



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:54 PM UTC

PDB ID : 8ZHK / pdb_00008zhk
EMDB ID : EMD-60106
Title : SARS-CoV-2 spike trimer (6P) in complex with three H18 Fabs, head-to-head aggregate (C3 symmetry)
Authors : Yan, Q.; Gao, X.; Liu, B.; Hou, R.; He, P.; Li, Z.; Chen, Q.; Wang, J.; He, J.; Chen, L.; Zhao, J.; Xiong, X.
Deposited on : 2024-05-11
Resolution : 6.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

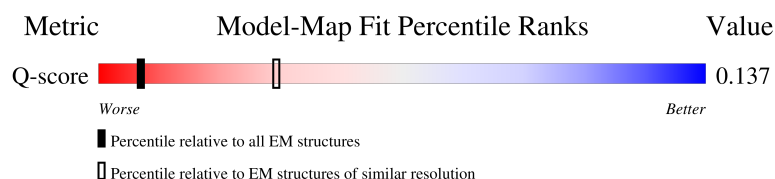
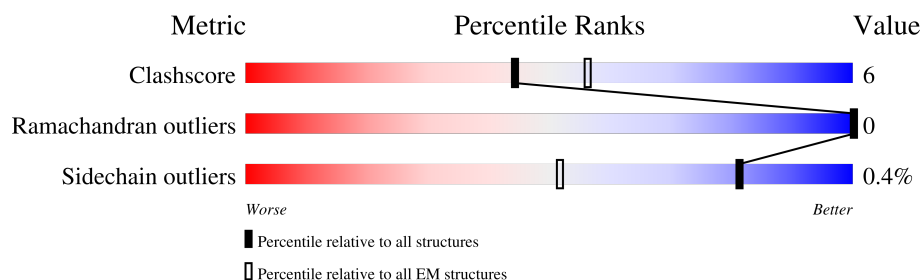
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

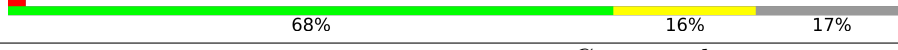
The reported resolution of this entry is 6.30 Å.

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



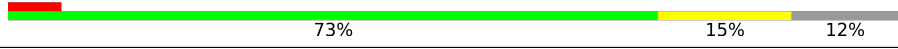
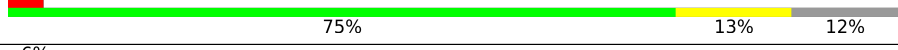
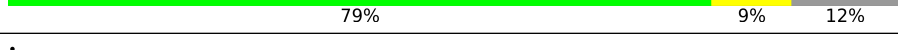
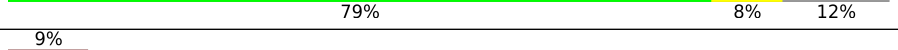
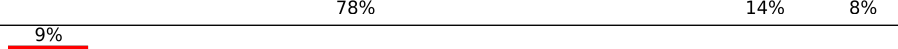
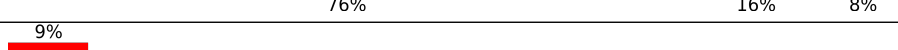
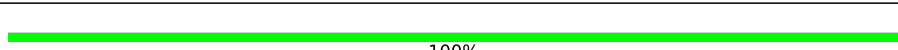
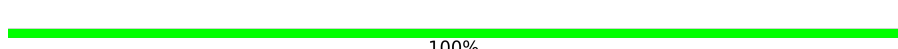
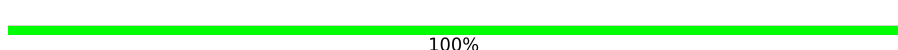
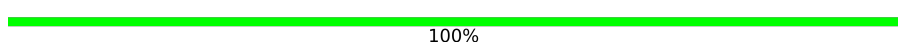
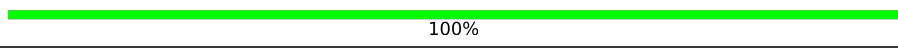
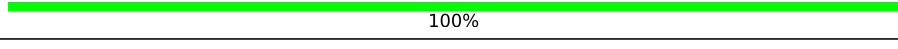
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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

Mol	Chain	Length	Quality of chain
1	A	1278	
1	B	1278	
1	C	1278	
1	G	1278	

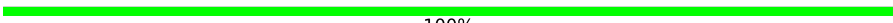
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Mol	Chain	Length	Quality of chain
1	H	1278	
1	I	1278	
2	D	243	
2	F	243	
2	K	243	
2	L	243	
2	O	243	
2	Q	243	
3	E	243	
3	J	243	
3	M	243	
3	N	243	
3	P	243	
3	R	243	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	c	2	

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Mol	Chain	Length	Quality of chain
4	d	2	 100%
4	e	2	 100%
4	f	2	 100%
4	g	2	 100%
4	h	2	 100%
4	i	2	 50%50%
4	j	2	 100%
4	k	2	 50%50%
4	l	2	 100%
4	m	2	 50%50%
4	n	2	 100%
4	o	2	 50%50%
4	p	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 71238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	B	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	C	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	G	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	H	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	I	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
G	682	GLY	ARG	conflict	UNP P0DTC2
G	683	SER	ARG	conflict	UNP P0DTC2
G	685	SER	ARG	conflict	UNP P0DTC2
G	817	PRO	PHE	conflict	UNP P0DTC2
G	892	PRO	ALA	conflict	UNP P0DTC2
G	899	PRO	ALA	conflict	UNP P0DTC2
G	942	PRO	ALA	conflict	UNP P0DTC2
G	986	PRO	LYS	variant	UNP P0DTC2
G	987	PRO	VAL	variant	UNP P0DTC2
G	1209	GLY	-	linker	UNP P0DTC2
G	1210	SER	-	linker	UNP P0DTC2
H	682	GLY	ARG	conflict	UNP P0DTC2
H	683	SER	ARG	conflict	UNP P0DTC2
H	685	SER	ARG	conflict	UNP P0DTC2
H	817	PRO	PHE	conflict	UNP P0DTC2
H	892	PRO	ALA	conflict	UNP P0DTC2
H	899	PRO	ALA	conflict	UNP P0DTC2
H	942	PRO	ALA	conflict	UNP P0DTC2
H	986	PRO	LYS	variant	UNP P0DTC2
H	987	PRO	VAL	variant	UNP P0DTC2
H	1209	GLY	-	linker	UNP P0DTC2
H	1210	SER	-	linker	UNP P0DTC2
I	682	GLY	ARG	conflict	UNP P0DTC2
I	683	SER	ARG	conflict	UNP P0DTC2
I	685	SER	ARG	conflict	UNP P0DTC2
I	817	PRO	PHE	conflict	UNP P0DTC2
I	892	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	899	PRO	ALA	conflict	UNP P0DTC2
I	942	PRO	ALA	conflict	UNP P0DTC2
I	986	PRO	LYS	variant	UNP P0DTC2
I	987	PRO	VAL	variant	UNP P0DTC2
I	1209	GLY	-	linker	UNP P0DTC2
I	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called Light chain of H18 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
2	F	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
2	K	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
2	L	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
2	O	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
2	Q	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		

- Molecule 3 is a protein called Heavy chain of H18 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
3	J	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
3	M	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
3	N	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
3	P	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
3	R	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		

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



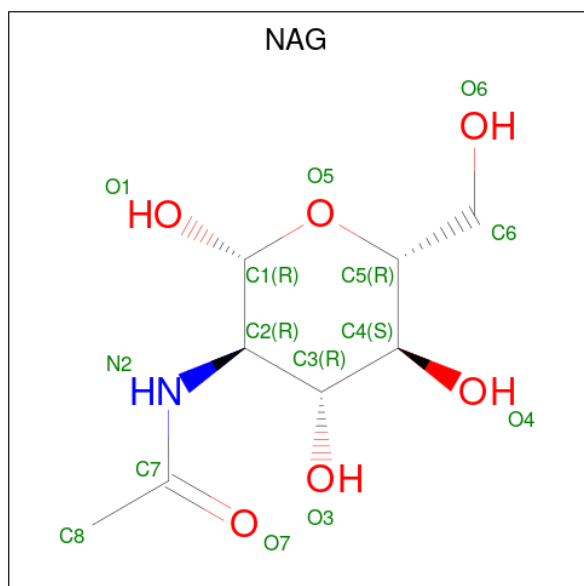
Mol	Chain	Residues	Atoms				AltConf	Trace
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	k	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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

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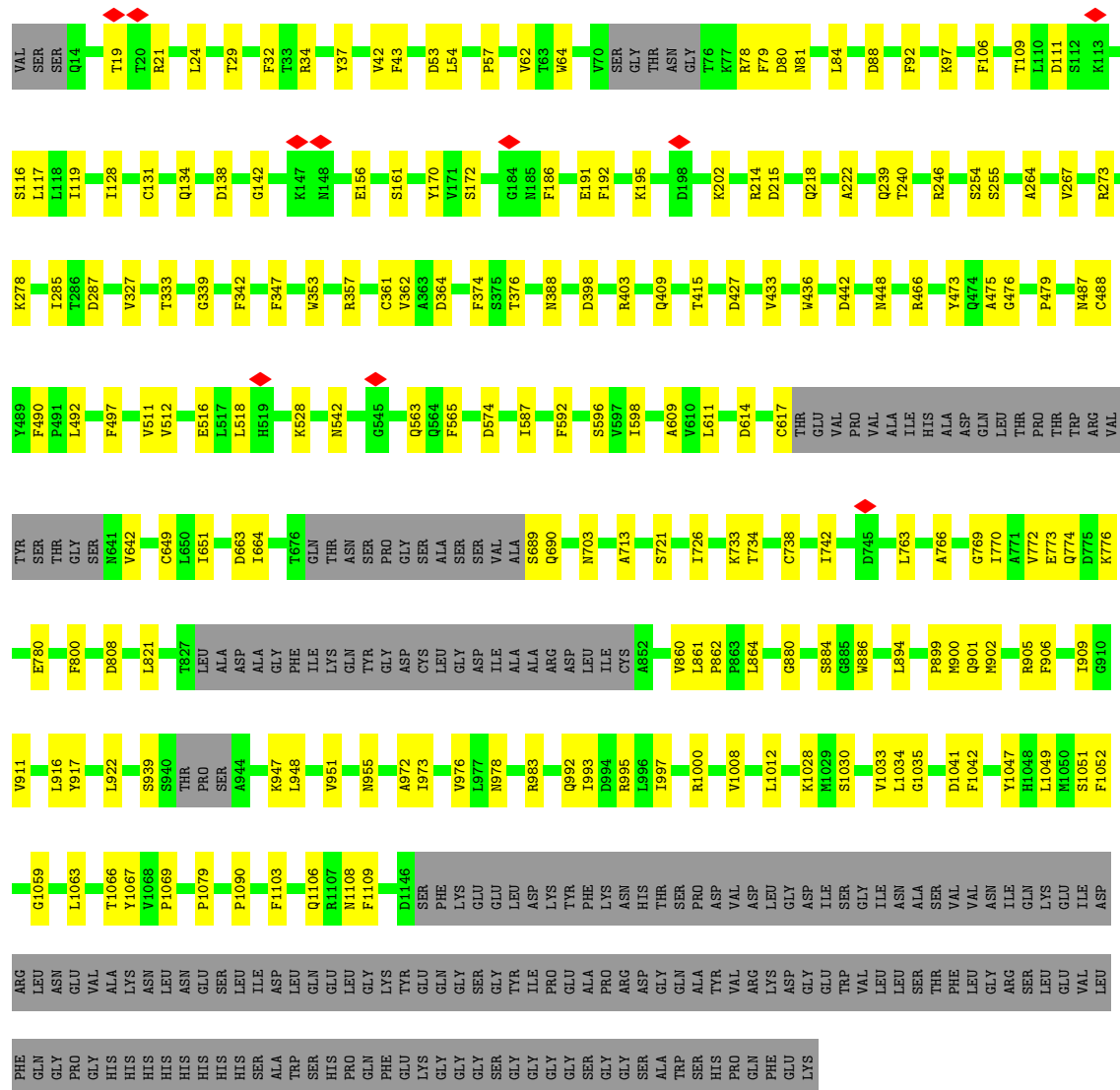
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5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

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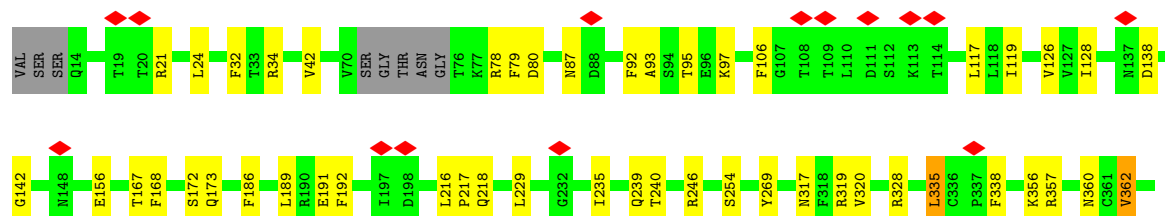
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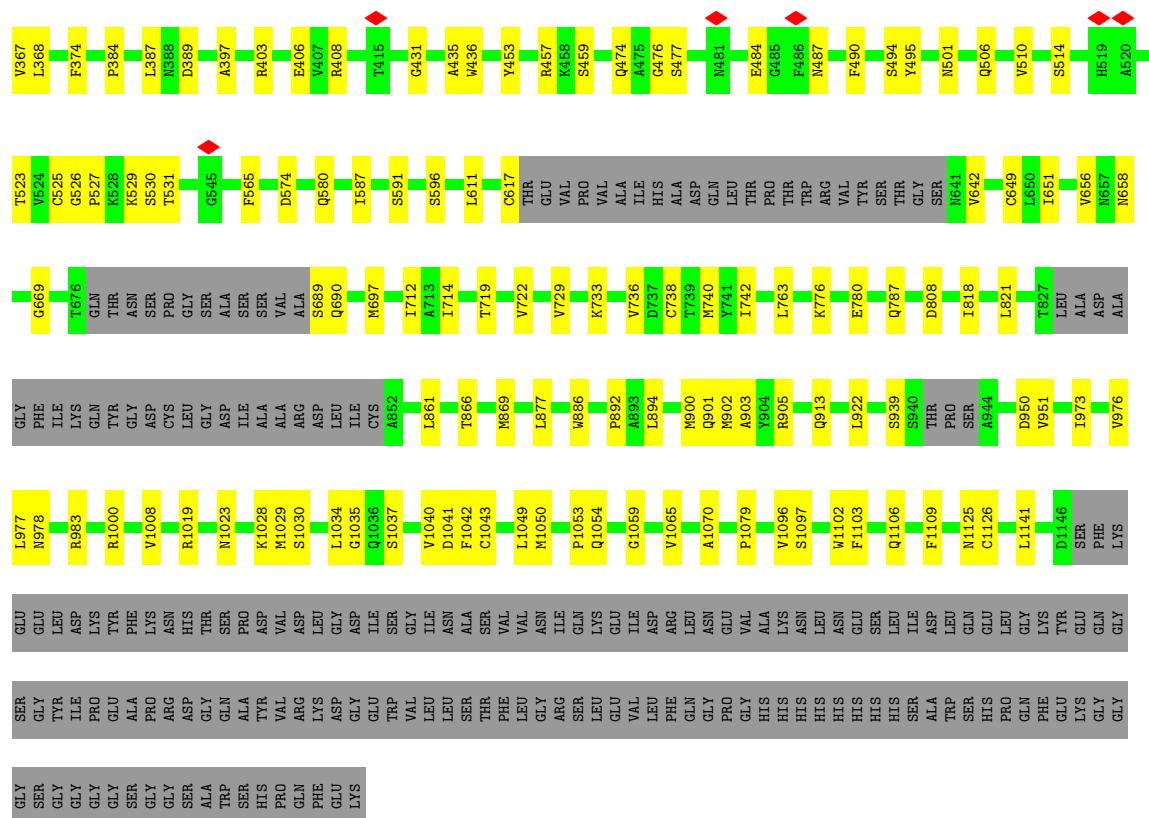
Mol	Chain	Residues	Atoms				AltConf
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5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

Chain B:

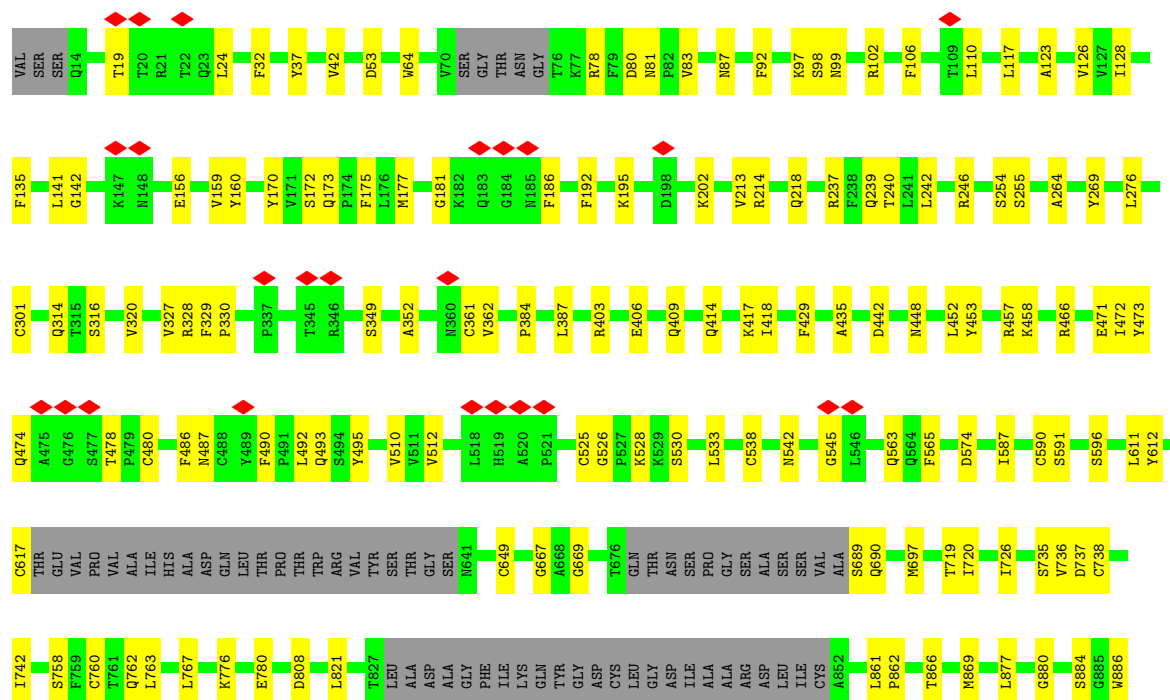


Chain C:

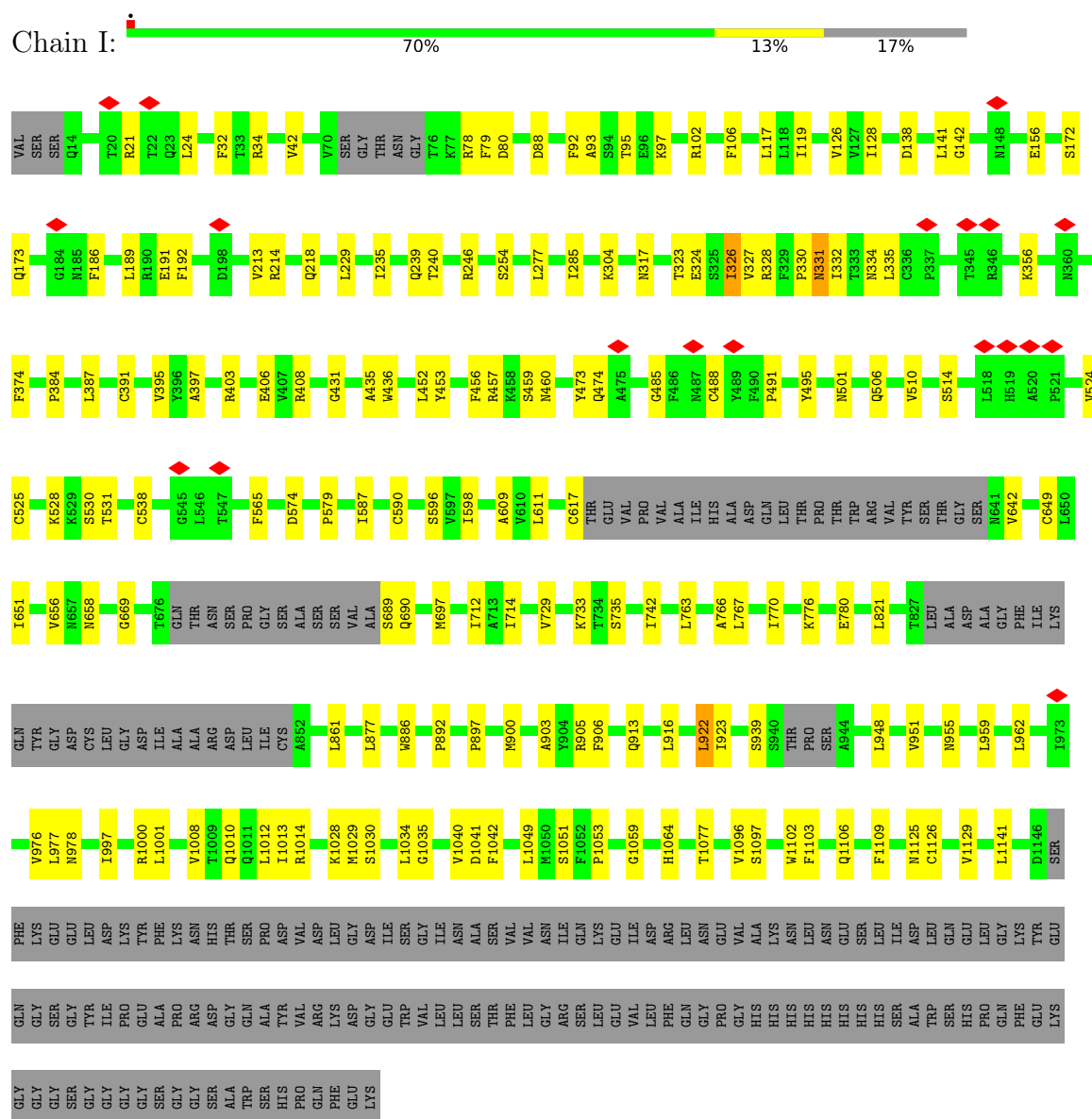




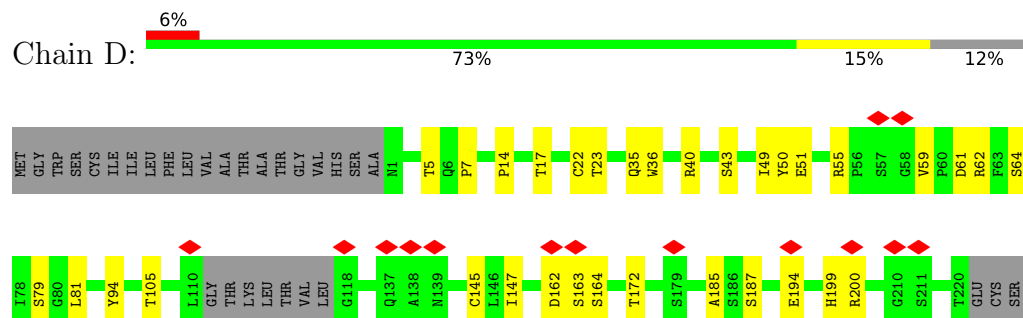
● Molecule 1: Spike glycoprotein,Fibrin,Expression Tag



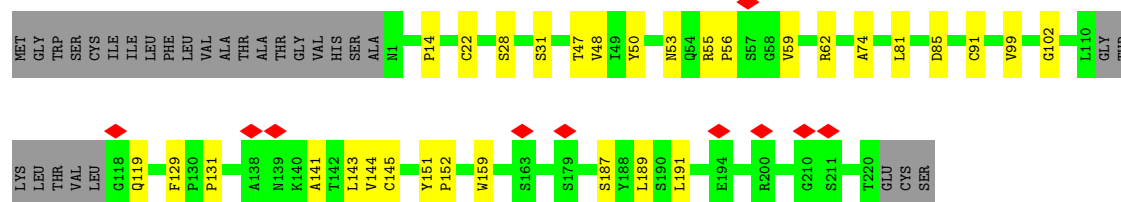
Chain I:



Chain D:

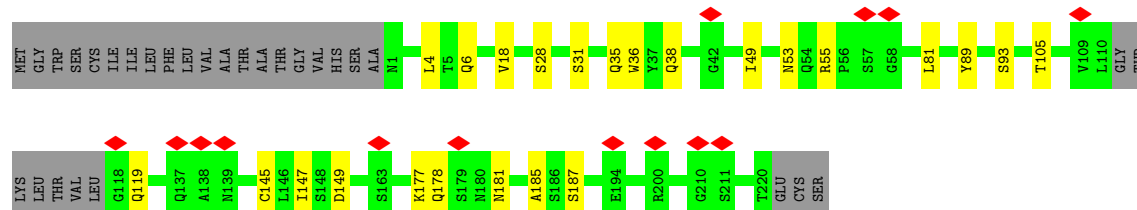


Chain F: 



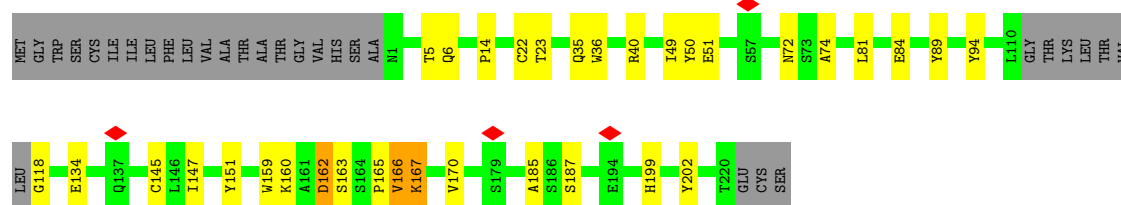
• Molecule 2: Light chain of H18 Fab

Chain K: 



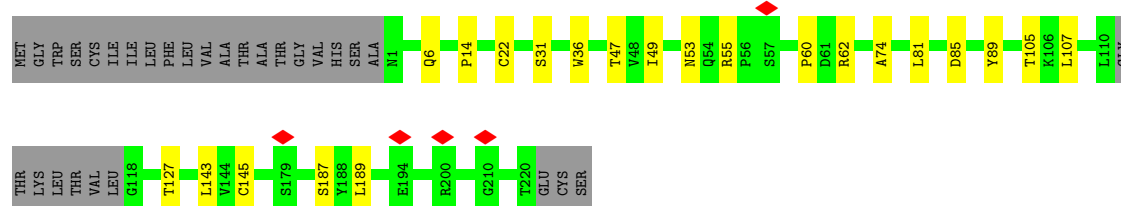
• Molecule 2: Light chain of H18 Fab

Chain L: 



• Molecule 2: Light chain of H18 Fab

Chain O: 



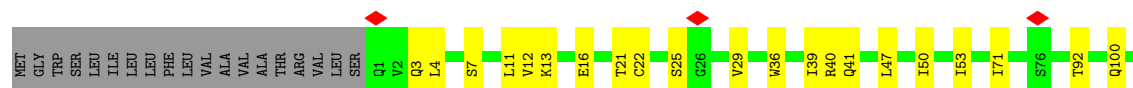
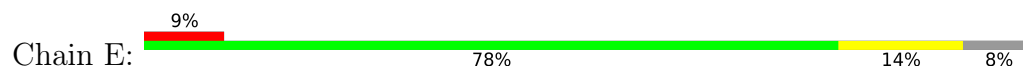
• Molecule 2: Light chain of H18 Fab

Chain Q: 

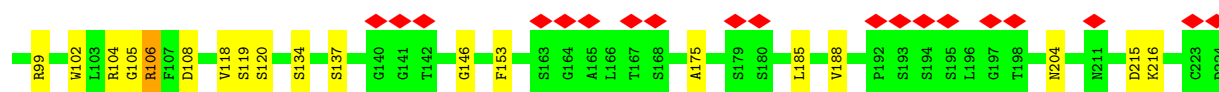
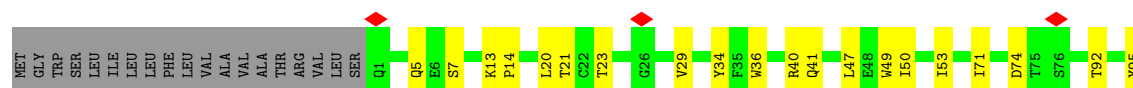
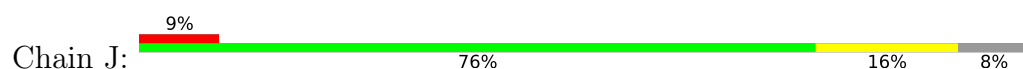




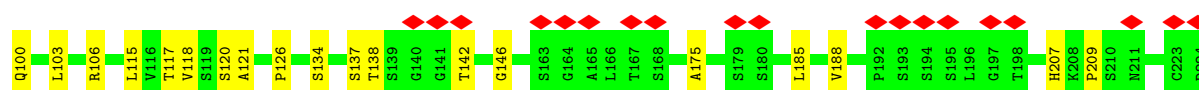
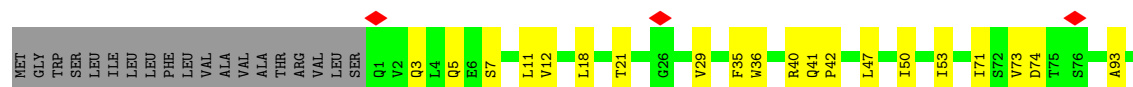
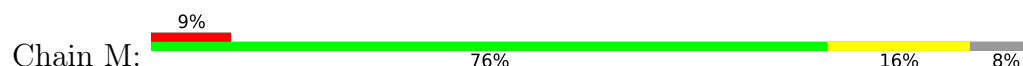
• Molecule 3: Heavy chain of H18 Fab



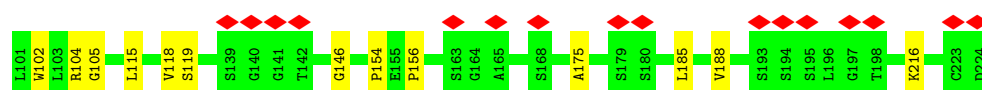
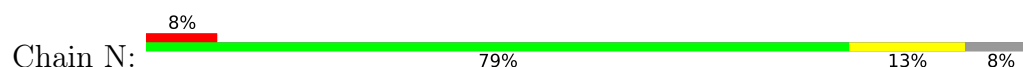
• Molecule 3: Heavy chain of H18 Fab



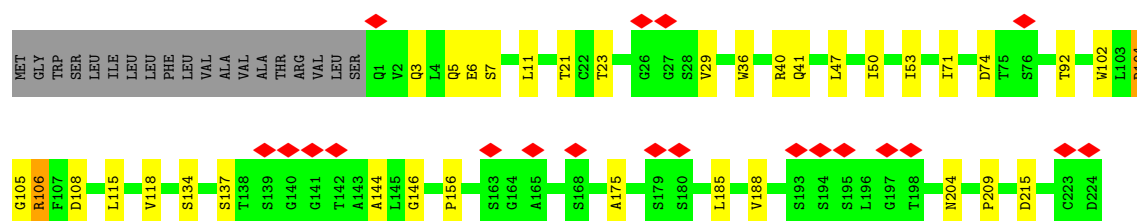
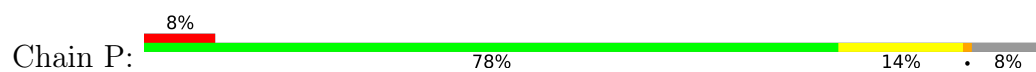
• Molecule 3: Heavy chain of H18 Fab



