



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:05 AM UTC

PDB ID : 7UOJ / pdb_00007uoj
EMDB ID : EMD-26648
Title : The CryoEM structure of N49-P9.6-FR3 and PGT121 Fabs in complex with BG505 SOSIP.664
Authors : Nguyen, D.N.; Tolbert, W.D.; Pazgier, M.
Deposited on : 2022-04-13
Resolution : 4.02 Å (reported)
Based on initial models : 6CDI, 5CEZ, 7SX7

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

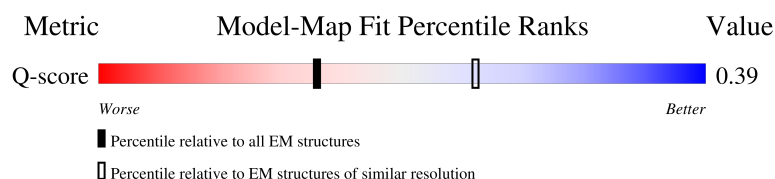
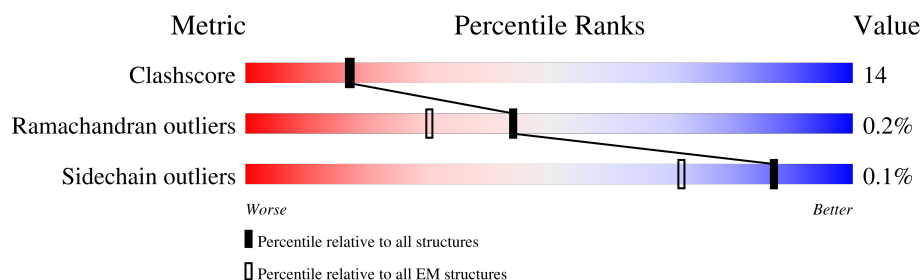
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.02 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6727 (3.52 - 4.52)

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

Mol	Chain	Length	Quality of chain
1	A	481	 69% 25% 6%
1	G	481	 66% 28% 6%
1	I	481	 67% 27% 6%
2	B	153	 61% 25% 14%

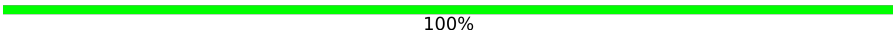
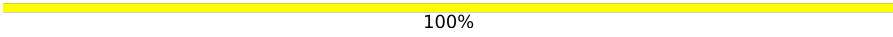
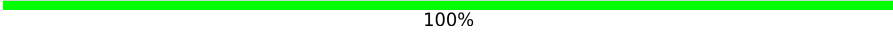
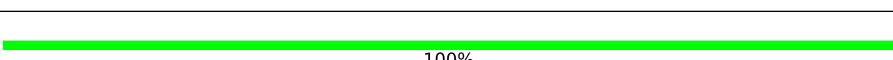
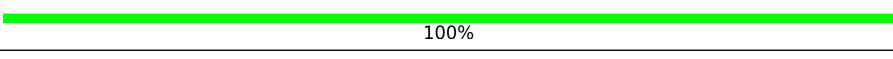
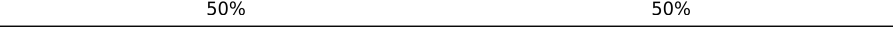
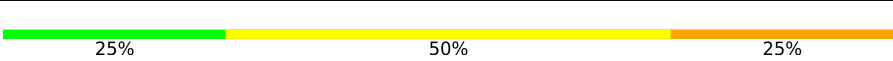
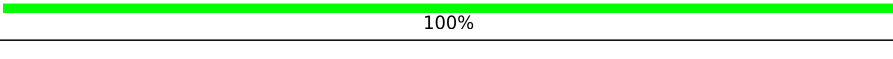
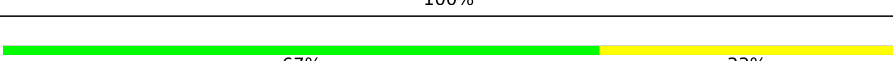
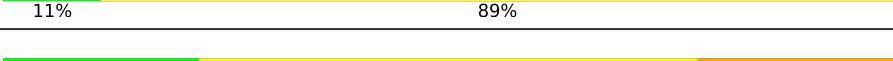
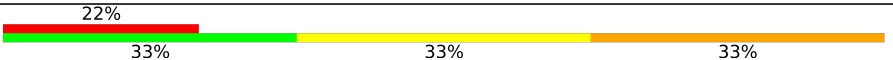
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Mol	Chain	Length	Quality of chain
2	C	153	
2	J	153	
3	D	230	
3	H	230	
3	K	230	
4	E	203	
4	L	203	
4	M	203	
5	e	213	
5	l	213	
5	m	213	
6	d	235	
6	h	235	
6	k	235	
7	F	2	
7	N	2	
7	P	2	
7	Q	2	
7	T	2	
7	V	2	
7	W	2	
7	X	2	
7	Y	2	
7	a	2	
7	b	2	

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Mol	Chain	Length	Quality of chain
7	g	2	
7	j	2	
7	n	2	
7	o	2	
7	p	2	
7	r	2	
7	s	2	
7	v	2	
7	x	2	
7	y	2	
8	O	4	
8	Z	4	
8	q	4	
9	R	3	
9	c	3	
9	t	3	
10	S	5	
10	f	5	
10	u	5	
11	U	9	
11	i	9	
11	w	9	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	W	1	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26133 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	452	Total	C	N	O	S	0	0
			3559	2233	629	669	28		
1	A	452	Total	C	N	O	S	0	0
			3559	2233	629	669	28		
1	I	452	Total	C	N	O	S	0	0
			3559	2233	629	669	28		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
I	332	ASN	THR	engineered mutation	UNP Q2N0S6
I	501	CYS	ALA	engineered mutation	UNP Q2N0S6
I	509	ARG	-	expression tag	UNP Q2N0S6
I	510	ARG	-	expression tag	UNP Q2N0S6
I	511	ARG	-	expression tag	UNP Q2N0S6
I	512	ARG	-	expression tag	UNP Q2N0S6
I	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	131	Total	C	N	O	S	0	0
			1029	651	177	195	6		
2	C	131	Total	C	N	O	S	0	0
			1029	651	177	195	6		
2	J	131	Total	C	N	O	S	0	0
			1029	651	177	195	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
C	559	PRO	ILE	engineered mutation	UNP Q2N0S6
C	605	CYS	THR	engineered mutation	UNP Q2N0S6
J	559	PRO	ILE	engineered mutation	UNP Q2N0S6
J	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called N49-P9.6-FR3 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	126	Total	C	N	O	S	0	0
			1010	642	180	181	7		
3	D	126	Total	C	N	O	S	0	0
			1010	642	180	181	7		
3	K	126	Total	C	N	O	S	0	0
			1010	642	180	181	7		

- Molecule 4 is a protein called N49-P9.6-FR3 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	98	Total	C	N	O	S	0	0
			737	464	124	146	3		
4	E	98	Total	C	N	O	S	0	0
			737	464	124	146	3		
4	M	98	Total	C	N	O	S	0	0
			737	464	124	146	3		

- Molecule 5 is a protein called PGT121 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	l	108	Total	C	N	O	S	0	0
			824	516	143	163	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	108	Total	C	N	O	S	0	0
			824	516	143	163	2		
5	m	108	Total	C	N	O	S	0	0
			824	516	143	163	2		

- Molecule 6 is a protein called PGT121 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	133	Total	C	N	O	S	0	0
			1031	652	176	199	4		
6	d	133	Total	C	N	O	S	0	0
			1031	652	176	199	4		
6	k	133	Total	C	N	O	S	0	0
			1031	652	176	199	4		

- Molecule 7 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
7	F	2	Total	C	N	O	0	0
			28	16	2	10		
7	N	2	Total	C	N	O	0	0
			28	16	2	10		
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		

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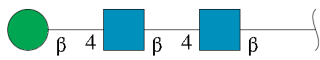
Mol	Chain	Residues	Atoms				AltConf	Trace
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	2	Total	C	N	O	0	0
			28	16	2	10		
7	n	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		
7	r	2	Total	C	N	O	0	0
			28	16	2	10		
7	s	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	x	2	Total	C	N	O	0	0
			28	16	2	10		
7	y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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.



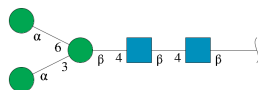
Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	4	Total	C	N	O	0	0
			50	28	2	20		
8	Z	4	Total	C	N	O	0	0
			50	28	2	20		
8	q	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 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.



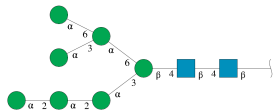
Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	3	Total	C	N	O	0	0
			39	22	2	15		
9	c	3	Total	C	N	O	0	0
			39	22	2	15		
9	t	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is an oligosaccharide called 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
10	S	5	Total	C	N	O	0	0
			61	34	2	25		
10	f	5	Total	C	N	O	0	0
			61	34	2	25		
10	u	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[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.



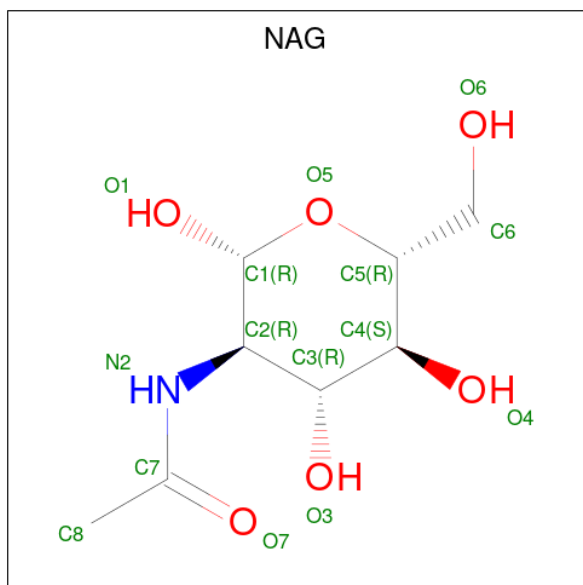
Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	9	Total	C	N	O	0	0
			105	58	2	45		
11	i	9	Total	C	N	O	0	0
			105	58	2	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	w	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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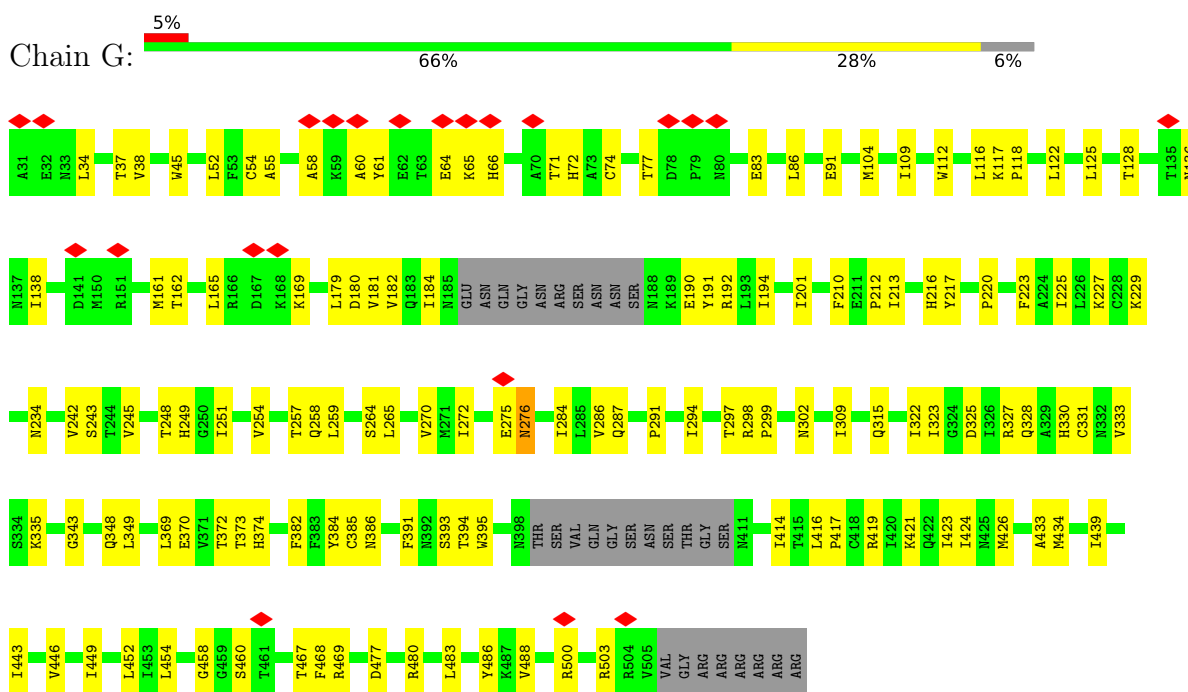
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Mol	Chain	Residues	Atoms				AltConf
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	

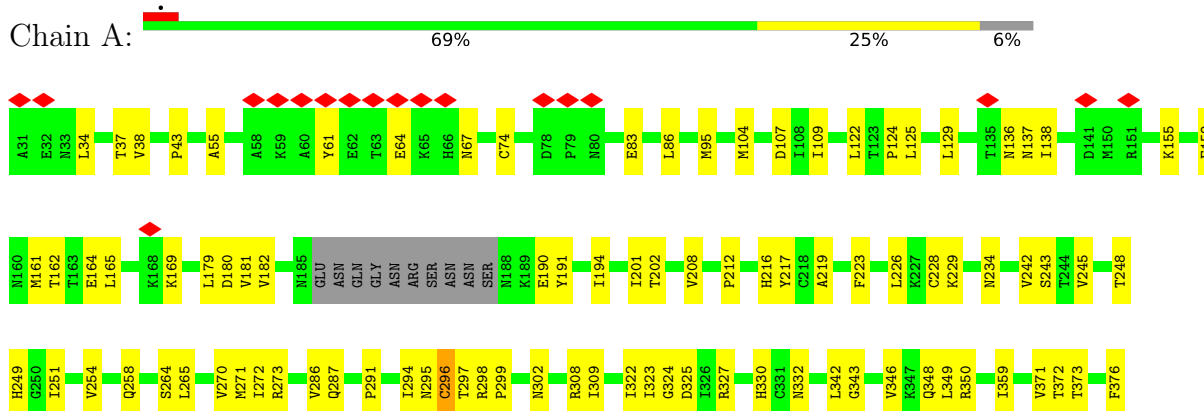
3 Residue-property plots

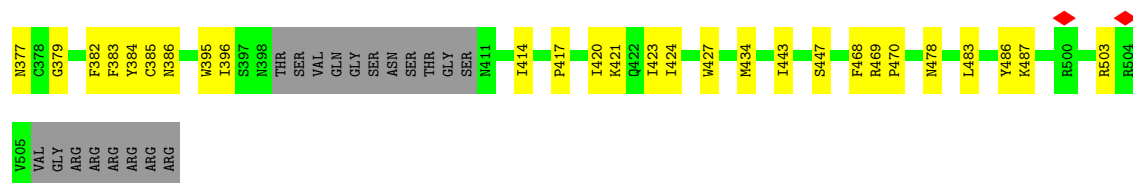
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Envelope glycoprotein gp120

