



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 10:40 PM EDT

PDB ID : 8CZZ  
EMDB ID : EMD-27103  
Title : Cryo-EM structure of T/F100 SOSIP.664 HIV-1 Env trimer with LMHS mutations in complex with Temsavir, 8ANC195, and 10-1074  
Authors : Chen, Y.; Pozharski, E.; Tolbert, W.; Pazgier, M.  
Deposited on : 2022-05-25  
Resolution : 3.14 Å (reported)  
Based on initial models : 6NQD, 4FQ2

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

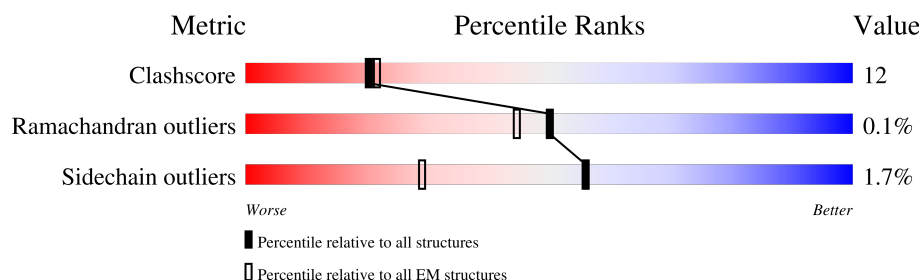
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.14 Å.

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



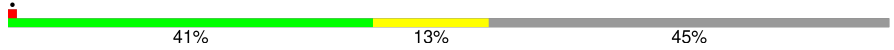


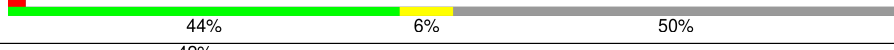
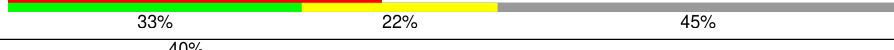
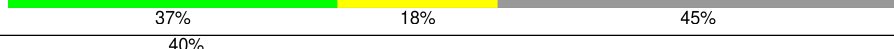
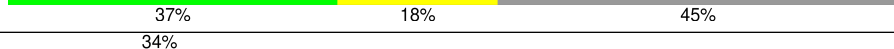
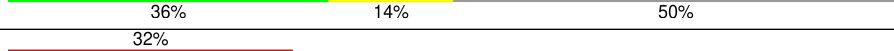
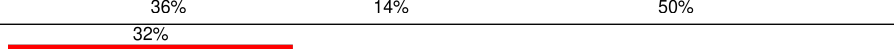
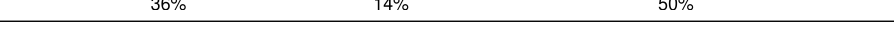
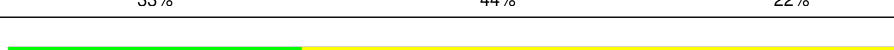



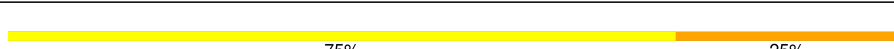





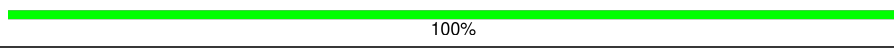
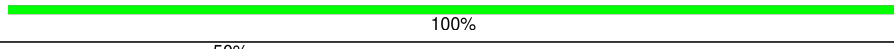
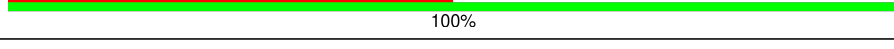


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	486	
1	E	486	
1	I	486	
2	B	155	
2	F	155	
2	J	155	
3	C	238	
3	G	238	


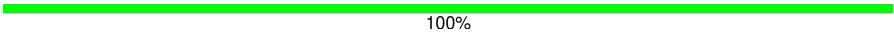
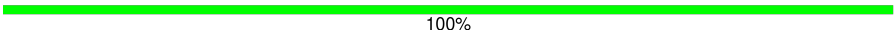




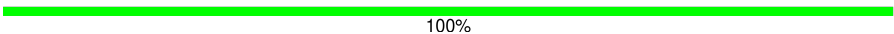

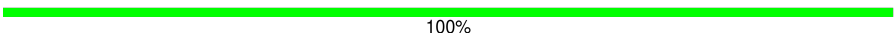
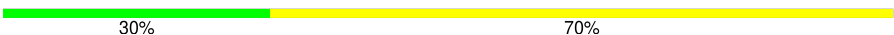

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Mol	Chain	Length	Quality of chain
3	K	238	
4	D	215	
4	H	215	
4	L	215	
5	M	238	
5	O	238	
5	Q	238	
6	N	214	
6	P	214	
6	R	214	
7	S	9	
7	j	9	
8	T	6	
8	b	6	
8	k	6	
9	U	4	
9	d	4	
9	n	4	
10	V	2	
10	W	2	
10	X	2	
10	c	2	
10	e	2	
10	f	2	
10	g	2	

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Mol	Chain	Length	Quality of chain
10	l	2	 50% 50%
10	m	2	 100%
10	o	2	 100%
10	p	2	 100%
10	q	2	 100%
11	Y	3	 100%
11	Z	3	 67% 33%
11	h	3	 100%
11	i	3	 100%
11	r	3	 100%
12	a	10	 30% 70%
13	s	4	 25% 75% 25%

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 26288 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 CRF01\_AE T/F100 HIV-1 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	440	Total	C	N	O	S	0	0
			3479	2197	612	642	28		
1	E	438	Total	C	N	O	S	0	0
			3462	2186	610	638	28		
1	I	437	Total	C	N	O	S	0	0
			3455	2182	609	636	28		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	TYR	HIS	engineered mutation	UNP A0A6C0ZY47
A	105	HIS	GLN	engineered mutation	UNP A0A6C0ZY47
A	108	ILE	VAL	engineered mutation	UNP A0A6C0ZY47
A	375	SER	HIS	conflict	UNP A0A6C0ZY47
A	474	ASP	ASN	engineered mutation	UNP A0A6C0ZY47
A	475	MET	ILE	engineered mutation	UNP A0A6C0ZY47
A	476	ARG	LYS	engineered mutation	UNP A0A6C0ZY47
A	501	CYS	ALA	conflict	UNP A0A6C0ZY47
A	508	ARG	-	expression tag	UNP A0A6C0ZY47
A	509	ARG	-	expression tag	UNP A0A6C0ZY47
A	510	ARG	-	expression tag	UNP A0A6C0ZY47
A	511	ARG	-	expression tag	UNP A0A6C0ZY47
A	512	ARG	-	expression tag	UNP A0A6C0ZY47
A	513	ARG	-	expression tag	UNP A0A6C0ZY47
E	61	TYR	HIS	engineered mutation	UNP A0A6C0ZY47
E	105	HIS	GLN	engineered mutation	UNP A0A6C0ZY47
E	108	ILE	VAL	engineered mutation	UNP A0A6C0ZY47
E	375	SER	HIS	conflict	UNP A0A6C0ZY47
E	474	ASP	ASN	engineered mutation	UNP A0A6C0ZY47
E	475	MET	ILE	engineered mutation	UNP A0A6C0ZY47
E	476	ARG	LYS	engineered mutation	UNP A0A6C0ZY47
E	501	CYS	ALA	conflict	UNP A0A6C0ZY47
E	508	ARG	-	expression tag	UNP A0A6C0ZY47
E	509	ARG	-	expression tag	UNP A0A6C0ZY47

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Chain	Residue	Modelled	Actual	Comment	Reference
E	510	ARG	-	expression tag	UNP A0A6C0ZY47
E	511	ARG	-	expression tag	UNP A0A6C0ZY47
E	512	ARG	-	expression tag	UNP A0A6C0ZY47
E	513	ARG	-	expression tag	UNP A0A6C0ZY47
I	61	TYR	HIS	engineered mutation	UNP A0A6C0ZY47
I	105	HIS	GLN	engineered mutation	UNP A0A6C0ZY47
I	108	ILE	VAL	engineered mutation	UNP A0A6C0ZY47
I	375	SER	HIS	conflict	UNP A0A6C0ZY47
I	474	ASP	ASN	engineered mutation	UNP A0A6C0ZY47
I	475	MET	ILE	engineered mutation	UNP A0A6C0ZY47
I	476	ARG	LYS	engineered mutation	UNP A0A6C0ZY47
I	501	CYS	ALA	conflict	UNP A0A6C0ZY47
I	508	ARG	-	expression tag	UNP A0A6C0ZY47
I	509	ARG	-	expression tag	UNP A0A6C0ZY47
I	510	ARG	-	expression tag	UNP A0A6C0ZY47
I	511	ARG	-	expression tag	UNP A0A6C0ZY47
I	512	ARG	-	expression tag	UNP A0A6C0ZY47
I	513	ARG	-	expression tag	UNP A0A6C0ZY47

- Molecule 2 is a protein called CRF-1\_AE T/F100 HIV-1 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	125	Total	C	N	O	S	0	0
			999	638	167	189	5		
2	F	119	Total	C	N	O	S	0	0
			956	610	160	181	5		
2	J	128	Total	C	N	O	S	0	0
			1034	660	174	195	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP A0A6C0ZY47
B	605	CYS	THR	conflict	UNP A0A6C0ZY47
B	665	ALA	-	expression tag	UNP A0A6C0ZY47
B	666	ALA	-	expression tag	UNP A0A6C0ZY47
F	559	PRO	ILE	conflict	UNP A0A6C0ZY47
F	605	CYS	THR	conflict	UNP A0A6C0ZY47
F	665	ALA	-	expression tag	UNP A0A6C0ZY47
F	666	ALA	-	expression tag	UNP A0A6C0ZY47
J	559	PRO	ILE	conflict	UNP A0A6C0ZY47
J	605	CYS	THR	conflict	UNP A0A6C0ZY47

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Chain	Residue	Modelled	Actual	Comment	Reference
J	665	ALA	-	expression tag	UNP A0A6C0ZY47
J	666	ALA	-	expression tag	UNP A0A6C0ZY47

- Molecule 3 is a protein called Heavy chain of 8ANC195 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		
3	G	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		
3	K	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		

- Molecule 4 is a protein called Light chain of 8ANC195 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total	C	N	O	S	0	0
			814	510	143	158	3		
4	H	108	Total	C	N	O	S	0	0
			823	516	145	159	3		
4	L	108	Total	C	N	O	S	0	0
			823	516	145	159	3		

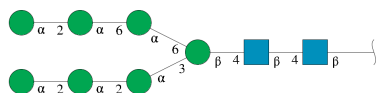
- Molecule 5 is a protein called Heavy chain of 10-1074 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		
5	O	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		
5	Q	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		

- Molecule 6 is a protein called Light chain of 10-1074 Fab.

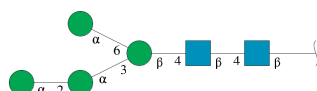
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	R	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	9	Total	C	N	O	0	0
			105	58	2	45		
7	j	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	6	Total	C	N	O	0	0
			72	40	2	30		
8	b	6	Total	C	N	O	0	0
			72	40	2	30		
8	k	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	4	Total	C	N	O	0	0
			56	32	4	20		
9	d	4	Total	C	N	O	0	0
			56	32	4	20		

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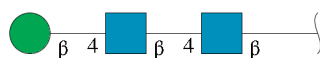
Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



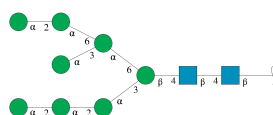
Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	2	Total	C	N	O	0	0
			28	16	2	10		
10	W	2	Total	C	N	O	0	0
			28	16	2	10		
10	X	2	Total	C	N	O	0	0
			28	16	2	10		
10	c	2	Total	C	N	O	0	0
			28	16	2	10		
10	e	2	Total	C	N	O	0	0
			28	16	2	10		
10	f	2	Total	C	N	O	0	0
			28	16	2	10		
10	g	2	Total	C	N	O	0	0
			28	16	2	10		
10	l	2	Total	C	N	O	0	0
			28	16	2	10		
10	m	2	Total	C	N	O	0	0
			28	16	2	10		
10	o	2	Total	C	N	O	0	0
			28	16	2	10		
10	p	2	Total	C	N	O	0	0
			28	16	2	10		
10	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	3	Total	C	N	O	0	0
			39	22	2	15		
11	Z	3	Total	C	N	O	0	0
			39	22	2	15		
11	h	3	Total	C	N	O	0	0
			39	22	2	15		
11	i	3	Total	C	N	O	0	0
			39	22	2	15		
11	r	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



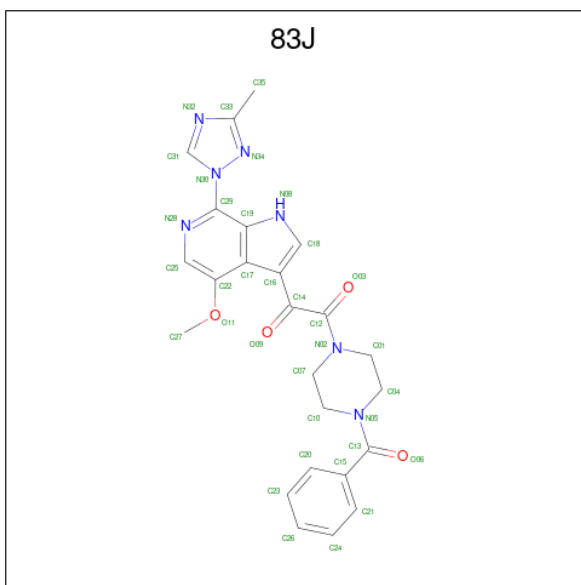
Mol	Chain	Residues	Atoms				AltConf	Trace
12	a	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



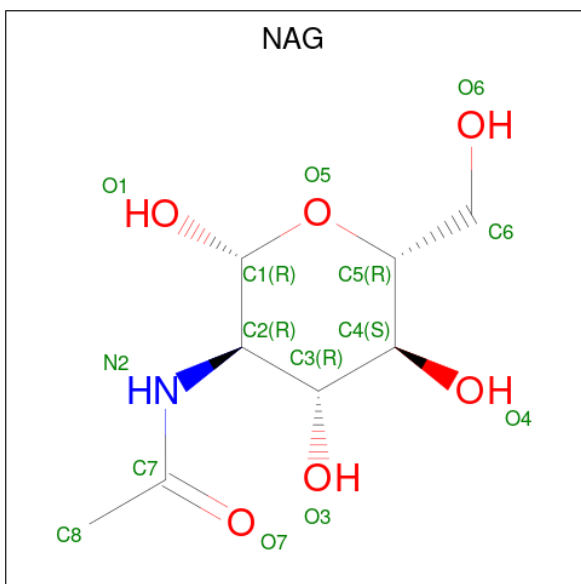
Mol	Chain	Residues	Atoms				AltConf	Trace
13	s	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 14 is 1-[4-(benzenecarbonyl)piperazin-1-yl]-2-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]ethane-1,2-dione (three-letter code: 83J) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>7</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			35	24	7	4	
14	E	1	Total	C	N	O	0
			35	24	7	4	
14	I	1	Total	C	N	O	0
			35	24	7	4	

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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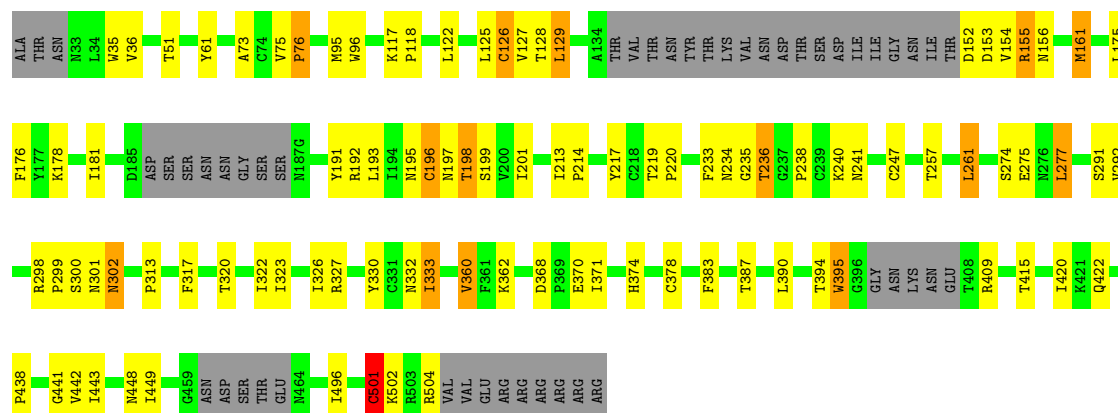
Mol	Chain	Residues	Atoms				AltConf
15	G	1	Total	C	N	O	0
			14	8	1	5	
15	I	1	Total	C	N	O	0
			14	8	1	5	
15	I	1	Total	C	N	O	0
			14	8	1	5	
15	I	1	Total	C	N	O	0
			14	8	1	5	
15	I	1	Total	C	N	O	0
			14	8	1	5	
15	I	1	Total	C	N	O	0
			14	8	1	5	
15	I	1	Total	C	N	O	0
			14	8	1	5	
15	J	1	Total	C	N	O	0
			14	8	1	5	
15	J	1	Total	C	N	O	0
			14	8	1	5	
15	J	1	Total	C	N	O	0
			14	8	1	5	
15	K	1	Total	C	N	O	0
			14	8	1	5	





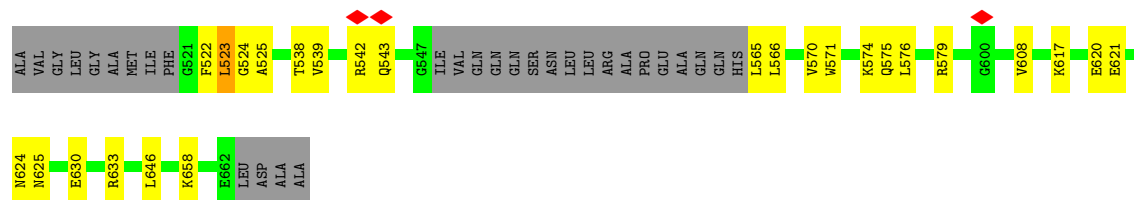
• Molecule 1: CRF01\_AE T/F100 HIV-1 gp120

Chain I: 70% 17% 10%



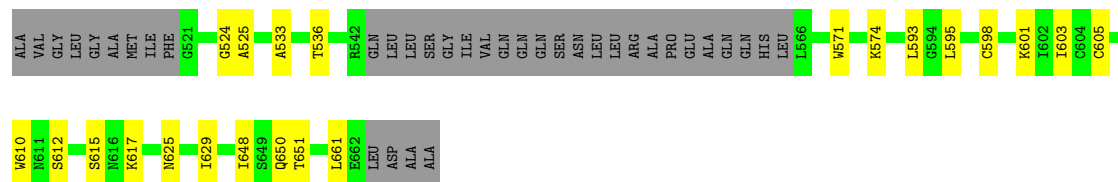
• Molecule 2: CRF-1\_AE T/F100 HIV-1 gp41

Chain B: 64% 16% 19%



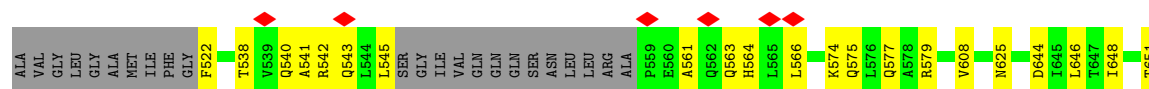
• Molecule 2: CRF-1\_AE T/F100 HIV-1 gp41

Chain F: 63% 14% 23%



• Molecule 2: CRF-1\_AE T/F100 HIV-1 gp41

Chain J: 69% 14% 17%

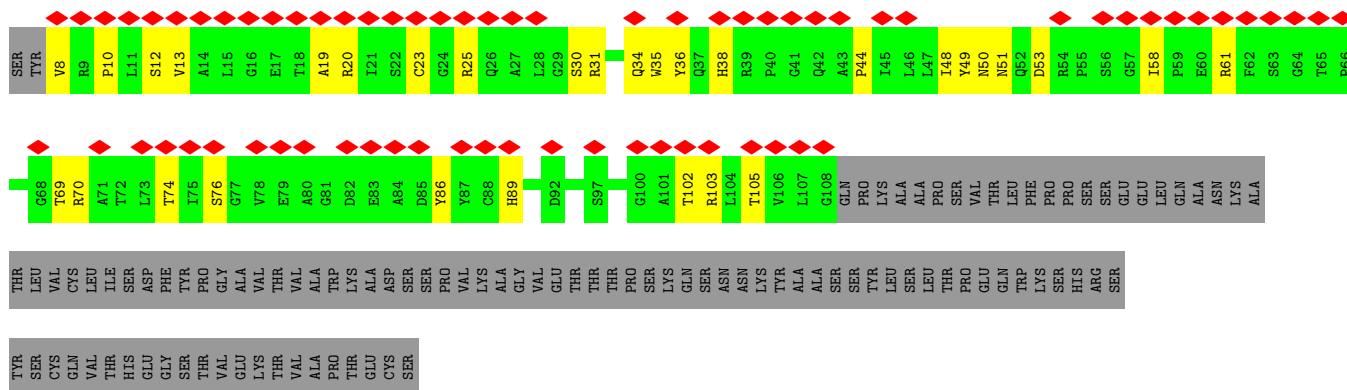




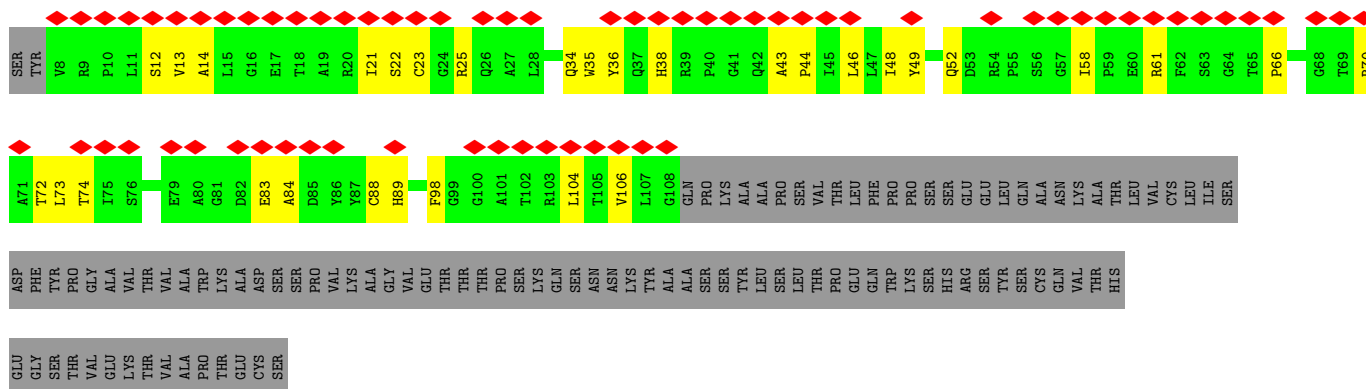
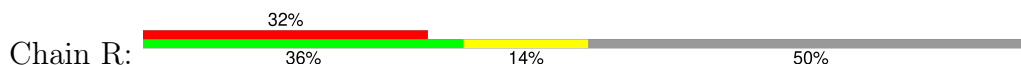








- Molecule 6: Light chain of 10-1074 Fab



- Molecule 7:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-6)- $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

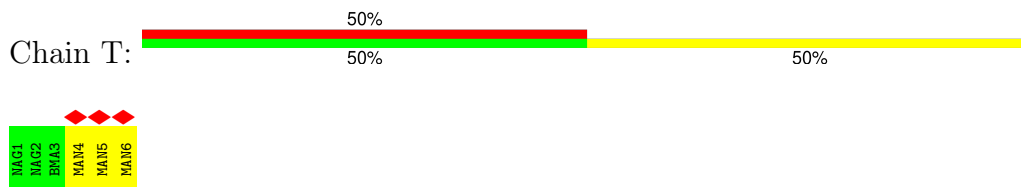


- Molecule 7:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-6)- $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

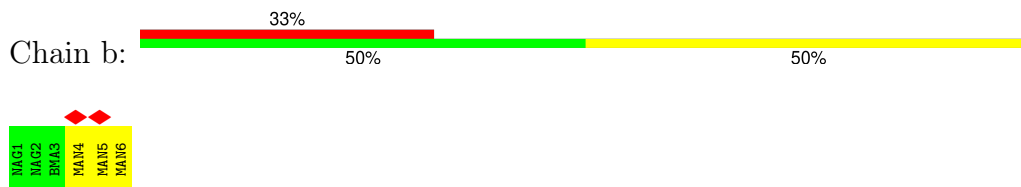


- Molecule 8:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetam

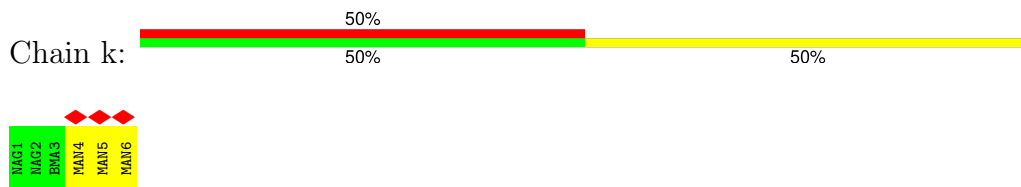
ido-2-deoxy-beta-D-glucopyranose



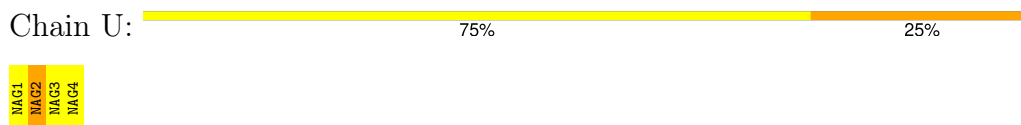
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



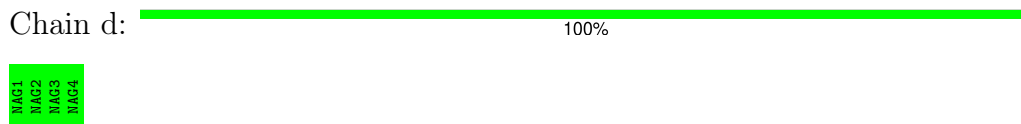
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  50% 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:  100%



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

IMG1  
IMG2  
BMA3

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  67% 33%

IMG1  
IMG2  
BMA3

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%

IMG1  
IMG2  
BMA3

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%

IMG1  
IMG2  
BMA3

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%


IMG1  
IMG2  
BMA3

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  30% 70%

IMG1  
IMG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 13: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  25% 75% 25%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	234547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.14	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.297	Depositor
Minimum map value	-0.876	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	288.1332, 288.1332, 288.1332	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88930005, 0.88930005, 0.88930005	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: MAN, NAG, BMA, 83J

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	0.62	0/3556	0.82	1/4823 (0.0%)
1	E	0.44	1/3539 (0.0%)	0.63	0/4800
1	I	0.53	0/3532	0.75	1/4790 (0.0%)
2	B	0.43	0/1018	0.59	0/1380
2	F	0.53	0/975	0.69	0/1322
2	J	0.29	0/1055	0.47	0/1431
3	C	0.35	0/1030	0.63	0/1403
3	G	0.46	0/1030	0.68	0/1403
3	K	0.29	0/1030	0.55	0/1403
4	D	0.32	0/832	0.62	0/1130
4	H	0.27	0/841	0.53	0/1141
4	L	0.25	0/841	0.54	0/1141
5	M	0.26	0/1055	0.50	0/1436
5	O	0.27	0/1055	0.51	0/1436
5	Q	0.27	0/1055	0.56	1/1436 (0.1%)
6	N	0.24	0/845	0.54	0/1148
6	P	0.24	0/845	0.55	0/1148
6	R	0.24	0/845	0.55	0/1148
All	All	0.43	1/24979 (0.0%)	0.65	3/33919 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	156	ASN	C-N	6.31	1.48	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PRO	N-CA-C	-7.23	93.31	112.10
5	Q	100(H)	GLY	N-CA-C	7.19	131.08	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	501	CYS	CB-CA-C	6.11	122.62	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3479	0	3416	105	0
1	E	3462	0	3399	74	0
1	I	3455	0	3393	116	0
2	B	999	0	983	46	0
2	F	956	0	934	23	0
2	J	1034	0	1013	33	0
3	C	1003	0	973	33	0
3	G	1003	0	973	11	0
3	K	1003	0	973	19	0
4	D	814	0	787	14	0
4	H	823	0	800	4	0
4	L	823	0	800	9	0
5	M	1030	0	995	41	0
5	O	1030	0	995	31	0
5	Q	1030	0	995	30	0
6	N	824	0	788	20	0
6	P	824	0	788	24	0
6	R	824	0	788	20	0
7	S	105	0	88	4	0
7	j	105	0	88	0	0
8	T	72	0	61	0	0
8	b	72	0	61	0	0
8	k	72	0	61	0	0
9	U	56	0	49	4	0
9	d	56	0	49	0	0
9	n	56	0	49	0	0
10	V	28	0	25	0	0
10	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	28	0	25	2	0
10	c	28	0	25	0	0
10	e	28	0	25	0	0
10	f	28	0	25	0	0
10	g	28	0	25	0	0
10	l	28	0	25	0	0
10	m	28	0	25	0	0
10	o	28	0	25	0	0
10	p	28	0	25	0	0
10	q	28	0	25	0	0
11	Y	39	0	34	0	0
11	Z	39	0	34	1	0
11	h	39	0	34	0	0
11	i	39	0	34	0	0
11	r	39	0	34	0	0
12	a	116	0	97	0	0
13	s	50	0	43	0	0
14	A	35	0	0	0	0
14	E	35	0	0	0	0
14	I	35	0	0	0	0
15	A	112	0	104	1	0
15	B	28	0	26	2	0
15	C	14	0	13	0	0
15	E	112	0	104	3	0
15	F	42	0	39	1	0
15	G	14	0	13	0	0
15	I	98	0	91	1	0
15	J	42	0	39	3	0
15	K	14	0	13	0	0
All	All	26288	0	25351	590	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 12.