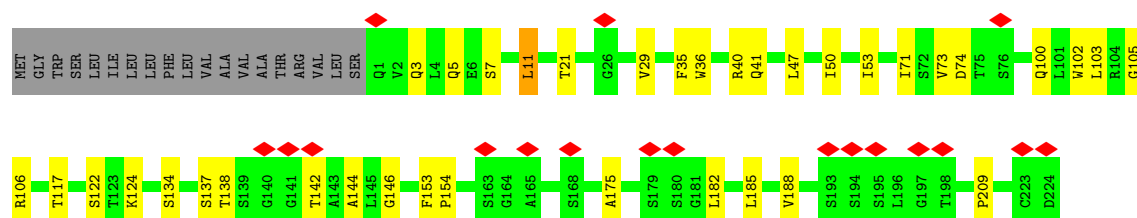
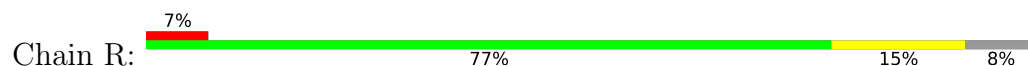
• Molecule 3: Heavy chain of H18 Fab



• Molecule 3: Heavy chain of H18 Fab



- Molecule 3: Heavy chain of H18 Fab



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



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



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



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





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

Chain W:  50% 50%



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

Chain X:  100%



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

Chain Y:  50% 50%



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

Chain Z:  100%

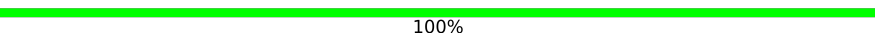


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%



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

Chain b:  100%



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

Chain c:  50% 50%



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

Chain d:  100%



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

Chain e:  100%



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

Chain f:  100%



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

Chain g:  100%



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

Chain h:  100%



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

Chain i:  50% 50%



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

Chain j:  100%



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

Chain k:  50% 50%



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

Chain l:  100%



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

Chain m:  50% 50%



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

Chain n:  100%



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

Chain o:  50% 50%



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

Chain p:  100%

EMC1
EMC2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.825	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2, 2.2, 2.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.20	0/8540	0.36	0/11624
1	B	0.13	0/8540	0.33	0/11624
1	C	0.18	0/8540	0.35	0/11624
1	G	0.13	0/8540	0.34	0/11624
1	H	0.17	0/8540	0.36	0/11624
1	I	0.17	0/8540	0.36	0/11624
2	D	0.13	0/1630	0.36	0/2225
2	F	0.12	0/1630	0.34	0/2225
2	K	0.15	0/1630	0.34	0/2225
2	L	0.16	0/1630	0.40	0/2225
2	O	0.12	0/1630	0.34	0/2225
2	Q	0.11	0/1630	0.32	0/2225
3	E	0.14	0/1713	0.36	0/2339
3	J	0.13	0/1713	0.37	0/2339
3	M	0.12	0/1713	0.35	0/2339
3	N	0.13	0/1713	0.37	0/2339
3	P	0.12	0/1713	0.35	0/2339
3	R	0.13	0/1713	0.37	0/2339
All	All	0.16	0/71298	0.35	0/97128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8344	0	8123	124	0
1	B	8344	0	8123	131	0
1	C	8344	0	8123	108	0
1	G	8344	0	8123	122	0
1	H	8344	0	8123	119	0
1	I	8344	0	8123	111	0
2	D	1593	0	1524	24	0
2	F	1593	0	1524	20	0
2	K	1593	0	1524	15	0
2	L	1593	0	1524	28	0
2	O	1593	0	1524	15	0
2	Q	1593	0	1524	13	0
3	E	1670	0	1643	19	0
3	J	1670	0	1643	29	0
3	M	1670	0	1643	24	0
3	N	1670	0	1643	21	0
3	P	1670	0	1643	22	0
3	R	1670	0	1643	23	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
4	Z	28	0	25	0	0
4	a	28	0	25	1	0
4	b	28	0	25	0	0
4	c	28	0	25	1	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
4	h	28	0	25	0	0
4	i	28	0	25	1	0
4	j	28	0	25	0	0
4	k	28	0	25	1	0
4	l	28	0	25	0	0
4	m	28	0	25	2	0
4	n	28	0	25	0	0
4	o	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	p	28	0	25	0	0
5	A	154	0	143	0	0
5	B	154	0	143	0	0
5	C	154	0	143	1	0
5	G	154	0	143	0	0
5	H	154	0	143	1	0
5	I	154	0	143	0	0
All	All	71238	0	69198	897	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (897) 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:I:330:PRO:HG2	1:I:579:PRO:HB2	1.50	0.93
1:A:577:ARG:HD3	1:A:582:LEU:HD12	1.64	0.80
1:C:738:CYS:HB3	1:C:742:ILE:HD12	1.61	0.80
3:P:11:LEU:HD22	3:P:209:PRO:HB3	1.62	0.79
1:H:902:MET:HG3	1:H:916:LEU:HD11	1.65	0.78
1:A:331:ASN:HB3	1:A:580:GLN:HA	1.65	0.77
3:J:102:TRP:HB3	3:J:105:GLY:HA3	1.66	0.76
1:B:902:MET:HG3	1:B:916:LEU:HD11	1.67	0.74
1:A:480:CYS:HA	1:A:487:ASN:HB3	1.71	0.73
3:P:102:TRP:HB3	3:P:105:GLY:HA3	1.71	0.72
1:I:922:LEU:HD21	4:m:1:NAG:H5	1.72	0.71
1:H:770:ILE:HD11	1:H:1012:LEU:HD23	1.73	0.71
1:G:328:ARG:HH21	1:G:533:LEU:HB2	1.56	0.71
1:A:328:ARG:HB3	1:A:531:THR:HG23	1.73	0.70
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.73	0.70
1:H:106:PHE:HB2	1:H:117:LEU:HB2	1.74	0.70
2:L:163:SER:H	2:L:199:HIS:CD2	2.10	0.69
1:B:333:THR:HG23	1:B:362:VAL:HG22	1.73	0.69
1:C:374:PHE:O	3:E:104:ARG:NH2	2.26	0.69
1:I:374:PHE:O	3:N:104:ARG:NH2	2.26	0.69
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.75	0.69
2:L:145:CYS:HB3	2:L:187:SER:HB3	1.75	0.69
1:C:362:VAL:HG23	1:C:526:GLY:HA2	1.75	0.68
2:L:163:SER:H	2:L:199:HIS:HD2	1.39	0.68
1:I:106:PHE:HB2	1:I:117:LEU:HB2	1.76	0.68
1:G:758:SER:O	1:G:762:GLN:NE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:119:SER:HB3	3:N:154:PRO:HG3	1.75	0.68
3:M:146:GLY:HA3	3:M:188:VAL:HG12	1.76	0.67
3:P:3:GLN:HE22	3:P:5:GLN:HB2	1.59	0.67
3:R:11:LEU:HD22	3:R:209:PRO:HB3	1.74	0.67
1:B:357:ARG:HH22	1:C:168:PHE:HB2	1.60	0.67
3:E:3:GLN:HE21	3:E:25:SER:HB2	1.60	0.66
3:M:29:VAL:HG13	3:M:36:TRP:HE1	1.61	0.66
1:A:328:ARG:HG3	1:A:531:THR:H	1.61	0.66
2:D:145:CYS:HB3	2:D:187:SER:HB3	1.75	0.66
3:R:146:GLY:HA3	3:R:188:VAL:HG12	1.77	0.66
2:K:145:CYS:HB3	2:K:187:SER:HB3	1.77	0.65
3:R:29:VAL:HG13	3:R:36:TRP:HE1	1.60	0.65
1:A:758:SER:O	1:A:762:GLN:NE2	2.29	0.65
1:G:742:ILE:O	1:G:1000:ARG:NH1	2.30	0.65
2:Q:145:CYS:HB3	2:Q:187:SER:HB3	1.79	0.65
3:E:146:GLY:HA3	3:E:188:VAL:HG12	1.78	0.65
2:F:143:LEU:HB2	2:F:189:LEU:HB3	1.80	0.64
1:A:87:ASN:HD21	1:A:269:TYR:HB3	1.62	0.64
3:N:146:GLY:HA3	3:N:188:VAL:HG12	1.78	0.64
3:R:11:LEU:HB2	3:R:117:THR:HB	1.80	0.64
3:R:35:PHE:HB2	3:R:100:GLN:HB3	1.79	0.64
1:C:459:SER:HA	1:G:487:ASN:H	1.63	0.64
1:B:479:PRO:HD2	1:H:494:SER:HB3	1.79	0.63
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.80	0.63
1:C:356:LYS:HB2	1:C:397:ALA:HB3	1.81	0.63
1:G:442:ASP:O	1:G:448:ASN:ND2	2.32	0.63
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.31	0.63
2:L:118:GLY:N	2:L:151:TYR:HH	1.97	0.62
3:P:41:GLN:HB2	3:P:47:LEU:HD23	1.82	0.62
1:B:1052:PHE:HB2	1:B:1063:LEU:HB3	1.80	0.62
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.64	0.62
1:A:213:VAL:HG13	1:A:214:ARG:HG2	1.82	0.62
2:O:14:PRO:HA	2:O:81:LEU:HB3	1.81	0.62
1:B:473:TYR:HE2	1:H:484:GLU:HB2	1.65	0.61
1:A:1030:SER:HB3	1:C:1041:ASP:HB3	1.82	0.61
3:J:41:GLN:HB2	3:J:47:LEU:HD23	1.83	0.61
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.83	0.61
1:G:1030:SER:HB3	1:I:1041:ASP:HB3	1.81	0.61
1:I:977:LEU:HD23	1:I:1000:ARG:HH12	1.66	0.61
1:I:742:ILE:O	1:I:1000:ARG:NH1	2.33	0.61
1:A:770:ILE:O	1:A:773:GLU:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:LEU:HD23	1:C:1000:ARG:HH12	1.66	0.60
1:I:356:LYS:HB2	1:I:397:ALA:HB3	1.81	0.60
3:J:40:ARG:HB3	3:J:50:ILE:HD11	1.84	0.60
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.83	0.60
1:G:173:GLN:HE22	1:G:175:PHE:HD2	1.50	0.60
1:H:442:ASP:O	1:H:448:ASN:ND2	2.35	0.60
3:N:175:ALA:HB2	3:N:185:LEU:HD23	1.83	0.60
3:E:41:GLN:HB2	3:E:47:LEU:HD23	1.84	0.60
1:G:458:LYS:NZ	1:G:471:GLU:OE1	2.34	0.60
1:H:1047:TYR:HB2	1:H:1067:TYR:HB3	1.84	0.60
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.66	0.59
2:F:14:PRO:HA	2:F:81:LEU:HB3	1.84	0.59
1:B:951:VAL:O	1:B:955:ASN:ND2	2.35	0.59
3:M:35:PHE:HB2	3:M:100:GLN:HB3	1.83	0.59
1:I:474:GLN:HE21	1:I:488:CYS:HB2	1.67	0.59
1:A:1041:ASP:HB3	1:B:1030:SER:HB3	1.84	0.59
1:B:239:GLN:NE2	1:B:240:THR:O	2.36	0.59
3:J:92:THR:HG22	3:J:118:VAL:H	1.66	0.59
3:J:146:GLY:HA3	3:J:188:VAL:HG12	1.84	0.59
1:G:983:ARG:HG3	1:G:984:LEU:HG	1.85	0.59
1:H:97:LYS:HB2	1:H:186:PHE:HA	1.83	0.59
1:H:776:LYS:NZ	1:H:780:GLU:OE2	2.36	0.59
3:R:175:ALA:HB2	3:R:185:LEU:HD23	1.84	0.59
1:B:776:LYS:NZ	1:B:780:GLU:OE2	2.36	0.59
3:R:11:LEU:HD13	3:R:154:PRO:HG3	1.85	0.59
1:B:466:ARG:HD2	5:C:1303:NAG:H82	1.84	0.59
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.35	0.59
3:E:92:THR:HG22	3:E:118:VAL:H	1.68	0.59
1:I:328:ARG:HA	1:I:530:SER:HA	1.83	0.59
3:N:13:LYS:O	3:N:16:GLU:HB2	2.03	0.59
1:B:278:LYS:HB3	1:B:287:ASP:H	1.68	0.59
1:H:278:LYS:HB3	1:H:287:ASP:H	1.68	0.59
1:I:119:ILE:HG12	1:I:128:ILE:HG23	1.85	0.59
1:A:173:GLN:HE22	1:A:175:PHE:HD2	1.49	0.59
1:B:922:LEU:HD11	4:W:1:NAG:H3	1.84	0.59
2:D:36:TRP:HB2	2:D:49:ILE:HG22	1.85	0.59
1:H:1029:MET:HE1	1:H:1053:PRO:HG3	1.85	0.59
1:A:97:LYS:HB2	1:A:186:PHE:HA	1.85	0.58
1:H:922:LEU:HD11	4:i:1:NAG:H3	1.84	0.58
1:B:773:GLU:OE2	1:B:774:GLN:NE2	2.33	0.58
1:A:861:LEU:HD12	1:A:862:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.35	0.58
1:C:239:GLN:NE2	1:C:240:THR:O	2.36	0.58
1:G:861:LEU:HD12	1:G:862:PRO:HD2	1.84	0.58
1:A:329:PHE:HB2	1:A:330:PRO:HD3	1.85	0.58
1:H:951:VAL:O	1:H:955:ASN:ND2	2.37	0.58
1:A:442:ASP:O	1:A:448:ASN:ND2	2.36	0.58
1:H:239:GLN:NE2	1:H:240:THR:O	2.36	0.58
1:H:64:TRP:HE1	1:H:264:ALA:HB1	1.67	0.58
1:H:330:PRO:HD2	1:H:528:LYS:HE2	1.84	0.58
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.86	0.58
1:I:770:ILE:HD11	1:I:1012:LEU:HD13	1.84	0.58
1:B:442:ASP:O	1:B:448:ASN:ND2	2.37	0.58
2:F:28:SER:HG	2:F:31:SER:HG	1.48	0.58
1:G:736:VAL:HG11	1:G:1004:LEU:HD11	1.86	0.58
1:H:905:ARG:NH1	1:H:1049:LEU:O	2.35	0.58
1:I:239:GLN:NE2	1:I:240:THR:O	2.37	0.58
2:Q:28:SER:OG	2:Q:31:SER:OG	2.21	0.58
2:K:28:SER:OG	2:K:31:SER:OG	2.21	0.57
1:H:119:ILE:HG23	1:H:128:ILE:HG12	1.86	0.57
2:L:160:LYS:HA	2:L:165:PRO:HA	1.85	0.57
2:Q:127:THR:HG21	3:R:144:ALA:HB3	1.86	0.57
1:H:246:ARG:HH22	1:H:254:SER:HB3	1.69	0.57
3:E:175:ALA:HB2	3:E:185:LEU:HD23	1.84	0.57
3:P:40:ARG:HB3	3:P:50:ILE:HD11	1.84	0.57
3:P:146:GLY:HA3	3:P:188:VAL:HG12	1.86	0.57
3:R:41:GLN:HB2	3:R:47:LEU:HD23	1.86	0.57
1:C:142:GLY:HA3	1:C:156:GLU:HB2	1.86	0.57
2:L:36:TRP:HB2	2:L:49:ILE:HG22	1.85	0.57
3:M:41:GLN:HB2	3:M:47:LEU:HD23	1.85	0.57
1:B:119:ILE:HG23	1:B:128:ILE:HG12	1.87	0.57
1:I:142:GLY:HA3	1:I:156:GLU:HB2	1.86	0.57
1:A:365:TYR:HA	1:A:368:LEU:HD13	1.86	0.57
1:H:142:GLY:HA3	1:H:156:GLU:HB2	1.87	0.57
1:H:336:CYS:HB2	1:H:338:PHE:HD1	1.69	0.57
1:G:327:VAL:HG23	1:G:542:ASN:HB3	1.87	0.57
1:H:24:LEU:HB2	1:H:78:ARG:HD3	1.87	0.56
1:A:352:ALA:HA	1:A:466:ARG:HD3	1.86	0.56
1:B:246:ARG:HH22	1:B:254:SER:HB3	1.69	0.56
2:K:119:GLN:HE21	2:K:177:LYS:HD2	1.70	0.56
1:B:726:ILE:HB	1:B:947:LYS:HE2	1.87	0.56
3:M:175:ALA:HB2	3:M:185:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:ARG:HH22	1:G:254:SER:HB3	1.69	0.56
1:B:361:CYS:SG	1:B:362:VAL:N	2.79	0.56
2:D:162:ASP:HB2	2:D:199:HIS:HD2	1.70	0.56
3:N:7:SER:OG	3:N:21:THR:OG1	2.23	0.56
3:R:7:SER:OG	3:R:21:THR:OG1	2.24	0.56
1:A:32:PHE:HB3	1:A:218:GLN:HG3	1.87	0.56
1:A:246:ARG:HH22	1:A:254:SER:HB3	1.70	0.56
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.88	0.56
3:P:92:THR:HG22	3:P:118:VAL:H	1.70	0.56
1:A:474:GLN:HA	1:A:488:CYS:HA	1.88	0.56
3:M:134:SER:H	3:M:137:SER:HB3	1.71	0.56
1:G:32:PHE:HB3	1:G:218:GLN:HG3	1.88	0.56
3:N:41:GLN:HB2	3:N:47:LEU:HD23	1.88	0.56
3:R:134:SER:H	3:R:137:SER:HB3	1.70	0.56
1:A:123:ALA:HA	1:A:177:MET:HB3	1.88	0.55
1:A:327:VAL:HG23	1:A:542:ASN:HB3	1.88	0.55
3:E:7:SER:OG	3:E:21:THR:OG1	2.23	0.55
3:J:175:ALA:HB2	3:J:185:LEU:HD23	1.88	0.55
1:G:667:GLY:HA2	1:H:864:LEU:HA	1.88	0.55
1:I:1010:GLN:OE1	1:I:1014:ARG:NH2	2.40	0.55
1:A:98:SER:HB3	1:A:181:GLY:HA2	1.87	0.55
1:C:526:GLY:N	1:C:527:PRO:HD2	2.21	0.55
1:B:119:ILE:HG12	1:B:128:ILE:HG23	1.89	0.55
1:G:1041:ASP:HB3	1:H:1030:SER:HB3	1.88	0.55
1:H:1030:SER:HA	1:H:1034:LEU:HD12	1.88	0.55
2:L:40:ARG:NH2	2:L:84:GLU:O	2.40	0.55
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.87	0.55
1:G:97:LYS:HB2	1:G:186:PHE:HA	1.88	0.55
1:H:1041:ASP:HB3	1:I:1030:SER:HB3	1.88	0.55
1:I:128:ILE:HG21	1:I:229:LEU:HD21	1.88	0.55
1:G:78:ARG:HE	1:G:80:ASP:HB2	1.71	0.55
1:I:763:LEU:HG	1:I:1008:VAL:HG21	1.89	0.55
2:O:143:LEU:HB2	2:O:189:LEU:HB3	1.87	0.55
1:B:81:ASN:HB3	1:B:239:GLN:HE21	1.72	0.55
3:M:11:LEU:HD22	3:M:118:VAL:HB	1.88	0.55
3:P:7:SER:OG	3:P:21:THR:OG1	2.24	0.55
3:P:175:ALA:HB2	3:P:185:LEU:HD23	1.89	0.55
1:A:1051:SER:HG	1:A:1064:HIS:HD1	1.53	0.55
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.88	0.55
2:D:5:THR:HB	2:D:23:THR:HB	1.88	0.55
3:N:52:CYS:SG	3:N:100:GLN:NE2	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HB2	1:A:202:LYS:HB2	1.89	0.55
1:C:246:ARG:HH22	1:C:254:SER:HB3	1.71	0.55
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.89	0.55
1:B:24:LEU:HB2	1:B:78:ARG:HD3	1.88	0.54
1:B:1090:PRO:O	1:C:913:GLN:NE2	2.40	0.54
1:H:328:ARG:HH21	1:H:533:LEU:HD13	1.73	0.54
3:N:4:LEU:HG	3:N:24:VAL:HG22	1.88	0.54
1:B:142:GLY:HA3	1:B:156:GLU:HB2	1.89	0.54
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.89	0.54
1:G:102:ARG:HG3	1:G:141:LEU:HD12	1.89	0.54
1:G:525:CYS:SG	1:G:526:GLY:N	2.81	0.54
1:C:87:ASN:HD21	1:C:269:TYR:HB3	1.72	0.54
2:F:62:ARG:NH2	2:F:85:ASP:OD2	2.40	0.54
2:K:36:TRP:HB2	2:K:49:ILE:HG22	1.87	0.54
1:G:352:ALA:HA	1:G:466:ARG:HD3	1.88	0.54
1:A:102:ARG:HG3	1:A:141:LEU:HD12	1.90	0.54
1:G:195:LYS:HB2	1:G:202:LYS:HB2	1.89	0.54
2:L:35:GLN:NE2	3:N:105:GLY:O	2.40	0.54
2:Q:36:TRP:HB2	2:Q:49:ILE:HG22	1.90	0.54
1:C:818:ILE:HD11	1:C:1054:GLN:HE21	1.71	0.54
2:D:35:GLN:NE2	3:E:105:GLY:O	2.41	0.54
3:M:7:SER:OG	3:M:21:THR:OG1	2.25	0.54
2:D:55:ARG:NH1	2:D:59:VAL:O	2.40	0.54
1:H:472:ILE:HD12	1:H:488:CYS:HB2	1.90	0.54
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.41	0.54
1:B:37:TYR:OH	1:B:54:LEU:O	2.26	0.54
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.88	0.54
3:J:7:SER:OG	3:J:21:THR:OG1	2.25	0.54
1:H:119:ILE:HG12	1:H:128:ILE:HG23	1.89	0.54
1:A:417:LYS:HG3	1:A:418:ILE:HG12	1.90	0.54
1:A:769:GLY:O	1:A:772:VAL:HG12	2.08	0.54
1:B:32:PHE:HB3	1:B:218:GLN:HG3	1.89	0.54
1:C:384:PRO:HA	1:C:387:LEU:HD23	1.90	0.54
1:G:42:VAL:HG12	1:I:565:PHE:HB2	1.89	0.54
1:C:319:ARG:NE	1:C:591:SER:OG	2.34	0.53
1:H:32:PHE:HB3	1:H:218:GLN:HG3	1.90	0.53
1:I:97:LYS:HB2	1:I:186:PHE:HA	1.88	0.53
1:I:246:ARG:HH22	1:I:254:SER:HB3	1.71	0.53
1:A:667:GLY:HA2	1:B:864:LEU:HA	1.91	0.53
1:B:1041:ASP:HB3	1:C:1030:SER:HB3	1.88	0.53
1:H:1028:LYS:NZ	1:H:1042:PHE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1028:LYS:NZ	1:G:1042:PHE:O	2.42	0.53
3:P:134:SER:H	3:P:137:SER:HB3	1.73	0.53
2:D:40:ARG:HB2	2:D:43:SER:HB2	1.90	0.53
1:G:980:ILE:HA	1:G:983:ARG:HG2	1.89	0.53
2:O:145:CYS:HB3	2:O:187:SER:HB3	1.91	0.53
1:B:29:THR:HG23	1:B:62:VAL:HG13	1.91	0.53
1:I:32:PHE:HB3	1:I:218:GLN:HG3	1.91	0.53
1:G:87:ASN:HD21	1:G:269:TYR:HB3	1.73	0.53
1:G:98:SER:HB3	1:G:181:GLY:HA2	1.89	0.53
1:G:574:ASP:HA	1:G:587:ILE:HB	1.91	0.53
1:I:922:LEU:HD11	4:m:1:NAG:H3	1.91	0.53
1:B:689:SER:OG	1:B:690:GLN:N	2.42	0.53
1:B:766:ALA:O	1:B:770:ILE:HG12	2.09	0.53
1:C:32:PHE:HB3	1:C:218:GLN:HG3	1.90	0.53
1:C:408:ARG:NH2	2:D:72:ASN:OD1	2.42	0.53
1:G:417:LYS:HG3	1:G:418:ILE:HG12	1.90	0.53
1:H:821:LEU:HD21	1:H:939:SER:HA	1.91	0.53
1:H:365:TYR:HA	1:H:368:LEU:HD13	1.91	0.53
1:H:1090:PRO:O	1:I:913:GLN:NE2	2.42	0.53
1:I:776:LYS:NZ	1:I:780:GLU:OE2	2.42	0.53
2:O:62:ARG:NH2	2:O:85:ASP:OD2	2.42	0.53
2:O:127:THR:HG21	3:P:144:ALA:HB3	1.91	0.53
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.90	0.52
1:G:110:LEU:HB3	1:G:135:PHE:HB2	1.90	0.52
3:P:29:VAL:HA	3:P:36:TRP:HZ2	1.74	0.52
3:R:122:SER:O	3:R:124:LYS:NZ	2.42	0.52
1:B:476:GLY:N	1:B:487:ASN:O	2.36	0.52
1:C:776:LYS:NZ	1:C:780:GLU:OE2	2.42	0.52
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.92	0.52
1:C:866:THR:N	1:C:869:MET:SD	2.82	0.52
1:I:501:ASN:HB2	1:I:506:GLN:HE22	1.75	0.52
1:I:951:VAL:O	1:I:955:ASN:ND2	2.42	0.52
3:P:115:LEU:HD23	3:P:156:PRO:HG3	1.92	0.52
1:A:314:GLN:NE2	1:A:316:SER:O	2.42	0.52
1:H:689:SER:OG	1:H:690:GLN:N	2.41	0.52
1:I:408:ARG:NH2	2:L:72:ASN:OD1	2.42	0.52
1:A:900:MET:HE1	1:C:1079:PRO:HB3	1.90	0.52
1:C:501:ASN:HB2	1:C:506:GLN:HE22	1.75	0.52
1:H:29:THR:HG23	1:H:62:VAL:HG13	1.91	0.52
1:H:37:TYR:OH	1:H:54:LEU:O	2.25	0.52
1:C:128:ILE:HG21	1:C:229:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:VAL:O	1:A:955:ASN:ND2	2.43	0.52
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.75	0.52
1:G:64:TRP:HE1	1:G:264:ALA:HB1	1.75	0.52
1:A:766:ALA:O	1:A:770:ILE:HG12	2.10	0.52
1:A:776:LYS:NZ	1:A:780:GLU:OE2	2.43	0.52
1:B:353:TRP:O	1:B:466:ARG:NH2	2.43	0.52
1:I:906:PHE:HE2	1:I:916:LEU:HD13	1.74	0.52
2:L:94:TYR:CG	3:N:104:ARG:HG2	2.44	0.52
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.91	0.51
1:B:861:LEU:HD12	1:B:862:PRO:HD2	1.91	0.51
1:H:906:PHE:HE1	1:H:1049:LEU:HD21	1.75	0.51
1:G:314:GLN:NE2	1:G:316:SER:O	2.43	0.51
1:H:565:PHE:HB2	1:I:42:VAL:HG12	1.93	0.51
1:B:374:PHE:HB2	3:J:104:ARG:NH2	2.26	0.51
2:D:94:TYR:CG	3:E:104:ARG:HG2	2.44	0.51
1:B:821:LEU:HD21	1:B:939:SER:HA	1.92	0.51
1:C:922:LEU:HD11	4:a:1:NAG:H3	1.93	0.51
1:C:973:ILE:HD12	1:C:983:ARG:HH12	1.74	0.51
3:J:108:ASP:OD1	3:J:108:ASP:N	2.43	0.51
1:G:776:LYS:NZ	1:G:780:GLU:OE2	2.44	0.51
3:R:3:GLN:HE22	3:R:5:GLN:HB3	1.76	0.51
1:G:128:ILE:HB	1:G:170:TYR:HB3	1.91	0.51
1:I:327:VAL:HB	1:I:528:LYS:HG2	1.93	0.51
1:A:349:SER:OG	1:A:452:LEU:O	2.29	0.51
1:B:906:PHE:HE1	1:B:1049:LEU:HD21	1.75	0.51
1:H:37:TYR:OH	1:H:53:ASP:OD2	2.29	0.51
1:A:42:VAL:HG12	1:C:565:PHE:HB2	1.93	0.51
1:B:973:ILE:HD12	1:B:983:ARG:HH12	1.76	0.51
2:F:99:VAL:HB	3:J:49:TRP:CG	2.46	0.51
1:H:356:LYS:HB2	1:H:397:ALA:HB3	1.91	0.51
2:D:55:ARG:NE	2:D:61:ASP:HA	2.26	0.51
2:L:5:THR:HB	2:L:23:THR:HB	1.92	0.51
1:A:689:SER:OG	1:A:690:GLN:N	2.44	0.51
1:C:821:LEU:HD21	1:C:939:SER:HA	1.93	0.51
1:I:689:SER:OG	1:I:690:GLN:N	2.42	0.51
1:A:1079:PRO:HB3	1:B:900:MET:HE1	1.92	0.50
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.29	0.50
1:B:565:PHE:HB2	1:C:42:VAL:HG12	1.93	0.50
1:C:689:SER:OG	1:C:690:GLN:N	2.42	0.50
1:H:574:ASP:HA	1:H:587:ILE:HB	1.93	0.50
3:N:92:THR:HG22	3:N:118:VAL:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HB	1:C:357:ARG:HD3	1.93	0.50
1:I:959:LEU:HD13	1:I:962:LEU:HD12	1.93	0.50
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.94	0.50
1:B:376:THR:HG22	2:F:31:SER:HB3	1.94	0.50
3:J:29:VAL:HA	3:J:36:TRP:HZ2	1.77	0.50
1:H:81:ASN:HB3	1:H:239:GLN:HE21	1.75	0.50
3:M:12:VAL:H	3:M:118:VAL:HG11	1.77	0.50
1:H:729:VAL:H	1:H:1059:GLY:HA2	1.77	0.50
1:A:735:SER:HA	1:A:767:LEU:HD13	1.94	0.50
1:B:339:GLY:HA2	1:B:342:PHE:CD2	2.47	0.50
1:G:349:SER:OG	1:G:452:LEU:O	2.30	0.50
1:G:992:GLN:OE1	1:G:995:ARG:NH2	2.42	0.50
3:P:108:ASP:OD1	3:P:108:ASP:N	2.44	0.50
1:B:563:GLN:NE2	1:C:42:VAL:O	2.44	0.50
1:G:1051:SER:OG	1:G:1064:HIS:ND1	2.39	0.50
1:H:1106:GLN:HE21	1:H:1109:PHE:HB3	1.75	0.50
1:A:384:PRO:HA	1:A:387:LEU:HD23	1.92	0.50
1:B:427:ASP:OD1	1:B:427:ASP:N	2.45	0.50
2:D:50:TYR:HD2	2:D:51:GLU:HG3	1.77	0.50
1:I:729:VAL:H	1:I:1059:GLY:HA2	1.77	0.50
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.94	0.50
1:G:821:LEU:HD21	1:G:939:SER:HA	1.94	0.50
2:Q:53:ASN:O	2:Q:55:ARG:NH1	2.45	0.50
1:A:454:ARG:NH1	1:A:469:SER:O	2.39	0.49
1:A:545:GLY:HA3	1:A:565:PHE:HZ	1.76	0.49
3:M:3:GLN:HE22	3:M:5:GLN:HB3	1.76	0.49
3:M:100:GLN:NE2	3:M:103:LEU:O	2.45	0.49
1:H:331:ASN:OD1	1:H:332:ILE:N	2.35	0.49
1:H:598:ILE:HB	1:H:609:ALA:HB3	1.94	0.49
1:A:126:VAL:HB	1:A:172:SER:HB3	1.94	0.49
1:A:328:ARG:HA	1:A:528:LYS:HG2	1.94	0.49
1:A:574:ASP:HA	1:A:587:ILE:HB	1.93	0.49
1:A:877:LEU:HD13	1:A:1029:MET:HE2	1.94	0.49
2:K:53:ASN:O	2:K:55:ARG:NH1	2.45	0.49
3:M:126:PRO:HG3	3:M:207:HIS:HB2	1.95	0.49
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.94	0.49
1:H:861:LEU:HD12	1:H:862:PRO:HD2	1.93	0.49
1:I:903:ALA:HB1	1:I:913:GLN:HB2	1.94	0.49
1:A:821:LEU:HD21	1:A:939:SER:HA	1.94	0.49
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.44	0.49
1:C:877:LEU:HD13	1:C:1029:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:916:LEU:HD12	1:G:923:ILE:HD12	1.95	0.49
1:H:352:ALA:HA	1:H:466:ARG:HD3	1.94	0.49
2:L:159:TRP:CD1	2:L:170:VAL:HG13	2.47	0.49
2:F:56:PRO:HB3	3:J:106:ARG:HH21	1.77	0.49
1:G:83:VAL:HG22	1:G:239:GLN:HG3	1.94	0.49
1:G:126:VAL:HB	1:G:172:SER:HB3	1.94	0.49
1:G:213:VAL:HG22	1:G:214:ARG:HD2	1.93	0.49
2:L:50:TYR:HD2	2:L:51:GLU:HG3	1.78	0.49
1:B:327:VAL:HG22	1:B:528:LYS:HZ1	1.78	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.94	0.49
3:M:40:ARG:HB3	3:M:50:ILE:HD11	1.94	0.49
1:G:726:ILE:HB	1:G:947:LYS:HE2	1.93	0.49
1:G:763:LEU:HD22	1:G:1008:VAL:HG21	1.93	0.49
1:A:472:ILE:HD12	1:A:488:CYS:SG	2.52	0.49
1:I:374:PHE:HD1	1:I:436:TRP:HB3	1.78	0.49
1:I:574:ASP:HA	1:I:587:ILE:HB	1.94	0.49
1:G:689:SER:OG	1:G:690:GLN:N	2.44	0.49
1:H:376:THR:HG22	2:O:31:SER:HB3	1.94	0.49
1:I:1010:GLN:HA	1:I:1013:ILE:HG12	1.95	0.49
1:A:403:ARG:NH2	1:A:406:GLU:OE2	2.46	0.49
1:G:877:LEU:HD13	1:G:1029:MET:HE2	1.94	0.49
1:B:574:ASP:HA	1:B:587:ILE:HB	1.94	0.49
1:G:490:PHE:O	1:G:493:GLN:NE2	2.46	0.49
1:H:195:LYS:HB2	1:H:202:LYS:HB2	1.94	0.49
1:I:1029:MET:HE1	1:I:1053:PRO:HG3	1.95	0.49
2:L:134:GLU:OE1	3:N:216:LYS:NZ	2.41	0.49
3:N:16:GLU:H	3:N:87:VAL:HG12	1.76	0.49
3:R:100:GLN:NE2	3:R:103:LEU:O	2.45	0.49
1:B:92:PHE:O	1:B:192:PHE:N	2.40	0.48
1:C:335:LEU:HD22	1:C:338:PHE:CD1	2.48	0.48
1:A:361:CYS:SG	1:A:362:VAL:N	2.86	0.48
1:H:976:VAL:HG22	1:H:978:ASN:H	1.78	0.48
1:A:617:CYS:N	1:A:649:CYS:SG	2.86	0.48
3:J:36:TRP:HB2	3:J:53:ILE:HG22	1.96	0.48
1:G:403:ARG:NH2	1:G:406:GLU:OE2	2.46	0.48
2:L:145:CYS:HB2	2:L:159:TRP:CH2	2.48	0.48
2:L:199:HIS:HB2	2:L:202:TYR:CE1	2.48	0.48
1:C:574:ASP:HA	1:C:587:ILE:HB	1.94	0.48
1:G:19:THR:OG1	1:G:255:SER:O	2.31	0.48
2:Q:6:GLN:NE2	2:Q:89:TYR:O	2.46	0.48
1:B:357:ARG:NH2	1:C:167:THR:HG22	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.79	0.48
2:K:38:GLN:NE2	2:K:89:TYR:OH	2.45	0.48
1:I:877:LEU:HD13	1:I:1029:MET:HE2	1.94	0.48
1:I:897:PRO:HB2	1:I:900:MET:HE3	1.95	0.48
2:Q:147:ILE:O	2:Q:185:ALA:N	2.41	0.48
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.46	0.48
1:C:328:ARG:NH1	1:C:531:THR:O	2.36	0.48
1:G:384:PRO:HA	1:G:387:LEU:HD23	1.94	0.48
1:G:738:CYS:HB3	1:G:760:CYS:HB2	1.59	0.48
1:H:57:PRO:HG3	1:H:273:ARG:HD2	1.96	0.48
1:H:663:ASP:OD1	1:H:663:ASP:N	2.44	0.48
1:I:92:PHE:O	1:I:192:PHE:N	2.43	0.48
1:A:320:VAL:H	1:A:591:SER:HB2	1.79	0.48
1:B:596:SER:HB2	1:B:611:LEU:HB3	1.95	0.48
1:H:409:GLN:NE2	1:H:415:THR:O	2.47	0.48
1:I:459:SER:OG	1:I:460:ASN:N	2.47	0.48
1:I:485:GLY:H	1:I:488:CYS:HB3	1.78	0.48
3:P:204:ASN:ND2	3:P:215:ASP:OD1	2.40	0.48
3:R:74:ASP:OD1	3:R:74:ASP:N	2.47	0.48
1:H:596:SER:HB2	1:H:611:LEU:HB3	1.95	0.48
1:I:384:PRO:HA	1:I:387:LEU:HD23	1.96	0.48
1:I:916:LEU:HD12	1:I:923:ILE:HD12	1.95	0.48
3:N:53:ILE:HD12	3:N:71:ILE:HG23	1.96	0.48
1:B:976:VAL:HG22	1:B:978:ASN:H	1.79	0.47
1:C:172:SER:OG	1:C:173:GLN:N	2.47	0.47
1:C:389:ASP:HA	1:C:527:PRO:HG3	1.94	0.47
3:J:204:ASN:ND2	3:J:215:ASP:OD1	2.39	0.47
1:G:361:CYS:SG	1:G:362:VAL:N	2.87	0.47
1:H:134:GLN:HB2	1:H:161:SER:HB2	1.95	0.47
3:P:36:TRP:HB2	3:P:53:ILE:HG22	1.96	0.47
2:Q:50:TYR:HB3	3:R:106:ARG:HG3	1.96	0.47