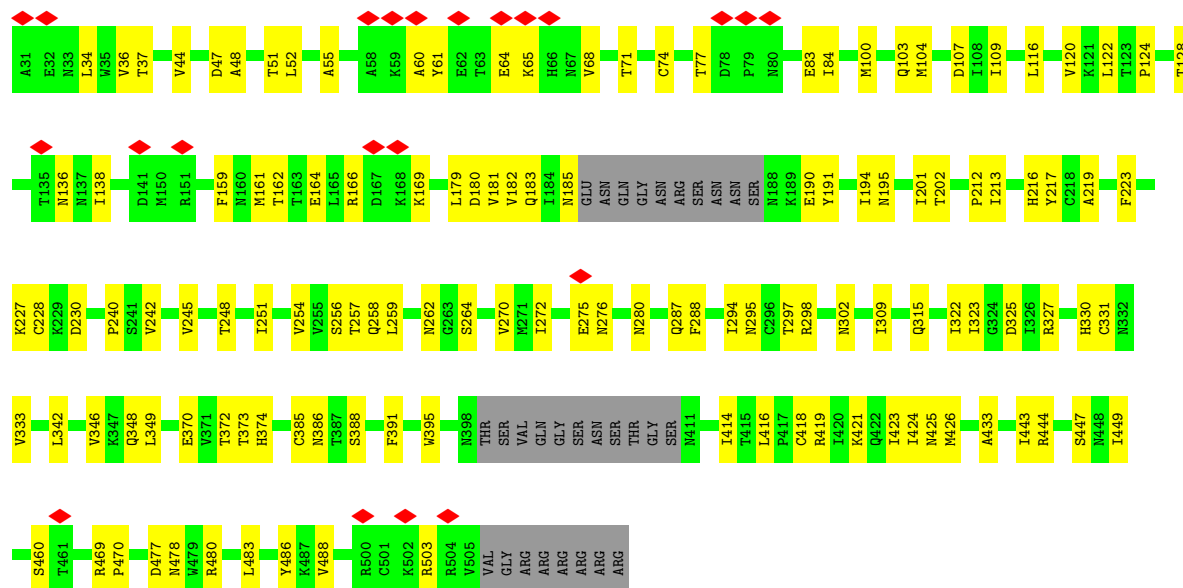


• Molecule 1: Envelope glycoprotein gp120

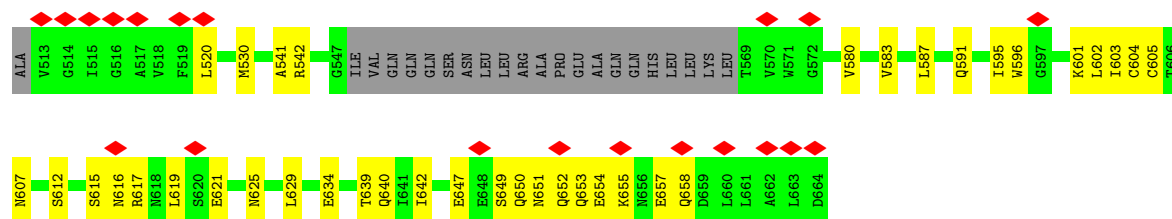




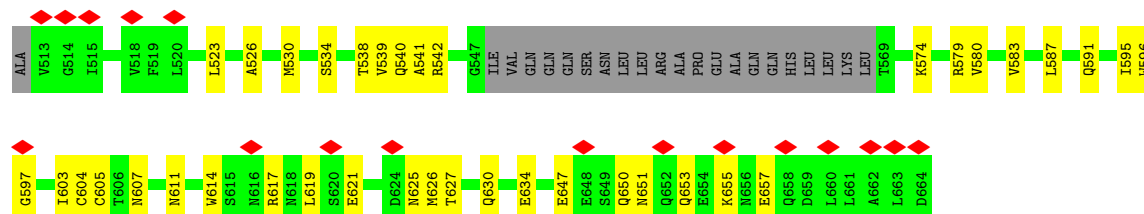
• Molecule 1: Envelope glycoprotein gp120



• Molecule 2: Envelope glycoprotein gp41



• Molecule 2: Envelope glycoprotein gp41



Chain J:

12% 58% 27% 14%

ALA V513 G514 I515 G516 F519 L520 G521 F522 L523 A526 G527 S528 T529 M530 S534 M535 L536 L537 A541 A542 G547 ILE VAL GLN GLN GLN SER ASN LEU LEU ARG ALA ALA GLN GLN HIS LEU LEU LYS LEU T569 G572 L573 K574 G576 L576 V580 V583

Y586 L587 Q591 G597 C605 T606 M607 W610 M616 R617 N618 L619 S620 E621 L622 W623 W628 G631 D632 K633 E634 T639 Q640 I641 I642 E648 M651 Q652 Q653 E654 K655 Q658 D659 L660 L661 A662 L663 D664

Chain H:

36% 19% 45%

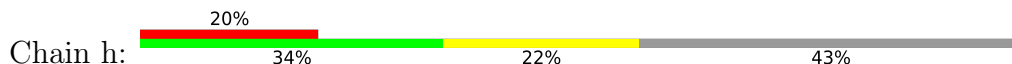
Position	Amino Acid	Conservation Score (approx.)
H1	SER	10
L4	GLY	10
V5	ALA	10
Q6	LEU	10
V11	THR	10
K12	SER	10
R19	GLY	10
E23	VAL	10
N28	HIS	10
F29	THR	10
Q32	PHE	10
F33	PRO	10
V37	ALA	10
A40	VAL	10
Q43	LEU	10
G44	SER	10
L45	SER	10
F46	VAL	10
W47	THR	10
N52	VAL	10
Y54	PRO	10
G55	SER	10
Q56	SER	10
W61	LEU	10
R62	THR	10
F63	GLN	10
Q64	THR	10
G65	ILE	10
R66	CYS	10
V67	ASN	10
T68	VAL	10
D76C	ASN	10
G76G	HIS	10
T77	LYS	10
A78	PRO	10
F79	SER	10
W80	ASN	10
E81	THR	10
L82	LYS	10
L82C	ASP	10
R83	VAL	10
V84	ARG	10
D85	GLU	10
D86	PRO	10

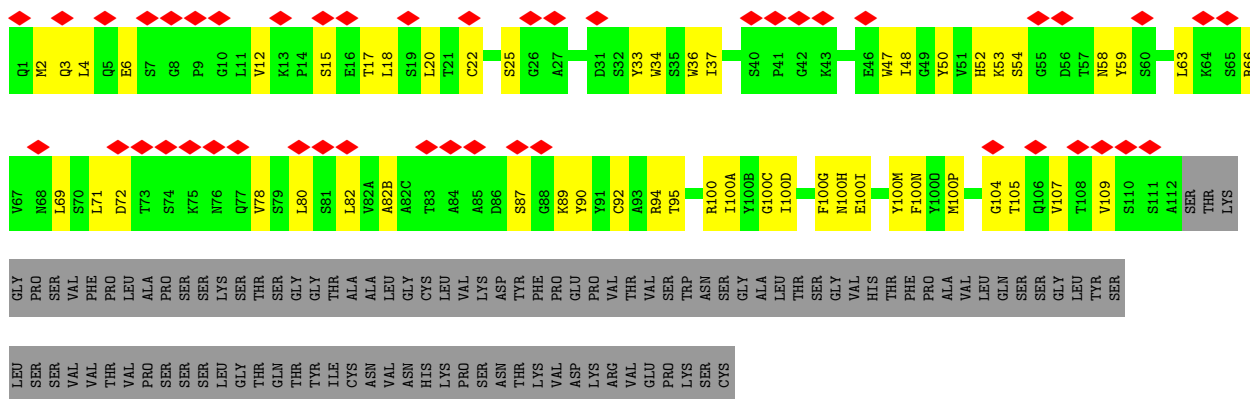
[illegible]

Chain K:

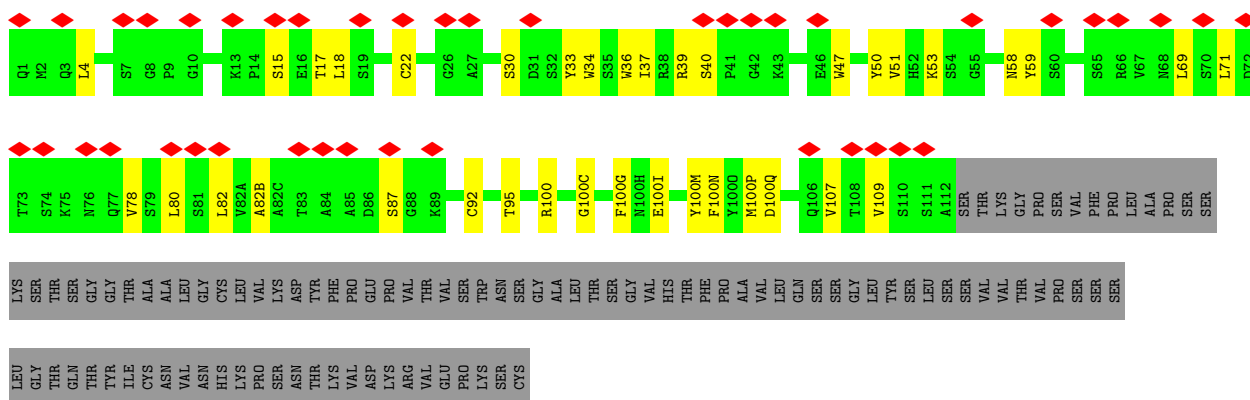
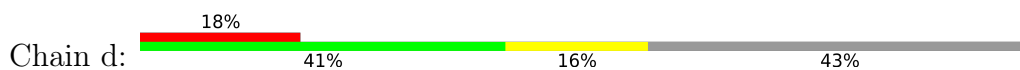
35% 20% 45%

Position	Residue	Category
1	T87	Yellow
2	Q32	Green
3	Y90	Yellow
4	Y91	Yellow
5	P96	Yellow
6	E99	Yellow
7	N100	Yellow
8	Y100A	Yellow
9	G106	Yellow
10	V107	Yellow
11	V110	Yellow
12	V111	Yellow
13	S112	Green
14	SER	Grey
15	ALA	Grey
16	SER	Grey
17	SER	Grey
18	THR	Grey
19	LYS	Grey
20	GLY	Grey
21	PRO	Grey
22	SER	Grey
23	VAL	Green
24	PHE	Grey
25	PRO	Grey
26	LEU	Grey
27	LEU	Grey
28	ALA	Grey
29	PRO	Grey
30	SER	Grey
31	SER	Grey
32	LYS	Grey
33	SER	Grey
34	THR	Grey
35	GLY	Grey
36	GLY	Grey
37	THR	Grey
38	ALA	Grey
39	ALA	Grey
40	LEU	Grey
41	CYS	Grey
42	LEU	Grey
43	VAL	Yellow
44	LYS	Yellow
45	ASP	Grey
46	THR	Grey
47	PHE	Grey
48	GLU	Grey
49	PRO	Grey
50	THR	Grey
51	VAL	Yellow
52	SER	Grey
53	TRP	Green

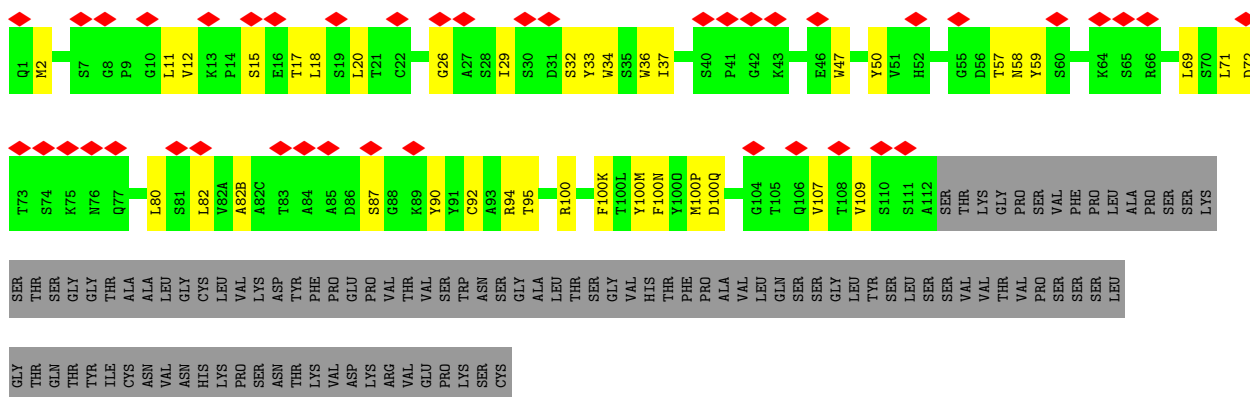




- Molecule 6: PGT121 Fab heavy chain



- Molecule 6: PGT121 Fab heavy chain



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



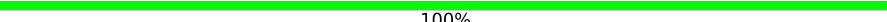
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

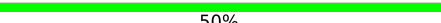
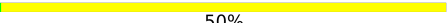


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50%
 100%

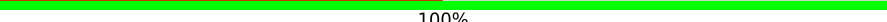


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50%
 50%

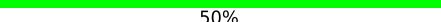
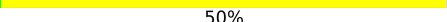


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50%
 100%

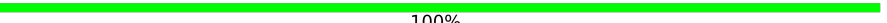


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  50%
 50%
 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  50% 50%



- Molecule 8: 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 O:  50% 25% 25%



- Molecule 8: 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 Z:  50% 50%



- Molecule 8: 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 q:  25% 50% 25%



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

Chain R:  100%



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

Chain c:  100%



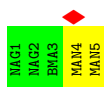
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t: 67% 33%



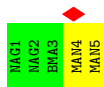
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 20% 60% 40%



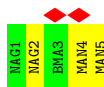
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 20% 60% 40%



- Molecule 10: 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 u: 40% 40% 60%

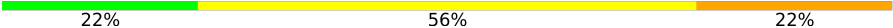


- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 11% 89%

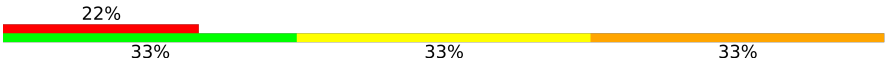


- Molecule 11: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain i: 



- Molecule 11: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain w: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	132055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	49.328	Depositor
Minimum map value	-48.408	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.8	Depositor
Map size ($\text{\AA}$)	355.72, 355.72, 355.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3895313, 1.3895313, 1.3895313	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/3633	0.43	0/4933
1	G	0.20	0/3633	0.45	1/4933 (0.0%)
1	I	0.16	0/3633	0.40	0/4933
2	B	0.13	0/1047	0.37	0/1420
2	C	0.14	0/1047	0.42	0/1420
2	J	0.14	0/1047	0.40	0/1420
3	D	0.20	0/1041	0.43	0/1414
3	H	0.17	0/1041	0.41	0/1414
3	K	0.19	0/1041	0.46	2/1414 (0.1%)
4	E	0.14	0/756	0.41	0/1029
4	L	0.17	0/756	0.41	0/1029
4	M	0.14	0/756	0.39	0/1029
5	e	0.16	0/845	0.34	0/1154
5	l	0.17	0/845	0.35	0/1154
5	m	0.14	0/845	0.34	0/1154
6	d	0.13	0/1057	0.35	0/1436
6	h	0.13	0/1057	0.36	0/1436
6	k	0.14	0/1057	0.35	0/1436
All	All	0.17	0/25137	0.41	3/34158 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	39	GLN	CA-C-N	5.56	129.34	121.61
3	K	39	GLN	C-N-CA	5.56	129.34	121.61
1	G	276	ASN	CA-CB-CG	5.10	117.70	112.60

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	3559	0	3491	93	0
1	G	3559	0	3491	120	0
1	I	3559	0	3492	95	0
2	B	1029	0	1009	29	0
2	C	1029	0	1009	36	0
2	J	1029	0	1009	36	0
3	D	1010	0	950	35	0
3	H	1010	0	950	34	0
3	K	1010	0	950	37	0
4	E	737	0	715	27	0
4	L	737	0	715	16	0
4	M	737	0	715	20	0
5	e	824	0	785	40	0
5	l	824	0	785	27	0
5	m	824	0	785	33	0
6	d	1031	0	999	27	0
6	h	1031	0	999	40	0
6	k	1031	0	999	32	0
7	F	28	0	25	0	0
7	N	28	0	25	0	0
7	P	28	0	25	0	0
7	Q	28	0	25	0	0
7	T	28	0	25	0	0
7	V	28	0	25	1	0
7	W	28	0	25	9	0
7	X	28	0	25	0	0
7	Y	28	0	25	0	0
7	a	28	0	25	2	0
7	b	28	0	25	0	0
7	g	28	0	25	0	0
7	j	28	0	25	0	0
7	n	28	0	25	3	0
7	o	28	0	25	0	0
7	p	28	0	25	1	0
7	r	28	0	25	1	0
7	s	28	0	25	0	0
7	v	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	x	28	0	25	0	0
7	y	28	0	25	3	0
8	O	50	0	43	1	0
8	Z	50	0	43	0	0
8	q	50	0	43	2	0
9	R	39	0	34	0	0
9	c	39	0	34	0	0
9	t	39	0	34	1	0
10	S	61	0	52	0	0
10	f	61	0	52	0	0
10	u	61	0	52	1	0
11	U	105	0	88	2	0
11	i	105	0	88	2	0
11	w	105	0	88	2	0
12	A	70	0	65	3	0
12	G	70	0	65	1	0
12	I	70	0	65	1	0
All	All	26133	0	25219	707	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 14.