All (590) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:CD1	1:A:390:LEU:HD21	1.57	1.33
1:I:156:ASN:HB3	1:I:175:LEU:CD1	1.67	1.23
2:B:566:LEU:CD1	1:I:51:THR:HG21	1.75	1.15
1:I:156:ASN:HB3	1:I:175:LEU:HD13	1.16	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:333:ILE:CD1	1:I:390:LEU:HD21	1.77	1.15
1:I:156:ASN:CB	1:I:175:LEU:HD13	1.78	1.14
1:A:383:PHE:CD1	1:A:420:ILE:HG22	1.83	1.13
1:A:383:PHE:HD1	1:A:420:ILE:HG22	1.15	1.11
1:A:37:THR:HG21	1:A:499:THR:OG1	1.52	1.09
1:I:302:ASN:N	1:I:302:ASN:HD22	1.49	1.06
5:O:71:ARG:HD2	5:O:78:LEU:HD22	1.35	1.06
2:B:566:LEU:HD11	1:I:51:THR:HG21	1.30	1.05
1:I:333:ILE:HD12	1:I:390:LEU:HD21	1.10	1.04
1:I:332:ASN:OD1	1:I:415:THR:HG22	1.58	1.01
1:A:333:ILE:HD12	1:A:390:LEU:CD2	1.89	1.01
1:E:501:CYS:O	1:E:502:LYS:HG3	1.61	1.00
1:A:332:ASN:OD1	1:A:415:THR:HG22	1.65	0.96
1:A:333:ILE:CD1	1:A:390:LEU:CD2	2.43	0.96
1:I:197:ASN:OD1	1:I:198:THR:HG22	1.67	0.95
5:O:28:SER:H	5:O:31:ASN:HD21	1.17	0.93
1:A:74:CYS:O	1:A:74:CYS:SG	2.25	0.93
1:A:333:ILE:HD12	1:A:390:LEU:HD21	0.92	0.91
1:I:327:ARG:NH2	1:I:330:TYR:HD1	1.70	0.90
1:A:383:PHE:CD1	1:A:420:ILE:CG2	2.58	0.86
1:A:37:THR:CG2	1:A:499:THR:OG1	2.24	0.85
1:I:154:VAL:O	1:I:155:ARG:O	1.95	0.85
1:A:45:TRP:CD1	1:A:489:VAL:HG11	2.12	0.84
1:I:333:ILE:HD12	1:I:390:LEU:CD2	2.03	0.84
3:C:93:THR:HG21	3:C:100(L):PHE:HB3	1.59	0.84
3:C:68:LEU:HA	7:S:9:MAN:H62	1.59	0.83
2:B:566:LEU:CD1	1:I:51:THR:CG2	2.56	0.83
1:I:302:ASN:N	1:I:302:ASN:ND2	2.26	0.82
1:A:198:THR:O	1:A:199:SER:OG	1.95	0.82
1:A:126:CYS:HG	1:A:196:CYS:HG	0.91	0.81
2:F:661:LEU:HD12	1:I:501:CYS:SG	2.20	0.81
1:A:128:THR:HG21	1:E:168:LYS:NZ	1.95	0.80
1:I:96:TRP:CG	1:I:275:GLU:OE2	2.35	0.79
1:A:232:LYS:HA	1:A:271:ILE:HD11	1.63	0.79
1:A:251:ILE:HG23	1:A:482:GLU:OE1	1.83	0.79
1:I:333:ILE:HD13	1:I:390:LEU:HD11	1.64	0.78
1:A:302:ASN:OD1	1:A:302:ASN:N	2.16	0.78
2:B:566:LEU:CD2	2:J:574:LYS:HA	2.14	0.78
3:C:6:GLN:HE22	3:C:104:GLY:HA3	1.48	0.78
1:I:327:ARG:HH21	1:I:330:TYR:HD1	1.32	0.77
1:I:129:LEU:N	1:I:129:LEU:HD23	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:71:ARG:HD2	5:O:78:LEU:CD2	2.16	0.75
5:M:18:LEU:HB2	5:M:82:LEU:HB2	1.68	0.74
2:F:574:LYS:HG2	2:J:566:LEU:HD21	1.68	0.74
1:I:127:VAL:O	1:I:129:LEU:HD23	1.86	0.74
1:I:333:ILE:CD1	1:I:390:LEU:CD2	2.63	0.74
2:B:539:VAL:HA	2:B:542:ARG:HB2	1.70	0.74
6:N:38:HIS:HB3	6:N:84:ALA:HB1	1.70	0.73
5:Q:40:SER:HB3	5:Q:43:LYS:HB3	1.71	0.73
1:I:155:ARG:NH2	1:I:178:LYS:HG3	2.03	0.73
6:N:34:GLN:HB2	6:N:89:HIS:HB3	1.70	0.72
4:L:89:GLN:HG3	4:L:97:THR:O	1.89	0.72
2:B:566:LEU:HD21	2:J:574:LYS:HA	1.70	0.72
1:I:152:ASP:CG	1:I:153:ASP:H	1.91	0.72
6:N:20:ARG:HH21	6:N:75:ILE:H	1.38	0.72
2:J:542:ARG:HG3	2:J:543:GLN:HG3	1.71	0.72
2:B:542:ARG:HE	2:J:651:THR:CG2	2.02	0.71
1:A:128:THR:HG21	1:E:168:LYS:HZ1	1.53	0.71
2:B:566:LEU:HD12	1:I:51:THR:HG21	1.72	0.71
1:A:275:GLU:HG3	1:A:275:GLU:O	1.89	0.71
1:E:501:CYS:HG	2:F:605:CYS:HG	0.77	0.71
3:K:23:LYS:HG2	3:K:77(D):ILE:HG12	1.73	0.71
3:C:95:THR:OG1	3:C:100(J):MET:SD	2.49	0.71
5:M:47:TRP:O	5:M:60:ASN:ND2	2.23	0.70
6:R:52:GLN:HE21	6:R:66:PRO:HA	1.57	0.70
4:D:4:MET:HE1	4:D:90:GLN:HB3	1.73	0.70
1:A:265:LEU:HD21	1:A:450:THR:HG22	1.74	0.70
1:I:127:VAL:O	1:I:129:LEU:CD2	2.39	0.69
1:I:156:ASN:HB2	1:I:175:LEU:HD13	1.72	0.69
6:N:83:GLU:HA	6:N:104:LEU:HB3	1.75	0.69
1:A:330:TYR:HE2	9:U:1:NAG:HN2	1.40	0.68
1:A:198:THR:C	1:A:199:SER:OG	2.31	0.68
1:A:428:GLN:HB3	1:A:430:VAL:HG23	1.75	0.67
1:A:261:LEU:HD23	1:A:449:ILE:HG22	1.75	0.67
1:I:298:ARG:NH1	1:I:302:ASN:OD1	2.28	0.67
1:I:333:ILE:CD1	1:I:390:LEU:HD11	2.24	0.67
6:N:10:PRO:HB3	6:N:103:ARG:HB3	1.75	0.67
3:K:6:GLN:HE22	3:K:104:GLY:HA3	1.59	0.67
6:N:59:PRO:HB2	6:N:61:ARG:HG3	1.77	0.67
1:E:291:SER:HB3	15:E:606:NAG:H82	1.76	0.67
3:C:87:THR:HG22	3:C:111:VAL:H	1.60	0.66
3:G:95:THR:HG22	3:G:100(L):PHE:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:CD1	1:A:489:VAL:CG1	2.78	0.66
3:K:12:LYS:HA	3:K:12:LYS:HE3	1.78	0.66
1:A:383:PHE:CE1	1:A:420:ILE:CG2	2.79	0.66
1:A:179:LEU:HG	1:A:421:LYS:HD3	1.78	0.66
1:E:501:CYS:O	1:E:502:LYS:CG	2.42	0.65
3:C:23:LYS:HG2	3:C:77(D):ILE:HG12	1.78	0.65
1:I:327:ARG:HD2	5:Q:100(G):PHE:HB2	1.78	0.65
3:K:95:THR:HG21	3:K:100(J):MET:SD	2.37	0.65
3:C:39:GLN:HA	3:C:45:LEU:HD23	1.78	0.65
5:M:38:ARG:HB2	5:M:48:ILE:HD13	1.79	0.65
1:I:274:SER:OG	1:I:277:LEU:HD23	1.97	0.64
1:I:327:ARG:NH2	1:I:330:TYR:CD1	2.60	0.64
6:P:34:GLN:HG3	6:P:49:TYR:HB2	1.78	0.64
1:I:213:ILE:HG23	1:I:214:PRO:HD2	1.80	0.63
1:A:333:ILE:HD13	1:A:390:LEU:CD2	2.28	0.63
2:B:630:GLU:OE2	2:B:633:ARG:NH2	2.31	0.63
2:J:644:ASP:O	2:J:648:ILE:HG12	1.98	0.63
5:Q:66:ARG:NH1	5:Q:82(B):SER:O	2.31	0.63
6:R:22:SER:HB2	6:R:70:ARG:HH21	1.63	0.63
1:A:75:VAL:HG12	1:A:75:VAL:O	1.96	0.63
2:F:593:LEU:HG	2:F:598:CYS:HB2	1.79	0.63
3:K:40:ALA:HB3	3:K:43:GLN:HB3	1.80	0.63
5:O:37:ILE:HB	5:O:91:TYR:HB2	1.81	0.63
6:R:38:HIS:HB3	6:R:84:ALA:HB1	1.81	0.63
3:C:12:LYS:NZ	3:C:17:SER:O	2.30	0.62
6:P:38:HIS:HA	6:P:44:PRO:HB3	1.81	0.62
5:Q:105:LYS:NZ	5:Q:107:THR:OG1	2.32	0.62
5:M:39:GLN:HB2	5:M:45:LEU:HG	1.82	0.62
1:A:201:ILE:HD13	1:A:423:ILE:HD12	1.80	0.62
1:I:154:VAL:O	1:I:155:ARG:C	2.35	0.62
2:F:661:LEU:CD1	1:I:501:CYS:SG	2.87	0.62
2:B:538:THR:C	2:B:542:ARG:HD2	2.20	0.62
1:A:74:CYS:HB3	2:B:571:TRP:CD1	2.35	0.62
1:I:152:ASP:OD1	1:I:153:ASP:N	2.33	0.61
5:O:47:TRP:HH2	6:P:89:HIS:HE1	1.48	0.61
3:C:45:LEU:HD11	4:D:44:PRO:HG3	1.82	0.61
5:M:29:MET:HG2	5:M:73:THR:HG23	1.82	0.61
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.35	0.61
1:I:302:ASN:HD22	1:I:302:ASN:H	1.40	0.61
1:E:363:PRO:O	1:E:469:ARG:NH1	2.34	0.61
4:L:4:MET:HG2	4:L:25:ALA:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:CG2	1:A:482:GLU:OE1	2.48	0.61
1:I:195:ASN:HB3	1:I:199:SER:OG	2.01	0.61
6:N:23:CYS:O	6:N:70:ARG:NH2	2.34	0.61
1:A:199:SER:CB	1:A:431:GLY:O	2.49	0.60
1:I:233:PHE:O	1:I:235:GLY:N	2.28	0.60
1:I:320:THR:CG2	1:I:422:GLN:HE22	2.13	0.60
1:A:502:LYS:HG3	1:A:502:LYS:O	1.99	0.60
1:A:501:CYS:O	1:A:502:LYS:HB3	2.00	0.60
3:G:95:THR:CG2	3:G:100(L):PHE:HA	2.31	0.60
2:B:617:LYS:HB3	2:B:621:GLU:HG3	1.83	0.60
1:E:75:VAL:O	1:E:76:PRO:C	2.38	0.60
5:O:4:LEU:HG	5:O:104:GLY:HA2	1.83	0.60
1:A:50:THR:HG21	1:A:223:TYR:CD2	2.36	0.60
1:E:129:LEU:HD21	1:E:193:LEU:CD2	2.31	0.60
1:E:300:SER:O	1:E:442:VAL:HG12	2.01	0.60
1:I:233:PHE:C	1:I:235:GLY:H	2.05	0.60
5:Q:100(C):GLY:HA3	5:Q:100(I):GLU:OE2	2.02	0.60
1:A:128:THR:CG2	1:E:168:LYS:NZ	2.65	0.60
4:D:21:ILE:HD11	4:D:73:LEU:HD23	1.82	0.60
1:I:301:ASN:HD22	1:I:323:ILE:HD11	1.66	0.60
1:A:383:PHE:CE1	1:A:420:ILE:HG21	2.36	0.59
1:A:75:VAL:HG12	1:A:77:THR:OG1	2.01	0.59
5:Q:39:GLN:HA	5:Q:45:LEU:HA	1.83	0.59
1:E:264:SER:O	1:E:287:HIS:NE2	2.28	0.59
3:G:7:SER:O	3:G:107:THR:HG22	2.03	0.59
6:R:34:GLN:HB2	6:R:89:HIS:HB3	1.84	0.59
2:B:625:ASN:HB3	15:B:702:NAG:N2	2.18	0.59
5:Q:35:THR:HA	5:Q:50:TYR:HB2	1.84	0.59
1:A:344:ARG:NH1	15:A:608:NAG:O7	2.35	0.59
6:R:83:GLU:HA	6:R:104:LEU:HB3	1.85	0.59
2:B:566:LEU:HD11	1:I:51:THR:CG2	2.18	0.59
2:B:566:LEU:HG	2:J:577:GLN:CB	2.33	0.59
1:A:111:LEU:HD11	2:B:571:TRP:CZ2	2.37	0.59
5:Q:63:LEU:HD12	5:Q:66:ARG:HH21	1.68	0.58
1:A:251:ILE:HG23	1:A:482:GLU:CD	2.23	0.58
1:A:333:ILE:CD1	1:A:390:LEU:HD11	2.33	0.58
1:A:395:TRP:HA	1:A:407:GLU:HG2	1.85	0.58
1:A:197:ASN:OD1	1:A:198:THR:HG22	2.03	0.58
5:M:68:VAL:O	5:M:81:LYS:N	2.35	0.58
1:I:333:ILE:HD13	1:I:390:LEU:HD21	1.80	0.58
1:E:127:VAL:O	1:E:129:LEU:CD1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:ARG:HB2	4:D:42:LYS:HD2	1.86	0.58
6:R:48:ILE:HD11	6:R:58:ILE:HG21	1.86	0.58
2:J:625:ASN:HB3	15:J:703:NAG:N2	2.18	0.58
2:F:612:SER:O	2:F:615:SER:O	2.22	0.58
1:A:45:TRP:HB2	1:A:489:VAL:HG12	1.85	0.57
5:Q:51:ILE:HG12	5:Q:71:ARG:HD3	1.84	0.57
1:E:61:TYR:HE1	1:E:66:HIS:CD2	2.22	0.57
1:I:152:ASP:CG	1:I:153:ASP:N	2.57	0.57
1:I:233:PHE:CE2	1:I:235:GLY:HA2	2.39	0.57
4:L:3:GLN:N	4:L:3:GLN:OE1	2.37	0.57
6:P:31:ARG:NH2	6:P:69:THR:OG1	2.33	0.57
1:I:128:THR:C	1:I:129:LEU:HD23	2.24	0.57
2:B:566:LEU:HG	2:J:577:GLN:HG2	1.86	0.57
1:I:96:TRP:CD2	1:I:275:GLU:OE2	2.56	0.57
6:P:48:ILE:HD11	6:P:58:ILE:HG21	1.85	0.57
6:R:61:ARG:O	6:R:74:THR:OG1	2.22	0.57
1:A:257:THR:HG21	1:A:370:GLU:O	2.04	0.57
2:J:561:ALA:HA	2:J:575:GLN:HE21	1.69	0.57
3:K:82(C):LEU:HD21	3:K:111:VAL:HG21	1.86	0.57
1:A:37:THR:HG21	1:A:499:THR:HG1	1.69	0.57
1:E:501:CYS:CB	2:F:605:CYS:HG	2.17	0.56
5:O:35:THR:HA	5:O:50:TYR:HB2	1.88	0.56
1:E:350:LYS:HE2	1:E:355:ASN:ND2	2.20	0.56
1:I:125:LEU:HD21	1:I:317:PHE:CE1	2.40	0.56
1:I:320:THR:HG23	1:I:422:GLN:HE22	1.71	0.56
1:I:333:ILE:HD13	1:I:390:LEU:CD1	2.35	0.56
6:N:35:TRP:HB3	6:N:47:LEU:HD12	1.88	0.56
1:A:199:SER:HB3	1:A:431:GLY:O	2.06	0.56
2:B:566:LEU:HD22	2:J:574:LYS:HA	1.88	0.56
6:R:23:CYS:O	6:R:70:ARG:NH2	2.38	0.56
6:R:35:TRP:CZ3	6:R:73:LEU:HB2	2.41	0.56
1:I:155:ARG:CZ	1:I:178:LYS:HG3	2.34	0.56
5:M:31:ASN:OD1	5:M:32:TYR:N	2.38	0.56
5:Q:37:ILE:HD12	5:Q:45:LEU:HD22	1.87	0.56
5:Q:43:LYS:NZ	5:Q:46:GLU:OE1	2.38	0.56
2:B:565:LEU:HD21	2:B:576:LEU:HA	1.87	0.56
1:A:265:LEU:CD2	1:A:450:THR:HG22	2.35	0.56
1:E:265:LEU:HD12	1:E:289:ASN:O	2.06	0.56
6:N:37:GLN:HB2	6:N:47:LEU:HD21	1.87	0.56
5:O:96:ARG:HG3	5:O:100(O):SER:HB2	1.87	0.56
1:I:291:SER:HB2	1:I:448:ASN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:292:VAL:HB	1:I:449:ILE:HD11	1.88	0.56
1:E:61:TYR:HB2	1:E:72:HIS:HD2	1.71	0.55
1:I:154:VAL:O	1:I:176:PHE:O	2.24	0.55
1:I:300:SER:O	1:I:442:VAL:HG12	2.06	0.55
6:N:38:HIS:HB3	6:N:85:ASP:H	1.71	0.55
2:B:566:LEU:HG	2:J:577:GLN:HB2	1.87	0.55
5:M:83:THR:HG23	5:M:85:ALA:H	1.71	0.55
6:P:34:GLN:HB2	6:P:89:HIS:HB3	1.89	0.55
1:A:50:THR:CG2	1:A:223:TYR:CE2	2.89	0.55
1:E:45:TRP:CD1	1:E:489:VAL:HG21	2.42	0.55
2:B:566:LEU:HG	2:J:577:GLN:CG	2.36	0.55
5:M:100:ARG:NH1	9:U:4:NAG:H2	2.21	0.55
1:E:84:MET:HG3	1:E:244:SER:HB3	1.89	0.55
3:K:19:THR:HA	3:K:81:GLU:HG2	1.88	0.55
3:K:100(I):VAL:HG12	4:L:91:TYR:HB2	1.88	0.55
5:O:71:ARG:CD	5:O:78:LEU:HD22	2.23	0.55
6:P:86:TYR:N	6:P:102:THR:O	2.40	0.55
9:U:2:NAG:H3	9:U:2:NAG:H83	1.89	0.55
3:G:87:THR:HG22	3:G:111:VAL:H	1.72	0.54
4:L:80:ALA:HA	4:L:83:PHE:HD2	1.71	0.54
5:O:103:TRP:CG	6:P:44:PRO:HD2	2.42	0.54
6:P:23:CYS:O	6:P:70:ARG:NH2	2.39	0.54
1:E:501:CYS:HG	2:F:605:CYS:CB	2.18	0.54
1:I:36:VAL:HG13	1:I:496:ILE:HG23	1.89	0.54
5:M:21:THR:HB	5:M:77:GLN:HB3	1.88	0.54
1:A:225:ILE:HG12	1:A:488:VAL:HG22	1.88	0.54
5:O:24:VAL:HG11	5:O:34:TRP:HH2	1.71	0.54
1:A:301:ASN:HB3	1:A:442:VAL:HG13	1.88	0.54
1:A:37:THR:OG1	1:A:499:THR:HG23	2.08	0.54
2:B:608:VAL:HG21	2:B:646:LEU:HD12	1.89	0.54
4:H:21:ILE:HG21	4:H:102:THR:HG21	1.88	0.54
1:E:196:CYS:HB2	1:I:313:PRO:HB3	1.90	0.54
1:E:501:CYS:HB2	2:F:605:CYS:SG	2.48	0.54
1:I:300:SER:HB3	1:I:326:ILE:HG22	1.88	0.54
1:I:299:PRO:HB2	1:I:326:ILE:HG12	1.90	0.54
1:E:501:CYS:CB	2:F:605:CYS:SG	2.96	0.53
5:O:53:ASP:HA	5:O:71:ARG:NH2	2.23	0.53
1:A:338:TRP:HZ3	1:A:449:ILE:CD1	2.21	0.53
1:E:251:ILE:HD13	1:E:483:LEU:HD21	1.89	0.53
6:P:61:ARG:NH1	6:P:76:SER:O	2.41	0.53
5:M:103:TRP:HB2	6:N:43:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:87:TYR:HB3	6:N:98:PHE:HB3	1.89	0.53
2:J:541:ALA:HA	2:J:545:LEU:HD22	1.90	0.53
5:Q:40:SER:HA	5:Q:88:ALA:HB1	1.90	0.53
1:I:387:THR:O	1:I:387:THR:OG1	2.24	0.53
1:A:474:ASP:OD1	1:A:476:ARG:HG3	2.08	0.53
1:E:129:LEU:CD1	1:E:129:LEU:N	2.72	0.53
3:C:39:GLN:HG3	3:C:45:LEU:HD23	1.91	0.53
4:H:24:ARG:NH2	4:H:70:ASP:OD1	2.42	0.53
5:Q:34:TRP:HE3	5:Q:78:LEU:HD21	1.74	0.53
6:R:21:ILE:O	6:R:72:THR:OG1	2.25	0.53
1:I:274:SER:OG	1:I:277:LEU:CD2	2.57	0.52
2:F:625:ASN:HB3	15:F:703:NAG:HN2	1.74	0.52
5:M:60:ASN:ND2	5:M:62:SER:OG	2.42	0.52
4:D:24:ARG:NH2	4:D:70:ASP:OD1	2.42	0.52
2:F:524:GLY:O	2:F:525:ALA:HB3	2.09	0.52
2:F:648:ILE:HD11	2:J:542:ARG:HD2	1.90	0.52
5:O:12:VAL:HB	5:O:18:LEU:HD21	1.92	0.52
1:A:122:LEU:HG	1:A:125:LEU:HD21	1.92	0.52
2:B:542:ARG:HE	2:J:651:THR:HG21	1.74	0.52
2:J:563:GLN:O	2:J:579:ARG:NH2	2.42	0.52
6:N:35:TRP:CE2	6:N:73:LEU:HD22	2.44	0.52
5:Q:36:TRP:CD1	5:Q:80:LEU:HD13	2.44	0.52
1:E:323:ILE:HD11	15:E:604:NAG:O5	2.10	0.52
1:A:300:SER:O	1:A:300:SER:OG	2.28	0.52
1:A:333:ILE:HD11	1:A:390:LEU:HD11	1.92	0.52
1:E:195:ASN:ND2	1:E:425:ASN:OD1	2.43	0.52
1:I:301:ASN:ND2	1:I:323:ILE:HD11	2.25	0.52
5:M:38:ARG:HD3	5:M:48:ILE:HD13	1.92	0.52
6:P:35:TRP:HB2	6:P:48:ILE:O	2.10	0.52
6:R:12:SER:HB2	6:R:104:LEU:HA	1.92	0.52
6:R:25:ARG:O	6:R:70:ARG:NH1	2.41	0.52
1:A:339:HIS:CE1	1:A:408:THR:HG23	2.45	0.52
2:B:658:LYS:HD2	2:F:603:ILE:HG21	1.90	0.51
1:I:129:LEU:N	1:I:129:LEU:CD2	2.72	0.51
5:M:4:LEU:HG	5:M:104:GLY:HA2	1.92	0.51
4:D:4:MET:HE1	4:D:90:GLN:CB	2.40	0.51
5:O:49:GLY:HA2	5:O:59:TYR:HA	1.91	0.51
1:I:298:ARG:NH2	1:I:441:GLY:O	2.44	0.51
5:M:51:ILE:HD11	5:M:55:GLU:HG3	1.93	0.51
1:A:278:THR:HG23	3:C:74:LEU:HD22	1.92	0.51
1:I:360:VAL:HB	1:I:394:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:CG1	10:X:2:NAG:H82	2.40	0.51
1:E:257:THR:HG21	1:E:370:GLU:O	2.10	0.51
1:E:122:LEU:HD11	1:E:203:GLN:HB2	1.92	0.51
1:E:154:VAL:HB	1:E:175:LEU:HD12	1.92	0.50
2:F:574:LYS:HA	2:J:566:LEU:HD11	1.92	0.50
5:M:70:SER:O	5:M:79:SER:N	2.44	0.50
6:P:25:ARG:O	6:P:70:ARG:NH1	2.43	0.50
1:I:320:THR:HG22	1:I:438:PRO:HG3	1.94	0.50
1:E:289:ASN:OD1	1:E:290:GLU:N	2.45	0.50
5:M:49:GLY:HA2	5:M:59:TYR:HA	1.93	0.50
1:A:182:VAL:HG12	10:X:2:NAG:H82	1.92	0.49
3:G:23:LYS:HG2	3:G:77(D):ILE:HG12	1.93	0.49
1:I:368:ASP:H	1:I:371:ILE:HD12	1.77	0.49
5:O:69:ILE:HD12	5:O:80:LEU:HG	1.94	0.49
6:P:34:GLN:NE2	6:P:49:TYR:O	2.39	0.49
1:A:54:CYS:SG	1:A:215:ILE:HG23	2.52	0.49
1:A:204:ALA:HB3	1:A:437:PRO:HD3	1.93	0.49
1:I:75:VAL:N	1:I:76:PRO:CD	2.75	0.49
1:I:327:ARG:HD2	5:Q:100(G):PHE:CB	2.41	0.49
5:M:100:ARG:HE	6:N:30:SER:HB2	1.76	0.49
5:M:18:LEU:HD13	5:M:82(C):VAL:HG11	1.94	0.49
5:M:29:MET:SD	5:M:29:MET:N	2.85	0.49
5:M:51:ILE:HD11	5:M:55:GLU:HA	1.95	0.49
6:P:20:ARG:HG2	6:P:74:THR:HB	1.95	0.49
1:E:61:TYR:CD1	1:E:72:HIS:HB2	2.47	0.49
1:I:327:ARG:HB2	5:Q:100(I):GLU:CD	2.32	0.49
1:E:215:ILE:HD12	1:E:253:PRO:HG3	1.94	0.49
2:J:625:ASN:HB3	15:J:703:NAG:HN2	1.77	0.49
5:Q:100(A):ILE:HG22	5:Q:100(J):PHE:HB3	1.95	0.49
1:E:154:VAL:O	1:E:155:ARG:O	2.30	0.49
1:E:322:ILE:HD11	1:E:326:ILE:HG12	1.94	0.49
1:A:45:TRP:CE3	2:B:523:LEU:HD11	2.47	0.49
3:C:68:LEU:HG	3:C:69:ILE:N	2.28	0.49
3:K:39:GLN:HB2	3:K:45:LEU:HD23	1.94	0.49
1:A:386:ASN:O	1:A:416:ILE:HB	2.13	0.48
2:B:566:LEU:CD2	2:J:577:GLN:HB2	2.43	0.48
4:D:88:CYS:O	4:D:99:GLY:N	2.46	0.48
1:A:276:ASN:OD1	1:A:278:THR:OG1	2.24	0.48
2:B:620:GLU:O	2:B:624:ASN:HB2	2.13	0.48
1:E:379:ARG:HE	1:E:443:ILE:HG22	1.77	0.48
2:B:566:LEU:HD21	2:J:577:GLN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:HIS:CE1	3:C:64:ARG:HH21	2.31	0.48
1:E:502:LYS:O	1:E:502:LYS:HD3	2.13	0.48
1:I:96:TRP:CB	1:I:275:GLU:OE2	2.62	0.48
6:P:36:TYR:HB2	6:P:38:HIS:CE1	2.48	0.48
2:B:542:ARG:NE	2:J:651:THR:HG21	2.28	0.48
1:E:122:LEU:CD1	1:E:203:GLN:HB2	2.43	0.48
3:G:75:THR:O	3:G:76:GLY:C	2.52	0.48
1:I:155:ARG:NH2	1:I:178:LYS:CG	2.75	0.48
2:J:522:PHE:O	2:J:540:GLN:NE2	2.37	0.48
3:K:35(A):ASN:O	3:K:93:THR:OG1	2.31	0.48
5:M:10:GLY:HA2	5:M:109:VAL:HA	1.96	0.48
5:O:67:VAL:HB	5:O:82:LEU:HA	1.94	0.48
4:D:89:GLN:HG2	4:D:90:GLN:N	2.29	0.48
1:E:36:VAL:HG13	1:E:496:ILE:HG23	1.95	0.48
1:I:300:SER:N	1:I:326:ILE:HG21	2.29	0.48
3:K:55:TRP:HH2	3:K:73:ASP:HB3	1.77	0.48
1:A:62:GLU:OE1	1:A:211:ASP:HB3	2.14	0.48
2:B:625:ASN:HB3	15:B:702:NAG:HN2	1.79	0.48
1:I:374:HIS:HB2	1:I:387:THR:HG21	1.96	0.48
1:E:50:THR:HG21	1:E:223:TYR:CZ	2.49	0.48
5:M:7:SER:OG	5:M:21:THR:OG1	2.32	0.48
5:M:38:ARG:NH2	5:M:86:ASP:O	2.47	0.48
1:E:128:THR:C	1:E:129:LEU:HD12	2.33	0.47
1:I:156:ASN:CB	1:I:175:LEU:CD1	2.54	0.47
5:O:24:VAL:HG11	5:O:34:TRP:CH2	2.48	0.47
1:E:129:LEU:HD21	1:E:193:LEU:HD22	1.97	0.47
1:E:129:LEU:N	1:E:129:LEU:HD12	2.28	0.47
1:I:127:VAL:O	1:I:129:LEU:HD21	2.15	0.47
5:M:12:VAL:HG21	5:M:18:LEU:HD21	1.96	0.47
2:J:575:GLN:O	2:J:579:ARG:HG3	2.15	0.47
6:R:34:GLN:NE2	6:R:49:TYR:HB2	2.29	0.47
6:R:35:TRP:CD1	6:R:88:CYS:HA	2.49	0.47
3:C:69:ILE:N	7:S:9:MAN:O6	2.45	0.47
5:O:21:THR:HB	5:O:77:GLN:HB3	1.97	0.47
2:B:542:ARG:NE	2:J:651:THR:CG2	2.75	0.47
1:E:59:LYS:O	1:E:60:ALA:C	2.50	0.47
1:E:111:LEU:HD11	2:F:571:TRP:CZ2	2.50	0.47
1:E:154:VAL:O	1:E:155:ARG:C	2.53	0.47
2:F:598:CYS:O	2:F:601:LYS:HG2	2.14	0.47
5:Q:45:LEU:HD21	6:R:98:PHE:CD1	2.50	0.47
1:A:449:ILE:HG13	1:A:449:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:595:LEU:O	2:F:650:GLN:HG2	2.15	0.47
5:Q:103:TRP:HB2	6:R:43:ALA:HB1	1.97	0.47
1:A:265:LEU:HD13	1:A:290:GLU:HA	1.96	0.47
1:I:122:LEU:HB2	1:I:201:ILE:O	2.16	0.46
3:C:39:GLN:O	3:C:88:ALA:HB1	2.16	0.46
2:B:524:GLY:O	2:B:525:ALA:HB3	2.15	0.46
1:E:127:VAL:O	1:E:129:LEU:HD13	2.14	0.46
1:I:238:PRO:HG3	3:K:54:ARG:HG2	1.97	0.46
2:B:566:LEU:HD21	2:J:577:GLN:CB	2.45	0.46
1:E:340:LYS:HE2	1:E:344:ARG:HH21	1.81	0.46
2:F:651:THR:HG21	2:J:538:THR:HA	1.96	0.46
1:I:126:CYS:SG	1:I:196:CYS:HA	2.55	0.46
15:J:702:NAG:H83	4:L:27:GLN:OE1	2.16	0.46
3:K:29:THR:HG23	3:K:31:GLY:H	1.79	0.46
5:M:40:SER:HB2	5:M:43:LYS:HB3	1.97	0.46
6:N:12:SER:HB2	6:N:105:THR:H	1.81	0.46
6:R:36:TYR:HA	6:R:46:LEU:HA	1.98	0.46
1:E:333:ILE:HG13	1:E:334:SER:N	2.31	0.46
1:I:395:TRP:CZ2	1:I:409:ARG:HD2	2.50	0.46
2:J:561:ALA:HA	2:J:575:GLN:NE2	2.30	0.46
3:C:67:VAL:CG2	3:C:82:ILE:HD13	2.45	0.46
3:K:32:LEU:HD12	3:K:33:TYR:HD1	1.79	0.46
1:A:75:VAL:CG1	1:A:77:THR:OG1	2.64	0.46
1:E:129:LEU:HD21	1:E:193:LEU:HD21	1.98	0.46
1:I:126:CYS:CB	1:I:196:CYS:HG	2.24	0.46
1:I:161:MET:HE2	1:I:161:MET:HB3	1.74	0.46
1:I:378:CYS:HB3	1:I:443:ILE:HD12	1.97	0.46
3:C:56:LYS:HE3	3:C:56:LYS:HA	1.98	0.45
1:E:265:LEU:HD23	1:E:265:LEU:H	1.81	0.45
5:O:4:LEU:HD12	5:O:92:CYS:HB3	1.99	0.45
1:A:179:LEU:HG	1:A:421:LYS:CD	2.45	0.45
2:J:608:VAL:HG21	2:J:646:LEU:HD23	1.97	0.45
6:N:20:ARG:HE	6:N:74:THR:HA	1.80	0.45
5:Q:33:TYR:O	5:Q:95:ALA:HB3	2.17	0.45
1:A:111:LEU:HD23	1:A:114:GLN:NE2	2.32	0.45
3:C:39:GLN:CA	3:C:45:LEU:HD23	2.46	0.45
3:C:39:GLN:CB	3:C:45:LEU:HD23	2.46	0.45
3:C:72:VAL:HG23	7:S:5:MAN:H61	1.99	0.45
5:M:47:TRP:CZ3	6:N:96:TRP:HD1	2.34	0.45
3:C:38:ARG:HG2	3:C:39:GLN:O	2.17	0.45
3:K:28:ASN:OD1	3:K:29:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:38:ARG:HB3	3:G:48:ILE:HD11	1.99	0.45
5:M:100(A):ILE:HG22	5:M:100(J):PHE:HB3	1.99	0.45
4:L:80:ALA:HA	4:L:83:PHE:CD2	2.51	0.45
5:M:15:SER:HA	5:M:82(B):SER:HA	1.98	0.45
5:O:89:VAL:HG22	5:O:106:GLY:HA3	1.98	0.45
1:E:229:ASN:O	15:E:602:NAG:H62	2.16	0.45
1:E:290:GLU:OE1	1:E:340:LYS:NZ	2.49	0.45
2:B:522:PHE:CE2	2:B:524:GLY:O	2.70	0.45
1:A:229:ASN:HB2	1:A:241:ASN:O	2.17	0.45
1:I:257:THR:HG21	1:I:370:GLU:O	2.16	0.45
5:Q:30:ASN:OD1	5:Q:31:ASN:N	2.50	0.45
3:C:48:ILE:O	3:C:60:SER:N	2.41	0.44
1:I:117:LYS:HG3	1:I:118:PRO:HD3	1.99	0.44
1:I:300:SER:HB2	1:I:322:ILE:CG2	2.46	0.44
6:R:14:ALA:HA	6:R:106:VAL:HG23	1.99	0.44
1:A:95:MET:HE3	1:A:273:ARG:HB3	2.00	0.44
1:A:227:ARG:HA	1:A:485:LYS:O	2.17	0.44
2:B:566:LEU:CG	2:J:577:GLN:CB	2.95	0.44
1:E:171:LYS:HE2	1:E:171:LYS:HB3	1.81	0.44
3:K:32:LEU:HD12	3:K:33:TYR:CD1	2.52	0.44
6:P:34:GLN:HA	6:P:49:TYR:HA	1.99	0.44
1:E:277:LEU:HD23	1:E:277:LEU:HA	1.77	0.44
5:M:36:TRP:HZ3	5:M:90:TYR:HB3	1.82	0.44
2:B:539:VAL:HG13	2:B:543:GLN:HG2	1.99	0.44
3:C:82(C):LEU:HD21	3:C:111:VAL:HG11	2.00	0.44
3:G:29:THR:HG23	3:G:32:LEU:H	1.82	0.44
1:I:362:LYS:HE2	1:I:362:LYS:HB3	1.66	0.44
1:A:383:PHE:HE1	1:A:420:ILE:HG21	1.80	0.44
2:F:629:ILE:HG21	3:G:100:ARG:HH21	1.83	0.44
5:M:52:SER:HB2	5:M:56:SER:HB2	1.99	0.44
4:D:36:TYR:HB2	4:D:87:TYR:HB2	1.99	0.44
6:N:38:HIS:HB2	6:N:85:ASP:HB2	1.99	0.44
5:Q:89:VAL:HG23	5:Q:107:THR:C	2.38	0.44
1:A:288:PHE:CE2	1:A:341:VAL:HG11	2.53	0.44
1:A:481:ASN:O	1:A:484:TYR:HD1	2.01	0.44
1:I:73:ALA:O	1:I:75:VAL:N	2.49	0.44
5:O:45:LEU:HD21	5:O:103:TRP:HH2	1.83	0.44
2:B:542:ARG:HG2	2:J:648:ILE:HD13	1.99	0.43
1:I:261:LEU:HD23	1:I:449:ILE:HG22	2.00	0.43
1:I:241:ASN:HB3	15:I:602:NAG:HN2	1.82	0.43
5:M:20:VAL:HG11	5:M:90:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:37:ILE:HG21	5:M:103:TRP:HZ3	1.83	0.43
3:C:29:THR:HG23	3:C:31:GLY:H	1.84	0.43
3:C:67:VAL:HG22	3:C:82:ILE:HD13	1.99	0.43
3:C:67:VAL:O	7:S:9:MAN:O4	2.23	0.43
1:E:129:LEU:CD2	1:E:193:LEU:HD22	2.49	0.43
3:G:93:THR:HG22	3:G:103:TRP:HA	1.99	0.43
5:O:13:LYS:HA	5:O:13:LYS:HD3	1.79	0.43
5:O:100:ARG:HE	6:P:30:SER:HB2	1.83	0.43
4:H:3:GLN:OE1	4:H:3:GLN:N	2.52	0.43
5:M:66:ARG:HH12	5:M:85:ALA:HB3	1.83	0.43
1:A:71:THR:HG21	1:A:213:ILE:HD11	1.99	0.43
2:B:565:LEU:HG	2:B:575:GLN:HB3	2.00	0.43
6:P:10:PRO:HG3	6:P:103:ARG:CZ	2.48	0.43
6:P:31:ARG:NH1	6:P:51:ASN:OD1	2.52	0.43
1:E:62:GLU:O	1:E:65:VAL:HG12	2.18	0.43
3:K:38:ARG:HB2	3:K:48:ILE:HD11	2.01	0.43
5:O:100(P):MET:HB3	6:P:36:TYR:CE2	2.54	0.43
6:R:12:SER:OG	6:R:13:VAL:N	2.52	0.43
1:I:240:LYS:HD3	1:I:240:LYS:HA	1.86	0.43
1:A:36:VAL:HG11	2:B:646:LEU:HD11	2.00	0.43
1:A:177:TYR:OH	1:A:420:ILE:HD11	2.18	0.43
1:I:181:ILE:CG2	1:I:191:TYR:HB3	2.49	0.43
1:A:290:GLU:OE2	1:A:340:LYS:NZ	2.52	0.42
1:E:153:ASP:HB2	1:E:178:LYS:HE3	2.00	0.42
1:E:382:PHE:CE2	1:E:424:ILE:HD13	2.54	0.42
1:I:326:ILE:HG23	1:I:327:ARG:O	2.18	0.42
1:I:333:ILE:CD1	1:I:390:LEU:CD1	2.97	0.42
5:M:2:VAL:HG13	5:M:24:VAL:HG13	2.02	0.42
1:A:321(A):ASP:OD1	1:A:322:ILE:N	2.52	0.42
1:A:333:ILE:CD1	1:A:390:LEU:CD1	2.98	0.42
3:C:69:ILE:HG12	3:C:80:LEU:HD12	2.01	0.42
1:I:96:TRP:HB3	1:I:275:GLU:OE2	2.19	0.42
2:J:564:HIS:HA	2:J:579:ARG:HH22	1.84	0.42
5:M:51:ILE:HB	5:M:69:ILE:HG12	2.02	0.42
5:Q:7:SER:O	5:Q:21:THR:OG1	2.29	0.42
1:A:325:ASP:OD1	1:A:325:ASP:O	2.36	0.42
1:A:392:ASN:O	1:A:393:SER:OG	2.34	0.42
1:I:213:ILE:CG2	1:I:214:PRO:HD2	2.47	0.42
5:Q:12:VAL:HB	5:Q:111:VAL:HG12	2.02	0.42
4:D:23:CYS:N	4:D:71:PHE:O	2.51	0.42
1:E:71:THR:HG21	1:E:213:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:PRO:HG2	1:E:254:VAL:HG12	2.02	0.42
1:E:431:GLY:O	1:E:432:GLN:HG3	2.19	0.42
3:C:55:TRP:HH2	3:C:73:ASP:HB3	1.84	0.42
4:D:4:MET:CE	4:D:90:GLN:HB3	2.47	0.42
1:I:217:TYR:O	1:I:247:CYS:HB2	2.19	0.42
5:M:66:ARG:HG3	5:M:86:ASP:HB3	2.01	0.42
1:I:192:ARG:HH11	1:I:196:CYS:CB	2.32	0.42
5:M:37:ILE:O	5:M:91:TYR:HB2	2.19	0.42
5:Q:103:TRP:CD2	6:R:44:PRO:HD2	2.54	0.42
1:A:45:TRP:HH2	1:A:89:VAL:HG11	1.85	0.42
1:A:293:LYS:HE2	1:A:293:LYS:HB3	1.84	0.42
2:B:538:THR:O	2:B:542:ARG:HG3	2.20	0.42
1:I:95:MET:HG2	1:I:235:GLY:O	2.20	0.42
1:A:333:ILE:HD13	1:A:390:LEU:HD11	2.01	0.42
1:E:196:CYS:HA	1:E:199:SER:O	2.20	0.42
1:A:350:LYS:HE3	1:A:355:ASN:OD1	2.20	0.42
1:E:61:TYR:CE1	1:E:66:HIS:CD2	3.04	0.42
1:I:298:ARG:HE	1:I:298:ARG:HB3	1.47	0.42
1:A:50:THR:HG21	1:A:223:TYR:CE2	2.55	0.41
2:B:570:VAL:O	2:B:574:LYS:HG3	2.20	0.41
1:E:36:VAL:HG22	2:F:610:TRP:CE3	2.55	0.41
1:I:73:ALA:C	1:I:75:VAL:N	2.73	0.41
1:I:235:GLY:O	1:I:236:THR:OG1	2.29	0.41
1:I:320:THR:CG2	1:I:422:GLN:NE2	2.83	0.41
1:A:178:LYS:HE3	1:A:178:LYS:HB2	1.92	0.41
3:C:39:GLN:HG2	3:C:40:ALA:N	2.35	0.41
3:C:95:THR:HG22	3:C:101:SER:H	1.85	0.41
1:E:368:ASP:H	1:E:371:ILE:HD12	1.85	0.41
4:D:31:ASN:ND2	11:Z:1:NAG:H82	2.36	0.41
1:E:340:LYS:HZ1	1:E:344:ARG:HH21	1.69	0.41
1:I:378:CYS:HB2	1:I:383:PHE:CE1	2.55	0.41
4:L:47:LEU:O	4:L:48:ILE:HD13	2.21	0.41
1:A:387:THR:HG23	1:A:387:THR:O	2.21	0.41
1:A:392:ASN:C	1:A:393:SER:OG	2.58	0.41
3:C:7:SER:OG	3:C:8:GLY:N	2.52	0.41
3:C:39:GLN:HG2	3:C:40:ALA:H	1.86	0.41
1:E:385:CYS:HA	1:E:418:CYS:HA	2.02	0.41
1:I:277:LEU:HD23	1:I:277:LEU:HA	1.92	0.41
5:M:51:ILE:HD13	5:M:71:ARG:HB3	2.02	0.41
5:O:53:ASP:OD1	5:O:53:ASP:N	2.54	0.41
1:A:340:LYS:HE2	1:A:344:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:480:ARG:O	1:E:484:TYR:HB3	2.20	0.41
1:I:129:LEU:HD11	1:I:193:LEU:CD1	2.51	0.41
5:O:71:ARG:HB3	5:O:79:SER:H	1.86	0.41
6:P:13:VAL:HG12	6:P:19:ALA:HB2	2.02	0.41
6:P:50:ASN:HB2	6:P:53:ASP:HB2	2.03	0.41
1:A:207:LYS:HE2	1:A:207:LYS:HB2	1.93	0.41
4:D:4:MET:HE3	4:D:4:MET:HB2	1.70	0.41
3:G:100(K):ALA:HB1	4:H:46:LEU:HD11	2.01	0.41
1:I:333:ILE:HD13	1:I:390:LEU:CD2	2.46	0.41
5:Q:34:TRP:CE3	5:Q:78:LEU:HD11	2.56	0.41
5:Q:38:ARG:HH21	5:Q:87:THR:HA	1.86	0.41
2:B:523:LEU:HD13	2:B:523:LEU:HA	1.69	0.41
1:E:112:TRP:HZ3	1:E:434:MET:SD	2.44	0.41
1:I:178:LYS:HE3	1:I:178:LYS:HB2	1.89	0.41
1:I:192:ARG:HH11	1:I:196:CYS:HB2	1.85	0.41
6:N:11:LEU:HD22	6:N:21:ILE:HD13	2.01	0.41
5:O:52:SER:HB2	5:O:56:SER:HB2	2.02	0.41
5:O:92:CYS:H	5:O:104:GLY:HA3	1.86	0.41
1:A:203:GLN:HG3	1:A:435:TYR:HD2	1.86	0.41
1:A:416:ILE:HA	1:A:417:PRO:HD3	1.96	0.41
2:B:565:LEU:HD21	2:B:579:ARG:HD2	2.03	0.41
1:E:163:THR:HG22	1:E:164:GLU:N	2.36	0.41
2:F:533:ALA:HA	2:F:536:THR:HG22	2.02	0.41
1:I:219:THR:HA	1:I:220:PRO:HD3	1.91	0.41
1:I:383:PHE:HA	1:I:420:ILE:HA	2.03	0.41
6:N:62:PHE:HB3	6:N:73:LEU:HD21	2.02	0.41
5:O:39:GLN:O	5:O:89:VAL:HG12	2.20	0.41
1:A:289:ASN:OD1	1:A:289:ASN:N	2.54	0.41
5:Q:32:TYR:HB2	5:Q:34:TRP:NE1	2.36	0.41
5:Q:69:ILE:HD12	5:Q:80:LEU:HD12	2.03	0.41
1:E:456:ARG:NH1	1:E:466:GLU:OE2	2.53	0.40
1:I:301:ASN:C	1:I:302:ASN:HD22	2.16	0.40
5:M:39:GLN:HA	5:M:45:LEU:HA	2.03	0.40
6:P:12:SER:OG	6:P:105:THR:OG1	2.24	0.40
5:Q:60:ASN:HB2	5:Q:63:LEU:HD23	2.03	0.40
2:B:522:PHE:CD2	2:B:524:GLY:O	2.74	0.40
2:B:542:ARG:CG	2:J:651:THR:HG21	2.52	0.40
2:F:661:LEU:HD11	1:I:504:ARG:HH22	1.86	0.40
3:K:37:VAL:HG11	3:K:103:TRP:CZ3	2.57	0.40
3:K:94:THR:OG1	3:K:102:SER:HB2	2.21	0.40
1:A:181:ILE:HG23	1:A:191:TYR:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HD13	1:A:390:LEU:CD1	2.51	0.40
3:C:36:TRP:CZ3	3:C:92:CYS:HB2	2.57	0.40
1:E:203:GLN:HG3	1:E:435:TYR:HD2	1.86	0.40
4:L:24:ARG:NH2	4:L:70:ASP:OD1	2.54	0.40
5:O:63:LEU:O	5:O:66:ARG:HG3	2.20	0.40
4:D:90:GLN:HG3	4:D:90:GLN:O	2.20	0.40
1:I:181:ILE:HG22	1:I:191:TYR:HB3	2.04	0.40
5:O:15:SER:HA	5:O:82(B):SER:HA	2.03	0.40
6:P:8:VAL:HG12	6:P:103:ARG:HE	1.87	0.40
2:B:658:LYS:HB3	2:B:658:LYS:HE2	1.81	0.40
1:I:35:TRP:CD1	1:I:502:LYS:HB2	2.56	0.40
5:M:100(A):ILE:O	9:U:3:NAG:H5	2.21	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	430/486 (88%)	415 (96%)	15 (4%)	0	100	100
1	E	428/486 (88%)	404 (94%)	24 (6%)	0	100	100
1	I	427/486 (88%)	403 (94%)	20 (5%)	4 (1%)	14	43
2	B	121/155 (78%)	117 (97%)	4 (3%)	0	100	100
2	F	115/155 (74%)	112 (97%)	3 (3%)	0	100	100
2	J	124/155 (80%)	121 (98%)	3 (2%)	0	100	100
3	C	128/238 (54%)	120 (94%)	8 (6%)	0	100	100
3	G	128/238 (54%)	126 (98%)	2 (2%)	0	100	100
3	K	128/238 (54%)	124 (97%)	4 (3%)	0	100	100
4	D	105/215 (49%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	106/215 (49%)	105 (99%)	1 (1%)	0	100	100
4	L	106/215 (49%)	105 (99%)	1 (1%)	0	100	100
5	M	129/238 (54%)	126 (98%)	3 (2%)	0	100	100
5	O	129/238 (54%)	127 (98%)	2 (2%)	0	100	100
5	Q	129/238 (54%)	124 (96%)	5 (4%)	0	100	100
6	N	105/214 (49%)	97 (92%)	8 (8%)	0	100	100
6	P	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
6	R	105/214 (49%)	96 (91%)	9 (9%)	0	100	100
All	All	3048/4638 (66%)	2925 (96%)	119 (4%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	234	ASN
1	I	155	ARG
1	I	236	THR
1	I	76	PRO