1:I:34:ARG:NH1	1:I:191:GLU:OE2	2.48	0.47
1:B:993:ILE:O	1:B:997:ILE:HG12	2.14	0.47
1:C:484:GLU:HG2	1:C:490:PHE:HB2	1.95	0.47
3:M:74:ASP:OD1	3:M:74:ASP:N	2.47	0.47
1:G:1035:GLY:HA3	1:I:1040:VAL:HG11	1.97	0.47
3:R:153:PHE:HB2	3:R:182:LEU:HD22	1.97	0.47
1:A:477:SER:HB3	1:I:452:LEU:HG	1.96	0.47
1:B:948:LEU:HD11	1:B:1059:GLY:HA3	1.96	0.47
1:B:1079:PRO:HB3	1:C:900:MET:HE1	1.95	0.47
1:G:490:PHE:HD2	1:G:492:LEU:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:735:SER:HA	1:H:767:LEU:HD13	1.97	0.47
1:H:737:ASP:HB3	1:H:740:MET:HE2	1.96	0.47
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.96	0.47
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.97	0.47
1:B:899:PRO:HA	1:B:902:MET:HG2	1.97	0.47
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.78	0.47
1:C:733:LYS:O	1:C:861:LEU:N	2.43	0.47
1:A:37:TYR:OH	1:A:53:ASP:OD1	2.33	0.47
1:B:134:GLN:HB2	1:B:161:SER:HB2	1.96	0.47
3:E:53:ILE:HD12	3:E:71:ILE:HG23	1.95	0.47
1:G:320:VAL:H	1:G:591:SER:HB2	1.79	0.47
1:G:435:ALA:HB2	1:G:510:VAL:HG23	1.95	0.47
1:G:617:CYS:N	1:G:649:CYS:SG	2.87	0.47
1:G:974:SER:HB3	1:G:980:ILE:HG23	1.97	0.47
1:G:993:ILE:O	1:G:997:ILE:HG12	2.15	0.47
1:I:106:PHE:HB3	1:I:235:ILE:HG21	1.96	0.47
2:L:159:TRP:HD1	2:L:170:VAL:HG13	1.80	0.47
1:A:335:LEU:HB3	1:A:338:PHE:HE1	1.80	0.47
1:A:435:ALA:HB2	1:A:510:VAL:HG23	1.96	0.47
1:G:669:GLY:HA2	1:G:697:MET:HE3	1.96	0.47
1:G:948:LEU:HD21	1:G:1059:GLY:HA3	1.96	0.47
1:C:95:THR:HA	1:C:189:LEU:HA	1.96	0.47
1:C:1030:SER:HA	1:C:1034:LEU:HD12	1.97	0.47
1:G:239:GLN:NE2	1:G:240:THR:O	2.48	0.47
1:G:493:GLN:N	1:G:493:GLN:OE1	2.48	0.47
1:I:669:GLY:HA2	1:I:697:MET:HE3	1.96	0.47
2:O:81:LEU:HD11	2:O:107:LEU:HD11	1.97	0.47
2:O:89:TYR:HB2	2:O:105:THR:HB	1.97	0.47
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.96	0.47
1:C:476:GLY:HA3	1:C:487:ASN:HB3	1.97	0.47
1:G:565:PHE:HB2	1:H:42:VAL:HG12	1.97	0.47
2:L:160:LYS:HE2	2:L:165:PRO:HB3	1.97	0.47
2:Q:147:ILE:HB	2:Q:185:ALA:HB3	1.97	0.47
1:B:721:SER:OG	1:B:1066:THR:OG1	2.32	0.46
1:B:742:ILE:HG12	1:B:1000:ARG:HB3	1.97	0.46
3:J:5:GLN:OE1	3:J:23:THR:OG1	2.32	0.46
1:I:453:TYR:HB3	1:I:495:TYR:HE1	1.81	0.46
1:I:457:ARG:HD2	1:I:457:ARG:HA	1.72	0.46
1:I:976:VAL:HG22	1:I:978:ASN:H	1.80	0.46
2:Q:145:CYS:O	2:Q:187:SER:N	2.48	0.46
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.48	0.46
1:H:476:GLY:HA3	1:H:487:ASN:HD21	1.80	0.46
1:I:403:ARG:NH2	1:I:406:GLU:OE2	2.48	0.46
1:A:948:LEU:HD21	1:A:1059:GLY:HA3	1.97	0.46
1:B:475:ALA:H	1:B:488:CYS:HA	1.81	0.46
1:B:703:ASN:ND2	1:C:787:GLN:OE1	2.45	0.46
1:G:92:PHE:O	1:G:192:PHE:N	2.41	0.46
1:H:866:THR:HG22	1:H:869:MET:HE1	1.97	0.46
1:H:880:GLY:O	1:H:884:SER:OG	2.30	0.46
1:H:886:TRP:HB3	1:H:1035:GLY:HA2	1.97	0.46
1:I:538:CYS:HB2	1:I:590:CYS:HB3	1.78	0.46
1:C:92:PHE:O	1:C:192:PHE:N	2.43	0.46
3:J:53:ILE:HD12	3:J:71:ILE:HG23	1.98	0.46
1:G:905:ARG:NH1	1:G:1049:LEU:O	2.44	0.46
3:N:115:LEU:HD23	3:N:156:PRO:HG3	1.98	0.46
1:C:431:GLY:HA2	1:C:514:SER:HA	1.97	0.46
1:C:886:TRP:HB3	1:C:1035:GLY:HA2	1.97	0.46
3:J:102:TRP:HB3	3:J:105:GLY:CA	2.41	0.46
2:K:145:CYS:O	2:K:187:SER:N	2.48	0.46
1:H:1033:VAL:HG22	1:H:1051:SER:HB2	1.97	0.46
1:I:886:TRP:HB3	1:I:1035:GLY:HA2	1.97	0.46
1:I:1103:PHE:HZ	4:O:1:NAG:H62	1.80	0.46
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.48	0.46
1:A:529:LYS:HB2	1:A:529:LYS:HE2	1.59	0.46
1:A:565:PHE:HB2	1:B:42:VAL:HG12	1.97	0.46
1:A:992:GLN:OE1	1:A:995:ARG:NH2	2.45	0.46
1:B:116:SER:N	1:B:131:CYS:O	2.46	0.46
1:B:409:GLN:NE2	1:B:415:THR:O	2.47	0.46
1:B:1103:PHE:HZ	4:Y:1:NAG:H62	1.80	0.46
1:G:329:PHE:CG	1:G:330:PRO:HD3	2.51	0.46
1:G:808:ASP:OD1	1:G:808:ASP:N	2.43	0.46
1:H:877:LEU:HD13	1:H:1029:MET:HE2	1.98	0.46
1:I:431:GLY:HA2	1:I:514:SER:HA	1.97	0.46
1:I:474:GLN:HB2	1:I:488:CYS:SG	2.56	0.46
1:A:669:GLY:HA2	1:A:697:MET:HE3	1.96	0.46
1:A:770:ILE:HA	1:A:773:GLU:CD	2.41	0.46
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	1.96	0.46
1:C:403:ARG:NH2	1:C:406:GLU:OE2	2.49	0.46
1:I:172:SER:OG	1:I:173:GLN:N	2.49	0.46
1:I:948:LEU:HD21	1:I:1059:GLY:HA3	1.98	0.46
3:P:74:ASP:OD1	3:P:74:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLN:NE2	1:B:42:VAL:O	2.49	0.46
3:E:13:LYS:HB2	3:E:16:GLU:HG3	1.98	0.46
1:H:734:THR:HG22	1:H:860:VAL:HG22	1.98	0.46
1:B:734:THR:HG22	1:B:860:VAL:HG22	1.97	0.46
1:C:1029:MET:HE1	1:C:1053:PRO:HG3	1.98	0.46
2:D:22:CYS:HB3	2:D:74:ALA:HB3	1.98	0.46
2:F:48:VAL:HA	2:F:59:VAL:HG11	1.98	0.46
2:K:6:GLN:NE2	2:K:89:TYR:O	2.49	0.46
1:G:142:GLY:HA3	1:G:156:GLU:HB2	1.97	0.46
1:H:766:ALA:O	1:H:770:ILE:HG12	2.16	0.46
1:H:993:ILE:O	1:H:997:ILE:HG12	2.15	0.46
1:H:1103:PHE:HZ	4:k:1:NAG:H62	1.80	0.46
1:B:403:ARG:HG2	1:B:497:PHE:HE1	1.81	0.46
2:D:162:ASP:CG	2:D:200:ARG:H	2.24	0.46
3:J:74:ASP:OD1	3:J:74:ASP:N	2.48	0.46
1:H:516:GLU:HG2	1:H:518:LEU:HD22	1.97	0.46
1:B:19:THR:OG1	1:B:255:SER:O	2.33	0.45
1:B:738:CYS:HB3	1:B:742:ILE:HD12	1.98	0.45
2:D:62:ARG:NE	2:D:79:SER:O	2.48	0.45
1:G:99:ASN:HB3	1:G:177:MET:HE3	1.97	0.45
1:H:109:THR:OG1	1:H:111:ASP:OD1	2.31	0.45
1:I:95:THR:HA	1:I:189:LEU:HA	1.97	0.45
1:A:974:SER:HB3	1:A:980:ILE:HG23	1.98	0.45
2:D:147:ILE:HB	2:D:185:ALA:HB3	1.98	0.45
1:A:972:ALA:HA	1:A:995:ARG:HH22	1.82	0.45
1:C:669:GLY:HA2	1:C:697:MET:HE3	1.97	0.45
1:G:474:GLN:HA	1:G:480:CYS:HB3	1.98	0.45
1:I:596:SER:N	1:I:611:LEU:O	2.50	0.45
2:L:162:ASP:HB2	2:L:199:HIS:HB3	1.97	0.45
1:C:78:ARG:NH2	1:C:80:ASP:OD2	2.40	0.45
1:C:596:SER:N	1:C:611:LEU:O	2.50	0.45
2:K:149:ASP:OD1	2:K:178:GLN:NE2	2.38	0.45
1:H:563:GLN:NE2	1:I:42:VAL:O	2.49	0.45
1:H:911:VAL:HG22	1:H:1108:ASN:HB2	1.99	0.45
1:I:733:LYS:O	1:I:861:LEU:N	2.46	0.45
1:A:961:THR:O	1:A:965:GLN:HG2	2.17	0.45
1:C:902:MET:HE1	1:C:1050:MET:HE2	1.98	0.45
1:G:37:TYR:OH	1:G:53:ASP:OD1	2.33	0.45
1:G:545:GLY:HA3	1:G:565:PHE:HZ	1.80	0.45
1:A:78:ARG:HE	1:A:80:ASP:HB2	1.81	0.45
1:A:821:LEU:HD11	1:A:939:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:ILE:O	1:A:997:ILE:HG12	2.16	0.45
1:B:80:ASP:N	1:B:80:ASP:OD1	2.48	0.45
1:B:592:PHE:HB3	1:B:614:ASP:HB3	1.98	0.45
1:C:320:VAL:H	1:C:591:SER:HB2	1.82	0.45
2:F:131:PRO:HD3	2:F:143:LEU:HD13	1.97	0.45
1:G:106:PHE:HB2	1:G:117:LEU:HB2	1.98	0.45
1:G:563:GLN:NE2	1:H:42:VAL:O	2.49	0.45
1:H:331:ASN:OD1	5:H:1306:NAG:N2	2.50	0.45
2:L:6:GLN:NE2	2:L:89:TYR:O	2.50	0.45
1:A:253:ASP:OD1	1:A:253:ASP:N	2.45	0.45
3:E:29:VAL:HA	3:E:36:TRP:HZ2	1.82	0.45
1:H:214:ARG:HH11	1:H:215:ASP:H	1.64	0.45
1:I:1030:SER:HA	1:I:1034:LEU:HD12	1.98	0.45
1:A:142:GLY:HA3	1:A:156:GLU:HB2	1.98	0.45
1:G:961:THR:O	1:G:965:GLN:HG2	2.17	0.45
1:G:1129:VAL:HG13	1:H:917:TYR:HB3	1.99	0.45
1:I:905:ARG:NH1	1:I:1049:LEU:O	2.50	0.45
3:P:53:ILE:HD12	3:P:71:ILE:HG23	1.97	0.45
1:A:525:CYS:SG	1:A:526:GLY:N	2.90	0.45
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.49	0.45
1:C:494:SER:OG	1:C:495:TYR:N	2.50	0.45
1:G:917:TYR:HB3	1:I:1129:VAL:HG13	1.99	0.45
1:I:735:SER:HA	1:I:767:LEU:HD13	1.97	0.45
2:L:14:PRO:HA	2:L:81:LEU:HB2	1.99	0.45
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.99	0.44
1:G:821:LEU:HD11	1:G:939:SER:HB3	1.98	0.44
1:H:34:ARG:NH1	1:H:191:GLU:OE2	2.49	0.44
1:H:403:ARG:HG2	1:H:497:PHE:HE1	1.81	0.44
1:H:617:CYS:N	1:H:649:CYS:SG	2.90	0.44
3:P:5:GLN:OE1	3:P:23:THR:OG1	2.32	0.44
1:B:214:ARG:HH11	1:B:215:ASP:H	1.66	0.44
1:C:1103:PHE:HZ	4:c:1:NAG:H62	1.82	0.44
1:G:1141:LEU:HD13	1:I:1141:LEU:HD11	1.99	0.44
1:H:80:ASP:OD1	1:H:80:ASP:N	2.50	0.44
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.48	0.44
1:C:1037:SER:OG	1:C:1043:CYS:SG	2.68	0.44
1:G:1030:SER:HA	1:G:1034:LEU:HD12	1.99	0.44
1:H:909:ILE:HG13	1:H:911:VAL:HG23	2.00	0.44
1:I:766:ALA:O	1:I:770:ILE:HG12	2.18	0.44
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.70	0.44
1:A:738:CYS:HB3	1:A:742:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD13	1:C:1141:LEU:HD11	1.99	0.44
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.98	0.44
1:B:195:LYS:HB2	1:B:202:LYS:HB2	1.98	0.44
1:B:374:PHE:HB2	3:J:104:ARG:HH22	1.81	0.44
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.99	0.44
2:F:91:CYS:O	2:F:102:GLY:N	2.51	0.44
2:K:147:ILE:O	2:K:185:ALA:N	2.42	0.44
1:I:656:VAL:HG22	1:I:658:ASN:H	1.83	0.44
1:B:327:VAL:HG23	1:B:542:ASN:HB2	2.00	0.44
3:M:138:THR:OG1	3:M:142:THR:O	2.34	0.44
1:H:821:LEU:HD11	1:H:939:SER:HB3	2.00	0.44
1:I:328:ARG:HG2	1:I:531:THR:H	1.82	0.44
1:I:331:ASN:OD1	1:I:331:ASN:N	2.50	0.44
1:I:1106:GLN:HE21	1:I:1109:PHE:HB3	1.82	0.44
2:D:145:CYS:O	2:D:187:SER:N	2.50	0.44
1:G:720:ILE:HG13	1:G:923:ILE:HG23	2.00	0.44
1:H:897:PRO:HB2	1:H:900:MET:HE3	1.99	0.44
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.99	0.44
1:A:1035:GLY:HA3	1:C:1040:VAL:HG11	2.00	0.44
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.94	0.44
1:B:911:VAL:HG22	1:B:1108:ASN:HB2	1.98	0.44
1:B:1033:VAL:HG22	1:B:1051:SER:HB2	2.00	0.44
1:G:596:SER:N	1:G:611:LEU:O	2.51	0.44
1:I:712:ILE:HB	1:I:1077:THR:HG21	1.99	0.44
3:R:40:ARG:HB3	3:R:50:ILE:HD11	1.99	0.44
3:R:53:ILE:HD12	3:R:71:ILE:HG23	2.00	0.44
1:B:642:VAL:HG22	1:B:651:ILE:HG22	1.99	0.44
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.82	0.44
2:F:145:CYS:O	2:F:187:SER:N	2.43	0.44
1:G:1052:PHE:HB2	1:G:1063:LEU:HB2	2.00	0.44
1:I:1051:SER:OG	1:I:1064:HIS:ND1	2.38	0.44
1:A:596:SER:N	1:A:611:LEU:O	2.51	0.43
1:A:886:TRP:HH2	1:A:904:TYR:HB3	1.83	0.43
2:D:22:CYS:N	2:D:74:ALA:O	2.51	0.43
2:D:162:ASP:HB2	2:D:199:HIS:CD2	2.51	0.43
1:H:459:SER:OG	1:H:460:ASN:N	2.51	0.43
1:I:395:VAL:HG23	1:I:524:VAL:HG21	2.00	0.43
1:C:976:VAL:HG22	1:C:978:ASN:H	1.82	0.43
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.83	0.43
2:F:129:PHE:HB2	2:F:144:VAL:HB	2.00	0.43
1:G:528:LYS:HA	1:G:528:LYS:HD2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:VAL:O	1:I:214:ARG:HD3	2.19	0.43
2:O:6:GLN:NE2	2:O:89:TYR:O	2.49	0.43
1:A:976:VAL:HG22	1:A:978:ASN:H	1.83	0.43
1:A:1029:MET:HE1	1:A:1053:PRO:HG3	1.99	0.43
1:C:656:VAL:HG22	1:C:658:ASN:H	1.83	0.43
1:G:886:TRP:HH2	1:G:904:TYR:HB3	1.83	0.43
1:G:1029:MET:HE1	1:G:1053:PRO:HG3	2.00	0.43
1:G:1097:SER:HB3	1:G:1102:TRP:CD2	2.54	0.43
3:N:29:VAL:HA	3:N:36:TRP:HZ2	1.83	0.43
3:R:36:TRP:HB2	3:R:53:ILE:HG22	2.00	0.43
1:A:1030:SER:HA	1:A:1034:LEU:HD12	1.99	0.43
1:B:906:PHE:CD2	1:B:916:LEU:HD12	2.53	0.43
1:B:1069:PRO:HG2	1:C:892:PRO:HD2	2.00	0.43
3:M:53:ILE:HD12	3:M:71:ILE:HG23	1.99	0.43
1:G:453:TYR:HB3	1:G:495:TYR:CE1	2.54	0.43
1:G:866:THR:H	1:G:869:MET:HE2	1.83	0.43
1:G:880:GLY:O	1:G:884:SER:OG	2.31	0.43
1:H:83:VAL:HG11	1:H:237:ARG:HE	1.84	0.43
1:A:726:ILE:HB	1:A:947:LYS:HE2	2.00	0.43
1:C:138:ASP:OD1	1:C:138:ASP:N	2.51	0.43
1:C:617:CYS:N	1:C:649:CYS:SG	2.91	0.43
3:M:36:TRP:HB2	3:M:53:ILE:HG22	2.01	0.43
1:G:972:ALA:HA	1:G:995:ARG:HH22	1.83	0.43
1:H:822:LEU:HB3	1:H:938:LEU:HD21	1.99	0.43
1:I:900:MET:HB3	1:I:900:MET:HE2	1.79	0.43
3:N:13:LYS:HD2	3:N:119:SER:OG	2.17	0.43
1:C:80:ASP:OD1	1:C:80:ASP:N	2.52	0.43
2:D:14:PRO:HA	2:D:81:LEU:HB2	2.01	0.43
2:K:4:LEU:HD11	2:K:93:SER:HB2	2.01	0.43
3:M:120:SER:OG	3:M:121:ALA:N	2.51	0.43
1:G:24:LEU:HB2	1:G:78:ARG:HH11	1.84	0.43
1:H:642:VAL:HG22	1:H:651:ILE:HG22	2.00	0.43
1:H:726:ILE:HB	1:H:947:LYS:HE2	1.99	0.43
1:I:391:CYS:HB3	1:I:525:CYS:HB3	1.65	0.43
2:L:159:TRP:O	2:L:166:VAL:N	2.51	0.43
1:B:901:GLN:O	1:B:905:ARG:HG2	2.18	0.43
2:F:47:THR:HG21	3:J:106:ARG:HG3	2.01	0.43
3:J:134:SER:H	3:J:137:SER:HB3	1.84	0.43
1:H:453:TYR:O	1:H:493:GLN:N	2.48	0.43
1:I:821:LEU:HD11	1:I:939:SER:HB3	1.99	0.43
1:B:138:ASP:OD1	1:B:138:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:PHE:CD1	1:B:511:VAL:HG11	2.54	0.43
2:F:141:ALA:HB3	2:F:191:LEU:HB3	2.01	0.43
1:G:719:THR:HG23	1:G:1070:ALA:HB2	1.99	0.43
1:H:116:SER:N	1:H:131:CYS:O	2.47	0.43
1:A:328:ARG:HB2	1:A:530:SER:HA	2.00	0.43
1:A:719:THR:HG23	1:A:1070:ALA:HB2	2.00	0.43
1:B:342:PHE:HA	1:B:347:PHE:HZ	1.83	0.43
1:B:516:GLU:HG2	1:B:518:LEU:HD22	2.01	0.43
1:G:457:ARG:HA	1:G:457:ARG:HD2	1.65	0.43
1:I:456:PHE:HB2	1:I:491:PRO:HB3	2.00	0.43
1:I:617:CYS:N	1:I:649:CYS:SG	2.91	0.43
1:A:458:LYS:NZ	1:A:471:GLU:OE1	2.52	0.43
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.50	0.43
1:G:538:CYS:HB2	1:G:590:CYS:HB3	1.69	0.43
1:I:277:LEU:HD12	1:I:285:ILE:HD13	2.01	0.43
1:C:126:VAL:HB	1:C:172:SER:HB3	2.01	0.42
2:F:22:CYS:HB3	2:F:74:ALA:HB3	2.01	0.42
2:K:35:GLN:HG2	3:M:106:ARG:HB3	2.01	0.42
1:G:328:ARG:HB2	1:G:530:SER:HA	2.00	0.42
1:A:358:ILE:HG22	1:A:524:VAL:HG21	2.01	0.42
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.54	0.42
3:E:12:VAL:HG13	3:E:118:VAL:HG13	2.00	0.42
1:G:409:GLN:O	1:G:414:GLN:NE2	2.52	0.42
1:G:735:SER:HA	1:G:767:LEU:HD13	2.01	0.42
1:G:909:ILE:HG13	1:G:911:VAL:HG23	2.01	0.42
1:H:84:LEU:HD22	1:H:267:VAL:HG11	2.02	0.42
1:I:93:ALA:HA	1:I:191:GLU:HA	2.02	0.42
2:L:22:CYS:N	2:L:74:ALA:O	2.53	0.42
2:Q:4:LEU:HD11	2:Q:93:SER:HB2	2.01	0.42
1:A:902:MET:HE1	1:A:1050:MET:HE2	2.01	0.42
1:A:1097:SER:HB3	1:A:1102:TRP:CD2	2.54	0.42
2:D:17:THR:HA	2:D:79:SER:HA	2.01	0.42
1:G:976:VAL:HG22	1:G:978:ASN:H	1.84	0.42
1:H:1037:SER:OG	1:H:1043:CYS:SG	2.72	0.42
1:I:1028:LYS:NZ	1:I:1042:PHE:O	2.49	0.42
1:B:364:ASP:HA	1:B:388:ASN:HD21	1.85	0.42
2:F:119:GLN:HG2	2:F:151:TYR:CD1	2.54	0.42
3:M:12:VAL:HG11	3:M:18:LEU:HD12	2.02	0.42
1:G:110:LEU:HD22	1:G:135:PHE:HD2	1.84	0.42
1:G:478:THR:HG21	1:G:486:PHE:HB2	2.01	0.42
1:H:808:ASP:OD1	1:H:808:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1045:LYS:HB2	1:H:1045:LYS:HE2	1.80	0.42
1:I:78:ARG:NH2	1:I:80:ASP:OD2	2.40	0.42
1:I:138:ASP:OD1	1:I:138:ASP:N	2.51	0.42
2:L:147:ILE:HB	2:L:185:ALA:HB3	2.01	0.42
1:A:720:ILE:HG13	1:A:923:ILE:HG23	2.01	0.42
1:A:909:ILE:HG13	1:A:911:VAL:HG23	2.02	0.42
1:B:342:PHE:HB3	1:B:436:TRP:CH2	2.55	0.42
1:C:93:ALA:HA	1:C:191:GLU:HA	2.02	0.42
1:G:886:TRP:HB3	1:G:1035:GLY:HA2	2.01	0.42
1:I:906:PHE:CE2	1:I:916:LEU:HD13	2.54	0.42
2:O:36:TRP:HB2	2:O:49:ILE:HG22	2.01	0.42
1:A:239:GLN:NE2	1:A:240:THR:O	2.52	0.42
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.31	0.42
1:A:472:ILE:HA	1:A:491:PRO:HD3	2.02	0.42
1:B:733:LYS:O	1:B:861:LEU:N	2.47	0.42
1:C:24:LEU:HB2	1:C:78:ARG:HH11	1.84	0.42
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	2.02	0.42
2:D:7:PRO:O	2:D:105:THR:OG1	2.31	0.42
2:F:50:TYR:HE1	3:J:105:GLY:HA2	1.84	0.42
1:H:138:ASP:OD1	1:H:138:ASP:N	2.52	0.42
1:H:1069:PRO:HG2	1:I:892:PRO:HD2	2.01	0.42
1:I:642:VAL:HG13	1:I:651:ILE:HG22	2.01	0.42
2:L:167:LYS:HD2	2:L:167:LYS:N	2.35	0.42
1:C:328:ARG:HE	1:C:580:GLN:HG3	1.85	0.42
1:C:642:VAL:HG13	1:C:651:ILE:HG22	2.01	0.42
2:F:53:ASN:O	2:F:55:ARG:NH1	2.53	0.42
3:M:207:HIS:CD2	3:M:209:PRO:HD2	2.55	0.42
1:H:170:TYR:CE2	1:H:172:SER:HB3	2.55	0.42
1:H:214:ARG:NH1	1:H:215:ASP:H	2.18	0.42
1:H:222:ALA:HB2	1:H:285:ILE:HB	2.01	0.42
1:I:126:VAL:HB	1:I:172:SER:HB3	2.00	0.42
2:Q:124:PRO:HA	2:Q:150:PHE:HB3	2.02	0.42
1:A:566:GLY:HA2	1:B:43:PHE:H	1.84	0.42
1:A:822:LEU:HD11	1:A:1061:VAL:HG11	2.02	0.42
1:B:880:GLY:O	1:B:884:SER:OG	2.30	0.42
1:C:435:ALA:HB2	1:C:510:VAL:HG22	2.02	0.42
2:K:119:GLN:HG3	2:K:181:ASN:OD1	2.20	0.42
1:H:1097:SER:HB3	1:H:1102:TRP:CD2	2.55	0.42
2:O:47:THR:HG21	3:P:106:ARG:NE	2.35	0.42
1:A:81:ASN:HD21	1:A:242:LEU:HD12	1.85	0.42
1:C:1019:ARG:NH1	1:C:1023:ASN:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:763:LEU:HD13	1:G:1004:LEU:HD23	2.02	0.42
1:I:714:ILE:HD12	1:I:1096:VAL:HG11	2.02	0.42
3:N:102:TRP:HD1	3:N:105:GLY:N	2.18	0.42
3:R:53:ILE:HD13	3:R:73:VAL:HG23	2.02	0.42
1:B:222:ALA:HB2	1:B:285:ILE:HB	2.01	0.41
1:B:476:GLY:HA3	1:B:487:ASN:HB3	2.01	0.41
1:B:808:ASP:OD1	1:B:808:ASP:N	2.53	0.41
1:B:972:ALA:HB2	1:B:995:ARG:HD2	2.02	0.41
1:C:216:LEU:HA	1:C:217:PRO:HD3	1.95	0.41
3:J:13:LYS:HA	3:J:13:LYS:HD3	1.74	0.41
1:G:612:TYR:HD2	1:G:649:CYS:HB2	1.85	0.41
1:H:733:LYS:HE2	1:H:861:LEU:HD23	2.00	0.41
1:I:1097:SER:HB3	1:I:1102:TRP:CD2	2.54	0.41
1:A:579:PRO:HA	1:A:582:LEU:HD13	2.01	0.41
1:C:21:ARG:HH21	1:C:79:PHE:HB3	1.85	0.41
2:F:151:TYR:CD1	2:F:152:PRO:HA	2.55	0.41
3:J:119:SER:HB2	3:J:153:PHE:HZ	1.85	0.41
1:G:995:ARG:HA	1:G:998:THR:HG22	2.01	0.41
1:H:92:PHE:O	1:H:192:PHE:N	2.40	0.41
2:L:22:CYS:HB3	2:L:74:ALA:HB3	2.01	0.41
2:L:145:CYS:O	2:L:187:SER:N	2.51	0.41
2:O:22:CYS:HB3	2:O:74:ALA:HB3	2.03	0.41
1:A:713:ALA:HB3	1:B:894:LEU:HB3	2.02	0.41
1:A:886:TRP:HB3	1:A:1035:GLY:HA2	2.01	0.41
2:D:172:THR:HA	2:D:187:SER:HA	2.03	0.41
3:J:20:LEU:HD12	3:J:95:TYR:HD2	1.85	0.41
2:K:18:VAL:HG12	2:K:81:LEU:HD21	2.02	0.41
1:G:737:ASP:OD2	1:I:317:ASN:ND2	2.50	0.41
1:G:1037:SER:OG	1:G:1043:CYS:SG	2.68	0.41
1:H:108:THR:HG22	1:H:236:THR:HG22	2.02	0.41
1:H:327:VAL:HG22	1:H:542:ASN:H	1.85	0.41
1:I:997:ILE:O	1:I:1001:LEU:HG	2.20	0.41
3:R:102:TRP:HD1	3:R:105:GLY:HA3	1.84	0.41
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.56	0.41
1:A:409:GLN:O	1:A:414:GLN:NE2	2.54	0.41
1:C:821:LEU:HD11	1:C:939:SER:HB3	2.02	0.41
2:D:64:SER:O	2:D:77:THR:N	2.49	0.41
3:J:34:TYR:HB2	3:J:99:ARG:NH2	2.35	0.41
1:G:902:MET:HE1	1:G:1050:MET:HE2	2.02	0.41
1:H:338:PHE:O	1:H:341:VAL:HG12	2.20	0.41
1:B:733:LYS:HE2	1:B:861:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:HB3	1:C:495:TYR:HE1	1.86	0.41
1:C:901:GLN:O	1:C:905:ARG:HG2	2.20	0.41
3:E:4:LEU:HD22	3:E:22:CYS:SG	2.60	0.41
3:E:11:LEU:HD21	3:E:209:PRO:HB3	2.02	0.41
3:E:40:ARG:HB3	3:E:50:ILE:HD11	2.02	0.41
1:H:454:ARG:HG3	1:H:491:PRO:HB2	2.01	0.41
1:A:480:CYS:HB2	1:A:488:CYS:HB3	1.82	0.41
1:A:612:TYR:HD2	1:A:649:CYS:HB2	1.85	0.41
1:A:995:ARG:HA	1:A:998:THR:HG22	2.02	0.41
1:B:84:LEU:HD22	1:B:267:VAL:HG11	2.01	0.41
1:B:342:PHE:HD1	1:B:511:VAL:HG11	1.85	0.41
3:J:216:LYS:HB2	3:J:216:LYS:HE2	1.87	0.41
2:K:89:TYR:HB2	2:K:105:THR:HB	2.02	0.41
1:H:1086:LYS:HD2	1:H:1122:VAL:HG11	2.03	0.41
1:I:473:TYR:H	1:I:491:PRO:HD3	1.86	0.41
2:O:53:ASN:O	2:O:55:ARG:NH1	2.53	0.41
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.30	0.41
1:G:472:ILE:HG13	1:G:480:CYS:SG	2.61	0.41
1:H:21:ARG:HH21	1:H:79:PHE:HB3	1.86	0.41
1:H:457:ARG:HD2	1:H:457:ARG:HA	1.70	0.41
1:H:472:ILE:HG23	1:H:488:CYS:HB2	2.02	0.41
1:I:21:ARG:HH21	1:I:79:PHE:HB3	1.86	0.41
1:I:24:LEU:HB2	1:I:78:ARG:HH11	1.85	0.41
1:I:102:ARG:HG3	1:I:141:LEU:HG	2.03	0.41
3:N:40:ARG:HB3	3:N:50:ILE:HD11	2.03	0.41
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.56	0.41
3:J:14:PRO:HG2	3:J:120:SER:HA	2.02	0.41
3:M:42:PRO:HA	3:M:93:ALA:HA	2.02	0.41
1:I:326:ILE:H	1:I:326:ILE:HG13	1.72	0.41
2:O:22:CYS:N	2:O:74:ALA:O	2.53	0.41
3:P:5:GLN:NE2	3:P:6:GLU:O	2.50	0.41
2:Q:18:VAL:HG12	2:Q:81:LEU:HD21	2.02	0.41
3:R:138:THR:OG1	3:R:142:THR:O	2.35	0.41
1:A:88:ASP:OD1	1:A:88:ASP:N	2.53	0.41
1:B:88:ASP:OD1	1:B:88:ASP:N	2.54	0.41
1:B:170:TYR:CE2	1:B:172:SER:HB3	2.55	0.41
1:B:214:ARG:NH1	1:B:215:ASP:H	2.18	0.41
1:C:317:ASN:HB3	1:C:319:ARG:NH1	2.36	0.41
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	2.03	0.41
1:C:808:ASP:OD1	1:C:808:ASP:N	2.51	0.41
3:E:138:THR:OG1	3:E:142:THR:O	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:LEU:HB3	2:F:159:TRP:CZ3	2.56	0.41
3:M:53:ILE:HD13	3:M:73:VAL:HG23	2.01	0.41
3:M:115:LEU:HD21	3:M:117:THR:HG22	2.03	0.41
1:G:81:ASN:HD21	1:G:242:LEU:HD12	1.86	0.41
1:G:159:VAL:HG23	1:G:160:TYR:CD1	2.56	0.41
1:G:429:PHE:HZ	1:G:512:VAL:HG11	1.85	0.41
1:G:974:SER:HB2	1:G:983:ARG:HH12	1.86	0.41
1:G:984:LEU:HB2	1:G:989:ALA:HB2	2.02	0.41
1:H:733:LYS:O	1:H:861:LEU:N	2.50	0.41
1:I:323:THR:OG1	1:I:324:GLU:OE1	2.33	0.41
1:I:332:ILE:H	1:I:332:ILE:HG12	1.69	0.41
1:I:598:ILE:HB	1:I:609:ALA:HB3	2.03	0.41
2:O:60:PRO:HB2	2:O:62:ARG:HG2	2.03	0.41
1:B:342:PHE:HA	1:B:347:PHE:CZ	2.56	0.41
1:B:769:GLY:HA2	1:B:772:VAL:HG12	2.02	0.41
3:E:39:ILE:HD11	3:E:107:PHE:CZ	2.56	0.41
3:E:119:SER:HB2	3:E:153:PHE:HE2	1.85	0.41
1:H:374:PHE:HB2	3:P:104:ARG:NH2	2.36	0.41
1:H:1090:PRO:HG2	1:I:913:GLN:HE22	1.86	0.41
1:B:21:ARG:HH21	1:B:79:PHE:HB3	1.86	0.40
1:C:950:ASP:OD1	1:C:951:VAL:N	2.55	0.40
1:G:123:ALA:HA	1:G:177:MET:HB3	2.03	0.40
1:I:88:ASP:OD1	1:I:88:ASP:N	2.55	0.40
1:A:896:ILE:HG13	1:C:712:ILE:HG13	2.03	0.40
1:B:357:ARG:NH2	1:C:168:PHE:HB2	2.33	0.40
1:C:474:GLN:HB3	1:C:477:SER:OG	2.21	0.40
2:D:194:GLU:OE2	2:D:194:GLU:N	2.36	0.40
1:G:458:LYS:HA	1:G:473:TYR:CE1	2.55	0.40
1:H:800:PHE:CE1	1:H:902:MET:HE1	2.56	0.40
1:I:304:LYS:HE2	1:I:304:LYS:HB3	1.90	0.40
1:B:800:PHE:CE1	1:B:902:MET:HE1	2.56	0.40
1:B:1090:PRO:HG2	1:C:913:GLN:HE22	1.86	0.40
1:C:457:ARG:HD2	1:C:457:ARG:HA	1.70	0.40
1:C:1125:ASN:OD1	1:C:1126:CYS:N	2.54	0.40
1:G:83:VAL:HG11	1:G:237:ARG:CZ	2.51	0.40
1:G:276:LEU:HD22	1:G:301:CYS:HA	2.03	0.40
1:H:153:MET:HE1	1:H:155:SER:HB3	2.02	0.40
1:H:384:PRO:HA	1:H:387:LEU:HD23	2.03	0.40
1:I:1125:ASN:OD1	1:I:1126:CYS:N	2.54	0.40
2:L:162:ASP:HB2	2:L:199:HIS:CD2	2.56	0.40
1:B:663:ASP:OD1	1:B:664:ILE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:VAL:HG13	1:C:368:LEU:HD12	2.04	0.40
3:J:119:SER:HB2	3:J:153:PHE:CZ	2.56	0.40
1:G:898:PHE:O	1:G:902:MET:HG2	2.21	0.40
1:G:950:ASP:OD1	1:G:951:VAL:N	2.55	0.40
3:N:13:LYS:HB2	3:N:16:GLU:OE1	2.20	0.40
1:B:617:CYS:N	1:B:649:CYS:SG	2.95	0.40
1:B:713:ALA:HB3	1:C:894:LEU:HB3	2.03	0.40
1:C:719:THR:HG23	1:C:1070:ALA:HB2	2.04	0.40
1:H:906:PHE:CD2	1:H:916:LEU:HD12	2.56	0.40
1:I:435:ALA:HB2	1:I:510:VAL:HG22	2.02	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	1054/1278 (82%)	1012 (96%)	42 (4%)	0	100	100
1	B	1054/1278 (82%)	1017 (96%)	37 (4%)	0	100	100
1	C	1054/1278 (82%)	1011 (96%)	43 (4%)	0	100	100
1	G	1054/1278 (82%)	1012 (96%)	42 (4%)	0	100	100
1	H	1054/1278 (82%)	1018 (97%)	36 (3%)	0	100	100
1	I	1054/1278 (82%)	1022 (97%)	32 (3%)	0	100	100
2	D	209/243 (86%)	197 (94%)	12 (6%)	0	100	100
2	F	209/243 (86%)	199 (95%)	10 (5%)	0	100	100
2	K	209/243 (86%)	197 (94%)	12 (6%)	0	100	100
2	L	209/243 (86%)	197 (94%)	12 (6%)	0	100	100
2	O	209/243 (86%)	198 (95%)	11 (5%)	0	100	100
2	Q	209/243 (86%)	199 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	222/243 (91%)	218 (98%)	4 (2%)	0	100	100
3	J	222/243 (91%)	215 (97%)	7 (3%)	0	100	100
3	M	222/243 (91%)	214 (96%)	8 (4%)	0	100	100
3	N	222/243 (91%)	216 (97%)	6 (3%)	0	100	100
3	P	222/243 (91%)	216 (97%)	6 (3%)	0	100	100
3	R	222/243 (91%)	215 (97%)	7 (3%)	0	100	100
All	All	8910/10584 (84%)	8573 (96%)	337 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	934/1106 (84%)	929 (100%)	5 (0%)	81	83
1	B	934/1106 (84%)	934 (100%)	0	100	100
1	C	934/1106 (84%)	925 (99%)	9 (1%)	68	78
1	G	934/1106 (84%)	933 (100%)	1 (0%)	88	89
1	H	934/1106 (84%)	931 (100%)	3 (0%)	86	85
1	I	934/1106 (84%)	929 (100%)	5 (0%)	81	83
2	D	184/208 (88%)	182 (99%)	2 (1%)	65	76
2	F	184/208 (88%)	184 (100%)	0	100	100
2	K	184/208 (88%)	184 (100%)	0	100	100
2	L	184/208 (88%)	181 (98%)	3 (2%)	55	70
2	O	184/208 (88%)	184 (100%)	0	100	100
2	Q	184/208 (88%)	184 (100%)	0	100	100
3	E	192/209 (92%)	191 (100%)	1 (0%)	81	83
3	J	192/209 (92%)	191 (100%)	1 (0%)	81	83
3	M	192/209 (92%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	192/209 (92%)	190 (99%)	2 (1%)	68	78
3	P	192/209 (92%)	190 (99%)	2 (1%)	68	78
3	R	192/209 (92%)	191 (100%)	1 (0%)	81	83
All	All	7860/9138 (86%)	7825 (100%)	35 (0%)	81	84