All (707) 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:G:276:ASN:CB	7:W:1:NAG:H62	1.36	1.54
1:G:276:ASN:HB3	7:W:1:NAG:C6	1.56	1.36
1:G:373:THR:HB	1:G:385:CYS:O	1.31	1.25
3:D:33:PHE:HB2	3:D:100:ASN:OD1	1.55	1.05
5:l:92:ASP:OD2	5:l:95:VAL:HG23	1.61	1.01
1:A:373:THR:HB	1:A:385:CYS:O	1.67	0.94
3:K:33:PHE:HB2	3:K:100:ASN:ND2	1.84	0.93
1:G:276:ASN:HB2	7:W:1:NAG:H62	1.47	0.93
3:D:100:ASN:O	3:D:100(A):TYR:HD1	1.52	0.91
1:G:373:THR:HG21	1:G:386:ASN:OD1	1.73	0.89
5:l:37:GLN:HB2	5:l:47:ILE:HD11	1.55	0.87
1:G:393:SER:HB3	1:G:395:TRP:HE1	1.40	0.84
4:M:86:TYR:O	4:M:101:GLY:HA2	1.78	0.84
1:A:182:VAL:HG13	1:A:194:ILE:HG22	1.57	0.83
1:G:161:MET:HE2	1:G:309:ILE:HG13	1.58	0.83
1:A:395:TRP:HE1	12:A:605:NAG:H83	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:ASN:CB	7:W:1:NAG:C6	2.32	0.81
6:h:37:ILE:HD11	6:h:100(P):MET:HE3	1.61	0.81
6:h:17:THR:HA	6:h:82:LEU:O	1.82	0.80
4:L:86:TYR:O	4:L:101:GLY:HA2	1.81	0.79
1:A:298:ARG:HG2	1:A:443:ILE:HG22	1.65	0.78
1:G:393:SER:HB3	1:G:395:TRP:NE1	1.99	0.78
6:d:17:THR:HA	6:d:82:LEU:O	1.84	0.77
6:k:17:THR:HA	6:k:82:LEU:O	1.86	0.76
4:L:3:LEU:N	4:L:23:CYS:SG	2.60	0.75
6:k:37:ILE:HD11	6:k:100(P):MET:HE3	1.69	0.75
4:E:86:TYR:O	4:E:101:GLY:HA2	1.87	0.74
1:I:280:ASN:ND2	4:M:96:GLU:OE1	2.20	0.74
1:I:298:ARG:NH1	1:I:302:ASN:OD1	2.20	0.74
4:E:3:LEU:N	4:E:23:CYS:SG	2.60	0.74
6:d:37:ILE:HD11	6:d:100(P):MET:HE3	1.69	0.74
1:G:272:ILE:HD13	1:G:349:LEU:HD23	1.69	0.73
4:L:46:LEU:HD21	4:L:49:PHE:HB3	1.70	0.73
4:L:38:GLN:HB2	4:L:44:PRO:HB3	1.71	0.73
1:G:276:ASN:HB3	7:W:1:NAG:C5	2.18	0.73
3:H:32:GLN:NE2	3:H:96:PRO:O	2.21	0.73
1:I:182:VAL:HG13	1:I:194:ILE:HG22	1.71	0.72
1:G:182:VAL:HG13	1:G:194:ILE:HG22	1.70	0.72
4:L:79:GLN:NE2	4:L:81:GLU:OE1	2.21	0.72
1:A:373:THR:CB	1:A:385:CYS:O	2.37	0.72
1:A:298:ARG:NH1	1:A:302:ASN:OD1	2.23	0.72
4:E:35:TRP:HB2	4:E:48:ILE:HB	1.71	0.71
1:G:227:LYS:HD3	1:G:486:TYR:HE1	1.55	0.71
1:G:424:ILE:HD12	1:G:426:MET:HG3	1.71	0.71
6:k:2:MET:HA	6:k:26:GLY:HA3	1.72	0.71
1:G:276:ASN:HB3	7:W:1:NAG:H62	0.73	0.71
2:C:617:ARG:HD3	2:C:626:MET:HE1	1.72	0.71
1:G:343:GLY:HA2	1:G:395:TRP:HZ3	1.55	0.70
4:E:32:ILE:HG13	7:n:2:NAG:H61	1.74	0.70
4:E:79:GLN:NE2	4:E:81:GLU:OE1	2.23	0.70
1:I:179:LEU:HD21	1:I:419:ARG:HH12	1.57	0.70
1:A:372:THR:HG23	1:A:373:THR:HG23	1.72	0.70
2:B:617:ARG:NE	2:B:634:GLU:OE1	2.24	0.70
1:A:254:VAL:O	1:A:478:ASN:ND2	2.25	0.70
4:M:79:GLN:NE2	4:M:81:GLU:OE1	2.24	0.70
1:G:64:GLU:HG2	1:G:65:LYS:HG3	1.72	0.69
3:K:32:GLN:NE2	3:K:96:PRO:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:m:46:LEU:HD22	6:k:100(Q):ASP:HA	1.73	0.69
1:I:227:LYS:HD3	1:I:486:TYR:HE1	1.58	0.69
1:G:327:ARG:HD2	6:h:100(C):GLY:HA2	1.75	0.69
1:I:373:THR:HB	1:I:386:ASN:HA	1.75	0.69
1:A:83:GLU:OE2	1:A:229:LYS:NZ	2.25	0.69
4:E:31:ILE:HA	7:n:2:NAG:H62	1.74	0.69
1:G:162:THR:HG22	1:G:169:LYS:HE2	1.75	0.68
3:D:38:ARG:NH1	3:D:86:ASP:OD1	2.27	0.68
1:G:343:GLY:HA2	1:G:395:TRP:CZ3	2.29	0.67
2:B:541:ALA:O	2:J:591:GLN:NE2	2.27	0.67
4:E:20:THR:HG22	4:E:74:THR:HG22	1.75	0.67
1:I:272:ILE:HD12	1:I:348:GLN:HG3	1.76	0.67
1:A:349:LEU:HD23	1:A:359:ILE:HD13	1.77	0.67
1:A:37:THR:HG22	2:C:605:CYS:HA	1.77	0.66
3:K:66:ARG:HH12	3:K:83:ARG:HH21	1.41	0.66
6:d:18:LEU:HD21	6:d:107:VAL:HG21	1.77	0.66
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.76	0.66
3:H:66:ARG:HH12	3:H:83:ARG:HH21	1.42	0.66
6:d:18:LEU:HB3	6:d:82:LEU:HB2	1.77	0.66
3:D:35:ASN:HD22	3:D:50:TRP:HB3	1.61	0.65
5:e:47:ILE:HG22	5:e:48:ILE:HG12	1.79	0.65
6:d:15:SER:HA	6:d:82(B):ALA:HA	1.76	0.65
1:A:95:MET:HE1	1:A:273:ARG:HD3	1.78	0.65
2:C:591:GLN:NE2	2:J:541:ALA:O	2.29	0.65
1:I:327:ARG:HH21	1:I:330:HIS:HE1	1.44	0.65
2:B:603:ILE:HG21	2:J:658:GLN:HG3	1.76	0.65
1:G:417:PRO:HB3	6:h:100(G):PHE:HE1	1.62	0.65
1:A:83:GLU:HG3	1:A:245:VAL:HB	1.79	0.64
1:G:136:ASN:HB3	1:G:138:ILE:HG23	1.78	0.64
1:G:190:GLU:OE2	1:G:190:GLU:N	2.29	0.64
5:m:35:TRP:HB2	5:m:48:ILE:HB	1.80	0.64
1:G:458:GLY:HA3	3:H:47:TRP:HZ3	1.63	0.64
1:I:34:LEU:HB3	2:J:610:TRP:HB3	1.79	0.64
6:h:18:LEU:HD21	6:h:107:VAL:HG21	1.79	0.64
1:G:373:THR:CB	1:G:385:CYS:O	2.27	0.64
1:A:155:LYS:NZ	12:A:602:NAG:O6	2.31	0.64
1:I:251:ILE:HD12	1:I:483:LEU:HD21	1.80	0.64
2:J:530:MET:HE1	2:J:631:TRP:HE1	1.63	0.64
1:A:190:GLU:OE2	1:A:190:GLU:N	2.26	0.63
6:k:18:LEU:HB3	6:k:82:LEU:HB2	1.80	0.63
6:k:100:ARG:NH2	11:w:4:MAN:O6	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:THR:C	1:G:395:TRP:HD1	2.05	0.63
2:B:612:SER:O	2:B:616:ASN:ND2	2.30	0.63
4:E:48:ILE:HA	4:E:54:ARG:HH12	1.63	0.63
1:I:322:ILE:O	5:m:94:ARG:NH1	2.30	0.63
1:G:298:ARG:HG2	1:G:443:ILE:HG22	1.81	0.63
5:m:51:ASN:ND2	5:m:65:SER:O	2.30	0.63
1:A:373:THR:HG21	1:A:386:ASN:OD1	1.99	0.62
4:M:35:TRP:HB2	4:M:48:ILE:HB	1.80	0.62
5:l:31:ARG:O	6:h:100:ARG:NH1	2.32	0.62
2:B:591:GLN:NE2	2:C:541:ALA:O	2.31	0.62
1:A:379:GLY:HA3	1:A:443:ILE:HD11	1.80	0.62
3:H:52:ASN:ND2	3:H:56:GLN:OE1	2.33	0.62
5:m:79:GLU:HG2	5:m:81:GLY:H	1.63	0.62
2:B:595:ILE:HD11	2:C:538:THR:HG22	1.82	0.62
4:E:48:ILE:HA	4:E:54:ARG:NH1	2.15	0.61
3:H:82:LEU:HD21	3:H:82(C):LEU:HD13	1.83	0.61
2:C:523:LEU:H	2:C:540:GLN:HE22	1.47	0.61
1:I:264:SER:O	1:I:287:GLN:NE2	2.33	0.61
1:I:372:THR:HG22	1:I:373:THR:HG23	1.83	0.61
3:D:80:MET:HE1	3:D:82:LEU:HB2	1.82	0.61
3:D:84:VAL:HA	3:D:111:VAL:HG11	1.83	0.61
1:G:83:GLU:OE2	1:G:229:LYS:NZ	2.28	0.60
1:I:162:THR:HG22	1:I:169:LYS:HE2	1.83	0.60
1:I:190:GLU:OE2	1:I:190:GLU:N	2.34	0.60
1:G:251:ILE:HD12	1:G:483:LEU:HD21	1.84	0.60
1:G:477:ASP:OD1	1:G:480:ARG:NH1	2.34	0.60
1:G:161:MET:CE	1:G:309:ILE:HG13	2.30	0.60
1:G:298:ARG:NH1	1:G:302:ASN:OD1	2.34	0.60
5:l:79:GLU:HG2	5:l:81:GLY:H	1.64	0.60
5:e:38:HIS:HB3	5:e:85:ASP:HB2	1.82	0.60
4:L:32:ILE:HD11	7:W:2:NAG:H62	1.83	0.60
2:B:520:LEU:HD22	2:B:542:ARG:HH12	1.65	0.60
3:D:36:TRP:CZ3	3:D:80:MET:HB2	2.37	0.60
5:m:67(A):SER:HB3	5:m:67(B):PRO:HD3	1.84	0.60
5:m:61:ARG:NH1	5:m:79:GLU:OE1	2.35	0.60
1:A:264:SER:O	1:A:287:GLN:NE2	2.35	0.60
6:d:100:ARG:NH2	11:i:4:MAN:O6	2.34	0.60
1:I:259:LEU:HD11	1:I:391:PHE:HZ	1.67	0.60
4:M:36:PHE:HB2	4:M:87:ILE:HB	1.83	0.60
3:D:66:ARG:HH12	3:D:83:ARG:HH21	1.49	0.59
1:G:264:SER:O	1:G:287:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:59:TYR:OH	6:h:69:LEU:N	2.35	0.59
4:E:5:GLN:NE2	4:E:22:SER:O	2.35	0.59
6:k:32:SER:HB2	6:k:94:ARG:NH2	2.17	0.59
6:d:59:TYR:OH	6:d:69:LEU:N	2.35	0.59
1:I:161:MET:HE1	1:I:309:ILE:HG13	1.84	0.59
4:M:46:LEU:HD21	4:M:49:PHE:HB3	1.85	0.59
6:h:4:LEU:HD12	6:h:22:CYS:SG	2.43	0.59
1:I:107:ASP:OD2	2:J:574:LYS:NZ	2.33	0.59
3:K:33:PHE:HB2	3:K:100:ASN:HD21	1.65	0.59
5:l:65:SER:HG	5:l:72:THR:HG1	1.48	0.58
1:A:64:GLU:O	1:A:67:ASN:ND2	2.35	0.58
1:I:61:TYR:OH	1:I:74:CYS:O	2.21	0.58
5:e:62:PHE:CE1	5:e:75:ILE:HG23	2.37	0.58
6:d:47:TRP:HH2	6:d:100(N):PHE:HB2	1.68	0.58
4:E:63:SER:OG	4:E:74:THR:OG1	2.21	0.58
3:H:54:TYR:HB2	3:H:56:GLN:NE2	2.18	0.58
1:G:165:LEU:HD12	1:I:128:THR:HG22	1.86	0.58
1:A:251:ILE:HD12	1:A:483:LEU:HD21	1.85	0.58
3:D:100:ASN:O	3:D:100(A):TYR:CD1	2.45	0.58
1:I:37:THR:HG22	2:J:605:CYS:HA	1.86	0.58
1:I:55:ALA:HB1	1:I:77:THR:HG22	1.86	0.58
1:G:61:TYR:OH	1:G:74:CYS:O	2.22	0.57
1:A:61:TYR:OH	1:A:74:CYS:O	2.22	0.57
1:A:161:MET:HE1	1:A:309:ILE:HG13	1.86	0.57
5:e:37:GLN:HE22	5:e:39:ARG:HD2	1.69	0.57
2:J:619:LEU:HA	2:J:622:ILE:HB	1.87	0.57
4:M:11:MET:HE3	4:M:102:THR:HG21	1.86	0.57
1:G:116:LEU:HD11	1:G:434:MET:HE2	1.86	0.57
1:A:86:LEU:HG	1:A:243:SER:HA	1.87	0.57
1:A:179:LEU:HD12	1:A:421:LYS:HG3	1.87	0.57
3:K:82:LEU:HD21	3:K:82(C):LEU:HD13	1.86	0.57
4:E:46:LEU:HD21	4:E:49:PHE:HB3	1.85	0.56
2:C:611:ASN:HB3	2:C:614:TRP:HE1	1.70	0.56
5:l:67(A):SER:HB3	5:l:67(B):PRO:HD3	1.88	0.56
1:A:164:GLU:OE2	1:A:308:ARG:HD3	2.05	0.56
1:A:503:ARG:HH12	2:C:650:GLN:HE22	1.52	0.56
6:k:34:TRP:CE2	6:k:94:ARG:NH1	2.73	0.56
5:e:54:ARG:NH2	5:e:62:PHE:O	2.36	0.56
4:L:26:THR:O	4:L:31:ILE:HG22	2.06	0.56
6:k:33:TYR:HB2	6:k:95:THR:OG1	2.06	0.56
1:G:503:ARG:HB3	2:B:607:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:96:GLU:HG3	4:M:97:PHE:CD1	2.41	0.56
1:I:179:LEU:HD12	1:I:421:LYS:HG3	1.87	0.55
1:G:291:PRO:HG2	7:V:1:NAG:H61	1.87	0.55
3:H:33:PHE:HB2	3:H:100:ASN:ND2	2.22	0.55
1:A:234:ASN:HB3	12:A:604:NAG:O5	2.06	0.55
1:G:225:ILE:HB	1:G:245:VAL:O	2.07	0.55
2:C:621:GLU:O	2:C:625:ASN:ND2	2.39	0.55
5:l:37:GLN:NE2	5:l:39:ARG:HD3	2.22	0.55
5:e:37:GLN:HG3	5:e:86:TYR:CE1	2.41	0.55
2:B:653:GLN:NE2	2:B:657:GLU:OE2	2.29	0.55
6:d:87:SER:HB2	6:d:109:VAL:H	1.72	0.55
4:E:26:THR:O	4:E:31:ILE:HG22	2.06	0.55
1:I:60:ALA:HB2	1:I:213:ILE:HG21	1.88	0.55
1:I:297:THR:OG1	1:I:443:ILE:O	2.22	0.55
1:A:136:ASN:HB3	1:A:138:ILE:HG23	1.88	0.55
5:m:91:TRP:CD1	6:k:100(M):TYR:HB2	2.42	0.55
1:I:122:LEU:HB2	1:I:201:ILE:HG13	1.86	0.55
2:B:655:LYS:NZ	2:C:534:SER:O	2.32	0.55
4:E:11:MET:HE1	4:E:19:VAL:HG21	1.89	0.55
5:e:19:ALA:HB3	5:e:75:ILE:HD12	1.88	0.55
1:I:460:SER:H	3:K:61:TRP:CD1	2.24	0.55
1:G:37:THR:HG22	2:B:605:CYS:HA	1.88	0.55
1:G:194:ILE:HG12	1:G:423:ILE:HD11	1.89	0.55
6:k:47:TRP:CH2	6:k:100(N):PHE:HB2	2.42	0.55
2:B:621:GLU:O	2:B:625:ASN:ND2	2.40	0.54
3:K:52:ASN:HB3	3:K:56:GLN:HB2	1.87	0.54
6:d:69:LEU:HD21	6:d:80:LEU:HD12	1.89	0.54
1:I:83:GLU:HG2	1:I:245:VAL:HG23	1.89	0.54
1:G:460:SER:HB2	3:H:61:TRP:HE1	1.73	0.54
1:I:259:LEU:HD11	1:I:391:PHE:CZ	2.42	0.54
1:I:460:SER:HB2	3:K:61:TRP:HE1	1.71	0.54
5:m:92:ASP:OD2	5:m:95(C):LYS:NZ	2.34	0.54
1:A:373:THR:HB	1:A:386:ASN:HA	1.89	0.54
1:I:136:ASN:HB3	1:I:138:ILE:HG23	1.89	0.54
5:m:39:ARG:HG3	5:m:42:GLN:HB2	1.87	0.54
1:A:377:ASN:HB3	1:A:382:PHE:CE1	2.42	0.54
5:e:30:SER:OG	5:e:93:SER:OG	2.22	0.54
3:K:11:VAL:HG22	3:K:110:VAL:HB	1.89	0.54
1:I:36:VAL:HG13	2:J:606:THR:HB	1.88	0.54
1:A:249:HIS:ND1	1:A:486:TYR:OH	2.29	0.54
3:D:54:TYR:HB2	3:D:56:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:39:ARG:NH1	6:d:40:SER:O	2.40	0.54
1:G:55:ALA:HB1	1:G:77:THR:HG22	1.90	0.54
6:d:4:LEU:HD12	6:d:22:CYS:SG	2.48	0.54
3:K:37:VAL:HG13	3:K:91:TYR:HB2	1.88	0.54
4:M:38:GLN:HB2	4:M:44:PRO:HB3	1.88	0.54
6:h:47:TRP:CH2	6:h:100(N):PHE:HB2	2.43	0.53
2:C:627:THR:O	2:C:630:GLN:HG3	2.07	0.53
7:r:1:NAG:HO6	7:r:2:NAG:HO6	1.56	0.53
1:A:272:ILE:HG12	1:A:286:VAL:HG22	1.90	0.53
3:K:84:VAL:HA	3:K:111:VAL:HG11	1.90	0.53
6:k:59:TYR:OH	6:k:69:LEU:N	2.36	0.53
1:G:384:TYR:CD2	1:G:421:LYS:HD3	2.43	0.53
1:G:384:TYR:CE2	1:G:421:LYS:HD3	2.43	0.53
3:H:96:PRO:HG2	3:H:99:GLU:HB2	1.90	0.53
5:l:91:TRP:CD1	6:h:100(M):TYR:HB2	2.44	0.53
4:E:54:ARG:HB3	4:E:58:VAL:HG11	1.89	0.53
5:m:30:SER:O	5:m:93:SER:OG	2.21	0.53
2:C:597:GLY:HA3	2:C:650:GLN:NE2	2.24	0.53
5:e:75:ILE:HG22	5:e:78:VAL:HG12	1.90	0.53
6:d:47:TRP:CH2	6:d:100(N):PHE:HB2	2.43	0.53
1:I:194:ILE:HG12	1:I:423:ILE:HD11	1.90	0.53