### 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	392/434 (90%)	380 (97%)	12 (3%)	35	60
1	E	390/434 (90%)	382 (98%)	8 (2%)	48	70
1	I	389/434 (90%)	376 (97%)	13 (3%)	33	59
2	B	108/130 (83%)	107 (99%)	1 (1%)	75	86
2	F	103/130 (79%)	102 (99%)	1 (1%)	73	85
2	J	112/130 (86%)	112 (100%)	0	100	100
3	C	111/204 (54%)	108 (97%)	3 (3%)	40	64
3	G	111/204 (54%)	106 (96%)	5 (4%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	111/204 (54%)	111 (100%)	0	100	100
4	D	85/182 (47%)	84 (99%)	1 (1%)	67	81
4	H	86/182 (47%)	86 (100%)	0	100	100
4	L	86/182 (47%)	86 (100%)	0	100	100
5	M	115/208 (55%)	115 (100%)	0	100	100
5	O	115/208 (55%)	115 (100%)	0	100	100
5	Q	115/208 (55%)	114 (99%)	1 (1%)	75	86
6	N	85/178 (48%)	85 (100%)	0	100	100
6	P	85/178 (48%)	85 (100%)	0	100	100
6	R	85/178 (48%)	85 (100%)	0	100	100
All	All	2684/4008 (67%)	2639 (98%)	45 (2%)	56	75

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	CYS
1	A	125	LEU
1	A	126	CYS
1	A	155	ARG
1	A	179	LEU
1	A	198	THR
1	A	261	LEU
1	A	277	LEU
1	A	302	ASN
1	A	333	ILE
1	A	387	THR
1	A	393	SER
2	B	523	LEU
3	C	38	ARG
3	C	67	VAL
3	C	68	LEU
4	D	89	GLN
1	E	61	TYR
1	E	68	VAL
1	E	76	PRO
1	E	261	LEU
1	E	275	GLU
1	E	277	LEU

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Mol	Chain	Res	Type
1	E	333	ILE
1	E	502	LYS
2	F	617	LYS
3	G	22	CYS
3	G	67	VAL
3	G	69	ILE
3	G	100(I)	VAL
3	G	100(L)	PHE
1	I	61	TYR
1	I	126	CYS
1	I	129	LEU
1	I	161	MET
1	I	196	CYS
1	I	198	THR
1	I	261	LEU
1	I	277	LEU
1	I	302	ASN
1	I	333	ILE
1	I	360	VAL
1	I	395	TRP
1	I	501	CYS
5	Q	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	169	GLN
1	A	195	ASN
1	A	203	GLN
1	A	229	ASN
1	A	339	HIS
1	A	425	ASN
3	C	61	HIS
4	D	38	GLN
1	E	66	HIS
1	E	67	ASN
1	E	72	HIS
1	E	99	ASN
1	E	203	GLN
3	G	61	HIS
1	I	33	ASN

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Mol	Chain	Res	Type
1	I	99	ASN
1	I	195	ASN
1	I	302	ASN
1	I	422	GLN
4	L	6	GLN
4	L	31	ASN
5	O	31	ASN
6	P	89	HIS
6	R	52	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

101 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	$\# Z  > 2$
7	NAG	S	1	1,7	14,14,15	0.16	0	17,19,21	0.41	0
7	NAG	S	2	7	14,14,15	0.34	0	17,19,21	0.50	0
7	BMA	S	3	7	11,11,12	0.57	0	15,15,17	0.97	0
7	MAN	S	4	7	11,11,12	0.57	0	15,15,17	0.93	2 (13%)
7	MAN	S	5	7	11,11,12	0.52	0	15,15,17	1.17	2 (13%)
7	MAN	S	6	7	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
7	MAN	S	7	7	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
7	MAN	S	8	7	11,11,12	0.59	0	15,15,17	1.04	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	S	9	7	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
8	NAG	T	1	1,8	14,14,15	0.33	0	17,19,21	0.41	0
8	NAG	T	2	8	14,14,15	0.25	0	17,19,21	0.45	0
8	BMA	T	3	8	11,11,12	0.55	0	15,15,17	0.80	0
8	MAN	T	4	8	11,11,12	0.75	0	15,15,17	1.00	2 (13%)
8	MAN	T	5	8	11,11,12	0.79	0	15,15,17	1.23	2 (13%)
8	MAN	T	6	8	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
9	NAG	U	1	9,1	14,14,15	0.35	0	17,19,21	0.41	0
9	NAG	U	2	9	14,14,15	0.40	0	17,19,21	1.38	2 (11%)
9	NAG	U	3	9	14,14,15	0.20	0	17,19,21	0.55	0
9	NAG	U	4	9	14,14,15	0.25	0	17,19,21	0.48	0
10	NAG	V	1	1,10	14,14,15	0.25	0	17,19,21	0.72	0
10	NAG	V	2	10	14,14,15	0.22	0	17,19,21	0.49	0
10	NAG	W	1	1,10	14,14,15	0.42	0	17,19,21	0.41	0
10	NAG	W	2	10	14,14,15	0.38	0	17,19,21	0.38	0
10	NAG	X	1	1,10	14,14,15	0.23	0	17,19,21	0.58	0
10	NAG	X	2	10	14,14,15	0.26	0	17,19,21	0.42	0
11	NAG	Y	1	1,11	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	Y	2	11	14,14,15	0.19	0	17,19,21	0.48	0
11	BMA	Y	3	11	11,11,12	0.53	0	15,15,17	0.67	0
11	NAG	Z	1	2,11	14,14,15	0.26	0	17,19,21	0.49	0
11	NAG	Z	2	11	14,14,15	0.26	0	17,19,21	0.43	0
11	BMA	Z	3	11	11,11,12	0.51	0	15,15,17	0.75	0
12	NAG	a	1	1,12	14,14,15	0.42	0	17,19,21	0.48	0
12	MAN	a	10	12	11,11,12	0.67	0	15,15,17	0.85	1 (6%)
12	NAG	a	2	12	14,14,15	0.20	0	17,19,21	0.48	0
12	BMA	a	3	12	11,11,12	0.56	0	15,15,17	0.97	0
12	MAN	a	4	12	11,11,12	0.58	0	15,15,17	0.96	1 (6%)
12	MAN	a	5	12	11,11,12	0.49	0	15,15,17	1.05	2 (13%)
12	MAN	a	6	12	11,11,12	0.54	0	15,15,17	1.04	2 (13%)
12	MAN	a	7	12	11,11,12	0.60	0	15,15,17	1.05	2 (13%)
12	MAN	a	8	12	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
12	MAN	a	9	12	11,11,12	0.57	0	15,15,17	0.98	2 (13%)
8	NAG	b	1	1,8	14,14,15	0.28	0	17,19,21	0.42	0
8	NAG	b	2	8	14,14,15	0.23	0	17,19,21	0.46	0
8	BMA	b	3	8	11,11,12	0.52	0	15,15,17	0.84	0
8	MAN	b	4	8	11,11,12	0.79	0	15,15,17	0.98	2 (13%)
8	MAN	b	5	8	11,11,12	0.82	0	15,15,17	1.25	2 (13%)
8	MAN	b	6	8	11,11,12	0.65	0	15,15,17	0.88	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	c	1	1,10	14,14,15	0.16	0	17,19,21	0.55	0
10	NAG	c	2	10	14,14,15	0.24	0	17,19,21	0.45	0
9	NAG	d	1	9,1	14,14,15	0.36	0	17,19,21	0.40	0
9	NAG	d	2	9	14,14,15	0.22	0	17,19,21	0.62	0
9	NAG	d	3	9	14,14,15	0.18	0	17,19,21	0.55	0
9	NAG	d	4	9	14,14,15	0.29	0	17,19,21	0.58	0
10	NAG	e	1	1,10	14,14,15	0.25	0	17,19,21	0.59	0
10	NAG	e	2	10	14,14,15	0.22	0	17,19,21	0.48	0
10	NAG	f	1	1,10	14,14,15	0.52	0	17,19,21	0.50	0
10	NAG	f	2	10	14,14,15	0.28	0	17,19,21	0.57	0
10	NAG	g	1	1,10	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	g	2	10	14,14,15	0.25	0	17,19,21	0.42	0
11	NAG	h	1	1,11	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	h	2	11	14,14,15	0.19	0	17,19,21	0.48	0
11	BMA	h	3	11	11,11,12	0.52	0	15,15,17	0.67	0
11	NAG	i	1	2,11	14,14,15	0.26	0	17,19,21	0.51	0
11	NAG	i	2	11	14,14,15	0.29	0	17,19,21	0.44	0
11	BMA	i	3	11	11,11,12	0.48	0	15,15,17	0.74	0
7	NAG	j	1	1,7	14,14,15	0.19	0	17,19,21	0.56	0
7	NAG	j	2	7	14,14,15	0.41	0	17,19,21	0.51	0
7	BMA	j	3	7	11,11,12	0.50	0	15,15,17	0.85	0
7	MAN	j	4	7	11,11,12	0.50	0	15,15,17	0.92	2 (13%)
7	MAN	j	5	7	11,11,12	0.58	0	15,15,17	1.13	2 (13%)
7	MAN	j	6	7	11,11,12	0.57	0	15,15,17	0.92	2 (13%)
7	MAN	j	7	7	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
7	MAN	j	8	7	11,11,12	0.61	0	15,15,17	1.07	2 (13%)
7	MAN	j	9	7	11,11,12	0.65	0	15,15,17	0.92	1 (6%)
8	NAG	k	1	1,8	14,14,15	0.27	0	17,19,21	0.44	0
8	NAG	k	2	8	14,14,15	0.25	0	17,19,21	0.46	0
8	BMA	k	3	8	11,11,12	0.56	0	15,15,17	0.83	0
8	MAN	k	4	8	11,11,12	0.71	0	15,15,17	0.95	2 (13%)
8	MAN	k	5	8	11,11,12	0.85	1 (9%)	15,15,17	1.30	2 (13%)
8	MAN	k	6	8	11,11,12	0.66	0	15,15,17	0.92	2 (13%)
10	NAG	l	1	1,10	14,14,15	0.80	1 (7%)	17,19,21	0.81	0
10	NAG	l	2	10	14,14,15	0.20	0	17,19,21	0.50	0
10	NAG	m	1	1,10	14,14,15	0.41	0	17,19,21	0.52	0
10	NAG	m	2	10	14,14,15	0.19	0	17,19,21	0.53	0
9	NAG	n	1	9,1	14,14,15	0.30	0	17,19,21	0.68	0
9	NAG	n	2	9	14,14,15	0.36	0	17,19,21	0.45	0
9	NAG	n	3	9	14,14,15	0.18	0	17,19,21	0.58	0
9	NAG	n	4	9	14,14,15	0.30	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	o	1	1,10	14,14,15	0.19	0	17,19,21	0.65	0
10	NAG	o	2	10	14,14,15	0.28	0	17,19,21	0.46	0
10	NAG	p	1	1,10	14,14,15	0.36	0	17,19,21	0.55	0
10	NAG	p	2	10	14,14,15	0.28	0	17,19,21	0.44	0
10	NAG	q	1	1,10	14,14,15	0.23	0	17,19,21	0.42	0
10	NAG	q	2	10	14,14,15	0.20	0	17,19,21	0.46	0
11	NAG	r	1	1,11	14,14,15	0.28	0	17,19,21	0.51	0
11	NAG	r	2	11	14,14,15	0.19	0	17,19,21	0.47	0
11	BMA	r	3	11	11,11,12	0.56	0	15,15,17	0.66	0
13	NAG	s	1	2,13	14,14,15	0.23	0	17,19,21	0.50	0
13	NAG	s	2	13	14,14,15	0.29	0	17,19,21	0.42	0
13	BMA	s	3	13	11,11,12	0.50	0	15,15,17	0.78	0
13	MAN	s	4	13	11,11,12	0.68	0	15,15,17	0.90	1 (6%)

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
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	0/2/19/22	0/1/1/1
7	MAN	S	7	7	-	0/2/19/22	0/1/1/1
7	MAN	S	8	7	-	2/2/19/22	0/1/1/1
7	MAN	S	9	7	-	0/2/19/22	0/1/1/1
8	NAG	T	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	MAN	T	5	8	-	0/2/19/22	0/1/1/1
8	MAN	T	6	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	6/6/23/26	0/1/1/1
9	NAG	U	3	9	-	3/6/23/26	0/1/1/1
9	NAG	U	4	9	-	2/6/23/26	0/1/1/1
10	NAG	V	1	1,10	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	NAG	W	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	4/6/23/26	0/1/1/1
10	NAG	X	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
11	NAG	Y	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	1/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	0/2/19/22	0/1/1/1
11	NAG	Z	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	Z	2	11	-	1/6/23/26	0/1/1/1
11	BMA	Z	3	11	-	1/2/19/22	0/1/1/1
12	NAG	a	1	1,12	-	1/6/23/26	0/1/1/1
12	MAN	a	10	12	-	0/2/19/22	0/1/1/1
12	NAG	a	2	12	-	0/6/23/26	0/1/1/1
12	BMA	a	3	12	-	2/2/19/22	0/1/1/1
12	MAN	a	4	12	-	0/2/19/22	0/1/1/1
12	MAN	a	5	12	-	2/2/19/22	0/1/1/1
12	MAN	a	6	12	-	2/2/19/22	0/1/1/1
12	MAN	a	7	12	-	0/2/19/22	0/1/1/1
12	MAN	a	8	12	-	2/2/19/22	0/1/1/1
12	MAN	a	9	12	-	0/2/19/22	0/1/1/1
8	NAG	b	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1
8	MAN	b	4	8	-	0/2/19/22	0/1/1/1
8	MAN	b	5	8	-	0/2/19/22	0/1/1/1
8	MAN	b	6	8	-	0/2/19/22	0/1/1/1
10	NAG	c	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	c	2	10	-	2/6/23/26	0/1/1/1
9	NAG	d	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	4/6/23/26	0/1/1/1
9	NAG	d	3	9	-	2/6/23/26	0/1/1/1
9	NAG	d	4	9	-	4/6/23/26	0/1/1/1
10	NAG	e	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	e	2	10	-	2/6/23/26	0/1/1/1
10	NAG	f	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	4/6/23/26	0/1/1/1
10	NAG	g	1	1,10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
11	NAG	h	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	h	2	11	-	1/6/23/26	0/1/1/1
11	BMA	h	3	11	-	0/2/19/22	0/1/1/1
11	NAG	i	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	i	2	11	-	1/6/23/26	0/1/1/1
11	BMA	i	3	11	-	1/2/19/22	0/1/1/1
7	NAG	j	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	BMA	j	3	7	-	2/2/19/22	0/1/1/1
7	MAN	j	4	7	-	0/2/19/22	0/1/1/1
7	MAN	j	5	7	-	2/2/19/22	0/1/1/1
7	MAN	j	6	7	-	0/2/19/22	0/1/1/1
7	MAN	j	7	7	-	0/2/19/22	0/1/1/1
7	MAN	j	8	7	-	2/2/19/22	0/1/1/1
7	MAN	j	9	7	-	0/2/19/22	0/1/1/1
8	NAG	k	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
8	BMA	k	3	8	-	0/2/19/22	0/1/1/1
8	MAN	k	4	8	-	0/2/19/22	0/1/1/1
8	MAN	k	5	8	-	0/2/19/22	0/1/1/1
8	MAN	k	6	8	-	0/2/19/22	0/1/1/1
10	NAG	l	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	l	2	10	-	2/6/23/26	0/1/1/1
10	NAG	m	1	1,10	-	3/6/23/26	0/1/1/1
10	NAG	m	2	10	-	2/6/23/26	0/1/1/1
9	NAG	n	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
9	NAG	n	3	9	-	2/6/23/26	0/1/1/1
9	NAG	n	4	9	-	4/6/23/26	0/1/1/1
10	NAG	o	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	o	2	10	-	2/6/23/26	0/1/1/1
10	NAG	p	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	p	2	10	-	0/6/23/26	0/1/1/1
10	NAG	q	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	2/6/23/26	0/1/1/1
11	NAG	r	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	r	2	11	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	r	3	11	-	0/2/19/22	0/1/1/1
13	NAG	s	1	2,13	-	0/6/23/26	0/1/1/1
13	NAG	s	2	13	-	2/6/23/26	0/1/1/1
13	BMA	s	3	13	-	2/2/19/22	0/1/1/1
13	MAN	s	4	13	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	l	1	NAG	O5-C1	-2.58	1.39	1.43
8	k	5	MAN	C1-C2	2.12	1.57	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	2	NAG	C2-N2-C7	4.65	129.13	122.90
8	k	5	MAN	C1-O5-C5	3.60	117.01	112.19
8	b	5	MAN	C1-O5-C5	3.52	116.91	112.19
8	T	5	MAN	C1-O5-C5	3.47	116.83	112.19
7	S	5	MAN	C1-O5-C5	3.02	116.23	112.19
12	a	5	MAN	C1-O5-C5	2.92	116.10	112.19
12	a	6	MAN	C1-O5-C5	2.80	115.94	112.19
7	j	8	MAN	C1-O5-C5	2.79	115.93	112.19
12	a	8	MAN	C1-O5-C5	2.78	115.91	112.19
7	S	8	MAN	C1-O5-C5	2.71	115.82	112.19
7	S	5	MAN	O2-C2-C3	-2.70	104.56	110.15
7	j	5	MAN	C1-O5-C5	2.67	115.77	112.19
12	a	7	MAN	C1-O5-C5	2.54	115.59	112.19
7	S	7	MAN	C1-O5-C5	2.47	115.50	112.19
12	a	9	MAN	C1-O5-C5	2.47	115.50	112.19
7	j	7	MAN	C1-O5-C5	2.43	115.44	112.19
7	j	8	MAN	O2-C2-C3	-2.43	105.12	110.15
12	a	4	MAN	C1-O5-C5	2.40	115.40	112.19
7	j	5	MAN	O2-C2-C3	-2.39	105.20	110.15
7	j	4	MAN	C1-O5-C5	2.36	115.35	112.19
8	T	6	MAN	C1-O5-C5	2.34	115.32	112.19
7	S	8	MAN	O2-C2-C3	-2.31	105.37	110.15
9	U	2	NAG	C1-C2-N2	2.30	114.06	110.43
12	a	5	MAN	O2-C2-C3	-2.28	105.44	110.15
7	S	4	MAN	C1-O5-C5	2.27	115.23	112.19
8	k	5	MAN	O2-C2-C3	-2.25	105.49	110.15
7	S	6	MAN	C1-O5-C5	2.24	115.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	7	MAN	O2-C2-C3	-2.23	105.52	110.15
8	T	6	MAN	O2-C2-C3	-2.22	105.54	110.15
8	k	6	MAN	O2-C2-C3	-2.22	105.55	110.15
8	b	5	MAN	O2-C2-C3	-2.21	105.57	110.15
7	S	6	MAN	O2-C2-C3	-2.20	105.59	110.15
8	b	6	MAN	O2-C2-C3	-2.20	105.59	110.15
7	j	6	MAN	O2-C2-C3	-2.19	105.62	110.15
12	a	9	MAN	O2-C2-C3	-2.19	105.62	110.15
7	S	7	MAN	O2-C2-C3	-2.18	105.63	110.15
7	j	7	MAN	O2-C2-C3	-2.18	105.63	110.15
8	T	4	MAN	C1-O5-C5	2.18	115.11	112.19
12	a	6	MAN	O2-C2-C3	-2.18	105.64	110.15
8	k	4	MAN	O2-C2-C3	-2.16	105.67	110.15
8	T	5	MAN	O2-C2-C3	-2.15	105.70	110.15
7	S	9	MAN	C1-O5-C5	2.14	115.06	112.19
7	j	6	MAN	C1-O5-C5	2.14	115.06	112.19
7	S	9	MAN	O2-C2-C3	-2.13	105.73	110.15
13	s	4	MAN	C1-O5-C5	2.13	115.04	112.19
12	a	10	MAN	O2-C2-C3	-2.13	105.75	110.15
8	k	6	MAN	C1-O5-C5	2.08	114.97	112.19
7	S	4	MAN	O2-C2-C3	-2.07	105.86	110.15
8	k	4	MAN	C1-O5-C5	2.07	114.97	112.19
8	T	4	MAN	O2-C2-C3	-2.07	105.87	110.15
8	b	4	MAN	O2-C2-C3	-2.06	105.89	110.15
7	j	9	MAN	O2-C2-C3	-2.05	105.90	110.15
7	j	4	MAN	O2-C2-C3	-2.04	105.92	110.15
8	b	4	MAN	C1-O5-C5	2.03	114.90	112.19
12	a	8	MAN	O2-C2-C3	-2.02	105.96	110.15

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	n	1	NAG	C3-C2-N2-C7
9	d	3	NAG	O5-C5-C6-O6
10	V	2	NAG	C4-C5-C6-O6
9	U	4	NAG	O5-C5-C6-O6
10	o	2	NAG	C4-C5-C6-O6
10	l	2	NAG	O5-C5-C6-O6
9	d	4	NAG	O5-C5-C6-O6
9	n	3	NAG	O5-C5-C6-O6
10	f	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	q	1	NAG	O5-C5-C6-O6
7	S	5	MAN	C4-C5-C6-O6
10	V	1	NAG	O5-C5-C6-O6
9	U	4	NAG	C4-C5-C6-O6
10	f	2	NAG	O5-C5-C6-O6
10	m	2	NAG	O5-C5-C6-O6
10	e	2	NAG	C4-C5-C6-O6
10	X	2	NAG	O5-C5-C6-O6
9	n	3	NAG	C4-C5-C6-O6
10	X	2	NAG	C4-C5-C6-O6
12	a	3	BMA	C4-C5-C6-O6
12	a	5	MAN	C4-C5-C6-O6
9	d	3	NAG	C4-C5-C6-O6
10	l	2	NAG	C4-C5-C6-O6
12	a	5	MAN	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
9	n	4	NAG	O5-C5-C6-O6
10	c	2	NAG	O5-C5-C6-O6
10	e	1	NAG	O5-C5-C6-O6
10	e	2	NAG	O5-C5-C6-O6
7	S	5	MAN	O5-C5-C6-O6
10	V	2	NAG	O5-C5-C6-O6
10	o	2	NAG	O5-C5-C6-O6
7	j	5	MAN	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
10	e	1	NAG	C4-C5-C6-O6
10	m	1	NAG	O5-C5-C6-O6
9	d	4	NAG	C4-C5-C6-O6
10	V	1	NAG	C4-C5-C6-O6
10	f	1	NAG	C4-C5-C6-O6
10	f	2	NAG	C4-C5-C6-O6
10	W	2	NAG	O5-C5-C6-O6
13	s	3	BMA	O5-C5-C6-O6
10	q	1	NAG	C4-C5-C6-O6
7	j	8	MAN	O5-C5-C6-O6
10	c	1	NAG	O5-C5-C6-O6
10	m	2	NAG	C4-C5-C6-O6
7	S	8	MAN	O5-C5-C6-O6
11	Z	1	NAG	O5-C5-C6-O6
10	W	2	NAG	C4-C5-C6-O6
9	U	1	NAG	C8-C7-N2-C2
9	U	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	U	2	NAG	C8-C7-N2-C2
9	U	2	NAG	O7-C7-N2-C2
9	U	3	NAG	C8-C7-N2-C2
9	U	3	NAG	O7-C7-N2-C2
9	n	2	NAG	C8-C7-N2-C2
9	n	2	NAG	O7-C7-N2-C2
9	n	4	NAG	C8-C7-N2-C2
9	n	4	NAG	O7-C7-N2-C2
10	W	1	NAG	C8-C7-N2-C2
10	W	1	NAG	O7-C7-N2-C2
10	W	2	NAG	C8-C7-N2-C2
10	W	2	NAG	O7-C7-N2-C2
11	r	1	NAG	O5-C5-C6-O6
10	c	1	NAG	C4-C5-C6-O6
9	U	2	NAG	O5-C5-C6-O6
7	j	3	BMA	C4-C5-C6-O6
11	Z	1	NAG	C4-C5-C6-O6
7	j	8	MAN	C4-C5-C6-O6
7	S	8	MAN	C4-C5-C6-O6
9	U	2	NAG	C4-C5-C6-O6
9	n	4	NAG	C4-C5-C6-O6
10	c	2	NAG	C4-C5-C6-O6
11	r	1	NAG	C4-C5-C6-O6
10	o	1	NAG	C4-C5-C6-O6
10	q	2	NAG	O5-C5-C6-O6
12	a	3	BMA	O5-C5-C6-O6
10	m	1	NAG	C4-C5-C6-O6
7	j	5	MAN	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
11	Z	3	BMA	O5-C5-C6-O6
10	o	1	NAG	O5-C5-C6-O6
9	U	3	NAG	O5-C5-C6-O6
7	S	3	BMA	C4-C5-C6-O6
11	Z	2	NAG	O5-C5-C6-O6
11	i	3	BMA	O5-C5-C6-O6
9	n	1	NAG	O5-C5-C6-O6
11	h	2	NAG	O5-C5-C6-O6
10	V	1	NAG	C3-C2-N2-C7
7	j	3	BMA	O5-C5-C6-O6
11	i	1	NAG	C4-C5-C6-O6
11	i	1	NAG	O5-C5-C6-O6
9	d	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	d	4	NAG	C1-C2-N2-C7
13	s	2	NAG	C4-C5-C6-O6
12	a	8	MAN	C4-C5-C6-O6
10	q	2	NAG	C4-C5-C6-O6
12	a	8	MAN	O5-C5-C6-O6
12	a	6	MAN	C4-C5-C6-O6
9	d	2	NAG	C3-C2-N2-C7
10	e	1	NAG	C3-C2-N2-C7
10	f	2	NAG	C3-C2-N2-C7
10	o	1	NAG	C3-C2-N2-C7
11	i	2	NAG	C4-C5-C6-O6
12	a	1	NAG	C4-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
10	X	1	NAG	C4-C5-C6-O6
13	s	2	NAG	O5-C5-C6-O6
9	U	2	NAG	C1-C2-N2-C7
10	e	1	NAG	C1-C2-N2-C7
10	f	2	NAG	C1-C2-N2-C7
10	o	1	NAG	C1-C2-N2-C7
10	p	1	NAG	C4-C5-C6-O6
9	U	2	NAG	C3-C2-N2-C7
9	d	4	NAG	C3-C2-N2-C7
10	m	1	NAG	C3-C2-N2-C7
10	X	1	NAG	O5-C5-C6-O6
10	p	1	NAG	O5-C5-C6-O6
12	a	6	MAN	O5-C5-C6-O6
13	s	3	BMA	C4-C5-C6-O6

