1.29	1.22
2	3	4	A1H10	O6A-C6	2.55	1.29	1.22
2	6	4	A1H10	O6A-C6	2.55	1.29	1.22
2	w	4	A1H10	O6A-C6	2.54	1.29	1.22
2	h	3	A1H1V	O6A-C6	2.54	1.29	1.22
2	q	3	A1H1V	O6A-C6	2.54	1.29	1.22
2	r	4	A1H10	O6A-C6	2.54	1.29	1.22
2	u	3	A1H1V	O6A-C6	2.54	1.29	1.22
2	f	4	A1H10	O6A-C6	2.54	1.29	1.22
2	a	4	A1H10	O6A-C6	2.54	1.29	1.22
2	s	4	A1H10	O6A-C6	2.54	1.29	1.22
2	h	4	A1H10	O6A-C6	2.54	1.29	1.22
2	JA	4	A1H10	O6A-C6	2.54	1.29	1.22
2	k	4	A1H10	O6A-C6	2.54	1.29	1.22
2	i	4	A1H10	O6A-C6	2.54	1.29	1.22
2	t	4	A1H10	O6A-C6	2.54	1.29	1.22
2	0	4	A1H10	O6A-C6	2.54	1.29	1.22
2	8	4	A1H10	O6A-C6	2.54	1.29	1.22
2	CA	3	A1H1V	O6A-C6	2.54	1.29	1.22
2	n	4	A1H10	O6A-C6	2.54	1.29	1.22
2	EA	4	A1H10	O6A-C6	2.54	1.29	1.22
2	GA	4	A1H10	O6A-C6	2.54	1.29	1.22
2	e	4	A1H10	O6A-C6	2.53	1.29	1.22
2	BA	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	x	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	9	4	A1H10	O6A-C6	2.53	1.29	1.22
2	HA	4	A1H10	O6A-C6	2.53	1.29	1.22
2	OA	4	A1H10	O6A-C6	2.53	1.29	1.22
2	AA	4	A1H10	O6A-C6	2.53	1.29	1.22
2	g	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	n	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	NA	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	p	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	1	4	A1H10	O6A-C6	2.53	1.29	1.22
2	3	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	e	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	i	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	r	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	l	4	A1H10	O6A-C6	2.53	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	y	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	4	4	A1H10	O6A-C6	2.53	1.29	1.22
2	p	4	A1H10	O6A-C6	2.53	1.29	1.22
2	v	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	9	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	o	4	A1H10	O6A-C6	2.53	1.29	1.22
2	4	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	y	4	A1H10	O6A-C6	2.53	1.29	1.22
2	PA	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	z	3	A1H1V	O6A-C6	2.53	1.29	1.22
2	c	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	j	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	2	4	A1H10	O6A-C6	2.52	1.29	1.22
2	7	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	c	4	A1H10	O6A-C6	2.52	1.29	1.22
2	u	4	A1H10	O6A-C6	2.52	1.29	1.22
2	MA	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	g	4	A1H10	O6A-C6	2.52	1.29	1.22
2	HA	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	m	4	A1H10	O6A-C6	2.52	1.29	1.22
2	z	4	A1H10	O6A-C6	2.52	1.29	1.22
2	OA	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	x	4	A1H10	O6A-C6	2.52	1.29	1.22
2	a	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	j	4	A1H10	O6A-C6	2.52	1.29	1.22
2	5	4	A1H10	O6A-C6	2.52	1.29	1.22
2	CA	4	A1H10	O6A-C6	2.52	1.29	1.22
2	k	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	m	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	FA	4	A1H10	O6A-C6	2.52	1.29	1.22
2	1	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	AA	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	f	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	2	3	A1H1V	O6A-C6	2.52	1.29	1.22
2	LA	4	A1H10	O6A-C6	2.51	1.29	1.22
2	GA	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	d	4	A1H10	O6A-C6	2.51	1.29	1.22
2	IA	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	NA	4	A1H10	O6A-C6	2.51	1.29	1.22
2	l	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	s	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	EA	3	A1H1V	O6A-C6	2.51	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	LA	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	JA	3	A1H1V	O6A-C6	2.51	1.29	1.22
2	b	4	A1H10	O6A-C6	2.50	1.29	1.22
2	DA	3	A1H1V	O6A-C6	2.50	1.29	1.22
2	d	3	A1H1V	O6A-C6	2.50	1.29	1.22
2	FA	3	A1H1V	O6A-C6	2.50	1.29	1.22
2	PA	4	A1H10	O6A-C6	2.50	1.29	1.22
2	o	3	A1H1V	O6A-C6	2.50	1.29	1.22
2	0	3	A1H1V	O6A-C6	2.50	1.29	1.22
2	w	3	A1H1V	O6A-C6	2.50	1.29	1.22
2	DA	4	A1H10	O6A-C6	2.49	1.29	1.22
2	t	3	A1H1V	O6A-C6	2.48	1.29	1.22
2	5	4	A1H10	O2-C2	-2.41	1.43	1.47
2	0	4	A1H10	O2-C2	-2.40	1.43	1.47
2	q	4	A1H10	O2-C2	-2.40	1.43	1.47
2	k	4	A1H10	O2-C2	-2.40	1.43	1.47
2	4	4	A1H10	O2-C2	-2.39	1.43	1.47
2	a	4	A1H10	O2-C2	-2.39	1.43	1.47
2	DA	4	A1H10	O2-C2	-2.39	1.43	1.47
2	y	4	A1H10	O2-C2	-2.38	1.43	1.47
2	w	4	A1H10	O2-C2	-2.38	1.43	1.47
2	m	4	A1H10	O2-C2	-2.38	1.43	1.47
2	CA	4	A1H10	O2-C2	-2.38	1.43	1.47
2	3	4	A1H10	O2-C2	-2.37	1.43	1.47
2	7	4	A1H10	O2-C2	-2.37	1.43	1.47
2	z	4	A1H10	O2-C2	-2.37	1.43	1.47
2	9	4	A1H10	O2-C2	-2.37	1.43	1.47
2	AA	4	A1H10	O2-C2	-2.37	1.43	1.47
2	v	4	A1H10	O2-C2	-2.37	1.43	1.47
2	f	4	A1H10	O2-C2	-2.37	1.43	1.47
2	i	4	A1H10	O2-C2	-2.37	1.43	1.47
2	JA	4	A1H10	O2-C2	-2.37	1.43	1.47
2	e	4	A1H10	O2-C2	-2.37	1.43	1.47
2	6	4	A1H10	O2-C2	-2.37	1.43	1.47
2	x	4	A1H10	O2-C2	-2.37	1.43	1.47
2	OA	4	A1H10	O2-C2	-2.37	1.43	1.47
2	LA	4	A1H10	O2-C2	-2.36	1.43	1.47
2	8	4	A1H10	O2-C2	-2.35	1.43	1.47
2	2	4	A1H10	O2-C2	-2.35	1.43	1.47
2	GA	4	A1H10	O2-C2	-2.35	1.43	1.47
2	IA	4	A1H10	O2-C2	-2.35	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	KA	4	A1H10	O2-C2	-2.35	1.43	1.47
2	n	4	A1H10	O2-C2	-2.35	1.43	1.47
2	b	4	A1H10	O2-C2	-2.34	1.43	1.47
2	o	4	A1H10	O2-C2	-2.34	1.43	1.47
2	j	4	A1H10	O2-C2	-2.34	1.43	1.47
2	u	4	A1H10	O2-C2	-2.34	1.43	1.47
2	FA	4	A1H10	O2-C2	-2.34	1.43	1.47
2	BA	4	A1H10	O2-C2	-2.34	1.43	1.47
2	NA	4	A1H10	O2-C2	-2.34	1.43	1.47
2	a	3	A1H1V	O24-S1	2.34	1.55	1.45
2	4	3	A1H1V	O24-S1	2.34	1.55	1.45
2	KA	3	A1H1V	O24-S1	2.34	1.55	1.45
2	1	4	A1H10	O2-C2	-2.34	1.43	1.47
2	HA	4	A1H10	O2-C2	-2.33	1.43	1.47
2	i	3	A1H1V	O24-S1	2.33	1.55	1.45
2	k	3	A1H1V	O24-S1	2.33	1.55	1.45
2	7	3	A1H1V	O24-S1	2.33	1.55	1.45
2	8	3	A1H1V	O24-S1	2.33	1.55	1.45
2	MA	3	A1H1V	O24-S1	2.33	1.55	1.45
2	y	3	A1H1V	O24-S1	2.33	1.55	1.45
2	o	3	A1H1V	O24-S1	2.33	1.55	1.45
2	2	3	A1H1V	O24-S1	2.33	1.55	1.45
2	0	3	A1H1V	O24-S1	2.33	1.55	1.45
2	q	3	A1H1V	O24-S1	2.32	1.55	1.45
2	g	3	A1H1V	O24-S1	2.32	1.55	1.45
2	w	3	A1H1V	O24-S1	2.32	1.55	1.45
2	p	4	A1H10	O2-C2	-2.32	1.43	1.47
2	AA	3	A1H1V	O24-S1	2.32	1.55	1.45
2	r	4	A1H10	O2-C2	-2.32	1.43	1.47
2	t	4	A1H10	O2-C2	-2.32	1.43	1.47
2	c	3	A1H1V	O24-S1	2.32	1.55	1.45
2	s	3	A1H1V	O24-S1	2.32	1.55	1.45
2	m	3	A1H1V	O24-S1	2.32	1.55	1.45
2	g	4	A1H10	O2-C2	-2.32	1.43	1.47
2	EA	3	A1H1V	O24-S1	2.32	1.55	1.45
2	c	4	A1H10	O2-C2	-2.32	1.43	1.47
2	u	3	A1H1V	O24-S1	2.32	1.55	1.45
2	e	3	A1H1V	O24-S1	2.32	1.55	1.45
2	CA	3	A1H1V	O24-S1	2.32	1.55	1.45
2	s	4	A1H10	O2-C2	-2.32	1.43	1.47
2	OA	3	A1H1V	O24-S1	2.31	1.55	1.45
2	GA	3	A1H1V	O24-S1	2.31	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	4	A1H10	O2-C2	-2.31	1.43	1.47
2	BA	3	A1H1V	O24-S1	2.31	1.55	1.45
2	6	3	A1H1V	O24-S1	2.31	1.55	1.45
2	h	4	A1H10	O2-C2	-2.30	1.43	1.47
2	IA	3	A1H1V	O24-S1	2.30	1.55	1.45
2	l	4	A1H10	O2-C2	-2.30	1.43	1.47
2	k	4	A1H10	O2S-S	2.30	1.55	1.45
2	m	4	A1H10	O2S-S	2.29	1.55	1.45
2	t	4	A1H10	O2S-S	2.29	1.55	1.45
2	i	4	A1H10	O2S-S	2.29	1.55	1.45
2	MA	4	A1H10	O2-C2	-2.29	1.43	1.47
2	w	4	A1H10	O2S-S	2.29	1.55	1.45
2	MA	4	A1H10	O2S-S	2.29	1.55	1.45
2	BA	4	A1H10	O2S-S	2.29	1.55	1.45
2	g	4	A1H10	O2S-S	2.29	1.55	1.45
2	FA	4	A1H10	O2S-S	2.29	1.55	1.45
2	PA	4	A1H10	O2-C2	-2.29	1.43	1.47
2	EA	4	A1H10	O2S-S	2.29	1.55	1.45
2	2	4	A1H10	O2S-S	2.29	1.55	1.45
2	n	4	A1H10	O2S-S	2.28	1.55	1.45
2	IA	4	A1H10	O2S-S	2.28	1.55	1.45
2	AA	4	A1H10	O2S-S	2.28	1.55	1.45
2	6	4	A1H10	O2S-S	2.28	1.55	1.45
2	EA	4	A1H10	O2-C2	-2.28	1.43	1.47
2	GA	4	A1H10	O2S-S	2.28	1.55	1.45
2	PA	4	A1H10	O2S-S	2.28	1.55	1.45
2	LA	4	A1H10	O2S-S	2.28	1.55	1.45
2	l	4	A1H10	O2S-S	2.28	1.55	1.45
2	DA	4	A1H10	O2S-S	2.28	1.55	1.45
2	e	4	A1H10	O2S-S	2.28	1.55	1.45
2	9	4	A1H10	O2S-S	2.28	1.55	1.45
2	NA	4	A1H10	O2S-S	2.28	1.55	1.45
2	x	4	A1H10	O2S-S	2.28	1.55	1.45
2	y	4	A1H10	O2S-S	2.28	1.55	1.45
2	b	4	A1H10	O2S-S	2.28	1.55	1.45
2	l	4	A1H10	O2S-S	2.28	1.55	1.45
2	3	4	A1H10	O2S-S	2.28	1.55	1.45
2	q	4	A1H10	O2S-S	2.28	1.55	1.45
2	CA	4	A1H10	O2S-S	2.28	1.55	1.45
2	f	4	A1H10	O2S-S	2.28	1.55	1.45
2	4	4	A1H10	O2S-S	2.28	1.55	1.45
2	p	4	A1H10	O2S-S	2.28	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	4	A1H10	O2S-S	2.27	1.55	1.45
2	s	4	A1H10	O2S-S	2.27	1.55	1.45
2	r	4	A1H10	O2S-S	2.27	1.55	1.45
2	0	4	A1H10	O2S-S	2.27	1.55	1.45
2	z	4	A1H10	O2S-S	2.27	1.55	1.45
2	c	4	A1H10	O2S-S	2.27	1.55	1.45
2	HA	4	A1H10	O2S-S	2.27	1.55	1.45
2	a	4	A1H10	O2S-S	2.27	1.55	1.45
2	OA	4	A1H10	O2S-S	2.27	1.55	1.45
2	v	4	A1H10	O2S-S	2.27	1.55	1.45
2	o	4	A1H10	O2S-S	2.27	1.55	1.45
2	u	4	A1H10	O2S-S	2.27	1.55	1.45
2	j	4	A1H10	O2S-S	2.27	1.55	1.45
2	7	4	A1H10	O2S-S	2.27	1.55	1.45
2	KA	4	A1H10	O2S-S	2.27	1.55	1.45
2	JA	4	A1H10	O2S-S	2.26	1.55	1.45
2	5	4	A1H10	O2S-S	2.26	1.55	1.45
2	8	4	A1H10	O2S-S	2.26	1.55	1.45
2	h	4	A1H10	O2S-S	2.26	1.54	1.45