3:K:1:HIS:NE2	3:K:3:GLN:OE1	2.36	0.53
1:I:477:ASP:OD1	1:I:480:ARG:NH1	2.41	0.53
1:I:64:GLU:HG2	1:I:65:LYS:HG3	1.89	0.53
1:I:298:ARG:HB3	1:I:443:ILE:HG22	1.91	0.53
3:K:82(C):LEU:HD21	3:K:86:ASP:HB3	1.91	0.53
6:k:32:SER:N	6:k:94:ARG:HH22	2.06	0.53
5:e:39:ARG:NH1	5:e:42:GLN:OE1	2.38	0.53
3:K:86:ASP:OD2	3:K:90:TYR:OH	2.26	0.53
5:m:27:SER:H	5:m:31:ARG:NH1	2.06	0.53
1:G:66:HIS:HA	1:G:71:THR:HG21	1.91	0.52
1:G:294:ILE:HD12	1:G:449:ILE:HD11	1.90	0.52
5:l:34:GLN:NE2	5:l:49:TYR:O	2.42	0.52
1:G:34:LEU:HG	2:B:619:LEU:HD21	1.92	0.52
4:L:23:CYS:O	4:L:70:THR:HA	2.08	0.52
6:k:95:THR:HG22	6:k:100(P):MET:SD	2.49	0.52
1:G:71:THR:HG23	1:G:72:HIS:ND1	2.24	0.52
3:D:35:ASN:ND2	3:D:50:TRP:HB3	2.25	0.52
3:H:86:ASP:OD2	3:H:90:TYR:OH	2.28	0.52
1:A:270:VAL:O	1:A:348:GLN:HG2	2.08	0.52
1:I:258:GLN:HB2	1:I:374:HIS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:VAL:HA	2:B:583:VAL:HG12	1.91	0.52
1:A:271:MET:HE3	1:A:272:ILE:H	1.75	0.52
3:D:82:LEU:HD21	3:D:82(C):LEU:HD13	1.92	0.52
5:e:46:LEU:HD22	6:d:100(Q):ASP:HA	1.90	0.52
4:L:35:TRP:CG	4:L:73:LEU:HD22	2.45	0.52
4:L:66:ARG:NH2	7:W:2:NAG:O4	2.42	0.52
2:C:580:VAL:HA	2:C:583:VAL:HG12	1.92	0.52
3:K:39:GLN:HB2	3:K:45:LEU:HD23	1.90	0.52
1:A:327:ARG:HD2	6:d:100(C):GLY:HA2	1.92	0.51
6:h:18:LEU:HB3	6:h:82:LEU:HB2	1.91	0.51
6:h:20:LEU:HD21	6:h:80:LEU:HD23	1.91	0.51
1:A:323:ILE:HD11	5:e:67(C):PHE:CZ	2.46	0.51
3:D:68:THR:OG1	3:D:81:GLU:HB3	2.10	0.51
1:I:424:ILE:HD12	1:I:426:MET:HG3	1.92	0.51
6:h:52:HIS:CD2	6:h:54:SER:H	2.28	0.51
1:A:350:ARG:NH2	1:A:396:ILE:O	2.42	0.51
2:C:653:GLN:NE2	2:C:657:GLU:OE2	2.44	0.51
3:D:11:VAL:HG22	3:D:110:VAL:HB	1.93	0.51
5:m:34:GLN:HB2	5:m:89:HIS:HB3	1.91	0.51
5:m:65:SER:HB2	5:m:72:THR:H	1.76	0.51
5:m:92:ASP:OD2	5:m:95:VAL:HG23	2.10	0.51
1:G:54:CYS:SG	1:G:55:ALA:N	2.84	0.51
1:G:179:LEU:HB2	1:G:421:LYS:HG2	1.90	0.51
1:A:332:ASN:HB2	7:a:1:NAG:H82	1.92	0.51
5:l:80:ALA:HA	5:l:106:VAL:HG11	1.92	0.51
3:K:68:THR:OG1	3:K:81:GLU:HB3	2.11	0.51
1:G:323:ILE:HD11	5:l:67(C):PHE:CZ	2.46	0.51
3:H:19:ARG:HH21	3:H:79:PHE:HB3	1.75	0.51
3:D:19:ARG:HH12	3:D:79:PHE:HB3	1.75	0.51
3:K:36:TRP:HB3	3:K:48:MET:HE2	1.92	0.51
1:G:66:HIS:H	1:G:72:HIS:HE1	1.59	0.50
3:H:23:GLU:HB2	3:H:77:THR:HG22	1.93	0.50
5:l:51:ASN:HB3	5:l:66:PRO:HA	1.92	0.50
6:h:6:GLU:HG3	6:h:105:THR:HB	1.92	0.50
3:D:51:MET:HE2	3:D:71:ARG:HB3	1.93	0.50
6:d:50:TYR:CE1	6:d:58:ASN:HB2	2.47	0.50
1:I:270:VAL:O	1:I:348:GLN:HG2	2.11	0.50
1:G:122:LEU:HD13	1:G:125:LEU:HD13	1.93	0.50
1:A:124:PRO:HD2	1:A:309:ILE:HD11	1.93	0.50
1:A:219:ALA:HB1	1:A:223:PHE:HB2	1.93	0.50
1:A:324:GLY:O	5:e:94:ARG:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:460:SER:H	3:K:61:TRP:HD1	1.60	0.50
6:k:20:LEU:HD21	6:k:80:LEU:HD23	1.92	0.50
1:G:234:ASN:HB3	12:G:604:NAG:O5	2.11	0.50
3:D:54:TYR:HB2	3:D:56:GLN:NE2	2.27	0.50
1:G:86:LEU:HG	1:G:243:SER:HA	1.94	0.50
2:C:611:ASN:HB3	2:C:614:TRP:NE1	2.26	0.50
1:I:469:ARG:NH1	3:K:64:GLN:OE1	2.44	0.50
2:J:520:LEU:HD22	2:J:542:ARG:HH12	1.77	0.50
6:k:12:VAL:HG21	6:k:18:LEU:HA	1.93	0.50
1:G:417:PRO:HB3	6:h:100(G):PHE:CE1	2.46	0.49
1:A:503:ARG:HB3	2:C:607:ASN:HD21	1.76	0.49
1:I:373:THR:HG21	1:I:386:ASN:OD1	2.12	0.49
1:G:258:GLN:HB2	1:G:374:HIS:HB3	1.94	0.49
1:G:270:VAL:O	1:G:348:GLN:HG2	2.13	0.49
4:L:54:ARG:HB2	4:L:58:VAL:HG11	1.94	0.49
5:e:80:ALA:HA	5:e:106:VAL:HG11	1.93	0.49
5:e:92:ASP:OD2	5:e:95:VAL:HG23	2.11	0.49
1:A:162:THR:HG22	1:A:169:LYS:HE2	1.94	0.49
1:I:256:SER:O	1:I:478:ASN:ND2	2.45	0.49
6:k:18:LEU:HD21	6:k:107:VAL:HG21	1.94	0.49
1:G:325:ASP:N	1:G:325:ASP:OD1	2.45	0.49
2:J:523:LEU:HD12	2:J:526:ALA:HB2	1.94	0.49
1:G:212:PRO:HG3	1:G:254:VAL:HG12	1.95	0.49
3:H:4:LEU:HD11	3:H:103:TRP:O	2.12	0.49
1:I:272:ILE:HD13	1:I:349:LEU:HD23	1.94	0.49
3:H:40:ALA:HB3	3:H:43:GLN:HE22	1.77	0.49
1:A:122:LEU:HD13	1:A:125:LEU:HD13	1.95	0.49
5:e:12:SER:HB3	5:e:107:LEU:HG	1.93	0.49
5:e:85:ASP:OD1	5:e:103:THR:HG22	2.13	0.49
5:e:67(A):SER:HB3	5:e:67(B):PRO:HD3	1.95	0.49
1:G:382:PHE:CE2	1:G:424:ILE:HD13	2.47	0.49
5:l:18:THR:HG22	5:l:76:THR:HA	1.95	0.49
1:A:503:ARG:HH12	2:C:650:GLN:NE2	2.11	0.49
3:D:47:TRP:CE3	4:E:96:GLU:HB2	2.48	0.49
1:I:460:SER:HA	4:M:97:PHE:CE1	2.48	0.49
1:G:373:THR:HG22	1:G:386:ASN:HA	1.95	0.48
3:D:81:GLU:OE2	3:D:82(A):ARG:NH1	2.42	0.48
1:G:331:CYS:HB2	1:G:416:LEU:CD1	2.43	0.48
6:h:90:TYR:O	6:h:104:GLY:HA2	2.13	0.48
5:e:35:TRP:HB2	5:e:48:ILE:HB	1.95	0.48
1:G:201:ILE:HA	1:G:433:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:372:THR:HG23	1:G:373:THR:HG23	1.96	0.48
3:H:82(C):LEU:HD11	3:H:86:ASP:HB3	1.95	0.48
1:A:299:PRO:HG3	1:A:327:ARG:CZ	2.43	0.48
1:G:122:LEU:HB2	1:G:201:ILE:HG13	1.95	0.48
5:l:54:ARG:CZ	5:l:60:GLU:HA	2.44	0.48
1:A:104:MET:HG3	1:A:217:TYR:OH	2.13	0.48
1:A:265:LEU:HD21	1:A:291:PRO:HG3	1.95	0.48
6:h:87:SER:HB2	6:h:109:VAL:HG12	1.96	0.48
2:J:642:ILE:H	2:J:642:ILE:HD12	1.79	0.48
5:m:32:ALA:O	5:m:91:TRP:HB2	2.14	0.48
5:l:34:GLN:HG3	5:l:49:TYR:HA	1.94	0.48
6:d:71:LEU:HG	6:d:78:VAL:HG12	1.94	0.48
1:G:52:LEU:HD21	1:G:488:VAL:HG21	1.95	0.48
1:A:194:ILE:HG12	1:A:423:ILE:HD11	1.95	0.48
1:I:47:ASP:OD1	1:I:48:ALA:N	2.46	0.48
1:I:228:CYS:HA	1:I:242:VAL:HA	1.94	0.48
3:H:29:PHE:CD2	3:H:76(G):GLY:HA3	2.49	0.48
1:A:384:TYR:CD2	1:A:421:LYS:HB2	2.48	0.48
1:I:180:ASP:OD1	1:I:423:ILE:HG12	2.13	0.48
2:J:651:ASN:HA	2:J:654:GLU:OE1	2.14	0.48
6:k:36:TRP:CD1	6:k:69:LEU:HD21	2.49	0.48
1:G:394:THR:C	1:G:395:TRP:CD1	2.90	0.48
2:J:530:MET:SD	2:J:623:TRP:HA	2.54	0.48
2:J:580:VAL:HA	2:J:583:VAL:HG12	1.95	0.48
1:G:83:GLU:HG3	1:G:245:VAL:HB	1.95	0.48
1:A:383:PHE:CD1	1:A:420:ILE:HG12	2.49	0.48
4:M:30:HIS:O	7:y:2:NAG:H61	2.13	0.48
6:h:34:TRP:CZ3	6:h:94:ARG:HG2	2.49	0.47
1:A:122:LEU:HB2	1:A:201:ILE:HG13	1.96	0.47
4:E:89:ASN:OD1	4:E:90:THR:N	2.48	0.47
6:d:33:TYR:HB2	6:d:95:THR:OG1	2.14	0.47
6:k:47:TRP:HH2	6:k:100(N):PHE:HB2	1.76	0.47
6:k:87:SER:HB2	6:k:109:VAL:HG12	1.97	0.47
8:q:1:NAG:H61	8:q:2:NAG:HN2	1.79	0.47
1:G:286:VAL:HB	1:G:452:LEU:HB2	1.95	0.47
1:G:335:LYS:HG3	1:G:414:ILE:HD11	1.96	0.47
5:l:98:PHE:HE1	6:h:47:TRP:HB2	1.78	0.47
6:h:100(A):ILE:HB	11:U:3:BMA:H61	1.96	0.47
1:A:383:PHE:HB3	1:A:385:CYS:SG	2.54	0.47
1:I:104:MET:HG3	1:I:217:TYR:OH	2.14	0.47
4:M:26:THR:O	4:M:31:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:ARG:HG2	1:G:443:ILE:CG2	2.44	0.47
1:A:228:CYS:HA	1:A:242:VAL:HA	1.96	0.47
2:C:655:LYS:NZ	2:J:534:SER:O	2.37	0.47
5:e:59:PRO:HG2	5:e:61:ARG:CZ	2.44	0.47
1:I:100:MET:SD	1:I:483:LEU:HD13	2.55	0.47
1:I:385:CYS:HA	1:I:418:CYS:HA	1.96	0.47
3:H:84:VAL:HA	3:H:111:VAL:HG11	1.97	0.47
6:h:47:TRP:HH2	6:h:100(N):PHE:HB2	1.80	0.47
3:H:43:GLN:N	3:H:43:GLN:OE1	2.47	0.47
1:A:136:ASN:OD1	1:A:137:ASN:N	2.44	0.47
1:A:202:THR:O	1:A:434:MET:HA	2.14	0.47
3:D:52:ASN:HB3	3:D:56:GLN:HB2	1.96	0.47
5:e:37:GLN:OE1	5:e:47:ILE:HD11	2.14	0.47
2:B:642:ILE:HD12	2:B:642:ILE:H	1.80	0.47
1:A:107:ASP:OD2	2:C:574:LYS:NZ	2.44	0.47
5:e:32:ALA:O	5:e:91:TRP:HB2	2.15	0.47
1:G:322:ILE:O	5:l:94:ARG:NH1	2.48	0.47
2:B:651:ASN:O	2:B:655:LYS:HG2	2.15	0.47
1:I:68:VAL:HG23	1:I:71:THR:HB	1.97	0.47
2:J:572:GLY:O	2:J:576:LEU:HD13	2.15	0.47
1:A:469:ARG:NH1	3:D:64:GLN:OE1	2.46	0.46
3:D:19:ARG:HH12	3:D:79:PHE:HD2	1.62	0.46
5:m:98:PHE:HE1	6:k:47:TRP:HB2	1.80	0.46
1:G:249:HIS:ND1	1:G:486:TYR:OH	2.37	0.46
1:A:212:PRO:HG3	1:A:254:VAL:HG12	1.96	0.46
4:E:23:CYS:HB2	4:E:35:TRP:CZ2	2.51	0.46
5:l:38:HIS:HB3	5:l:85:ASP:HB2	1.96	0.46
5:l:61:ARG:HB2	5:l:76:THR:O	2.15	0.46
6:h:36:TRP:CH2	6:h:92:CYS:HB3	2.51	0.46
1:A:109:ILE:HD13	1:A:427:TRP:CD1	2.50	0.46
4:M:37:GLN:HB2	4:M:47:ILE:HD13	1.97	0.46
4:M:88:CYS:O	4:M:99:GLY:N	2.47	0.46
1:G:331:CYS:HB2	1:G:416:LEU:HD11	1.97	0.46
4:E:96:GLU:HG2	4:E:97:PHE:CD1	2.50	0.46
1:I:201:ILE:HG22	1:I:433:ALA:HB3	1.98	0.46
1:I:212:PRO:HG3	1:I:254:VAL:HG12	1.97	0.46
3:H:76(C):ASP:OD1	3:H:76(C):ASP:N	2.48	0.46
1:G:179:LEU:HD21	1:G:419:ARG:NH2	2.31	0.46
3:D:29:PHE:HD2	3:D:73:LEU:HD23	1.80	0.46
5:m:37:GLN:CD	5:m:47:ILE:HD11	2.40	0.46
1:G:276:ASN:HB3	7:W:1:NAG:O5	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:30:SER:O	5:e:93:SER:OG	2.25	0.46
5:m:12:SER:HB3	5:m:107:LEU:HG	1.98	0.46
2:C:630:GLN:O	2:C:634:GLU:OE1	2.33	0.46
1:I:295:ASN:HD21	1:I:444:ARG:HH21	1.63	0.46
6:k:50:TYR:O	6:k:57:THR:OG1	2.21	0.46
1:G:104:MET:HG3	1:G:217:TYR:OH	2.16	0.46
1:A:385:CYS:HB3	1:A:417:PRO:O	2.16	0.46
3:D:11:VAL:HA	3:D:110:VAL:O	2.16	0.46
1:I:84:ILE:HD11	2:J:521:GLY:HA3	1.98	0.46
1:I:276:ASN:OD1	7:y:1:NAG:N2	2.49	0.46
2:J:530:MET:HE2	2:J:530:MET:HB3	1.78	0.46
3:K:54:TYR:HB2	3:K:56:GLN:NE2	2.31	0.46
4:L:77:ASN:O	4:L:77:ASN:ND2	2.39	0.46
5:l:35:TRP:HB2	5:l:48:ILE:HG22	1.98	0.46
1:G:369:LEU:O	1:G:369:LEU:HD23	2.16	0.45
3:H:68:THR:OG1	3:H:81:GLU:HB3	2.15	0.45
6:h:100(D):ILE:HD13	11:U:1:NAG:H5	1.97	0.45
5:m:85:ASP:OD1	5:m:103:THR:HG22	2.16	0.45
1:I:124:PRO:HD2	1:I:309:ILE:HD11	1.98	0.45
1:I:327:ARG:HH21	1:I:330:HIS:CE1	2.28	0.45
2:B:649:SER:O	2:B:652:GLN:HG3	2.15	0.45
3:H:87:THR:HG22	3:H:111:VAL:H	1.81	0.45
4:L:42:LYS:HD2	4:L:42:LYS:HA	1.80	0.45
1:I:77:THR:HG21	1:I:216:HIS:CD2	2.52	0.45
5:m:33:VAL:O	5:m:34:GLN:NE2	2.49	0.45
6:k:50:TYR:CE1	6:k:58:ASN:HB2	2.51	0.45
3:H:29:PHE:CE2	3:H:76(G):GLY:HA3	2.52	0.45
1:A:180:ASP:OD1	1:A:423:ILE:HG12	2.17	0.45
2:C:587:LEU:HD21	2:J:586:TYR:CD2	2.52	0.45
3:K:87:THR:HG22	3:K:111:VAL:H	1.82	0.45
6:h:36:TRP:HB3	6:h:48:ILE:HD11	1.97	0.45
4:E:65:SER:OG	4:E:66:ARG:N	2.49	0.45
5:e:91:TRP:CD1	6:d:100(M):TYR:HB2	2.52	0.45
7:y:1:NAG:H4	7:y:2:NAG:H2	1.68	0.45
4:L:89:ASN:OD1	4:L:90:THR:N	2.49	0.45
6:h:100(C):GLY:HA3	6:h:100(I):GLU:HB3	1.97	0.45
5:e:35:TRP:HD1	5:e:88:CYS:HA	1.81	0.45
5:m:54:ARG:HH22	5:m:59:PRO:C	2.24	0.45
1:G:298:ARG:NH2	1:G:439:ILE:O	2.47	0.45
1:G:460:SER:H	3:H:61:TRP:CD1	2.34	0.45
3:D:4:LEU:HD11	3:D:103:TRP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:11:VAL:HA	3:K:110:VAL:O	2.16	0.45
6:h:33:TYR:HB2	6:h:95:THR:OG1	2.16	0.45
1:A:296:CYS:O	1:A:297:THR:HB	2.16	0.45
5:e:89:HIS:HB2	5:e:98:PHE:CD2	2.52	0.45
1:A:38:VAL:HG12	2:C:604:CYS:HB3	1.98	0.45
3:D:1:HIS:NE2	3:D:3:GLN:OE1	2.37	0.45
3:D:17:ALA:HA	3:D:82:LEU:O	2.16	0.45
2:B:580:VAL:HG23	2:C:579:ARG:HH21	1.81	0.45
3:D:38:ARG:HB2	3:D:48:MET:SD	2.57	0.45
2:J:522:PHE:CD1	2:J:523:LEU:HD23	2.52	0.45
3:K:47:TRP:CZ2	3:K:50:TRP:HD1	2.35	0.44
3:K:96:PRO:HG2	3:K:99:GLU:HB2	1.99	0.44
11:w:7:MAN:H62	11:w:9:MAN:H2	1.59	0.44
2:B:530:MET:SD	2:B:530:MET:N	2.90	0.44
3:D:29:PHE:CE2	3:D:76(G):GLY:HA3	2.52	0.44
3:D:52:ASN:ND2	3:D:56:GLN:OE1	2.51	0.44
4:E:42:LYS:HA	4:E:42:LYS:HD2	1.78	0.44
1:I:181:VAL:HB	1:I:191:TYR:HB3	2.00	0.44
5:m:61:ARG:HB3	5:m:76:THR:O	2.17	0.44
1:G:328:GLN:O	1:G:330:HIS:ND1	2.41	0.44