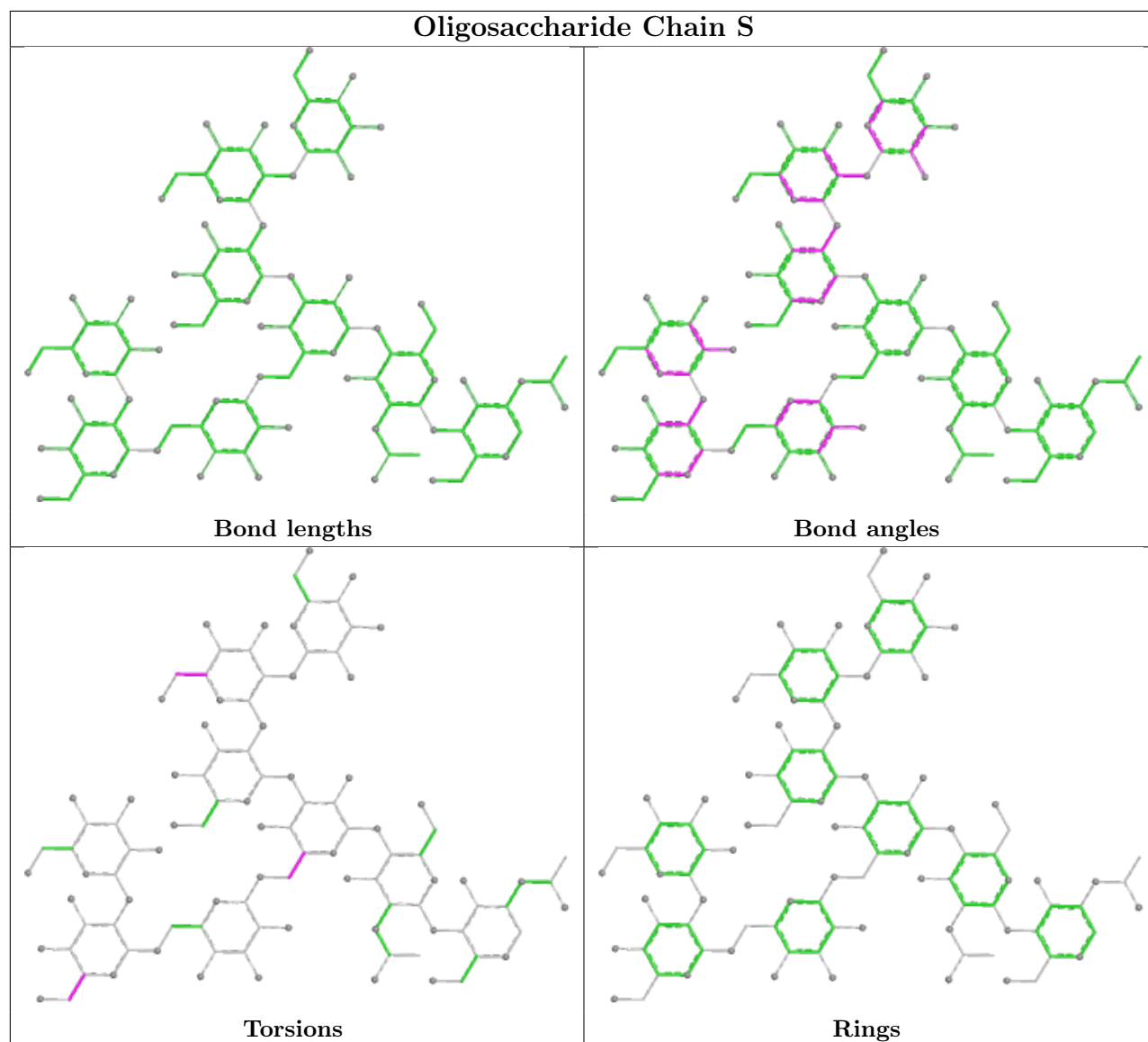
There are no ring outliers.

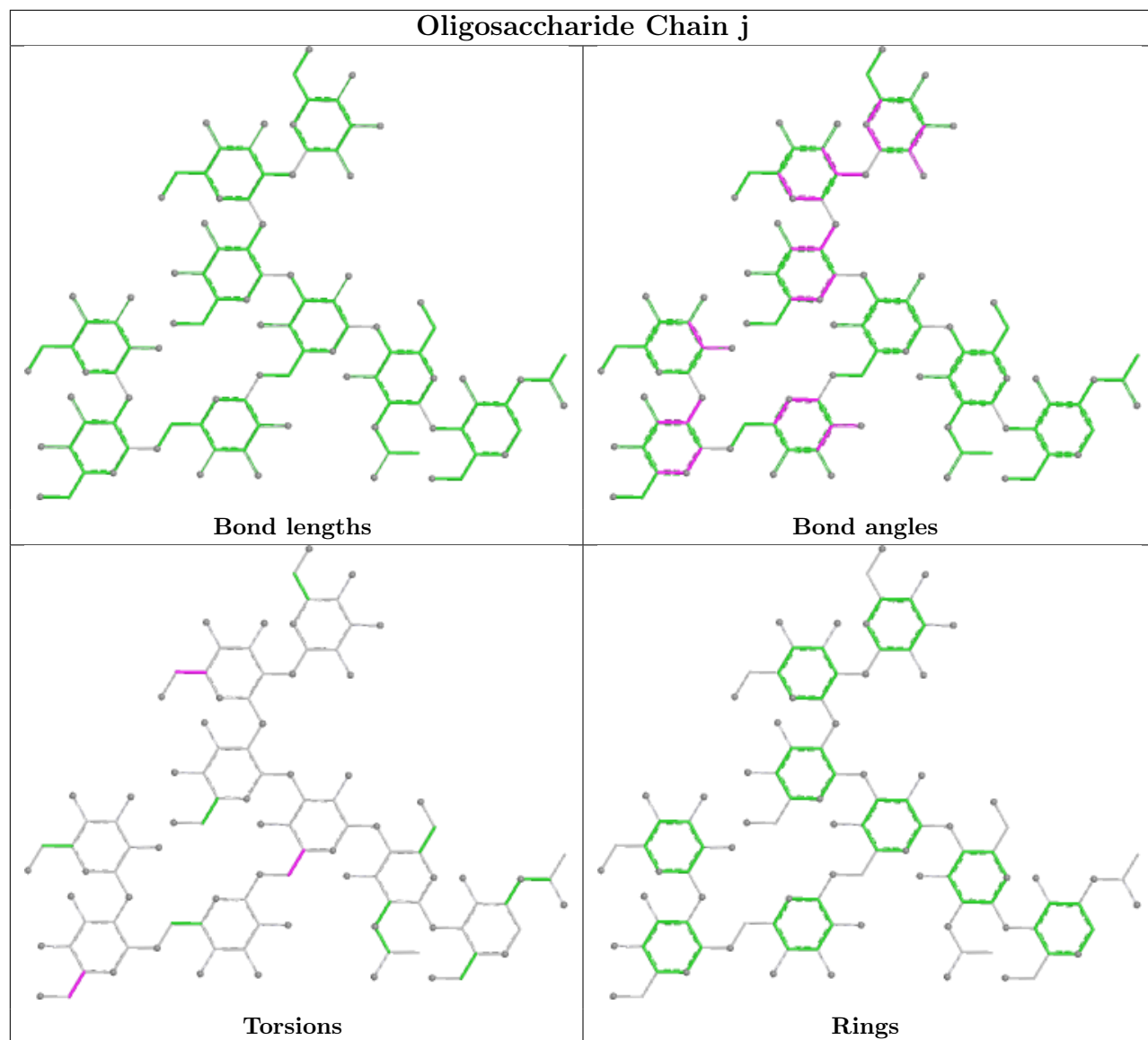
8 monomers are involved in 11 short contacts:

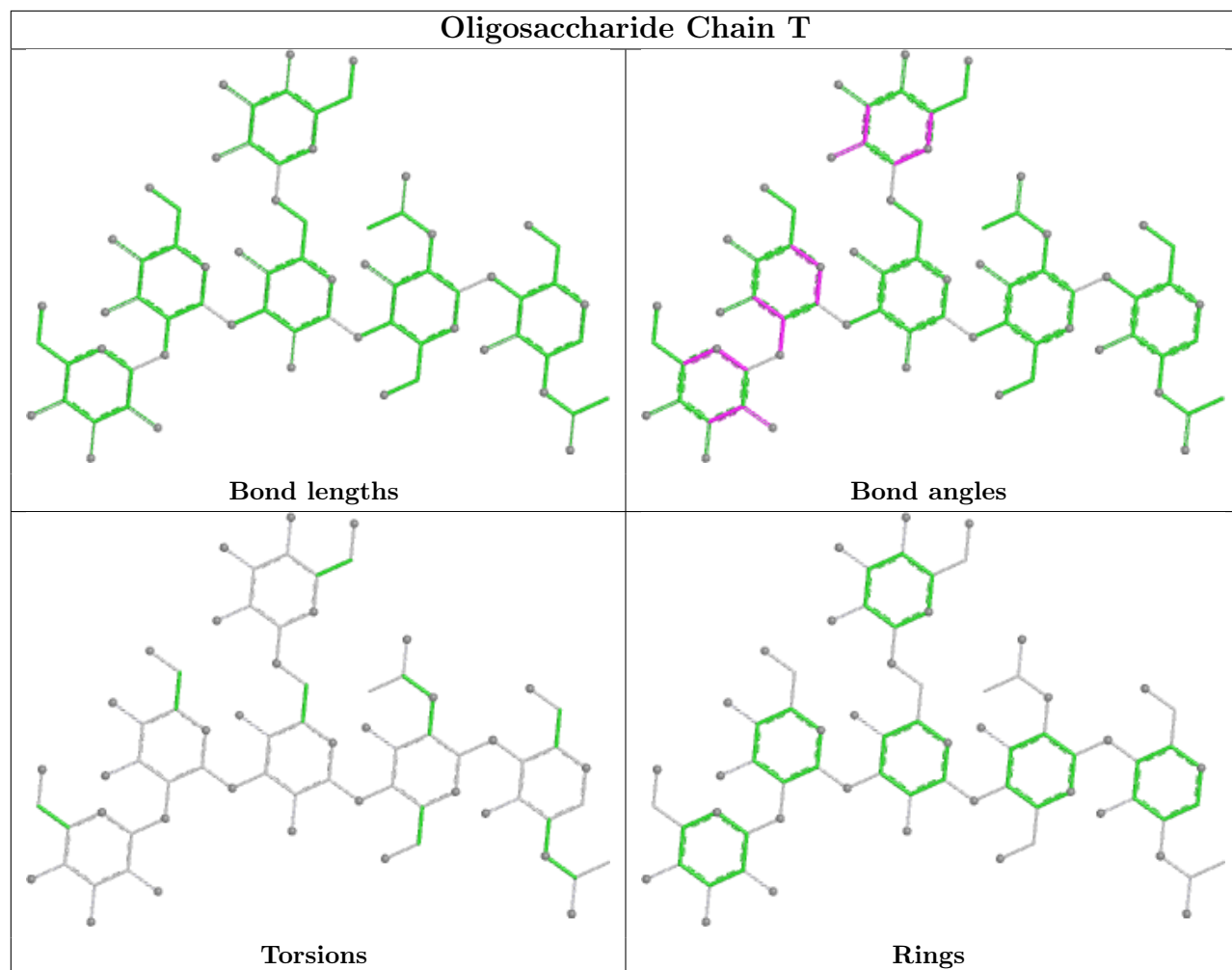
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	2	NAG	2	0
9	U	2	NAG	1	0
9	U	3	NAG	1	0
7	S	9	MAN	3	0
11	Z	1	NAG	1	0
9	U	1	NAG	1	0
9	U	4	NAG	1	0
7	S	5	MAN	1	0

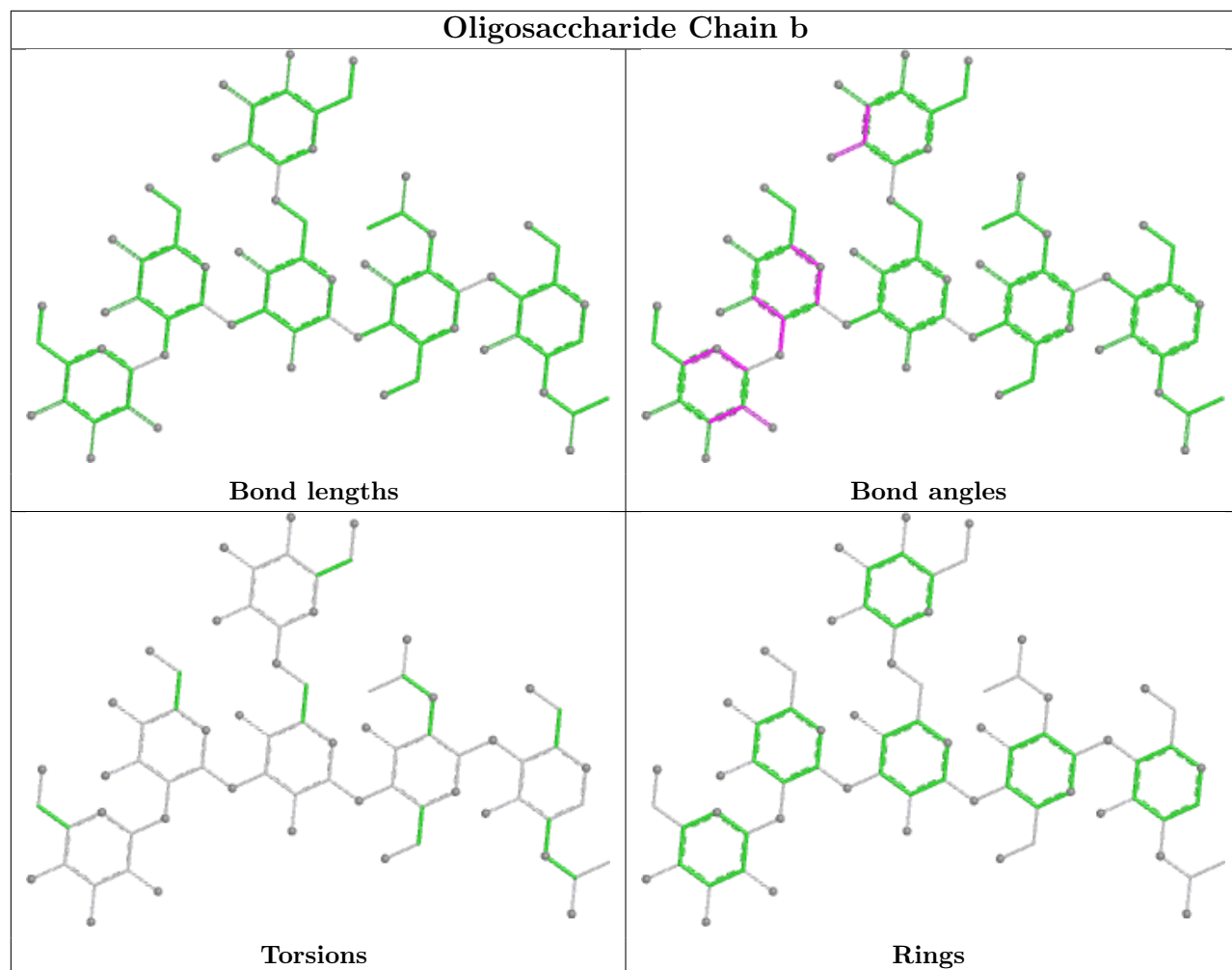
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

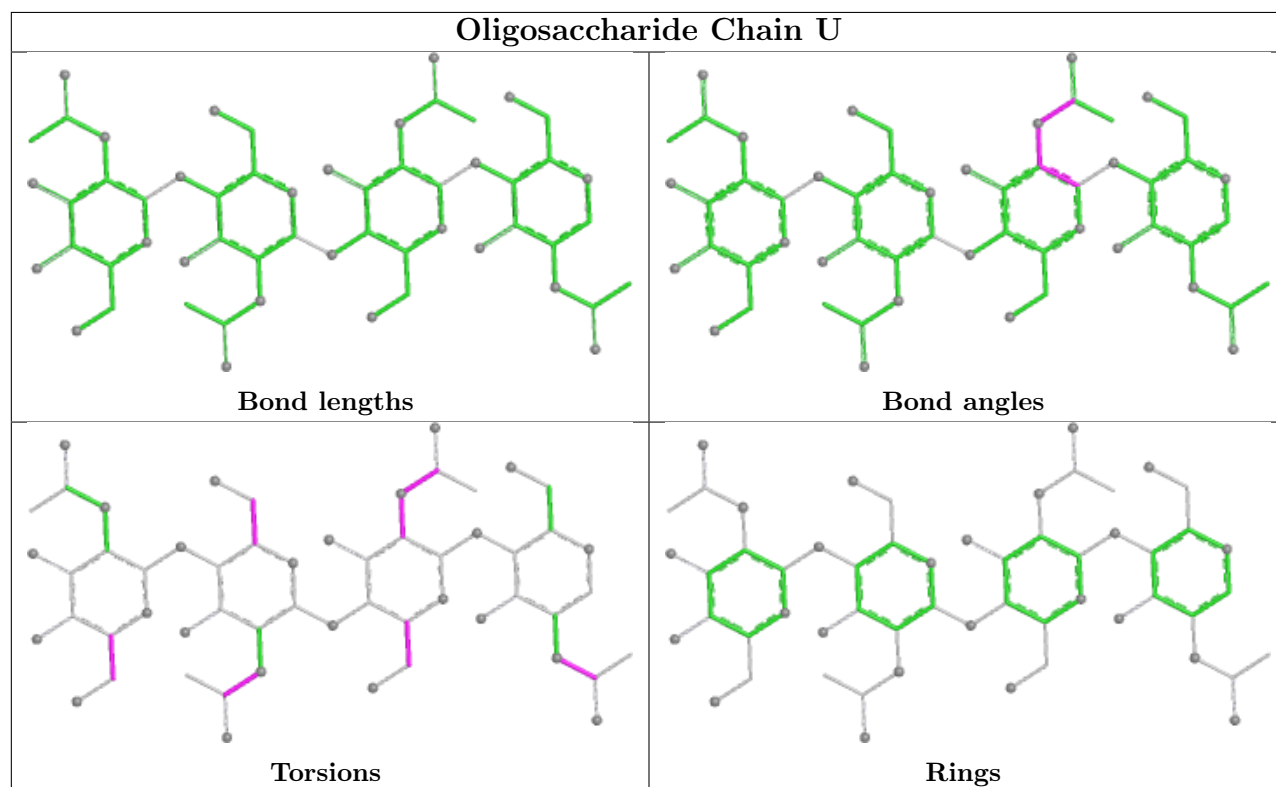
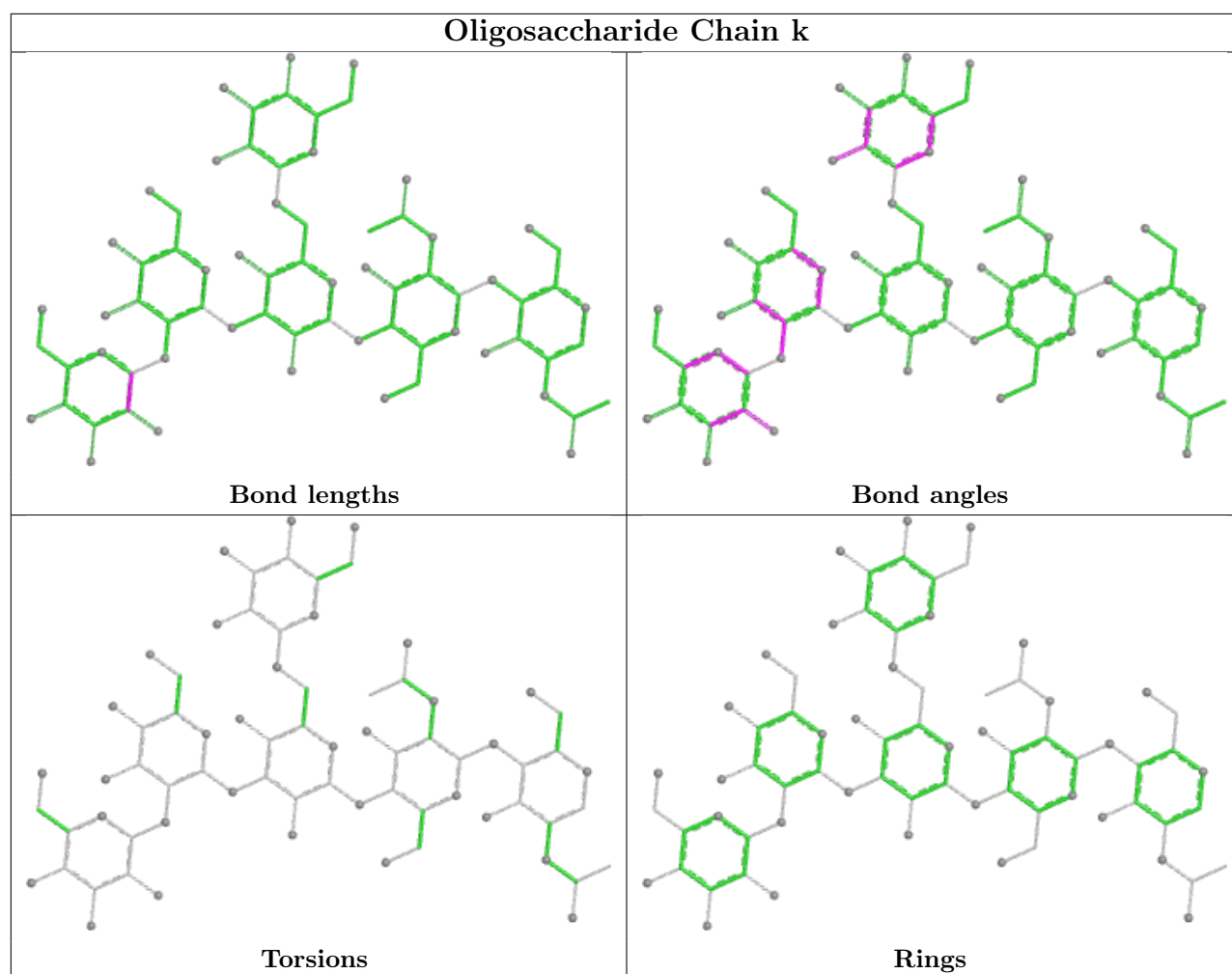
bond angles, torsion angles, and ring geometry for oligosaccharide.

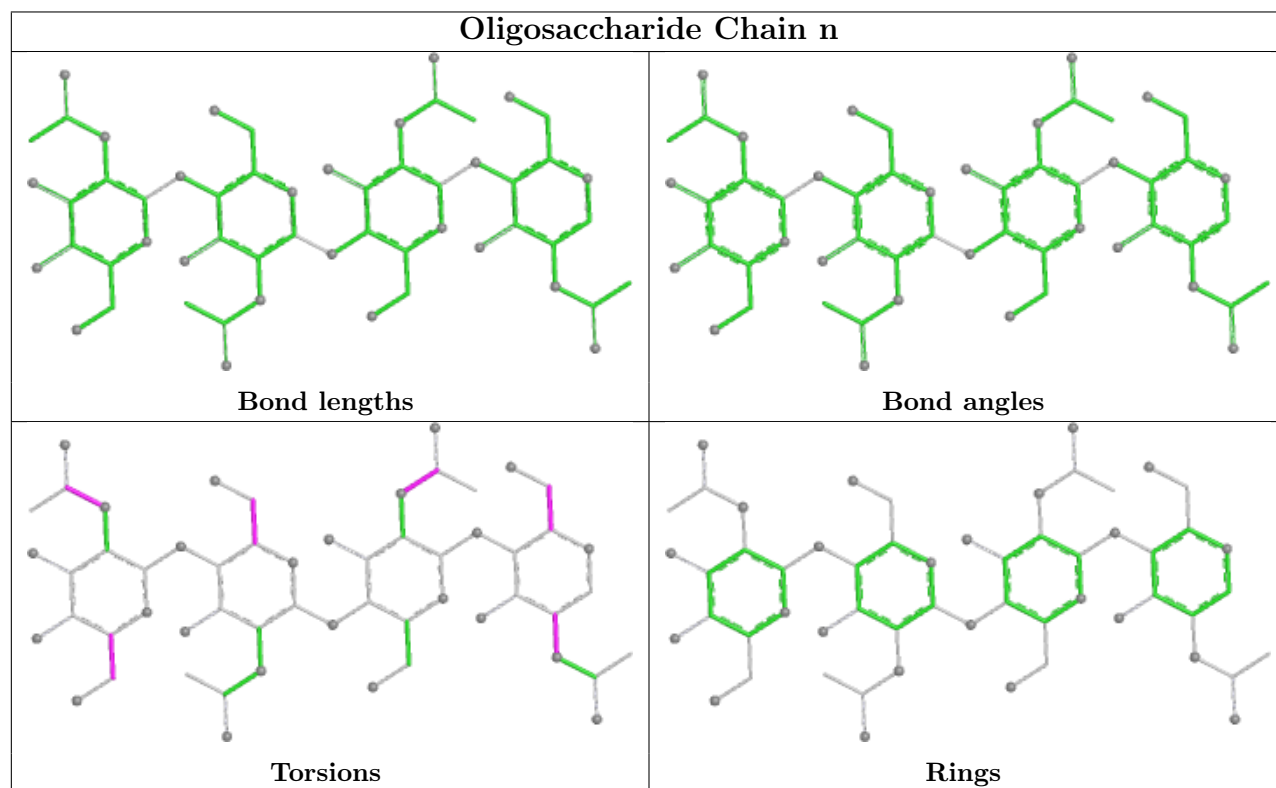
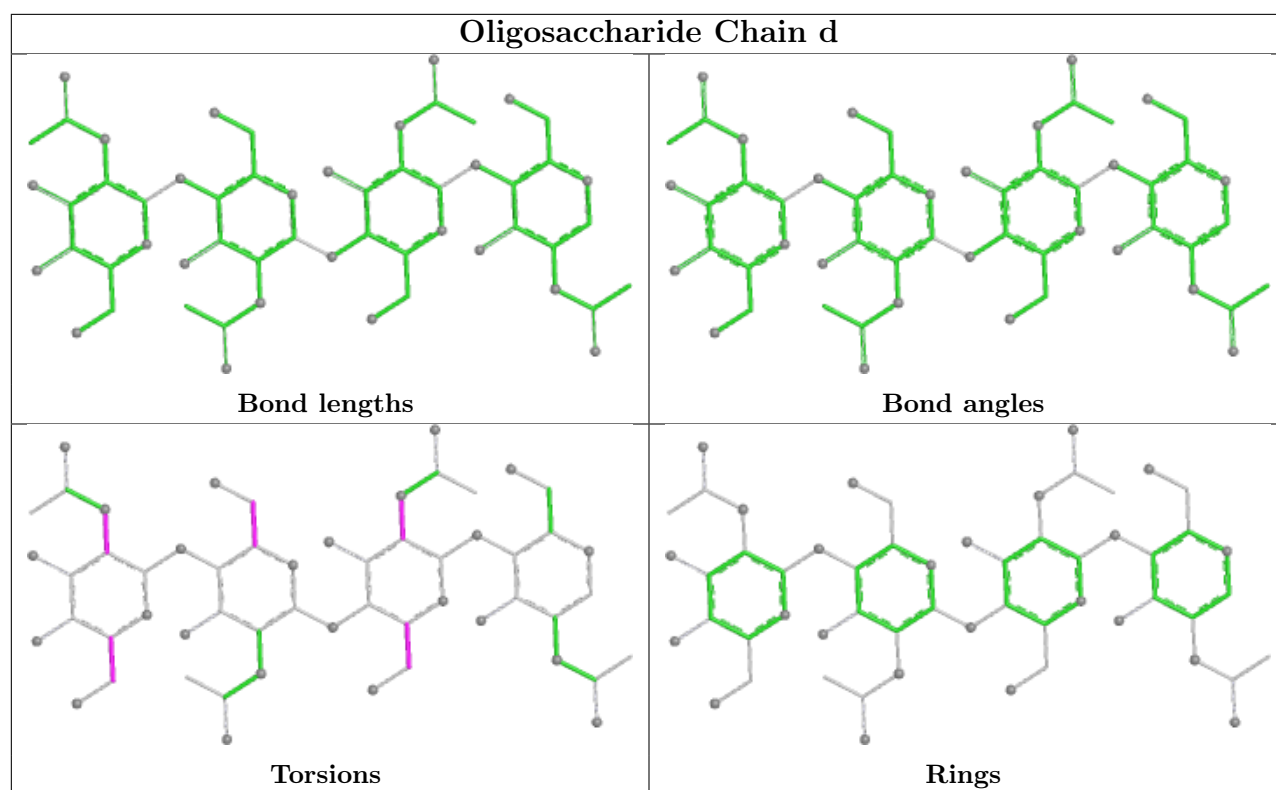