All (536) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	4	A1H10	C2-O2-S	4.91	124.31	117.91
2	NA	4	A1H10	C2-O2-S	4.76	124.11	117.91
2	t	4	A1H10	C2-O2-S	4.71	124.06	117.91
2	h	4	A1H10	C2-O2-S	4.70	124.04	117.91
2	z	4	A1H10	C2-O2-S	4.69	124.03	117.91
2	PA	4	A1H10	C2-O2-S	4.68	124.02	117.91
2	r	1	BGC	O4-C4-C3	-4.67	99.56	110.35
2	AA	4	A1H10	C2-O2-S	4.65	123.98	117.91
2	v	4	A1H10	C2-O2-S	4.61	123.93	117.91
2	b	4	A1H10	C2-O2-S	4.60	123.91	117.91
2	r	4	A1H10	C2-O2-S	4.56	123.86	117.91
2	HA	4	A1H10	C2-O2-S	4.56	123.86	117.91
2	f	4	A1H10	C2-O2-S	4.55	123.85	117.91
2	l	4	A1H10	C2-O2-S	4.55	123.84	117.91
2	x	4	A1H10	C2-O2-S	4.55	123.84	117.91
2	JA	4	A1H10	C2-O2-S	4.54	123.83	117.91
2	DA	4	A1H10	C2-O2-S	4.53	123.82	117.91
2	n	4	A1H10	C2-O2-S	4.49	123.77	117.91
2	FA	4	A1H10	C2-O2-S	4.49	123.77	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LA	4	A1H10	C2-O2-S	4.48	123.76	117.91
2	j	4	A1H10	C2-O2-S	4.47	123.74	117.91
2	EA	4	A1H10	C2-O2-S	4.47	123.74	117.91
2	BA	4	A1H10	C2-O2-S	4.46	123.72	117.91
2	s	4	A1H10	C2-O2-S	4.44	123.70	117.91
2	3	4	A1H10	C2-O2-S	4.41	123.66	117.91
2	MA	4	A1H10	C2-O2-S	4.40	123.65	117.91
2	7	4	A1H10	C2-O2-S	4.38	123.62	117.91
2	p	4	A1H10	C2-O2-S	4.37	123.62	117.91
2	1	4	A1H10	C2-O2-S	4.37	123.61	117.91
2	9	4	A1H10	C2-O2-S	4.35	123.58	117.91
2	KA	4	A1H10	C2-O2-S	4.34	123.58	117.91
2	IA	4	A1H10	C2-O2-S	4.32	123.55	117.91
2	g	4	A1H10	C2-O2-S	4.28	123.49	117.91
2	5	4	A1H10	C2-O2-S	4.28	123.49	117.91
2	m	4	A1H10	C2-O2-S	4.22	123.41	117.91
2	c	4	A1H10	C2-O2-S	4.21	123.41	117.91
2	8	4	A1H10	C2-O2-S	4.13	123.30	117.91
2	6	4	A1H10	C2-O2-S	4.10	123.25	117.91
2	u	4	A1H10	C2-O2-S	4.08	123.23	117.91
2	o	4	A1H10	C2-O2-S	4.07	123.21	117.91
2	CA	4	A1H10	C2-O2-S	4.03	123.17	117.91
2	GA	4	A1H10	C2-O2-S	4.03	123.16	117.91
2	4	4	A1H10	C2-O2-S	4.00	123.13	117.91
2	e	4	A1H10	C2-O2-S	4.00	123.13	117.91
2	i	4	A1H10	C2-O2-S	3.99	123.11	117.91
2	OA	4	A1H10	C2-O2-S	3.99	123.11	117.91
2	k	4	A1H10	C2-O2-S	3.97	123.09	117.91
2	BA	1	BGC	O4-C4-C3	-3.95	101.23	110.35
2	a	4	A1H10	C2-O2-S	3.94	123.05	117.91
2	0	4	A1H10	C2-O2-S	3.77	122.83	117.91
2	6	2	BDP	O6B-C6-O6A	-3.76	115.55	124.09
2	1	3	A1H1V	O6B-C6-O6A	-3.76	115.56	124.09
2	2	4	A1H10	C2-O2-S	3.75	122.80	117.91
2	LA	2	BDP	O6B-C6-O6A	-3.74	115.59	124.09
2	4	4	A1H10	O6B-C6-O6A	-3.74	115.59	124.09
2	AA	3	A1H1V	O6B-C6-O6A	-3.74	115.60	124.09
2	9	3	A1H1V	O6B-C6-O6A	-3.73	115.62	124.09
2	o	2	BDP	O6B-C6-O6A	-3.73	115.62	124.09
2	n	3	A1H1V	O6B-C6-O6A	-3.73	115.62	124.09
2	e	2	BDP	O6B-C6-O6A	-3.73	115.62	124.09
2	i	2	BDP	O6B-C6-O6A	-3.73	115.63	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	w	4	A1H10	C2-O2-S	3.73	122.77	117.91
2	g	2	BDP	O6B-C6-O6A	-3.73	115.63	124.09
2	y	4	A1H10	C2-O2-S	3.72	122.77	117.91
2	DA	3	A1H1V	O6B-C6-O6A	-3.72	115.64	124.09
2	c	3	A1H1V	O6B-C6-O6A	-3.72	115.65	124.09
2	CA	3	A1H1V	O6B-C6-O6A	-3.72	115.65	124.09
2	a	3	A1H1V	O6B-C6-O6A	-3.72	115.65	124.09
2	3	3	A1H1V	O6B-C6-O6A	-3.72	115.65	124.09
2	1	4	A1H10	O6B-C6-O6A	-3.72	115.65	124.09
2	d	3	A1H1V	O6B-C6-O6A	-3.71	115.66	124.09
2	u	3	A1H1V	O6B-C6-O6A	-3.71	115.66	124.09
2	FA	4	A1H10	O6B-C6-O6A	-3.71	115.66	124.09
2	n	4	A1H10	O6B-C6-O6A	-3.71	115.66	124.09
2	z	3	A1H1V	O6B-C6-O6A	-3.71	115.66	124.09
2	AA	4	A1H10	O6B-C6-O6A	-3.71	115.67	124.09
2	HA	2	BDP	O6B-C6-O6A	-3.71	115.67	124.09
2	g	3	A1H1V	O6B-C6-O6A	-3.71	115.67	124.09
2	4	2	BDP	O6B-C6-O6A	-3.71	115.67	124.09
2	PA	2	BDP	O6B-C6-O6A	-3.71	115.67	124.09
2	h	4	A1H10	O6B-C6-O6A	-3.71	115.67	124.09
2	k	4	A1H10	O6B-C6-O6A	-3.71	115.67	124.09
2	IA	2	BDP	O6B-C6-O6A	-3.71	115.67	124.09
2	j	4	A1H10	O6B-C6-O6A	-3.71	115.68	124.09
2	q	3	A1H1V	O6B-C6-O6A	-3.71	115.68	124.09
2	3	4	A1H10	O6B-C6-O6A	-3.71	115.68	124.09
2	6	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.09
2	HA	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.09
2	d	2	BDP	O6B-C6-O6A	-3.70	115.68	124.09
2	h	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.09
2	MA	4	A1H10	O6B-C6-O6A	-3.70	115.68	124.09
2	JA	3	A1H1V	O6B-C6-O6A	-3.70	115.68	124.09
2	LA	4	A1H10	O6B-C6-O6A	-3.70	115.68	124.09
2	CA	4	A1H10	O6B-C6-O6A	-3.70	115.68	124.09
2	KA	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.09
2	m	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.09
2	p	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.09
2	4	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.09
2	q	4	A1H10	C2-O2-S	3.70	122.74	117.91
2	v	2	BDP	O6B-C6-O6A	-3.70	115.69	124.09
2	8	4	A1H10	O6B-C6-O6A	-3.70	115.69	124.09
2	NA	3	A1H1V	O6B-C6-O6A	-3.70	115.69	124.09
2	e	4	A1H10	O6B-C6-O6A	-3.70	115.69	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8	3	A1H1V	O6B-C6-O6A	-3.70	115.70	124.09
2	9	4	A1H10	O6B-C6-O6A	-3.69	115.70	124.09
2	j	2	BDP	O6B-C6-O6A	-3.69	115.70	124.09
2	p	4	A1H10	O6B-C6-O6A	-3.69	115.70	124.09
2	u	4	A1H10	O6B-C6-O6A	-3.69	115.70	124.09
2	p	2	BDP	O6B-C6-O6A	-3.69	115.70	124.09
2	BA	2	BDP	O6B-C6-O6A	-3.69	115.70	124.09
2	BA	4	A1H10	O6B-C6-O6A	-3.69	115.70	124.09
2	v	3	A1H1V	O6B-C6-O6A	-3.69	115.70	124.09
2	LA	3	A1H1V	O6B-C6-O6A	-3.69	115.70	124.09
2	HA	4	A1H10	O6B-C6-O6A	-3.69	115.71	124.09
2	JA	4	A1H10	O6B-C6-O6A	-3.69	115.71	124.09
2	t	3	A1H1V	O6B-C6-O6A	-3.69	115.71	124.09
2	m	2	BDP	O6B-C6-O6A	-3.69	115.71	124.09
2	l	3	A1H1V	O6B-C6-O6A	-3.69	115.72	124.09
2	GA	3	A1H1V	O6B-C6-O6A	-3.69	115.72	124.09
2	q	4	A1H10	O6B-C6-O6A	-3.69	115.72	124.09
2	w	2	BDP	O6B-C6-O6A	-3.69	115.72	124.09
2	JA	2	BDP	O6B-C6-O6A	-3.69	115.72	124.09
2	l	4	A1H10	O6B-C6-O6A	-3.69	115.72	124.09
2	n	2	BDP	O6B-C6-O6A	-3.69	115.72	124.09
2	h	2	BDP	O6B-C6-O6A	-3.69	115.72	124.09
2	0	3	A1H1V	O6B-C6-O6A	-3.68	115.72	124.09
2	s	2	BDP	O6B-C6-O6A	-3.68	115.72	124.09
2	w	3	A1H1V	O6B-C6-O6A	-3.68	115.72	124.09
2	0	4	A1H10	O6B-C6-O6A	-3.68	115.72	124.09
2	8	2	BDP	O6B-C6-O6A	-3.68	115.72	124.09
2	2	2	BDP	O6B-C6-O6A	-3.68	115.72	124.09
2	DA	2	BDP	O6B-C6-O6A	-3.68	115.72	124.09
2	BA	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.09
2	EA	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.09
2	FA	2	BDP	O6B-C6-O6A	-3.68	115.73	124.09
2	IA	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.09
2	f	3	A1H1V	O6B-C6-O6A	-3.68	115.73	124.09
2	o	4	A1H10	O6B-C6-O6A	-3.68	115.73	124.09
2	v	4	A1H10	O6B-C6-O6A	-3.68	115.73	124.09
2	y	3	A1H1V	O6B-C6-O6A	-3.68	115.74	124.09
2	FA	3	A1H1V	O6B-C6-O6A	-3.68	115.74	124.09
2	l	2	BDP	O6B-C6-O6A	-3.68	115.74	124.09
2	0	2	BDP	O6B-C6-O6A	-3.68	115.74	124.09
2	o	3	A1H1V	O6B-C6-O6A	-3.68	115.74	124.09
2	t	4	A1H10	O6B-C6-O6A	-3.68	115.74	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	4	A1H10	O6B-C6-O6A	-3.68	115.74	124.09
2	x	2	BDP	O6B-C6-O6A	-3.68	115.74	124.09
2	CA	2	BDP	O6B-C6-O6A	-3.68	115.74	124.09
2	PA	4	A1H10	O6B-C6-O6A	-3.68	115.74	124.09
2	a	4	A1H10	O6B-C6-O6A	-3.68	115.74	124.09
2	2	4	A1H10	O6B-C6-O6A	-3.68	115.74	124.09
2	IA	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	1	2	BDP	O6B-C6-O6A	-3.67	115.75	124.09
2	b	3	A1H1V	O6B-C6-O6A	-3.67	115.75	124.09
2	DA	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	GA	2	BDP	O6B-C6-O6A	-3.67	115.75	124.09
2	c	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	s	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	NA	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	g	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	w	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	z	2	BDP	O6B-C6-O6A	-3.67	115.75	124.09
2	OA	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	f	2	BDP	O6B-C6-O6A	-3.67	115.75	124.09
2	f	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	7	2	BDP	O6B-C6-O6A	-3.67	115.75	124.09
2	7	3	A1H1V	O6B-C6-O6A	-3.67	115.75	124.09
2	r	4	A1H10	O6B-C6-O6A	-3.67	115.75	124.09
2	q	2	BDP	O6B-C6-O6A	-3.67	115.76	124.09
2	y	2	BDP	O6B-C6-O6A	-3.67	115.76	124.09
2	a	2	BDP	O6B-C6-O6A	-3.67	115.76	124.09
2	r	3	A1H1V	O6B-C6-O6A	-3.67	115.76	124.09
2	PA	3	A1H1V	O6B-C6-O6A	-3.67	115.76	124.09
2	b	2	BDP	O6B-C6-O6A	-3.67	115.76	124.09
2	z	4	A1H10	O6B-C6-O6A	-3.67	115.76	124.09
2	MA	3	A1H1V	O6B-C6-O6A	-3.67	115.77	124.09
2	x	3	A1H1V	O6B-C6-O6A	-3.67	115.77	124.09
2	i	3	A1H1V	O6B-C6-O6A	-3.67	115.77	124.09
2	6	4	A1H10	O6B-C6-O6A	-3.67	115.77	124.09
2	9	2	BDP	O6B-C6-O6A	-3.66	115.77	124.09
2	GA	4	A1H10	O6B-C6-O6A	-3.66	115.77	124.09
2	y	4	A1H10	O6B-C6-O6A	-3.66	115.77	124.09
2	t	2	BDP	O6B-C6-O6A	-3.66	115.77	124.09
2	2	3	A1H1V	O6B-C6-O6A	-3.66	115.77	124.09
2	k	3	A1H1V	O6B-C6-O6A	-3.66	115.77	124.09
2	b	4	A1H10	O6B-C6-O6A	-3.66	115.77	124.09
2	d	4	A1H10	O6B-C6-O6A	-3.66	115.77	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4	A1H10	O6B-C6-O6A	-3.66	115.77	124.09
2	AA	2	BDP	O6B-C6-O6A	-3.66	115.77	124.09
2	KA	4	A1H10	O6B-C6-O6A	-3.66	115.78	124.09
2	5	3	A1H1V	O6B-C6-O6A	-3.66	115.78	124.09
2	7	4	A1H10	O6B-C6-O6A	-3.66	115.78	124.09
2	s	3	A1H1V	O6B-C6-O6A	-3.66	115.78	124.09
2	5	2	BDP	O6B-C6-O6A	-3.66	115.79	124.09
2	c	2	BDP	O6B-C6-O6A	-3.66	115.79	124.09
2	m	4	A1H10	O6B-C6-O6A	-3.66	115.79	124.09
2	EA	4	A1H10	O6B-C6-O6A	-3.66	115.79	124.09
2	j	3	A1H1V	O6B-C6-O6A	-3.65	115.79	124.09
2	e	3	A1H1V	O6B-C6-O6A	-3.65	115.80	124.09
2	i	4	A1H10	O6B-C6-O6A	-3.65	115.80	124.09
2	OA	2	BDP	O6B-C6-O6A	-3.65	115.80	124.09
2	NA	2	BDP	O6B-C6-O6A	-3.65	115.81	124.09
2	OA	3	A1H1V	O6B-C6-O6A	-3.64	115.82	124.09
2	EA	2	BDP	O6B-C6-O6A	-3.64	115.83	124.09
2	MA	2	BDP	O6B-C6-O6A	-3.64	115.83	124.09
2	r	2	BDP	O6B-C6-O6A	-3.63	115.84	124.09
2	3	2	BDP	O6B-C6-O6A	-3.63	115.84	124.09
2	k	2	BDP	O6B-C6-O6A	-3.63	115.85	124.09
2	KA	2	BDP	O6B-C6-O6A	-3.62	115.86	124.09
2	u	2	BDP	O6B-C6-O6A	-3.57	115.97	124.09
2	j	3	A1H1V	C1-C2-C3	3.44	113.33	109.17
2	t	3	A1H1V	C1-C2-C3	3.42	113.30	109.17
2	1	2	BDP	C3-C4-C5	3.29	114.88	109.25
2	DA	3	A1H1V	C1-C2-C3	3.19	113.03	109.17
2	OA	2	BDP	C1-C2-C3	-3.16	105.78	109.67
2	BA	3	A1H1V	C1-C2-C3	3.15	112.98	109.17
2	r	3	A1H1V	C1-C2-C3	3.15	112.98	109.17
2	AA	3	A1H1V	C3-O3-S1	3.15	124.95	118.88
2	KA	3	A1H1V	C1-C2-C3	3.13	112.95	109.17
2	7	3	A1H1V	C1-C2-C3	3.10	112.92	109.17
2	e	3	A1H1V	C3-O3-S1	3.07	124.80	118.88
2	IA	3	A1H1V	C3-O3-S1	3.06	124.80	118.88
2	c	3	A1H1V	C3-O3-S1	3.06	124.79	118.88
2	OA	3	A1H1V	C3-O3-S1	3.05	124.77	118.88
2	l	3	A1H1V	C3-O3-S1	3.03	124.73	118.88
2	o	3	A1H1V	C3-O3-S1	3.02	124.71	118.88
2	d	3	A1H1V	C3-O3-S1	3.02	124.70	118.88
2	5	2	BDP	O4-C4-C5	-2.99	103.04	109.74
2	u	4	A1H10	O6A-C6-C5	-2.97	109.92	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3	A1H1V	O6A-C6-C5	-2.97	109.92	120.81
2	r	3	A1H1V	O6A-C6-C5	-2.96	109.95	120.81
2	OA	3	A1H1V	O6A-C6-C5	-2.96	109.96	120.81
2	KA	4	A1H10	O6A-C6-C5	-2.95	109.98	120.81
2	6	4	A1H10	O6A-C6-C5	-2.95	109.99	120.81
2	3	2	BDP	O4-C4-C5	-2.95	103.13	109.74
2	7	3	A1H1V	O6A-C6-C5	-2.95	110.00	120.81
2	BA	3	A1H1V	O6A-C6-C5	-2.95	110.00	120.81
2	a	3	A1H1V	O6A-C6-C5	-2.95	110.00	120.81
2	9	4	A1H10	O6A-C6-C5	-2.95	110.01	120.81
2	3	3	A1H1V	O6A-C6-C5	-2.94	110.01	120.81
2	9	2	BDP	C1-C2-C3	-2.94	106.05	109.67
2	w	3	A1H1V	O6A-C6-C5	-2.94	110.02	120.81
2	AA	4	A1H10	O6A-C6-C5	-2.94	110.02	120.81
2	5	4	A1H10	O6A-C6-C5	-2.94	110.02	120.81
2	a	4	A1H10	O6A-C6-C5	-2.94	110.02	120.81
2	w	4	A1H10	O6A-C6-C5	-2.94	110.02	120.81
2	9	3	A1H1V	O6A-C6-C5	-2.94	110.03	120.81
2	k	3	A1H1V	O6A-C6-C5	-2.94	110.04	120.81
2	n	3	A1H1V	O6A-C6-C5	-2.94	110.04	120.81
2	0	3	A1H1V	O6A-C6-C5	-2.94	110.04	120.81
2	IA	4	A1H10	O6A-C6-C5	-2.94	110.04	120.81
2	v	4	A1H10	O6A-C6-C5	-2.94	110.04	120.81
2	8	4	A1H10	O6A-C6-C5	-2.93	110.05	120.81
2	JA	4	A1H10	O6A-C6-C5	-2.93	110.05	120.81
2	EA	4	A1H10	O6A-C6-C5	-2.93	110.05	120.81
2	6	3	A1H1V	O6A-C6-C5	-2.93	110.05	120.81
2	GA	3	A1H1V	O6A-C6-C5	-2.93	110.05	120.81
2	2	4	A1H10	O6A-C6-C5	-2.93	110.06	120.81
2	y	4	A1H10	O6A-C6-C5	-2.93	110.06	120.81
2	CA	4	A1H10	O6A-C6-C5	-2.93	110.06	120.81
2	LA	3	A1H1V	O6A-C6-C5	-2.93	110.06	120.81
2	x	3	A1H1V	O6A-C6-C5	-2.93	110.07	120.81
2	b	3	A1H1V	O6A-C6-C5	-2.93	110.07	120.81
2	e	3	A1H1V	O6A-C6-C5	-2.93	110.08	120.81
2	e	4	A1H10	O6A-C6-C5	-2.93	110.08	120.81
2	l	3	A1H1V	O6A-C6-C5	-2.92	110.08	120.81
2	FA	3	A1H1V	O6A-C6-C5	-2.92	110.08	120.81
2	PA	3	A1H1V	O6A-C6-C5	-2.92	110.08	120.81
2	4	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	t	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	n	4	A1H10	O6A-C6-C5	-2.92	110.09	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	v	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	j	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	o	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	i	4	A1H10	O6A-C6-C5	-2.92	110.09	120.81
2	u	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	l	3	A1H1V	O6A-C6-C5	-2.92	110.09	120.81
2	JA	3	A1H1V	O6A-C6-C5	-2.92	110.10	120.81
2	g	3	A1H1V	C3-O3-S1	2.92	124.52	118.88
2	m	3	A1H1V	O6A-C6-C5	-2.92	110.10	120.81
2	g	4	A1H10	O6A-C6-C5	-2.92	110.10	120.81
2	s	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	x	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	z	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	l	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	HA	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	3	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	GA	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	f	4	A1H10	O6A-C6-C5	-2.92	110.11	120.81
2	4	4	A1H10	O6A-C6-C5	-2.92	110.12	120.81
2	NA	3	A1H1V	O6A-C6-C5	-2.91	110.12	120.81
2	b	4	A1H10	O6A-C6-C5	-2.91	110.12	120.81
2	8	3	A1H1V	O6A-C6-C5	-2.91	110.12	120.81
2	h	4	A1H10	O6A-C6-C5	-2.91	110.12	120.81
2	LA	4	A1H10	O6A-C6-C5	-2.91	110.13	120.81
2	DA	3	A1H1V	O6A-C6-C5	-2.91	110.13	120.81
2	EA	3	A1H1V	O6A-C6-C5	-2.91	110.13	120.81
2	DA	4	A1H10	O6A-C6-C5	-2.91	110.13	120.81
2	f	3	A1H1V	O6A-C6-C5	-2.91	110.13	120.81
2	2	3	A1H1V	O6A-C6-C5	-2.91	110.13	120.81
2	c	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	d	3	A1H1V	O6A-C6-C5	-2.91	110.14	120.81
2	MA	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	FA	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	k	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	NA	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	l	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	HA	3	A1H1V	C1-C2-C3	2.91	112.69	109.17
2	p	4	A1H10	O6A-C6-C5	-2.91	110.14	120.81
2	i	3	A1H1V	O6A-C6-C5	-2.91	110.15	120.81
2	p	3	A1H1V	O6A-C6-C5	-2.91	110.15	120.81
2	CA	3	A1H1V	O6A-C6-C5	-2.91	110.15	120.81
2	MA	3	A1H1V	O6A-C6-C5	-2.90	110.16	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	4	A1H10	O6A-C6-C5	-2.90	110.17	120.81
2	2	3	A1H1V	C3-O3-S1	2.90	124.48	118.88
2	d	4	A1H10	O6A-C6-C5	-2.90	110.17	120.81
2	8	3	A1H1V	C3-O3-S1	2.90	124.48	118.88
2	0	4	A1H10	O6A-C6-C5	-2.90	110.17	120.81
2	h	3	A1H1V	O6A-C6-C5	-2.90	110.18	120.81
2	AA	3	A1H1V	O6A-C6-C5	-2.90	110.18	120.81
2	BA	4	A1H10	O6A-C6-C5	-2.90	110.18	120.81
2	EA	3	A1H1V	C3-O3-S1	2.90	124.47	118.88
2	PA	4	A1H10	O6A-C6-C5	-2.90	110.18	120.81
2	o	4	A1H10	O6A-C6-C5	-2.90	110.18	120.81
2	c	3	A1H1V	O6A-C6-C5	-2.90	110.19	120.81
2	IA	3	A1H1V	O6A-C6-C5	-2.90	110.19	120.81
2	s	3	A1H1V	O6A-C6-C5	-2.90	110.19	120.81
2	OA	4	A1H10	O6A-C6-C5	-2.90	110.19	120.81
2	g	3	A1H1V	O6A-C6-C5	-2.90	110.19	120.81
2	HA	3	A1H1V	O6A-C6-C5	-2.90	110.19	120.81
2	m	4	A1H10	O6A-C6-C5	-2.89	110.21	120.81
2	z	3	A1H1V	O6A-C6-C5	-2.89	110.21	120.81
2	3	2	BDP	C1-C2-C3	-2.89	106.11	109.67
2	KA	3	A1H1V	O6A-C6-C5	-2.89	110.22	120.81
2	q	4	A1H10	O6A-C6-C5	-2.89	110.22	120.81
2	t	4	A1H10	O6A-C6-C5	-2.89	110.22	120.81
2	4	3	A1H1V	C3-O3-S1	2.88	124.45	118.88
2	y	3	A1H1V	O6A-C6-C5	-2.88	110.23	120.81
2	5	3	A1H1V	C1-C2-C3	2.88	112.66	109.17
2	PA	3	A1H1V	C3-O3-S1	2.88	124.44	118.88
2	r	4	A1H10	O6A-C6-C5	-2.88	110.24	120.81
2	w	3	A1H1V	C3-O3-S1	2.88	124.44	118.88
2	7	4	A1H10	O6A-C6-C5	-2.88	110.24	120.81
2	n	3	A1H1V	C3-O3-S1	2.88	124.43	118.88
2	h	3	A1H1V	C1-C2-C3	2.87	112.64	109.17
2	b	3	A1H1V	C3-O3-S1	2.87	124.41	118.88
2	q	3	A1H1V	O6A-C6-C5	-2.86	110.31	120.81
2	1	2	BDP	O4-C4-C5	-2.86	103.33	109.74
2	9	3	A1H1V	C1-C2-C3	2.85	112.62	109.17
2	LA	3	A1H1V	C1-C2-C3	2.83	112.59	109.17
2	3	3	A1H1V	C1-C2-C3	2.83	112.59	109.17
2	u	3	A1H1V	C3-O3-S1	2.82	124.33	118.88
2	1	3	A1H1V	C1-C2-C3	2.82	112.58	109.17
2	f	3	A1H1V	C3-O3-S1	2.81	124.31	118.88
2	1	3	A1H1V	C3-O3-S1	2.80	124.29	118.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	v	3	A1H1V	C1-C2-C3	2.80	112.56	109.17
2	r	2	BDP	O6A-C6-C5	-2.79	110.57	120.81
2	JA	3	A1H1V	C3-O3-S1	2.79	124.27	118.88
2	i	3	A1H1V	C3-O3-S1	2.79	124.26	118.88
2	CA	2	BDP	C1-C2-C3	-2.79	106.24	109.67
2	p	2	BDP	O6A-C6-C5	-2.79	110.59	120.81
2	j	3	A1H1V	C3-O3-S1	2.78	124.25	118.88
2	h	2	BDP	O6A-C6-C5	-2.78	110.62	120.81
2	q	2	BDP	O6A-C6-C5	-2.77	110.64	120.81
2	8	2	BDP	O6A-C6-C5	-2.77	110.64	120.81
2	FA	3	A1H1V	C1-C2-C3	2.77	112.52	109.17
2	NA	3	A1H1V	C3-O3-S1	2.77	124.23	118.88
2	k	2	BDP	C1-C2-C3	-2.77	106.26	109.67
2	m	3	A1H1V	C3-O3-S1	2.77	124.22	118.88
2	b	2	BDP	O6A-C6-C5	-2.76	110.67	120.81
2	6	3	A1H1V	C3-O3-S1	2.76	124.21	118.88
2	1	2	BDP	C1-C2-C3	-2.76	106.27	109.67
2	y	2	BDP	O6A-C6-C5	-2.76	110.70	120.81
2	p	1	BGC	O4-C4-C5	-2.76	102.45	109.30
2	i	3	A1H1V	C1-C2-C3	2.75	112.50	109.17
2	BA	2	BDP	O6A-C6-C5	-2.75	110.72	120.81
2	j	2	BDP	O6A-C6-C5	-2.75	110.73	120.81
2	m	2	BDP	O6A-C6-C5	-2.75	110.73	120.81
2	x	3	A1H1V	C1-C2-C3	2.75	112.49	109.17
2	KA	2	BDP	O6A-C6-C5	-2.74	110.75	120.81
2	GA	2	BDP	O6A-C6-C5	-2.74	110.76	120.81
2	HA	2	BDP	O6A-C6-C5	-2.74	110.76	120.81
2	g	2	BDP	O6A-C6-C5	-2.74	110.76	120.81
2	LA	3	A1H1V	C3-O3-S1	2.74	124.17	118.88
2	9	2	BDP	O6A-C6-C5	-2.74	110.76	120.81
2	n	2	BDP	O6A-C6-C5	-2.74	110.77	120.81
2	CA	3	A1H1V	C3-O3-S1	2.74	124.16	118.88
2	l	2	BDP	O6A-C6-C5	-2.73	110.78	120.81
2	5	2	BDP	O6A-C6-C5	-2.73	110.78	120.81
2	9	2	BDP	O4-C4-C5	-2.73	103.61	109.74
2	w	2	BDP	O6A-C6-C5	-2.73	110.78	120.81
2	7	2	BDP	O6A-C6-C5	-2.73	110.78	120.81
2	z	3	A1H1V	C3-O3-S1	2.73	124.15	118.88
2	MA	2	BDP	O6A-C6-C5	-2.73	110.79	120.81
2	z	2	BDP	O6A-C6-C5	-2.73	110.80	120.81
2	CA	2	BDP	O6A-C6-C5	-2.73	110.80	120.81
2	i	2	BDP	O6A-C6-C5	-2.73	110.80	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	JA	2	BDP	O6A-C6-C5	-2.73	110.80	120.81
2	OA	2	BDP	O6A-C6-C5	-2.73	110.81	120.81
2	NA	2	BDP	O6A-C6-C5	-2.73	110.81	120.81
2	6	2	BDP	O6A-C6-C5	-2.72	110.82	120.81
2	s	2	BDP	O6A-C6-C5	-2.72	110.82	120.81
2	x	2	BDP	O6A-C6-C5	-2.72	110.82	120.81
2	2	2	BDP	O6A-C6-C5	-2.72	110.83	120.81
2	4	2	BDP	O6A-C6-C5	-2.72	110.84	120.81
2	0	2	BDP	O6A-C6-C5	-2.72	110.85	120.81
2	PA	2	BDP	O6A-C6-C5	-2.72	110.85	120.81
2	t	2	BDP	O6A-C6-C5	-2.72	110.85	120.81
2	u	2	BDP	O6A-C6-C5	-2.71	110.85	120.81
2	AA	2	BDP	O6A-C6-C5	-2.71	110.85	120.81
2	FA	3	A1H1V	C3-O3-S1	2.71	124.12	118.88
2	c	2	BDP	O6A-C6-C5	-2.71	110.86	120.81
2	v	3	A1H1V	C3-O3-S1	2.71	124.11	118.88
2	DA	2	BDP	O6A-C6-C5	-2.71	110.87	120.81
2	p	3	A1H1V	C1-C2-C3	2.71	112.45	109.17
2	o	2	BDP	O6A-C6-C5	-2.71	110.88	120.81
2	h	3	A1H1V	C3-O3-S1	2.71	124.10	118.88
2	1	2	BDP	O6A-C6-C5	-2.70	110.89	120.81
2	x	3	A1H1V	C3-O3-S1	2.70	124.10	118.88
2	k	2	BDP	O6A-C6-C5	-2.70	110.89	120.81
2	EA	2	BDP	O6A-C6-C5	-2.70	110.89	120.81
2	b	3	A1H1V	C1-C2-C3	2.70	112.44	109.17
2	MA	3	A1H1V	C3-O3-S1	2.70	124.09	118.88
2	e	2	BDP	O6A-C6-C5	-2.70	110.91	120.81
2	d	2	BDP	O6A-C6-C5	-2.70	110.91	120.81
2	3	2	BDP	O6A-C6-C5	-2.70	110.91	120.81
2	f	2	BDP	O6A-C6-C5	-2.70	110.92	120.81
2	FA	2	BDP	O6A-C6-C5	-2.69	110.95	120.81
2	v	2	BDP	O6A-C6-C5	-2.69	110.95	120.81
2	a	2	BDP	O6A-C6-C5	-2.68	110.96	120.81
2	IA	2	BDP	O6A-C6-C5	-2.68	110.97	120.81
2	s	3	A1H1V	C1-C2-C3	2.68	112.41	109.17
2	LA	2	BDP	O6A-C6-C5	-2.67	111.03	120.81
2	a	3	A1H1V	C3-O3-S1	2.66	124.02	118.88
2	GA	3	A1H1V	C3-O3-S1	2.66	124.01	118.88
2	q	3	A1H1V	C3-O3-S1	2.66	124.01	118.88
2	k	3	A1H1V	C3-O3-S1	2.64	123.97	118.88
2	BA	3	A1H1V	C3-O3-S1	2.63	123.95	118.88
2	t	3	A1H1V	C3-O3-S1	2.62	123.94	118.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	2	BDP	C3-C4-C5	2.62	113.73	109.25
2	HA	3	A1H1V	C3-O3-S1	2.62	123.93	118.88
2	z	3	A1H1V	C1-C2-C3	2.62	112.34	109.17
2	DA	3	A1H1V	C3-O3-S1	2.62	123.93	118.88
2	s	3	A1H1V	C3-O3-S1	2.61	123.93	118.88
2	0	3	A1H1V	C1-C2-C3	2.59	112.30	109.17
2	PA	3	A1H1V	C1-C2-C3	2.57	112.28	109.17
2	9	3	A1H1V	C3-O3-S1	2.57	123.84	118.88
2	n	3	A1H1V	C1-C2-C3	2.56	112.26	109.17
2	p	2	BDP	C3-C4-C5	2.53	113.57	109.25
2	7	3	A1H1V	C3-O3-S1	2.53	123.75	118.88
2	l	3	A1H1V	C1-C2-C3	2.52	112.22	109.17
2	y	3	A1H1V	C3-O3-S1	2.52	123.74	118.88
2	8	3	A1H1V	C1-C2-C3	2.51	112.20	109.17
2	5	3	A1H1V	C3-O3-S1	2.48	123.68	118.88
2	p	3	A1H1V	C3-O3-S1	2.48	123.67	118.88
2	3	3	A1H1V	C3-O3-S1	2.47	123.64	118.88
2	9	2	BDP	C3-C4-C5	2.47	113.46	109.25
2	JA	3	A1H1V	C1-C2-C3	2.46	112.15	109.17
2	KA	3	A1H1V	C3-O3-S1	2.46	123.62	118.88
2	o	3	A1H1V	C1-C2-C3	2.45	112.14	109.17
2	r	1	BGC	O4-C4-C5	2.45	115.39	109.30
2	r	3	A1H1V	C3-O3-S1	2.45	123.61	118.88
2	5	1	BGC	O4-C4-C5	-2.45	103.21	109.30
2	4	2	BDP	C1-C2-C3	-2.45	106.66	109.67
2	0	3	A1H1V	C3-O3-S1	2.45	123.60	118.88
2	OA	2	BDP	O4-C4-C5	-2.44	104.26	109.74
2	5	2	BDP	C1-C2-C3	-2.44	106.66	109.67
2	d	3	A1H1V	C1-C2-C3	2.42	112.10	109.17
2	e	3	A1H1V	C1-C2-C3	2.40	112.07	109.17
2	p	2	BDP	O4-C4-C5	-2.40	104.37	109.74
2	u	3	A1H1V	C1-C2-C3	2.39	112.06	109.17
2	2	3	A1H1V	C1-C2-C3	2.39	112.06	109.17
2	9	1	BGC	O4-C4-C3	-2.38	104.85	110.35
2	MA	3	A1H1V	C1-C2-C3	2.37	112.04	109.17
2	EA	3	A1H1V	C1-C2-C3	2.37	112.03	109.17
2	u	2	BDP	C1-C2-C3	-2.36	106.76	109.67
2	a	3	A1H1V	C1-C2-C3	2.35	112.01	109.17
2	NA	3	A1H1V	C1-C2-C3	2.34	112.01	109.17
2	f	3	A1H1V	C1-C2-C3	2.34	112.00	109.17
2	y	3	A1H1V	O22-S1-O23	2.34	116.61	108.49
2	c	2	BDP	O4-C4-C5	-2.33	104.51	109.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	3	A1H1V	O22-S1-O23	2.33	116.60	108.49
2	q	3	A1H1V	O22-S1-O23	2.33	116.60	108.49
2	0	3	A1H1V	O22-S1-O23	2.33	116.59	108.49
2	k	3	A1H1V	O22-S1-O23	2.33	116.59	108.49
2	GA	3	A1H1V	O22-S1-O23	2.33	116.58	108.49
2	2	3	A1H1V	O22-S1-O23	2.32	116.55	108.49
2	6	3	A1H1V	C1-C2-C3	2.31	111.97	109.17
2	m	3	A1H1V	O22-S1-O23	2.31	116.51	108.49
2	w	3	A1H1V	O22-S1-O23	2.30	116.49	108.49
2	i	3	A1H1V	O22-S1-O23	2.29	116.47	108.49
2	o	2	BDP	C1-C2-C3	-2.29	106.85	109.67
2	MA	3	A1H1V	O22-S1-O23	2.29	116.45	108.49
2	KA	3	A1H1V	O22-S1-O23	2.29	116.44	108.49
2	CA	3	A1H1V	O22-S1-O23	2.29	116.44	108.49
2	CA	3	A1H1V	C1-C2-C3	2.28	111.94	109.17
2	w	3	A1H1V	C1-C2-C3	2.28	111.93	109.17
2	s	3	A1H1V	O22-S1-O23	2.27	116.38	108.49
2	6	3	A1H1V	O22-S1-O23	2.27	116.37	108.49
2	g	3	A1H1V	O22-S1-O23	2.26	116.35	108.49
2	e	3	A1H1V	O22-S1-O23	2.25	116.30	108.49
2	OA	3	A1H1V	O22-S1-O23	2.24	116.29	108.49
2	p	2	BDP	C1-C2-C3	-2.24	106.91	109.67
2	EA	3	A1H1V	O22-S1-O23	2.24	116.28	108.49
2	c	3	A1H1V	O22-S1-O23	2.24	116.28	108.49
2	GA	3	A1H1V	C1-C2-C3	2.23	111.87	109.17
2	o	3	A1H1V	O22-S1-O23	2.23	116.24	108.49
2	BA	3	A1H1V	O22-S1-O23	2.23	116.22	108.49
2	IA	3	A1H1V	O22-S1-O23	2.21	116.17	108.49
2	8	3	A1H1V	O22-S1-O23	2.21	116.17	108.49
2	7	3	A1H1V	O22-S1-O23	2.21	116.16	108.49
2	4	3	A1H1V	O22-S1-O23	2.21	116.16	108.49
2	k	2	BDP	O4-C4-C5	-2.20	104.80	109.74
2	u	3	A1H1V	O22-S1-O23	2.20	116.15	108.49
2	AA	3	A1H1V	C1-C2-C3	2.20	111.84	109.17
2	OA	3	A1H1V	C1-C2-C3	2.20	111.83	109.17
2	k	3	A1H1V	C1-C2-C3	2.19	111.83	109.17
2	q	3	A1H1V	C1-C2-C3	2.17	111.80	109.17
2	6	2	BDP	C1-C2-C3	-2.16	107.01	109.67
2	KA	2	BDP	C1-C2-C3	-2.16	107.02	109.67
2	y	2	BDP	O4-C4-C3	2.15	115.32	110.35
2	AA	3	A1H1V	O22-S1-O23	2.15	115.95	108.49
2	m	3	A1H1V	C1-C2-C3	2.14	111.76	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	y	3	A1H1V	C1-C2-C3	2.13	111.75	109.17
2	4	3	A1H1V	C1-C2-C3	2.13	111.75	109.17
2	q	2	BDP	O4-C4-C5	-2.13	104.97	109.74
2	r	1	BGC	O5-C1-C2	-2.11	107.51	110.77
2	4	2	BDP	O4-C4-C5	-2.11	105.01	109.74
2	IA	3	A1H1V	C1-C2-C3	2.09	111.70	109.17
2	BA	1	BGC	O4-C4-C5	2.07	114.44	109.30
2	g	3	A1H1V	C1-C2-C3	2.05	111.65	109.17
2	BA	1	BGC	O5-C1-C2	-2.04	107.62	110.77
2	p	1	BGC	O3-C3-C2	-2.03	106.11	109.99
2	p	2	BDP	O3-C3-C2	-2.03	106.11	109.99
2	MA	2	BDP	O4-C4-C3	2.03	115.03	110.35
2	a	2	BDP	C1-C2-C3	-2.02	107.19	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	OA	1	BGC	C1