1:I:276:ASN:HD22	1:I:276:ASN:HA	1.59	0.44
1:G:469:ARG:NH1	3:H:64:GLN:OE1	2.50	0.44
5:l:65:SER:HB2	5:l:72:THR:H	1.82	0.44
1:A:327:ARG:HH12	1:A:330:HIS:CE1	2.36	0.44
5:e:37:GLN:NE2	5:e:39:ARG:HD2	2.31	0.44
5:e:65:SER:OG	5:e:72:THR:OG1	2.23	0.44
3:H:37:VAL:HG13	3:H:91:TYR:HB2	2.00	0.44
6:h:4:LEU:HD11	6:h:34:TRP:CZ3	2.52	0.44
2:C:530:MET:HE1	2:C:626:MET:HG3	1.98	0.44
3:K:27:TYR:O	3:K:76(E):ASP:HB2	2.18	0.44
1:G:180:ASP:OD1	1:G:423:ILE:HG12	2.18	0.44
5:l:12:SER:HB3	5:l:107:LEU:HG	2.00	0.44
4:E:5:GLN:HE22	4:E:23:CYS:HA	1.82	0.44
1:I:116:LEU:HB3	1:I:202:THR:HG21	1.98	0.44
1:I:333:VAL:HG23	1:I:414:ILE:HB	1.99	0.44
4:E:31:ILE:CA	7:n:2:NAG:H62	2.47	0.44
1:A:503:ARG:H	2:C:607:ASN:HD21	1.65	0.44
5:e:34:GLN:HG3	5:e:49:TYR:HA	1.99	0.44
6:d:30:SER:C	6:d:53:LYS:HE3	2.43	0.44
1:I:325:ASP:OD1	1:I:325:ASP:N	2.46	0.44
3:K:52:ASN:ND2	3:K:56:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:TRP:HE1	1:G:91:GLU:CD	2.26	0.44
1:G:297:THR:OG1	1:G:443:ILE:O	2.24	0.44
1:G:395:TRP:CD1	1:G:395:TRP:N	2.86	0.44
3:H:37:VAL:CG1	3:H:91:TYR:HB2	2.48	0.44
1:A:343:GLY:HA2	1:A:395:TRP:CZ3	2.53	0.44
1:I:275:GLU:CD	12:I:604:NAG:HN2	2.26	0.44
1:G:128:THR:HG22	1:A:165:LEU:HD12	1.99	0.43
1:G:234:ASN:HD21	1:G:275:GLU:HG2	1.83	0.43
1:I:388:SER:OG	10:u:2:NAG:O7	2.33	0.43
1:G:284:ILE:HG22	1:G:454:LEU:O	2.18	0.43
3:H:11:VAL:HG22	3:H:110:VAL:HB	1.98	0.43
1:I:346:VAL:HG21	1:I:395:TRP:CD1	2.52	0.43
1:G:60:ALA:HB2	1:G:213:ILE:HG21	1.99	0.43
1:G:184:ILE:HD11	1:G:192:ARG:HD3	1.99	0.43
6:h:47:TRP:NE1	6:h:100(P):MET:HE1	2.34	0.43
6:h:50:TYR:CE1	6:h:58:ASN:HB2	2.54	0.43
1:A:327:ARG:HH22	1:A:330:HIS:HE1	1.66	0.43
5:e:37:GLN:HE21	5:e:39:ARG:HG3	1.84	0.43
6:d:100(C):GLY:HA3	6:d:100(I):GLU:HB3	2.00	0.43
1:I:34:LEU:HG	2:J:619:LEU:HD21	1.99	0.43
6:k:100:ARG:HD3	6:k:100(K):PHE:CZ	2.53	0.43
1:G:112:TRP:HH2	1:G:210:PHE:HD1	1.65	0.43
1:G:265:LEU:HD21	1:G:291:PRO:HG3	2.00	0.43
1:G:299:PRO:HG3	1:G:327:ARG:NH2	2.33	0.43
2:B:639:THR:HG23	2:B:640:GLN:OE1	2.18	0.43
6:h:15:SER:HA	6:h:82(B):ALA:HA	1.99	0.43
1:A:332:ASN:HA	1:A:414:ILE:O	2.18	0.43
5:e:27:SER:H	5:e:31:ARG:NH1	2.15	0.43
1:I:373:THR:HG21	1:I:386:ASN:CG	2.43	0.43
1:I:386:ASN:O	1:I:416:LEU:HD13	2.18	0.43
5:l:75:ILE:HD11	5:l:86:TYR:HE2	1.84	0.43
5:e:37:GLN:HG2	5:e:38:HIS:N	2.33	0.43
5:e:67:ASP:HA	5:e:69:THR:OG1	2.18	0.43
6:d:36:TRP:CH2	6:d:92:CYS:HB3	2.53	0.43
5:m:34:GLN:OE1	5:m:49:TYR:HA	2.19	0.43
6:k:71:LEU:HD12	6:k:72:ASP:N	2.33	0.43
6:k:90:TYR:CE1	6:k:107:VAL:HG11	2.53	0.43
5:l:9:ILE:O	5:l:103:THR:OG1	2.34	0.43
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.82	0.43
5:e:59:PRO:HG2	5:e:61:ARG:NE	2.34	0.43
1:I:503:ARG:HH12	2:J:597:GLY:HA3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:THR:HG21	1:G:216:HIS:CD2	2.53	0.43
1:G:309:ILE:HG22	1:G:315:GLN:O	2.18	0.43
3:K:50:TRP:NE1	3:K:58:ASN:HB3	2.34	0.43
1:A:327:ARG:HH22	1:A:330:HIS:CE1	2.37	0.43
5:e:65:SER:HB2	5:e:72:THR:H	1.83	0.43
6:d:95:THR:HG22	6:d:100(P):MET:SD	2.59	0.43
1:I:183:GLN:NE2	1:I:185:ASN:O	2.39	0.43
2:J:530:MET:CE	2:J:631:TRP:HE1	2.30	0.43
3:K:6:GLN:HB3	3:K:107:VAL:HG13	2.00	0.43
3:K:45:LEU:HD12	4:M:87:ILE:HG21	2.01	0.43
3:K:54:TYR:HA	3:K:71:ARG:HH21	1.84	0.43
3:K:100(A):TYR:HD2	4:M:91:TYR:HD1	1.65	0.43
6:h:2:MET:HG2	6:h:94:ARG:HD3	2.01	0.43
6:h:12:VAL:HG21	6:h:18:LEU:HA	1.99	0.43
6:d:4:LEU:HD11	6:d:34:TRP:CZ3	2.53	0.43
1:I:51:THR:HG23	1:I:103:GLN:HE22	1.84	0.43
1:I:159:PHE:HA	7:p:1:NAG:H83	2.00	0.43
1:I:217:TYR:O	1:I:248:THR:HG23	2.19	0.43
1:I:323:ILE:HD11	5:m:67(C):PHE:CZ	2.54	0.43
6:k:29:ILE:HA	6:k:34:TRP:HZ2	1.83	0.43
5:l:27:SER:H	5:l:31:ARG:NH1	2.17	0.43
6:h:3:GLN:O	6:h:25:SER:OG	2.35	0.43
3:D:100:ASN:C	3:D:100(A):TYR:HD1	2.22	0.43
1:G:272:ILE:HD12	1:G:348:GLN:HG3	2.00	0.42
1:G:45:TRP:CZ3	2:B:629:LEU:HD21	2.54	0.42
3:H:12:LYS:NZ	3:H:82(C):LEU:HB3	2.34	0.42
1:A:43:PRO:HB2	2:C:526:ALA:HA	2.01	0.42
6:d:100(G):PHE:HB2	6:d:100(I):GLU:OE1	2.19	0.42
6:k:15:SER:HA	6:k:82(B):ALA:HA	1.99	0.42
1:G:217:TYR:O	1:G:248:THR:HG23	2.19	0.42
2:B:595:ILE:HG23	2:B:596:TRP:CD1	2.54	0.42
4:L:5:GLN:HE22	4:L:23:CYS:HA	1.84	0.42
1:A:55:ALA:HB3	1:A:216:HIS:HB2	2.01	0.42
1:A:371:VAL:HG11	3:D:56:GLN:HE21	1.84	0.42
1:I:52:LEU:HD21	1:I:488:VAL:HG21	2.02	0.42
1:I:294:ILE:HG23	1:I:447:SER:HB2	2.00	0.42
2:C:595:ILE:HG23	2:C:596:TRP:CD1	2.54	0.42
5:m:80:ALA:HA	5:m:106:VAL:HG11	2.01	0.42
1:G:58:ALA:HA	1:G:61:TYR:HB2	2.00	0.42
3:K:52(A):PRO:HA	3:K:71:ARG:HD3	2.01	0.42
6:h:63:LEU:HB3	6:h:66:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:GLU:O	1:I:166:ARG:HD3	2.19	0.42
5:m:59:PRO:HG2	5:m:61:ARG:HH21	1.83	0.42
3:H:45:LEU:HD11	3:H:103:TRP:HH2	1.85	0.42
2:J:639:THR:C	2:J:641:ILE:H	2.27	0.42
6:k:32:SER:H	6:k:94:ARG:HH22	1.66	0.42
6:k:36:TRP:CH2	6:k:92:CYS:HB3	2.55	0.42
1:G:284:ILE:CG2	1:G:454:LEU:HB2	2.48	0.42
1:G:298:ARG:CG	1:G:443:ILE:HG22	2.50	0.42
6:h:94:ARG:HE	6:h:94:ARG:HB3	1.72	0.42
1:A:226:LEU:HB2	1:A:487:LYS:HG2	2.00	0.42
4:M:66:ARG:HG2	4:M:68:GLY:O	2.20	0.42
1:G:38:VAL:HG13	2:B:604:CYS:HB3	2.00	0.42
1:G:382:PHE:CD2	1:G:424:ILE:HG21	2.55	0.42
1:G:500:ARG:HH21	2:J:663:LEU:HA	1.84	0.42
4:E:46:LEU:HD11	4:E:49:PHE:HB3	2.02	0.42
1:I:331:CYS:HB2	1:I:416:LEU:CD1	2.50	0.42
2:C:587:LEU:HD21	2:J:586:TYR:HD2	1.84	0.42
5:e:91:TRP:HE1	6:d:100(N):PHE:H	1.67	0.42
5:m:50:ASN:HB2	5:m:53:ASP:HB2	2.01	0.42
2:B:650:GLN:O	2:B:654:GLU:OE1	2.38	0.41
2:B:658:GLN:HG3	2:C:603:ILE:HD13	2.01	0.41
3:H:62:ARG:HG3	3:H:63:PHE:CD2	2.55	0.41
1:A:181:VAL:HB	1:A:191:TYR:HB3	2.02	0.41
1:A:258:GLN:NE2	1:A:470:PRO:HB2	2.34	0.41
1:A:325:ASP:OD1	1:A:325:ASP:N	2.50	0.41
2:C:595:ILE:HD12	2:C:595:ILE:HA	1.93	0.41
2:C:597:GLY:HA3	2:C:650:GLN:HE22	1.84	0.41
1:I:109:ILE:HD12	1:I:109:ILE:HA	1.92	0.41
1:G:117:LYS:HB2	1:G:118:PRO:HD3	2.02	0.41
1:G:181:VAL:HB	1:G:191:TYR:HB3	2.03	0.41
1:I:195:ASN:ND2	1:I:425:ASN:HD21	2.17	0.41
2:J:628:TRP:HA	2:J:631:TRP:HD1	1.85	0.41
2:B:601:LYS:O	2:B:603:ILE:N	2.53	0.41
3:H:91:TYR:CE1	3:H:106:GLY:HA3	2.54	0.41
5:e:18:THR:HA	5:e:75:ILE:O	2.20	0.41
2:J:528:SER:OG	2:J:529:THR:N	2.53	0.41
4:M:62:PHE:HZ	4:M:86:TYR:OH	2.04	0.41
5:m:30:SER:OG	5:m:93:SER:OG	2.24	0.41
1:G:109:ILE:HD12	1:G:109:ILE:HA	1.91	0.41
3:H:82(C):LEU:HD11	3:H:86:ASP:CB	2.50	0.41
6:h:71:LEU:HD12	6:h:72:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:89:LYS:HD3	6:h:105:THR:O	2.20	0.41
1:A:129:LEU:HD23	1:A:159:PHE:HB3	2.03	0.41
1:A:383:PHE:HD1	1:A:420:ILE:HG12	1.85	0.41
6:d:51:VAL:HG11	6:d:71:LEU:HD13	2.01	0.41
3:K:47:TRP:NE1	3:K:49:GLY:O	2.52	0.41
4:M:63:SER:O	4:M:73:LEU:HD12	2.20	0.41
1:G:467:THR:C	1:G:468:PHE:HD1	2.28	0.41
1:A:217:TYR:O	1:A:248:THR:HG23	2.21	0.41
1:A:376:PHE:CE1	1:A:383:PHE:HB2	2.55	0.41
1:I:262:ASN:HB2	8:q:1:NAG:HN2	1.86	0.41
1:I:322:ILE:HD13	1:I:322:ILE:HA	1.92	0.41
2:J:658:GLN:HA	2:J:661:LEU:HG	2.02	0.41
3:K:12:LYS:HG2	3:K:18:VAL:HG22	2.01	0.41
5:m:9:ILE:O	5:m:103:THR:OG1	2.34	0.41
5:l:67:ASP:HA	5:l:69:THR:OG1	2.20	0.41
2:J:617:ARG:HD2	2:J:634:GLU:OE1	2.20	0.41
3:K:82(C):LEU:HD11	3:K:86:ASP:CB	2.51	0.41
4:M:23:CYS:O	4:M:70:THR:HA	2.21	0.41
11:i:3:BMA:H62	11:i:7:MAN:H2	1.81	0.41
1:G:257:THR:HG21	1:G:370:GLU:O	2.20	0.41
1:A:295:ASN:HB3	7:a:1:NAG:HN2	1.86	0.41
1:A:323:ILE:HD12	1:A:323:ILE:HA	1.86	0.41
4:E:18:SER:HA	4:E:75:ILE:O	2.21	0.41
5:m:27:SER:OG	5:m:31:ARG:NH1	2.54	0.41
5:m:51:ASN:ND2	5:m:67:ASP:OD1	2.54	0.41
1:G:220:PRO:HG2	1:G:223:PHE:HD2	1.86	0.41
1:A:34:LEU:HD21	2:C:619:LEU:HD11	2.03	0.41
1:A:346:VAL:HG13	1:A:359:ILE:HD12	2.03	0.41
4:E:88:CYS:O	4:E:99:GLY:N	2.44	0.41
5:e:29:GLY:O	5:e:31:ARG:HG3	2.20	0.41
1:I:44:VAL:HG21	2:J:632:ASP:HB3	2.03	0.41
1:G:446:VAL:O	8:O:1:NAG:H5	2.21	0.41
6:h:36:TRP:CD1	6:h:69:LEU:HD21	2.56	0.41
1:A:294:ILE:HG23	1:A:447:SER:HB2	2.03	0.41
2:C:539:VAL:HG23	2:C:540:GLN:HE21	1.86	0.41
1:I:219:ALA:HB1	1:I:223:PHE:HB2	2.03	0.41
9:t:1:NAG:H62	7:v:1:NAG:H81	2.03	0.41
1:G:259:LEU:HD21	1:G:391:PHE:CZ	2.55	0.41
1:G:299:PRO:HB3	1:G:327:ARG:HH21	1.85	0.41
6:h:52:HIS:CG	6:h:53:LYS:N	2.89	0.41
1:A:349:LEU:HD21	1:A:468:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:ARG:HG3	3:D:63:PHE:CD2	2.56	0.41
1:G:86:LEU:HD12	1:G:242:VAL:HG23	2.04	0.40
3:D:12:LYS:NZ	3:D:82(C):LEU:HB3	2.36	0.40
1:I:120:VAL:HG13	1:I:315:GLN:HG2	2.03	0.40
2:B:615:SER:O	2:B:617:ARG:HD2	2.21	0.40
2:B:647:GLU:OE1	2:C:542:ARG:NH2	2.53	0.40
5:l:30:SER:OG	5:l:93:SER:OG	2.26	0.40
6:h:71:LEU:HD13	6:h:78:VAL:HG12	2.03	0.40
1:A:34:LEU:HG	2:C:619:LEU:HD21	2.03	0.40
2:C:647:GLU:O	2:C:651:ASN:HB2	2.21	0.40
4:E:3:LEU:N	4:E:5:GLN:OE1	2.53	0.40
5:e:26:LYS:HG2	5:e:27:SER:O	2.21	0.40
1:I:201:ILE:HA	1:I:433:ALA:O	2.21	0.40
5:m:28:LEU:O	5:m:94:ARG:HD3	2.21	0.40
1:G:424:ILE:HG12	1:G:434:MET:HG2	2.02	0.40
1:G:460:SER:H	3:H:61:TRP:HD1	1.68	0.40
1:A:322:ILE:O	5:e:94:ARG:NH1	2.53	0.40
3:D:37:VAL:CG1	3:D:91:TYR:HB2	2.51	0.40
2:J:534:SER:HA	2:J:537:LEU:HD21	2.03	0.40
6:k:11:LEU:HD12	6:k:11:LEU:O	2.22	0.40
2:B:587:LEU:HD11	2:J:587:LEU:HD11	2.03	0.40
3:H:6:GLN:OE1	3:H:105:GLN:N	2.55	0.40
1:I:230:ASP:HB2	1:I:240:PRO:HD2	2.03	0.40
1:I:288:PHE:HZ	1:I:449:ILE:HG22	1.86	0.40
1:I:342:LEU:HD23	1:I:342:LEU:HA	1.82	0.40
1:I:503:ARG:HH21	2:J:607:ASN:ND2	2.20	0.40
2:J:536:THR:C	2:J:537:LEU:HD22	2.47	0.40
3:K:20:ILE:HG23	3:K:107:VAL:HG21	2.02	0.40
3:K:91:TYR:CE1	3:K:106:GLY:HA3	2.56	0.40
6:k:29:ILE:HA	6:k:34:TRP:CZ2	2.56	0.40
1:G:333:VAL:HG23	1:G:414:ILE:HB	2.03	0.40
1:A:248:THR:HB	1:A:486:TYR:HE2	1.86	0.40
1:A:424:ILE:HG13	1:A:434:MET:HG2	2.04	0.40
1:I:257:THR:HG21	1:I:370:GLU:O	2.22	0.40
1:I:258:GLN:NE2	1:I:470:PRO:HB2	2.37	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	446/481 (93%)	407 (91%)	38 (8%)	1 (0%)	43	75
1	G	446/481 (93%)	411 (92%)	35 (8%)	0	100	100
1	I	446/481 (93%)	403 (90%)	43 (10%)	0	100	100
2	B	127/153 (83%)	119 (94%)	7 (6%)	1 (1%)	16	51
2	C	127/153 (83%)	118 (93%)	9 (7%)	0	100	100
2	J	127/153 (83%)	119 (94%)	8 (6%)	0	100	100
3	D	124/230 (54%)	116 (94%)	8 (6%)	0	100	100
3	H	124/230 (54%)	117 (94%)	7 (6%)	0	100	100
3	K	124/230 (54%)	116 (94%)	8 (6%)	0	100	100
4	E	96/203 (47%)	82 (85%)	13 (14%)	1 (1%)	12	45
4	L	96/203 (47%)	86 (90%)	9 (9%)	1 (1%)	12	45
4	M	96/203 (47%)	84 (88%)	11 (12%)	1 (1%)	12	45
5	e	106/213 (50%)	97 (92%)	9 (8%)	0	100	100
5	l	106/213 (50%)	98 (92%)	8 (8%)	0	100	100
5	m	106/213 (50%)	98 (92%)	8 (8%)	0	100	100
6	d	131/235 (56%)	127 (97%)	4 (3%)	0	100	100
6	h	131/235 (56%)	126 (96%)	4 (3%)	1 (1%)	16	51
6	k	131/235 (56%)	127 (97%)	4 (3%)	0	100	100
All	All	3090/4545 (68%)	2851 (92%)	233 (8%)	6 (0%)	44	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	602	LEU
1	A	208	VAL
4	L	32	ILE
4	E	32	ILE