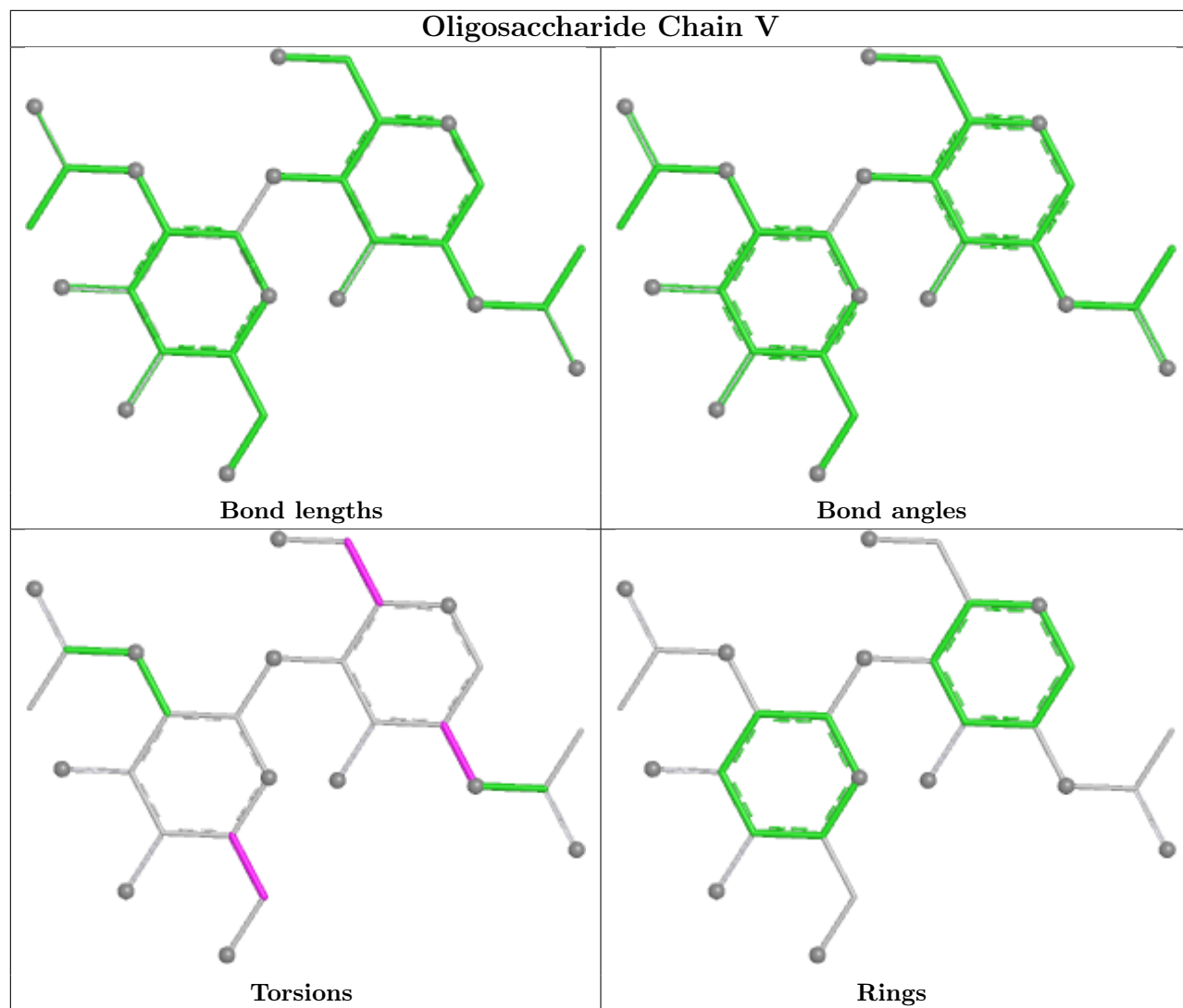




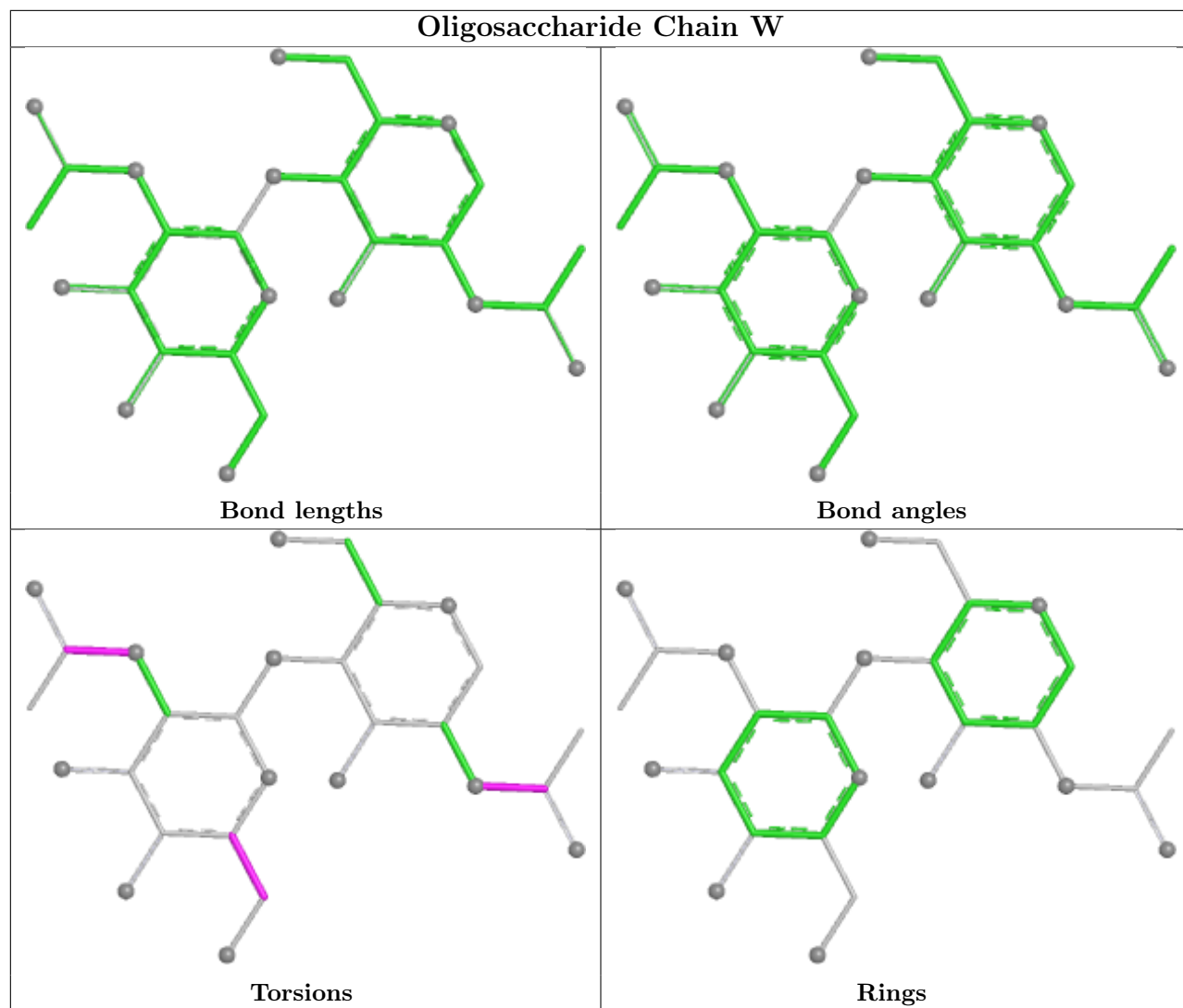


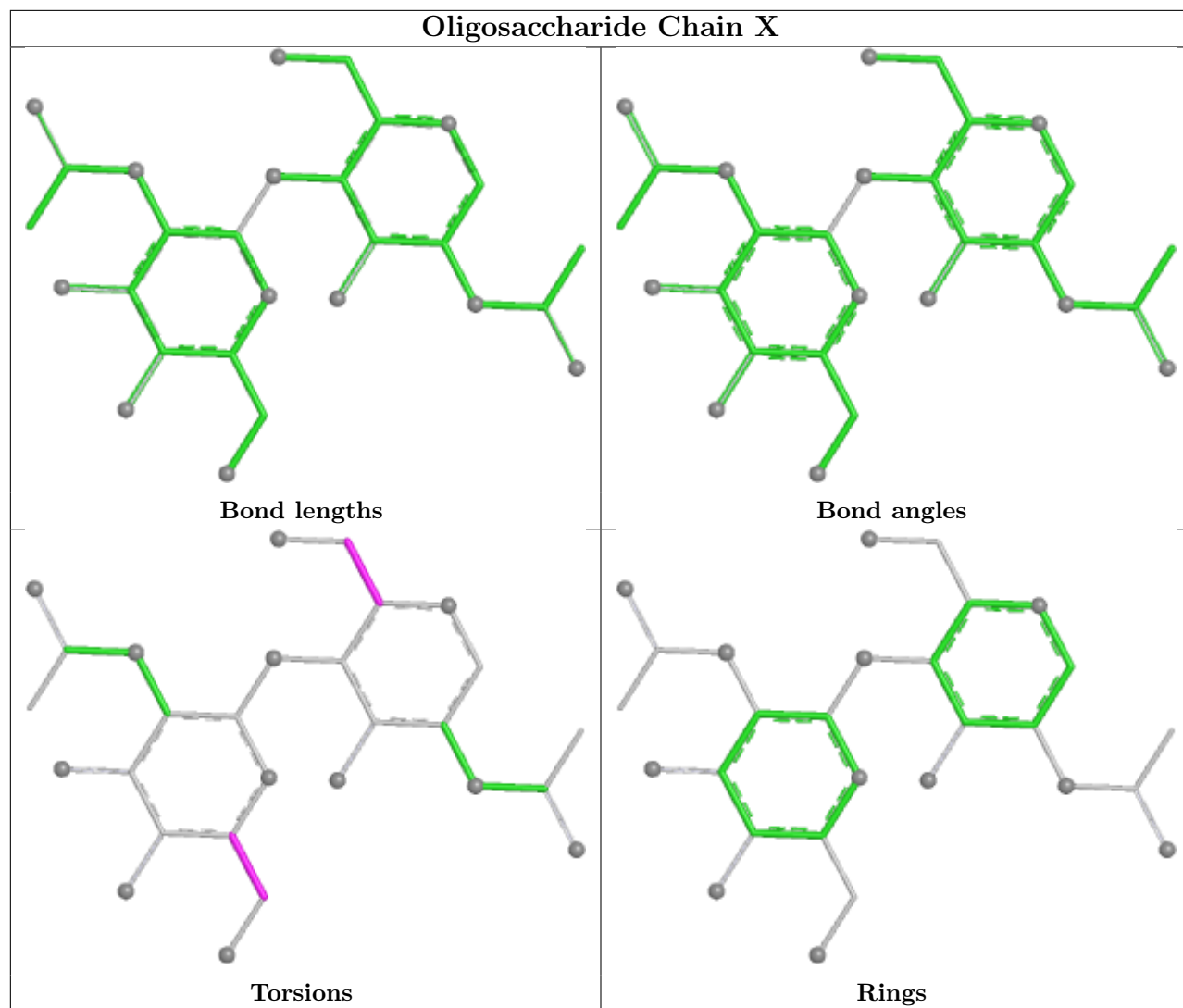


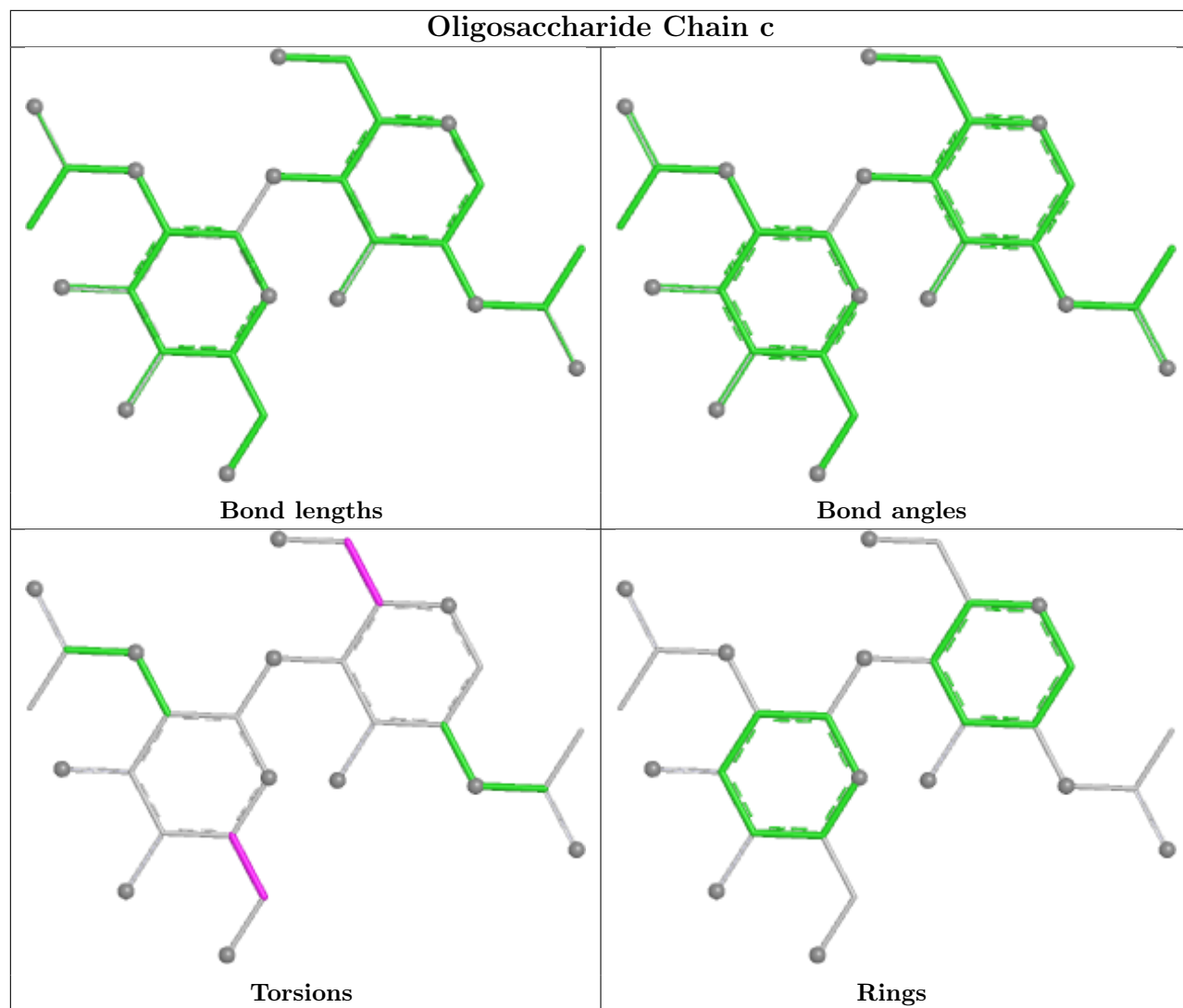


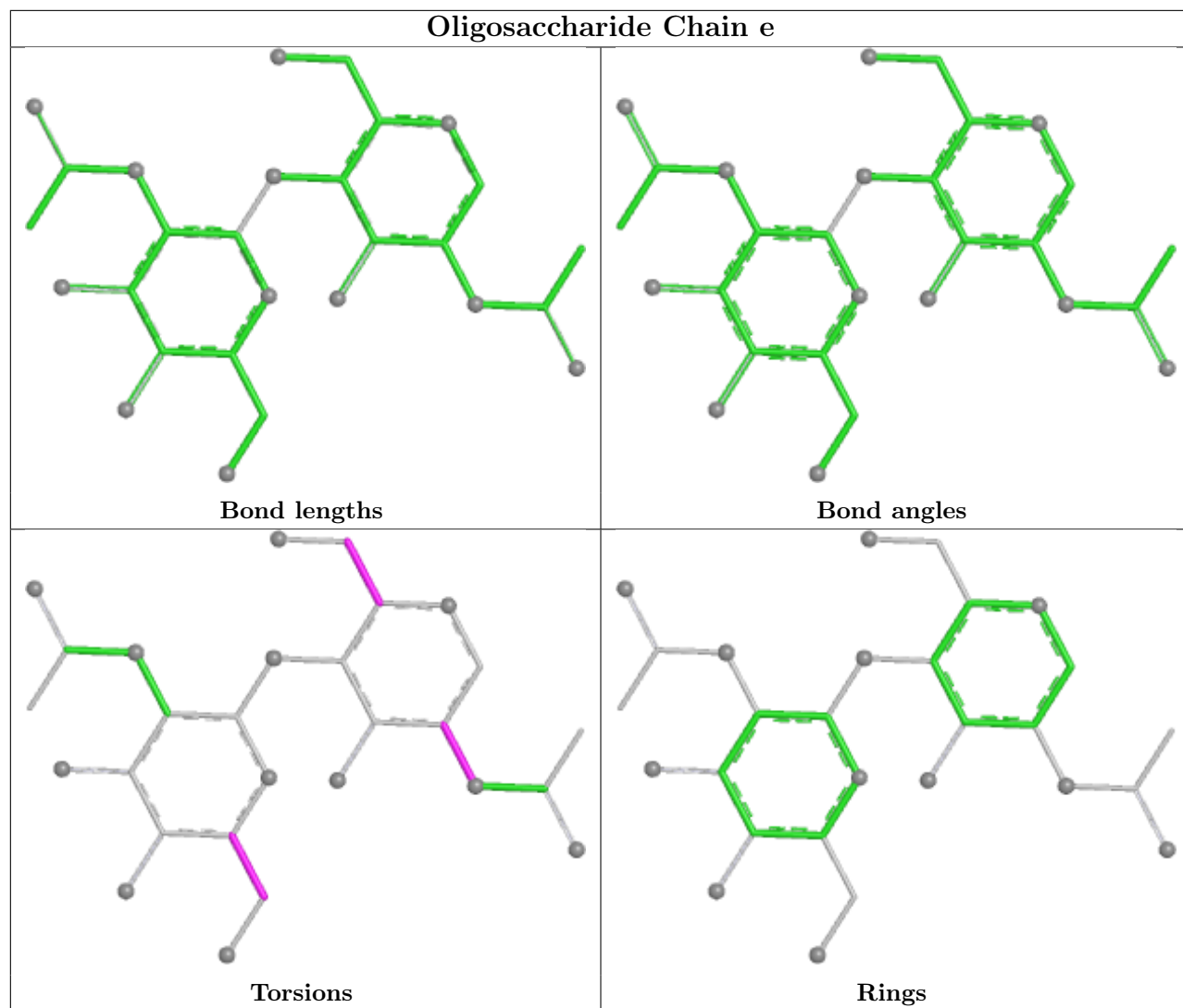


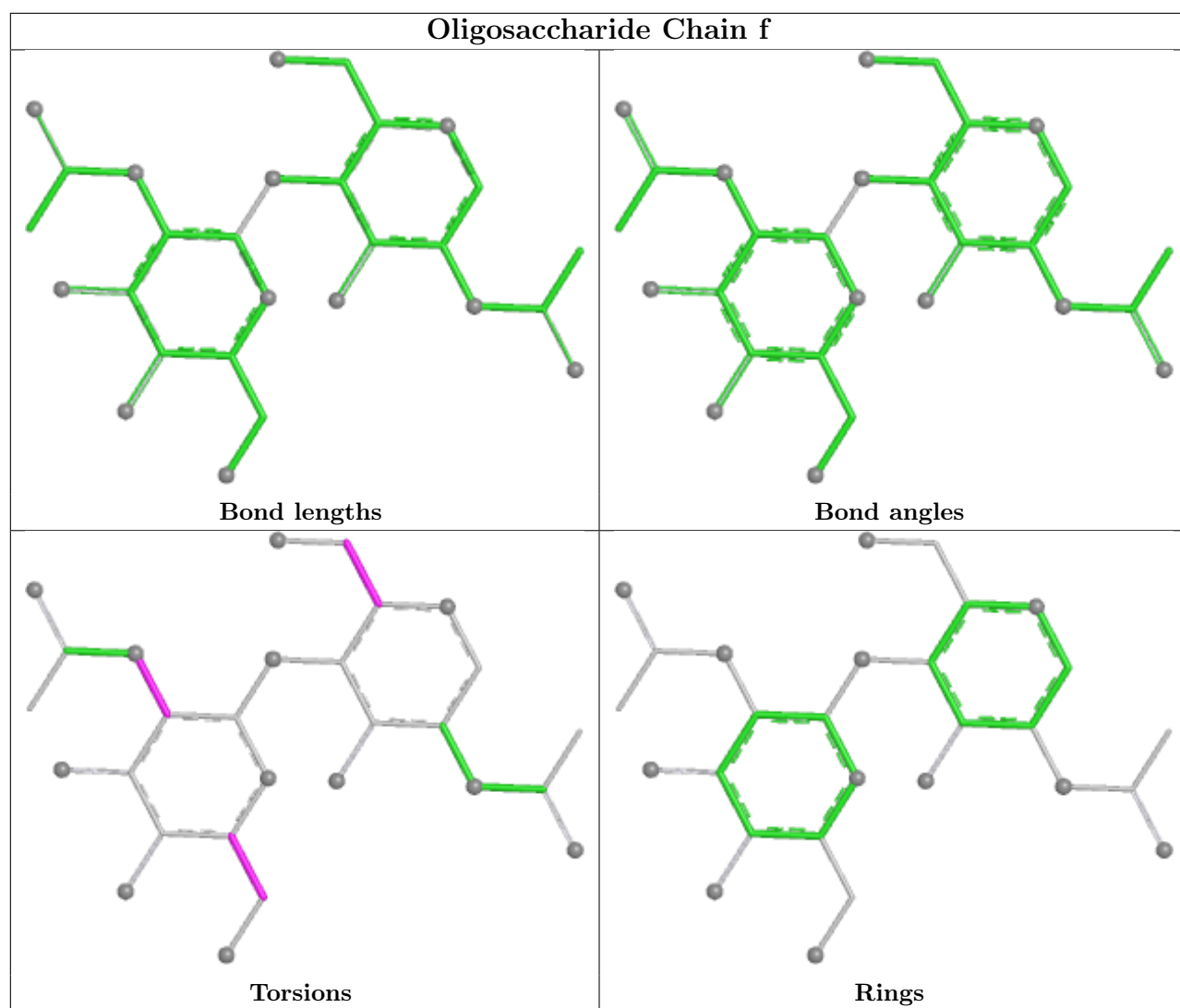


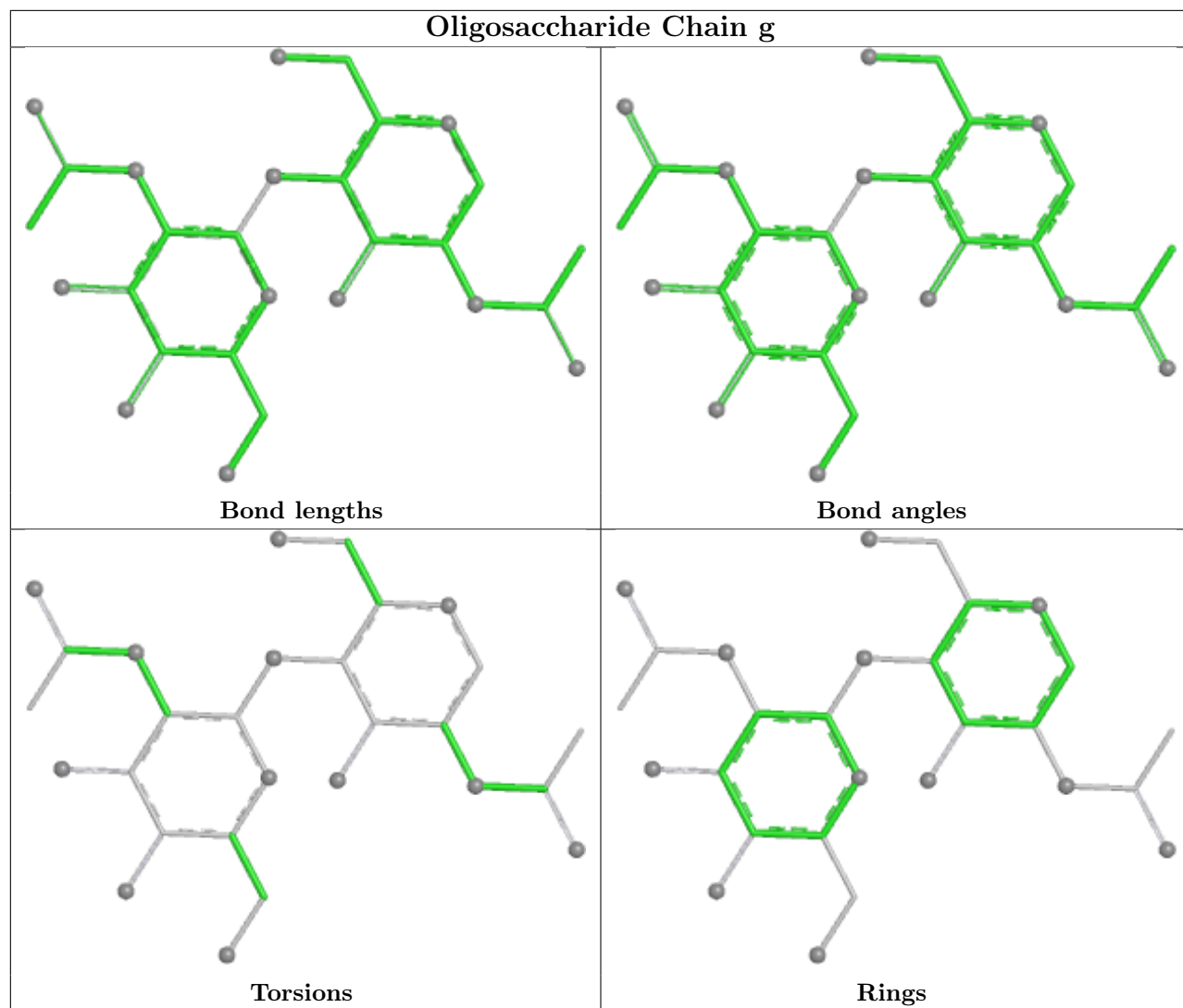


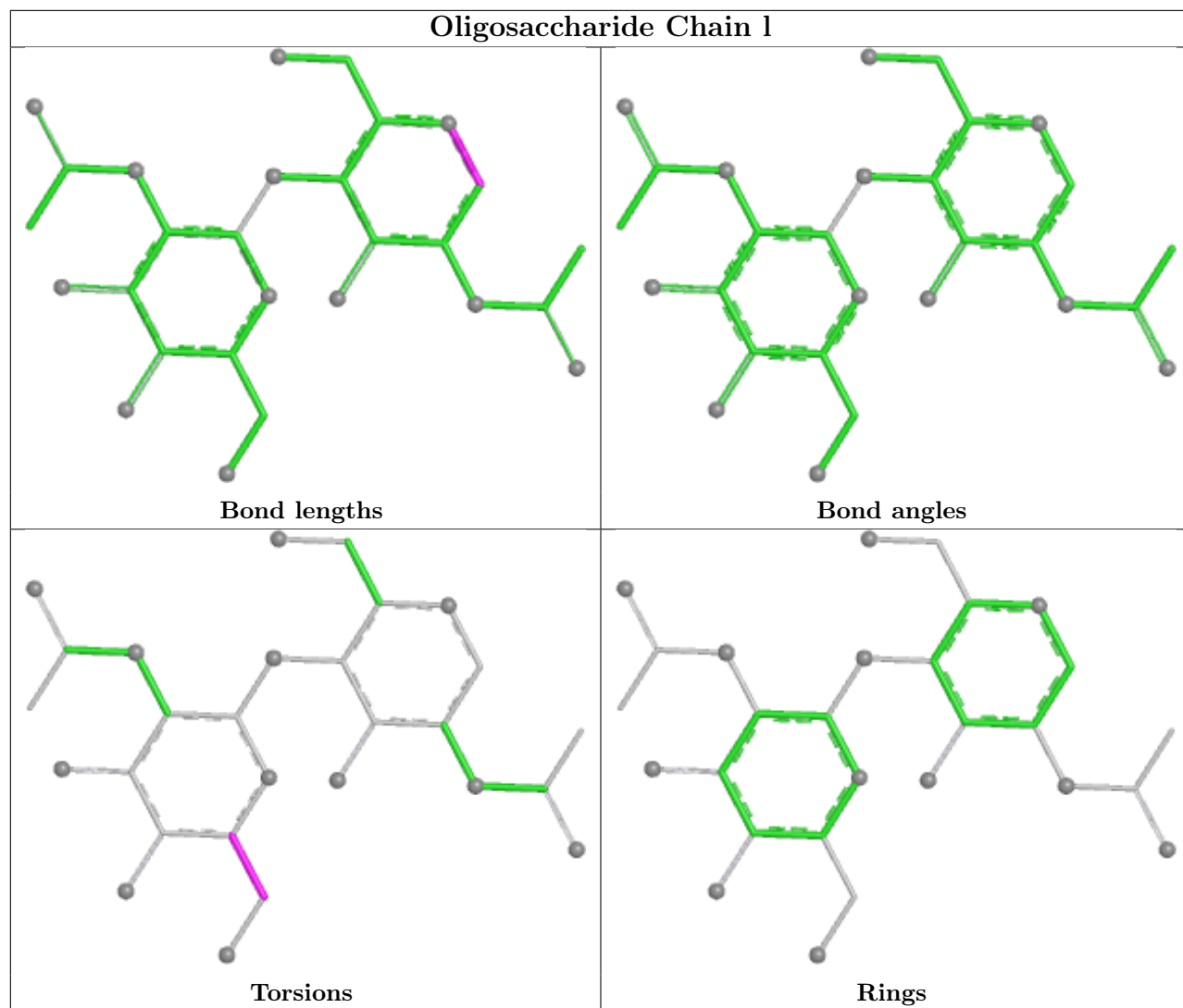


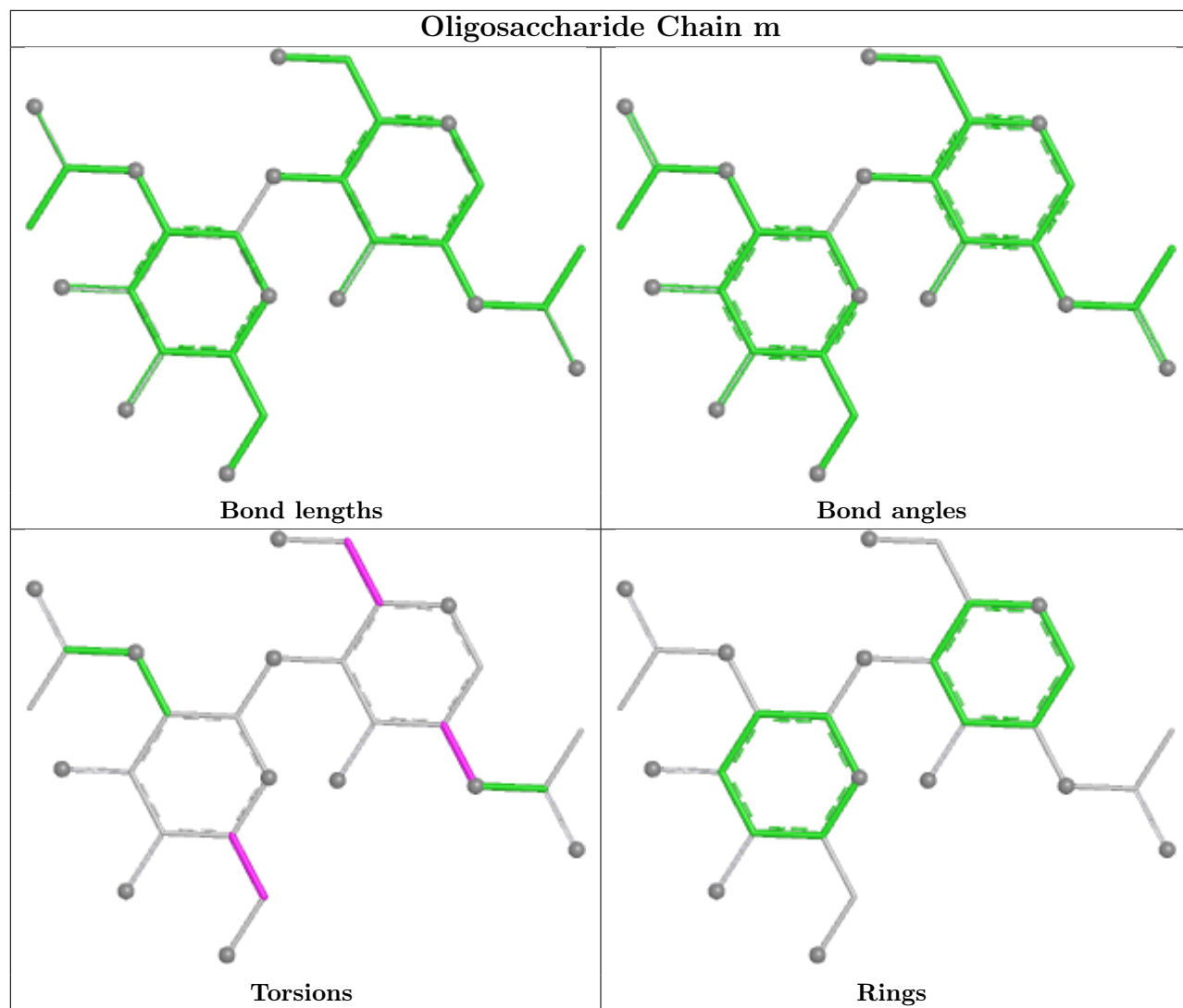




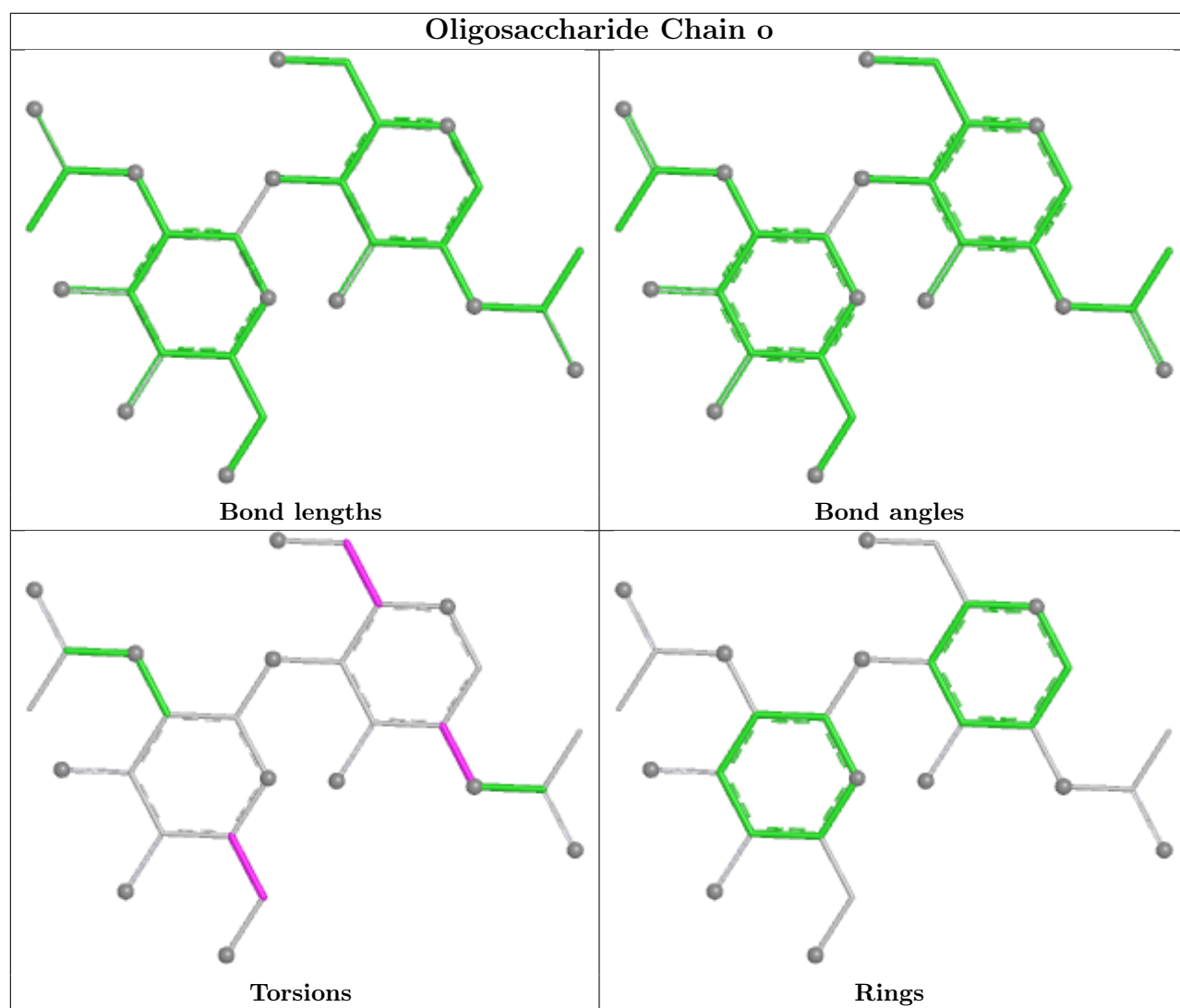


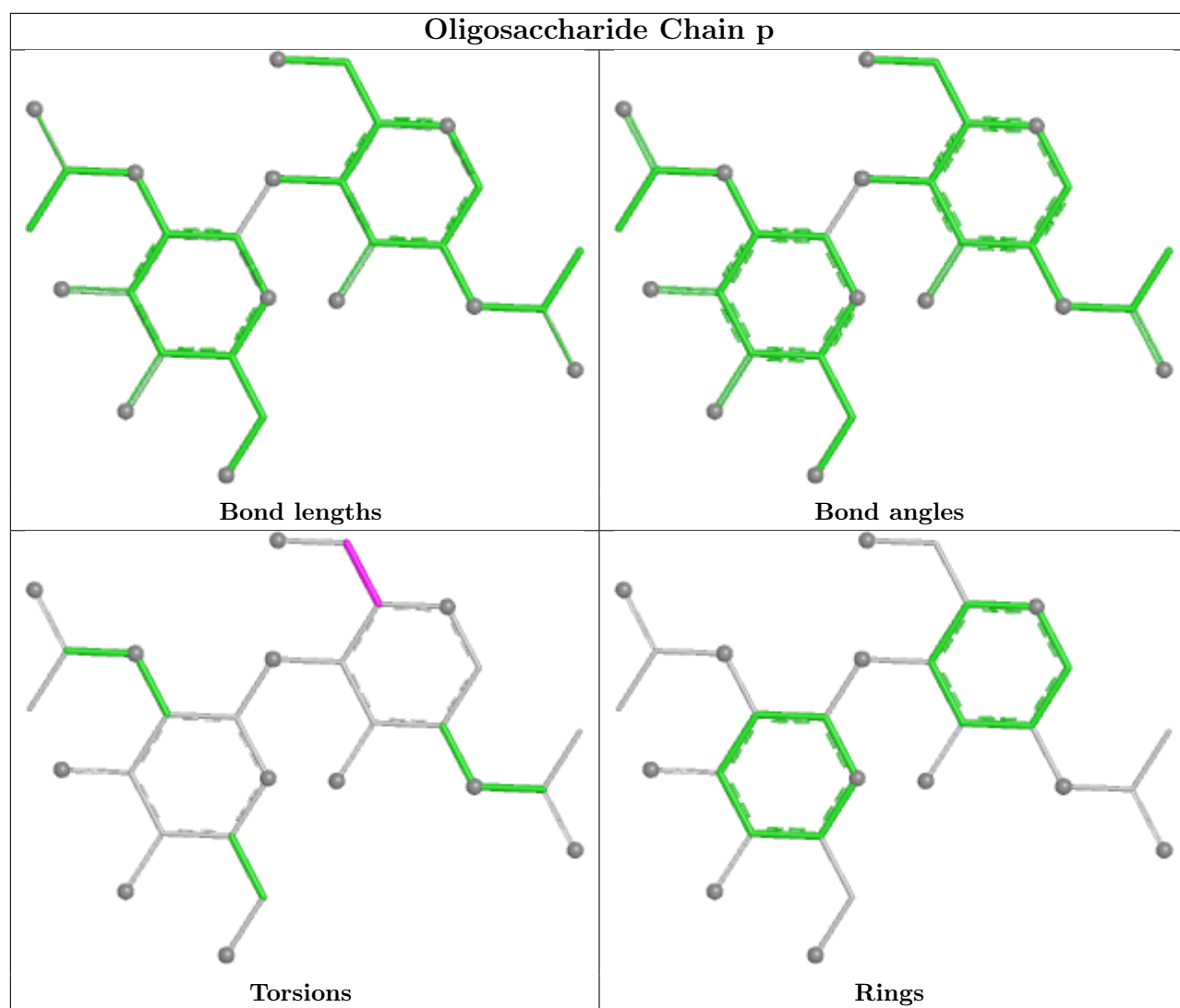


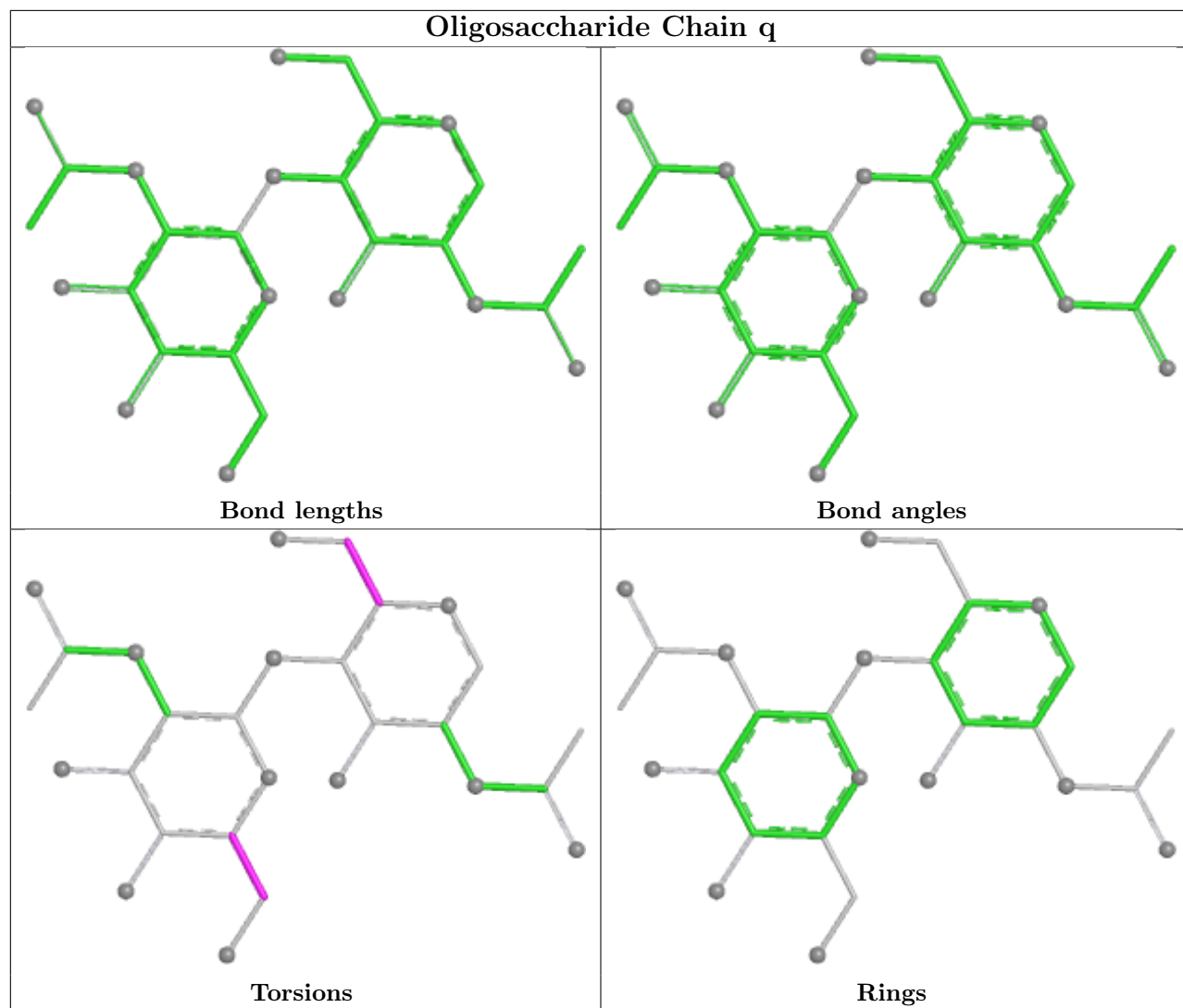


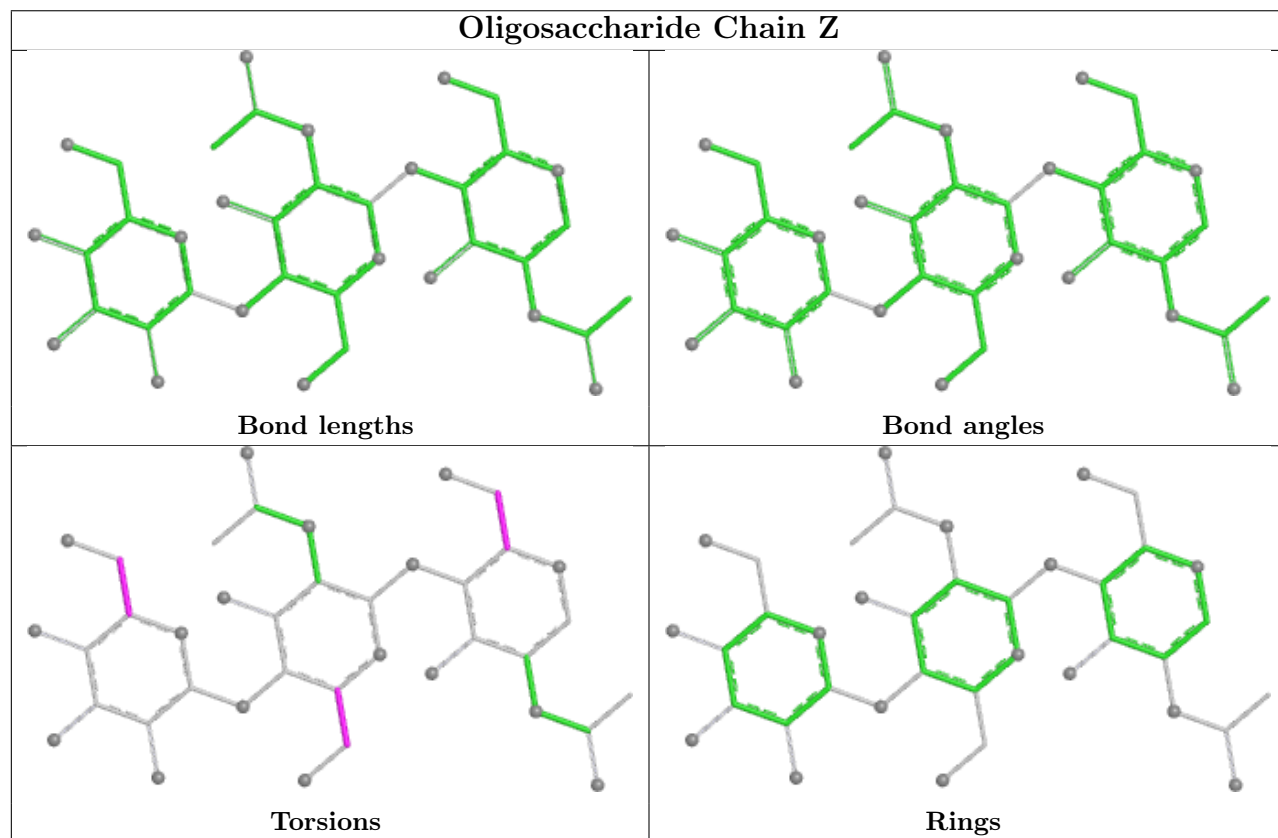
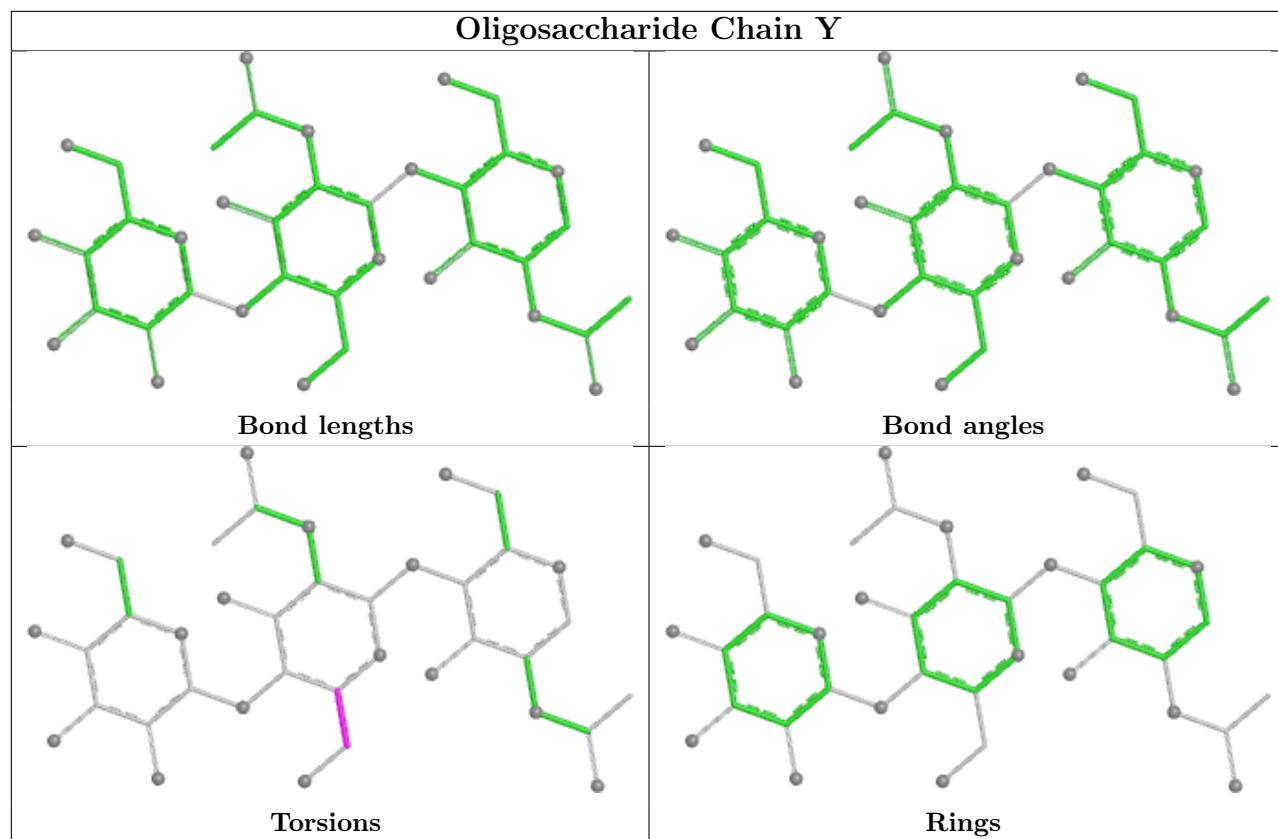


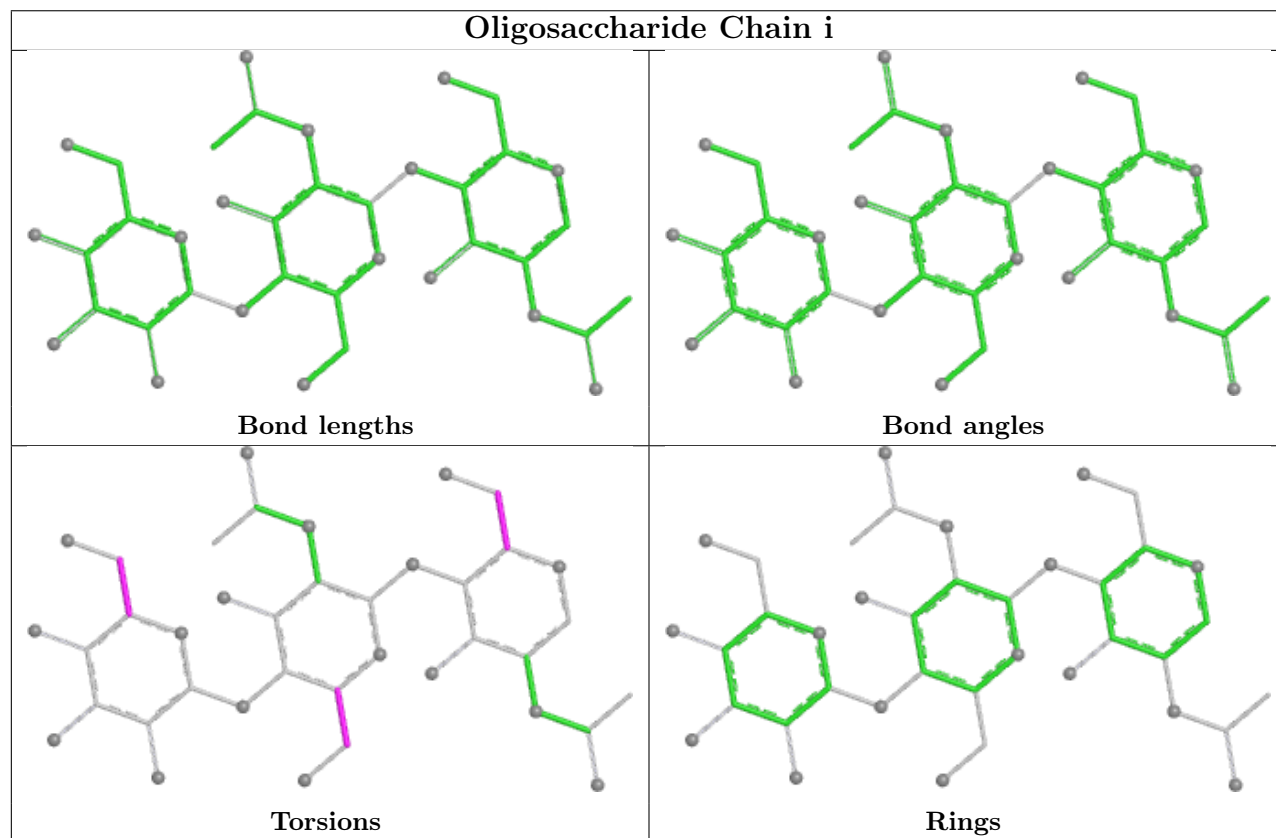
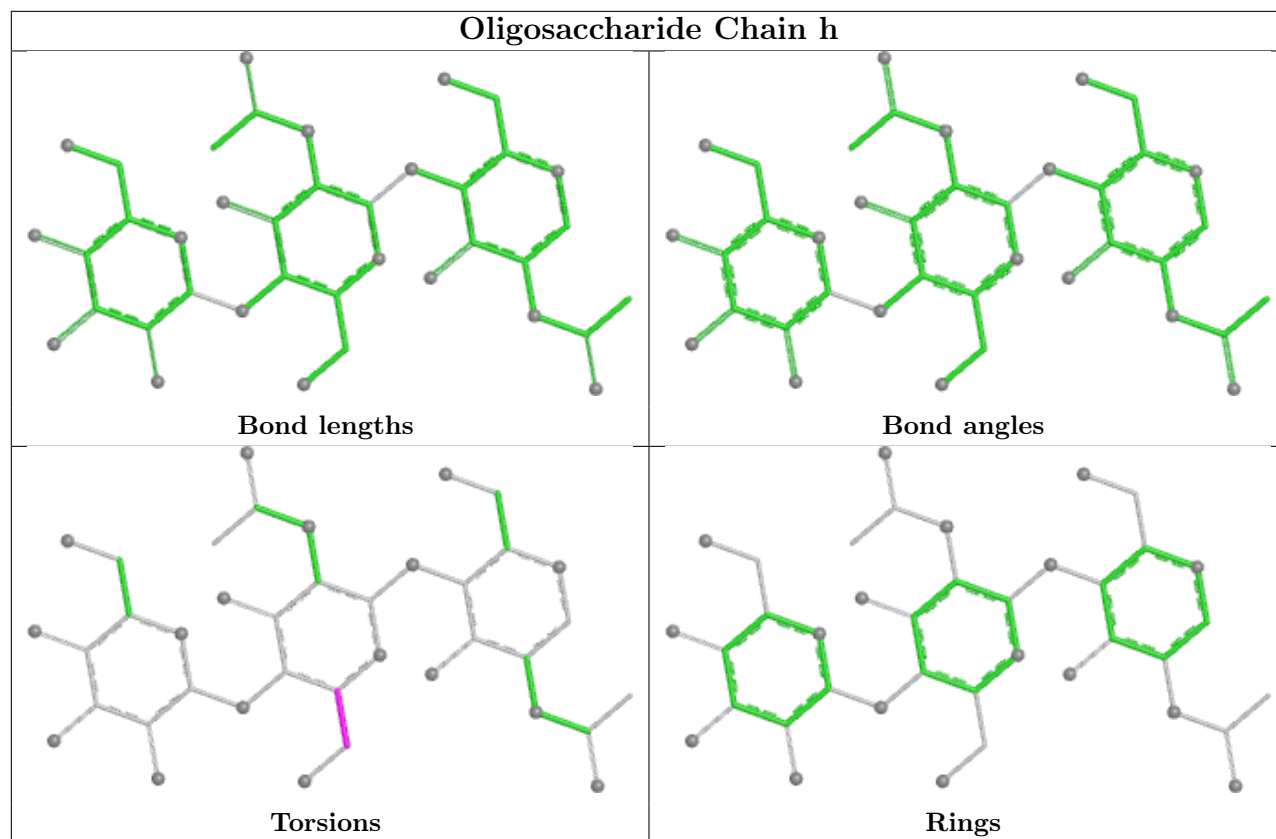


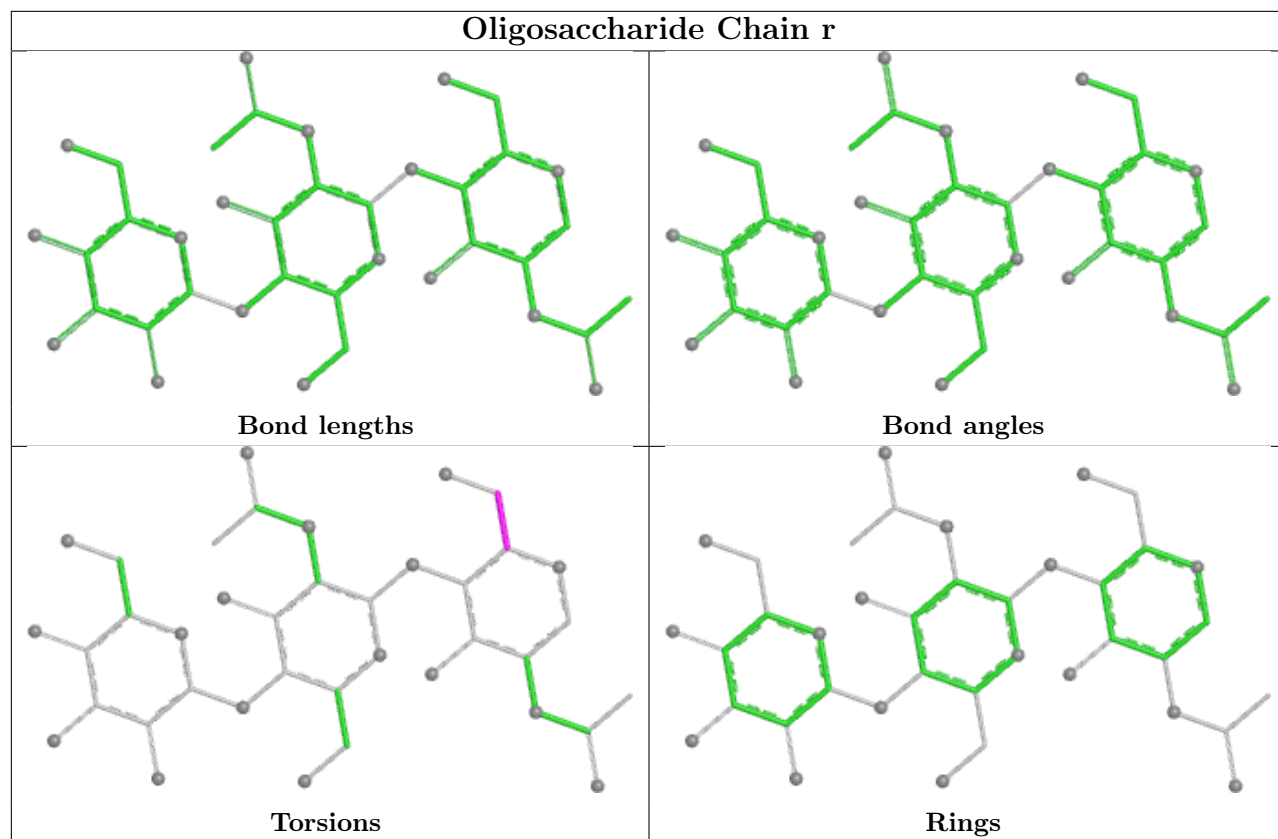


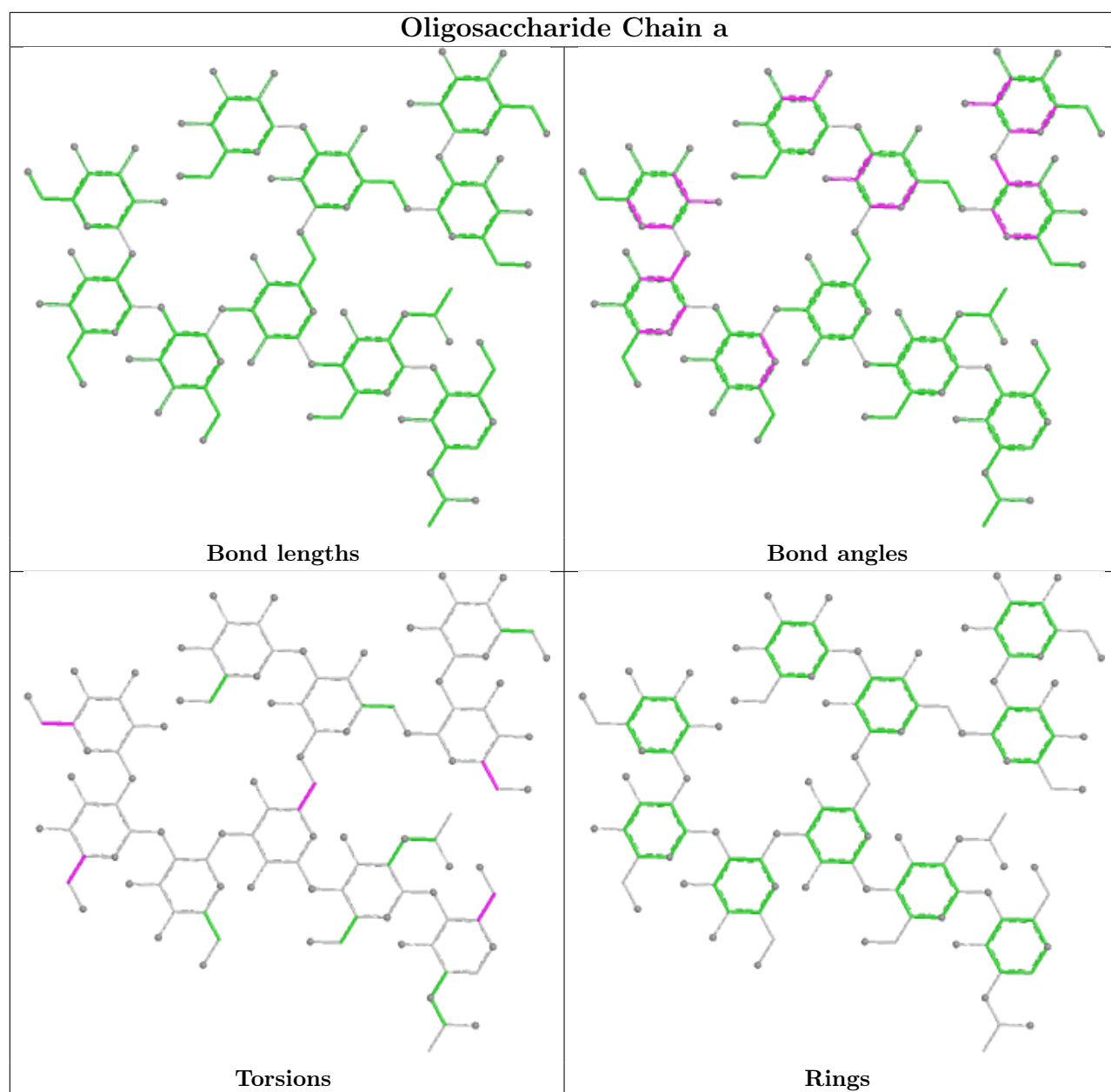


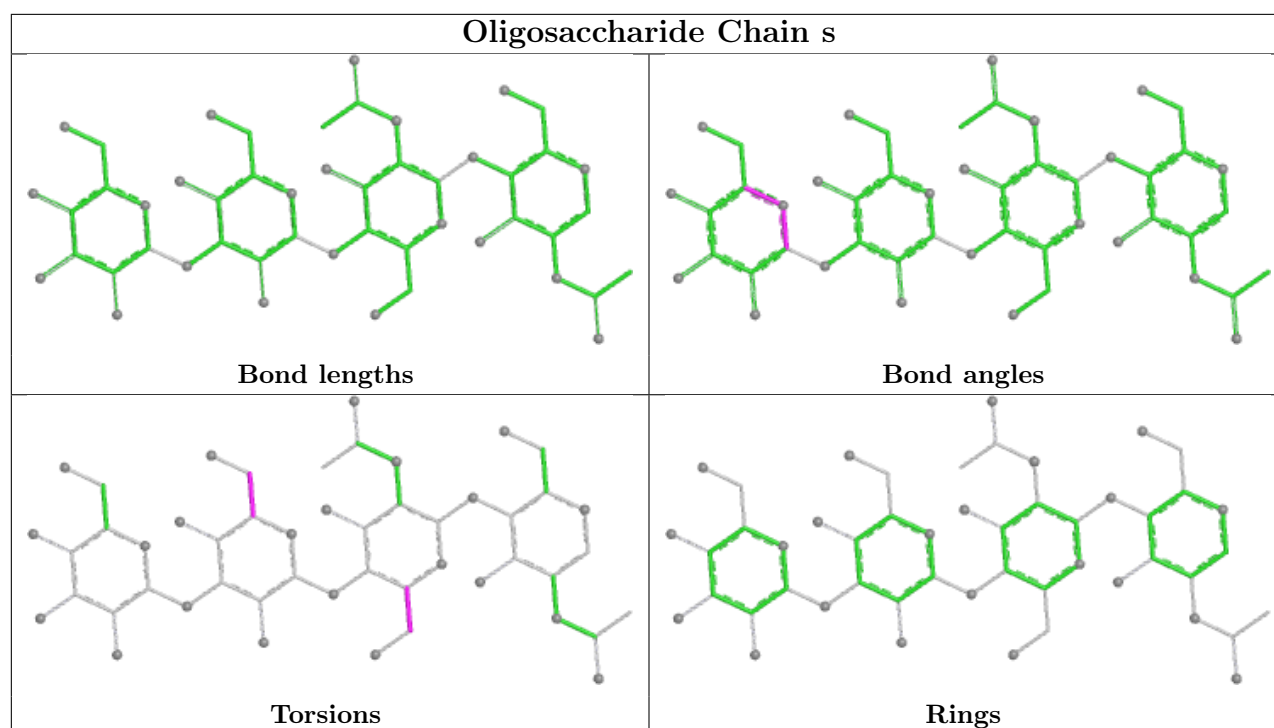












## 5.6 Ligand geometry [i](#)

37 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
15	NAG	A	606	1	14,14,15	0.26	0	17,19,21	0.51	0
15	NAG	E	609	1	14,14,15	0.22	0	17,19,21	0.36	0
15	NAG	F	701	2	14,14,15	0.23	0	17,19,21	0.51	0
15	NAG	I	602	1	14,14,15	0.26	0	17,19,21	0.45	0
15	NAG	I	604	1	14,14,15	0.22	0	17,19,21	0.46	0
15	NAG	C	301	3	14,14,15	0.27	0	17,19,21	0.44	0
15	NAG	B	702	2	14,14,15	0.64	1 (7%)	17,19,21	0.73	1 (5%)
15	NAG	A	609	1	14,14,15	0.26	0	17,19,21	0.70	0
15	NAG	I	601	1	14,14,15	0.22	0	17,19,21	0.40	0
15	NAG	I	603	1	14,14,15	0.26	0	17,19,21	0.45	0
15	NAG	K	301	3	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
14	83J	I	607	-	35,39,39	2.15	10 (28%)	42,56,56	4.23	20 (47%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	NAG	F	703	2	14,14,15	0.34	0	17,19,21	0.49	0
15	NAG	I	606	1	14,14,15	0.32	0	17,19,21	0.35	0
15	NAG	E	605	1	14,14,15	0.21	0	17,19,21	0.57	0
15	NAG	E	602	1	14,14,15	0.24	0	17,19,21	0.37	0
15	NAG	E	604	1	14,14,15	0.23	0	17,19,21	0.45	0
15	NAG	A	603	1	14,14,15	0.25	0	17,19,21	0.46	0
15	NAG	G	301	3	14,14,15	0.26	0	17,19,21	0.47	0
14	83J	A	601	-	35,39,39	2.04	11 (31%)	42,56,56	4.28	20 (47%)
15	NAG	F	702	2	14,14,15	0.30	0	17,19,21	0.42	0
15	NAG	E	606	1	14,14,15	0.55	0	17,19,21	0.46	0
15	NAG	E	608	1	14,14,15	1.01	1 (7%)	17,19,21	1.29	1 (5%)
15	NAG	E	601	1	14,14,15	0.23	0	17,19,21	0.41	0
15	NAG	I	605	1	14,14,15	0.21	0	17,19,21	0.40	0
15	NAG	J	701	2	14,14,15	0.27	0	17,19,21	0.50	0
15	NAG	A	605	1	14,14,15	0.25	0	17,19,21	0.49	0
15	NAG	B	701	2	14,14,15	0.64	0	17,19,21	0.50	0
14	83J	E	607	-	35,39,39	2.10	10 (28%)	42,56,56	4.39	17 (40%)
15	NAG	J	702	2	14,14,15	0.29	0	17,19,21	0.54	0
15	NAG	I	608	1	14,14,15	0.70	1 (7%)	17,19,21	0.92	1 (5%)
15	NAG	A	604	1	14,14,15	0.29	0	17,19,21	0.47	0
15	NAG	A	608	1	14,14,15	0.27	0	17,19,21	0.58	0
15	NAG	E	603	1	14,14,15	0.23	0	17,19,21	0.46	0
15	NAG	A	607	1	14,14,15	0.39	0	17,19,21	1.81	4 (23%)
15	NAG	J	703	2	14,14,15	0.64	1 (7%)	17,19,21	0.75	1 (5%)