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	529	LYS
1	A	532	ASN
1	A	582	LEU
1	A	1106	GLN
1	C	335	LEU
1	C	360	ASN
1	C	362	VAL
1	C	523	THR
1	C	525	CYS
1	C	529	LYS
1	C	530	SER
1	C	736	VAL
1	C	740	MET
2	D	163	SER
2	D	164	SER
3	E	100	GLN
3	J	106	ARG
1	G	1106	GLN
1	H	528	LYS
1	H	529	LYS
1	H	530	SER
1	I	326	ILE
1	I	331	ASN
1	I	334	ASN
1	I	335	LEU
1	I	922	LEU
2	L	162	ASP
2	L	166	VAL
2	L	167	LYS
3	N	3	GLN
3	N	16	GLU
3	P	104	ARG

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Mol	Chain	Res	Type
3	P	106	ARG
3	R	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	146	HIS
1	A	173	GLN
1	A	188	ASN
1	A	314	GLN
1	A	450	ASN
1	A	481	ASN
1	A	498	GLN
1	A	563	GLN
1	A	580	GLN
1	A	613	GLN
1	A	655	HIS
1	A	804	GLN
1	A	955	ASN
1	A	957	GLN
1	A	1106	GLN
1	A	1108	ASN
1	B	148	ASN
1	B	239	GLN
1	B	271	GLN
1	B	314	GLN
1	B	354	ASN
1	B	675	GLN
1	B	895	GLN
1	B	901	GLN
1	B	913	GLN
1	B	919	ASN
1	B	955	ASN
1	B	957	GLN
1	B	969	ASN
1	C	87	ASN
1	C	134	GLN
1	C	354	ASN
1	C	439	ASN
1	C	448	ASN
1	C	450	ASN

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Mol	Chain	Res	Type
1	C	506	GLN
1	C	655	HIS
1	C	675	GLN
1	C	762	GLN
1	C	895	GLN
1	C	913	GLN
1	C	969	ASN
1	C	1108	ASN
2	D	8	HIS
2	D	137	GLN
3	E	3	GLN
2	F	8	HIS
2	F	39	GLN
3	J	41	GLN
2	K	1	ASN
2	K	137	GLN
3	M	3	GLN
3	M	100	GLN
1	G	134	GLN
1	G	173	GLN
1	G	314	GLN
1	G	354	ASN
1	G	450	ASN
1	G	498	GLN
1	G	563	GLN
1	G	580	GLN
1	G	613	GLN
1	G	655	HIS
1	G	755	GLN
1	G	804	GLN
1	G	1083	HIS
1	G	1106	GLN
1	G	1108	ASN
1	H	239	GLN
1	H	314	GLN
1	H	354	ASN
1	H	409	GLN
1	H	448	ASN
1	H	450	ASN
1	H	493	GLN
1	H	675	GLN
1	H	895	GLN

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Mol	Chain	Res	Type
1	H	913	GLN
1	H	919	ASN
1	H	955	ASN
1	H	957	GLN
1	H	969	ASN
1	I	87	ASN
1	I	134	GLN
1	I	354	ASN
1	I	439	ASN
1	I	448	ASN
1	I	450	ASN
1	I	460	ASN
1	I	474	GLN
1	I	481	ASN
1	I	506	GLN
1	I	655	HIS
1	I	762	GLN
1	I	764	ASN
1	I	895	GLN
1	I	913	GLN
1	I	920	GLN
1	I	935	GLN
1	I	955	ASN
1	I	969	ASN
1	I	1108	ASN
2	L	119	GLN
3	N	171	HIS
2	O	8	HIS
2	O	35	GLN
2	O	72	ASN
3	P	3	GLN
3	P	79	GLN
2	Q	1	ASN
2	Q	8	HIS
2	Q	139	ASN
2	Q	195	GLN
3	R	3	GLN
3	R	100	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

48 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	$\# Z > 2$
4	NAG	S	1	1,4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	S	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	T	1	1,4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	T	2	4	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	U	1	1,4	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	U	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	V	1	1,4	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	V	2	4	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	W	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	W	2	4	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	X	1	1,4	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	X	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	Y	1	1,4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	Y	2	4	14,14,15	0.29	0	17,19,21	0.42	0
4	NAG	Z	1	1,4	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	Z	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	a	1	1,4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	a	2	4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	b	1	1,4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	b	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	c	1	1,4	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	c	2	4	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	d	1	1,4	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	d	2	4	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	e	1	1,4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	e	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	f	1	1,4	14,14,15	0.26	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	f	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	g	1	1,4	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	g	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	h	1	1,4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	h	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	i	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	i	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	j	1	1,4	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	j	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	k	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	k	2	4	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	l	1	1,4	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	l	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	m	1	1,4	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	m	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	n	1	1,4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	n	2	4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	o	1	1,4	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	o	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	p	1	1,4	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	p	2	4	14,14,15	0.27	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
4	NAG	c	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
4	NAG	d	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	2/6/23/26	0/1/1/1
4	NAG	e	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
4	NAG	f	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
4	NAG	g	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	h	2	4	-	2/6/23/26	0/1/1/1
4	NAG	i	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
4	NAG	j	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	2/6/23/26	0/1/1/1
4	NAG	k	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	k	2	4	-	2/6/23/26	0/1/1/1
4	NAG	l	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	NAG	m	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
4	NAG	n	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	n	2	4	-	2/6/23/26	0/1/1/1
4	NAG	o	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	V	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	p	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	l	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	k	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	l	2	NAG	C4-C5-C6-O6
4	o	2	NAG	C4-C5-C6-O6
4	p	1	NAG	O5-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
4	l	1	NAG	O5-C5-C6-O6
4	p	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
4	d	2	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	n	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
4	l	1	NAG	C4-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6

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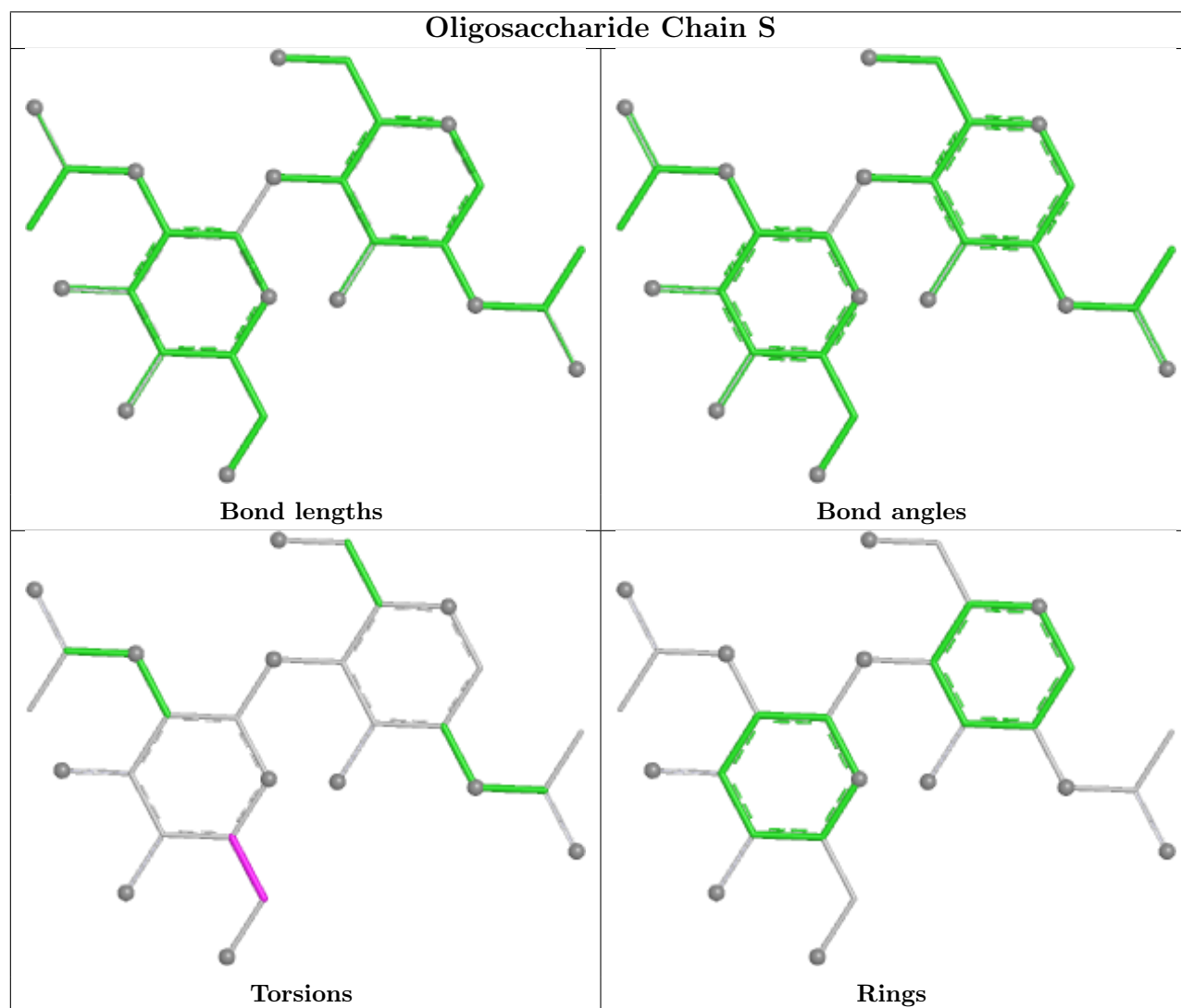
Mol	Chain	Res	Type	Atoms
4	p	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	j	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
4	n	1	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	k	2	NAG	O5-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	o	2	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	n	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	n	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6

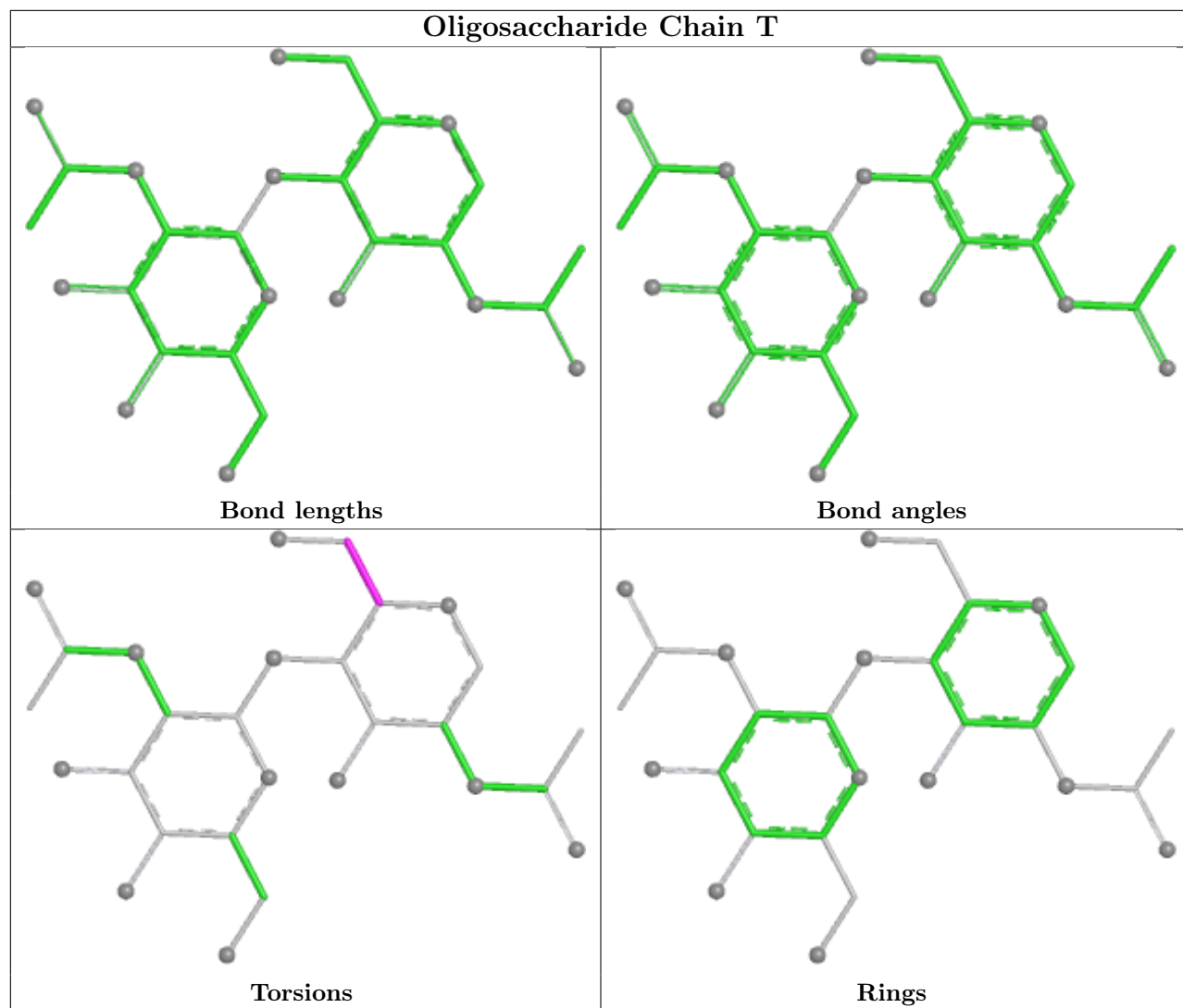
There are no ring outliers.