All (363) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	a	4	A1H10	C1-C2-O2-S
2	a	4	A1H10	C3-C2-O2-S
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	b	4	A1H10	C1-C2-O2-S
2	b	4	A1H10	C3-C2-O2-S
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	c	4	A1H10	C1-C2-O2-S
2	c	4	A1H10	C3-C2-O2-S
2	d	2	BDP	C4-C5-C6-O6B
2	d	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	d	3	A1H1V	C4-C3-O3-S1
2	d	3	A1H1V	C2-C3-O3-S1
2	d	4	A1H10	C1-C2-O2-S
2	d	4	A1H10	C3-C2-O2-S
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	e	4	A1H10	C1-C2-O2-S
2	e	4	A1H10	C3-C2-O2-S
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	f	4	A1H10	C1-C2-O2-S
2	f	4	A1H10	C3-C2-O2-S
2	g	2	BDP	C4-C5-C6-O6B
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	g	4	A1H10	C1-C2-O2-S
2	g	4	A1H10	C3-C2-O2-S
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	h	4	A1H10	C1-C2-O2-S
2	h	4	A1H10	C3-C2-O2-S
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	i	4	A1H10	C1-C2-O2-S
2	i	4	A1H10	C3-C2-O2-S
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	j	4	A1H10	C1-C2-O2-S
2	j	4	A1H10	C3-C2-O2-S
2	k	2	BDP	C4-C5-C6-O6B
2	k	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	k	3	A1H1V	C4-C3-O3-S1
2	k	3	A1H1V	C2-C3-O3-S1
2	k	4	A1H10	C1-C2-O2-S
2	k	4	A1H10	C3-C2-O2-S
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	l	4	A1H10	C1-C2-O2-S
2	l	4	A1H10	C3-C2-O2-S
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	m	4	A1H10	C1-C2-O2-S
2	m	4	A1H10	C3-C2-O2-S
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	n	4	A1H10	C1-C2-O2-S
2	n	4	A1H10	C3-C2-O2-S
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	o	4	A1H10	C1-C2-O2-S
2	o	4	A1H10	C3-C2-O2-S
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	p	4	A1H10	C1-C2-O2-S
2	p	4	A1H10	C3-C2-O2-S
2	q	2	BDP	C4-C5-C6-O6B
2	q	3	A1H1V	C4-C5-C6-O6A
2	q	3	A1H1V	C4-C3-O3-S1
2	q	3	A1H1V	C2-C3-O3-S1
2	q	4	A1H10	C1-C2-O2-S
2	q	4	A1H10	C3-C2-O2-S
2	r	2	BDP	C4-C5-C6-O6B
2	r	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	r	3	A1H1V	C4-C3-O3-S1
2	r	3	A1H1V	C2-C3-O3-S1
2	r	4	A1H10	C1-C2-O2-S
2	r	4	A1H10	C3-C2-O2-S
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	s	4	A1H10	C1-C2-O2-S
2	s	4	A1H10	C3-C2-O2-S
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	t	4	A1H10	C1-C2-O2-S
2	t	4	A1H10	C3-C2-O2-S
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	u	4	A1H10	C1-C2-O2-S
2	u	4	A1H10	C3-C2-O2-S
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	v	4	A1H10	C1-C2-O2-S
2	v	4	A1H10	C3-C2-O2-S
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	w	4	A1H10	C1-C2-O2-S
2	w	4	A1H10	C3-C2-O2-S
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	x	4	A1H10	C1-C2-O2-S
2	x	4	A1H10	C3-C2-O2-S
2	y	2	BDP	C4-C5-C6-O6B
2	y	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	y	3	A1H1V	C4-C3-O3-S1
2	y	3	A1H1V	C2-C3-O3-S1
2	y	4	A1H10	C1-C2-O2-S
2	y	4	A1H10	C3-C2-O2-S
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	z	4	A1H10	C1-C2-O2-S
2	z	4	A1H10	C3-C2-O2-S
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	0	4	A1H10	C1-C2-O2-S
2	0	4	A1H10	C3-C2-O2-S
2	1	2	BDP	C4-C5-C6-O6B
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	1	4	A1H10	C1-C2-O2-S
2	1	4	A1H10	C3-C2-O2-S
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	2	4	A1H10	C1-C2-O2-S
2	2	4	A1H10	C3-C2-O2-S
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	3	4	A1H10	C1-C2-O2-S
2	3	4	A1H10	C3-C2-O2-S
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	4	4	A1H10	C1-C2-O2-S
2	4	4	A1H10	C3-C2-O2-S
2	5	2	BDP	C4-C5-C6-O6B
2	5	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	5	3	A1H1V	C4-C3-O3-S1
2	5	3	A1H1V	C2-C3-O3-S1
2	5	4	A1H10	C1-C2-O2-S
2	5	4	A1H10	C3-C2-O2-S
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	6	4	A1H10	C1-C2-O2-S
2	6	4	A1H10	C3-C2-O2-S
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	7	4	A1H10	C1-C2-O2-S
2	7	4	A1H10	C3-C2-O2-S
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	8	4	A1H10	C1-C2-O2-S
2	8	4	A1H10	C3-C2-O2-S
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	9	4	A1H10	C1-C2-O2-S
2	9	4	A1H10	C3-C2-O2-S
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	AA	4	A1H10	C1-C2-O2-S
2	AA	4	A1H10	C3-C2-O2-S
2	BA	2	BDP	C4-C5-C6-O6B
2	BA	3	A1H1V	C4-C5-C6-O6A
2	BA	3	A1H1V	C4-C3-O3-S1
2	BA	3	A1H1V	C2-C3-O3-S1
2	BA	4	A1H10	C1-C2-O2-S
2	BA	4	A1H10	C3-C2-O2-S
2	CA	2	BDP	C4-C5-C6-O6B
2	CA	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	CA	3	A1H1V	C4-C3-O3-S1
2	CA	3	A1H1V	C2-C3-O3-S1
2	CA	4	A1H10	C1-C2-O2-S
2	CA	4	A1H10	C3-C2-O2-S
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	DA	4	A1H10	C1-C2-O2-S
2	DA	4	A1H10	C3-C2-O2-S
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	EA	4	A1H10	C1-C2-O2-S
2	EA	4	A1H10	C3-C2-O2-S
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	FA	4	A1H10	C1-C2-O2-S
2	FA	4	A1H10	C3-C2-O2-S
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	GA	4	A1H10	C1-C2-O2-S
2	GA	4	A1H10	C3-C2-O2-S
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	HA	4	A1H10	C1-C2-O2-S
2	HA	4	A1H10	C3-C2-O2-S
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	IA	4	A1H10	C1-C2-O2-S
2	IA	4	A1H10	C3-C2-O2-S
2	JA	2	BDP	C4-C5-C6-O6B
2	JA	3	A1H1V	C4-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	JA	3	A1H1V	C4-C3-O3-S1
2	JA	3	A1H1V	C2-C3-O3-S1
2	JA	4	A1H10	C1-C2-O2-S
2	JA	4	A1H10	C3-C2-O2-S
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	KA	4	A1H10	C1-C2-O2-S
2	KA	4	A1H10	C3-C2-O2-S
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	LA	4	A1H10	C1-C2-O2-S
2	LA	4	A1H10	C3-C2-O2-S
2	MA	2	BDP	C4-C5-C6-O6B
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	MA	4	A1H10	C1-C2-O2-S
2	MA	4	A1H10	C3-C2-O2-S
2	NA	2	BDP	C4-C5-C6-O6B
2	NA	3	A1H1V	C4-C5-C6-O6A
2	NA	3	A1H1V	C4-C3-O3-S1
2	NA	3	A1H1V	C2-C3-O3-S1
2	NA	4	A1H10	C1-C2-O2-S
2	NA	4	A1H10	C3-C2-O2-S
2	OA	2	BDP	C4-C5-C6-O6B
2	OA	3	A1H1V	C4-C5-C6-O6A
2	OA	3	A1H1V	C4-C3-O3-S1
2	OA	3	A1H1V	C2-C3-O3-S1
2	OA	4	A1H10	C1-C2-O2-S
2	OA	4	A1H10	C3-C2-O2-S
2	PA	2	BDP	C4-C5-C6-O6B
2	PA	3	A1H1V	C4-C5-C6-O6A
2	PA	3	A1H1V	C4-C3-O3-S1
2	PA	3	A1H1V	C2-C3-O3-S1
2	PA	4	A1H10	C1-C2-O2-S
2	PA	4	A1H10	C3-C2-O2-S
2	r	1	BGC	O5-C5-C6-O6
2	BA	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	c	1	BGC	O5-C5-C6-O6
2	e	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	v	1	BGC	O5-C5-C6-O6
2	w	1	BGC	O5-C5-C6-O6
2	y	1	BGC	O5-C5-C6-O6
2	0	1	BGC	O5-C5-C6-O6
2	2	1	BGC	O5-C5-C6-O6
2	5	1	BGC	O5-C5-C6-O6
2	6	1	BGC	O5-C5-C6-O6
2	AA	1	BGC	O5-C5-C6-O6
2	DA	1	BGC	O5-C5-C6-O6
2	EA	1	BGC	O5-C5-C6-O6
2	GA	1	BGC	O5-C5-C6-O6
2	JA	1	BGC	O5-C5-C6-O6
2	a	1	BGC	O5-C5-C6-O6
2	b	1	BGC	O5-C5-C6-O6
2	d	1	BGC	O5-C5-C6-O6
2	f	1	BGC	O5-C5-C6-O6
2	g	1	BGC	O5-C5-C6-O6
2	i	1	BGC	O5-C5-C6-O6
2	m	1	BGC	O5-C5-C6-O6
2	o	1	BGC	O5-C5-C6-O6
2	q	1	BGC	O5-C5-C6-O6
2	s	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	4	1	BGC	O5-C5-C6-O6
2	8	1	BGC	O5-C5-C6-O6
2	CA	1	BGC	O5-C5-C6-O6
2	FA	1	BGC	O5-C5-C6-O6
2	HA	1	BGC	O5-C5-C6-O6
2	LA	1	BGC	O5-C5-C6-O6
2	MA	1	BGC	O5-C5-C6-O6
2	NA	1	BGC	O5-C5-C6-O6
2	PA	1	BGC	O5-C5-C6-O6
2	j	1	BGC	O5-C5-C6-O6
2	k	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	IA	1	BGC	O5-C5-C6-O6
2	KA	1	BGC	O5-C5-C6-O6
2	7	1	BGC	O5-C5-C6-O6
2	OA	1	BGC	O5-C5-C6-O6
2	1	1	BGC	O5-C5-C6-O6
2	3	1	BGC	O5-C5-C6-O6
2	9	1	BGC	O5-C5-C6-O6

There are no ring outliers.

32 monomers are involved in 36 short contacts:

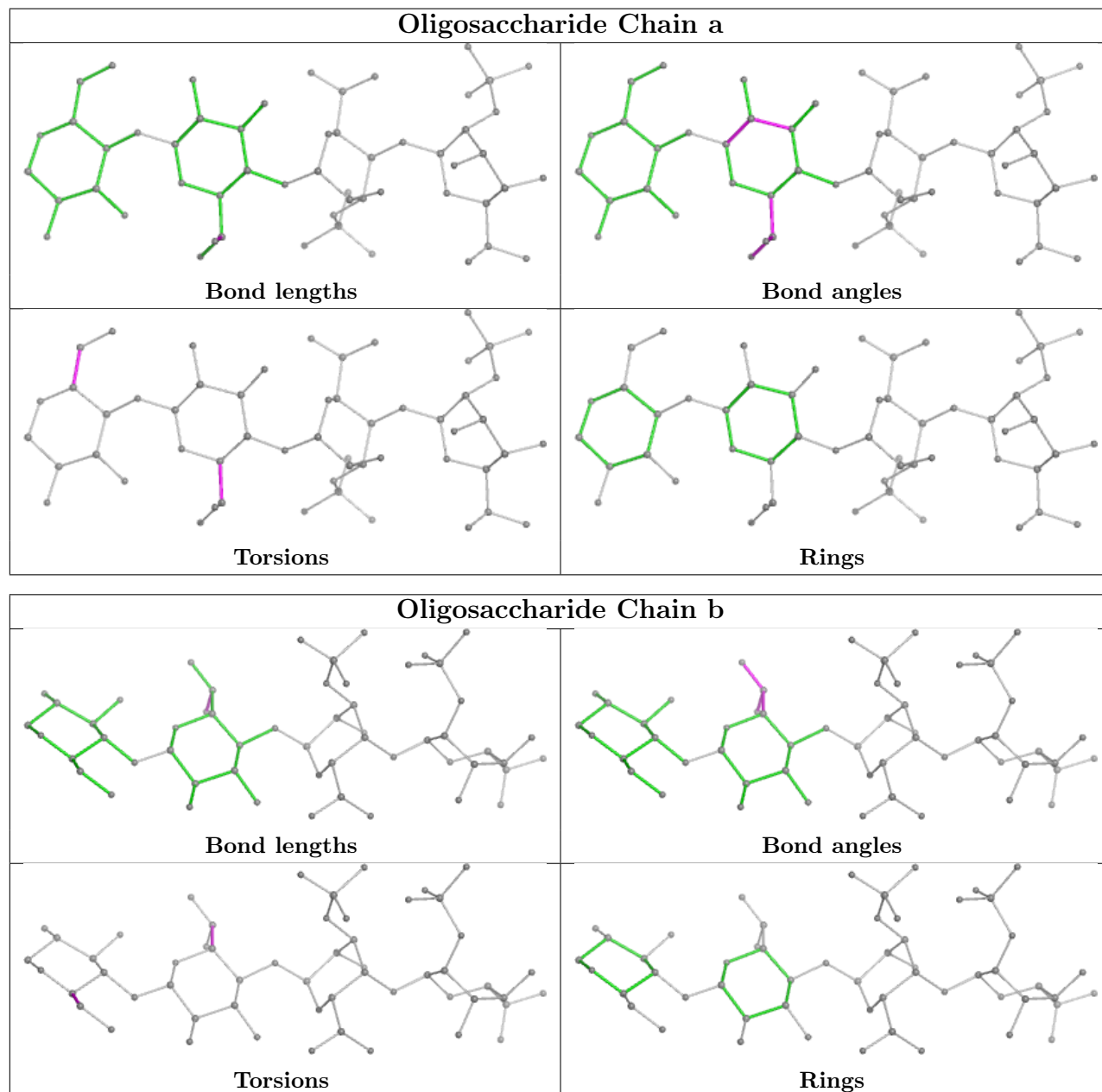
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	HA	4	A1H10	2	0
2	LA	3	A1H1V	1	0
2	NA	4	A1H10	3	0
2	7	3	A1H1V	2	0
2	DA	3	A1H1V	1	0
2	AA	1	BGC	1	0
2	OA	1	BGC	1	0
2	7	4	A1H10	2	0
2	PA	3	A1H1V	3	0
2	OA	2	BDP	1	0
2	PA	4	A1H10	3	0
2	BA	3	A1H1V	1	0
2	3	4	A1H10	3	0
2	8	1	BGC	1	0
2	JA	1	BGC	2	0
2	9	4	A1H10	2	0
2	NA	3	A1H1V	3	0
2	LA	4	A1H10	1	0
2	JA	4	A1H10	3	0
2	JA	3	A1H1V	3	0
2	1	3	A1H1V	1	0
2	5	4	A1H10	5	0
2	3	3	A1H1V	3	0
2	FA	4	A1H10	2	0
2	HA	3	A1H1V	2	0
2	1	4	A1H10	1	0
2	BA	4	A1H10	1	0
2	DA	4	A1H10	1	0
2	9	3	A1H1V	2	0
2	FA	3	A1H1V	2	0

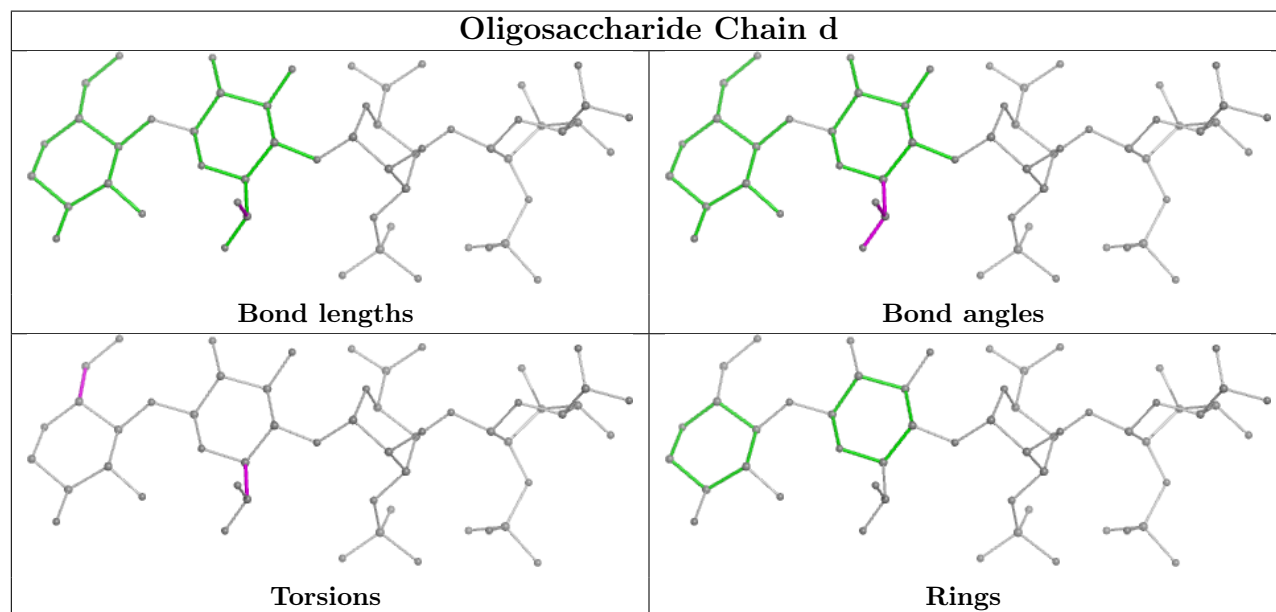
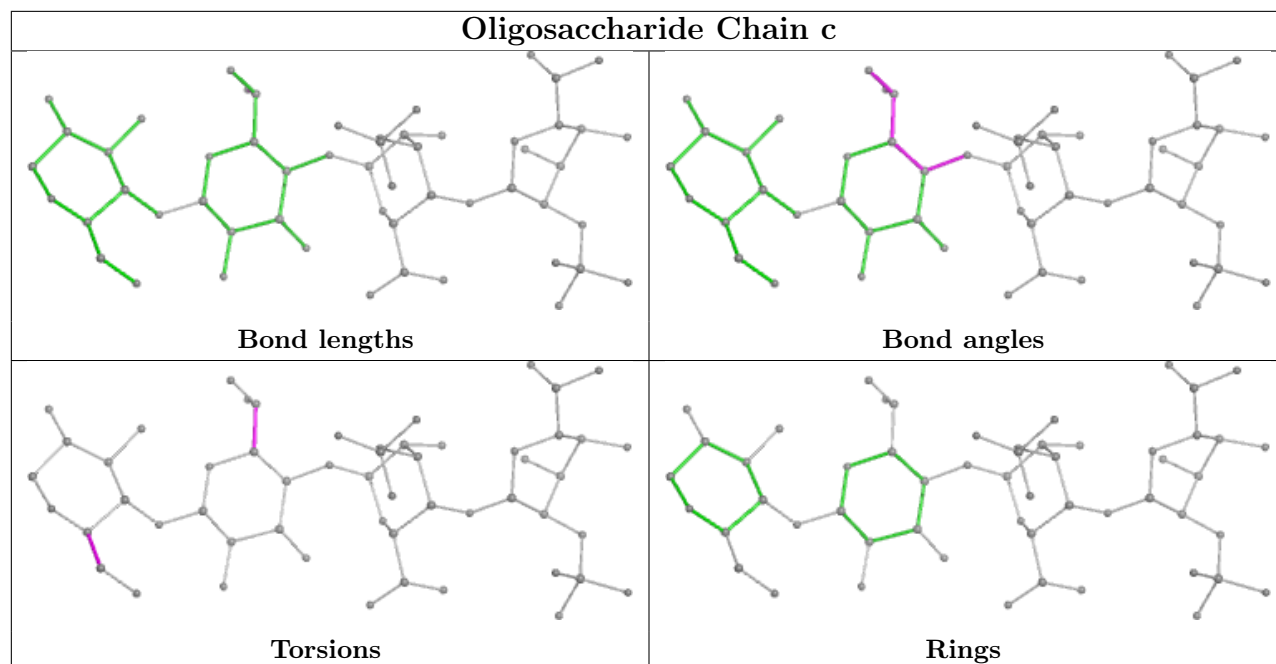
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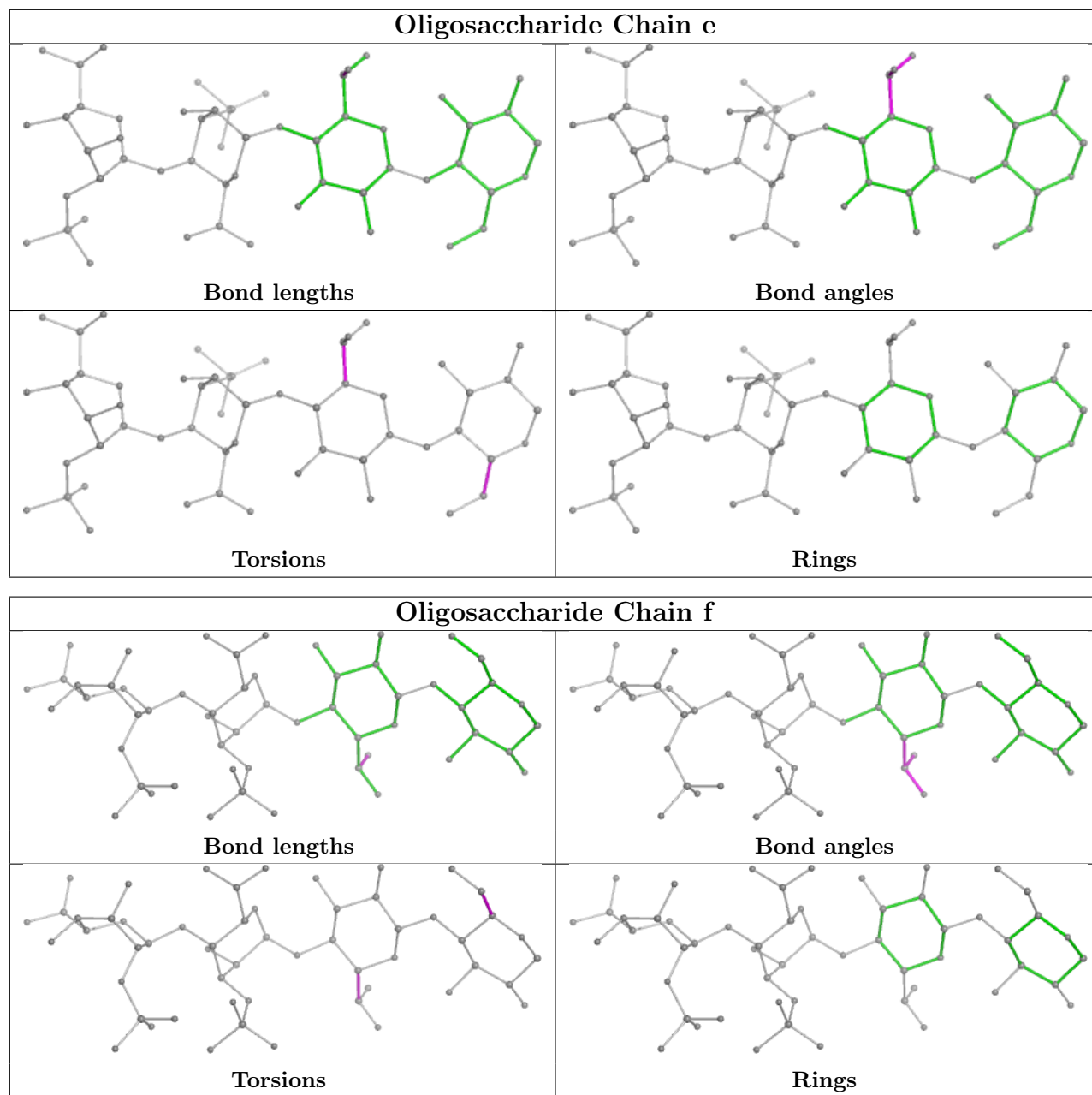
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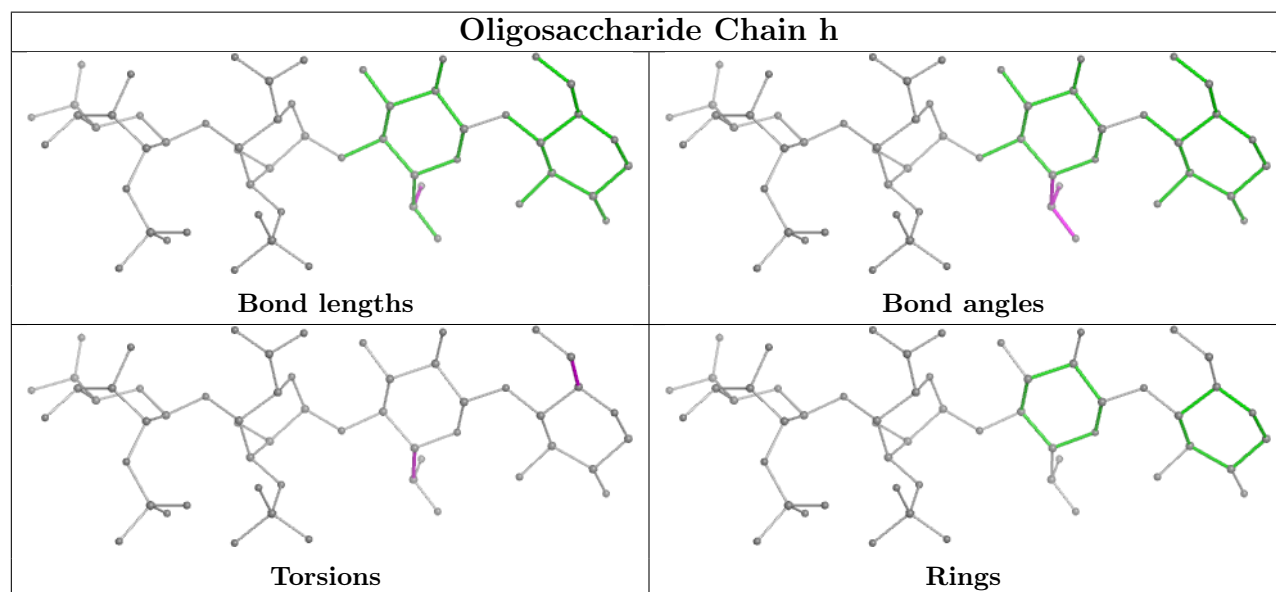
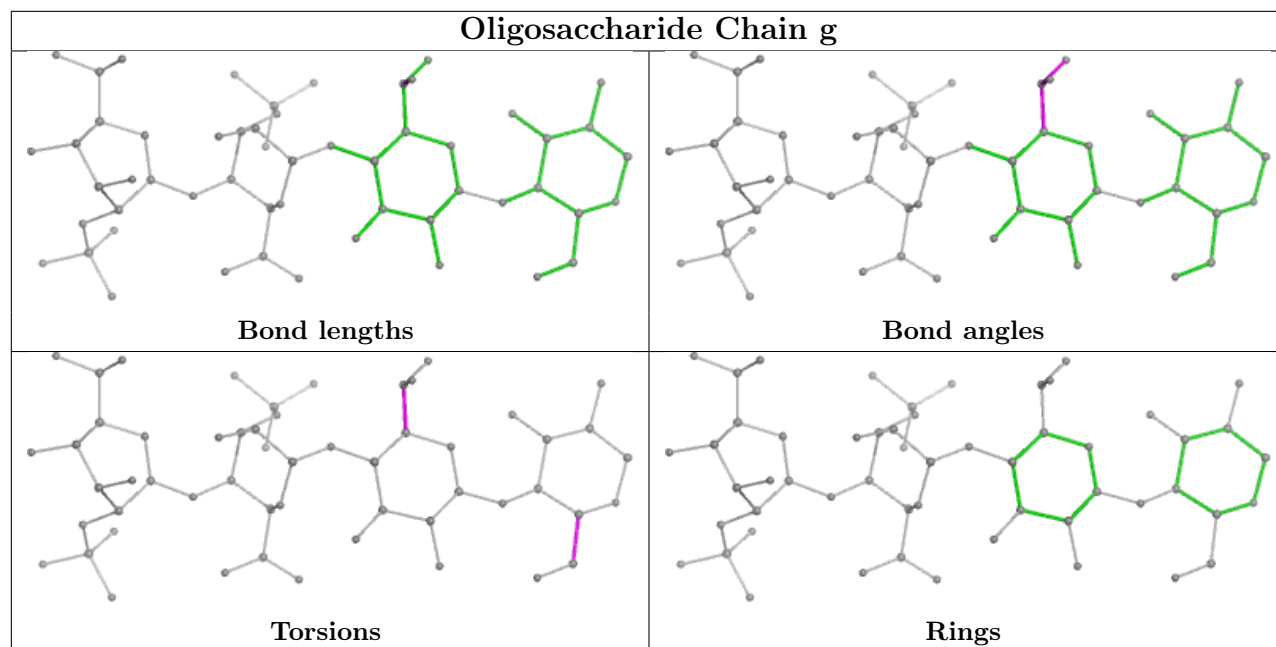
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	3	A1H1V	5	0
2	KA	1	BGC	1	0

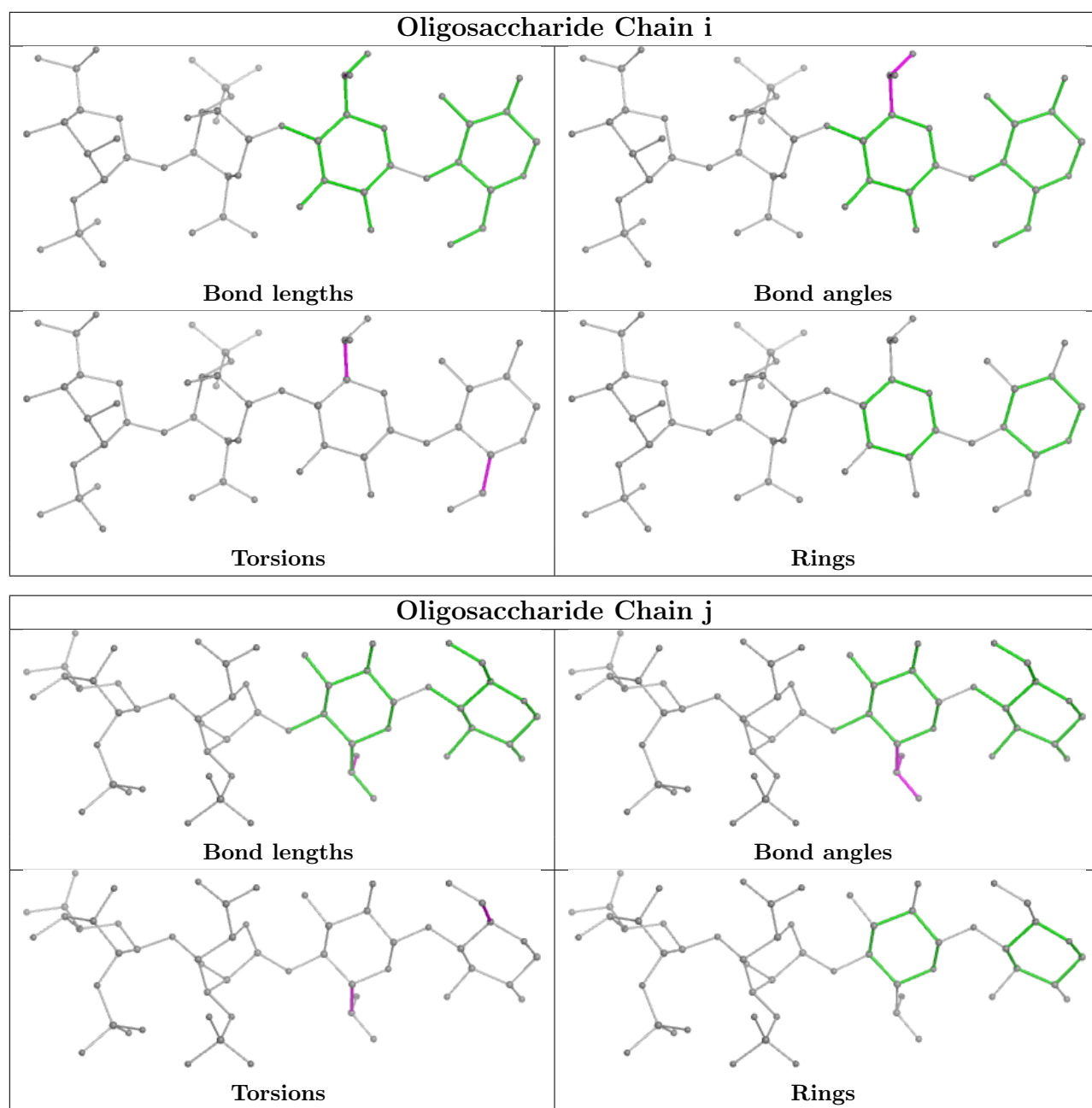
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