15	NAG	A	602	1	14,14,15	0.23	0	17,19,21	0.42	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
15	NAG	A	606	1	-	2/6/23/26	0/1/1/1
15	NAG	E	609	1	-	0/6/23/26	0/1/1/1
15	NAG	F	701	2	-	2/6/23/26	0/1/1/1
15	NAG	I	602	1	-	2/6/23/26	0/1/1/1
15	NAG	I	604	1	-	2/6/23/26	0/1/1/1
15	NAG	C	301	3	-	0/6/23/26	0/1/1/1
15	NAG	B	702	2	-	2/6/23/26	0/1/1/1
15	NAG	A	609	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	I	601	1	-	2/6/23/26	0/1/1/1
15	NAG	I	603	1	-	2/6/23/26	0/1/1/1
15	NAG	K	301	3	-	2/6/23/26	0/1/1/1
14	83J	I	607	-	-	2/18/36/36	0/5/5/5
15	NAG	F	703	2	-	2/6/23/26	0/1/1/1
15	NAG	I	606	1	-	2/6/23/26	0/1/1/1
15	NAG	E	605	1	-	2/6/23/26	0/1/1/1
15	NAG	E	602	1	-	2/6/23/26	0/1/1/1
15	NAG	E	604	1	-	2/6/23/26	0/1/1/1
15	NAG	A	603	1	-	2/6/23/26	0/1/1/1
15	NAG	G	301	3	-	2/6/23/26	0/1/1/1
14	83J	A	601	-	-	2/18/36/36	0/5/5/5
15	NAG	F	702	2	-	2/6/23/26	0/1/1/1
15	NAG	E	606	1	-	3/6/23/26	0/1/1/1
15	NAG	E	608	1	-	2/6/23/26	0/1/1/1
15	NAG	E	601	1	-	2/6/23/26	0/1/1/1
15	NAG	I	605	1	-	2/6/23/26	0/1/1/1
15	NAG	J	701	2	-	2/6/23/26	0/1/1/1
15	NAG	A	605	1	-	0/6/23/26	0/1/1/1
15	NAG	B	701	2	-	2/6/23/26	0/1/1/1
14	83J	E	607	-	-	2/18/36/36	0/5/5/5
15	NAG	J	702	2	-	2/6/23/26	0/1/1/1
15	NAG	I	608	1	-	3/6/23/26	0/1/1/1
15	NAG	A	604	1	-	2/6/23/26	0/1/1/1
15	NAG	A	608	1	-	2/6/23/26	0/1/1/1
15	NAG	E	603	1	-	2/6/23/26	0/1/1/1
15	NAG	A	607	1	-	4/6/23/26	0/1/1/1
15	NAG	J	703	2	-	2/6/23/26	0/1/1/1
15	NAG	A	602	1	-	2/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	607	83J	C12-N02	6.19	1.45	1.34
14	I	607	83J	C12-N02	6.14	1.45	1.34
14	I	607	83J	C13-N05	5.61	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	607	83J	C13-N05	5.40	1.46	1.34
14	A	601	83J	C12-N02	5.34	1.44	1.34
14	A	601	83J	C13-N05	5.15	1.45	1.34
14	I	607	83J	C16-C17	-4.69	1.35	1.42
14	A	601	83J	C16-C17	-4.46	1.35	1.42
14	E	607	83J	C16-C17	-4.31	1.36	1.42
15	E	608	NAG	O5-C1	3.43	1.49	1.43
14	A	601	83J	N34-N30	-2.91	1.33	1.39
14	I	607	83J	N34-N30	-2.87	1.34	1.39
14	E	607	83J	N34-N30	-2.79	1.34	1.39
14	A	601	83J	O09-C14	-2.75	1.17	1.23
14	I	607	83J	O09-C14	-2.73	1.17	1.23
14	E	607	83J	O09-C14	-2.72	1.17	1.23
14	A	601	83J	C29-N28	2.71	1.34	1.31
14	I	607	83J	C29-N28	2.69	1.34	1.31
14	E	607	83J	C29-N28	2.66	1.34	1.31
14	I	607	83J	C15-C13	2.64	1.54	1.50
14	I	607	83J	C22-C17	-2.50	1.37	1.42
14	A	601	83J	O03-C12	-2.46	1.18	1.23
14	E	607	83J	C22-C17	-2.43	1.37	1.42
14	E	607	83J	O03-C12	-2.42	1.18	1.23
14	E	607	83J	C15-C13	2.40	1.54	1.50
14	I	607	83J	O03-C12	-2.38	1.18	1.23
14	A	601	83J	C22-C17	-2.35	1.37	1.42
15	I	608	NAG	O5-C1	2.32	1.47	1.43
14	A	601	83J	C15-C13	2.26	1.53	1.50
14	E	607	83J	C07-N02	-2.18	1.43	1.47
15	B	702	NAG	C1-C2	2.17	1.55	1.52
14	A	601	83J	C04-N05	-2.15	1.43	1.47
15	J	703	NAG	C1-C2	2.12	1.55	1.52
14	I	607	83J	C07-N02	-2.12	1.43	1.47
14	A	601	83J	O06-C13	-2.02	1.18	1.22