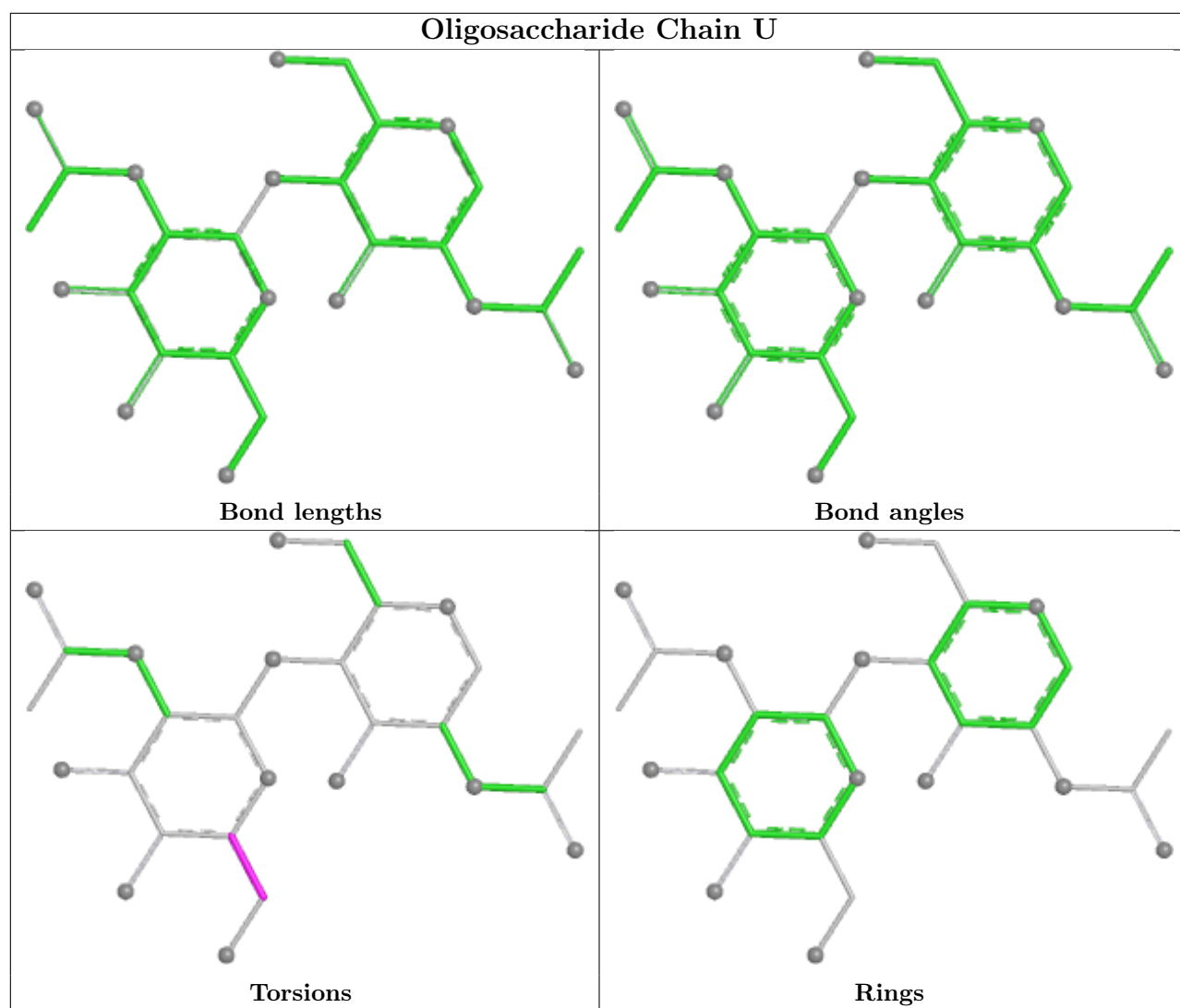
8 monomers are involved in 9 short contacts:

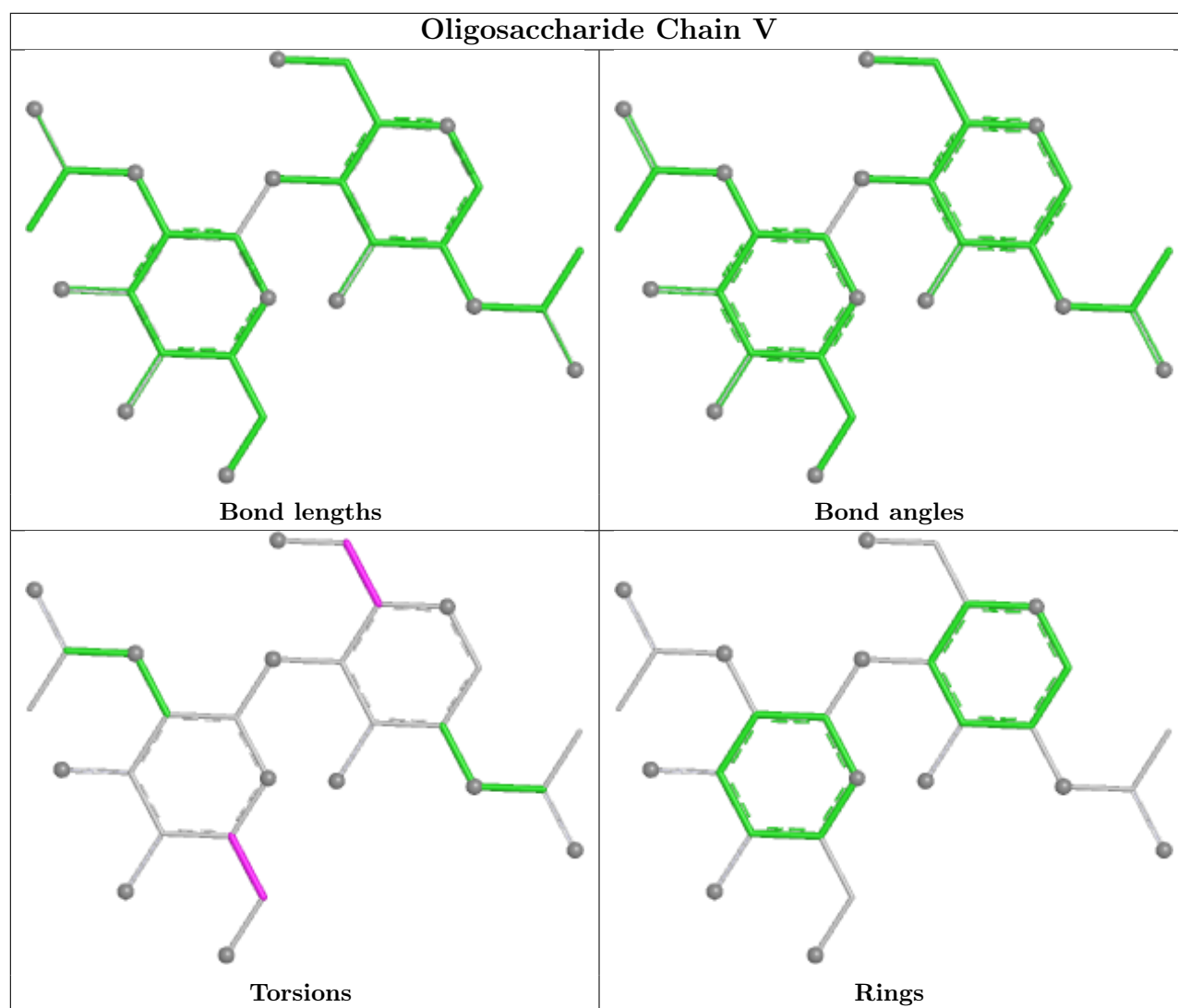
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	k	1	NAG	1	0
4	m	1	NAG	2	0
4	i	1	NAG	1	0
4	o	1	NAG	1	0
4	W	1	NAG	1	0
4	Y	1	NAG	1	0
4	a	1	NAG	1	0
4	c	1	NAG	1	0

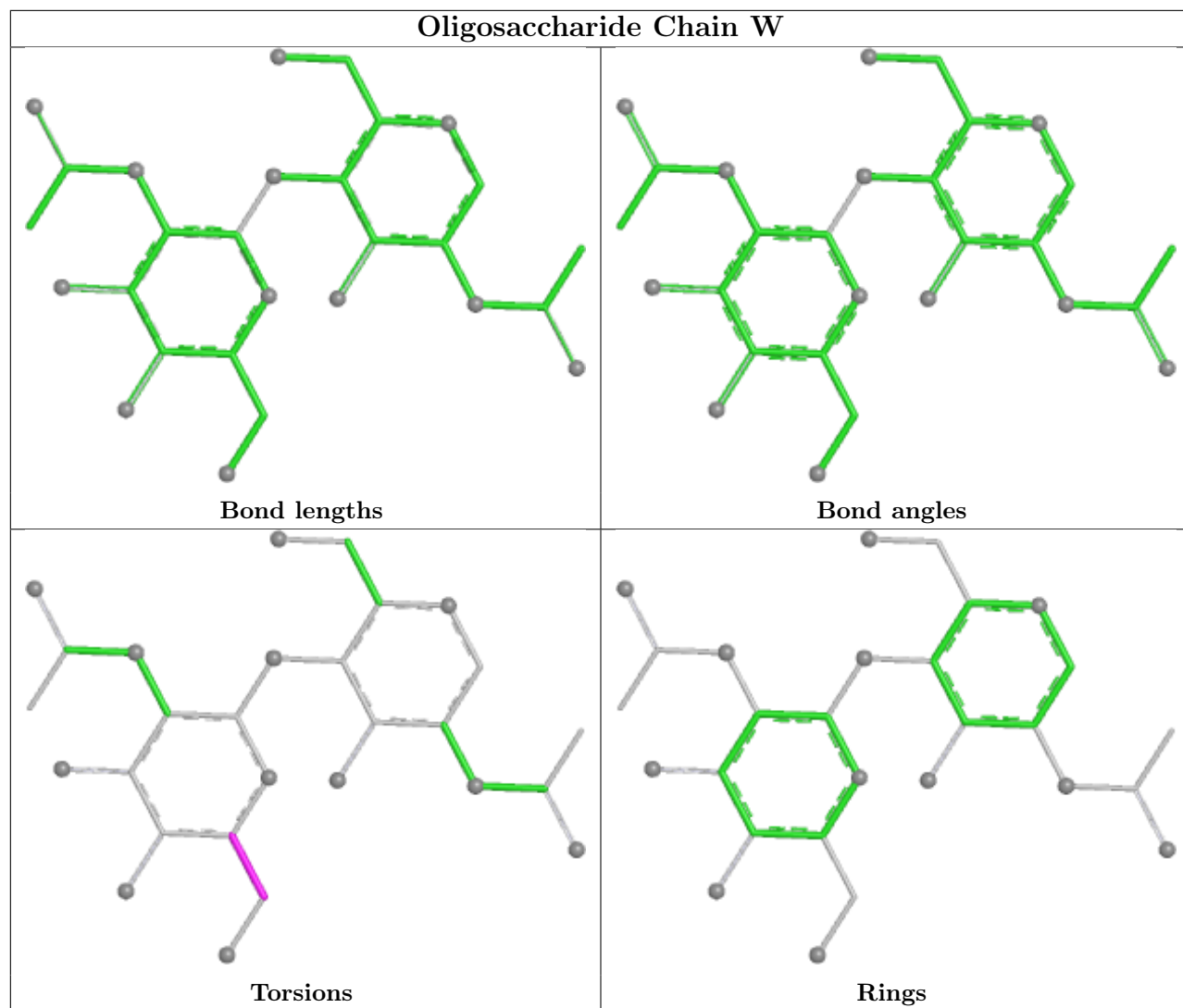
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