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Mol	Chain	Res	Type
4	M	32	ILE
6	h	100(H)	ASN

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	403/428 (94%)	402 (100%)	1 (0%)	87	87
1	G	403/428 (94%)	403 (100%)	0	100	100
1	I	403/428 (94%)	403 (100%)	0	100	100
2	B	110/129 (85%)	110 (100%)	0	100	100
2	C	110/129 (85%)	110 (100%)	0	100	100
2	J	110/129 (85%)	110 (100%)	0	100	100
3	D	104/194 (54%)	104 (100%)	0	100	100
3	H	104/194 (54%)	104 (100%)	0	100	100
3	K	104/194 (54%)	104 (100%)	0	100	100
4	E	83/173 (48%)	83 (100%)	0	100	100
4	L	83/173 (48%)	82 (99%)	1 (1%)	63	73
4	M	83/173 (48%)	83 (100%)	0	100	100
5	e	89/179 (50%)	89 (100%)	0	100	100
5	l	89/179 (50%)	89 (100%)	0	100	100
5	m	89/179 (50%)	89 (100%)	0	100	100
6	d	113/202 (56%)	113 (100%)	0	100	100
6	h	113/202 (56%)	113 (100%)	0	100	100
6	k	113/202 (56%)	113 (100%)	0	100	100
All	All	2706/3915 (69%)	2704 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	77	ASN
1	A	296	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	283	ASN
1	G	432	GLN
2	B	591	GLN
2	B	656	ASN
3	H	75	GLN
5	l	52	GLN
5	l	89	HIS
6	h	58	ASN
1	A	67	ASN
1	A	130	GLN
1	A	188	ASN
1	A	432	GLN
2	C	540	GLN
2	C	577	GLN
2	C	591	GLN
2	C	630	GLN
2	C	640	GLN
2	C	650	GLN
5	e	37	GLN
6	d	97	HIS
6	d	103	ASN
1	I	82	GLN
1	I	99	ASN
1	I	103	GLN
1	I	246	GLN
1	I	283	ASN
1	I	422	GLN
1	I	425	ASN
1	I	428	GLN
1	I	432	GLN
2	J	591	GLN
3	K	32	GLN
5	m	52	GLN
6	k	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