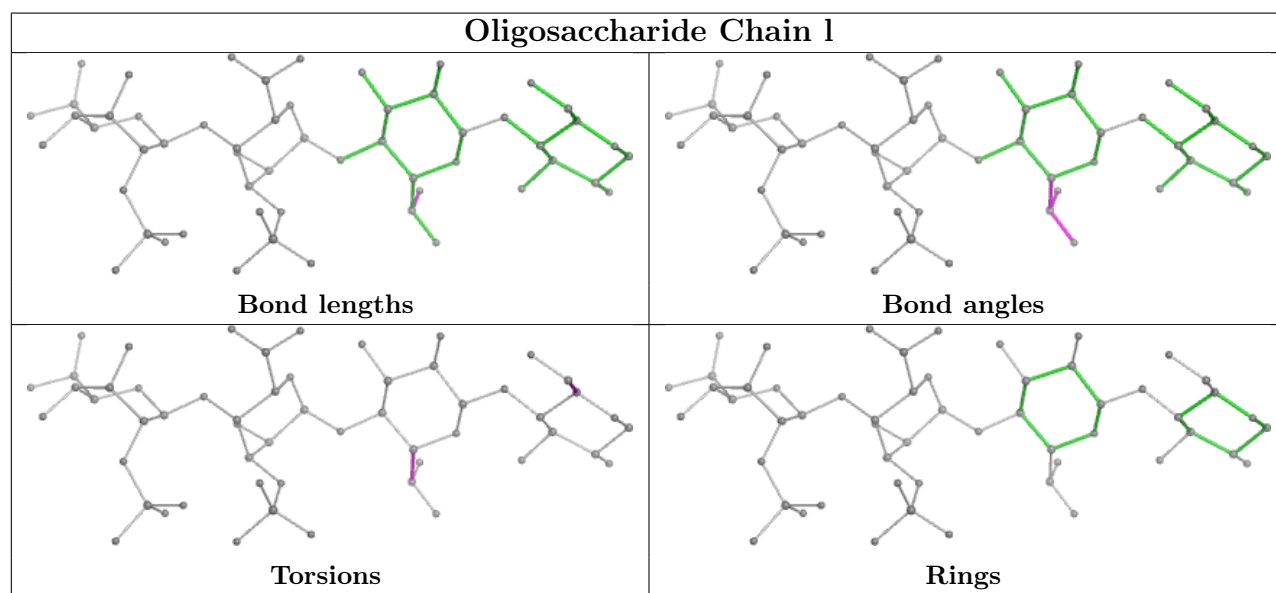
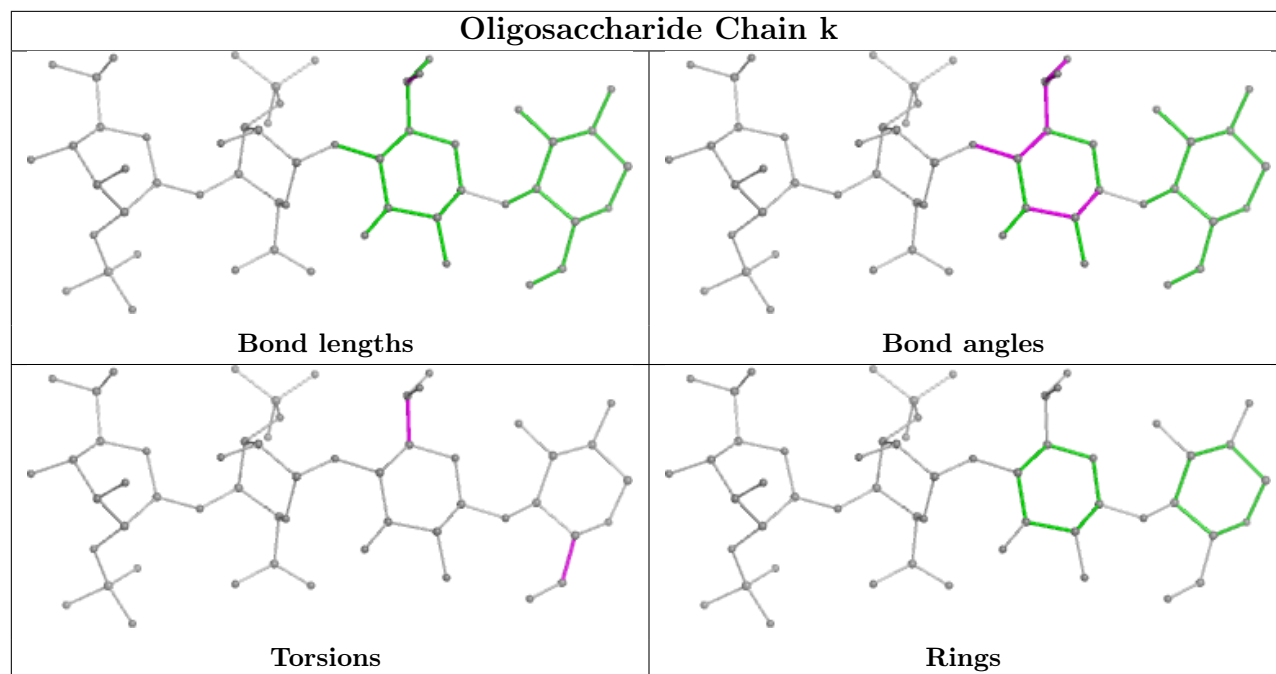


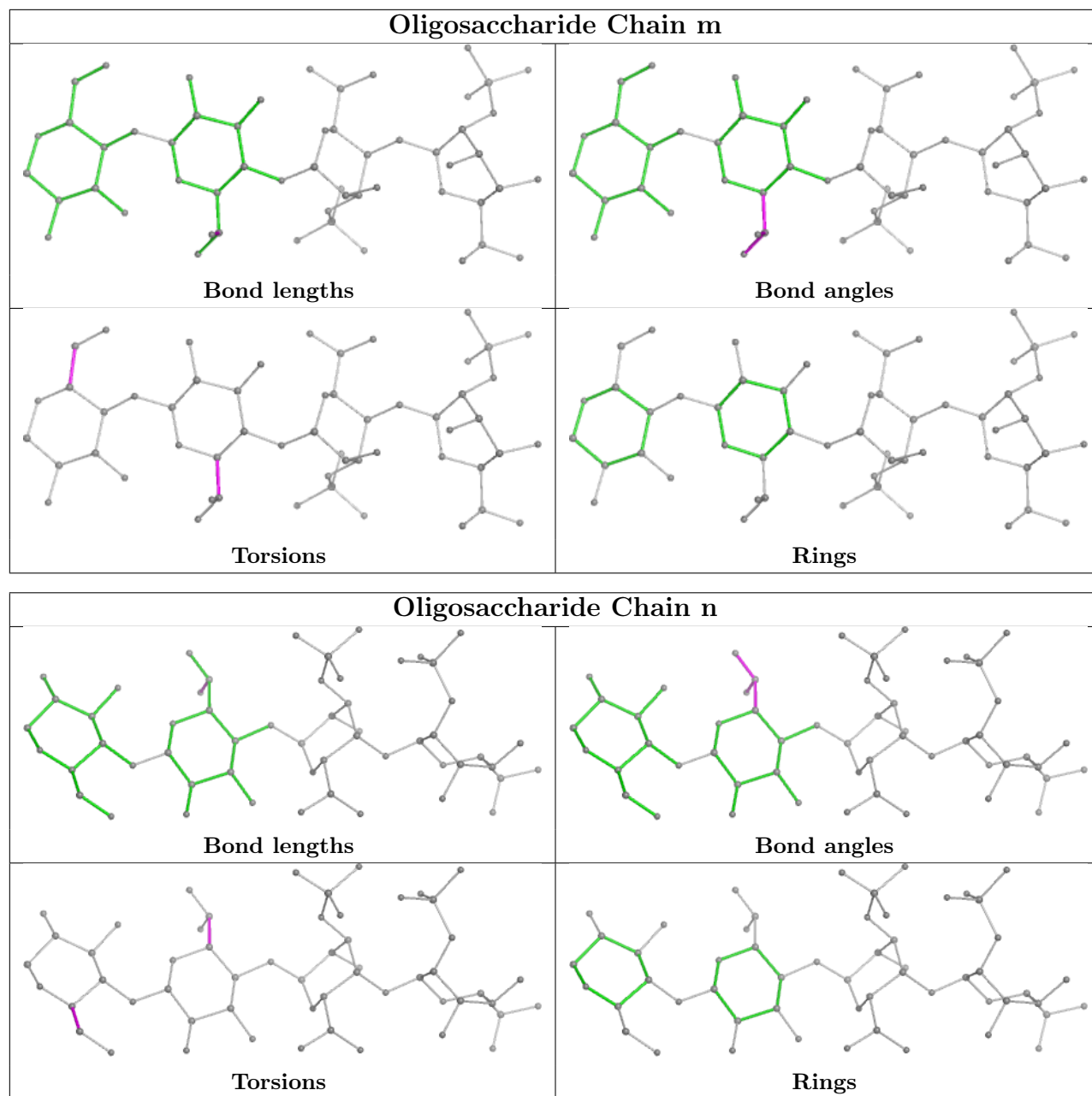




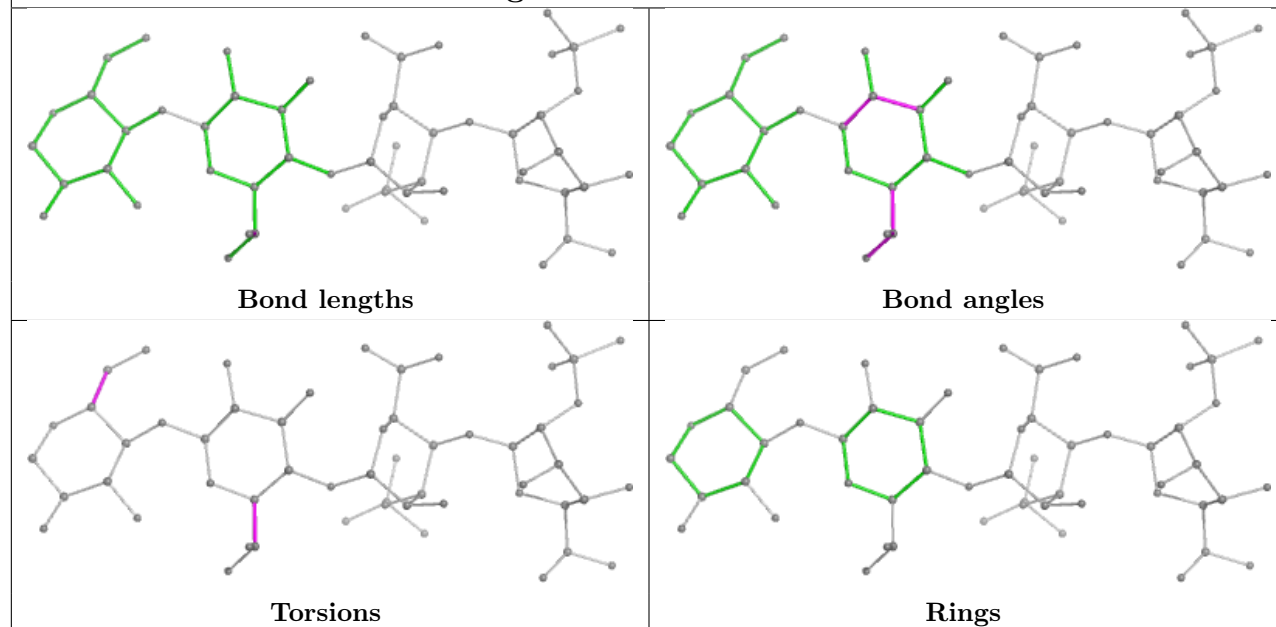




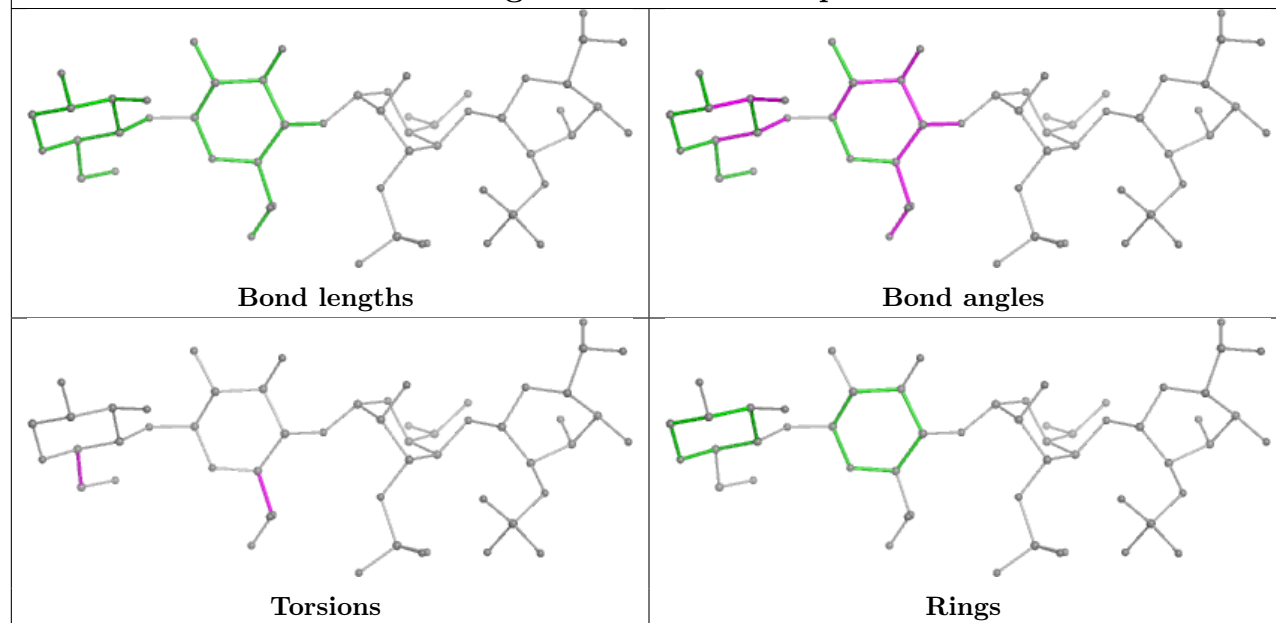


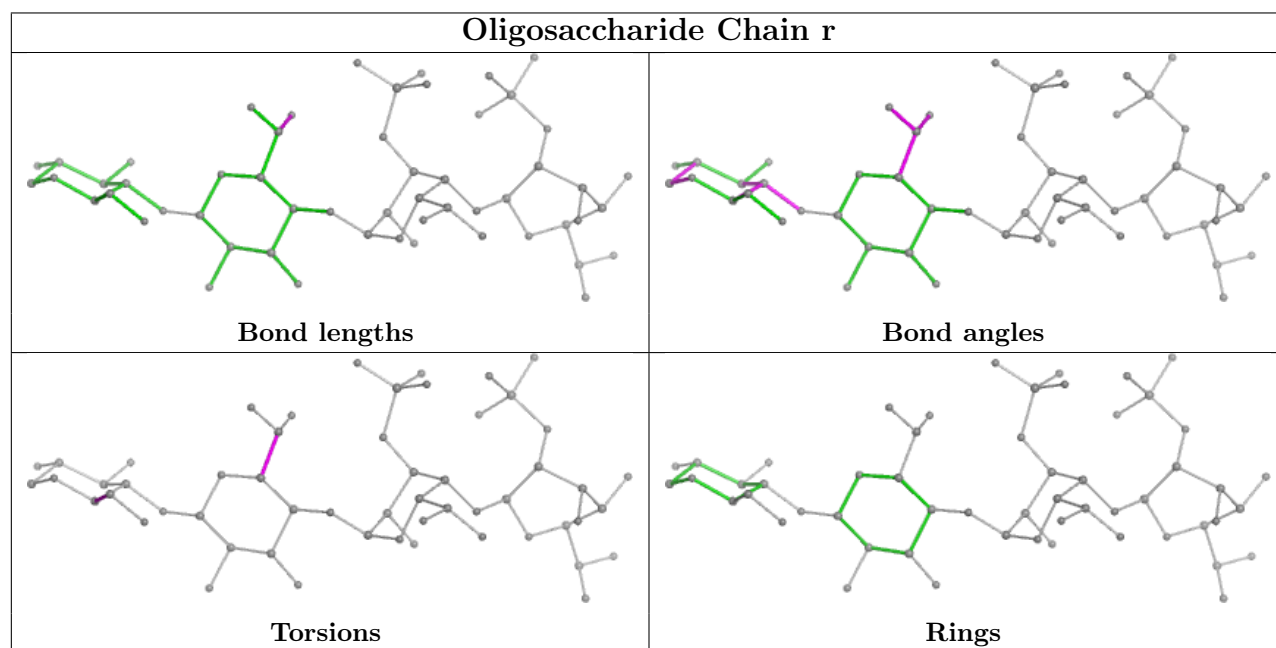
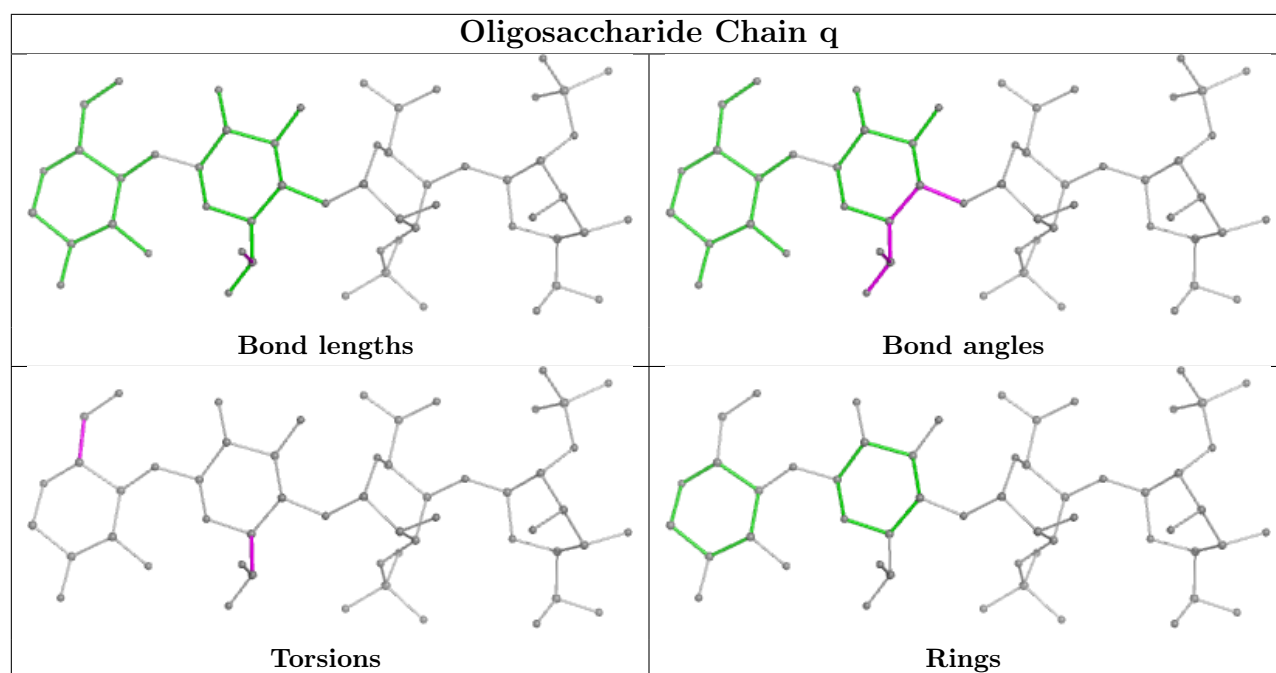


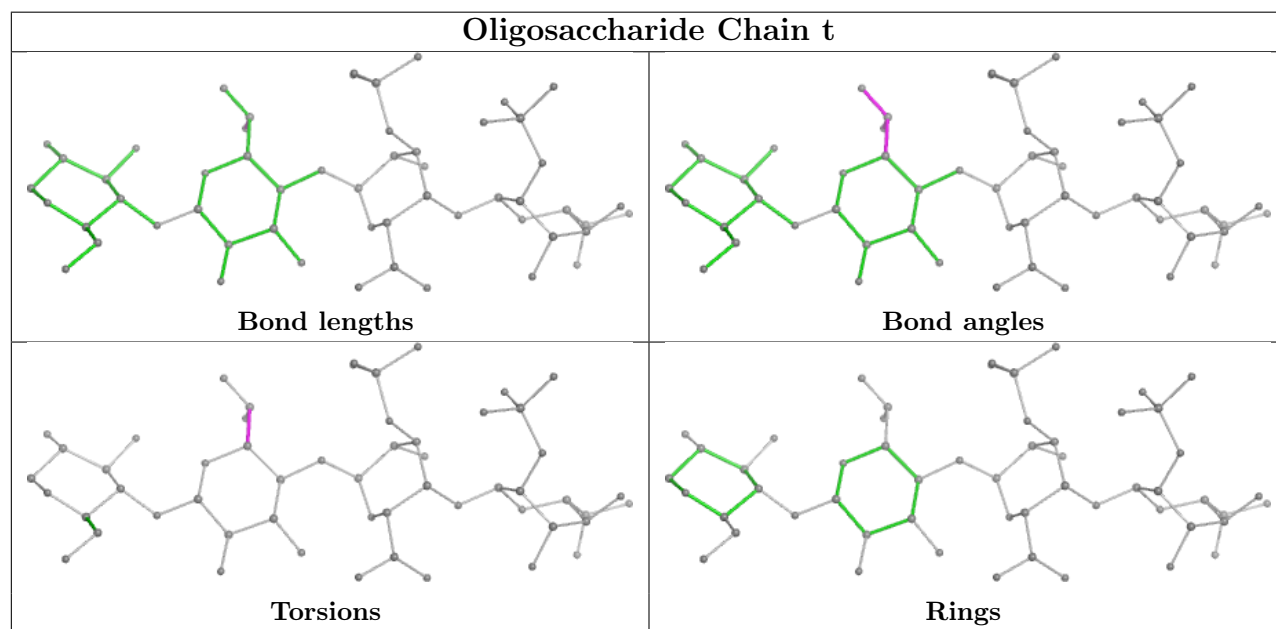
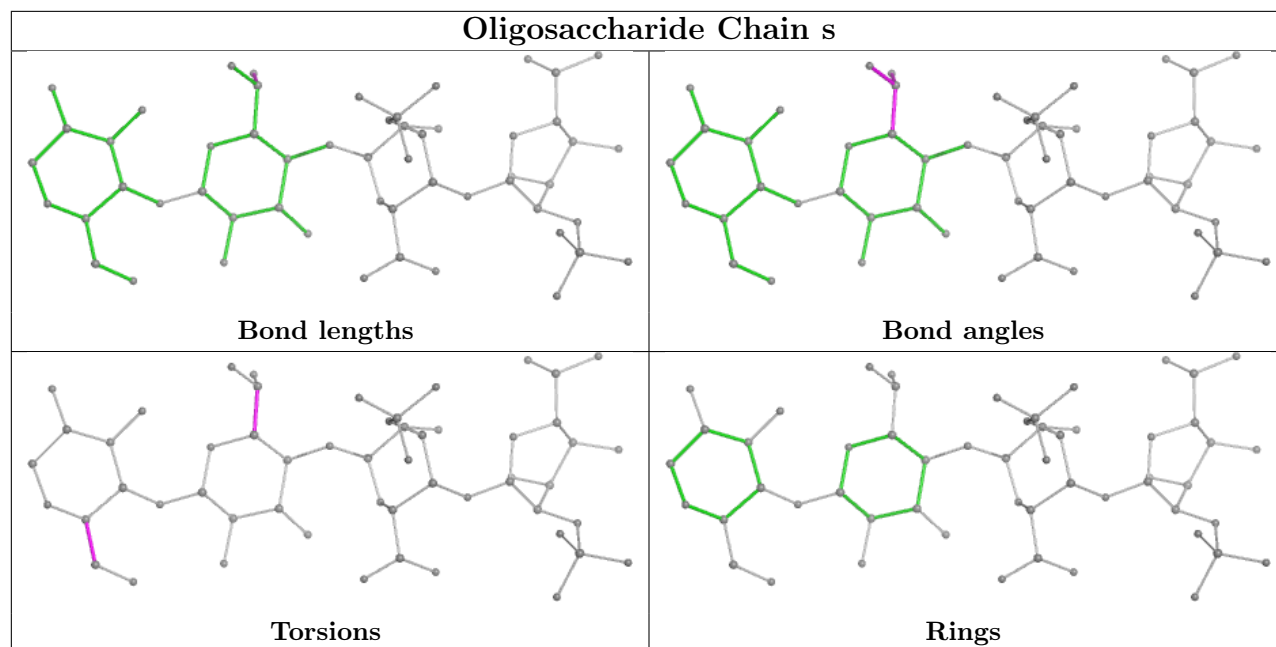
## Oligosaccharide Chain o