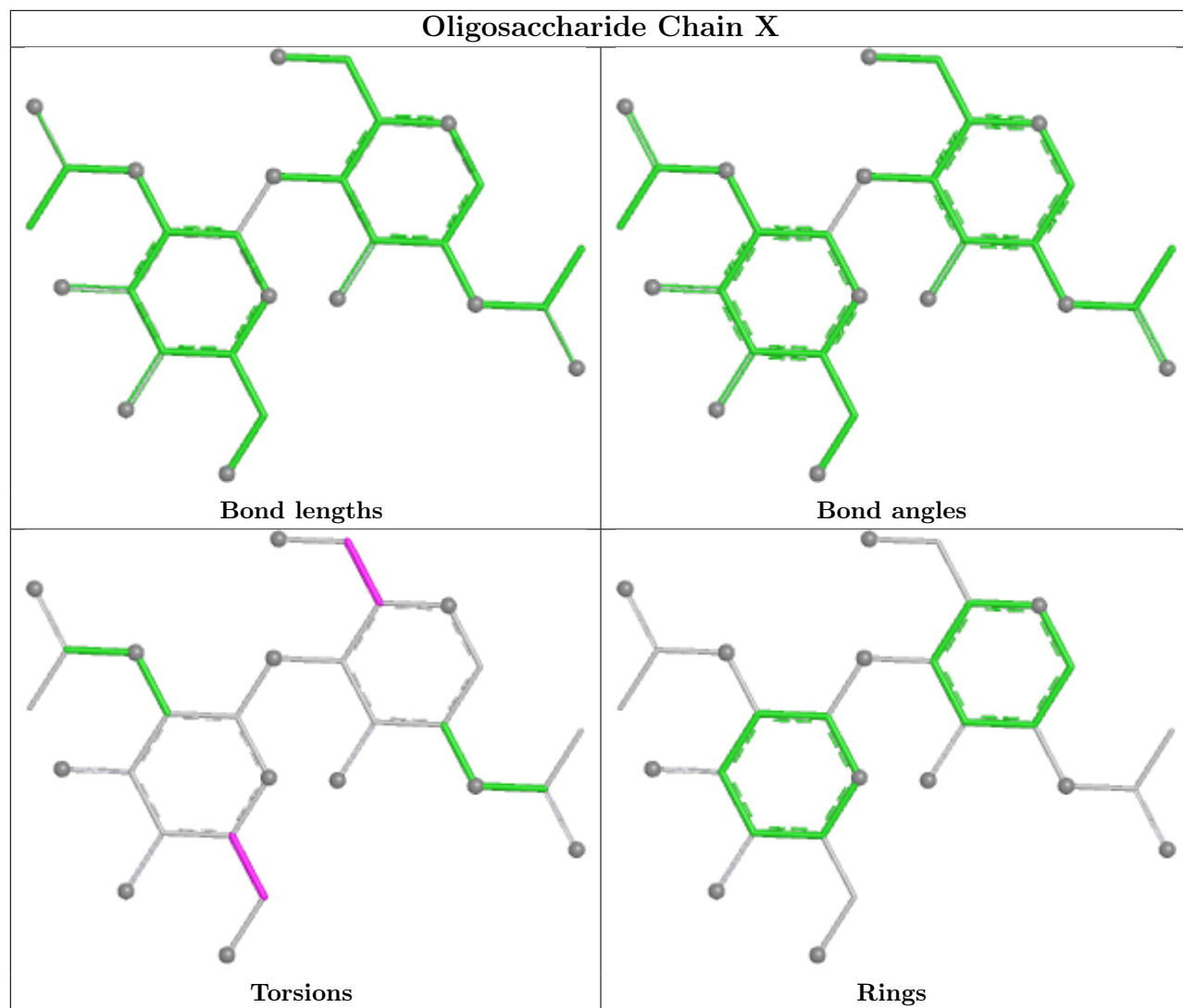


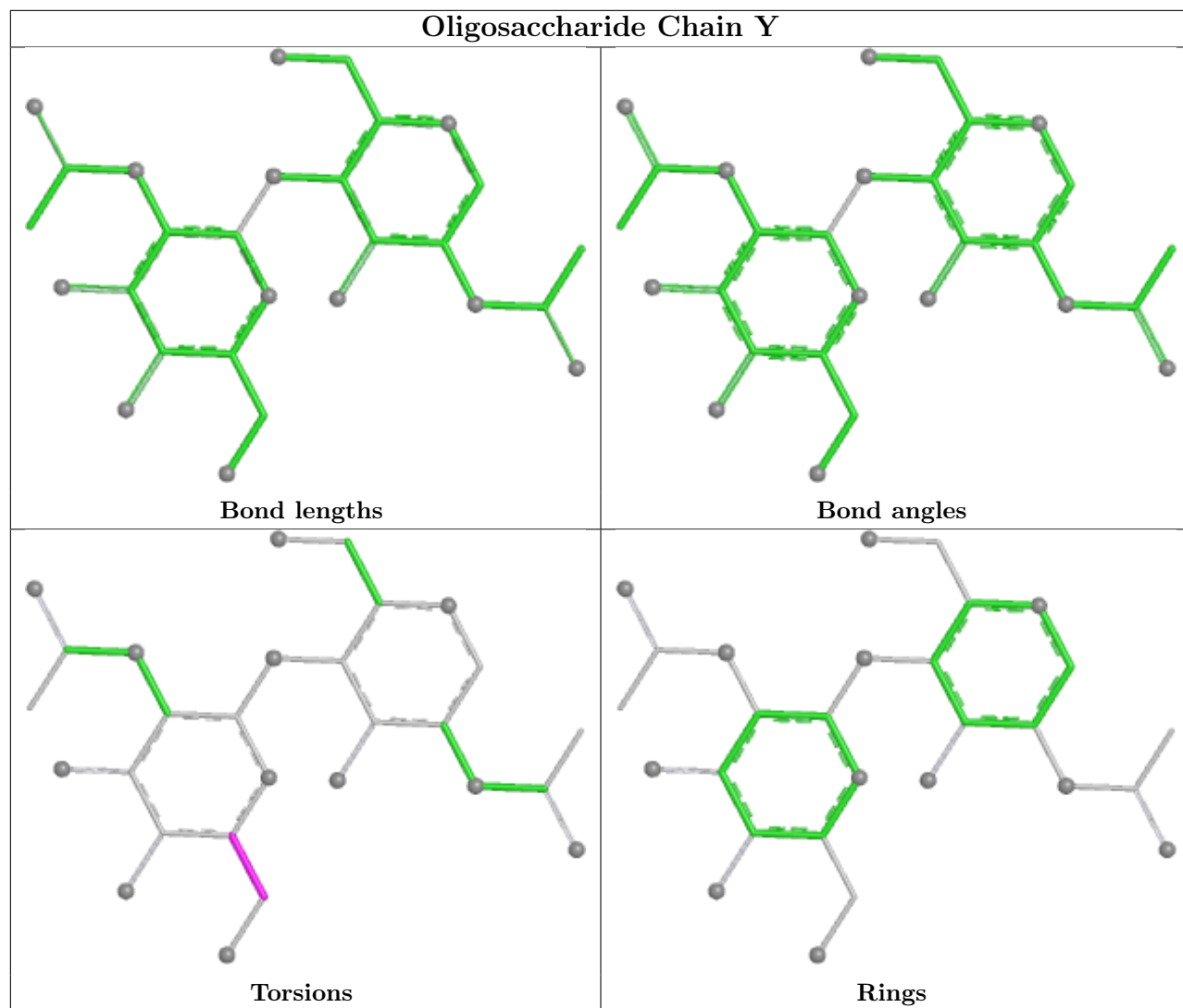


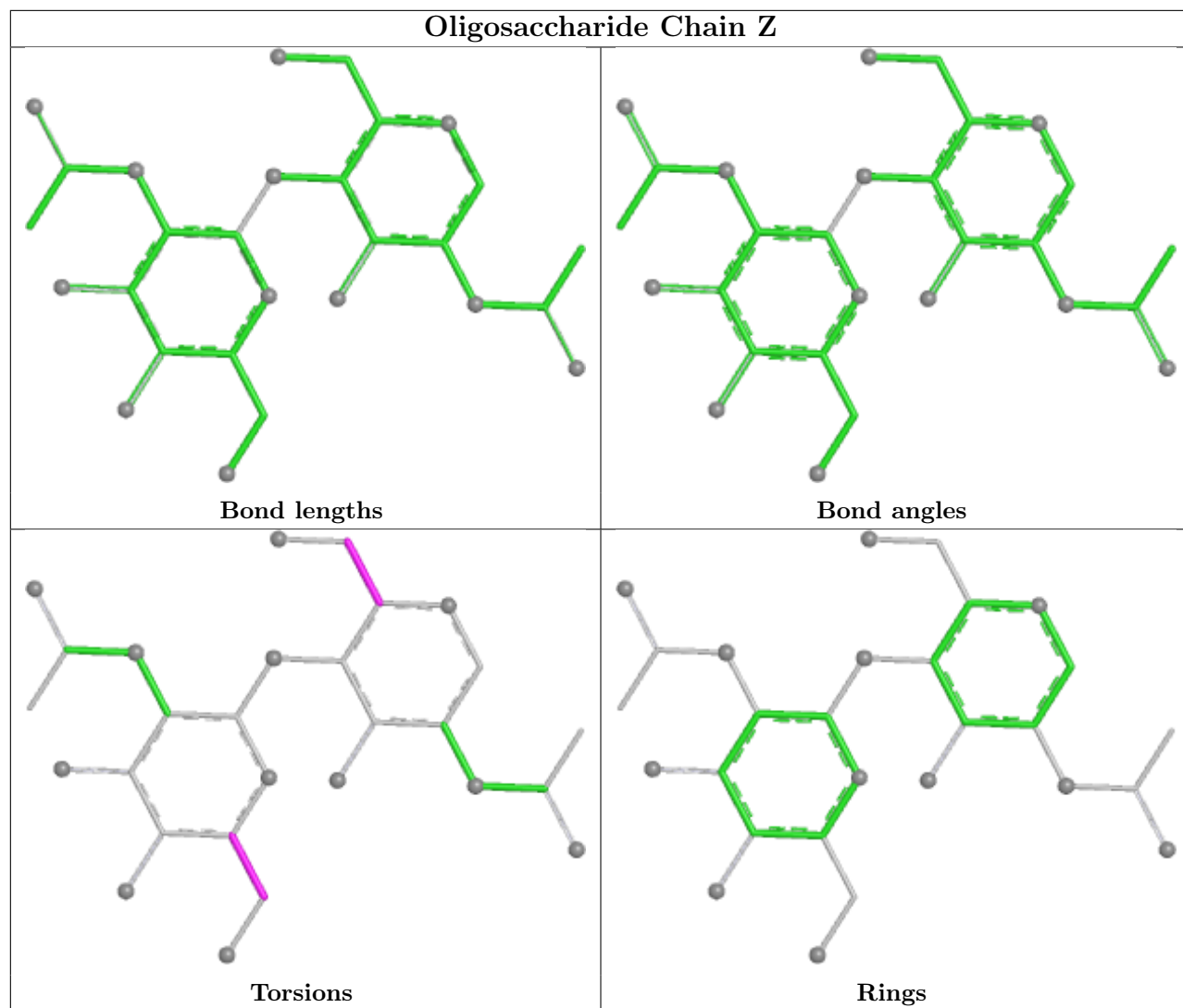


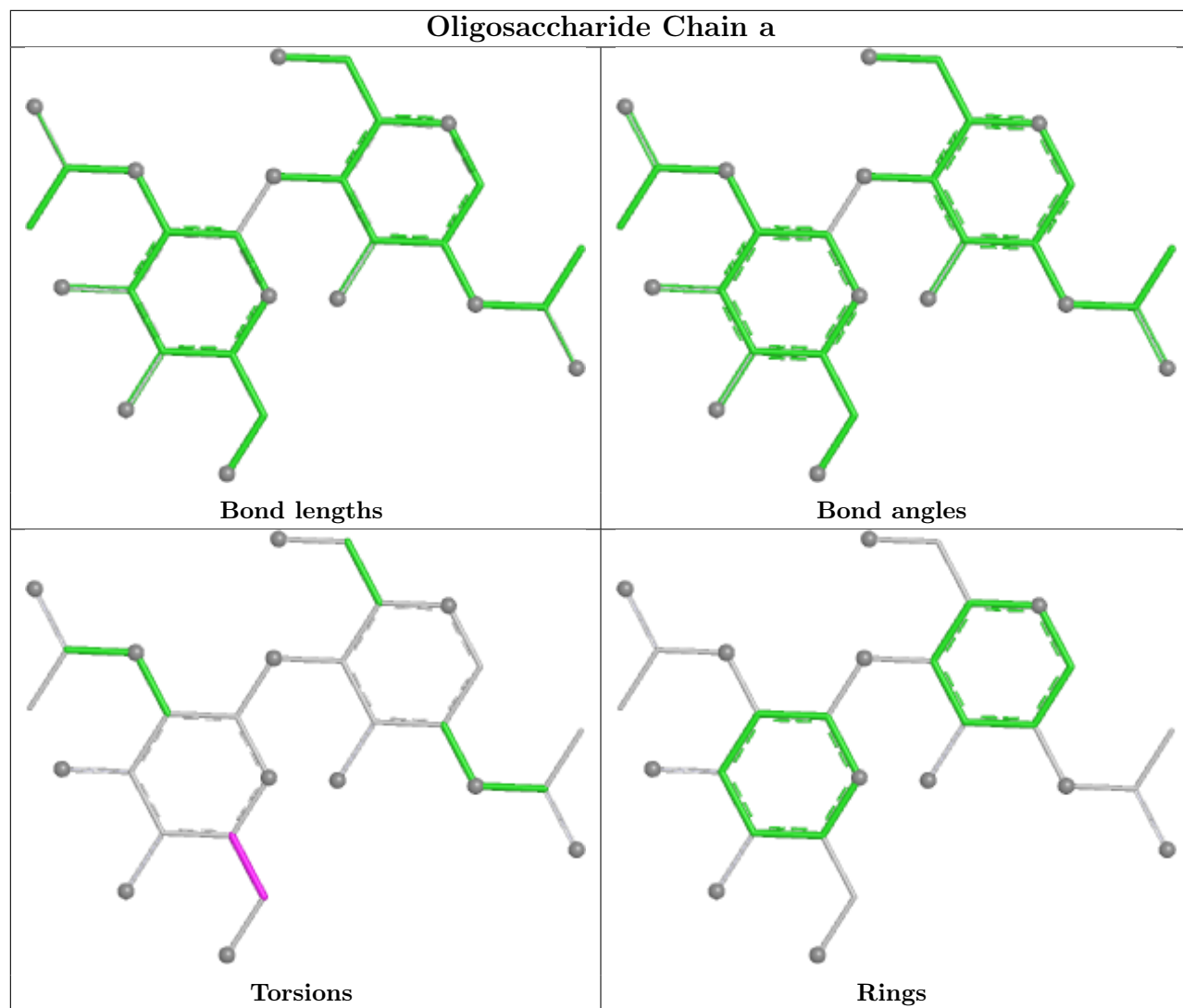


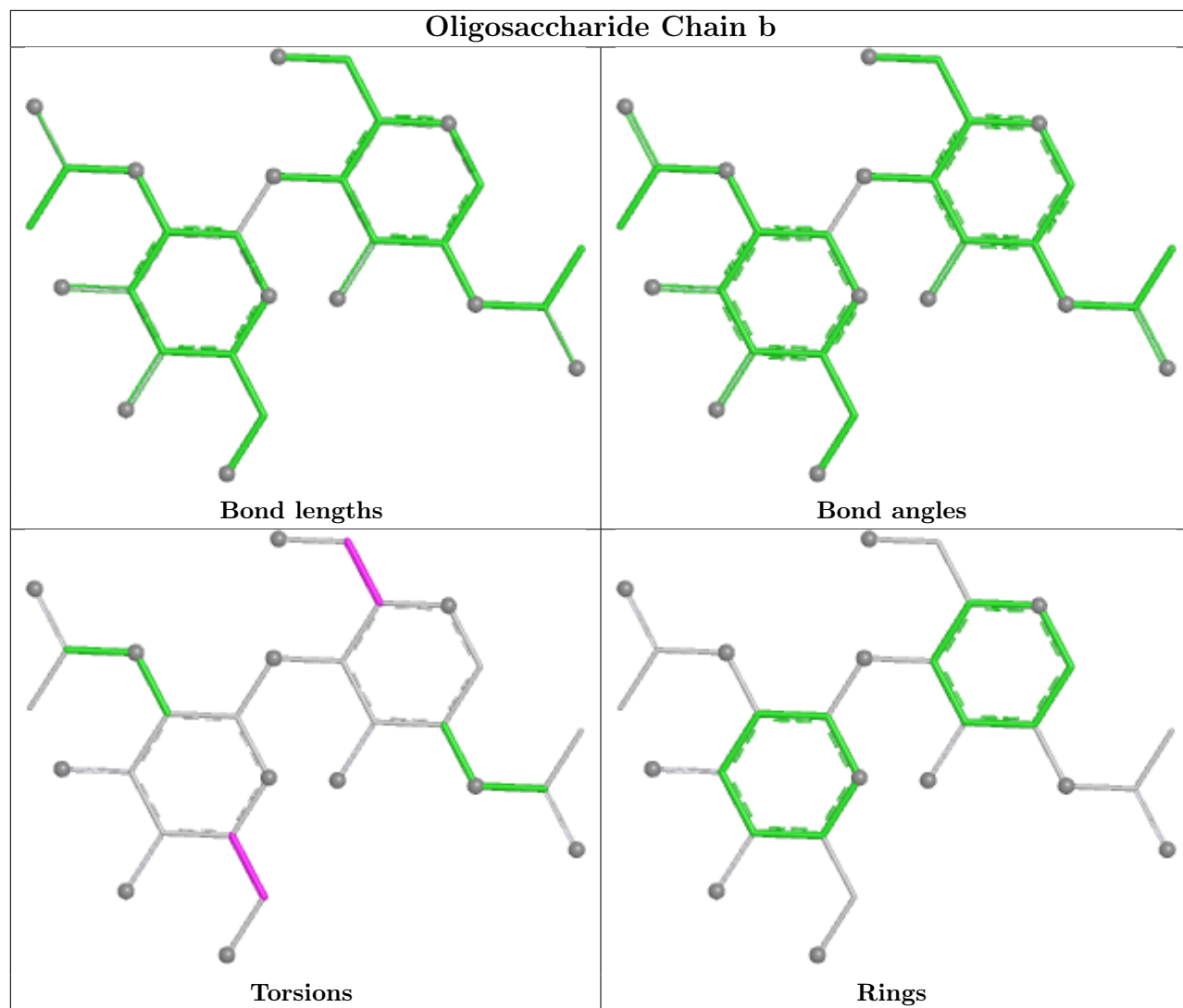


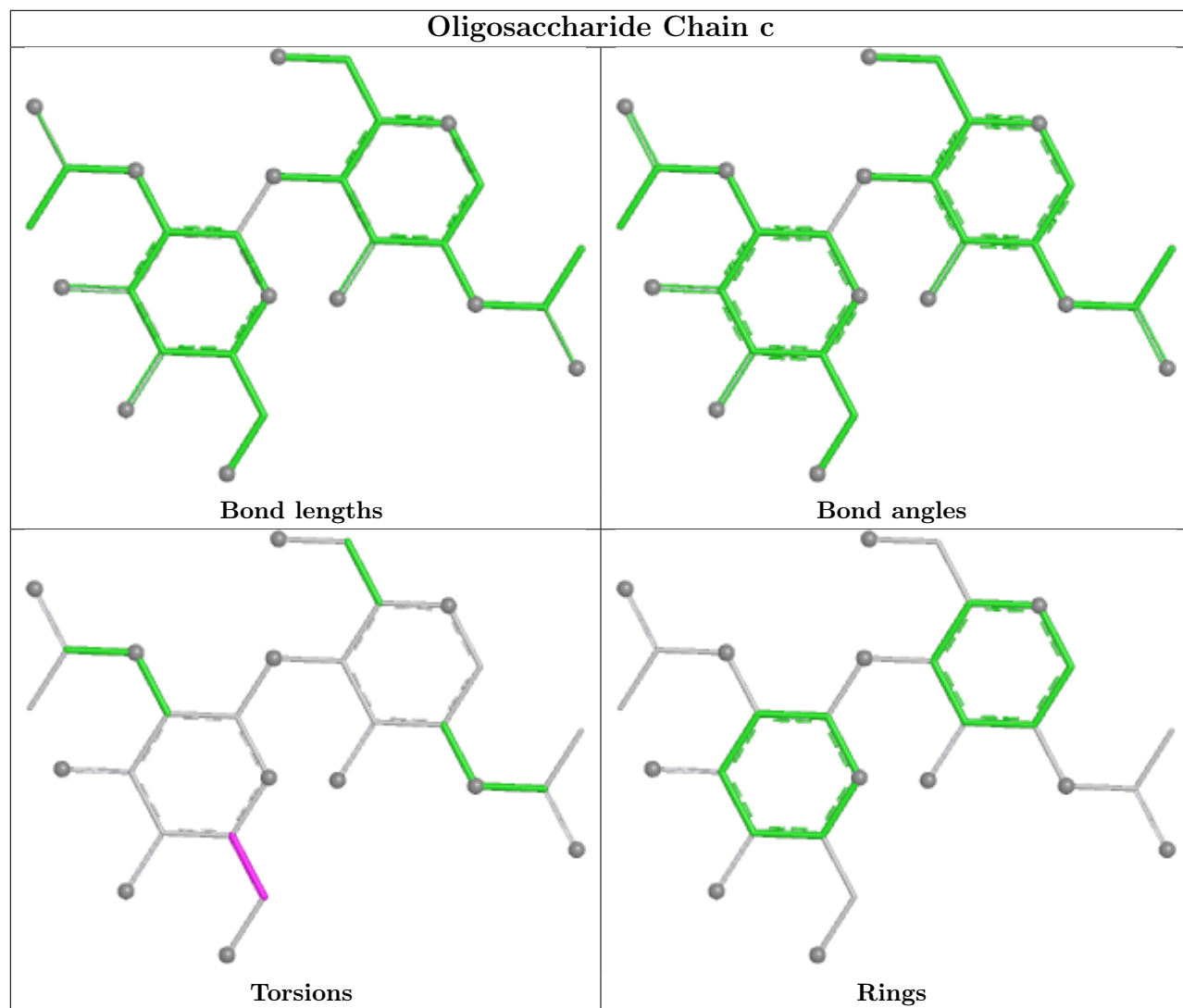


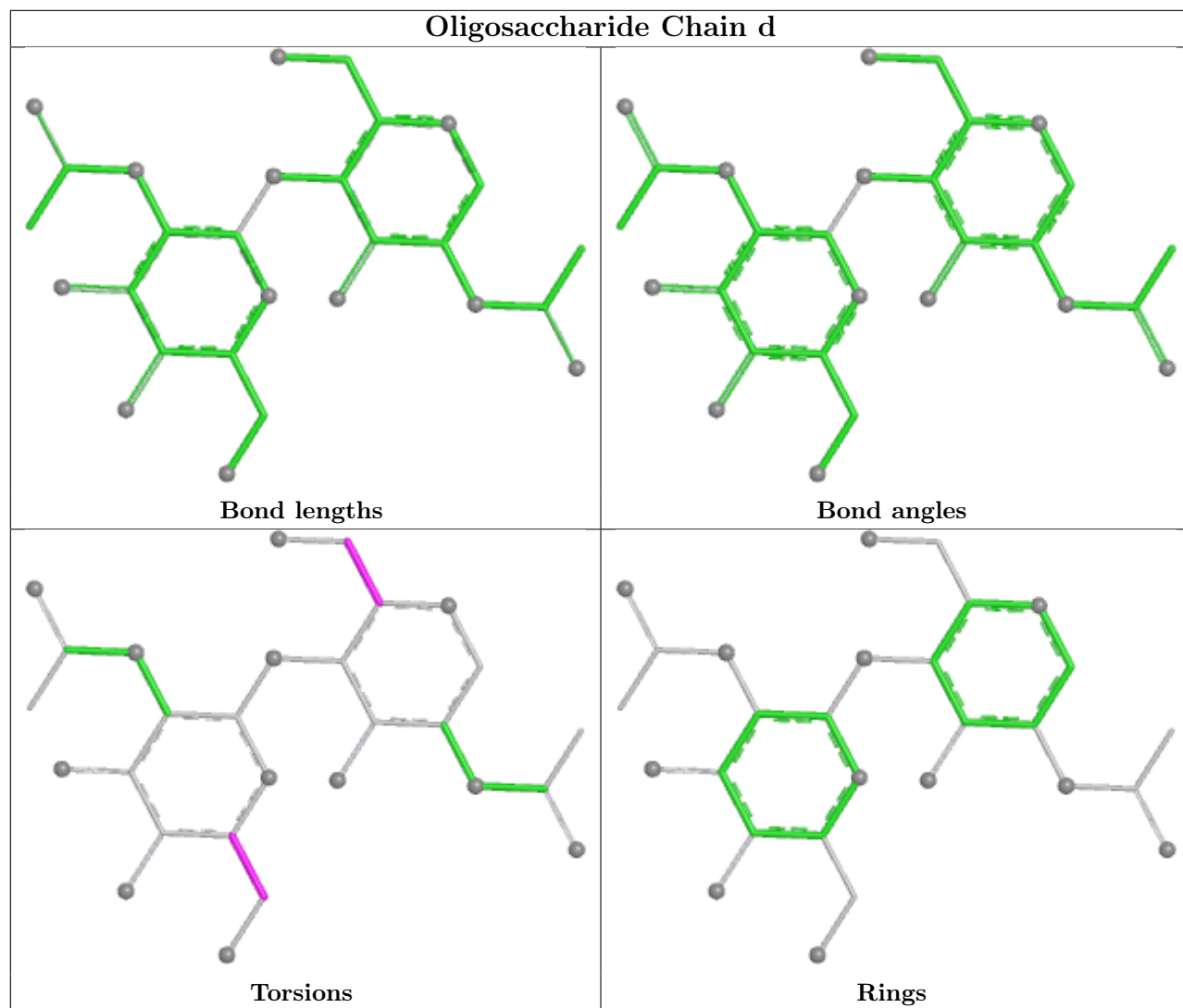


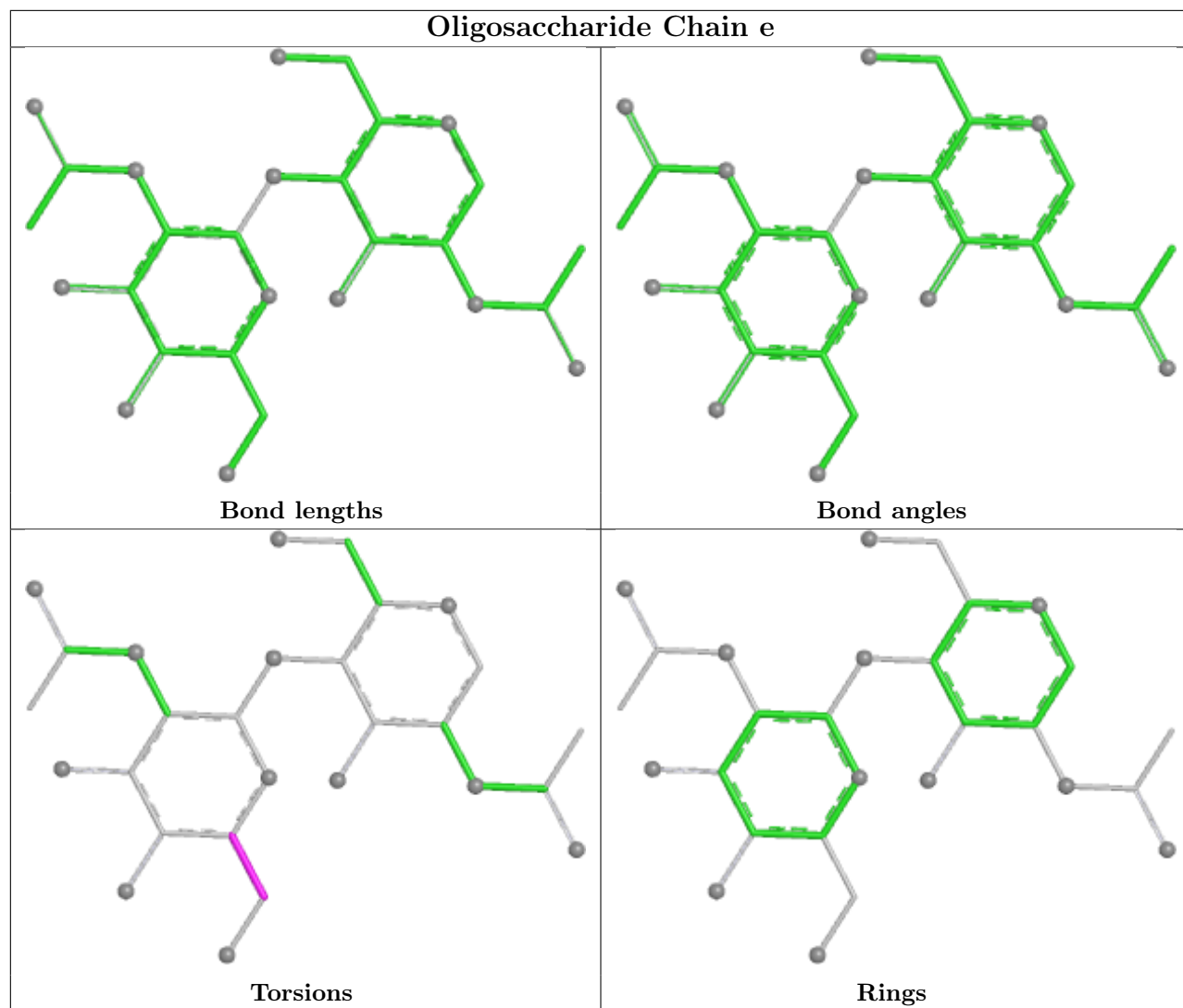


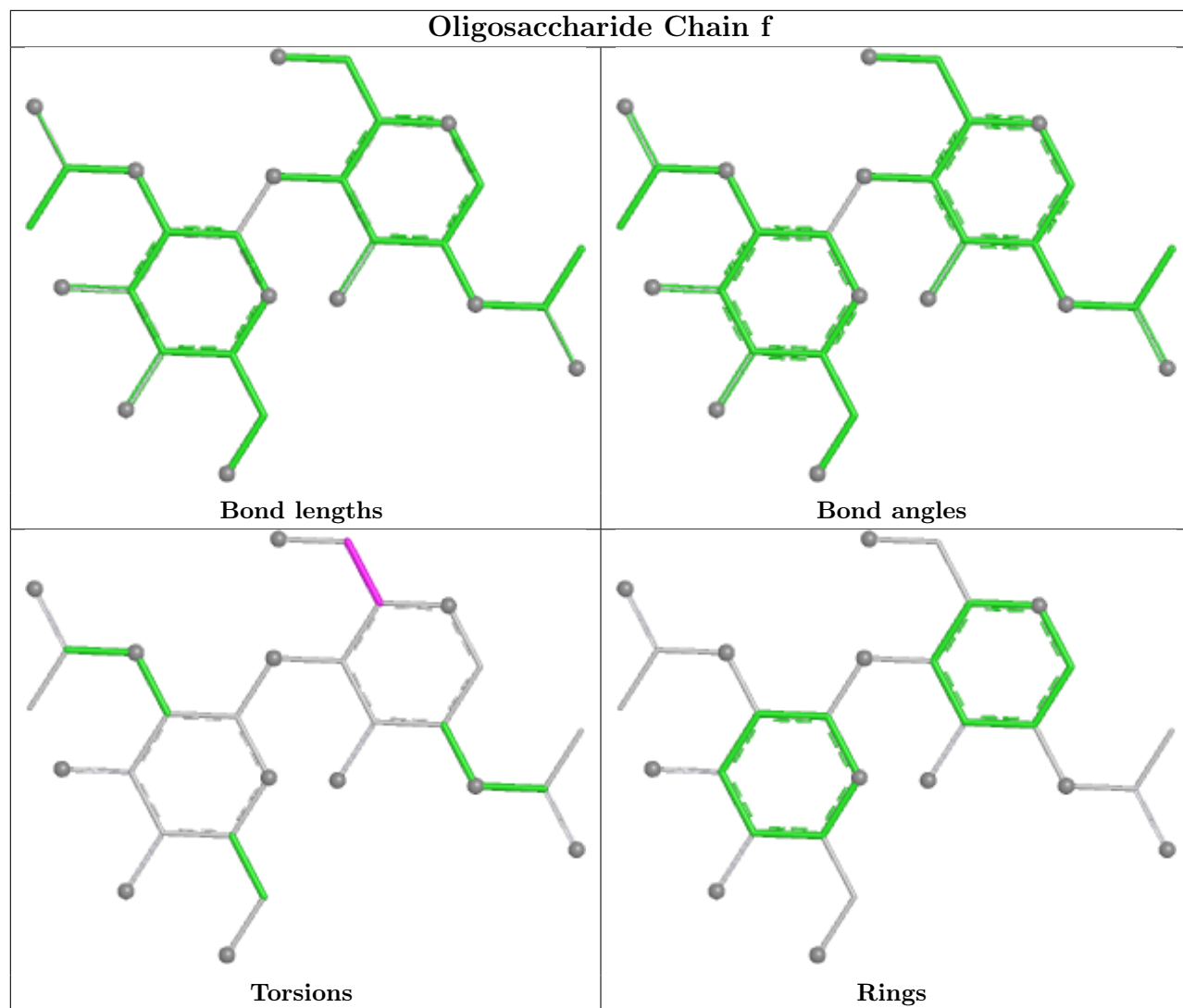


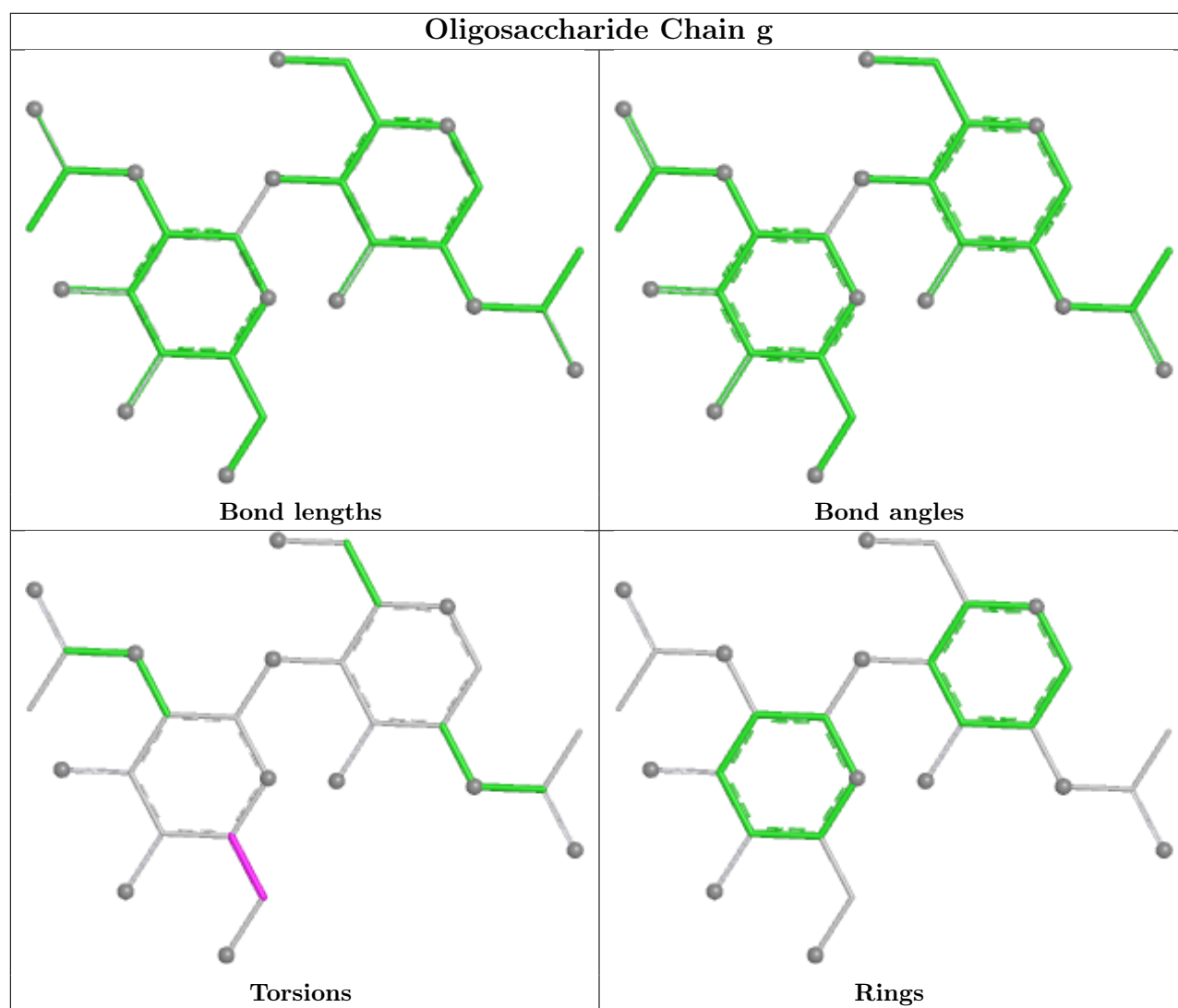


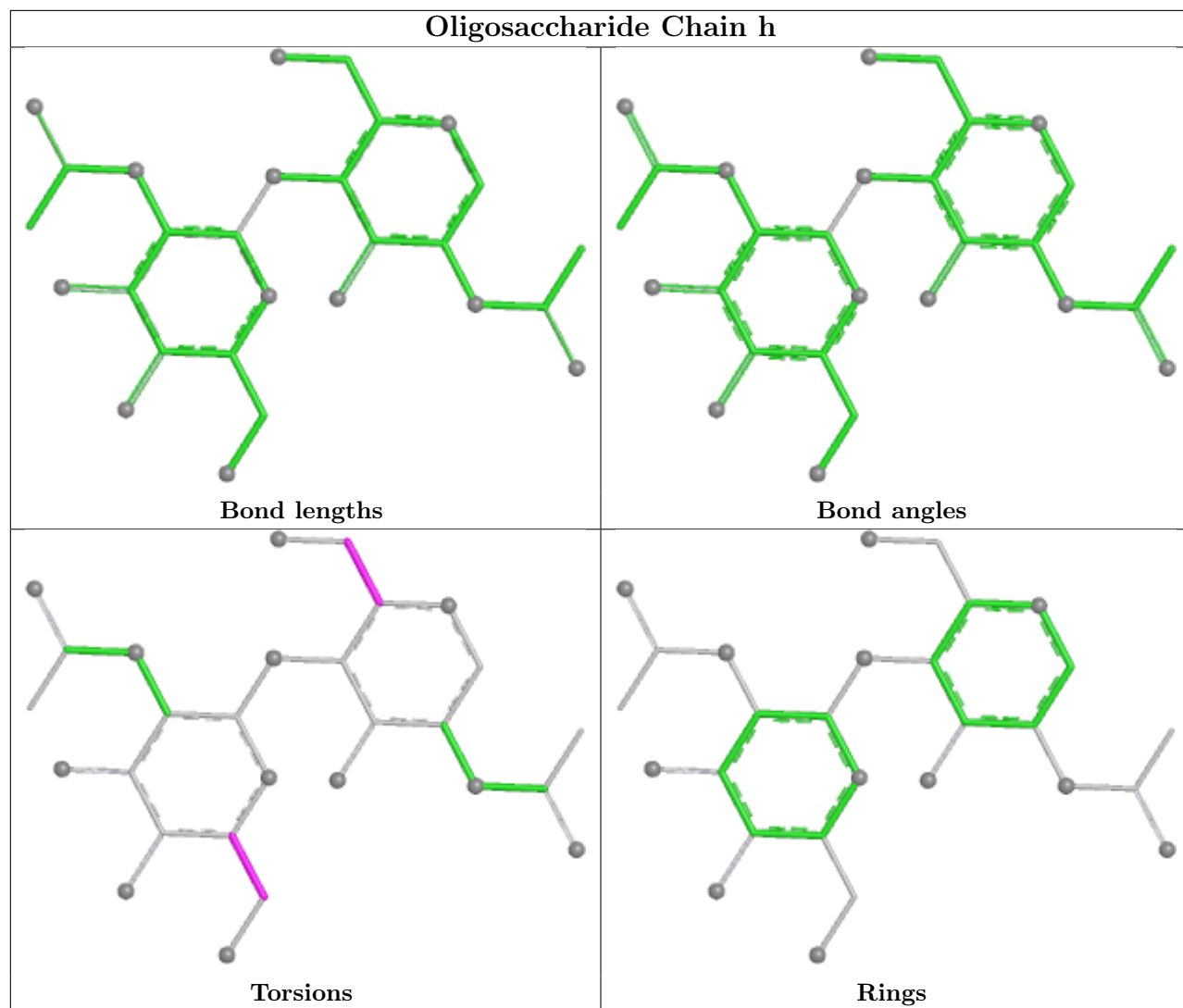


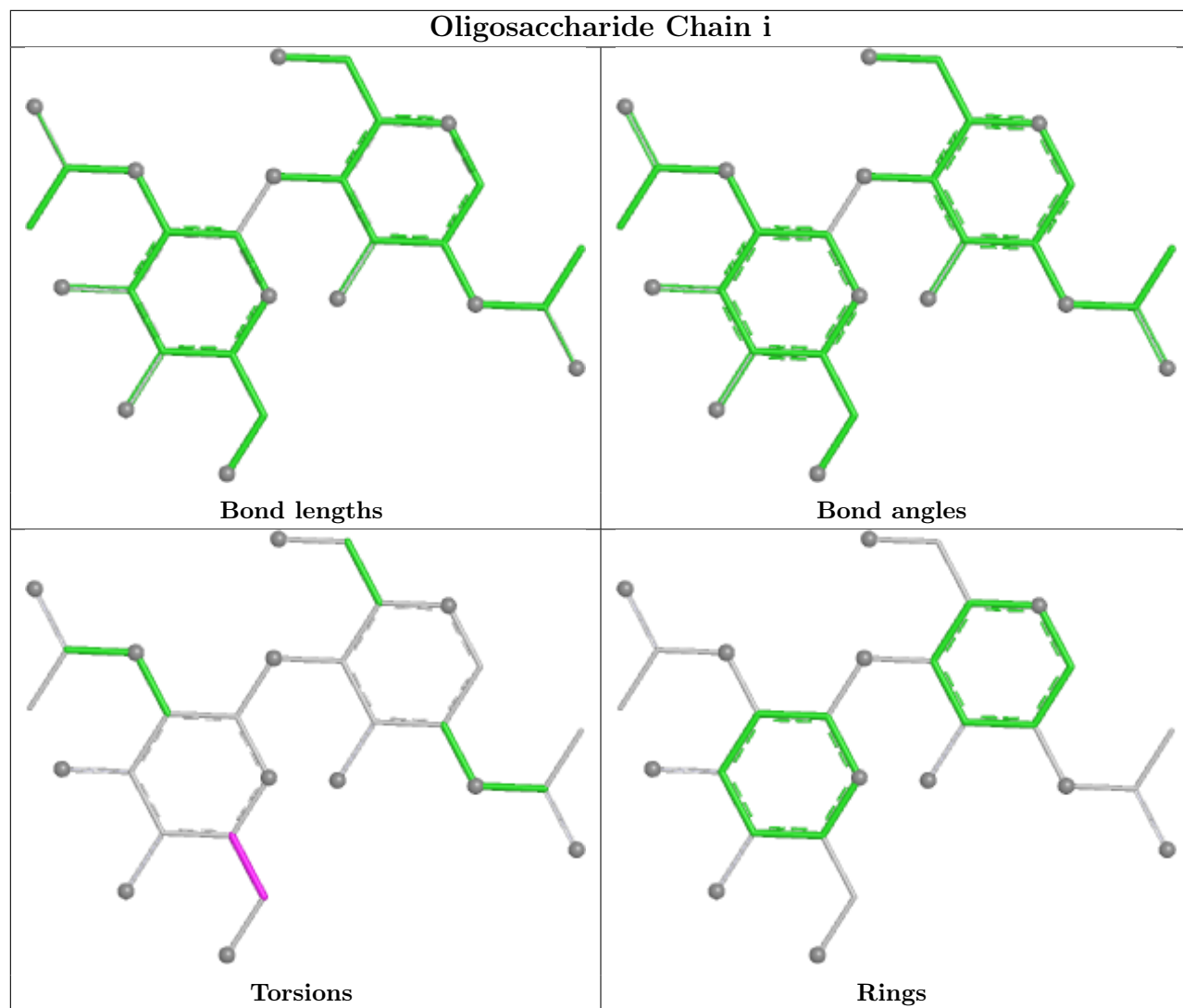


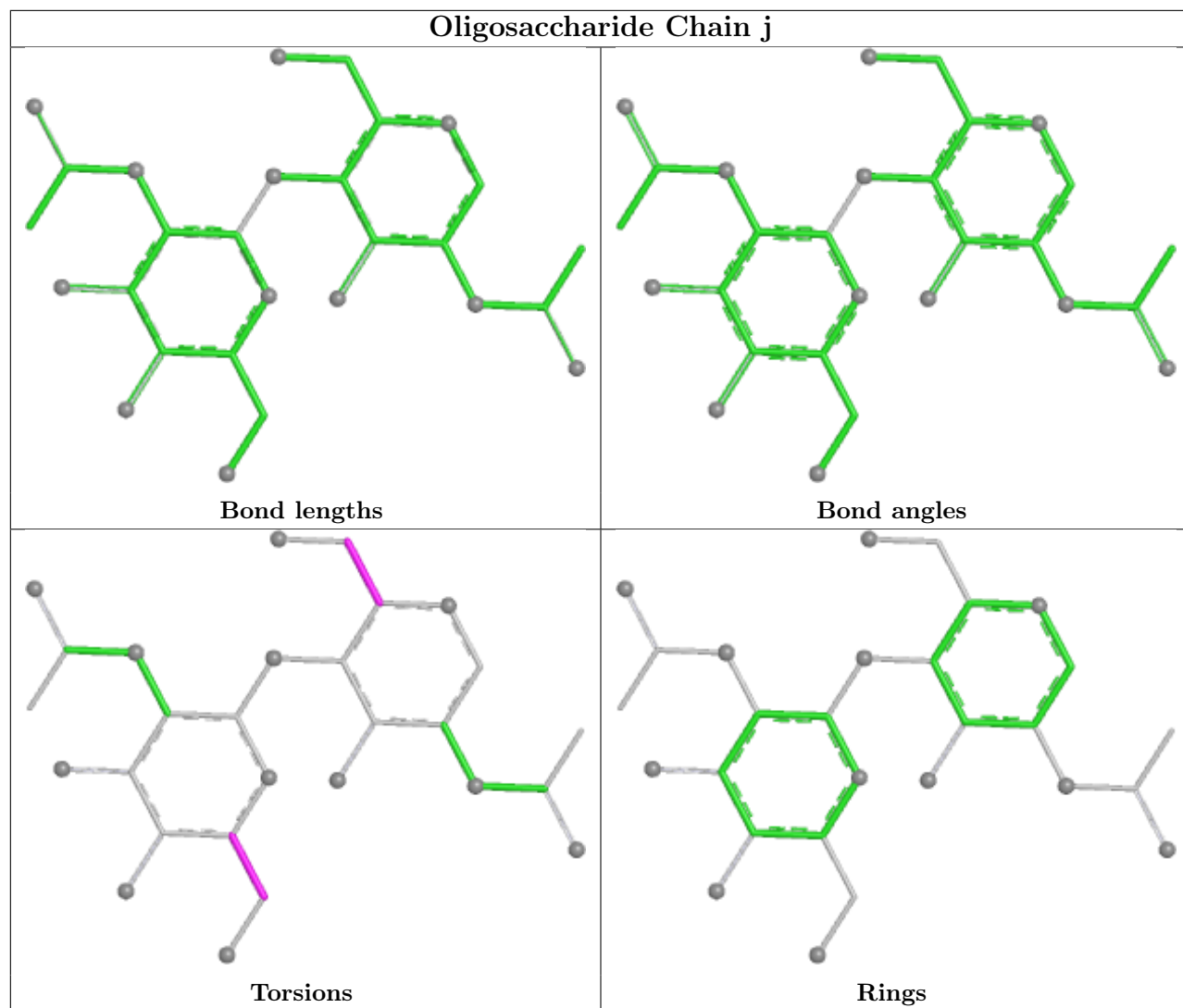


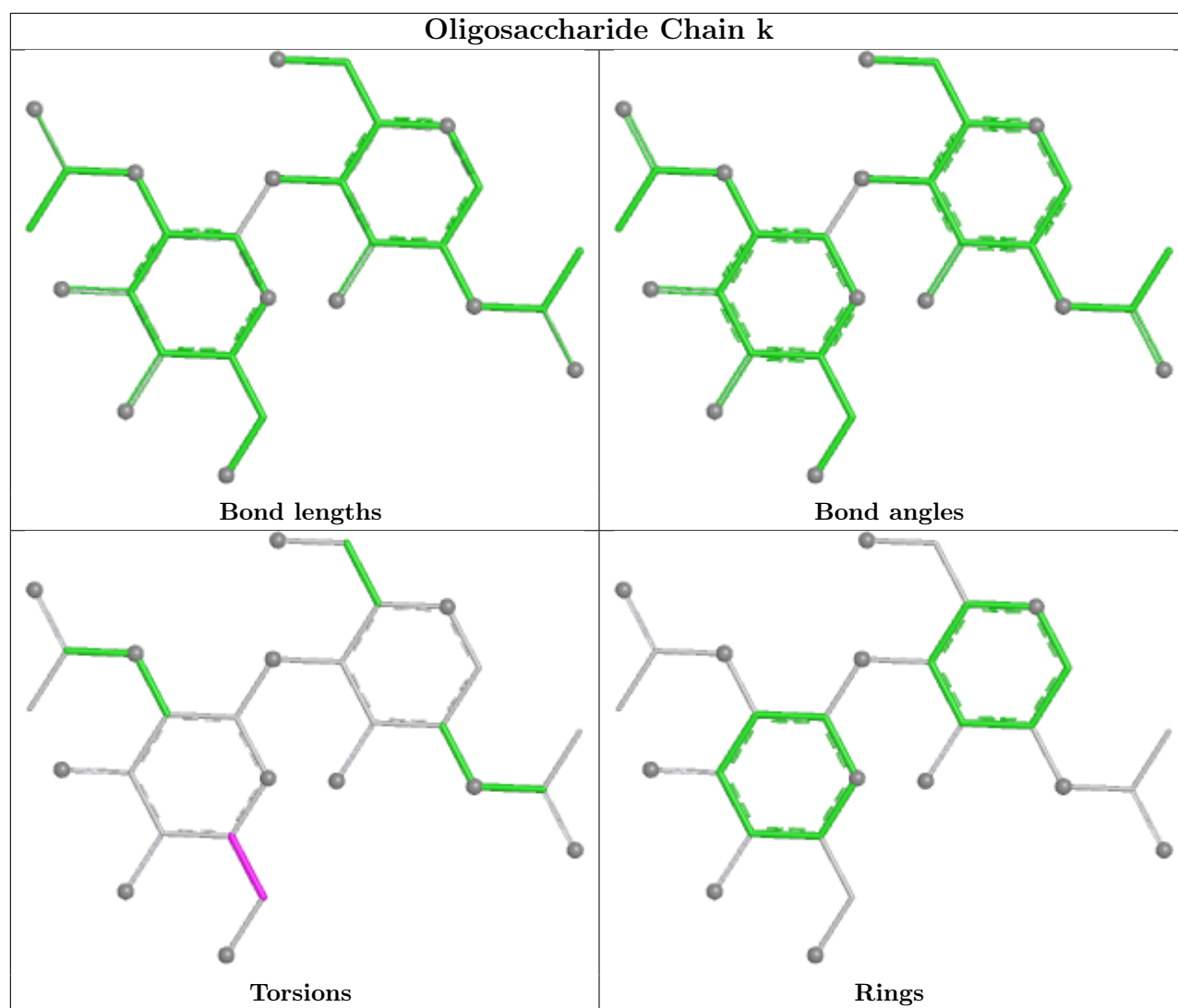


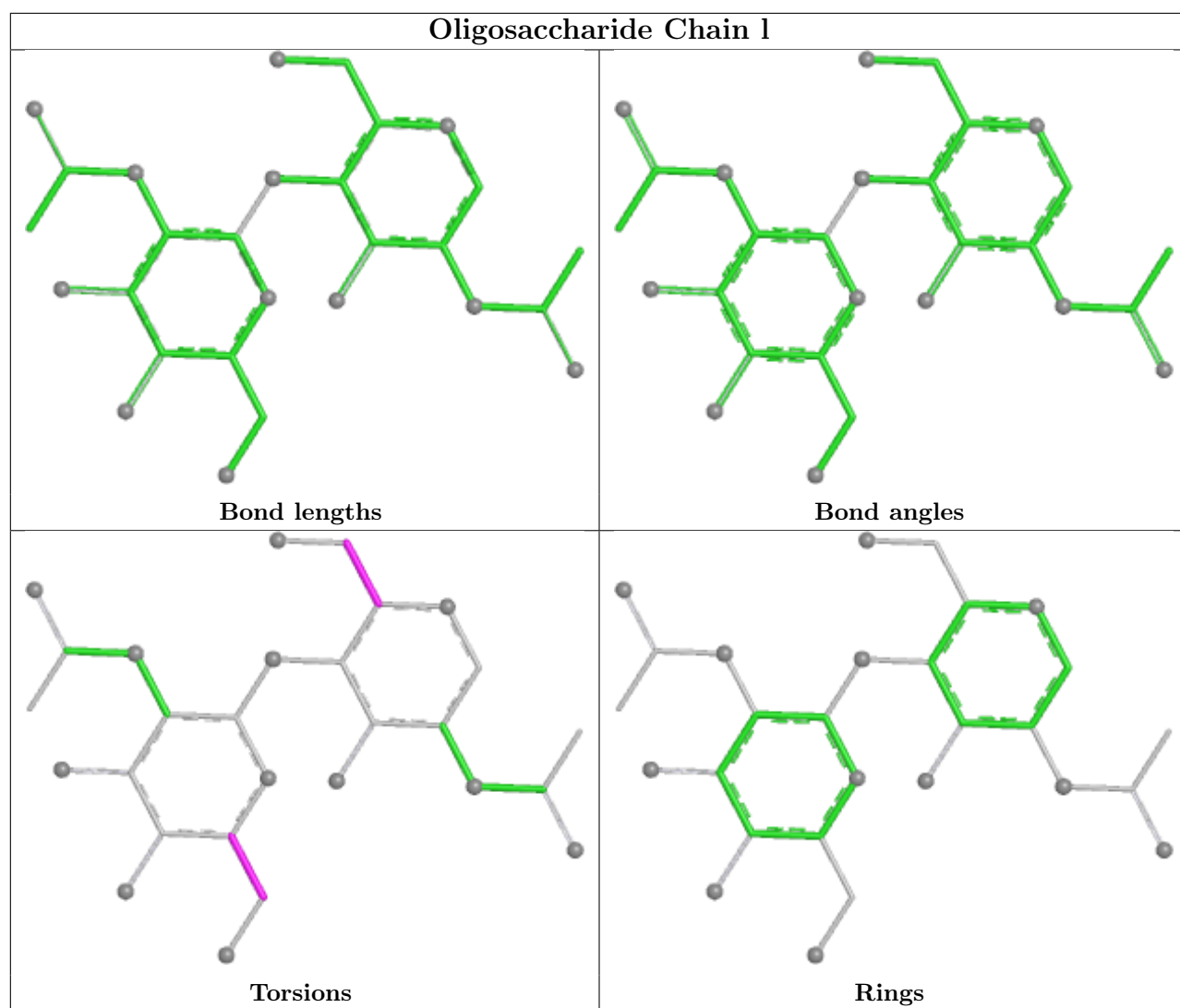


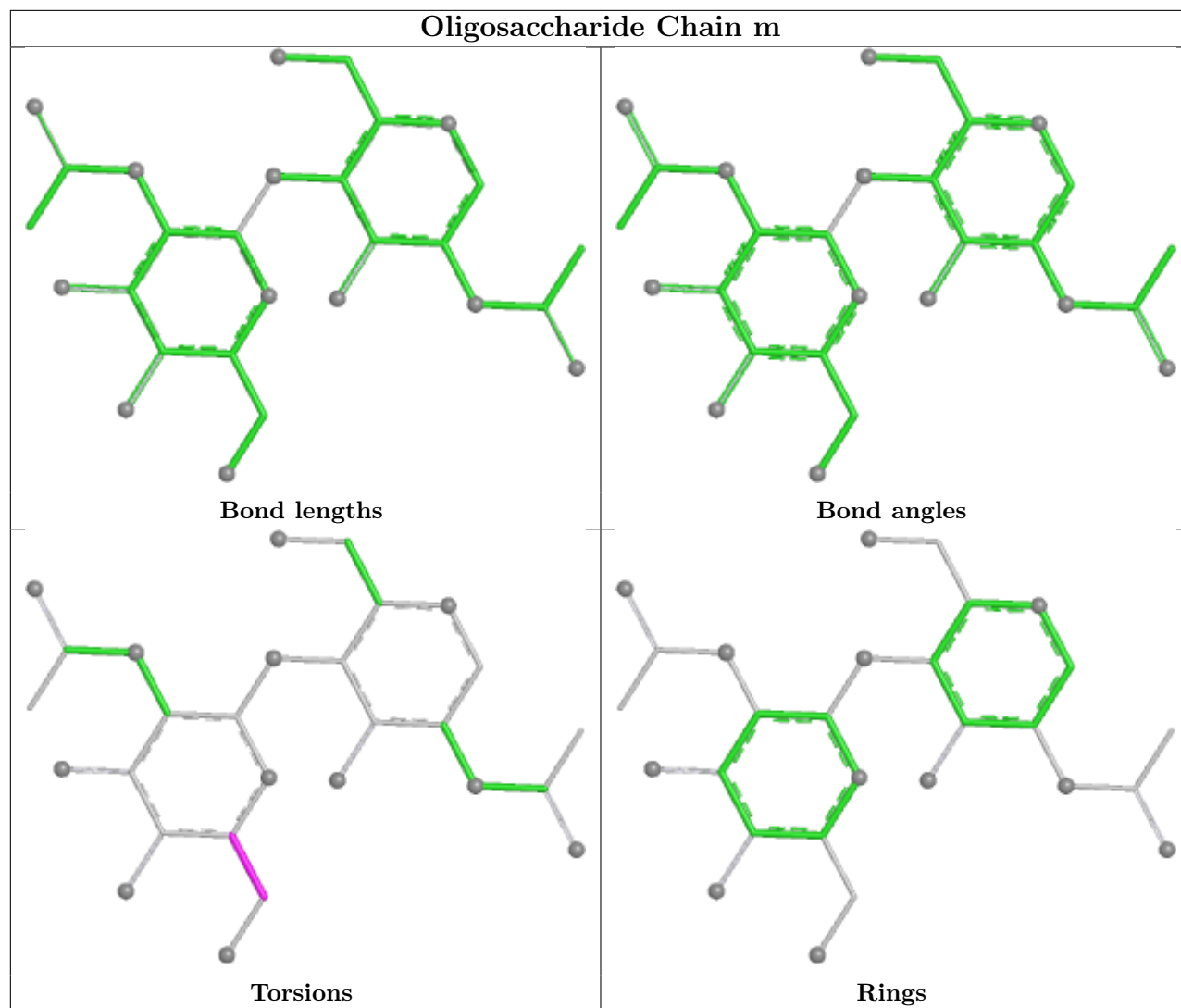


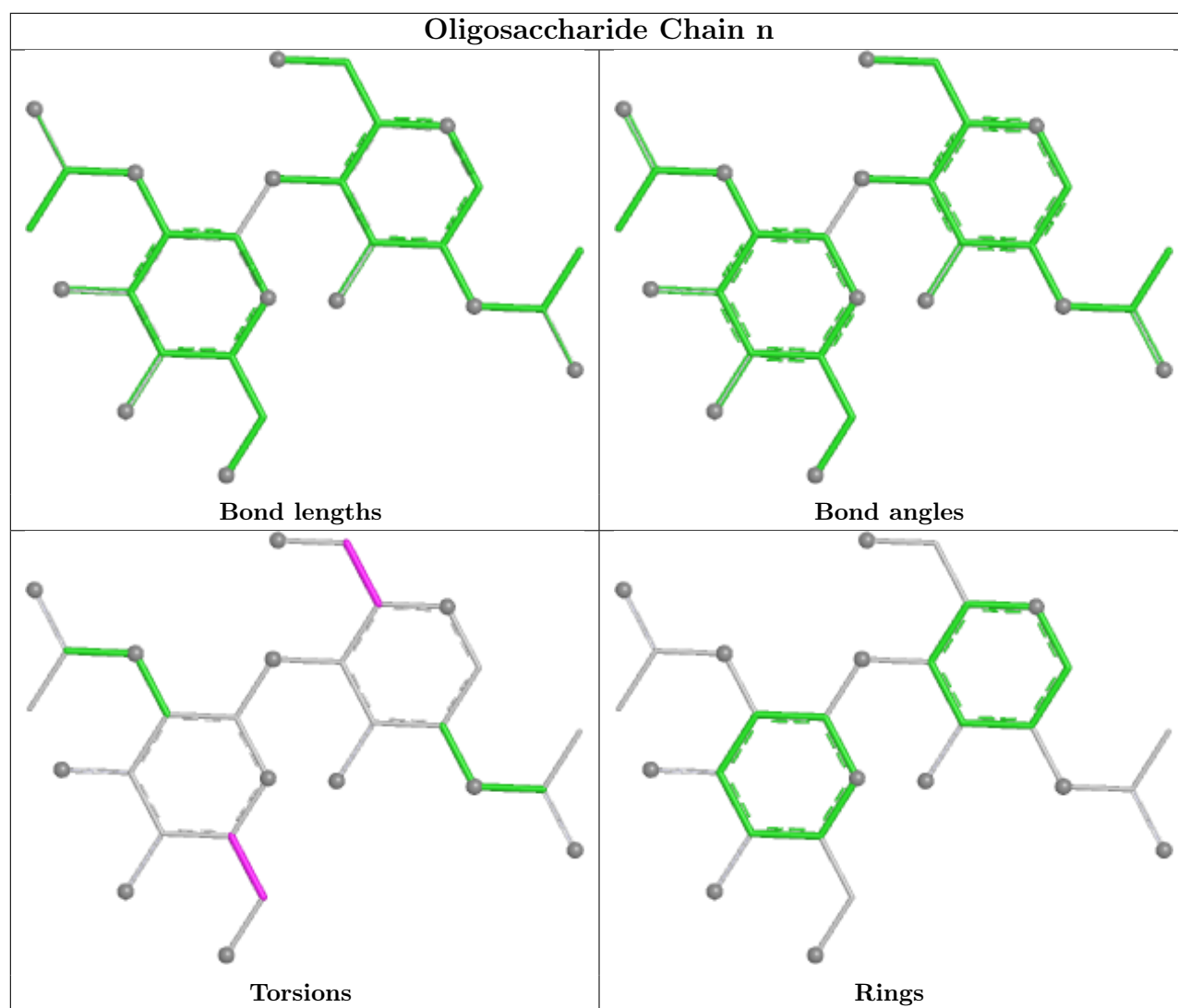


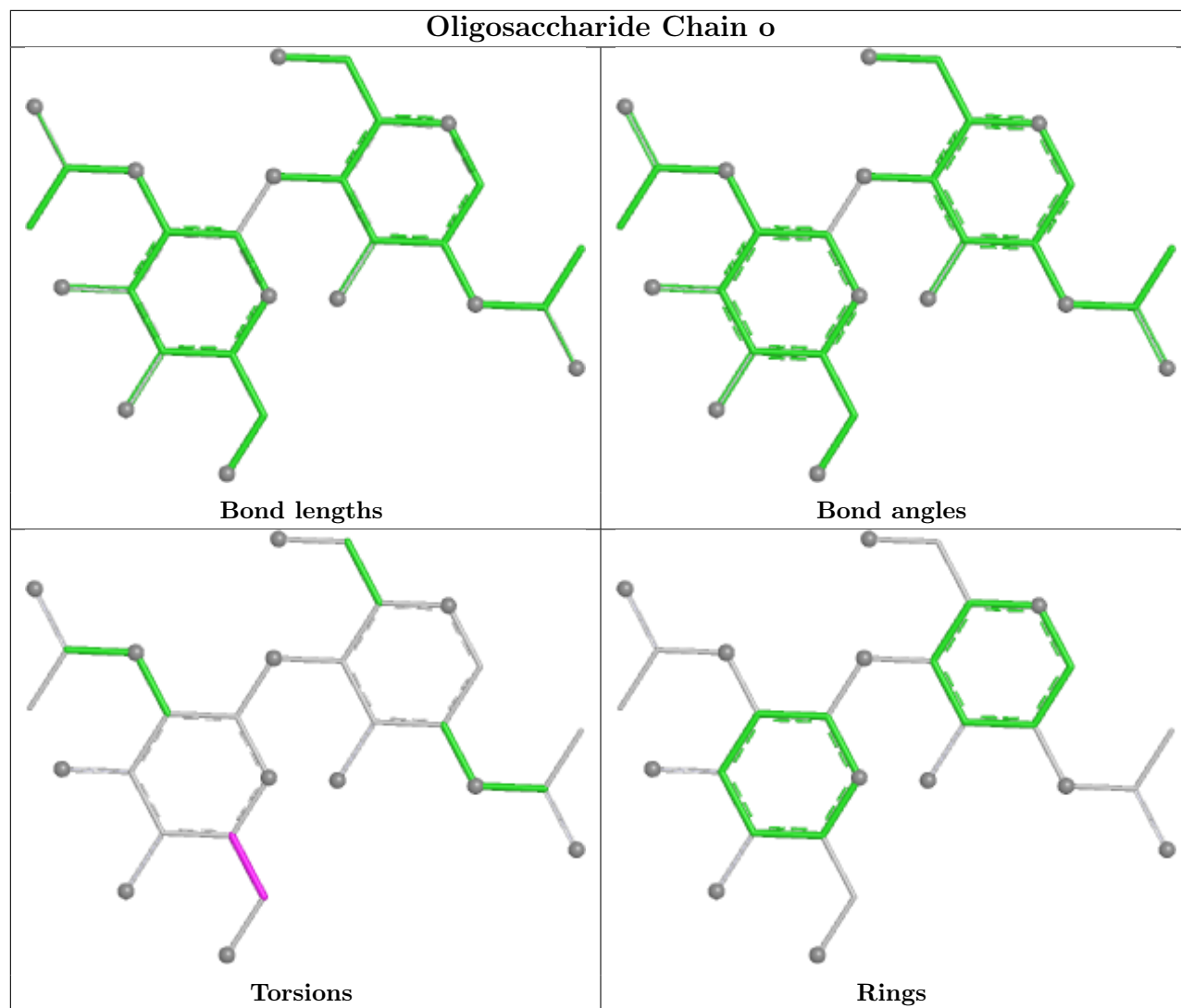


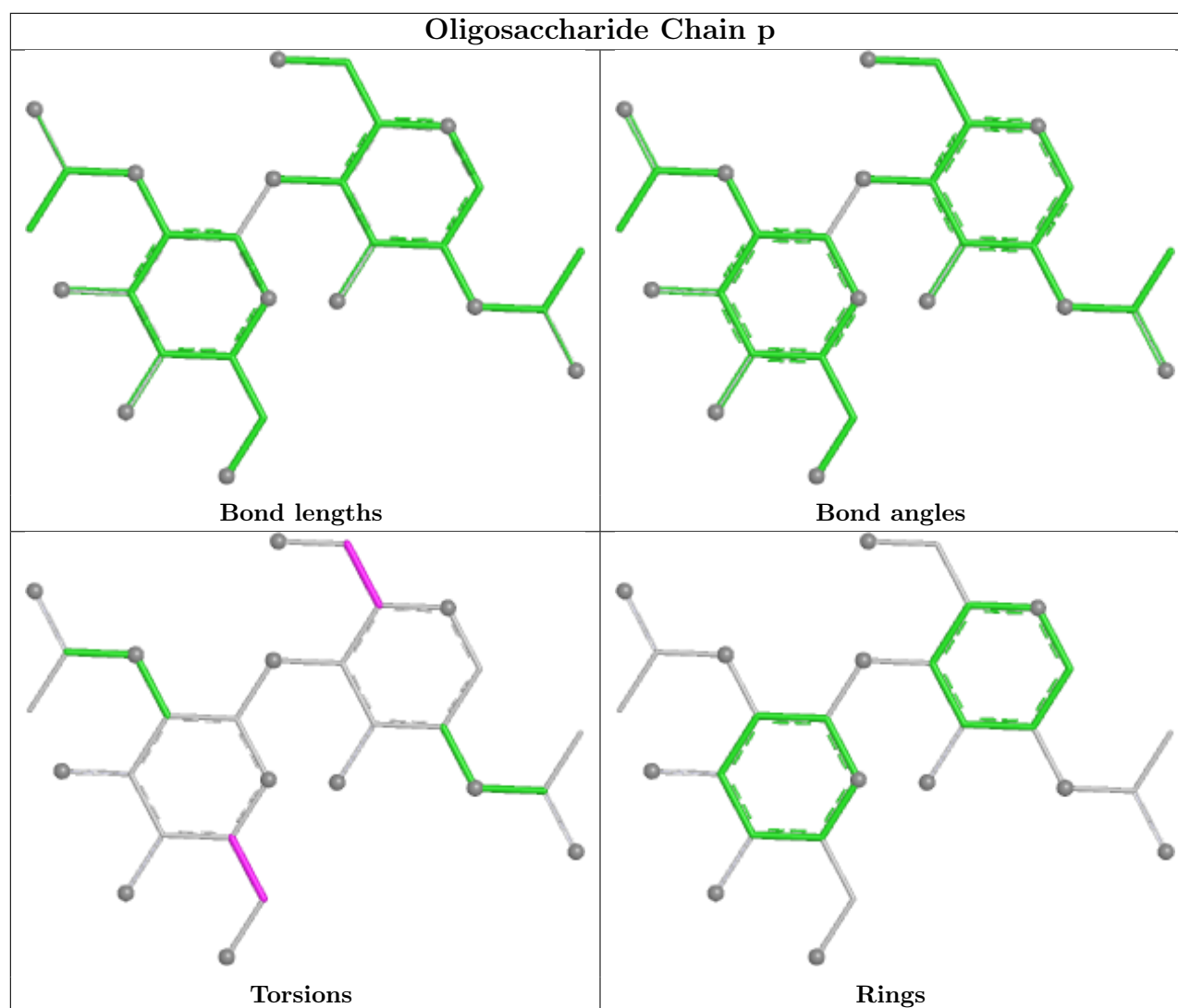












5.6 Ligand geometry [i](#)

66 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	H	1302	1	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	I	1301	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	G	1311	1	14,14,15	0.25	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	H	1311	1	14,14,15	0.29	0	17,19,21	0.50	0
5	NAG	I	1307	1	14,14,15	0.41	0	17,19,21	0.77	1 (5%)
5	NAG	H	1306	1	14,14,15	0.58	0	17,19,21	0.64	0
5	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	G	1302	1	14,14,15	0.25	0	17,19,21	0.50	0
5	NAG	A	1301	1	14,14,15	0.30	0	17,19,21	0.48	0
5	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	I	1306	1	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	G	1304	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	1303	1	14,14,15	0.50	0	17,19,21	0.54	0
5	NAG	B	1305	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	G	1310	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	I	1305	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	C	1308	1	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	A	1308	1	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	C	1307	1	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
5	NAG	C	1305	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	H	1303	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	I	1310	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	A	1311	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	C	1302	1	14,14,15	0.42	0	17,19,21	0.35	0
5	NAG	C	1304	1	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	C	1309	1	14,14,15	0.30	0	17,19,21	0.47	0
5	NAG	H	1308	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	I	1304	1	14,14,15	0.37	0	17,19,21	0.49	0
5	NAG	G	1307	1	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
5	NAG	A	1306	1	14,14,15	0.36	0	17,19,21	0.51	0
5	NAG	I	1303	1	14,14,15	0.41	0	17,19,21	0.36	0
5	NAG	B	1304	1	14,14,15	0.33	0	17,19,21	0.58	0
5	NAG	I	1309	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	B	1310	1	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	H	1307	1	14,14,15	0.59	0	17,19,21	0.84	2 (11%)
5	NAG	H	1309	1	14,14,15	0.29	0	17,19,21	0.45	0
5	NAG	C	1301	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	H	1304	1	14,14,15	0.34	0	17,19,21	0.59	1 (5%)
5	NAG	A	1310	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	B	1311	1	14,14,15	0.30	0	17,19,21	0.50	0
5	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	C	1303	1	14,14,15	0.43	0	17,19,21	0.45	0
5	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1310	1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	A	1307	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
5	NAG	G	1301	1	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	I	1311	1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
5	NAG	H	1310	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	G	1303	1	14,14,15	0.53	0	17,19,21	0.54	0
5	NAG	G	1308	1	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	I	1302	1	14,14,15	0.42	0	17,19,21	0.35	0
5	NAG	H	1301	1	14,14,15	0.42	0	17,19,21	0.40	0
5	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	B	1307	1	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
5	NAG	G	1305	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	C	1311	1	14,14,15	0.55	0	17,19,21	0.74	1 (5%)
5	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	H	1305	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	G	1306	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	G	1309	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	B	1301	1	14,14,15	0.43	0	17,19,21	0.40	0
5	NAG	I	1308	1	14,14,15	0.29	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	G	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	G	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1306	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	G	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	H	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	G	1307	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	H	1307	1	-	4/6/23/26	0/1/1/1
5	NAG	H	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