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	607	83J	C18-C16-C14	-12.92	100.44	127.72
14	I	607	83J	C18-C16-C14	-12.88	100.53	127.72
14	A	601	83J	C18-C16-C14	-12.60	101.11	127.72
14	A	601	83J	O11-C22-C17	11.29	132.00	115.91
14	E	607	83J	O11-C22-C17	11.26	131.96	115.91
14	I	607	83J	O11-C22-C17	11.10	131.73	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	607	83J	O11-C22-C25	-9.72	104.22	125.15
14	A	601	83J	O11-C22-C25	-9.58	104.51	125.15
14	I	607	83J	O11-C22-C25	-9.41	104.89	125.15
14	E	607	83J	C20-C15-C13	-9.05	97.06	120.28
14	E	607	83J	C21-C15-C13	8.67	142.53	120.28
14	A	601	83J	C20-C15-C13	-8.62	98.16	120.28
14	E	607	83J	C31-N32-C33	8.15	107.66	101.74
14	A	601	83J	C21-C15-C13	8.11	141.08	120.28
14	I	607	83J	C31-N32-C33	8.02	107.56	101.74
14	A	601	83J	C31-N32-C33	8.01	107.56	101.74
14	I	607	83J	C20-C15-C13	-7.72	100.47	120.28
14	I	607	83J	C21-C15-C13	7.54	139.62	120.28
14	E	607	83J	N28-C29-N30	-6.32	107.82	114.12
14	A	601	83J	C16-C17-C19	-5.95	102.79	107.54
14	I	607	83J	N28-C29-N30	-5.92	108.21	114.12
14	A	601	83J	N28-C29-N30	-5.60	108.54	114.12
14	I	607	83J	C16-C17-C19	-5.50	103.14	107.54
14	E	607	83J	C16-C17-C19	-5.45	103.19	107.54
15	E	608	NAG	C1-O5-C5	5.04	118.94	112.19
15	A	607	NAG	O5-C1-C2	-4.88	103.74	111.29
14	E	607	83J	C01-C04-N05	4.63	119.61	110.42
14	I	607	83J	C15-C13-N05	4.06	123.73	118.66
14	A	601	83J	C16-C18-N08	-3.63	101.89	108.91
14	E	607	83J	C14-C12-N02	3.59	121.97	118.46
15	I	608	NAG	C1-O5-C5	3.47	116.84	112.19
14	A	601	83J	C22-C25-N28	-3.45	117.90	122.76
14	I	607	83J	C22-C25-N28	-3.42	117.93	122.76
14	I	607	83J	C01-C04-N05	3.39	117.16	110.42
14	I	607	83J	C16-C18-N08	-3.34	102.45	108.91
14	E	607	83J	C22-C25-N28	-3.29	118.12	122.76
14	E	607	83J	C27-O11-C22	-3.19	112.37	117.67
14	E	607	83J	C16-C18-N08	-3.19	102.75	108.91
14	E	607	83J	C19-C29-N28	3.12	127.69	118.92
15	A	607	NAG	C4-C3-C2	-3.10	106.48	111.02
14	A	601	83J	O09-C14-C12	3.08	121.94	117.68
15	A	607	NAG	C2-N2-C7	-3.06	118.80	122.90
15	K	301	NAG	C1-O5-C5	3.04	116.27	112.19
14	A	601	83J	C19-C29-N28	3.01	127.38	118.92
14	E	607	83J	O03-C12-N02	-2.98	117.96	122.67
14	I	607	83J	C19-C29-N28	2.96	127.25	118.92
14	A	601	83J	O03-C12-C14	2.89	121.79	117.24
14	A	601	83J	C27-O11-C22	-2.75	113.10	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	I	607	83J	O06-C13-N05	-2.67	118.14	122.35
14	I	607	83J	C07-C10-N05	2.66	115.70	110.42
15	J	703	NAG	C1-O5-C5	2.65	115.73	112.19
15	A	607	NAG	C1-O5-C5	2.62	115.70	112.19
14	A	601	83J	C35-C33-N32	2.61	127.01	120.49
14	I	607	83J	C14-C12-N02	2.58	120.98	118.46
15	B	702	NAG	C1-O5-C5	2.54	115.59	112.19
14	I	607	83J	C35-C33-N32	2.53	126.83	120.49
14	I	607	83J	C27-O11-C22	-2.46	113.57	117.67
14	A	601	83J	C04-N05-C10	-2.45	107.69	112.68
14	I	607	83J	O03-C12-N02	-2.43	118.83	122.67
14	A	601	83J	C04-C01-N02	2.36	115.11	110.42
14	I	607	83J	C07-N02-C01	-2.35	107.89	112.68
14	E	607	83J	C35-C33-N32	2.34	126.36	120.49
14	A	601	83J	O03-C12-N02	-2.30	119.04	122.67
14	E	607	83J	C07-N02-C01	-2.28	108.03	112.68
14	A	601	83J	O06-C13-N05	-2.14	118.98	122.35
14	A	601	83J	C07-C10-N05	-2.00	106.43	110.42

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	83J	C25-C22-O11-C27
14	E	607	83J	C25-C22-O11-C27
14	I	607	83J	C25-C22-O11-C27
15	A	609	NAG	C8-C7-N2-C2
15	A	609	NAG	O7-C7-N2-C2
15	E	602	NAG	C4-C5-C6-O6
15	I	608	NAG	C4-C5-C6-O6
15	A	607	NAG	C8-C7-N2-C2
15	A	607	NAG	O7-C7-N2-C2
14	A	601	83J	C17-C22-O11-C27
14	E	607	83J	C17-C22-O11-C27
15	I	608	NAG	O5-C5-C6-O6
15	I	601	NAG	O5-C5-C6-O6
15	J	702	NAG	O5-C5-C6-O6
15	E	601	NAG	O5-C5-C6-O6
15	A	603	NAG	O5-C5-C6-O6
15	B	702	NAG	O5-C5-C6-O6
15	E	602	NAG	O5-C5-C6-O6
15	F	703	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	I	605	NAG	O5-C5-C6-O6
15	E	601	NAG	C4-C5-C6-O6
15	E	604	NAG	C4-C5-C6-O6
15	A	607	NAG	O5-C5-C6-O6
15	I	602	NAG	O5-C5-C6-O6
15	I	601	NAG	C4-C5-C6-O6
15	J	702	NAG	C4-C5-C6-O6
15	A	602	NAG	O5-C5-C6-O6
15	F	701	NAG	O5-C5-C6-O6
15	I	604	NAG	O5-C5-C6-O6
15	A	606	NAG	O5-C5-C6-O6
15	I	606	NAG	O5-C5-C6-O6
15	A	602	NAG	C4-C5-C6-O6
15	E	608	NAG	C4-C5-C6-O6
15	J	703	NAG	O5-C5-C6-O6
15	G	301	NAG	O5-C5-C6-O6
14	I	607	83J	C17-C22-O11-C27
15	E	606	NAG	O5-C5-C6-O6
15	E	606	NAG	C4-C5-C6-O6
15	I	602	NAG	C4-C5-C6-O6
15	B	702	NAG	C4-C5-C6-O6
15	F	701	NAG	C4-C5-C6-O6
15	F	702	NAG	O5-C5-C6-O6
15	I	603	NAG	O5-C5-C6-O6
15	F	703	NAG	C4-C5-C6-O6
15	G	301	NAG	C4-C5-C6-O6
15	I	605	NAG	C4-C5-C6-O6
15	A	603	NAG	C4-C5-C6-O6
15	A	607	NAG	C4-C5-C6-O6
15	A	608	NAG	O5-C5-C6-O6
15	E	608	NAG	O5-C5-C6-O6
15	E	604	NAG	O5-C5-C6-O6
15	I	606	NAG	C4-C5-C6-O6
15	K	301	NAG	C8-C7-N2-C2
15	E	605	NAG	O5-C5-C6-O6
15	I	603	NAG	C4-C5-C6-O6
15	A	604	NAG	O5-C5-C6-O6
15	E	605	NAG	C4-C5-C6-O6
15	E	603	NAG	O5-C5-C6-O6
15	A	604	NAG	C4-C5-C6-O6
15	I	604	NAG	C4-C5-C6-O6
15	E	603	NAG	C4-C5-C6-O6

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
15	J	701	NAG	C4-C5-C6-O6
15	K	301	NAG	O7-C7-N2-C2
15	F	702	NAG	C4-C5-C6-O6
15	J	703	NAG	C4-C5-C6-O6
15	B	701	NAG	C4-C5-C6-O6
15	J	701	NAG	O5-C5-C6-O6
15	A	608	NAG	C4-C5-C6-O6
15	B	701	NAG	O5-C5-C6-O6
15	A	609	NAG	C4-C5-C6-O6
15	A	606	NAG	C4-C5-C6-O6
15	I	608	NAG	C3-C2-N2-C7
15	E	606	NAG	C3-C2-N2-C7

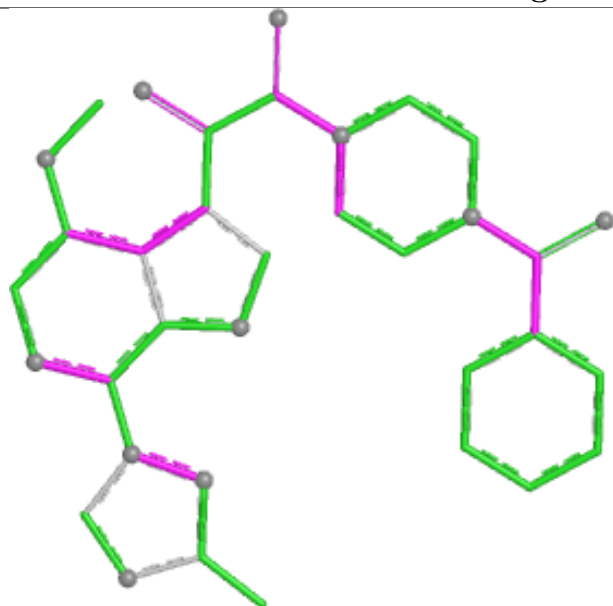
There are no ring outliers.

9 monomers are involved in 11 short contacts:

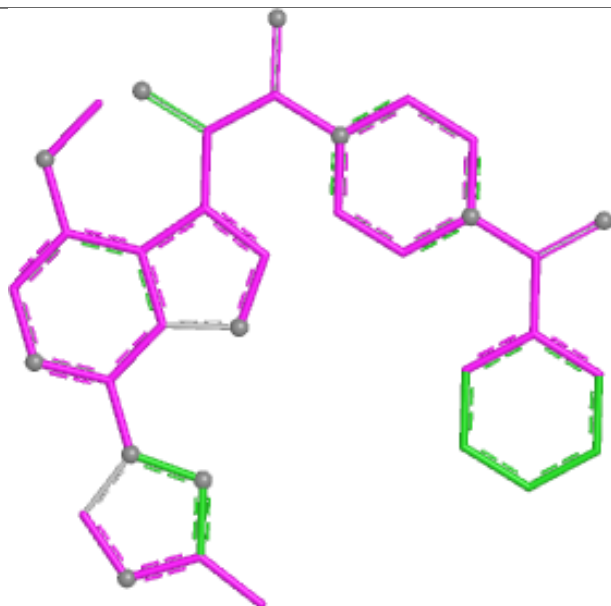
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	I	602	NAG	1	0
15	B	702	NAG	2	0
15	F	703	NAG	1	0
15	E	602	NAG	1	0
15	E	604	NAG	1	0
15	E	606	NAG	1	0
15	J	702	NAG	1	0
15	A	608	NAG	1	0
15	J	703	NAG	2	0

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

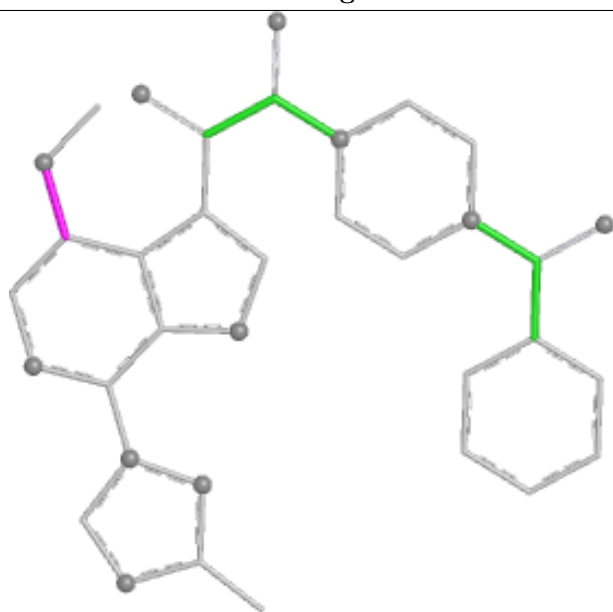
## Ligand 83J I 607



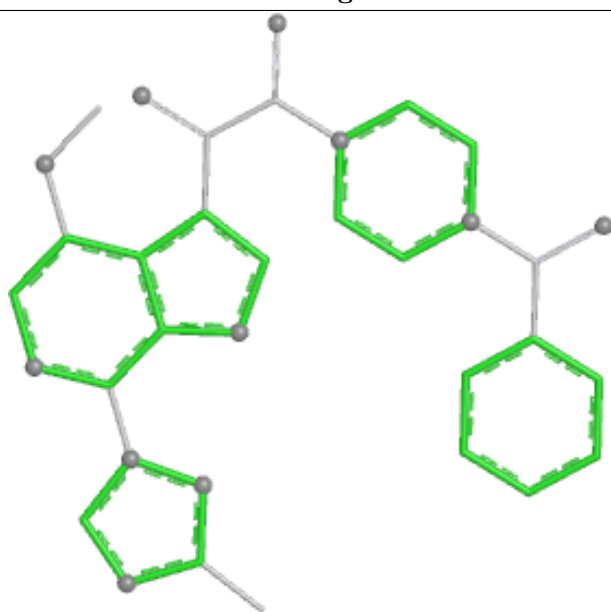
Bond lengths



Bond angles



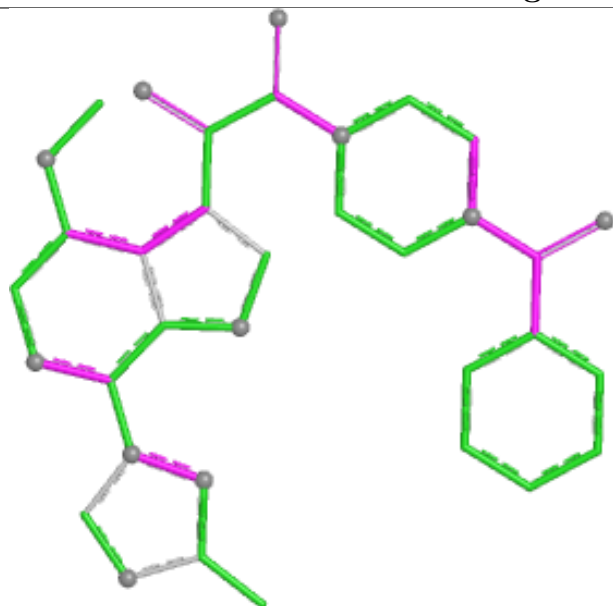
Torsions



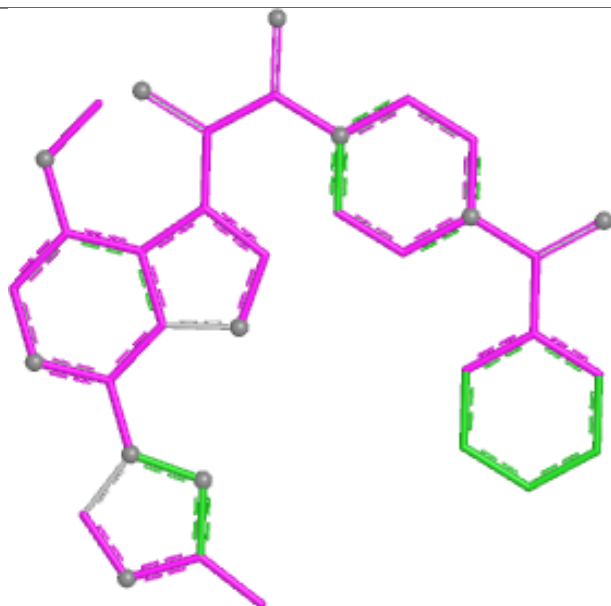
Rings



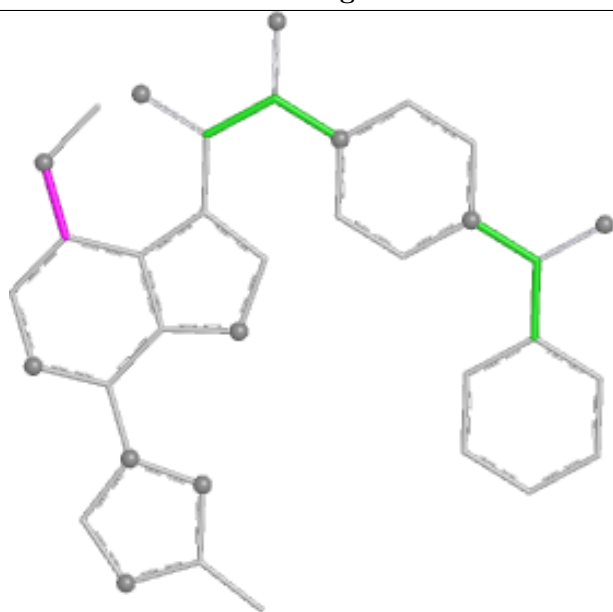
## Ligand 83J A 601



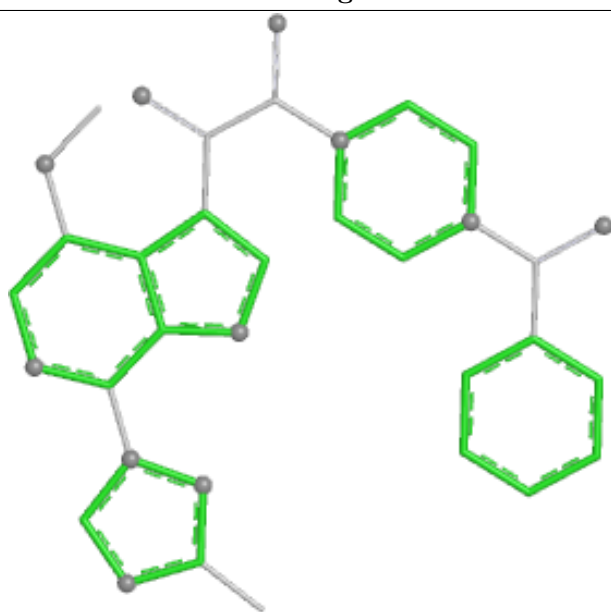
Bond lengths



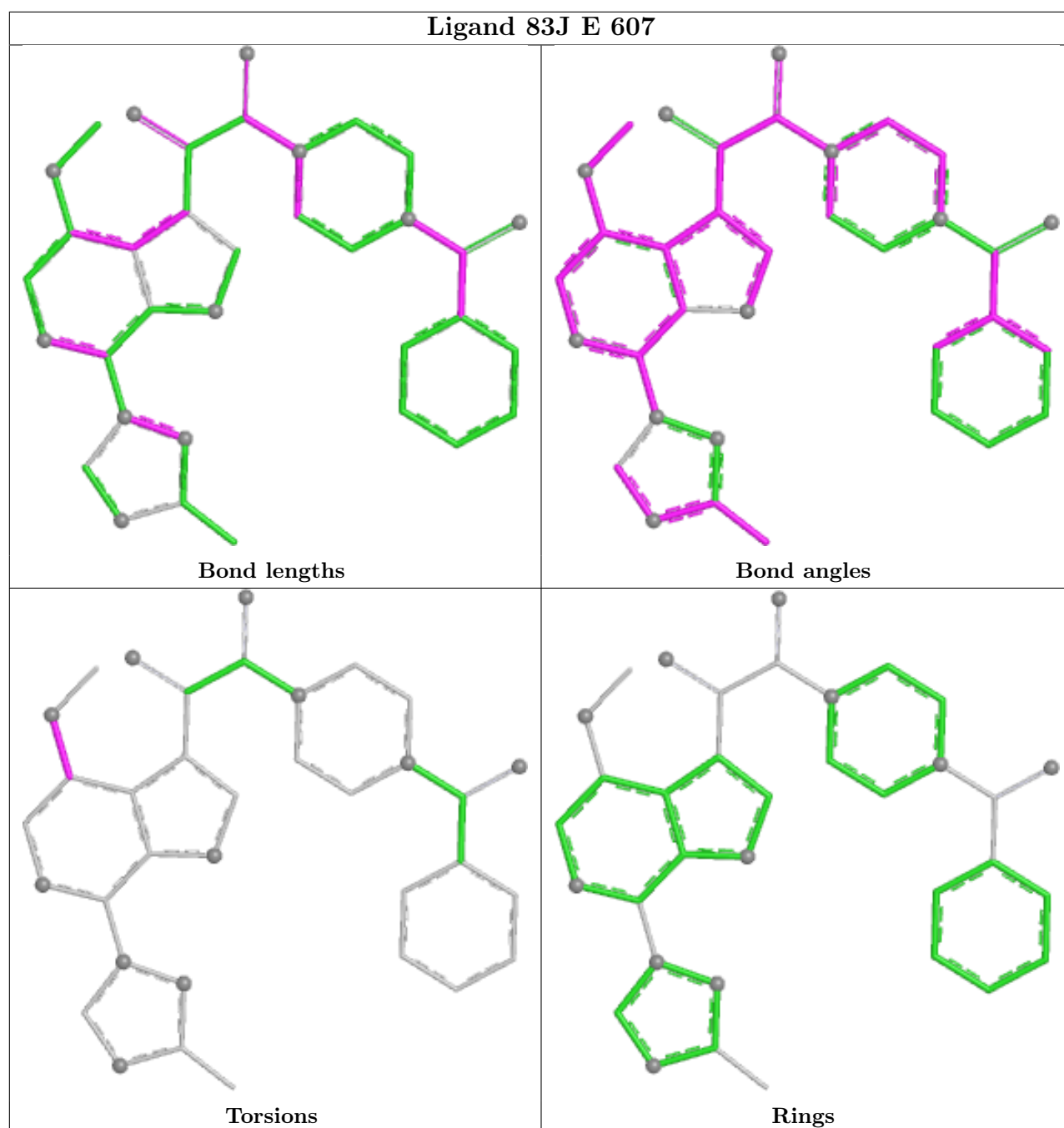
Bond angles



Torsions



Rings



## 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.

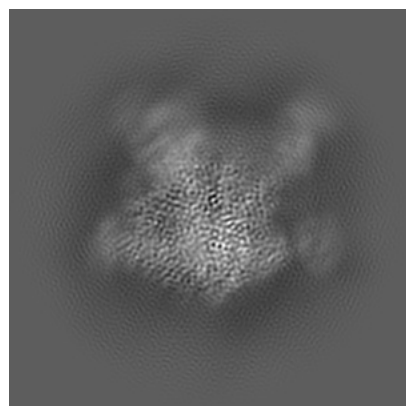
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27103. These allow visual inspection of the internal detail of the map and identification of artifacts.

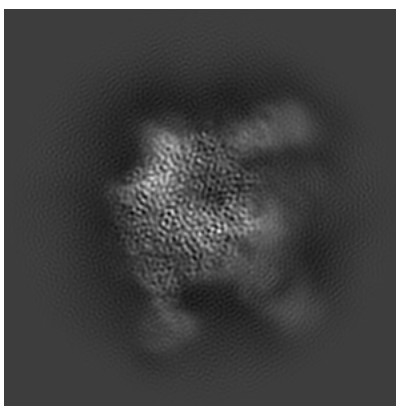
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

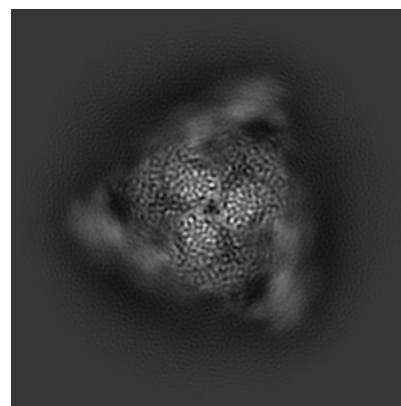
#### 6.1.1 Primary map



X

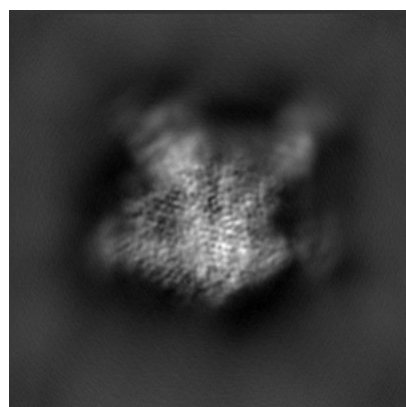


Y

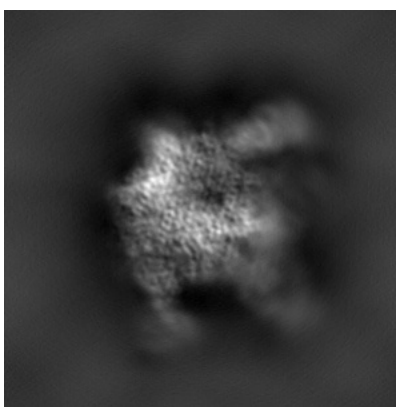


Z

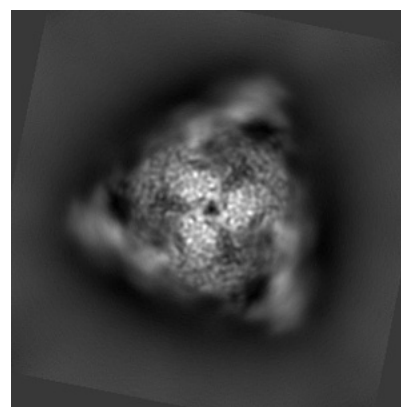
#### 6.1.2 Raw map



X



Y

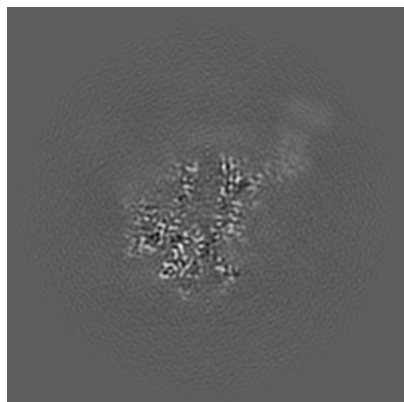


Z

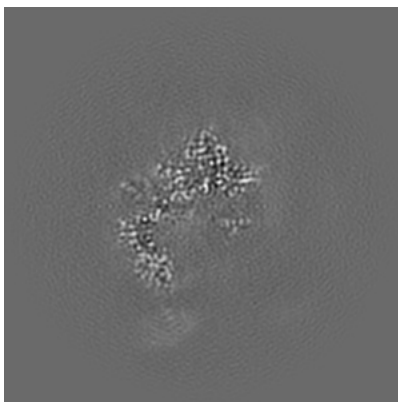
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

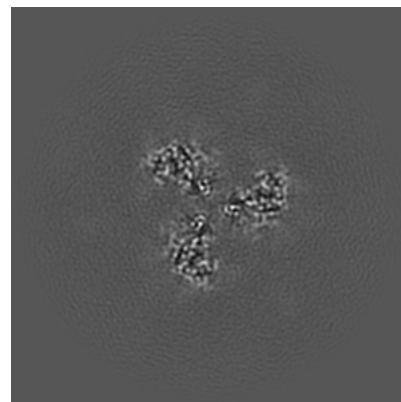
### 6.2.1 Primary map



X Index: 162

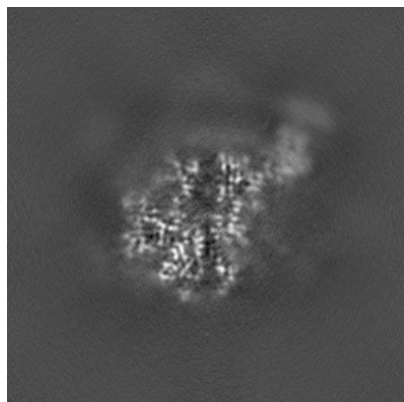


Y Index: 162

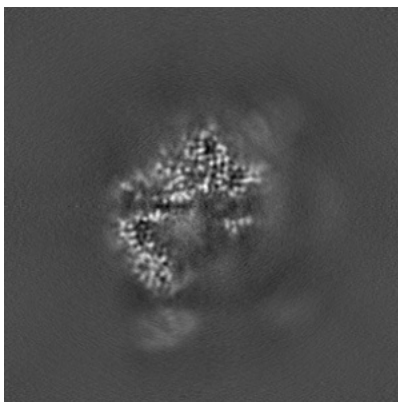


Z Index: 162

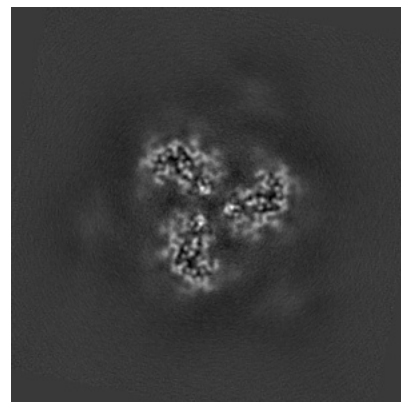
### 6.2.2 Raw map



X Index: 162



Y Index: 162

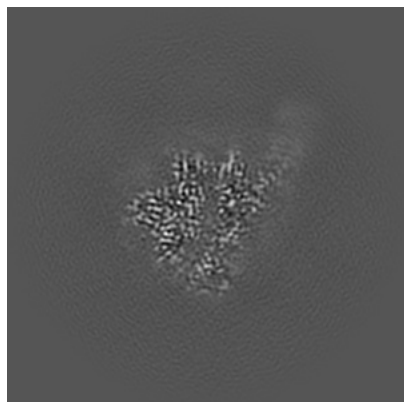


Z Index: 162

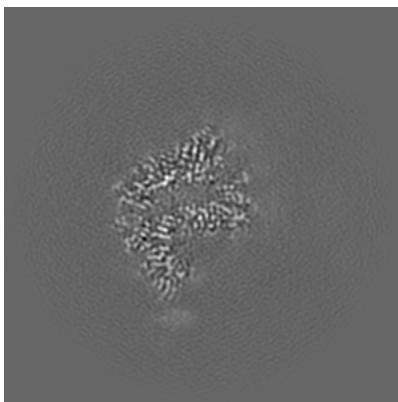
The images above show central slices of the map in three orthogonal directions.