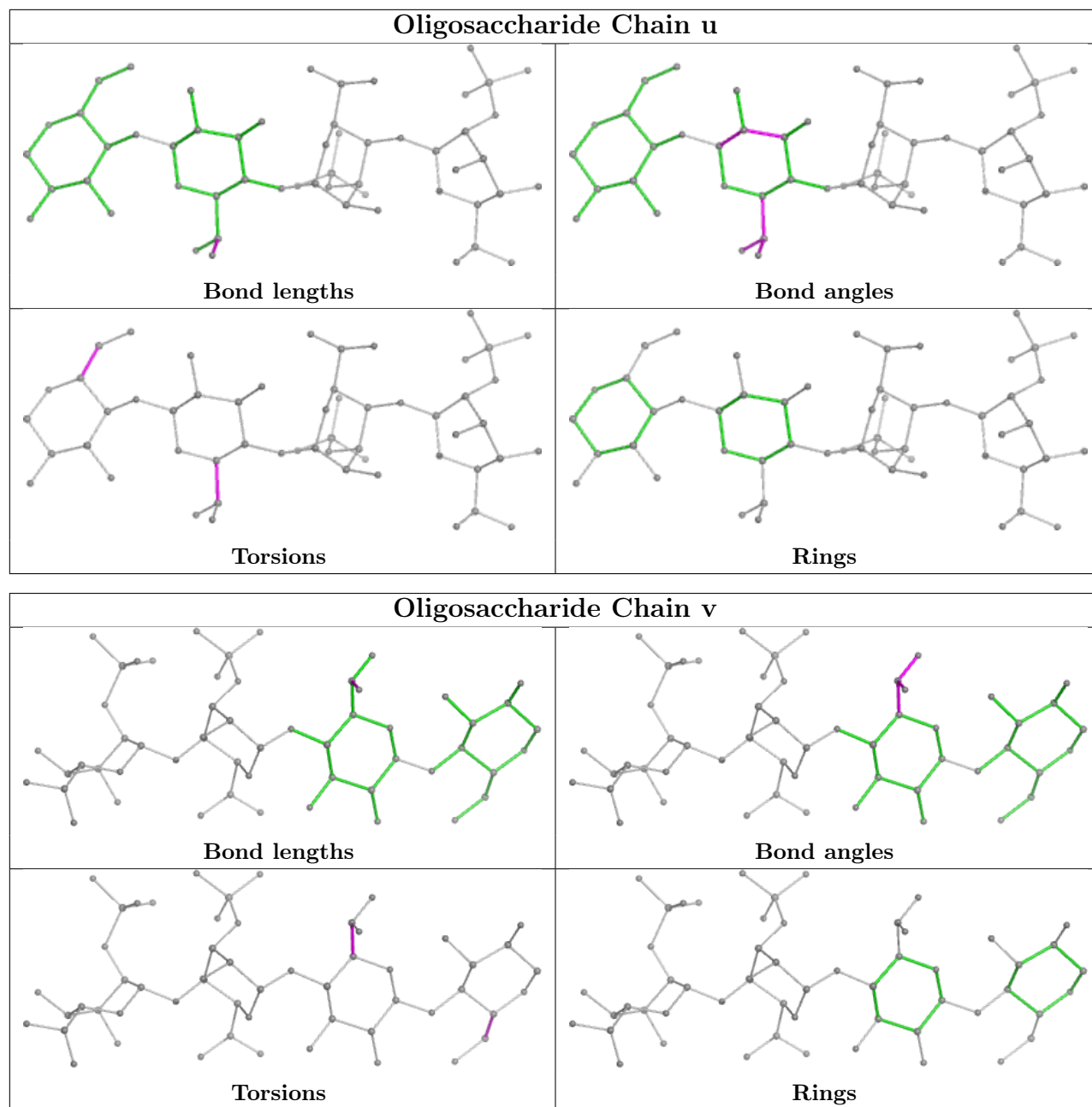


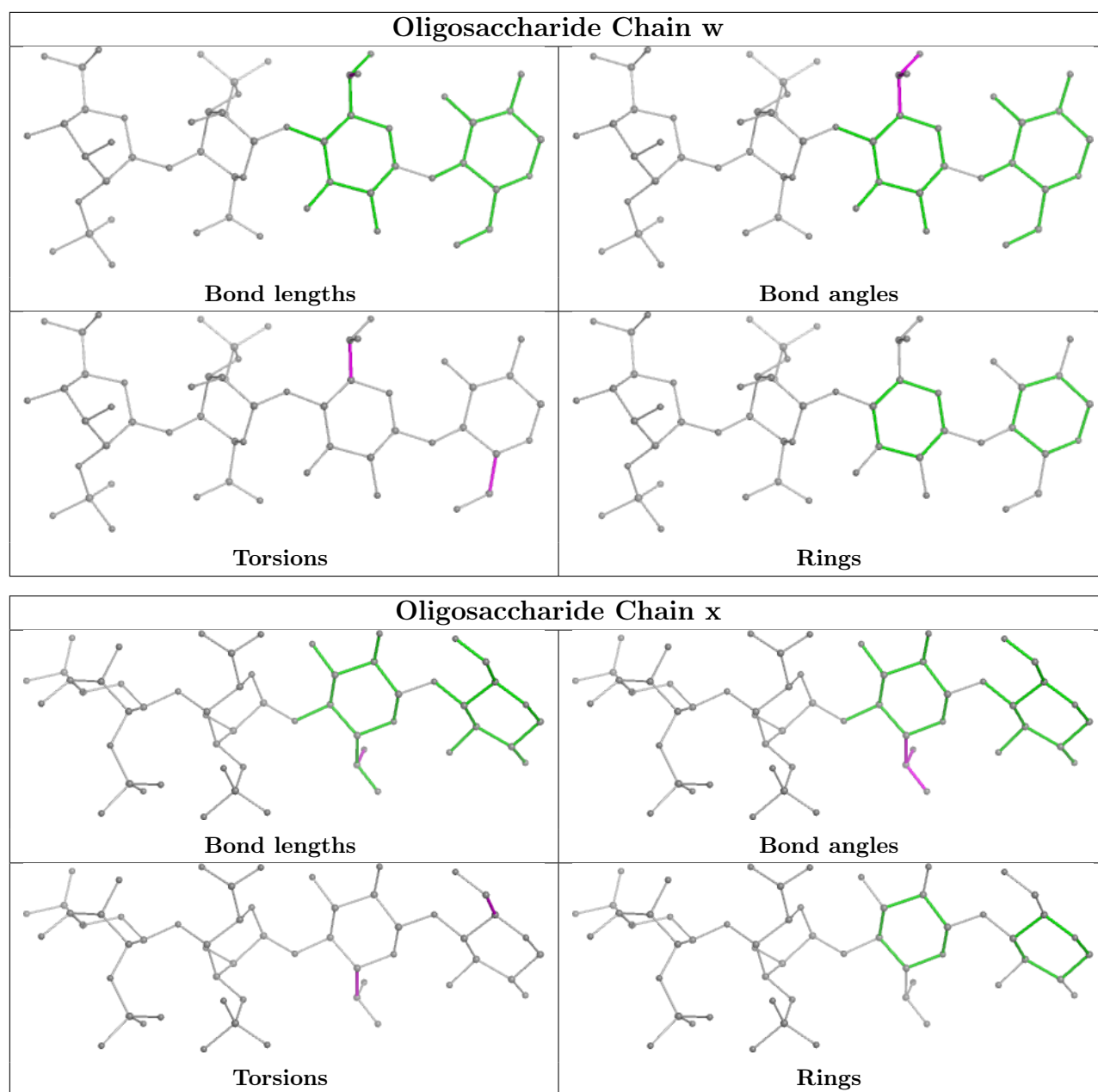
## Oligosaccharide Chain p

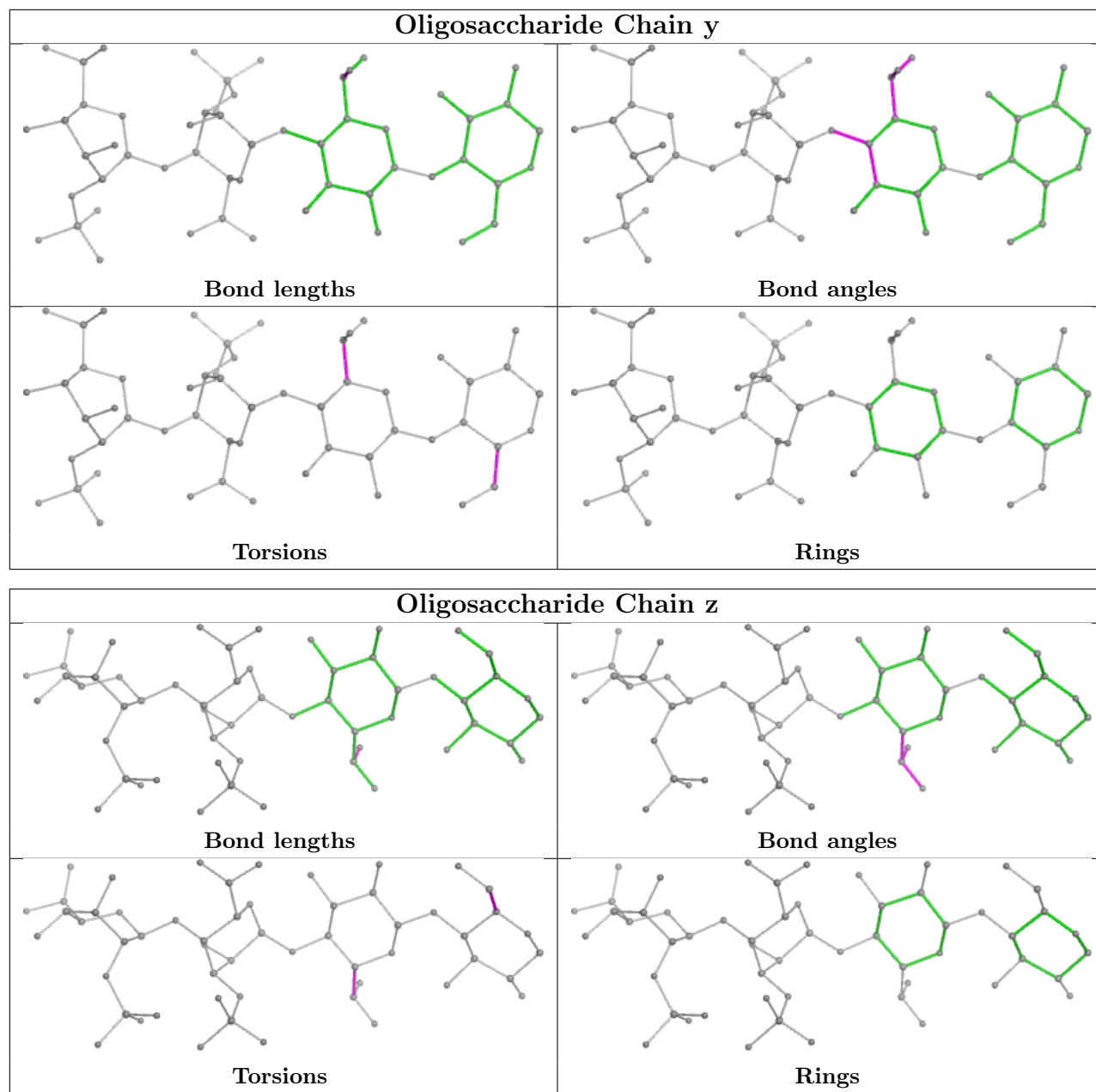


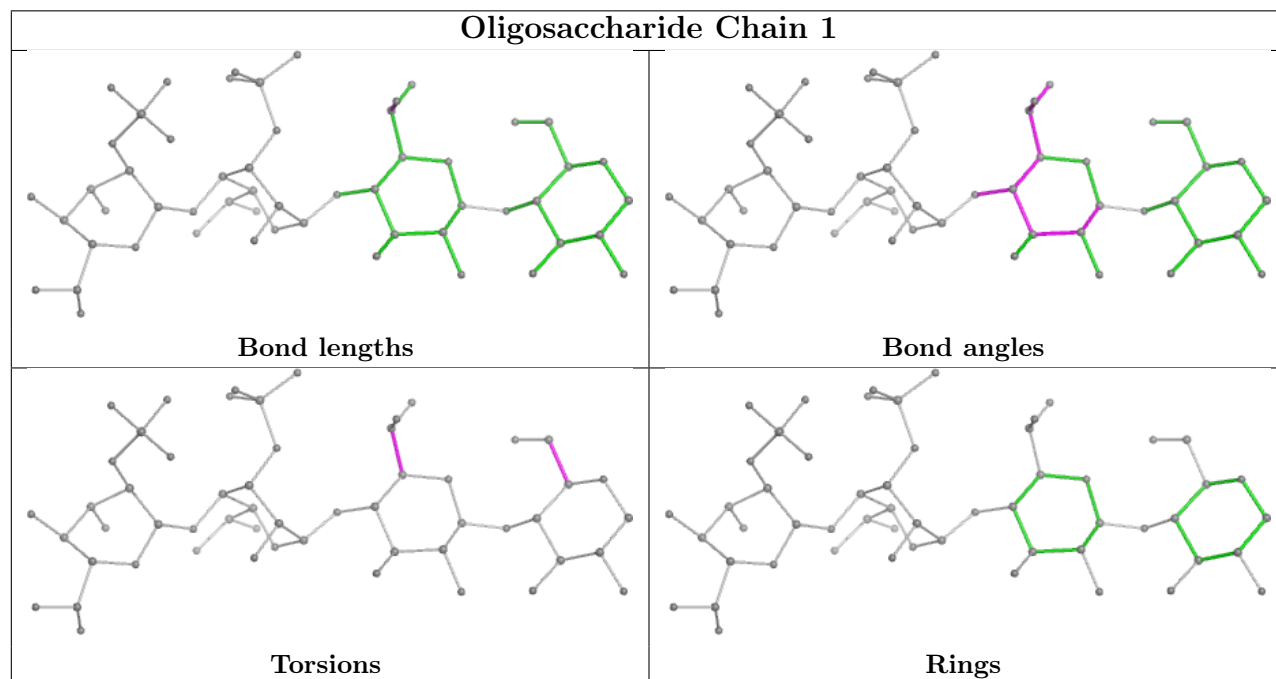
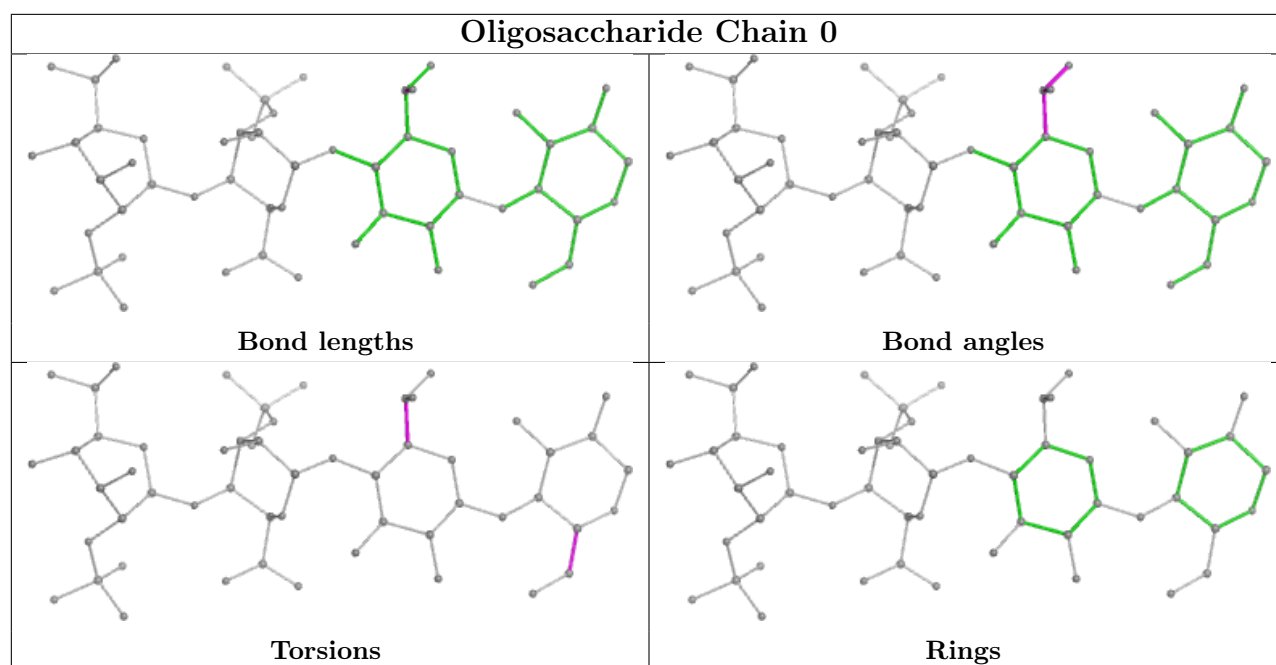


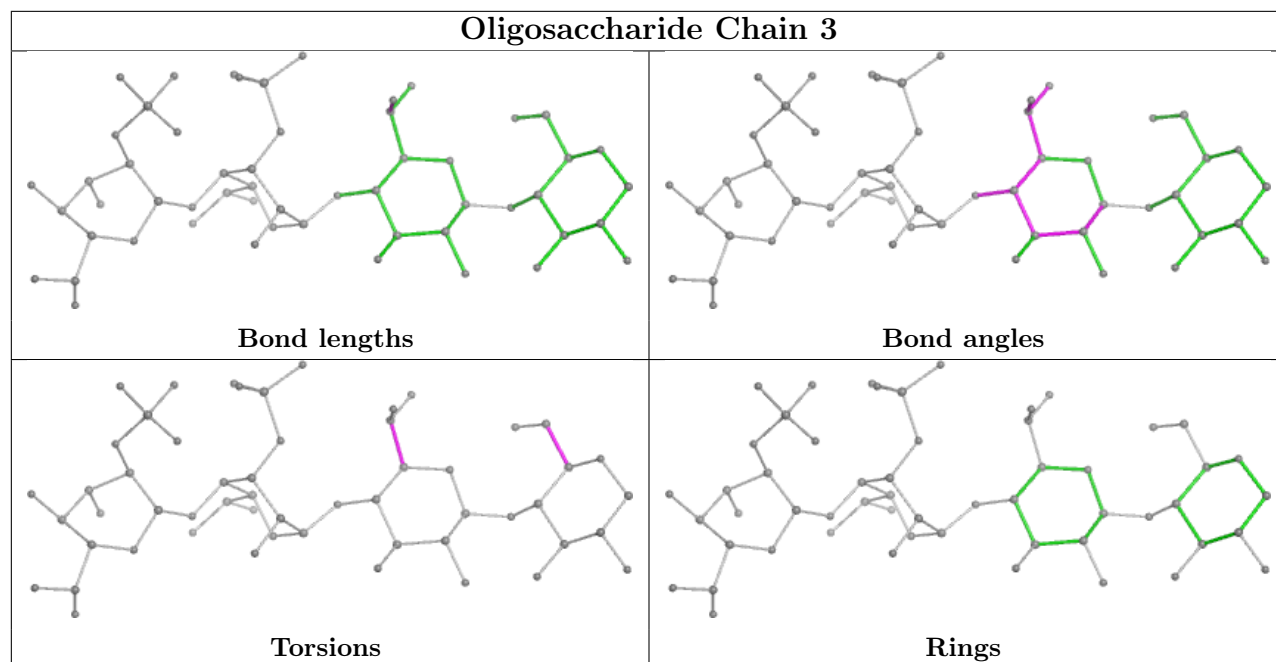
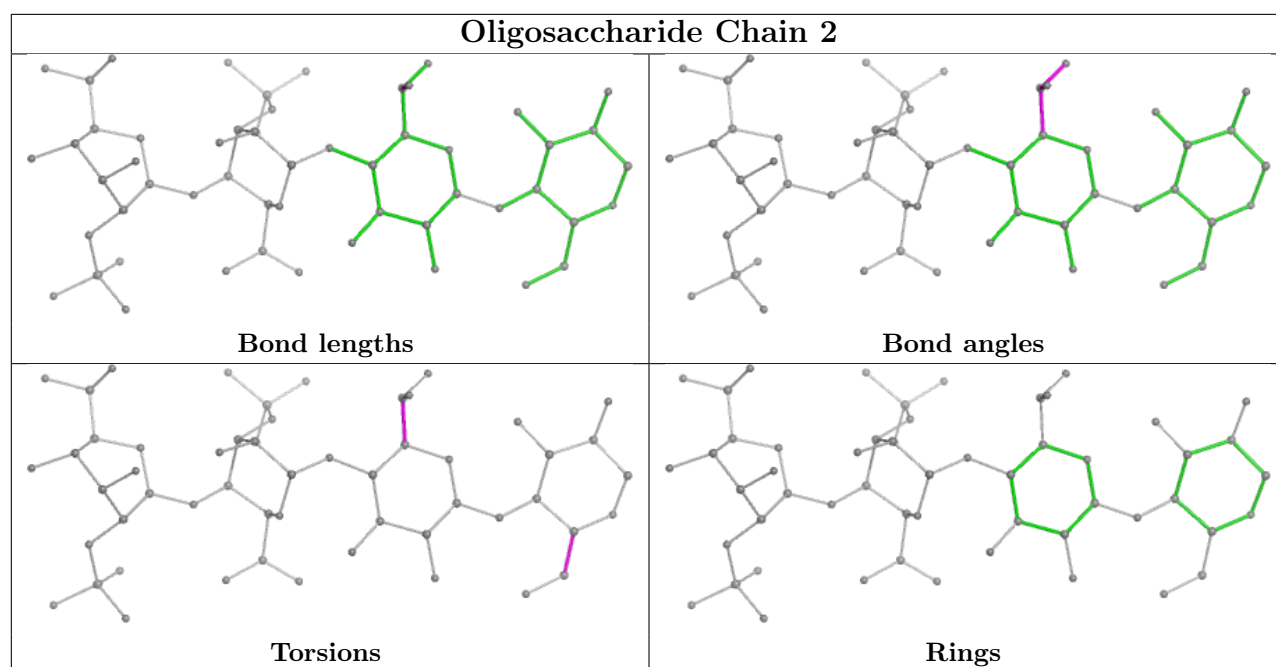