5	NAG	G	1301	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	H	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	G	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	G	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
5	NAG	G	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	G	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	G	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1308	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1307	NAG	C1-O5-C5	2.66	115.75	112.19
5	I	1311	NAG	C1-O5-C5	2.66	115.75	112.19
5	C	1311	NAG	C1-O5-C5	2.65	115.73	112.19
5	H	1307	NAG	C1-O5-C5	2.11	115.02	112.19
5	I	1307	NAG	C2-N2-C7	2.10	125.72	122.90
5	C	1307	NAG	C2-N2-C7	2.09	125.70	122.90
5	A	1307	NAG	C2-N2-C7	2.08	125.69	122.90
5	G	1307	NAG	C2-N2-C7	2.07	125.67	122.90
5	H	1307	NAG	C2-N2-C7	2.03	125.62	122.90
5	H	1304	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	1302	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	G	1301	NAG	O5-C5-C6-O6
5	I	1301	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	G	1308	NAG	O5-C5-C6-O6
5	G	1301	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	G	1307	NAG	O5-C5-C6-O6
5	I	1308	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	H	1308	NAG	O5-C5-C6-O6
5	H	1309	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1311	NAG	O5-C5-C6-O6
5	G	1304	NAG	O5-C5-C6-O6
5	H	1303	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	G	1302	NAG	O5-C5-C6-O6
5	H	1311	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	H	1301	NAG	O5-C5-C6-O6
5	H	1303	NAG	O5-C5-C6-O6
5	H	1308	NAG	C4-C5-C6-O6
5	H	1301	NAG	C4-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	G	1307	NAG	C4-C5-C6-O6
5	I	1301	NAG	C4-C5-C6-O6
5	I	1308	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	G	1304	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1308	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	G	1308	NAG	C4-C5-C6-O6
5	H	1306	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	I	1305	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	A	1306	NAG	C8-C7-N2-C2
5	A	1306	NAG	O7-C7-N2-C2
5	B	1306	NAG	C8-C7-N2-C2
5	B	1306	NAG	O7-C7-N2-C2
5	C	1306	NAG	C8-C7-N2-C2
5	C	1306	NAG	O7-C7-N2-C2
5	G	1306	NAG	C8-C7-N2-C2
5	G	1306	NAG	O7-C7-N2-C2
5	H	1306	NAG	C8-C7-N2-C2
5	H	1306	NAG	O7-C7-N2-C2
5	I	1306	NAG	C8-C7-N2-C2
5	I	1306	NAG	O7-C7-N2-C2
5	H	1304	NAG	O5-C5-C6-O6
5	H	1306	NAG	C4-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	I	1309	NAG	O5-C5-C6-O6
5	B	1311	NAG	C4-C5-C6-O6
5	H	1311	NAG	C4-C5-C6-O6
5	I	1302	NAG	O5-C5-C6-O6
5	I	1305	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	G	1309	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	H	1307	NAG	O5-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	H	1309	NAG	C4-C5-C6-O6
5	H	1307	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	G	1305	NAG	C4-C5-C6-O6
5	H	1304	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	G	1305	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	G	1311	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1311	NAG	C4-C5-C6-O6
5	A	1307	NAG	C3-C2-N2-C7
5	B	1307	NAG	C3-C2-N2-C7
5	C	1307	NAG	C3-C2-N2-C7
5	G	1307	NAG	C3-C2-N2-C7
5	H	1307	NAG	C3-C2-N2-C7
5	I	1307	NAG	C3-C2-N2-C7
5	G	1311	NAG	O5-C5-C6-O6
5	A	1311	NAG	O5-C5-C6-O6
5	A	1307	NAG	C1-C2-N2-C7
5	B	1307	NAG	C1-C2-N2-C7
5	C	1307	NAG	C1-C2-N2-C7
5	G	1307	NAG	C1-C2-N2-C7
5	H	1307	NAG	C1-C2-N2-C7
5	I	1307	NAG	C1-C2-N2-C7
5	I	1302	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1306	NAG	1	0
5	C	1303	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

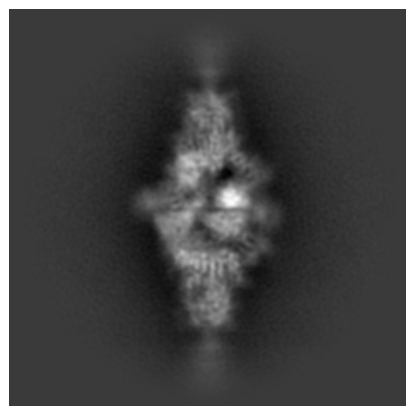
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60106. These allow visual inspection of the internal detail of the map and identification of artifacts.

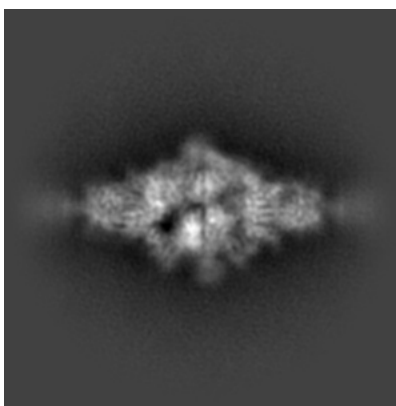
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

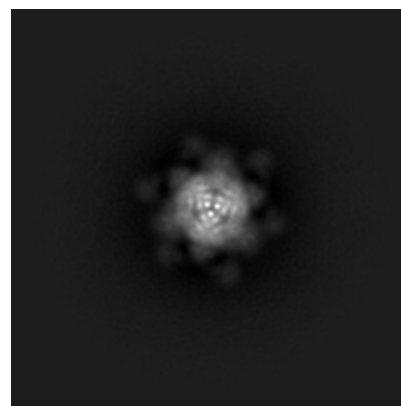
6.1.1 Primary map



X

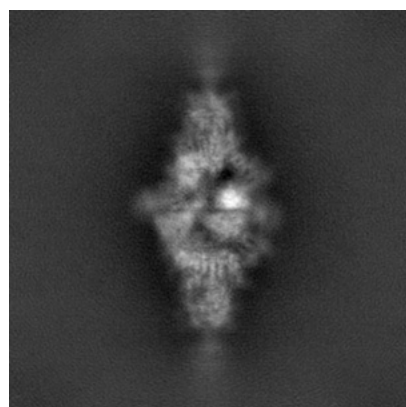


Y

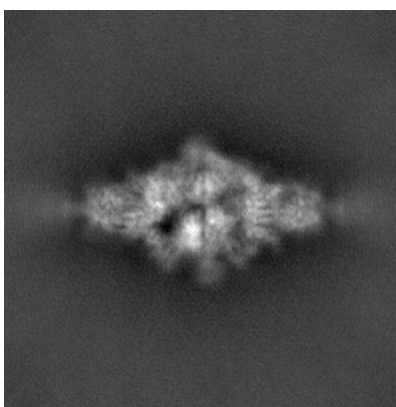


Z

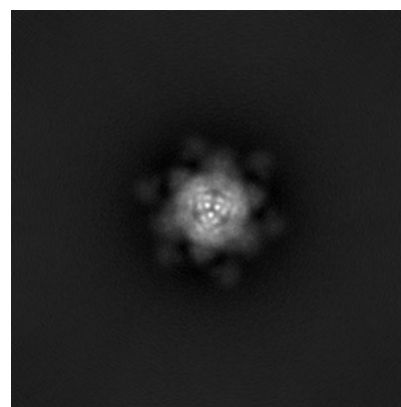
6.1.2 Raw map



X



Y

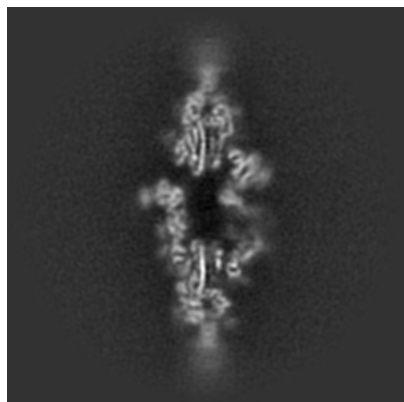


Z

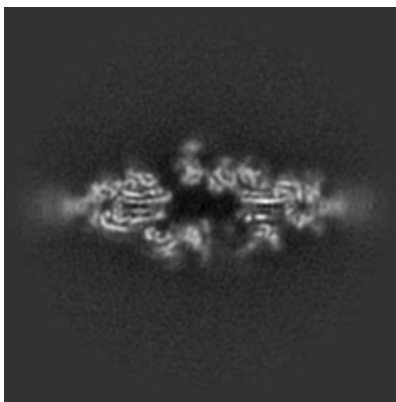
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

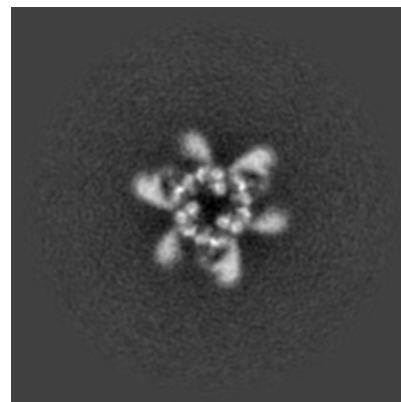
6.2.1 Primary map



X Index: 120

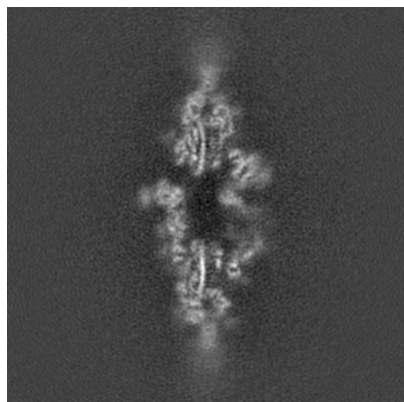


Y Index: 120

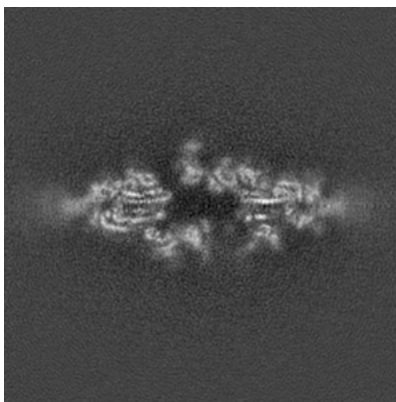


Z Index: 120

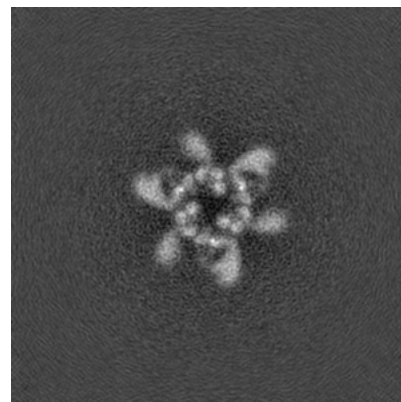
6.2.2 Raw map



X Index: 120



Y Index: 120

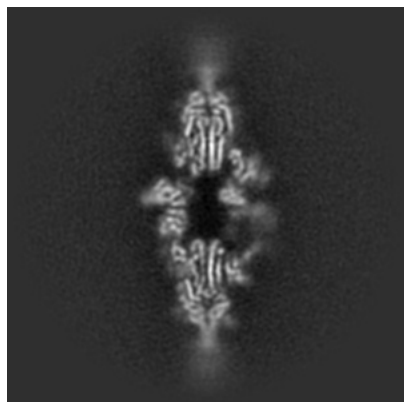


Z Index: 120

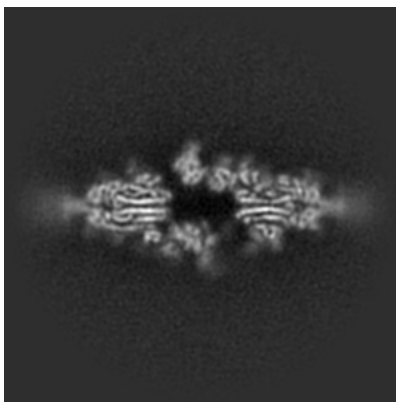
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

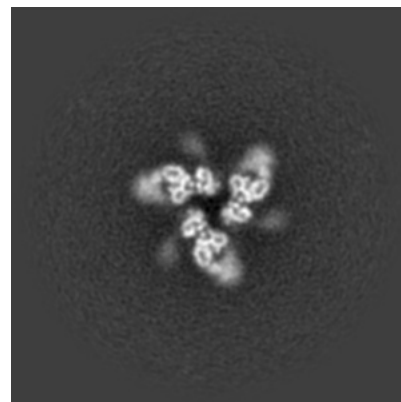
6.3.1 Primary map



X Index: 118

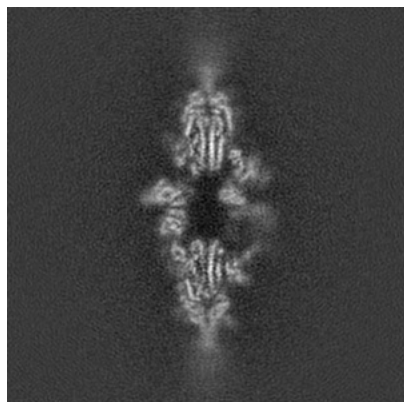


Y Index: 122

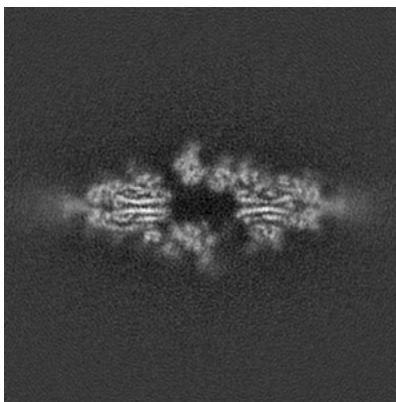


Z Index: 125

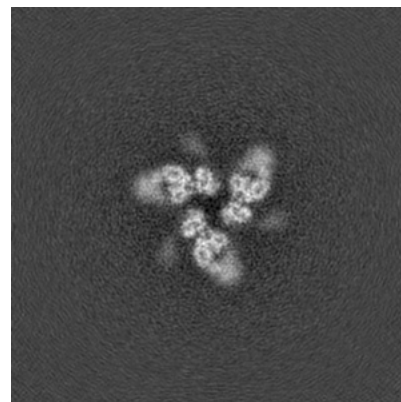
6.3.2 Raw map



X Index: 118



Y Index: 122

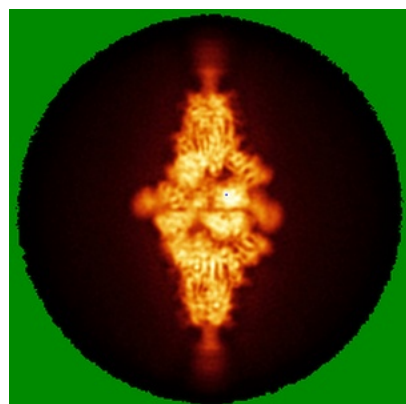


Z Index: 125

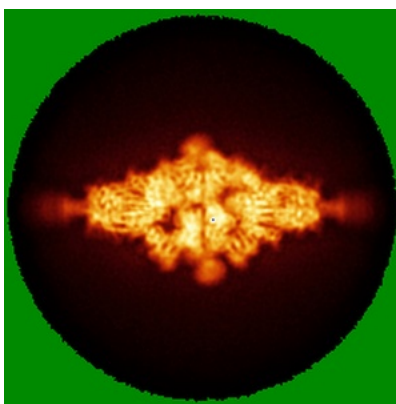
The images above show the largest variance slices of the map in three orthogonal directions.