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

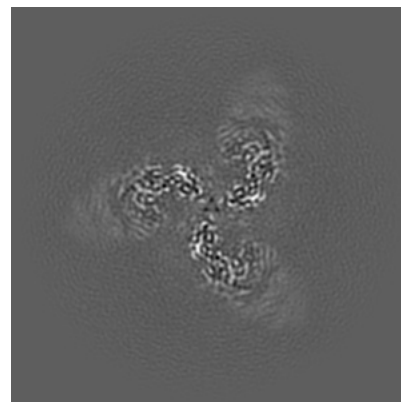
### 6.3.1 Primary map



X Index: 152

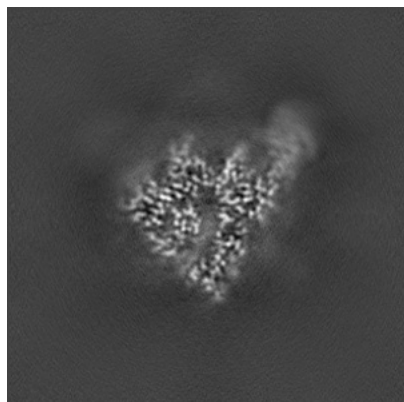


Y Index: 173

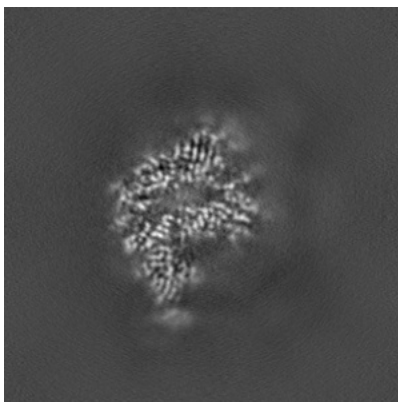


Z Index: 134

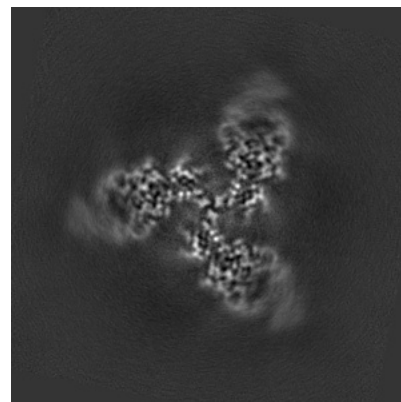
### 6.3.2 Raw map



X Index: 146



Y Index: 174

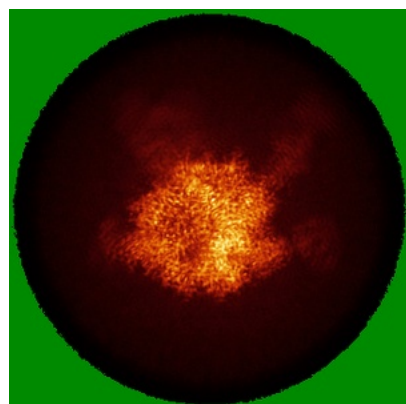


Z Index: 129

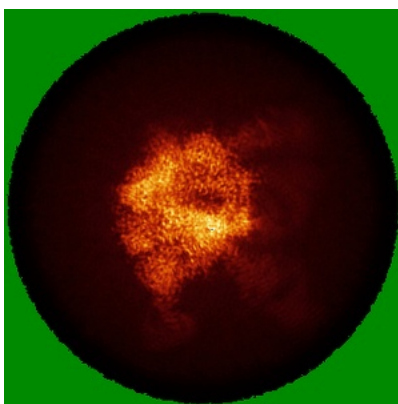
The images above show the largest variance slices of the map in three orthogonal directions.

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

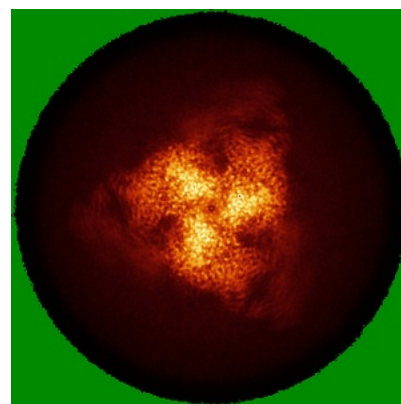
### 6.4.1 Primary map



X

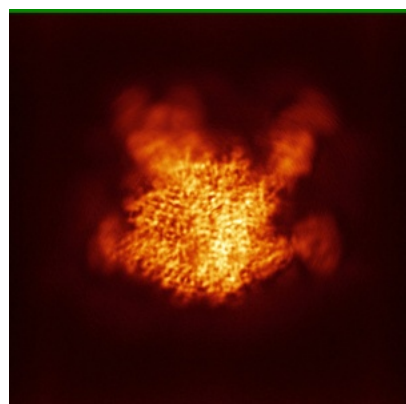


Y

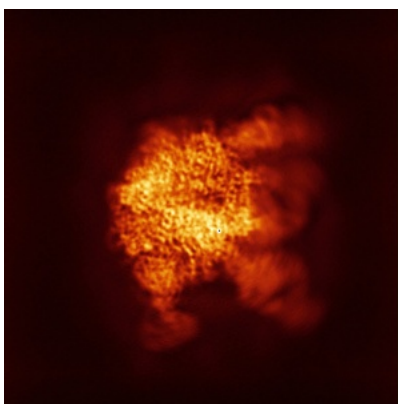


Z

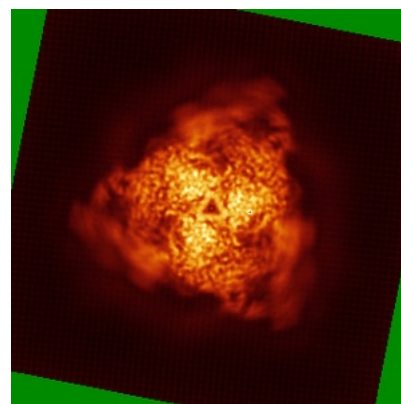
### 6.4.2 Raw map



X



Y



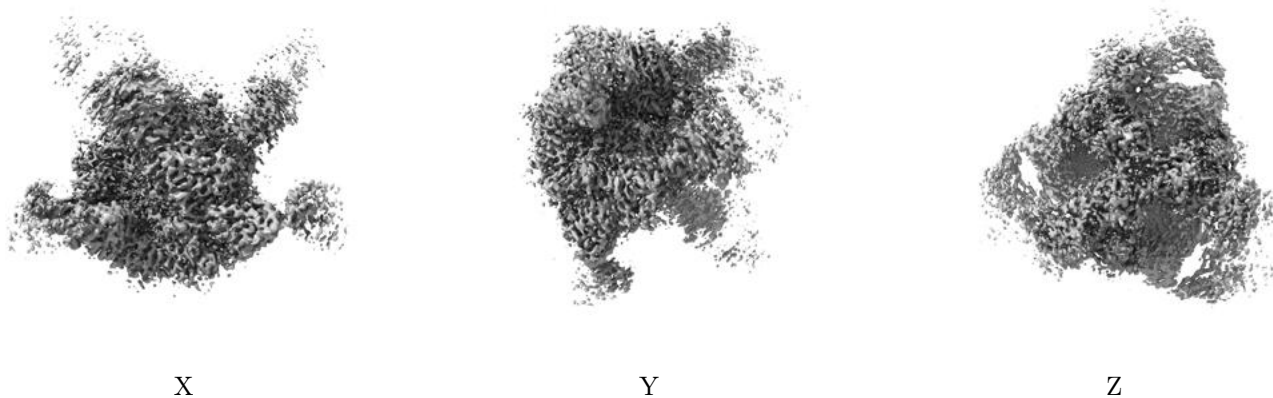
Z

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.



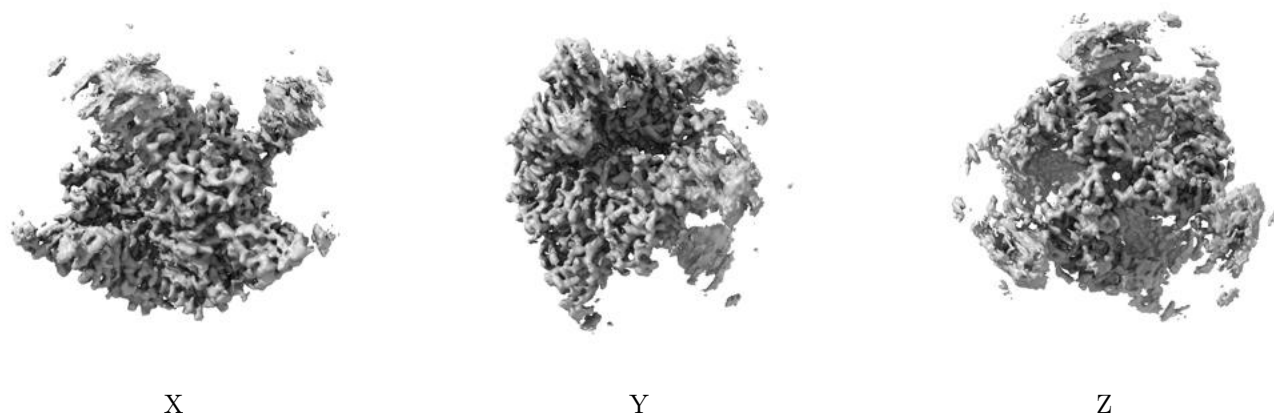
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

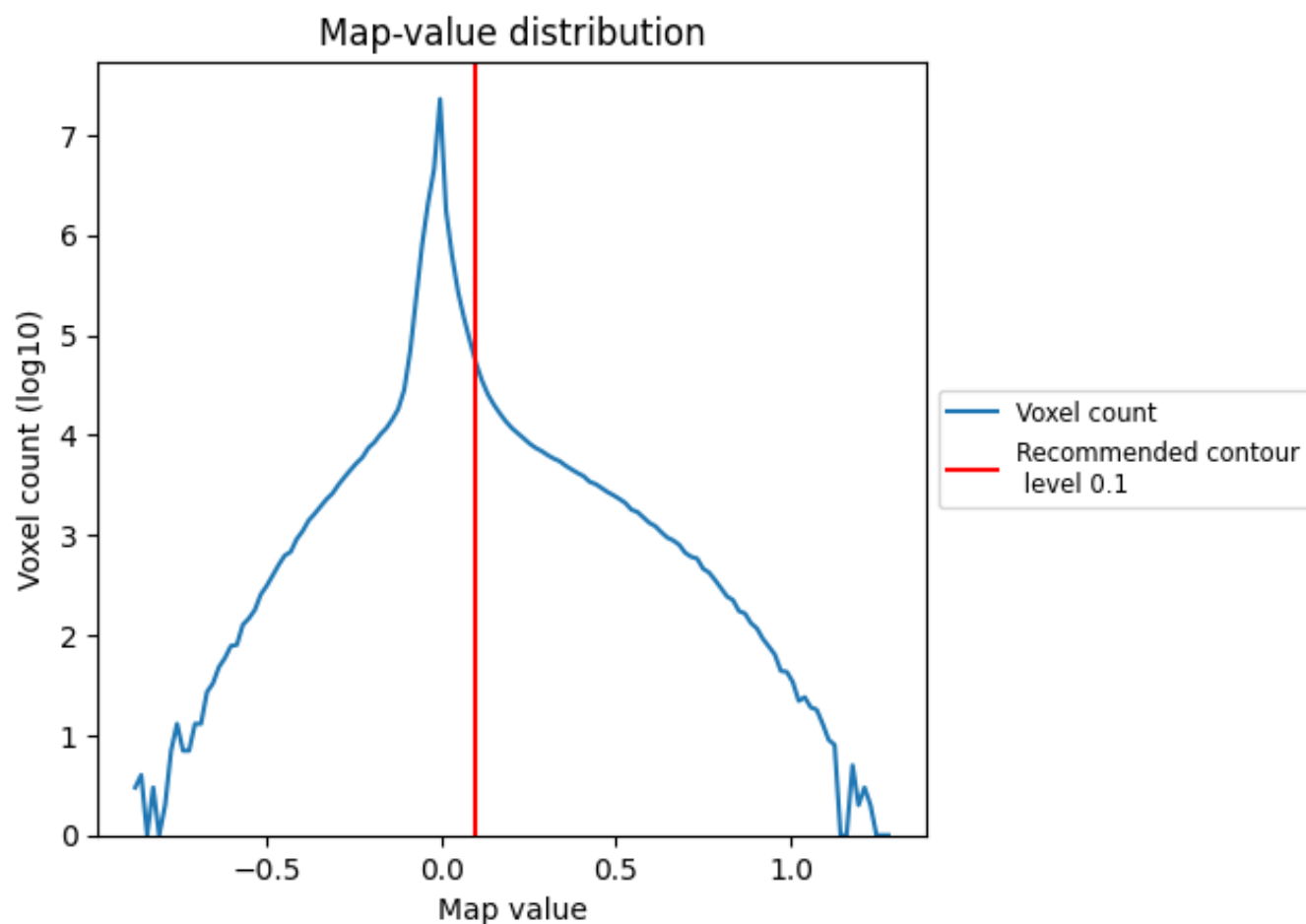
## 6.6 Mask visualisation [i](#)

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.

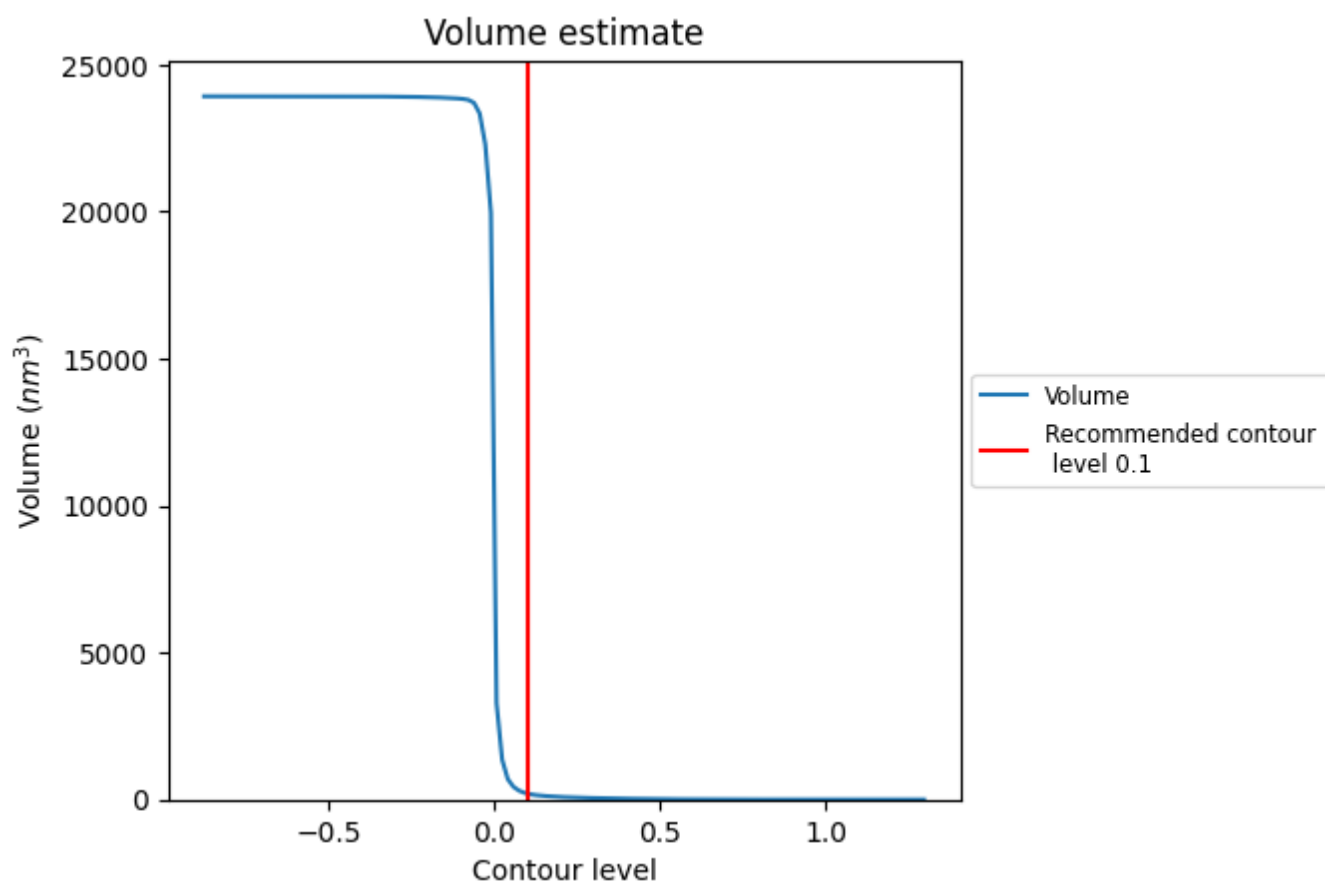
### 7.1 Map-value distribution [i](#)



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.



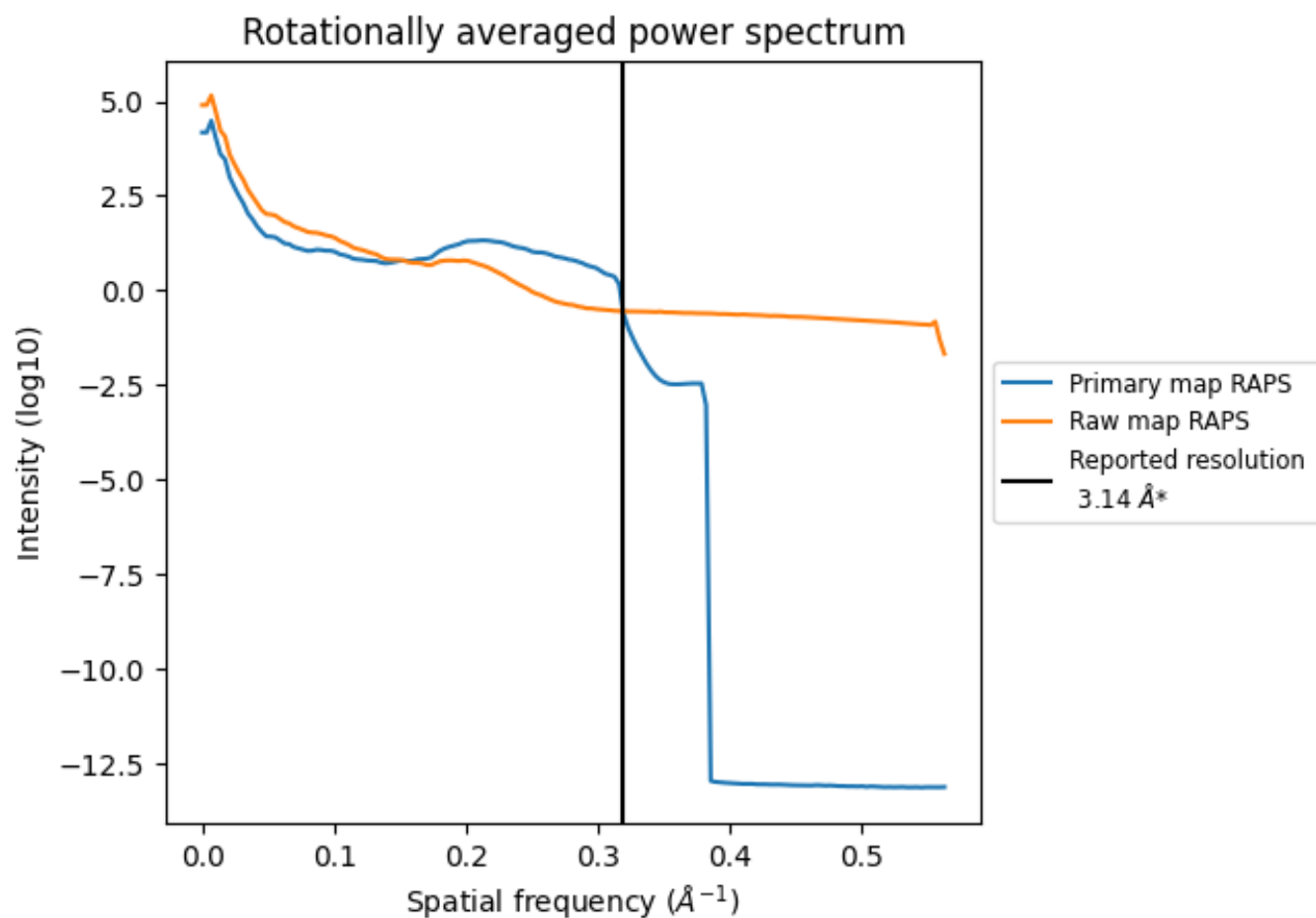
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm<sup>3</sup>; this corresponds to an approximate mass of 184 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 ⓘ

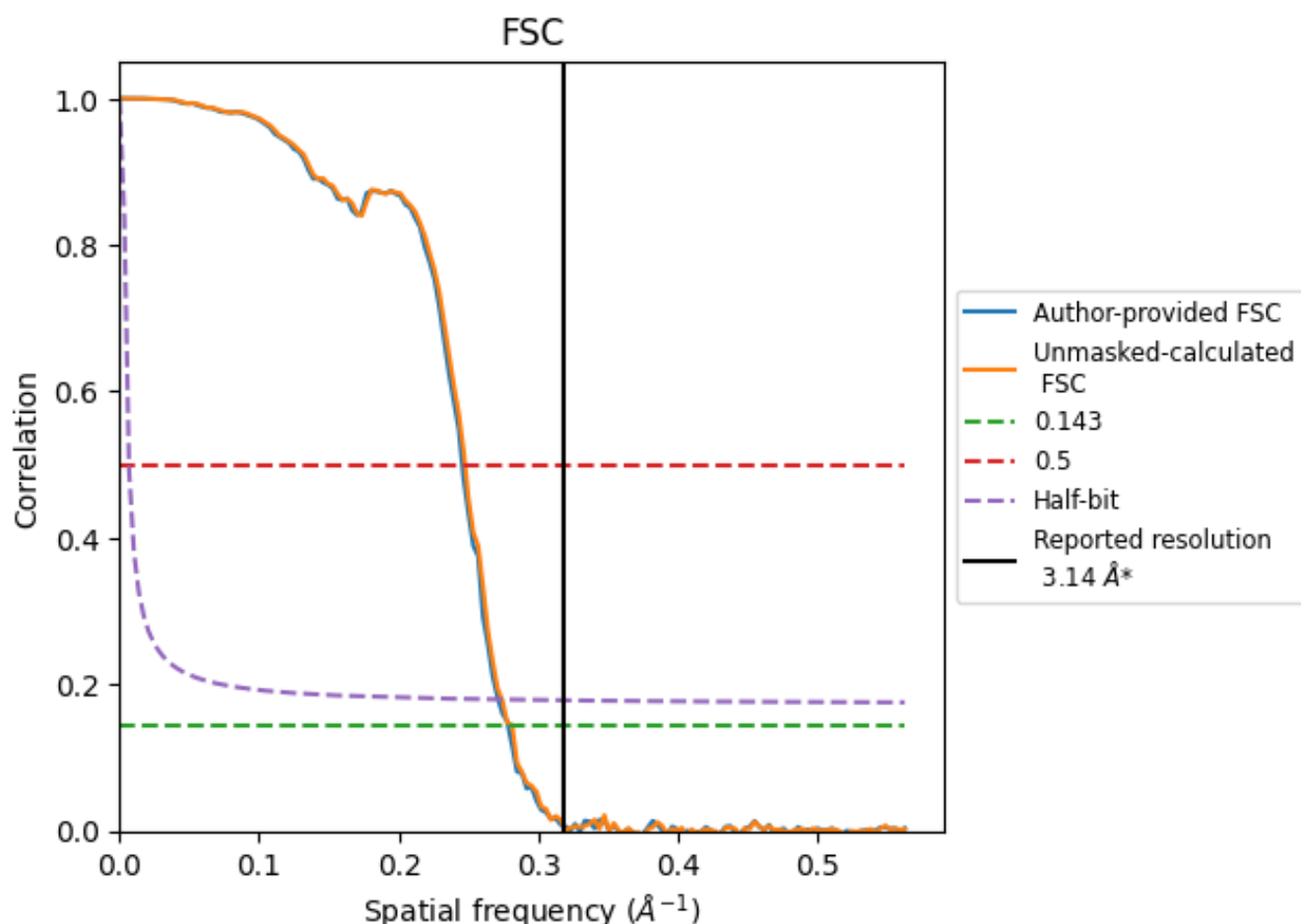


\*Reported resolution corresponds to spatial frequency of 0.318 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.59	4.07	3.69
Unmasked-calculated*	3.56	4.04	3.65

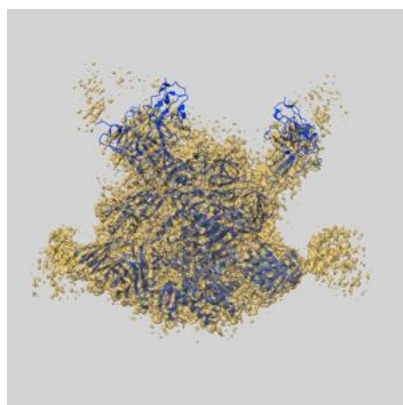
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.14 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 3.14 by more than 10 %

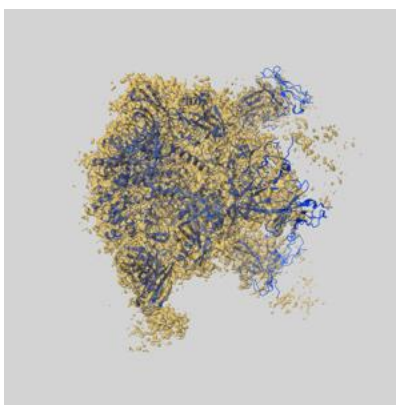
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27103 and PDB model 8CZZ. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

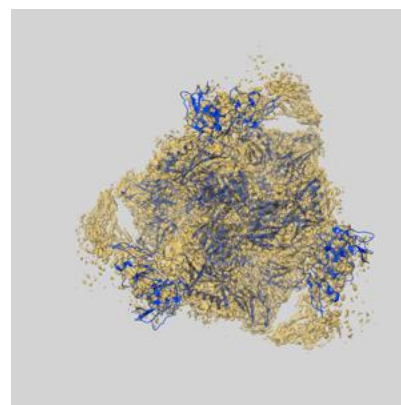
### 9.1 Map-model overlay [i](#)



X



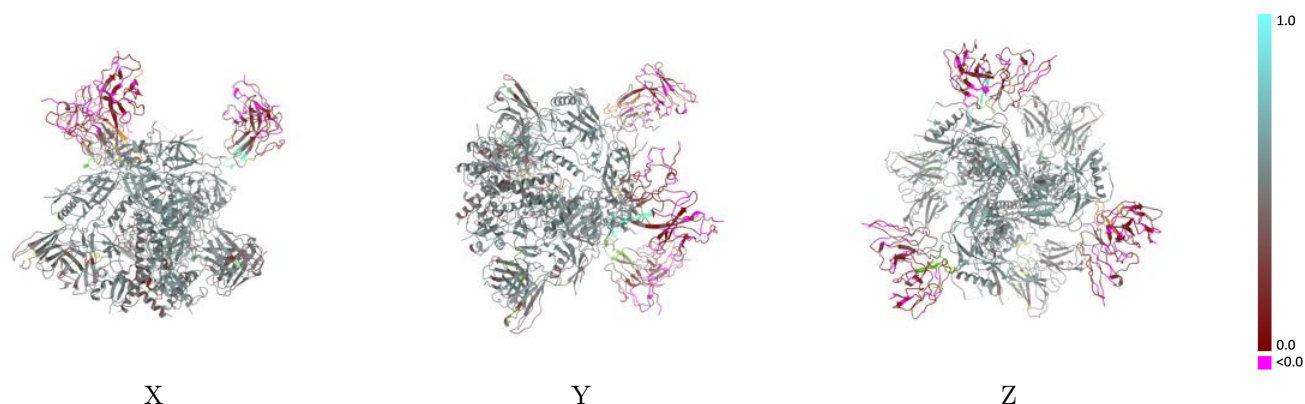
Y



Z

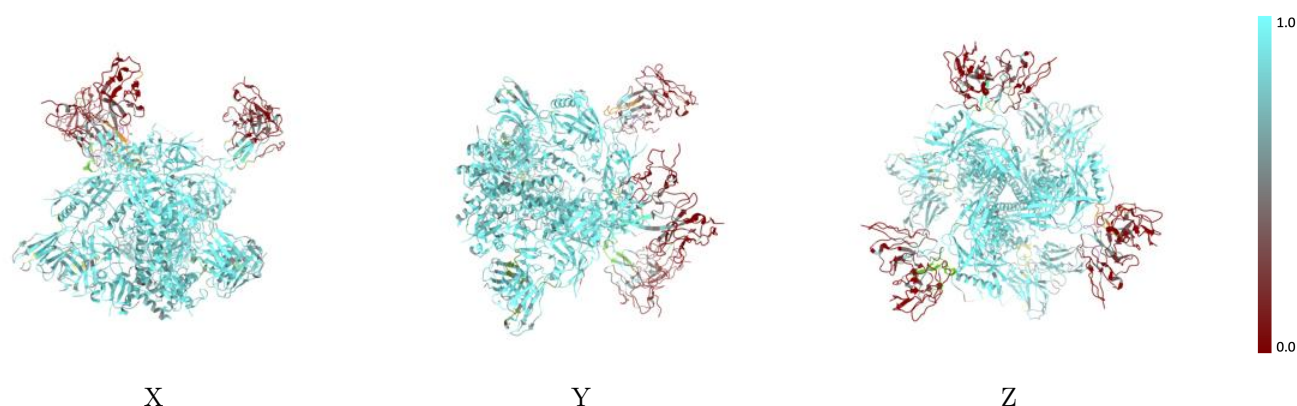
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



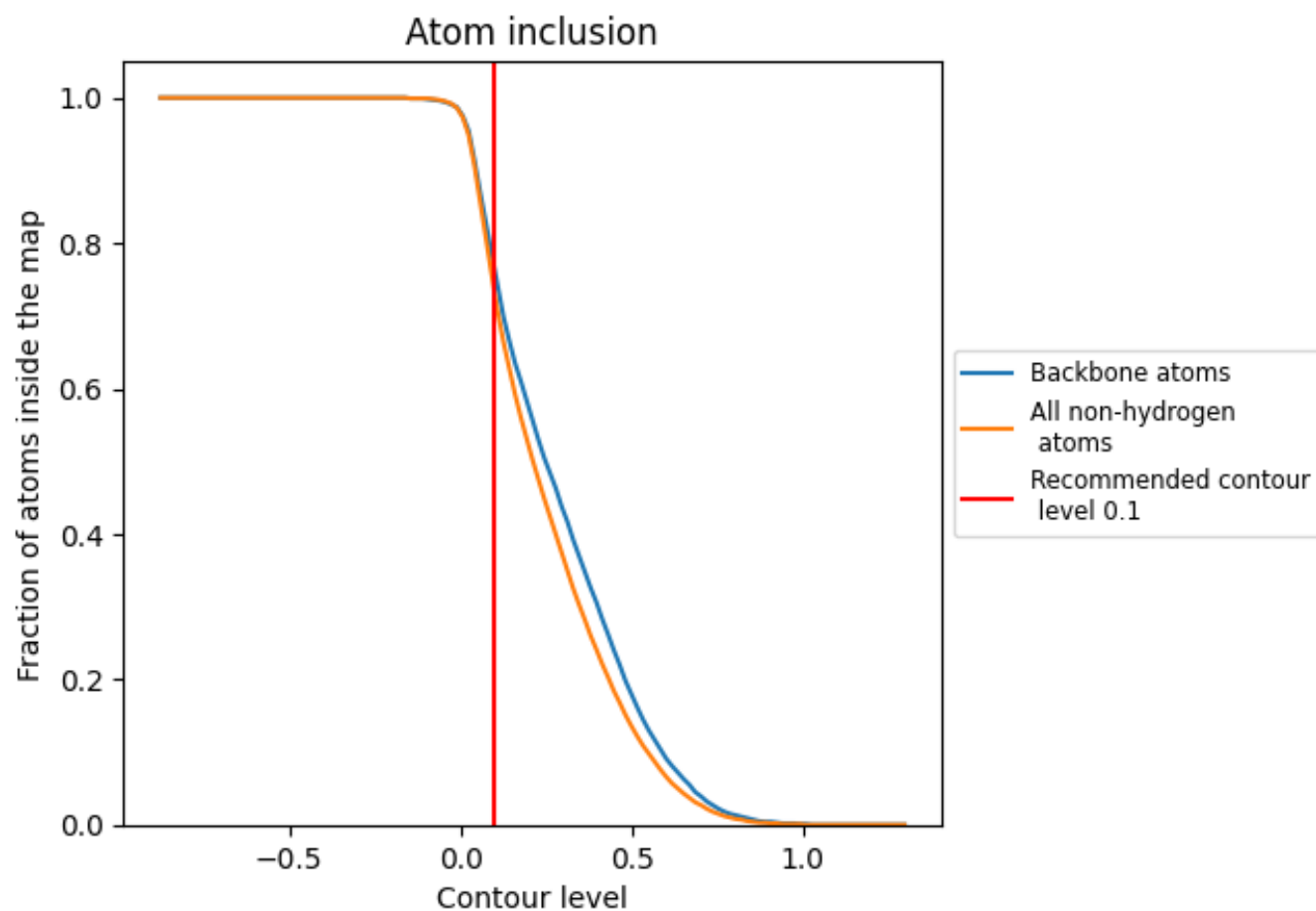
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.1) and Q-score for the entire model and for each chain.























Chain	Atom inclusion	Q-score
All	 0.7300	 0.4280
A	 0.8970	 0.5340
B	 0.8430	 0.4850
C	 0.8410	 0.4890
D	 0.8010	 0.4750
E	 0.8770	 0.5150
F	 0.8550	 0.5050
G	 0.8420	 0.5010
H	 0.7980	 0.4760
I	 0.8870	 0.5260
J	 0.7970	 0.4600
K	 0.8320	 0.4860
L	 0.7850	 0.4610
M	 0.2410	 0.1530
N	 0.3070	 0.1710
O	 0.2450	 0.1420
P	 0.3060	 0.1620
Q	 0.2370	 0.1430
R	 0.3210	 0.1630
S	 0.8480	 0.5110
T	 0.5970	 0.4000
U	 0.7320	 0.3570
V	 0.7500	 0.4280
W	 0.2140	 0.1030
X	 0.6430	 0.4180
Y	 0.9230	 0.5140
Z	 0.9230	 0.5320
a	 0.8280	 0.4820
b	 0.5970	 0.3920
c	 0.6790	 0.4590
d	 0.7680	 0.3770
e	 0.7860	 0.3900
f	 0.3210	 0.2260
g	 0.5710	 0.3490
h	 0.9230	 0.5050



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*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.9230	 0.5240
j	 0.8570	 0.5040
k	 0.5420	 0.3840
l	 0.6430	 0.4160
m	 0.6430	 0.3320
n	 0.7500	 0.3570
o	 0.7500	 0.4240
p	 0.7140	 0.4140
q	 0.7860	 0.3870
r	 0.8720	 0.4920
s	 0.7200	 0.4560