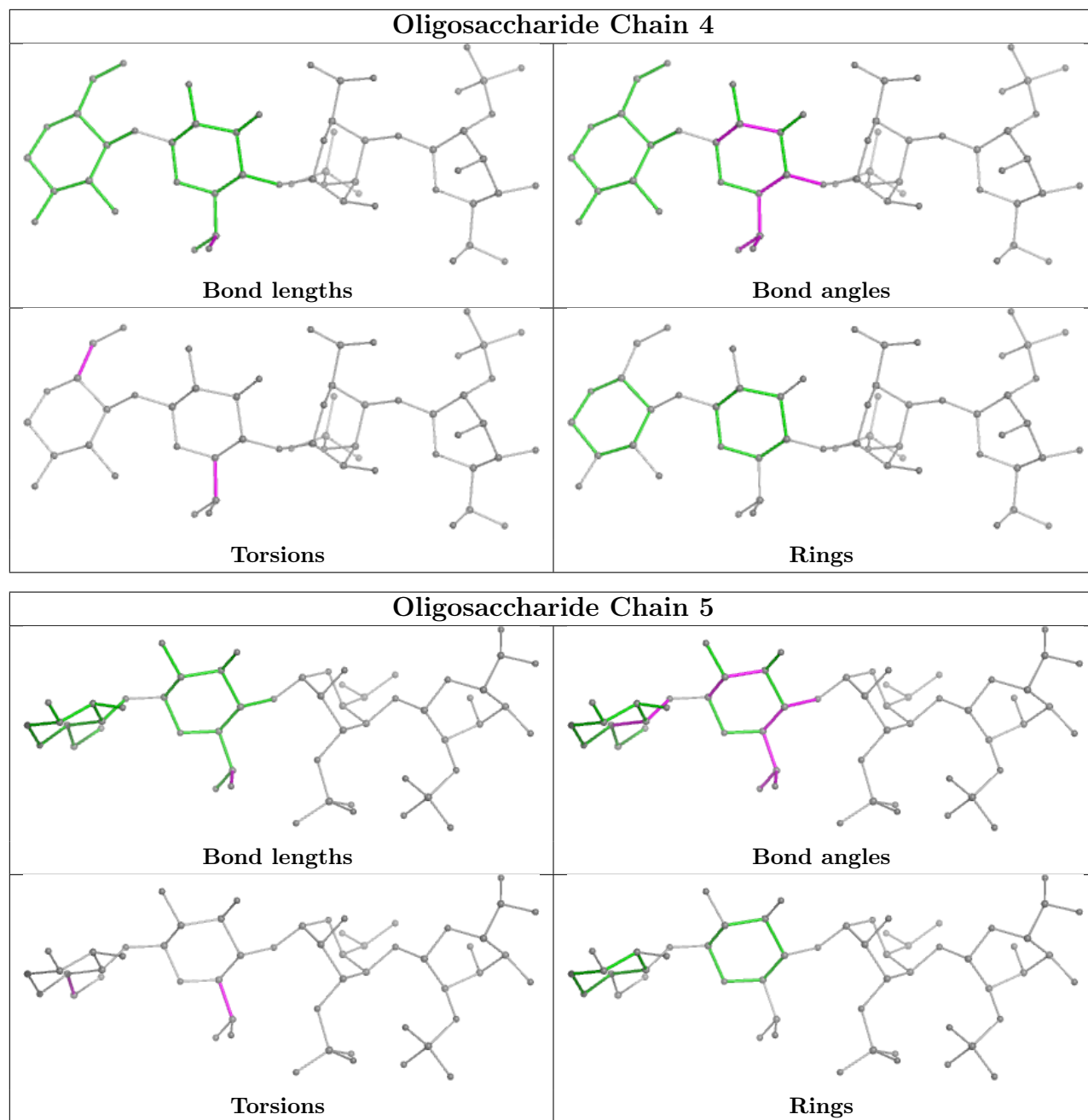




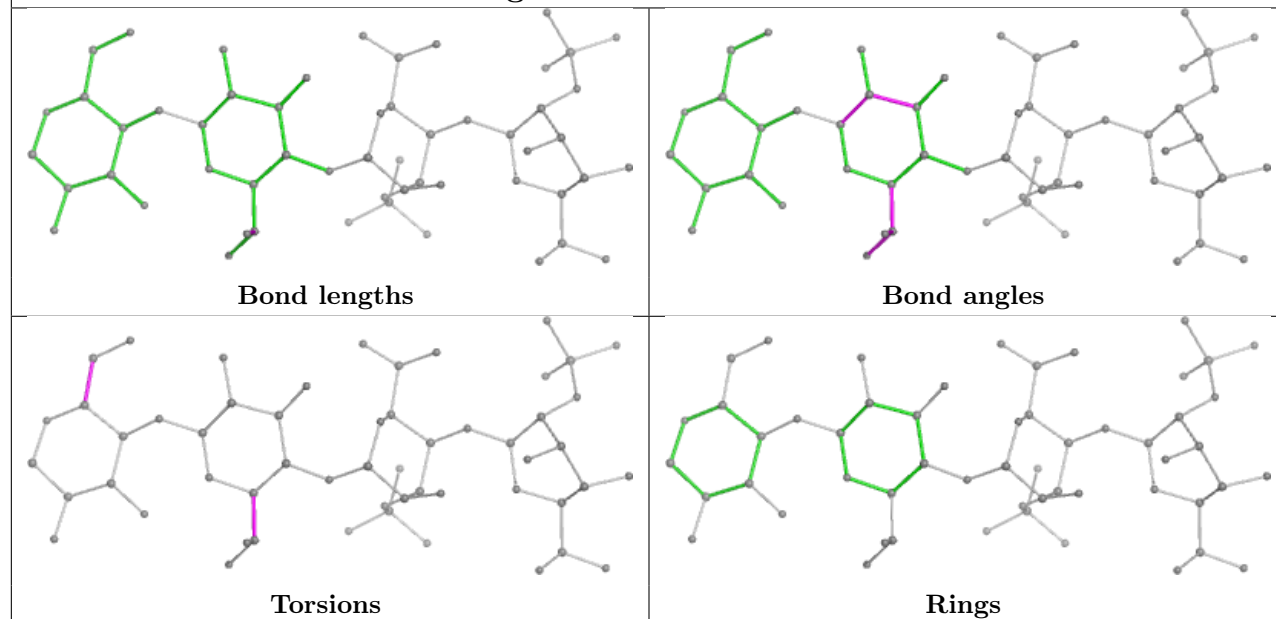




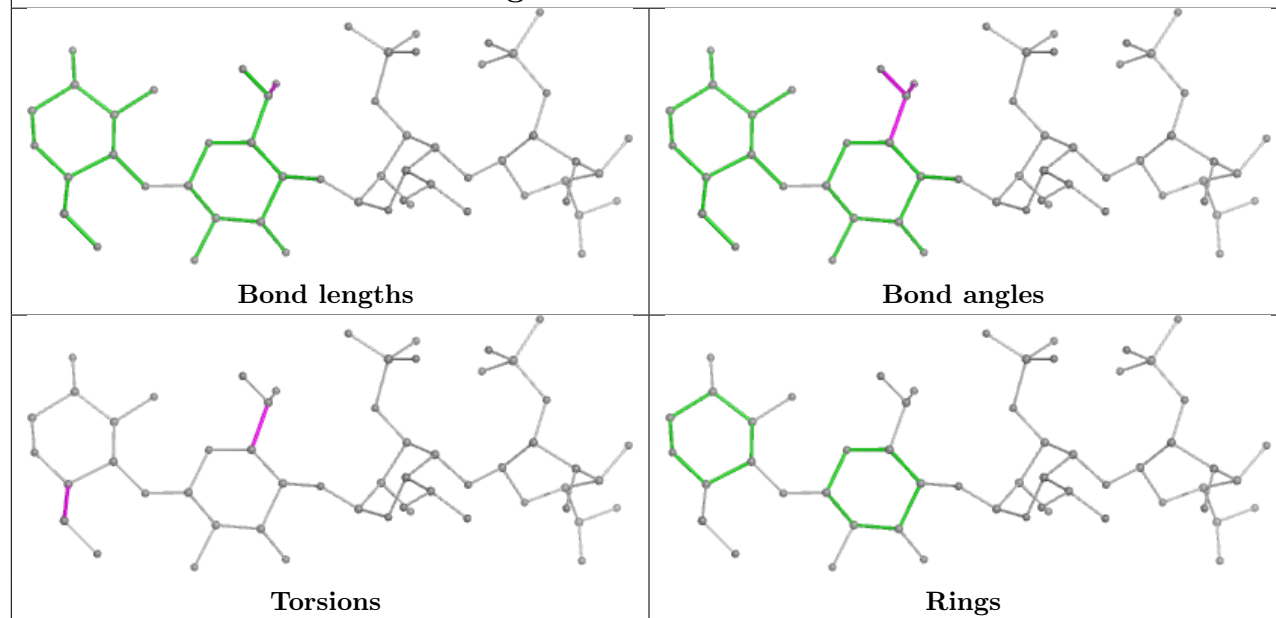




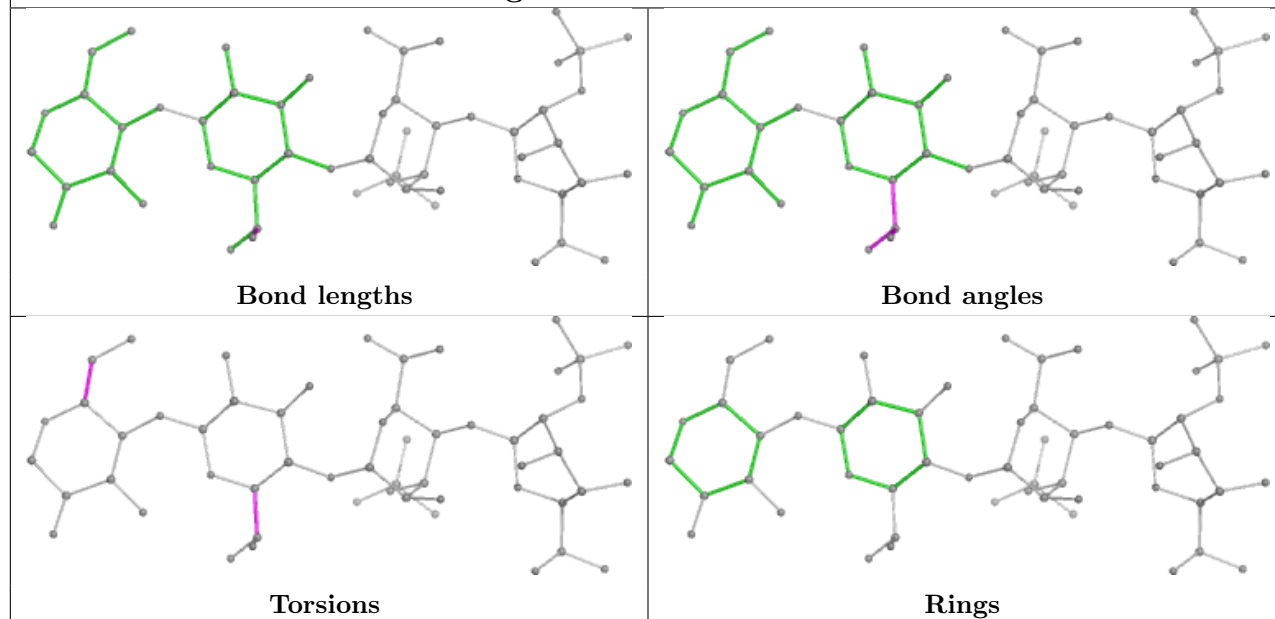
## Oligosaccharide Chain 6



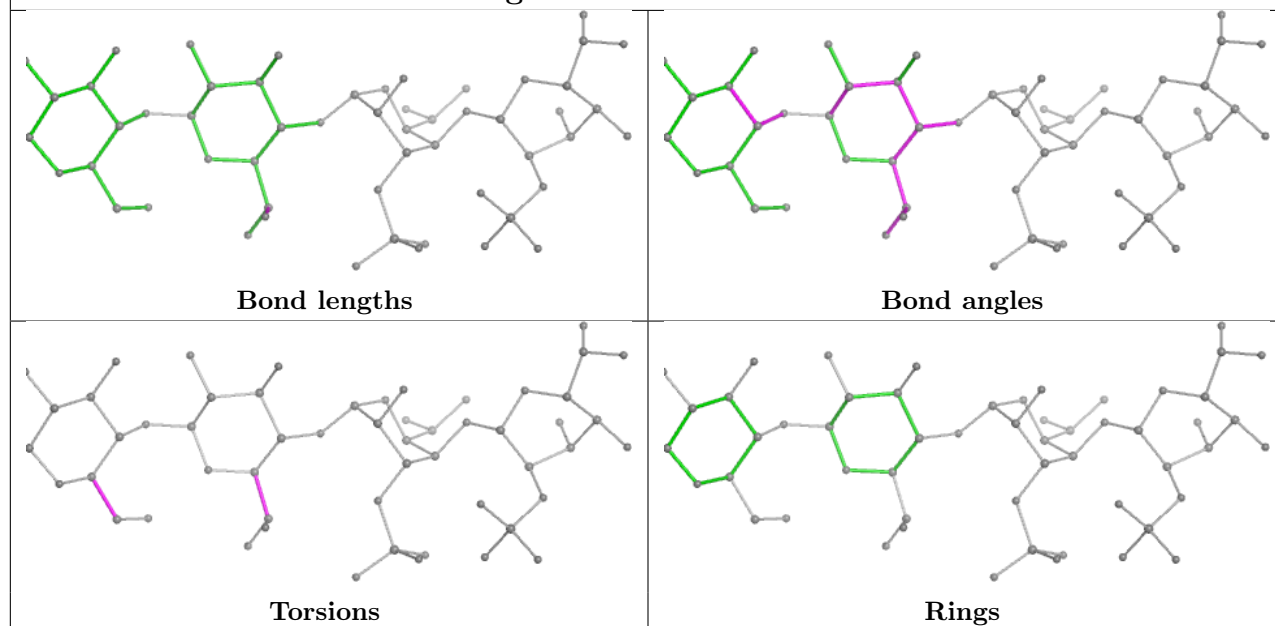
## Oligosaccharide Chain 7

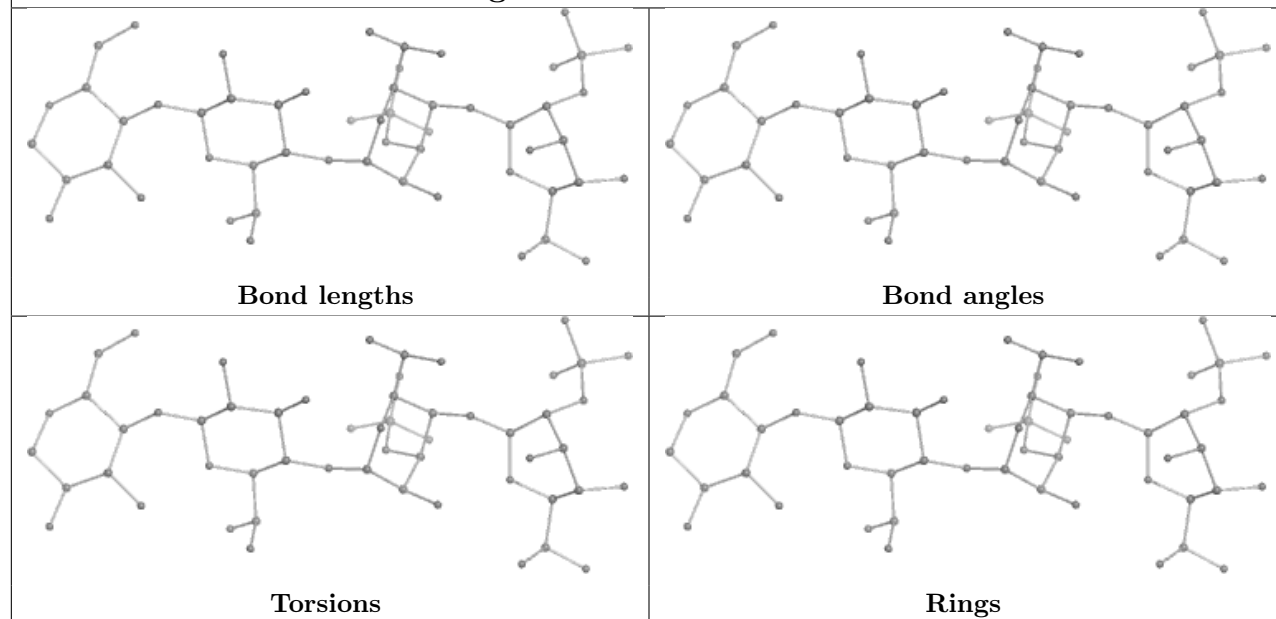
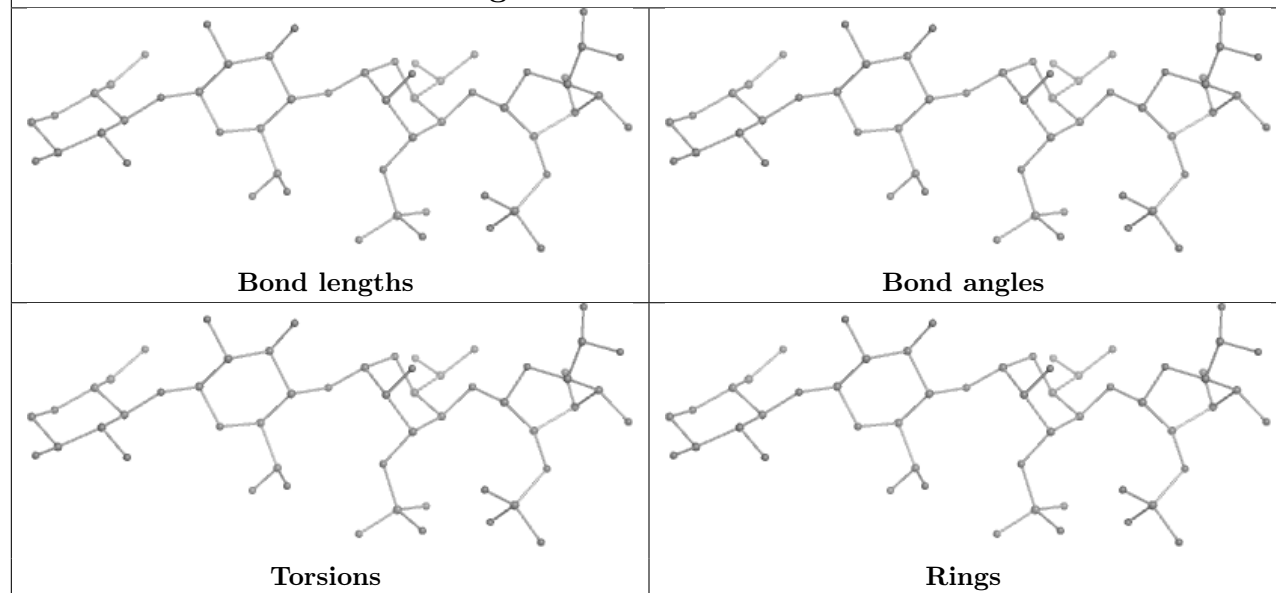


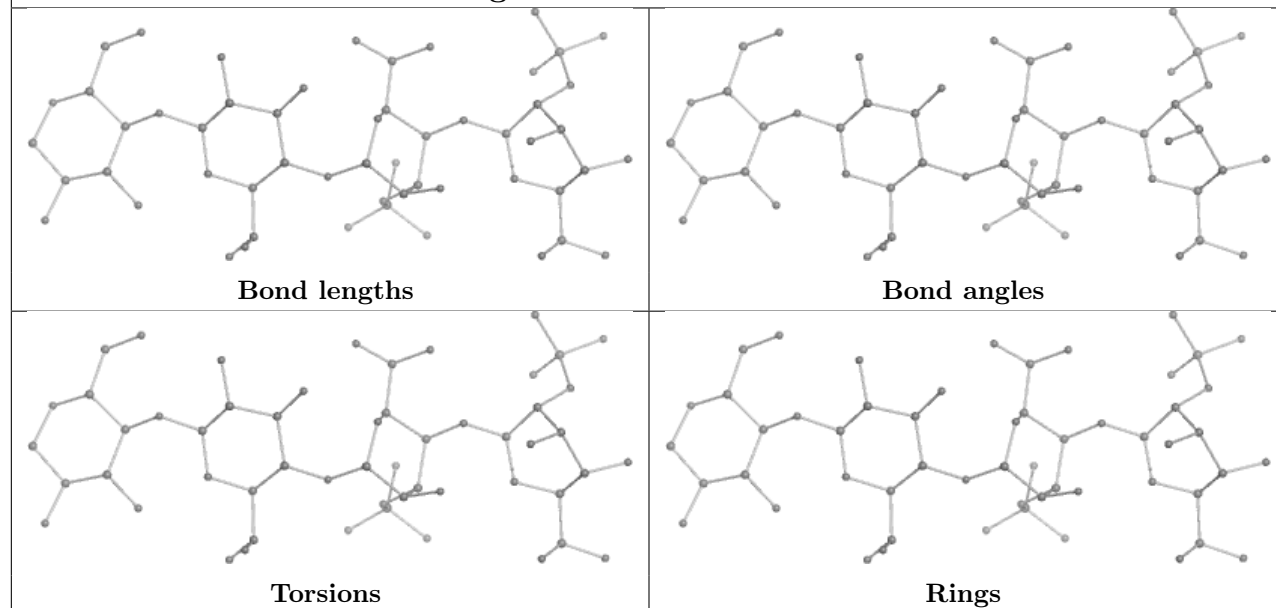
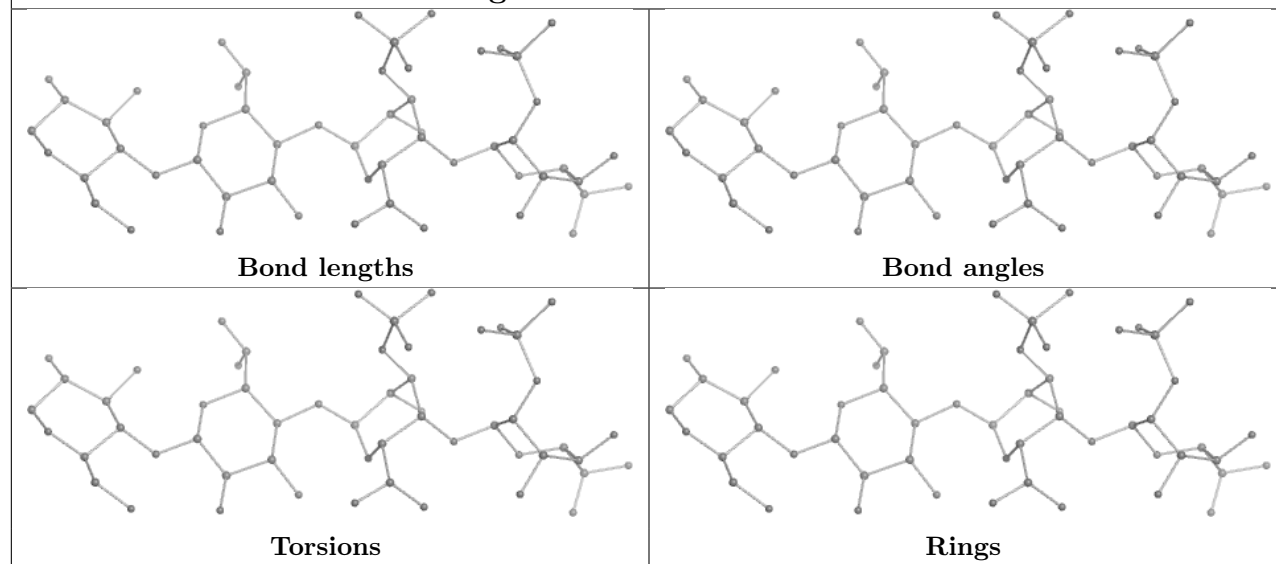
## Oligosaccharide Chain 8

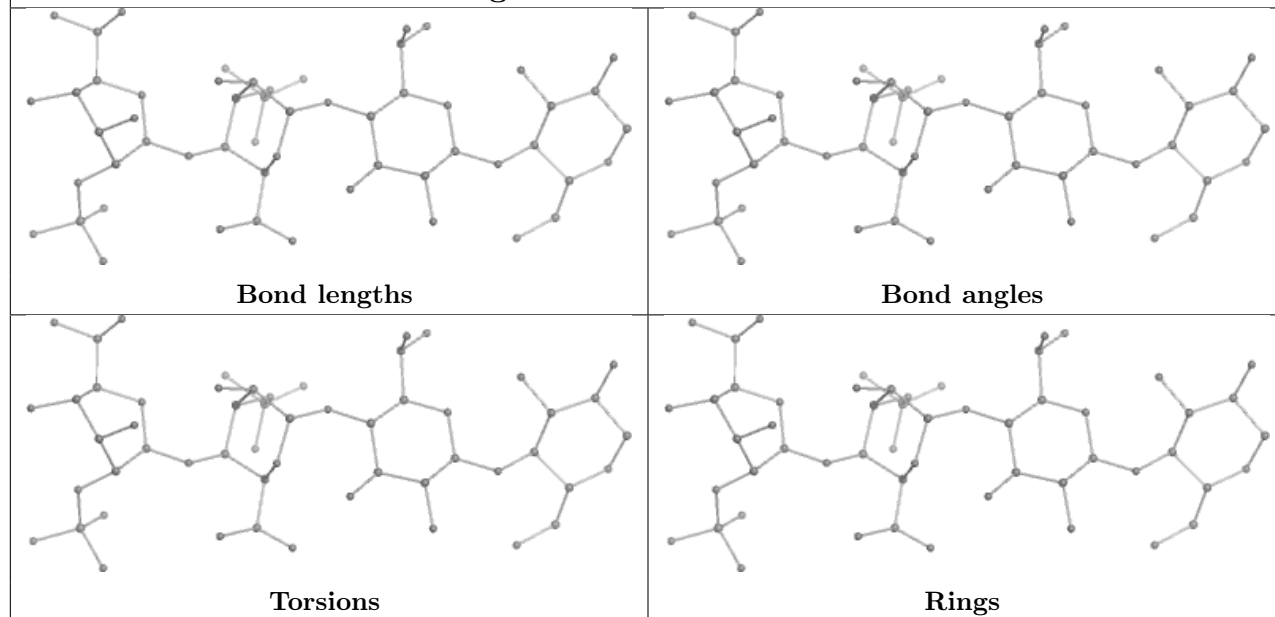
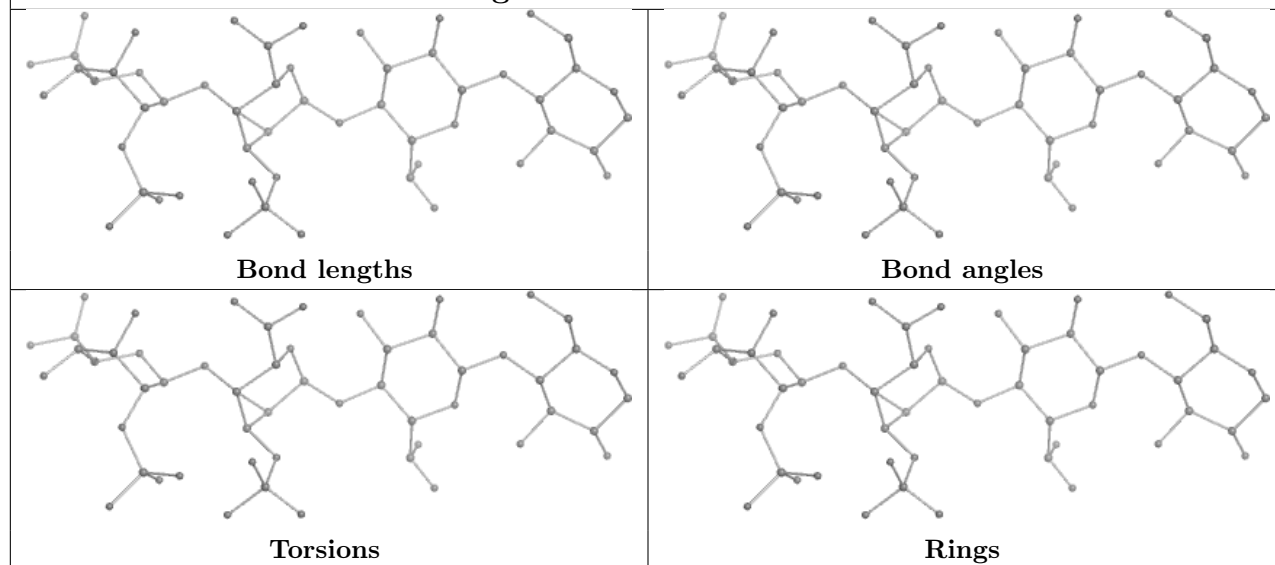


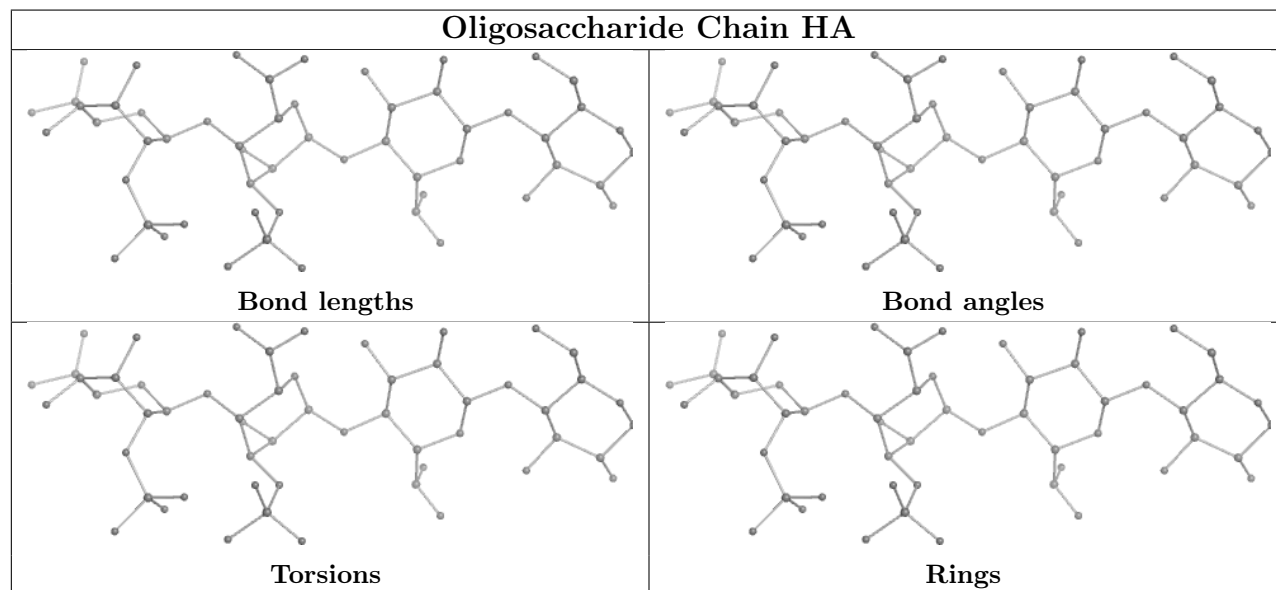
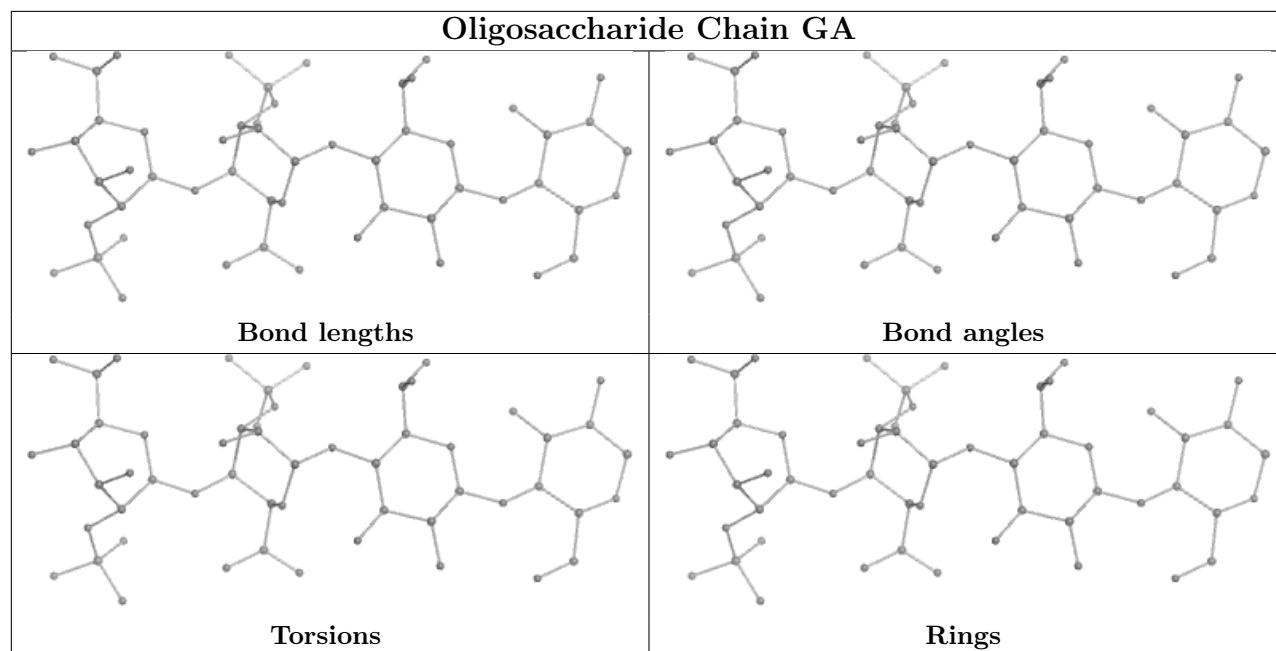
## Oligosaccharide Chain 9

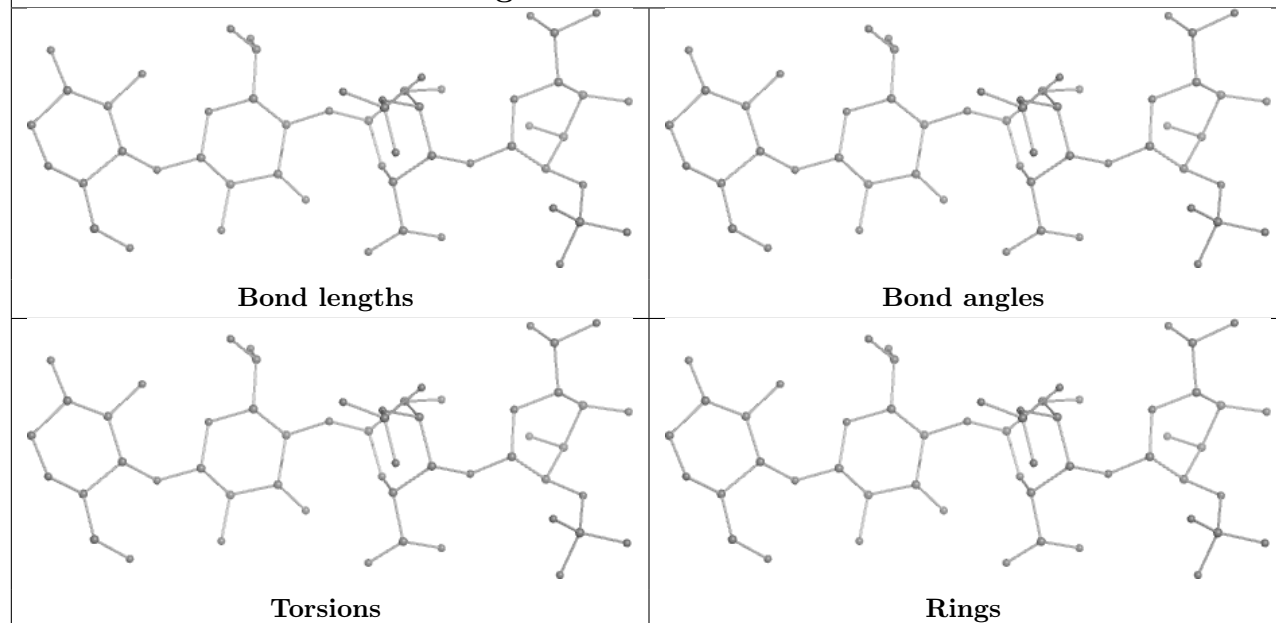
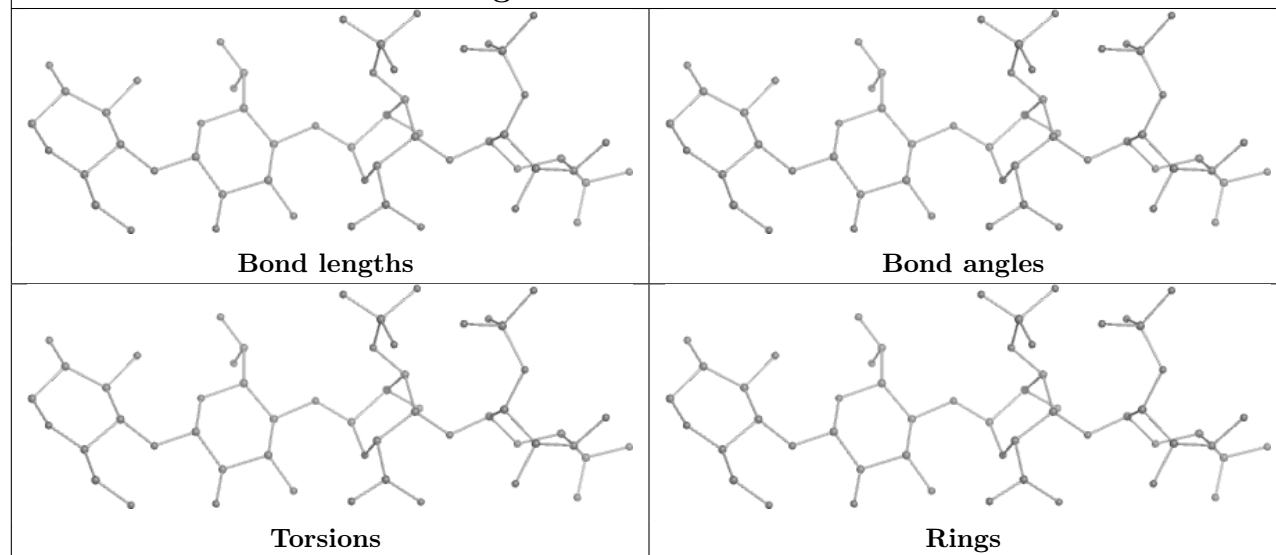