105 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	F	1	1,7	14,14,15	0.21	0	17,19,21	0.40	0
7	NAG	F	2	7	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	N	1	1,7	14,14,15	0.32	0	17,19,21	0.50	0
7	NAG	N	2	7	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	O	1	1,8	14,14,15	0.63	1 (7%)	17,19,21	0.67	1 (5%)
8	NAG	O	2	8	14,14,15	0.25	0	17,19,21	0.50	0
8	BMA	O	3	8	11,11,12	0.45	0	15,15,17	0.80	0
8	MAN	O	4	8	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
7	NAG	P	1	1,7	14,14,15	0.43	0	17,19,21	0.49	0
7	NAG	P	2	7	14,14,15	0.22	0	17,19,21	0.43	0
7	NAG	Q	1	1,7	14,14,15	0.32	0	17,19,21	0.53	0
7	NAG	Q	2	7	14,14,15	0.23	0	17,19,21	0.46	0
9	NAG	R	1	1,9	14,14,15	0.17	0	17,19,21	0.41	0
9	NAG	R	2	9	14,14,15	0.19	0	17,19,21	0.53	0
9	BMA	R	3	9	11,11,12	0.58	0	15,15,17	0.69	0
10	NAG	S	1	1,10	14,14,15	0.20	0	17,19,21	0.49	0
10	NAG	S	2	10	14,14,15	0.38	0	17,19,21	0.38	0
10	BMA	S	3	10	11,11,12	0.61	0	15,15,17	0.76	0
10	MAN	S	4	10	11,11,12	0.82	0	15,15,17	1.16	2 (13%)
10	MAN	S	5	10	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
7	NAG	T	1	1,7	14,14,15	0.44	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	T	2	7	14,14,15	0.25	0	17,19,21	0.52	0
11	NAG	U	1	1,11	14,14,15	0.24	0	17,19,21	0.41	0
11	NAG	U	2	11	14,14,15	0.27	0	17,19,21	0.64	0
11	BMA	U	3	11	11,11,12	0.96	0	15,15,17	0.91	0
11	MAN	U	4	11	11,11,12	0.65	0	15,15,17	1.09	2 (13%)
11	MAN	U	5	11	11,11,12	0.70	0	15,15,17	0.97	1 (6%)
11	MAN	U	6	11	11,11,12	0.80	0	15,15,17	1.30	2 (13%)
11	MAN	U	7	11	11,11,12	0.72	0	15,15,17	1.03	2 (13%)
11	MAN	U	8	11	11,11,12	0.64	0	15,15,17	0.92	1 (6%)
11	MAN	U	9	11	11,11,12	0.83	1 (9%)	15,15,17	1.32	2 (13%)
7	NAG	V	1	1,7	14,14,15	0.25	0	17,19,21	0.75	1 (5%)
7	NAG	V	2	7	14,14,15	0.30	0	17,19,21	0.41	0
7	NAG	W	1	1,7	14,14,15	0.31	0	17,19,21	0.52	0
7	NAG	W	2	7	14,14,15	0.31	0	17,19,21	0.55	0
7	NAG	X	1	1,7	14,14,15	0.20	0	17,19,21	0.44	0
7	NAG	X	2	7	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	Y	1	1,7	14,14,15	0.28	0	17,19,21	0.50	0
7	NAG	Y	2	7	14,14,15	0.19	0	17,19,21	0.43	0
8	NAG	Z	1	1,8	14,14,15	0.63	1 (7%)	17,19,21	0.69	1 (5%)
8	NAG	Z	2	8	14,14,15	0.26	0	17,19,21	0.49	0
8	BMA	Z	3	8	11,11,12	0.48	0	15,15,17	0.81	0
8	MAN	Z	4	8	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
7	NAG	a	1	1,7	14,14,15	0.37	0	17,19,21	0.59	0
7	NAG	a	2	7	14,14,15	0.32	0	17,19,21	0.40	0
7	NAG	b	1	1,7	14,14,15	0.32	0	17,19,21	0.53	0
7	NAG	b	2	7	14,14,15	0.24	0	17,19,21	0.41	0
9	NAG	c	1	1,9	14,14,15	0.19	0	17,19,21	0.40	0
9	NAG	c	2	9	14,14,15	0.20	0	17,19,21	0.50	0
9	BMA	c	3	9	11,11,12	0.57	0	15,15,17	0.66	0
10	NAG	f	1	1,10	14,14,15	0.26	0	17,19,21	0.51	0
10	NAG	f	2	10	14,14,15	0.24	0	17,19,21	0.56	0
10	BMA	f	3	10	11,11,12	0.66	0	15,15,17	0.75	0
10	MAN	f	4	10	11,11,12	0.81	1 (9%)	15,15,17	1.08	2 (13%)
10	MAN	f	5	10	11,11,12	0.58	0	15,15,17	0.92	2 (13%)
7	NAG	g	1	1,7	14,14,15	0.58	1 (7%)	17,19,21	0.48	0
7	NAG	g	2	7	14,14,15	0.38	0	17,19,21	0.59	0
11	NAG	i	1	1,11	14,14,15	0.25	0	17,19,21	0.63	0
11	NAG	i	2	11	14,14,15	0.41	0	17,19,21	0.71	0
11	BMA	i	3	11	11,11,12	0.92	0	15,15,17	1.00	0
11	MAN	i	4	11	11,11,12	0.66	0	15,15,17	1.14	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	i	5	11	11,11,12	0.72	0	15,15,17	0.93	1 (6%)
11	MAN	i	6	11	11,11,12	0.79	1 (9%)	15,15,17	1.34	2 (13%)
11	MAN	i	7	11	11,11,12	0.67	0	15,15,17	0.89	2 (13%)
11	MAN	i	8	11	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
11	MAN	i	9	11	11,11,12	0.78	1 (9%)	15,15,17	1.17	2 (13%)
7	NAG	j	1	1,7	14,14,15	0.29	0	17,19,21	0.69	0
7	NAG	j	2	7	14,14,15	0.32	0	17,19,21	0.42	0
7	NAG	n	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	0.68	0
7	NAG	n	2	7	14,14,15	0.47	0	17,19,21	0.54	0
7	NAG	o	1	1,7	14,14,15	0.15	0	17,19,21	0.45	0
7	NAG	o	2	7	14,14,15	0.25	0	17,19,21	0.44	0
7	NAG	p	1	1,7	14,14,15	0.28	0	17,19,21	0.56	0
7	NAG	p	2	7	14,14,15	0.26	0	17,19,21	0.44	0
8	NAG	q	1	1,8	14,14,15	0.62	1 (7%)	17,19,21	0.69	1 (5%)
8	NAG	q	2	8	14,14,15	0.26	0	17,19,21	0.48	0
8	BMA	q	3	8	11,11,12	0.48	0	15,15,17	0.82	0
8	MAN	q	4	8	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
7	NAG	r	1	1,7	14,14,15	0.64	1 (7%)	17,19,21	0.84	1 (5%)
7	NAG	r	2	7	14,14,15	0.47	0	17,19,21	0.47	0
7	NAG	s	1	1,7	14,14,15	0.27	0	17,19,21	0.52	0
7	NAG	s	2	7	14,14,15	0.26	0	17,19,21	0.53	0
9	NAG	t	1	1,9	14,14,15	0.22	0	17,19,21	0.37	0
9	NAG	t	2	9	14,14,15	0.19	0	17,19,21	0.54	0
9	BMA	t	3	9	11,11,12	0.61	0	15,15,17	0.67	0
10	NAG	u	1	1,10	14,14,15	0.31	0	17,19,21	0.62	0
10	NAG	u	2	10	14,14,15	0.33	0	17,19,21	0.37	0
10	BMA	u	3	10	11,11,12	0.65	0	15,15,17	0.80	0
10	MAN	u	4	10	11,11,12	0.75	0	15,15,17	1.20	2 (13%)
10	MAN	u	5	10	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
7	NAG	v	1	1,7	14,14,15	0.52	0	17,19,21	0.42	0
7	NAG	v	2	7	14,14,15	0.27	0	17,19,21	0.55	0
11	NAG	w	1	1,11	14,14,15	0.20	0	17,19,21	0.51	0
11	NAG	w	2	11	14,14,15	0.29	0	17,19,21	0.69	0
11	BMA	w	3	11	11,11,12	0.97	0	15,15,17	0.96	0
11	MAN	w	4	11	11,11,12	0.72	0	15,15,17	1.11	1 (6%)
11	MAN	w	5	11	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
11	MAN	w	6	11	11,11,12	0.83	0	15,15,17	1.32	2 (13%)
11	MAN	w	7	11	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
11	MAN	w	8	11	11,11,12	0.92	1 (9%)	15,15,17	1.50	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	w	9	11	11,11,12	0.94	1 (9%)	15,15,17	0.97	1 (6%)
7	NAG	x	1	1,7	14,14,15	0.30	0	17,19,21	0.69	0
7	NAG	x	2	7	14,14,15	0.29	0	17,19,21	0.42	0
7	NAG	y	1	1,7	14,14,15	0.69	1 (7%)	17,19,21	1.77	1 (5%)
7	NAG	y	2	7	14,14,15	0.51	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	F	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	0/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
8	NAG	O	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	O	2	8	-	0/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
8	MAN	O	4	8	-	0/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
9	NAG	R	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	2/6/23/26	0/1/1/1
9	BMA	R	3	9	-	2/2/19/22	0/1/1/1
10	NAG	S	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	BMA	S	3	10	-	1/2/19/22	0/1/1/1
10	MAN	S	4	10	-	0/2/19/22	1/1/1/1
10	MAN	S	5	10	-	1/2/19/22	0/1/1/1
7	NAG	T	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
11	NAG	U	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	4/6/23/26	0/1/1/1
11	BMA	U	3	11	-	1/2/19/22	0/1/1/1
11	MAN	U	4	11	-	2/2/19/22	0/1/1/1
11	MAN	U	5	11	-	1/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	i	8	11	-	1/2/19/22	0/1/1/1
11	MAN	i	9	11	-	0/2/19/22	0/1/1/1
7	NAG	j	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	NAG	n	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	n	2	7	-	3/6/23/26	0/1/1/1
7	NAG	o	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	-	2/6/23/26	0/1/1/1
7	NAG	p	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	p	2	7	-	2/6/23/26	0/1/1/1
8	NAG	q	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	q	3	8	-	0/2/19/22	0/1/1/1
8	MAN	q	4	8	-	1/2/19/22	0/1/1/1
7	NAG	r	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	r	2	7	-	2/6/23/26	0/1/1/1
7	NAG	s	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	s	2	7	-	2/6/23/26	0/1/1/1
9	NAG	t	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	BMA	t	3	9	-	2/2/19/22	0/1/1/1
10	NAG	u	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
10	BMA	u	3	10	-	2/2/19/22	0/1/1/1
10	MAN	u	4	10	-	1/2/19/22	1/1/1/1
10	MAN	u	5	10	-	2/2/19/22	0/1/1/1
7	NAG	v	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	v	2	7	-	4/6/23/26	0/1/1/1
11	NAG	w	1	1,11	-	1/6/23/26	0/1/1/1
11	NAG	w	2	11	-	4/6/23/26	0/1/1/1
11	BMA	w	3	11	-	1/2/19/22	0/1/1/1
11	MAN	w	4	11	-	0/2/19/22	0/1/1/1
11	MAN	w	5	11	-	1/2/19/22	0/1/1/1
11	MAN	w	6	11	-	1/2/19/22	1/1/1/1
11	MAN	w	7	11	-	1/2/19/22	0/1/1/1
11	MAN	w	8	11	-	1/2/19/22	0/1/1/1
11	MAN	w	9	11	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	x	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	x	2	7	-	2/6/23/26	0/1/1/1
7	NAG	y	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	y	2	7	-	4/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	n	1	NAG	O5-C1	-2.74	1.39	1.43
7	y	1	NAG	O5-C1	2.46	1.47	1.43
11	w	8	MAN	C1-C2	2.43	1.58	1.52
11	i	9	MAN	C1-C2	2.41	1.57	1.52
10	f	4	MAN	C1-C2	2.38	1.57	1.52
7	r	1	NAG	C1-C2	2.30	1.55	1.52
11	i	6	MAN	C1-C2	2.23	1.57	1.52
8	q	1	NAG	C1-C2	2.15	1.55	1.52
8	O	1	NAG	C1-C2	2.15	1.55	1.52
8	Z	1	NAG	C1-C2	2.14	1.55	1.52
11	U	9	MAN	C1-C2	2.12	1.57	1.52
11	w	9	MAN	C1-C2	2.04	1.57	1.52
7	g	1	NAG	O5-C1	-2.01	1.40	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	y	1	NAG	C1-O5-C5	6.71	121.19	112.19
11	w	8	MAN	C1-O5-C5	4.25	117.89	112.19
11	i	6	MAN	C1-O5-C5	4.05	117.61	112.19
11	U	6	MAN	C1-O5-C5	3.97	117.51	112.19
11	w	6	MAN	C1-O5-C5	3.97	117.50	112.19
10	u	4	MAN	C1-O5-C5	3.65	117.08	112.19
11	U	9	MAN	C1-O5-C5	3.48	116.86	112.19
10	S	4	MAN	C1-O5-C5	3.29	116.60	112.19
11	i	4	MAN	C1-O5-C5	3.10	116.34	112.19
11	w	4	MAN	C1-O5-C5	2.99	116.19	112.19
11	U	4	MAN	C1-O5-C5	2.88	116.05	112.19
11	i	9	MAN	C1-O5-C5	2.83	115.98	112.19
11	w	5	MAN	C1-O5-C5	2.73	115.85	112.19
8	q	4	MAN	C1-O5-C5	2.64	115.73	112.19
11	i	5	MAN	C1-O5-C5	2.61	115.69	112.19
10	f	4	MAN	C1-O5-C5	2.54	115.60	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Z	4	MAN	C1-O5-C5	2.52	115.56	112.19
11	U	7	MAN	C1-O5-C5	2.51	115.55	112.19
7	r	1	NAG	C1-O5-C5	2.50	115.54	112.19
10	u	5	MAN	C1-O5-C5	2.49	115.52	112.19
11	U	5	MAN	C1-O5-C5	2.47	115.50	112.19
11	i	8	MAN	C1-O5-C5	2.46	115.48	112.19
7	V	1	NAG	C1-O5-C5	2.37	115.37	112.19
8	O	4	MAN	C1-O5-C5	2.37	115.37	112.19
11	w	6	MAN	O2-C2-C3	-2.36	105.27	110.15
11	U	6	MAN	O2-C2-C3	-2.35	105.28	110.15
8	q	1	NAG	C1-O5-C5	2.35	115.33	112.19
10	S	5	MAN	C1-O5-C5	2.30	115.27	112.19
11	w	8	MAN	O2-C2-C3	-2.28	105.42	110.15
8	Z	1	NAG	C1-O5-C5	2.28	115.24	112.19
11	U	7	MAN	O2-C2-C3	-2.26	105.47	110.15
11	i	7	MAN	O2-C2-C3	-2.26	105.48	110.15
11	U	9	MAN	O2-C2-C3	-2.25	105.49	110.15
11	i	6	MAN	O2-C2-C3	-2.25	105.49	110.15
11	w	5	MAN	O2-C2-C3	-2.25	105.50	110.15
8	O	1	NAG	C1-O5-C5	2.23	115.17	112.19
10	u	5	MAN	O2-C2-C3	-2.20	105.60	110.15
11	U	8	MAN	O2-C2-C3	-2.20	105.60	110.15
11	w	7	MAN	O2-C2-C3	-2.20	105.60	110.15
10	f	5	MAN	O2-C2-C3	-2.19	105.61	110.15
11	U	4	MAN	O2-C2-C3	-2.19	105.62	110.15
8	Z	4	MAN	O2-C2-C3	-2.18	105.64	110.15
8	q	4	MAN	O2-C2-C3	-2.17	105.65	110.15
11	i	7	MAN	C1-O5-C5	2.16	115.09	112.19
10	S	5	MAN	O2-C2-C3	-2.16	105.68	110.15
10	u	4	MAN	O2-C2-C3	-2.14	105.72	110.15
11	i	8	MAN	O2-C2-C3	-2.14	105.72	110.15
11	w	9	MAN	O2-C2-C3	-2.11	105.78	110.15
11	i	9	MAN	O2-C2-C3	-2.11	105.78	110.15
10	f	5	MAN	C1-O5-C5	2.11	115.01	112.19
11	i	4	MAN	O2-C2-C3	-2.10	105.81	110.15
10	S	4	MAN	O2-C2-C3	-2.08	105.85	110.15
8	O	4	MAN	O2-C2-C3	-2.07	105.86	110.15
10	f	4	MAN	O2-C2-C3	-2.04	105.92	110.15