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

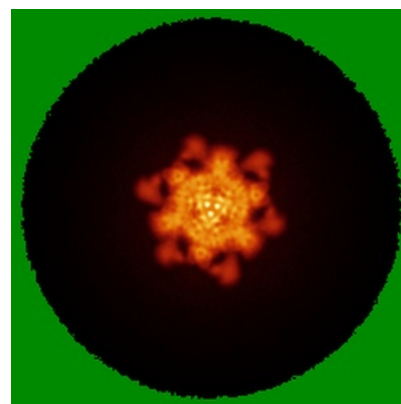
6.4.1 Primary map



X

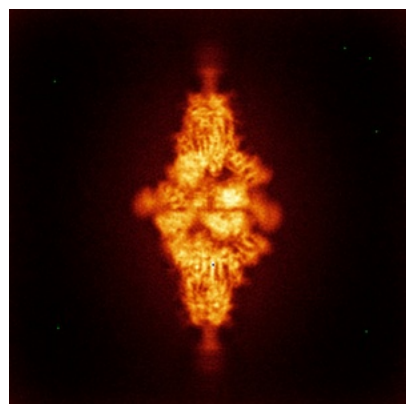


Y

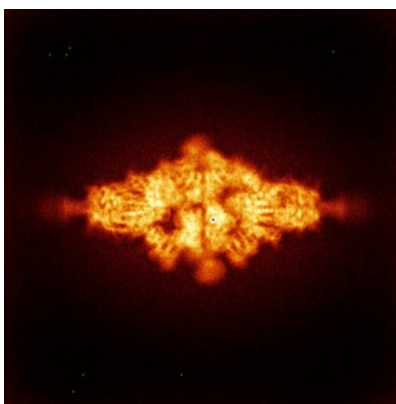


Z

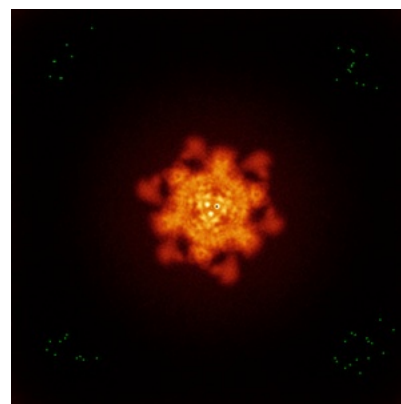
6.4.2 Raw map



X



Y

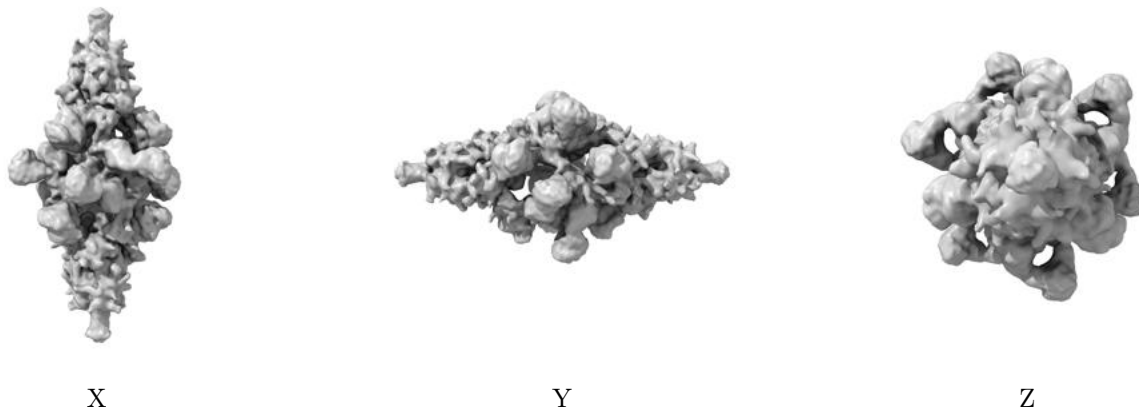


Z

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.

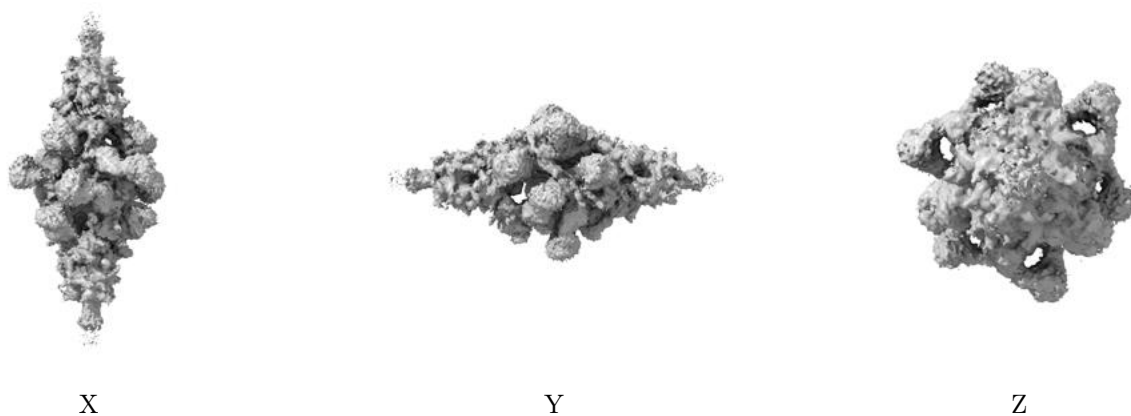
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

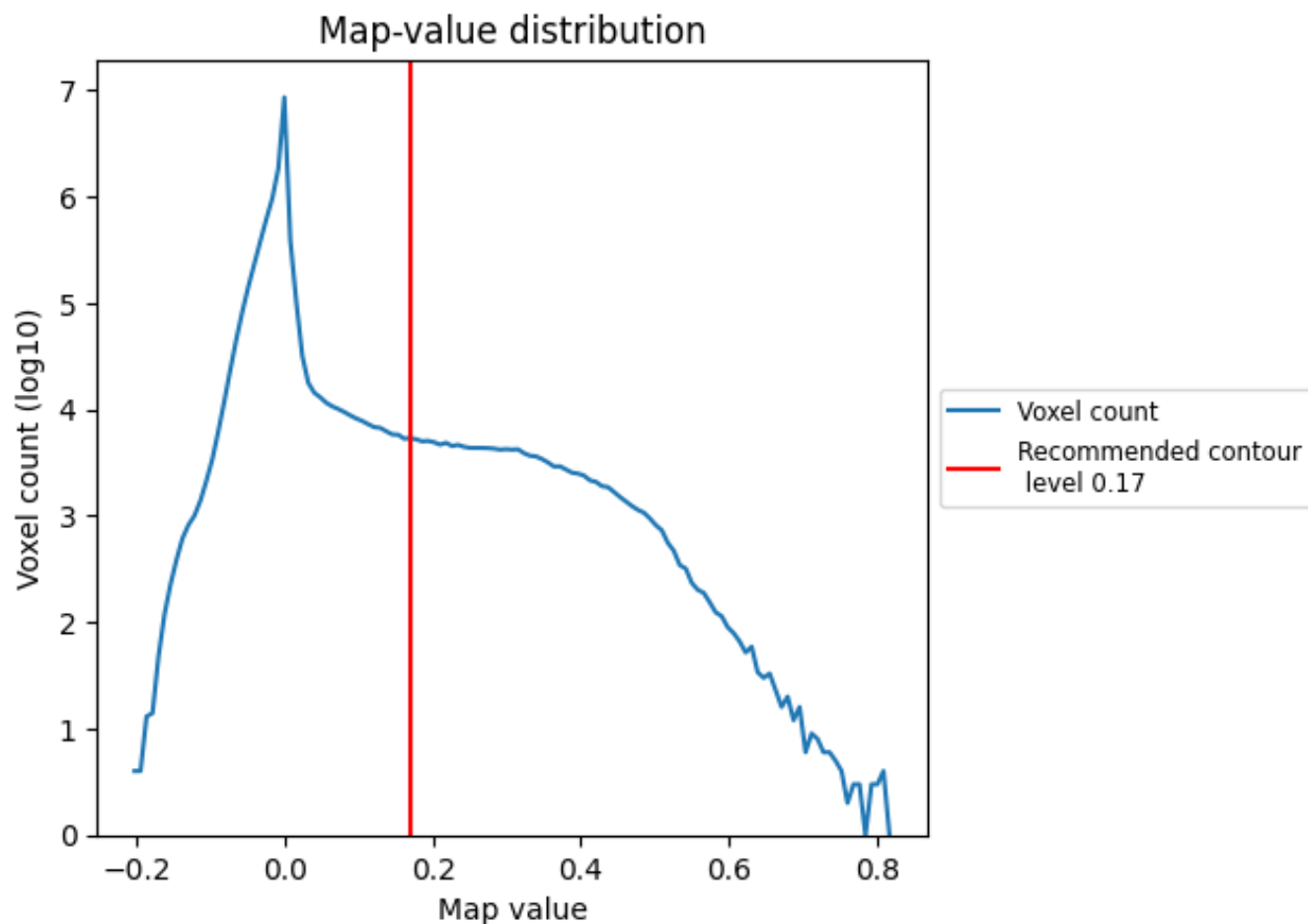
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

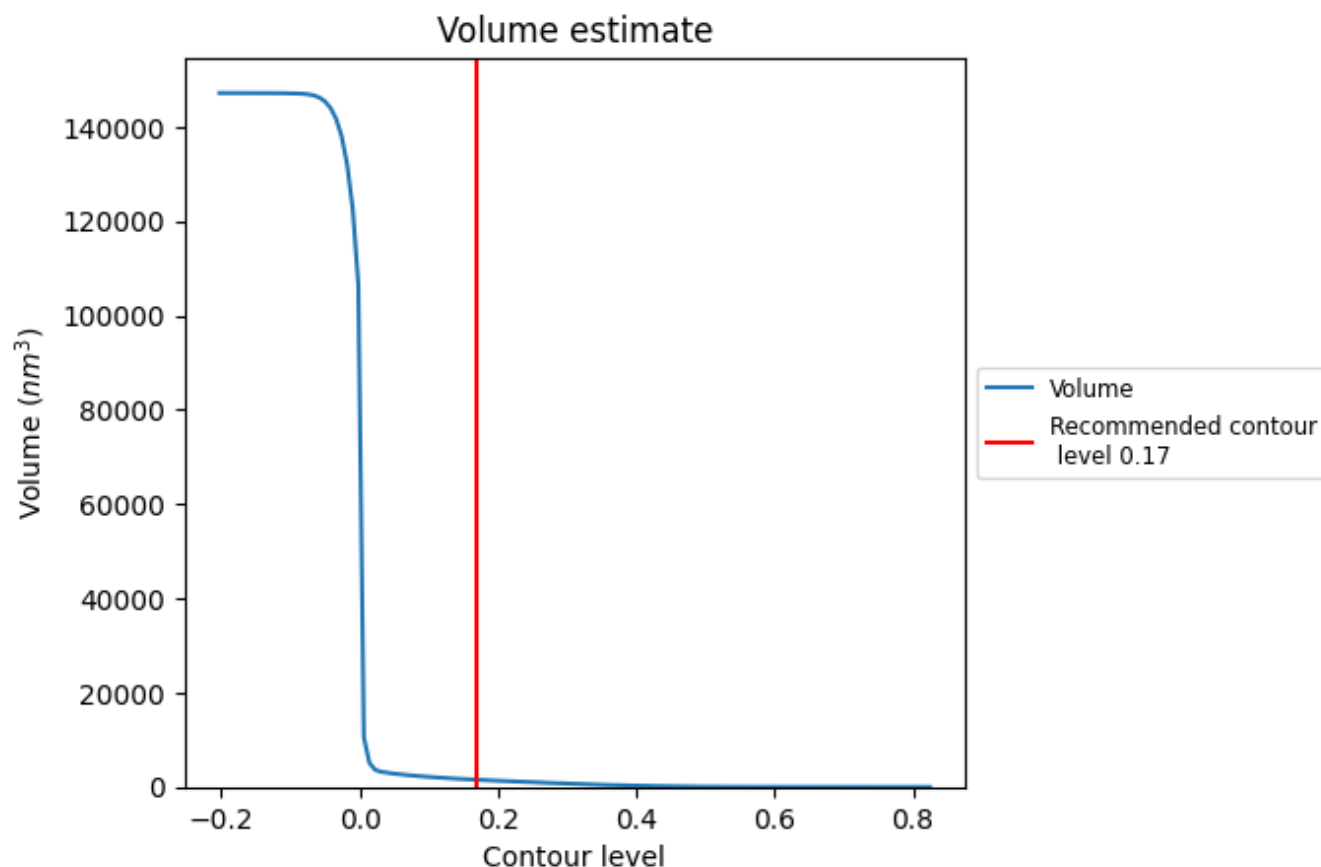
This section contains the results of statistical analysis of the map.

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.

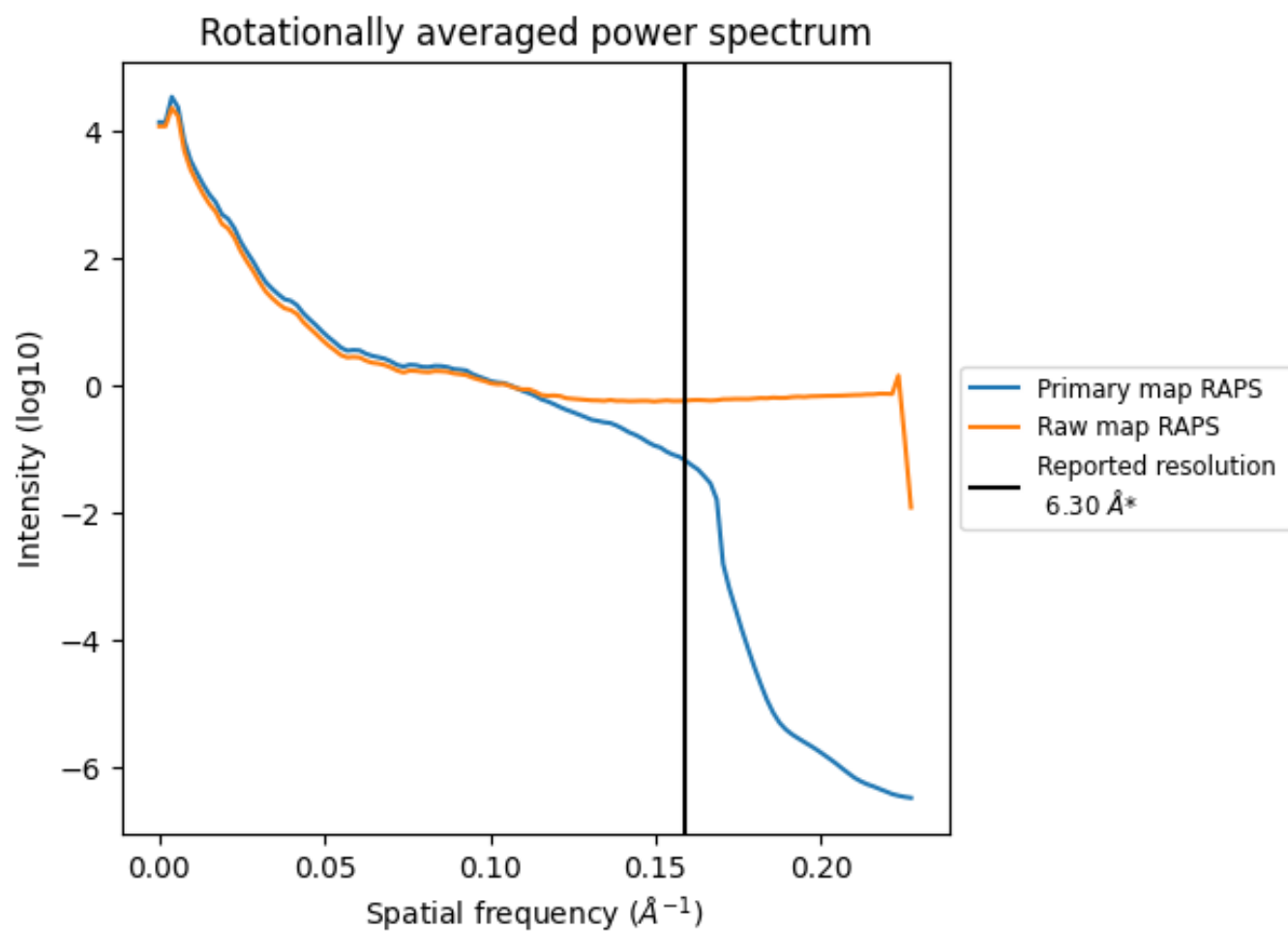
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1521 nm^3 ; this corresponds to an approximate mass of 1374 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 ⓘ

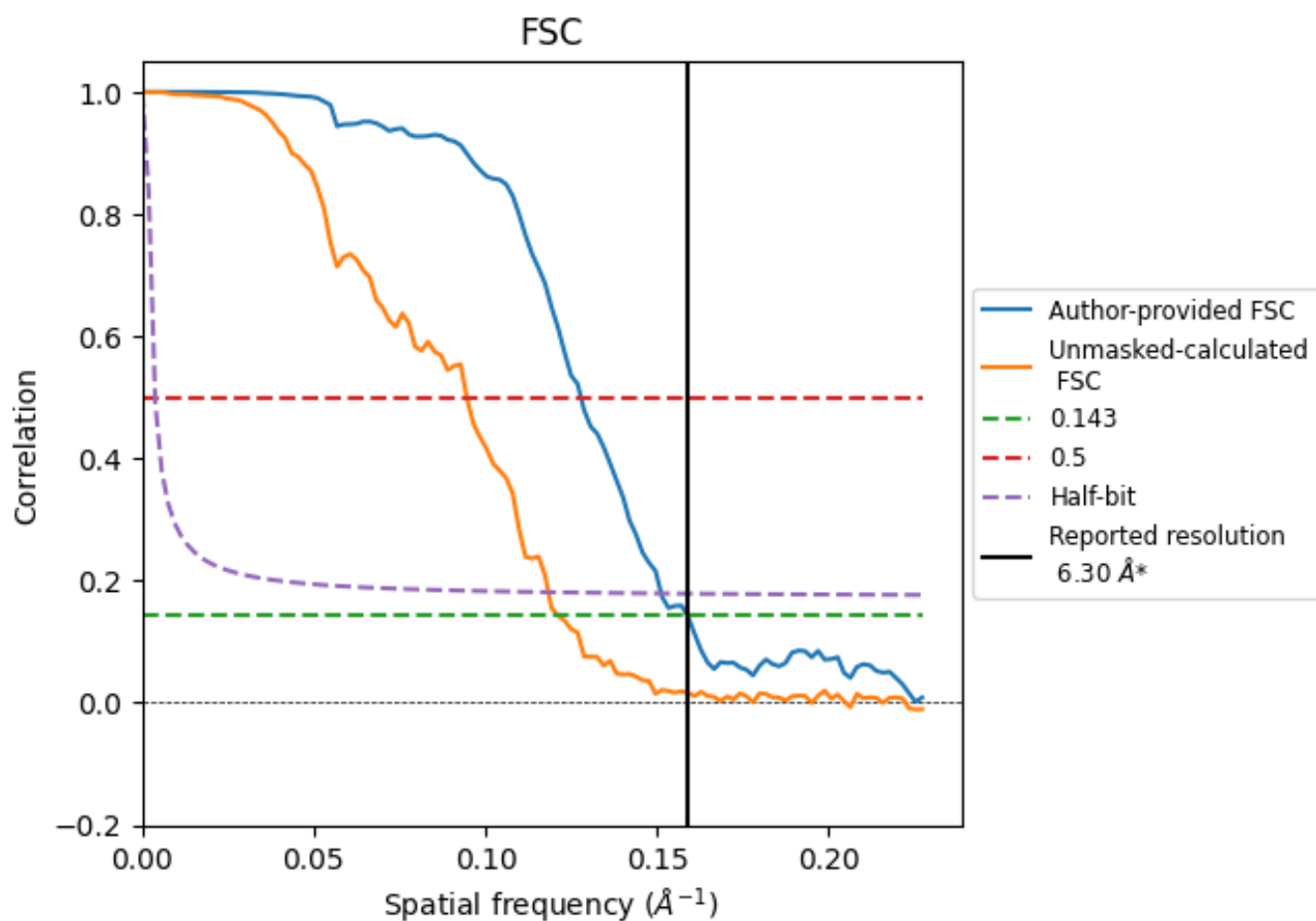


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.159 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

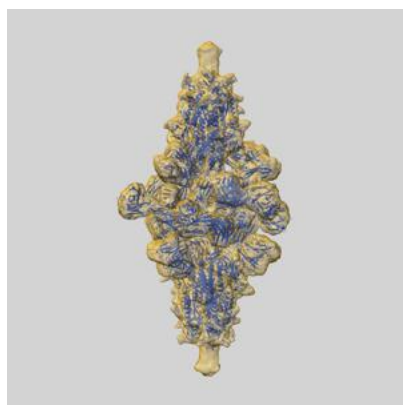
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.30	7.82	6.61
Unmasked-calculated*	8.25	10.57	8.45

*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 8.25 differs from the reported value 6.3 by more than 10 %

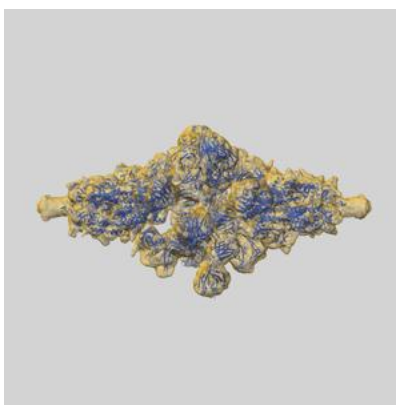
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60106 and PDB model 8ZHK. Per-residue inclusion information can be found in section 3 on page 13.

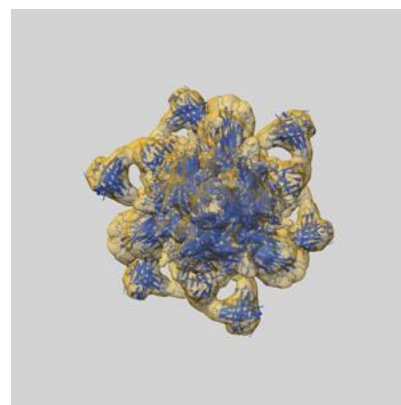
9.1 Map-model overlay [i](#)



X



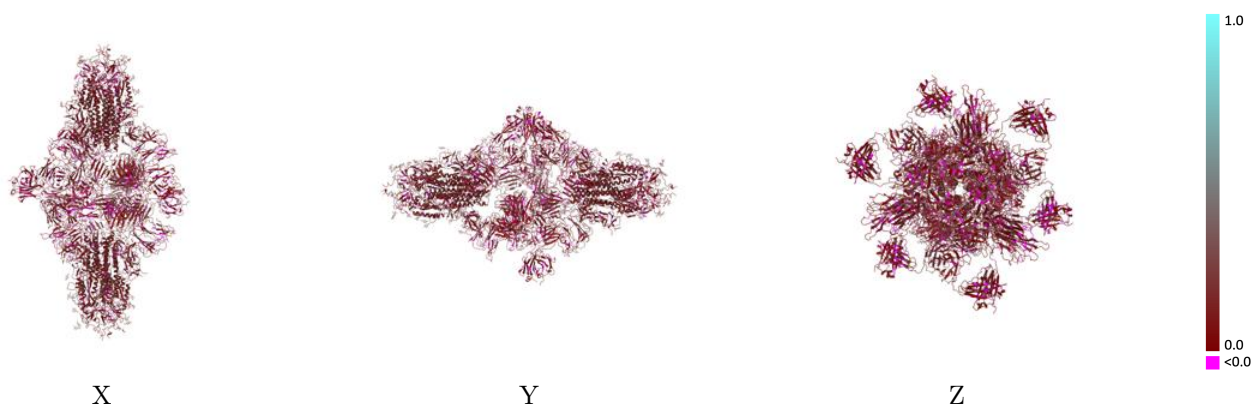
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

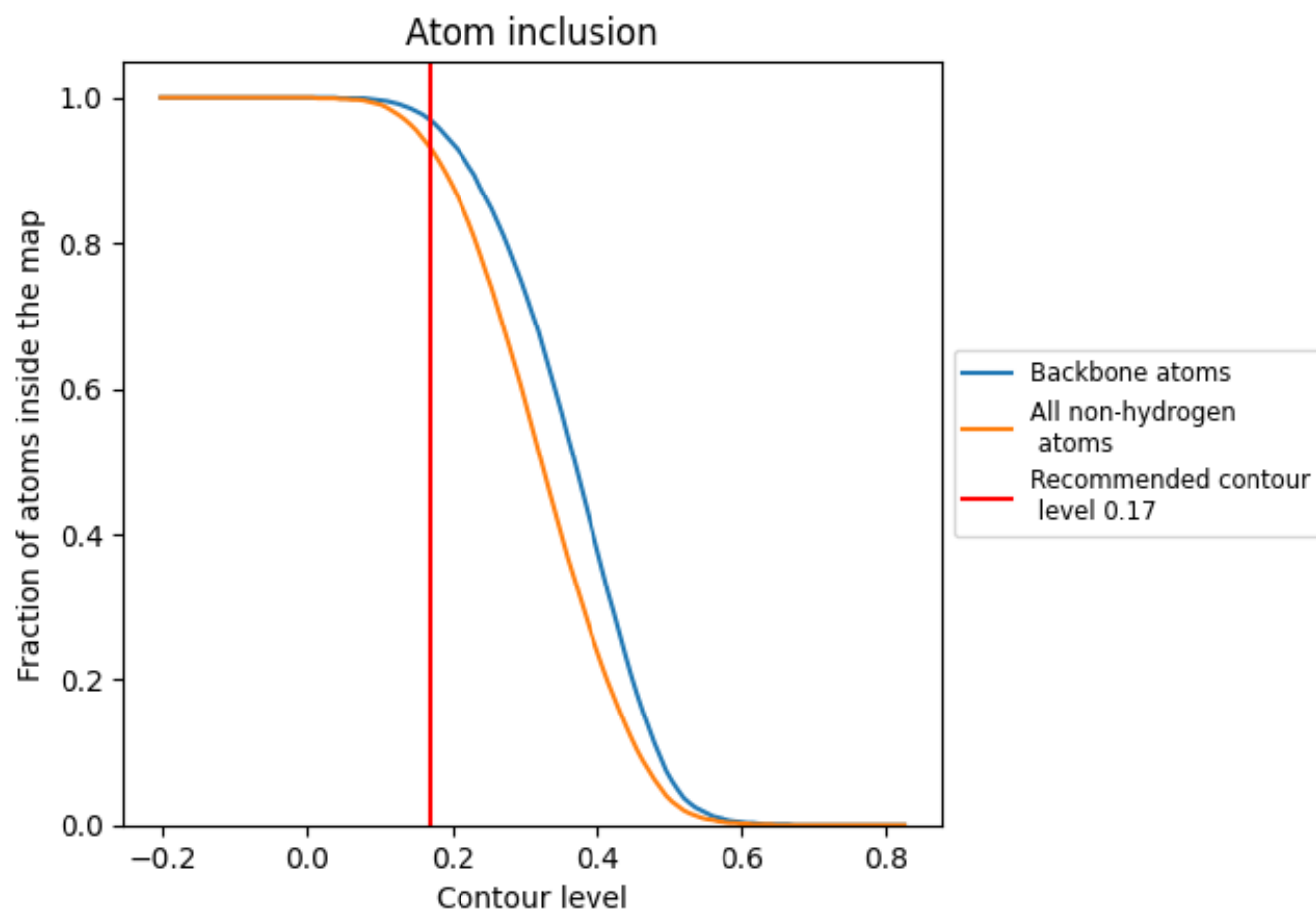


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.1370
A	 0.9330	 0.1440
B	 0.9500	 0.1510
C	 0.9350	 0.1460
D	 0.9130	 0.1130
E	 0.8990	 0.1100
F	 0.9220	 0.1170
G	 0.9340	 0.1400
H	 0.9360	 0.1410
I	 0.9340	 0.1370
J	 0.8980	 0.1080
K	 0.9160	 0.1160
L	 0.9420	 0.1310
M	 0.8990	 0.1110
N	 0.9060	 0.1190
O	 0.9390	 0.1240
P	 0.9010	 0.1130
Q	 0.9410	 0.1250
R	 0.9090	 0.1170
S	 0.9640	 0.2310
T	 0.8930	 0.2480
U	 0.9640	 0.1920
V	 0.9640	 0.3130
W	 0.9640	 0.2360
X	 0.8930	 0.2230
Y	 0.9290	 0.1900
Z	 0.9290	 0.2480
a	 0.8930	 0.1870
b	 0.8930	 0.2370
c	 0.8930	 0.1640
d	 0.9290	 0.3170
e	 0.8570	 0.1670
f	 0.7860	 0.1530
g	 1.0000	 0.2500
h	 0.8930	 0.1540



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Chain	Atom inclusion	Q-score
i	 0.8210	 0.1610
j	 0.7500	 0.1560
k	 1.0000	 0.2830
l	 0.8930	 0.1190
m	 0.9640	 0.1550
n	 0.7500	 0.1490
o	 0.9640	 0.2240
p	 0.9290	 0.1690