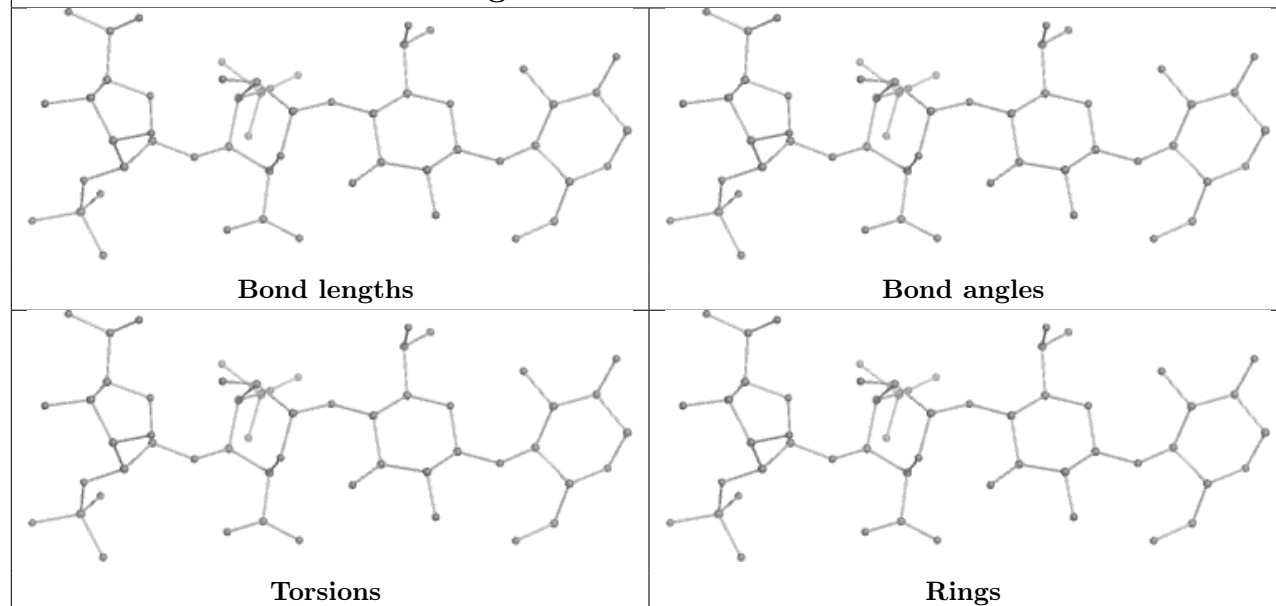
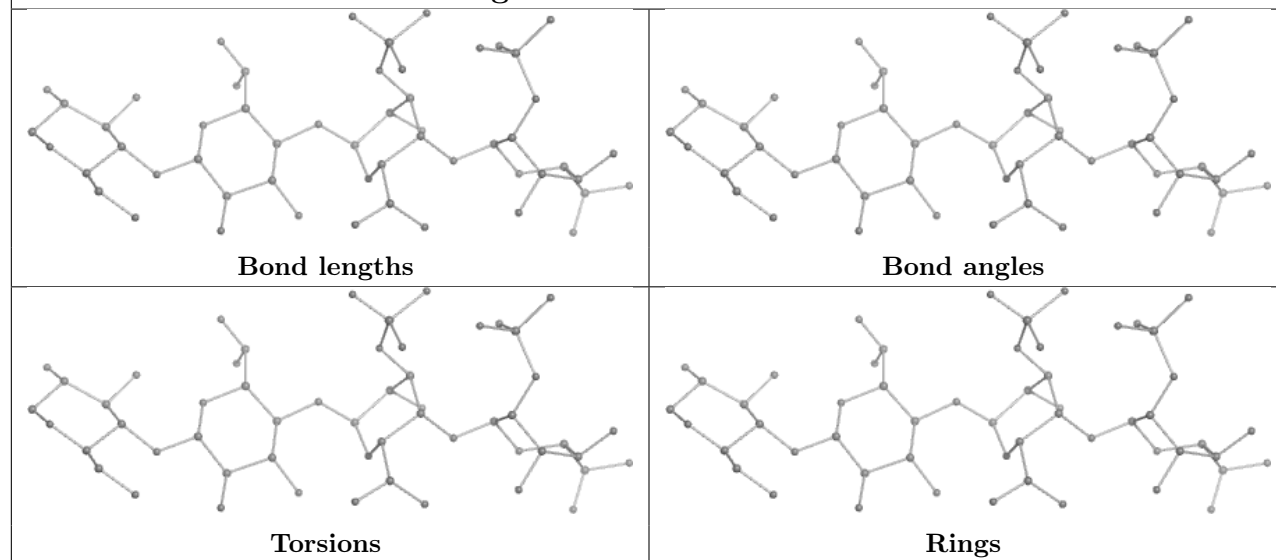
**Oligosaccharide Chain AA****Oligosaccharide Chain BA**

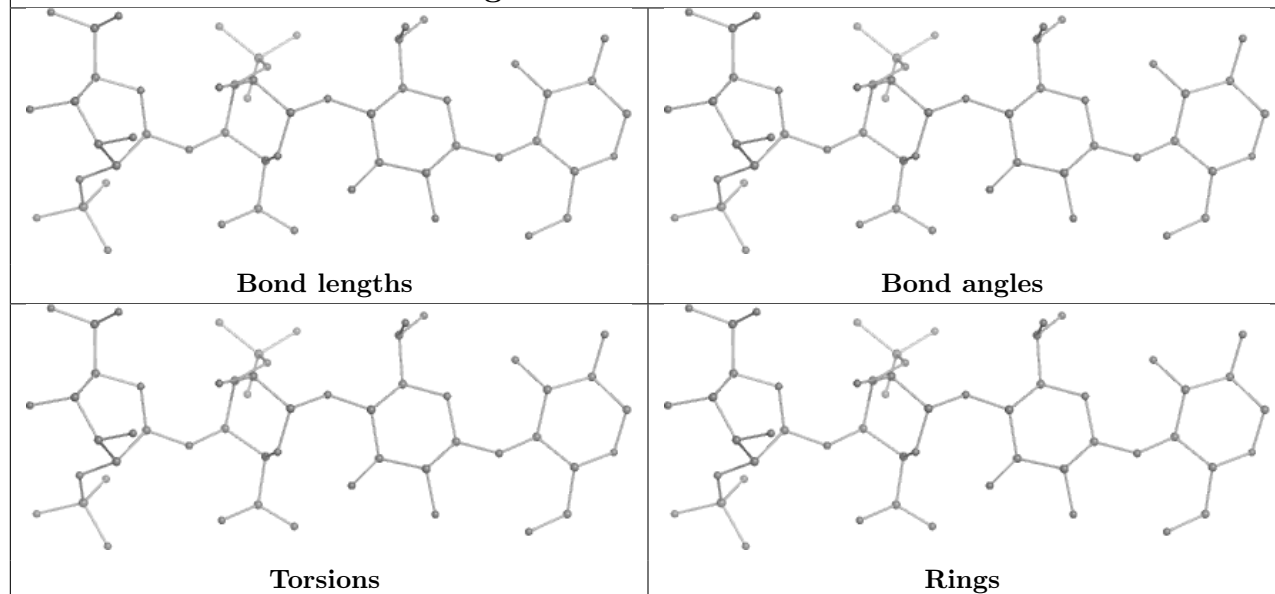
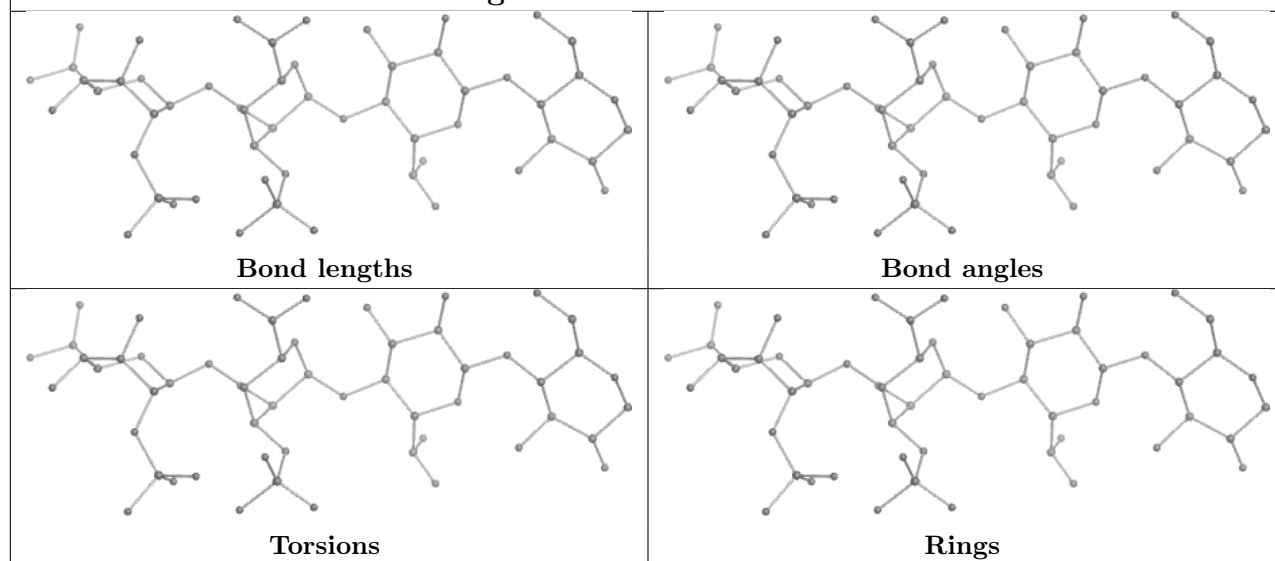
**Oligosaccharide Chain CA****Oligosaccharide Chain DA**

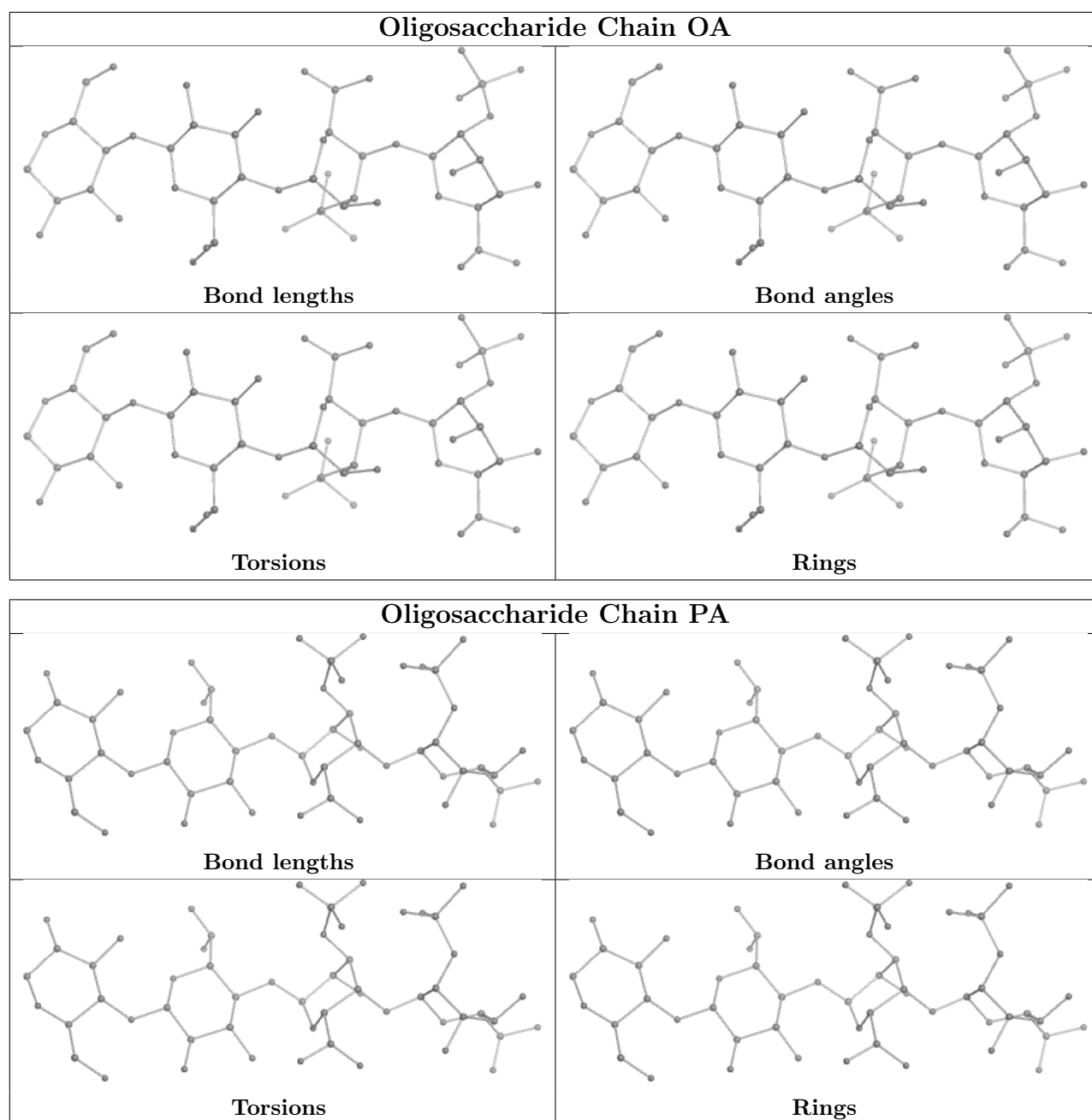
**Oligosaccharide Chain EA****Oligosaccharide Chain FA**



**Oligosaccharide Chain IA****Oligosaccharide Chain JA**

**Oligosaccharide Chain KA****Oligosaccharide Chain LA**

**Oligosaccharide Chain MA****Oligosaccharide Chain NA**



## 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.

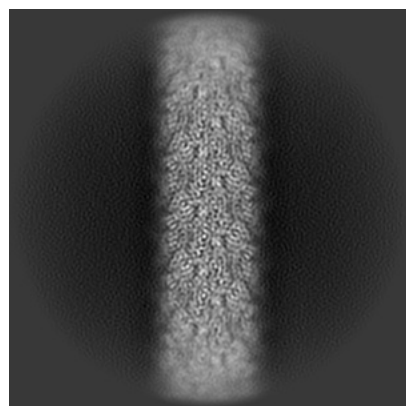
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19905. These allow visual inspection of the internal detail of the map and identification of artifacts.

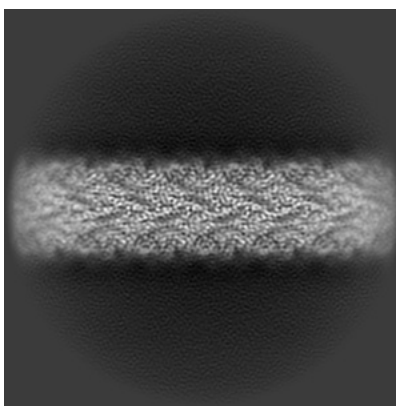
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

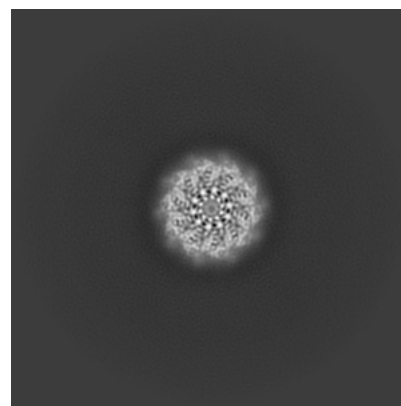
#### 6.1.1 Primary map



X

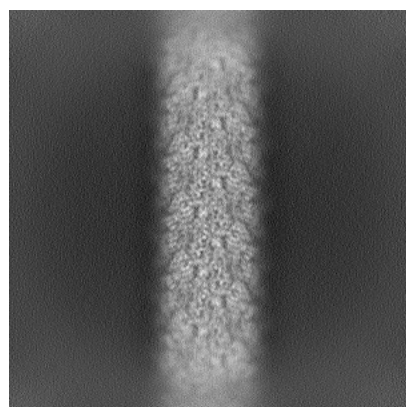


Y

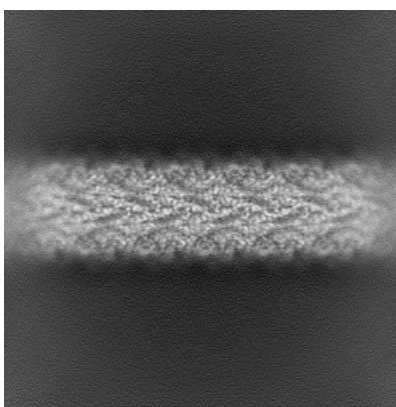


Z

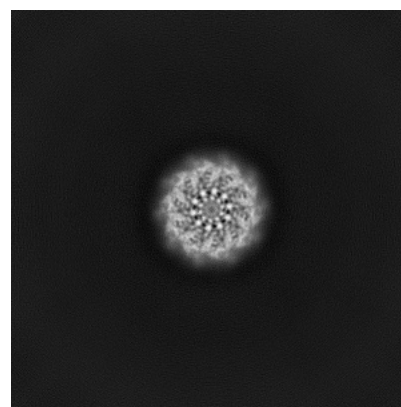
#### 6.1.2 Raw map



X



Y

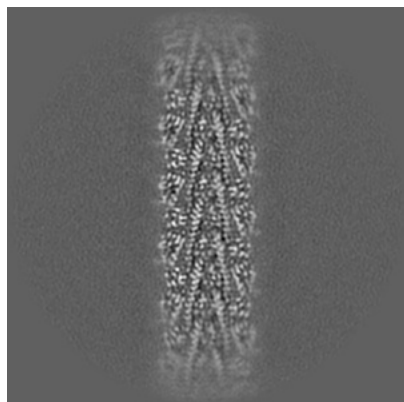


Z

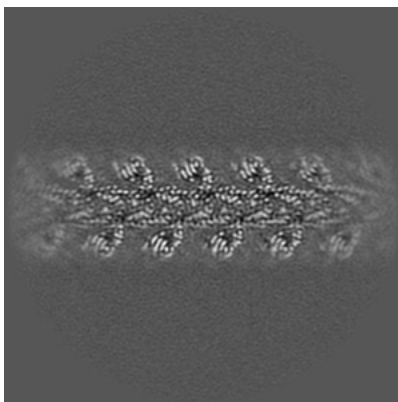
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

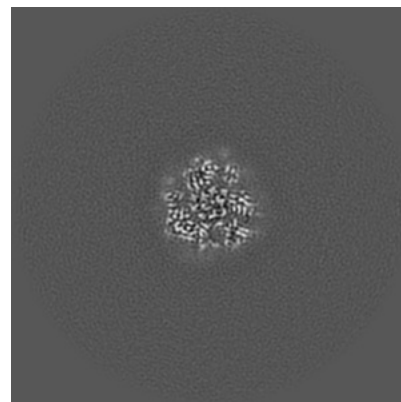
### 6.2.1 Primary map



X Index: 208

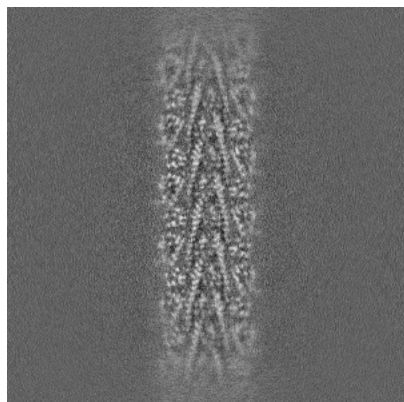


Y Index: 208

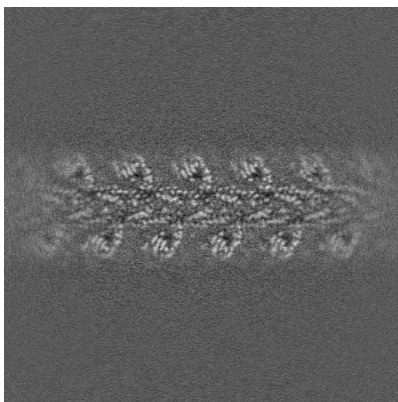


Z Index: 208

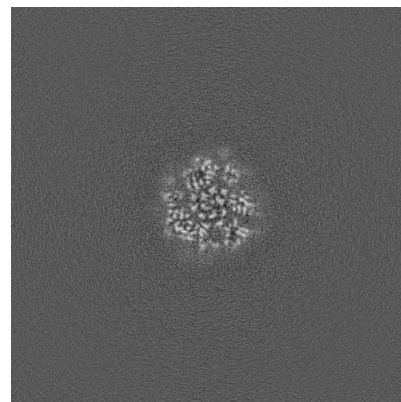
### 6.2.2 Raw map



X Index: 208



Y Index: 208

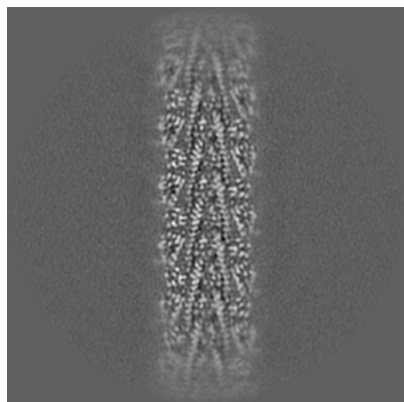


Z Index: 208

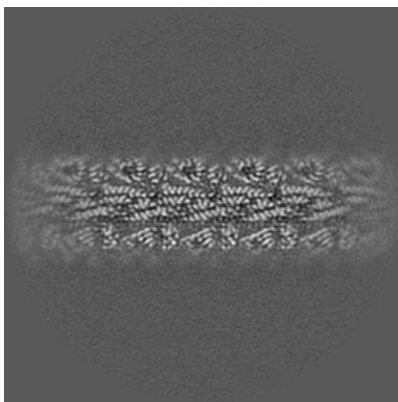
The images above show central slices of the map in three orthogonal directions.

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

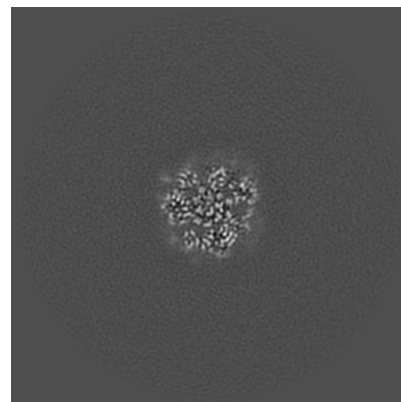
### 6.3.1 Primary map



X Index: 208

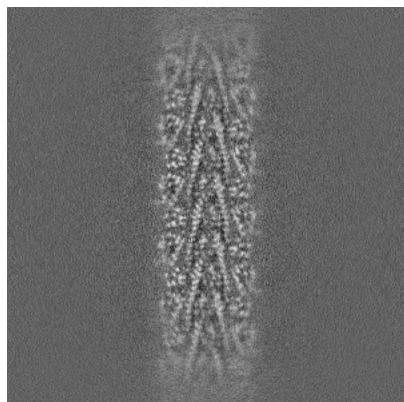


Y Index: 199

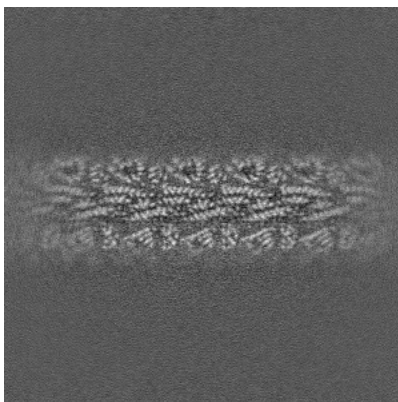


Z Index: 172

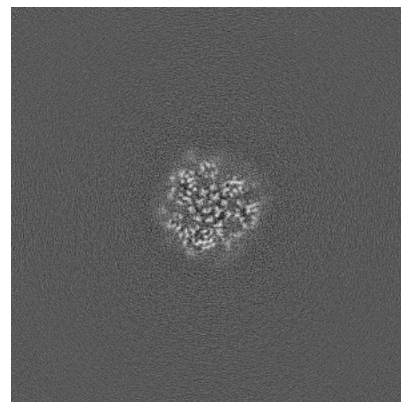
### 6.3.2 Raw map



X Index: 208



Y Index: 199

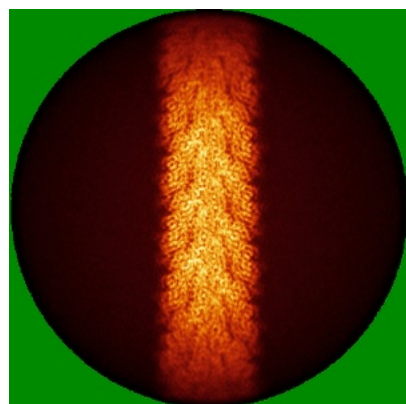


Z Index: 190

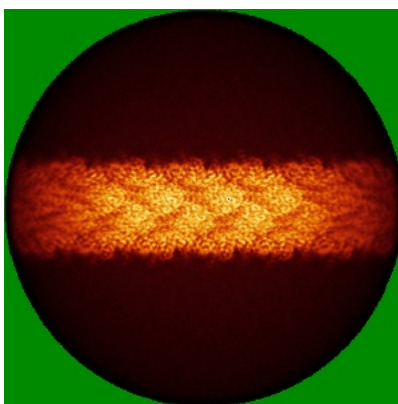
The images above show the largest variance slices of the map in three orthogonal directions.

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

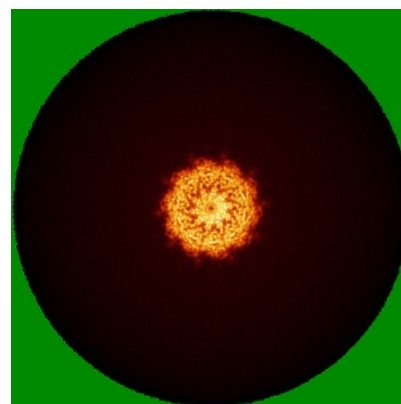
### 6.4.1 Primary map



X

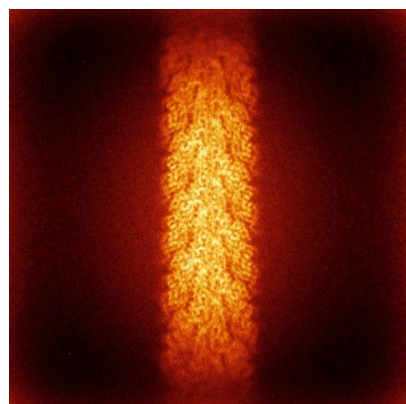


Y

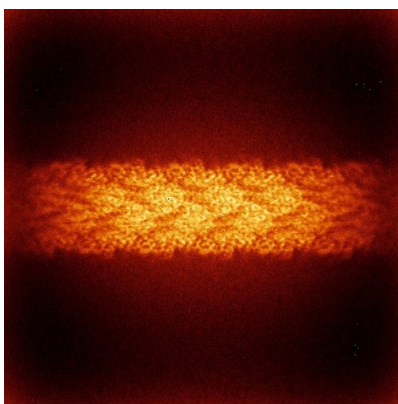


Z

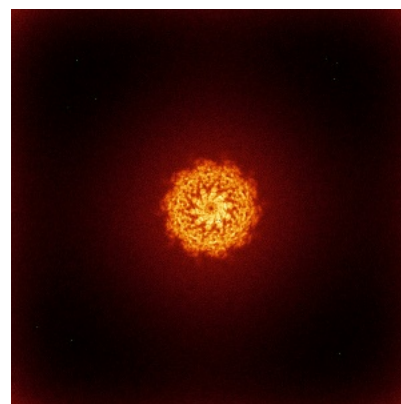
### 6.4.2 Raw map



X



Y

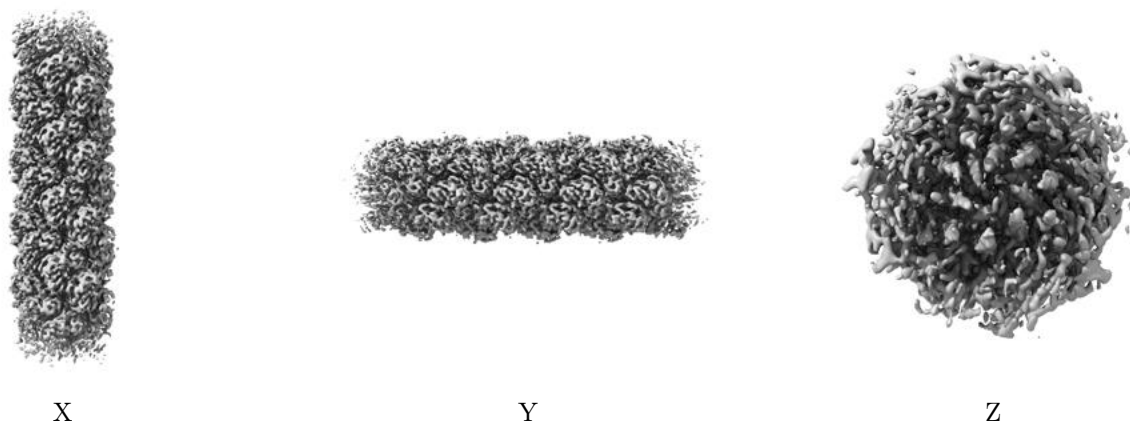


Z

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.

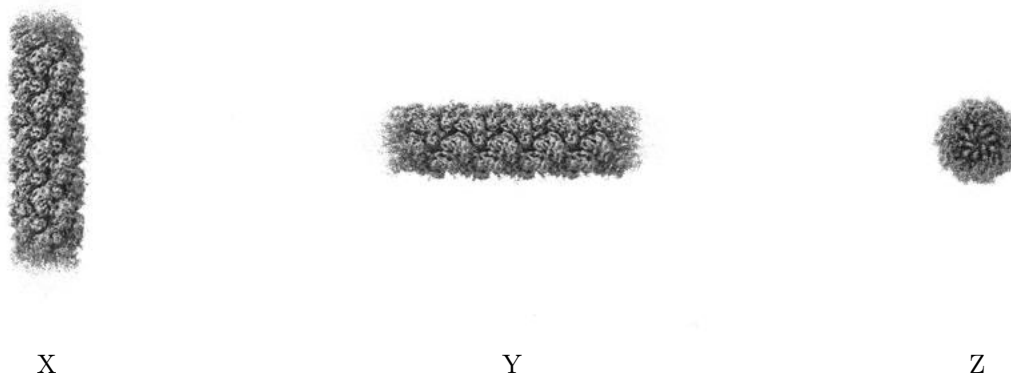
## 6.5 Orthogonal surface views [i](#)

### 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.

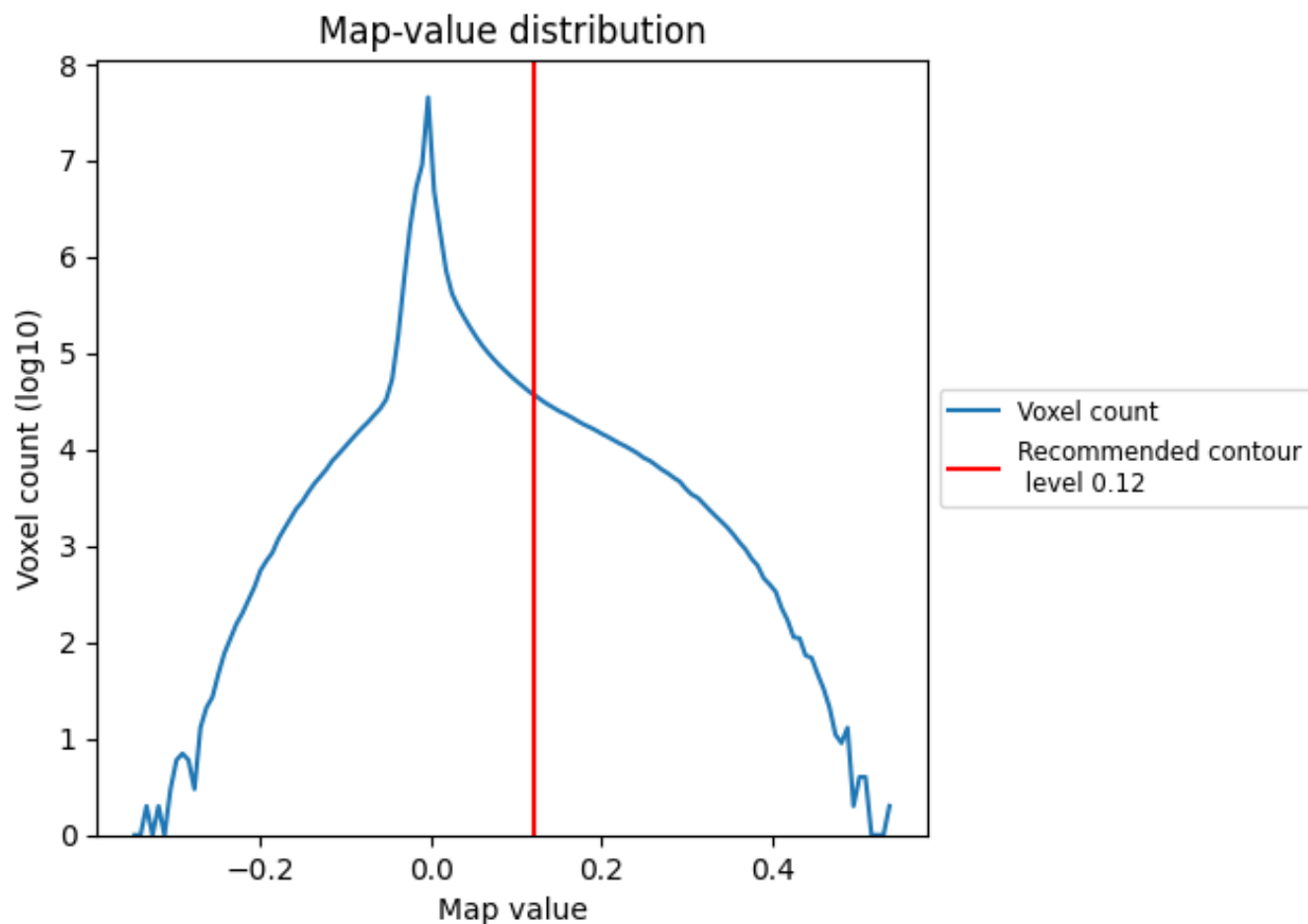
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

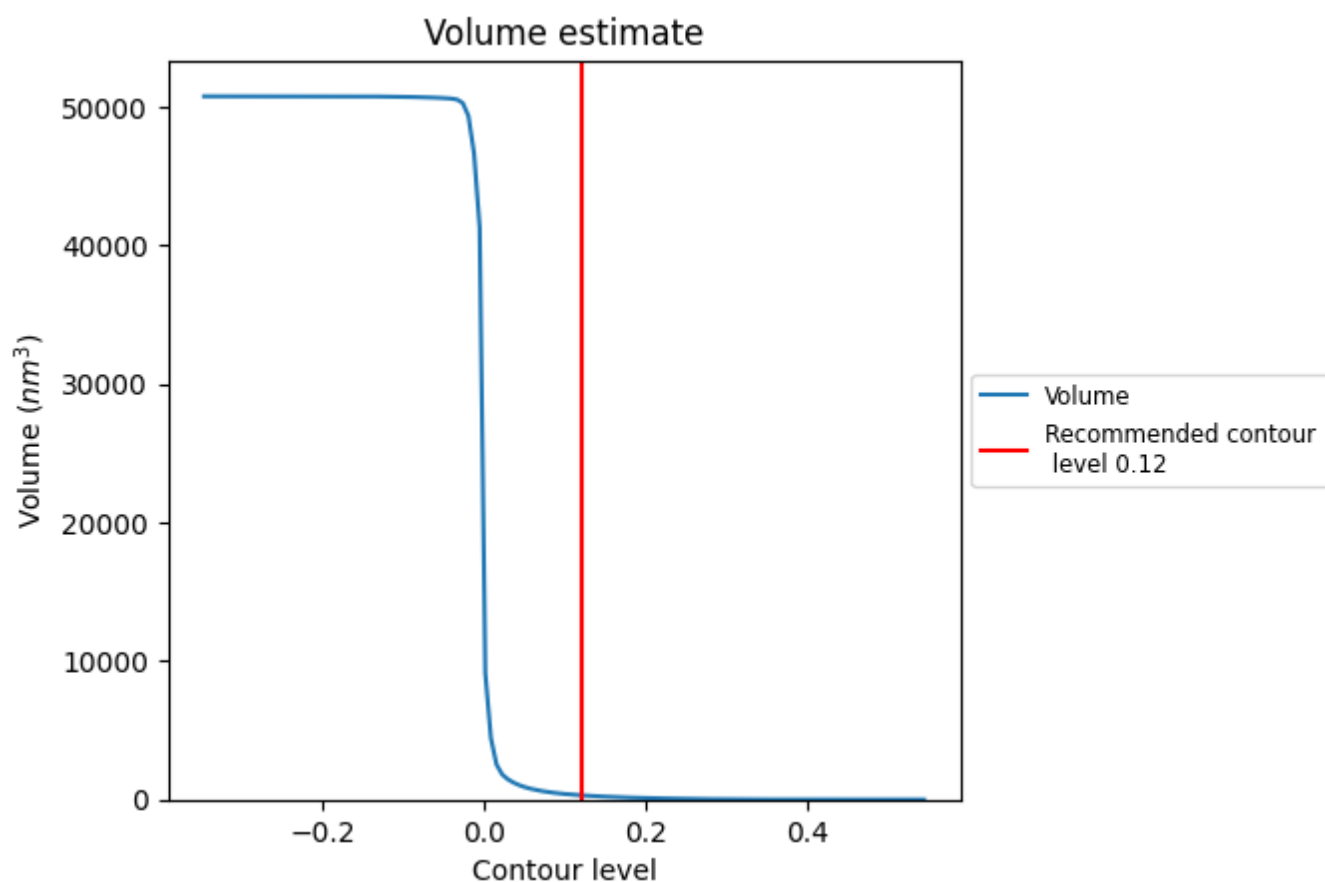
This section contains the results of statistical analysis of the map.

### 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.

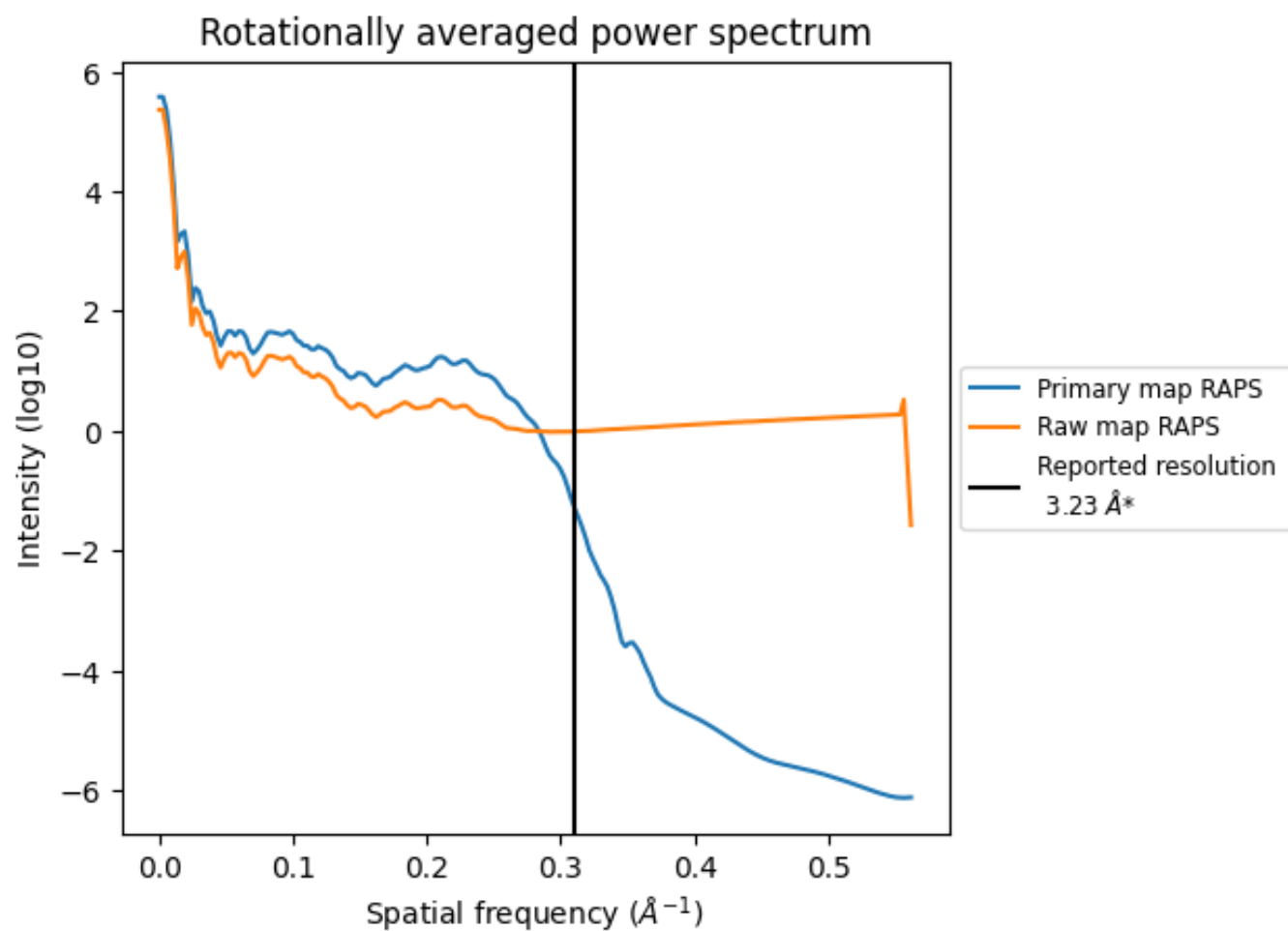
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm<sup>3</sup>; this corresponds to an approximate mass of 278 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 ⓘ

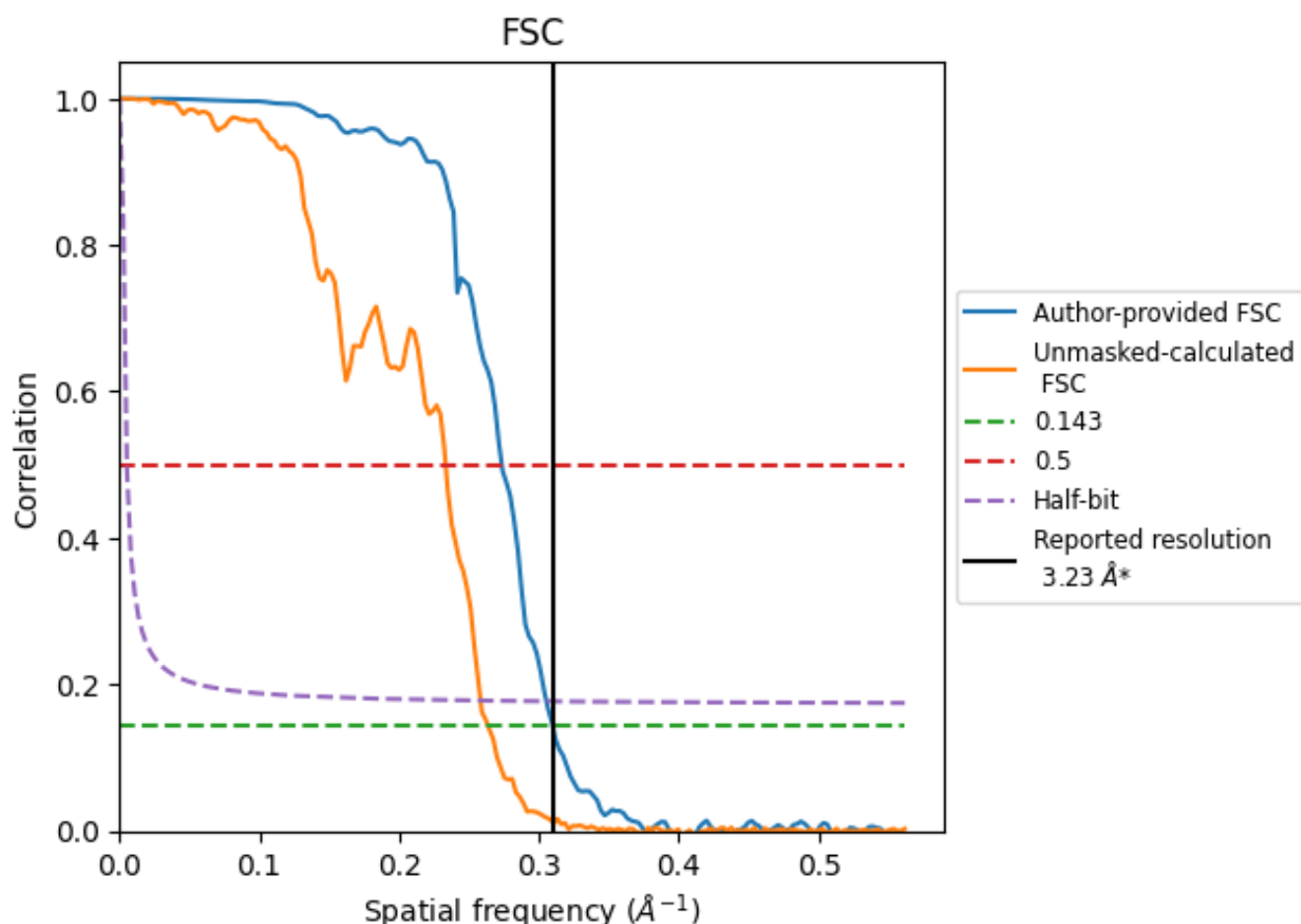


\*Reported resolution corresponds to spatial frequency of 0.310  $\text{\AA}^{-1}$

## 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 0.310 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

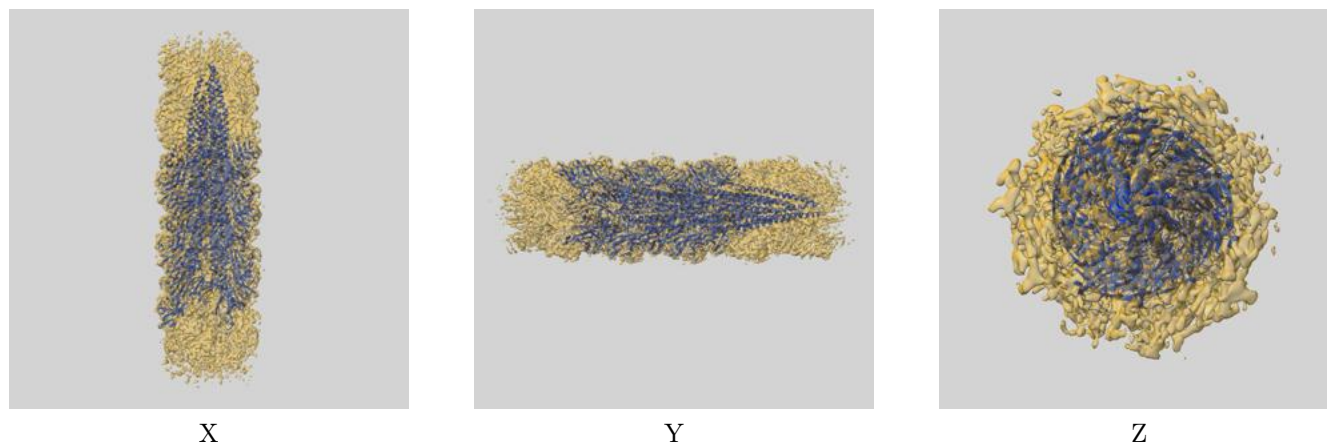
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.66	3.27
Unmasked-calculated*	3.79	4.29	3.87

\*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 3.79 differs from the reported value 3.23 by more than 10 %

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

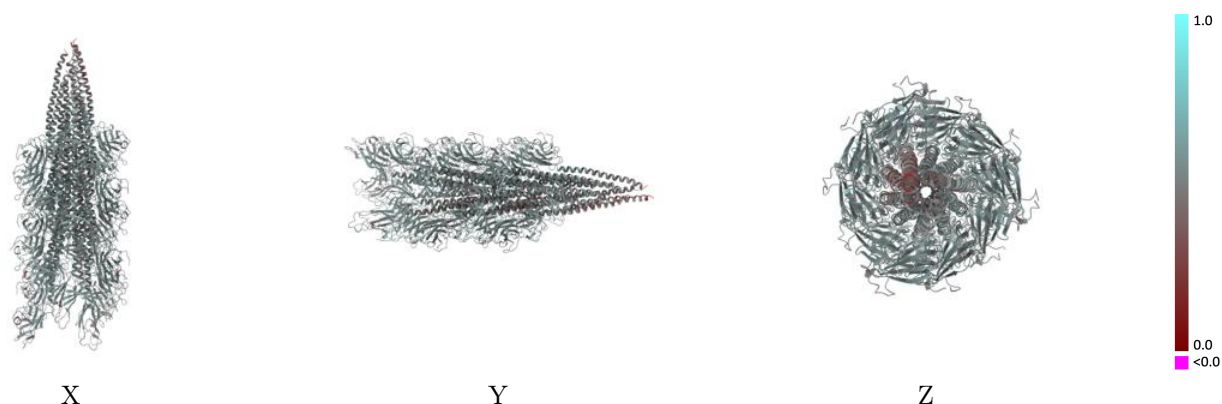
This section contains information regarding the fit between EMDB map EMD-19905 and PDB model 9EQ7. Per-residue inclusion information can be found in section 3 on page 11.

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



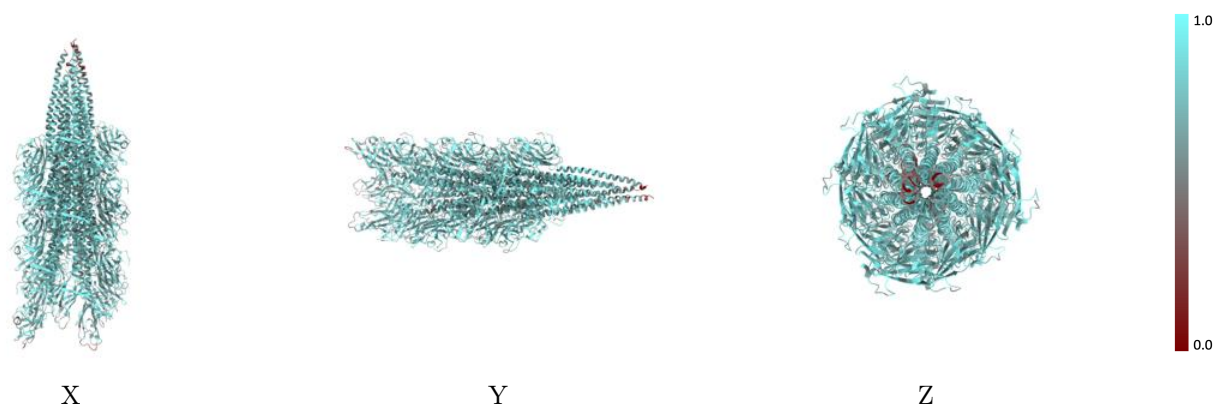
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



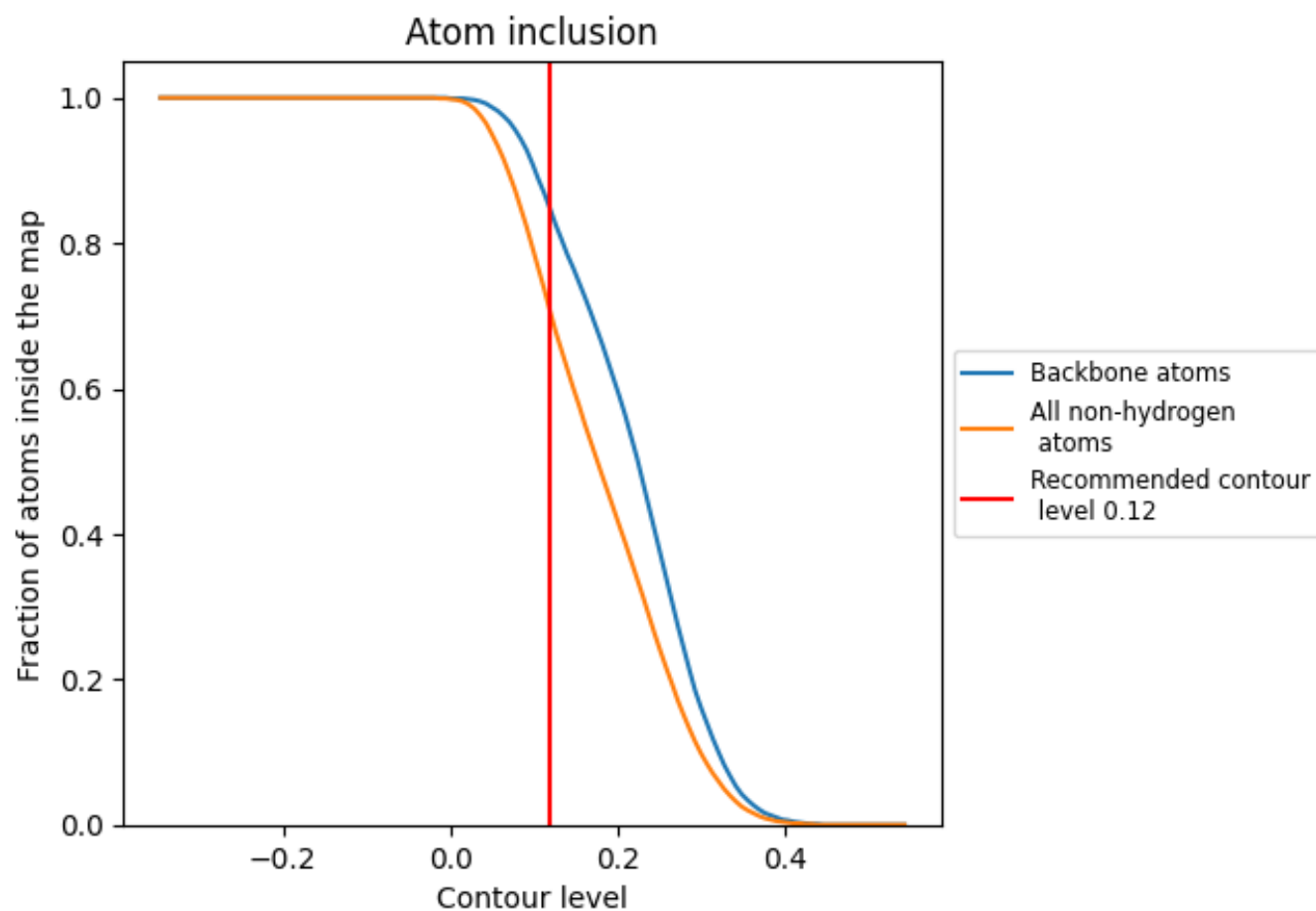
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 71% 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	 0.7060	 0.5070
0	 0.3090	 0.3420
1	 0.2360	 0.3960
2	 0.2550	 0.3480
3	 0.2180	 0.3190
4	 0.2180	 0.3570
5	 0.2180	 0.2830
6	 0.2360	 0.4220
7	 0.2000	 0.2860
8	 0.2910	 0.3430
9	 0.2550	 0.3190
A	 0.7370	 0.5250
AA	 0.2730	 0.3370
B	 0.7460	 0.5260
BA	 0.2360	 0.3460
C	 0.7510	 0.5310
CA	 0.2360	 0.3080
D	 0.7190	 0.5040
DA	 0.2000	 0.2930
E	 0.7220	 0.5040
EA	 0.2360	 0.4020
F	 0.7350	 0.5220
FA	 0.2000	 0.3540
G	 0.6960	 0.5130
GA	 0.2730	 0.3910
H	 0.7480	 0.5260
HA	 0.1820	 0.3570
I	 0.7590	 0.5220
IA	 0.2910	 0.3290
J	 0.7760	 0.5360
JA	 0.2360	 0.3110
K	 0.7790	 0.5330
KA	 0.2910	 0.3260
L	 0.7690	 0.5330
LA	 0.1820	 0.3500







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Chain	Atom inclusion	Q-score
M	 0.7750	 0.5260
MA	 0.2550	 0.3760
N	 0.7650	 0.5130
NA	 0.1820	 0.3020
O	 0.7450	 0.5150
OA	 0.1640	 0.2190
P	 0.7540	 0.5330
PA	 0.1450	 0.2540
Q	 0.7660	 0.5350
R	 0.7710	 0.5290
S	 0.7550	 0.5260
T	 0.7440	 0.5260
U	 0.7640	 0.5220
V	 0.7460	 0.5080
W	 0.7800	 0.5330
X	 0.7490	 0.5300
Y	 0.7080	 0.5010
Z	 0.6880	 0.5080
a	 0.2910	 0.3860
b	 0.1640	 0.3010
c	 0.2550	 0.3950
d	 0.1820	 0.2920
e	 0.2730	 0.3730
f	 0.2000	 0.3110
g	 0.1820	 0.3210
h	 0.2000	 0.3000
i	 0.1820	 0.3480
j	 0.1820	 0.3750
k	 0.2550	 0.3710
l	 0.2000	 0.3060
m	 0.2360	 0.3990
n	 0.1820	 0.2970
o	 0.2550	 0.3270
p	 0.2180	 0.3430
q	 0.2000	 0.3260
r	 0.1820	 0.3140
s	 0.2910	 0.3830
t	 0.2180	 0.2790
u	 0.3090	 0.3530
v	 0.2000	 0.2670
w	 0.2360	 0.3560
x	 0.2180	 0.2330

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Chain	Atom inclusion	Q-score
y	 0.3090	 0.3550
z	 0.1820	 0.2810