There are no chirality outliers.

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	g	1	NAG	O5-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
11	i	3	BMA	O5-C5-C6-O6
7	x	2	NAG	C4-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	r	2	NAG	O5-C5-C6-O6
8	q	1	NAG	O5-C5-C6-O6
11	U	7	MAN	O5-C5-C6-O6
11	i	2	NAG	O5-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
7	n	2	NAG	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	n	1	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
11	U	8	MAN	O5-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
7	Y	2	NAG	O5-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
10	u	2	NAG	O5-C5-C6-O6
11	i	7	MAN	O5-C5-C6-O6
11	w	2	NAG	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	x	1	NAG	O5-C5-C6-O6
11	i	1	NAG	O5-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	v	1	NAG	O5-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
11	i	2	NAG	C4-C5-C6-O6
7	F	1	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	y	2	NAG	O5-C5-C6-O6
10	u	3	BMA	O5-C5-C6-O6
11	U	4	MAN	O5-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
7	x	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	v	2	NAG	C4-C5-C6-O6
11	U	7	MAN	C4-C5-C6-O6
11	U	4	MAN	C4-C5-C6-O6
7	Y	2	NAG	C4-C5-C6-O6
7	x	1	NAG	C4-C5-C6-O6
10	u	3	BMA	C4-C5-C6-O6
11	U	8	MAN	C4-C5-C6-O6
11	i	7	MAN	C4-C5-C6-O6
11	w	9	MAN	C4-C5-C6-O6
8	Z	4	MAN	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
8	q	1	NAG	C4-C5-C6-O6
7	v	1	NAG	C4-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
11	w	9	MAN	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	r	2	NAG	C4-C5-C6-O6
7	y	1	NAG	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
8	Z	4	MAN	C4-C5-C6-O6
9	t	3	BMA	O5-C5-C6-O6
11	U	2	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6
11	w	2	NAG	C4-C5-C6-O6
7	n	1	NAG	C4-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
7	y	2	NAG	C4-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
8	Z	1	NAG	C4-C5-C6-O6
10	u	2	NAG	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
9	R	3	BMA	O5-C5-C6-O6
7	s	1	NAG	C4-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	W	1	NAG	O5-C5-C6-O6
7	v	2	NAG	O5-C5-C6-O6
9	R	3	BMA	C4-C5-C6-O6
11	w	8	MAN	O5-C5-C6-O6
8	O	1	NAG	C4-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
11	w	1	NAG	O5-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6
10	u	5	MAN	C4-C5-C6-O6
11	i	3	BMA	C4-C5-C6-O6
11	i	1	NAG	C4-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
8	q	4	MAN	O5-C5-C6-O6
10	u	5	MAN	O5-C5-C6-O6
11	w	7	MAN	O5-C5-C6-O6
11	w	6	MAN	O5-C5-C6-O6
10	S	3	BMA	O5-C5-C6-O6
11	i	8	MAN	O5-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
10	f	5	MAN	O5-C5-C6-O6
11	i	5	MAN	O5-C5-C6-O6
11	U	6	MAN	C4-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
9	t	1	NAG	O5-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
10	f	3	BMA	O5-C5-C6-O6
10	u	4	MAN	O5-C5-C6-O6
10	u	1	NAG	O5-C5-C6-O6
10	f	1	NAG	O5-C5-C6-O6
10	f	2	NAG	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
11	w	5	MAN	O5-C5-C6-O6
11	U	2	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
9	t	3	BMA	C4-C5-C6-O6
8	O	1	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	N	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	T	2	NAG	C1-C2-N2-C7
7	v	2	NAG	C1-C2-N2-C7
7	y	2	NAG	C1-C2-N2-C7
7	Q	2	NAG	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
11	w	3	BMA	C4-C5-C6-O6
7	p	2	NAG	C4-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6
7	N	1	NAG	C3-C2-N2-C7
7	V	1	NAG	C3-C2-N2-C7
7	W	2	NAG	C3-C2-N2-C7
7	Y	1	NAG	C3-C2-N2-C7
7	g	2	NAG	C3-C2-N2-C7
7	j	1	NAG	C3-C2-N2-C7
7	p	1	NAG	C3-C2-N2-C7
7	v	2	NAG	C3-C2-N2-C7
7	x	1	NAG	C3-C2-N2-C7
10	f	2	NAG	C3-C2-N2-C7
11	U	2	NAG	C3-C2-N2-C7
11	i	2	NAG	C3-C2-N2-C7
11	w	2	NAG	C3-C2-N2-C7
9	t	2	NAG	O5-C5-C6-O6
11	U	3	BMA	C4-C5-C6-O6
7	y	1	NAG	C4-C5-C6-O6
11	U	6	MAN	O5-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
7	V	1	NAG	C1-C2-N2-C7
7	Y	1	NAG	C1-C2-N2-C7
7	g	2	NAG	C1-C2-N2-C7
7	j	1	NAG	C1-C2-N2-C7
7	n	2	NAG	C1-C2-N2-C7
7	p	1	NAG	C1-C2-N2-C7
7	x	1	NAG	C1-C2-N2-C7
11	U	2	NAG	C1-C2-N2-C7
11	i	2	NAG	C1-C2-N2-C7
11	w	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
7	y	2	NAG	C3-C2-N2-C7
8	O	1	NAG	C3-C2-N2-C7
8	Z	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	q	1	NAG	C3-C2-N2-C7
9	c	3	BMA	O5-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
9	c	3	BMA	C4-C5-C6-O6
10	S	5	MAN	C4-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6

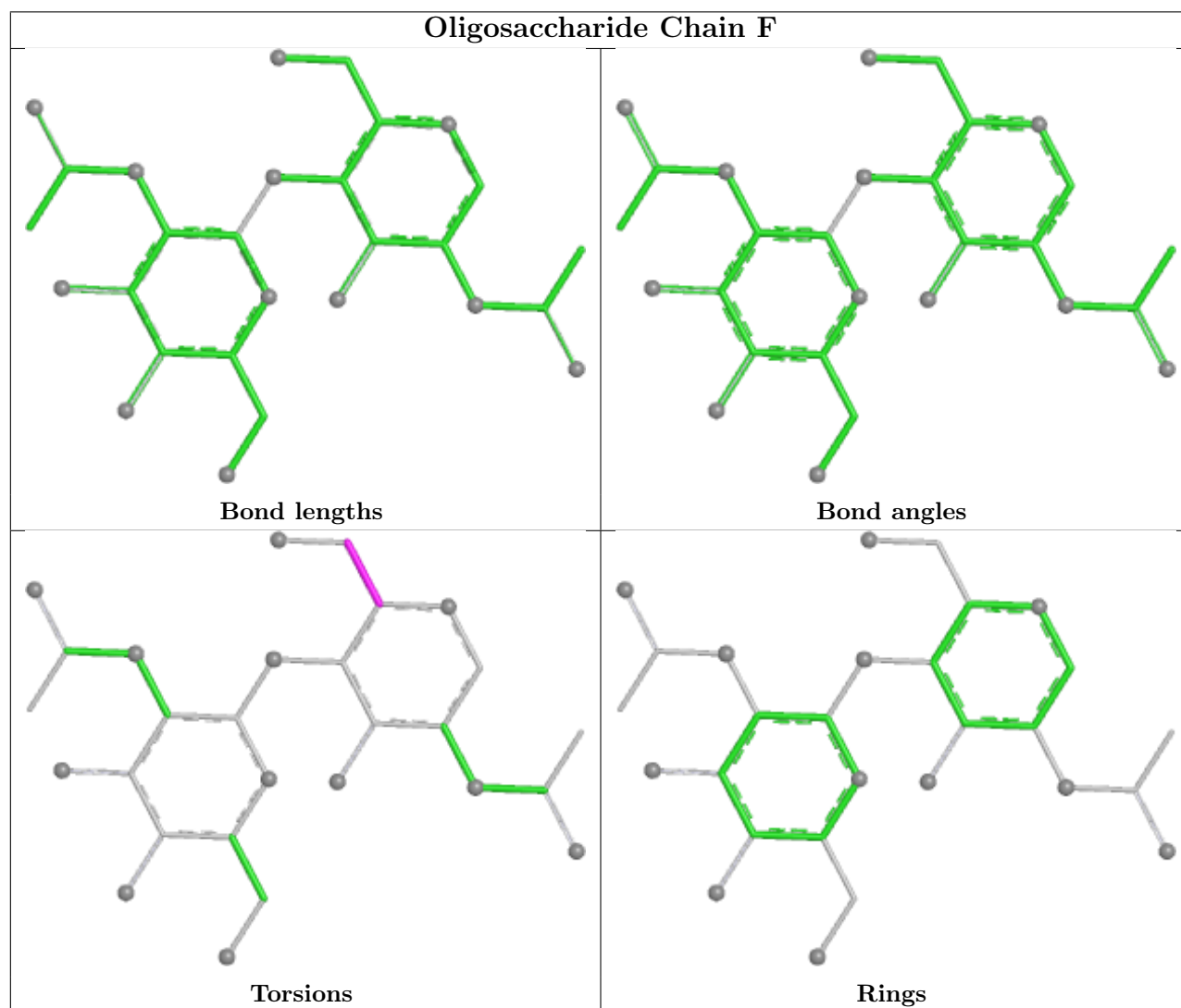
All (4) ring outliers are listed below:

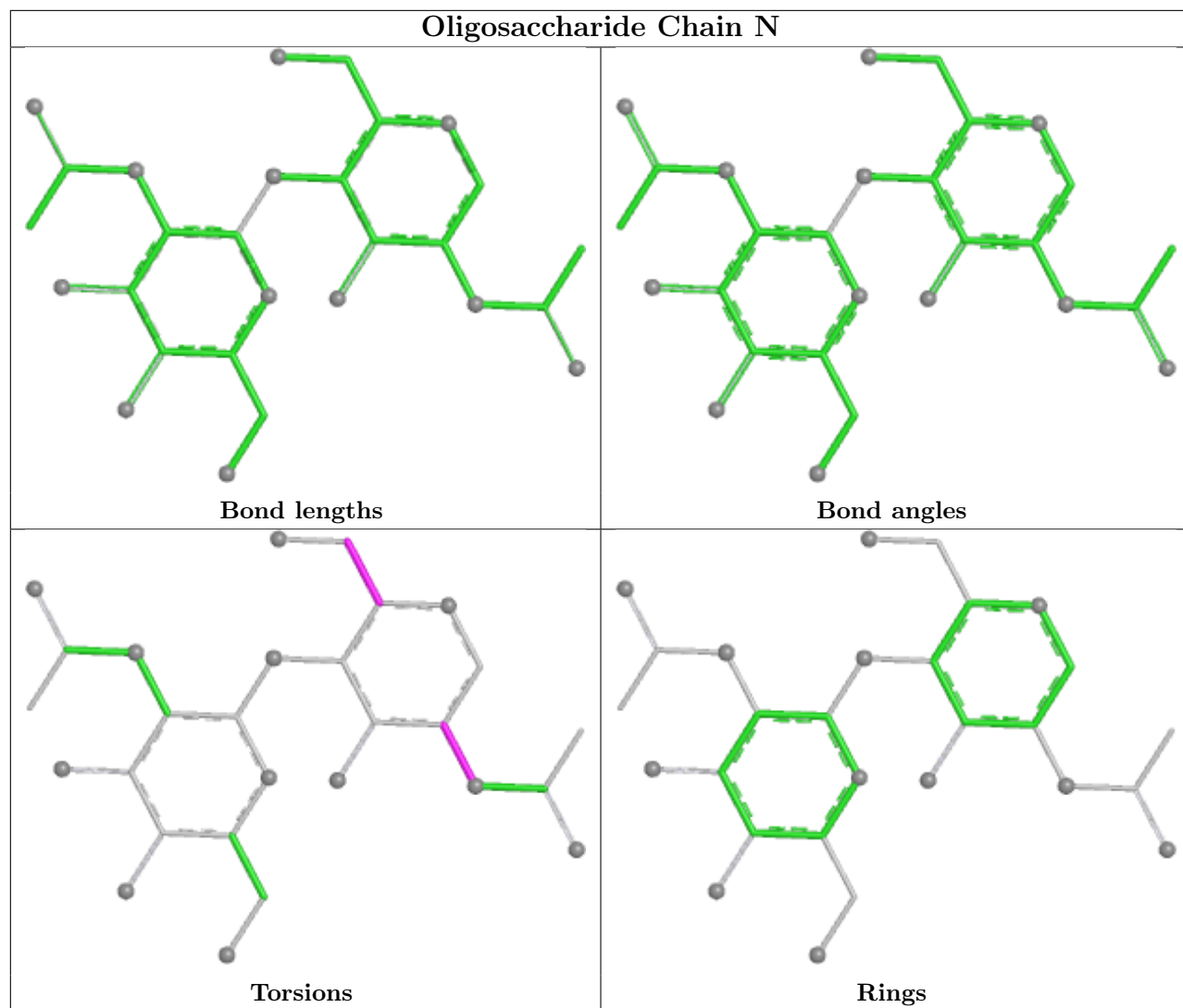
Mol	Chain	Res	Type	Atoms
10	S	4	MAN	C1-C2-C3-C4-C5-O5
11	w	6	MAN	C1-C2-C3-C4-C5-O5
11	U	6	MAN	C1-C2-C3-C4-C5-O5
10	u	4	MAN	C1-C2-C3-C4-C5-O5

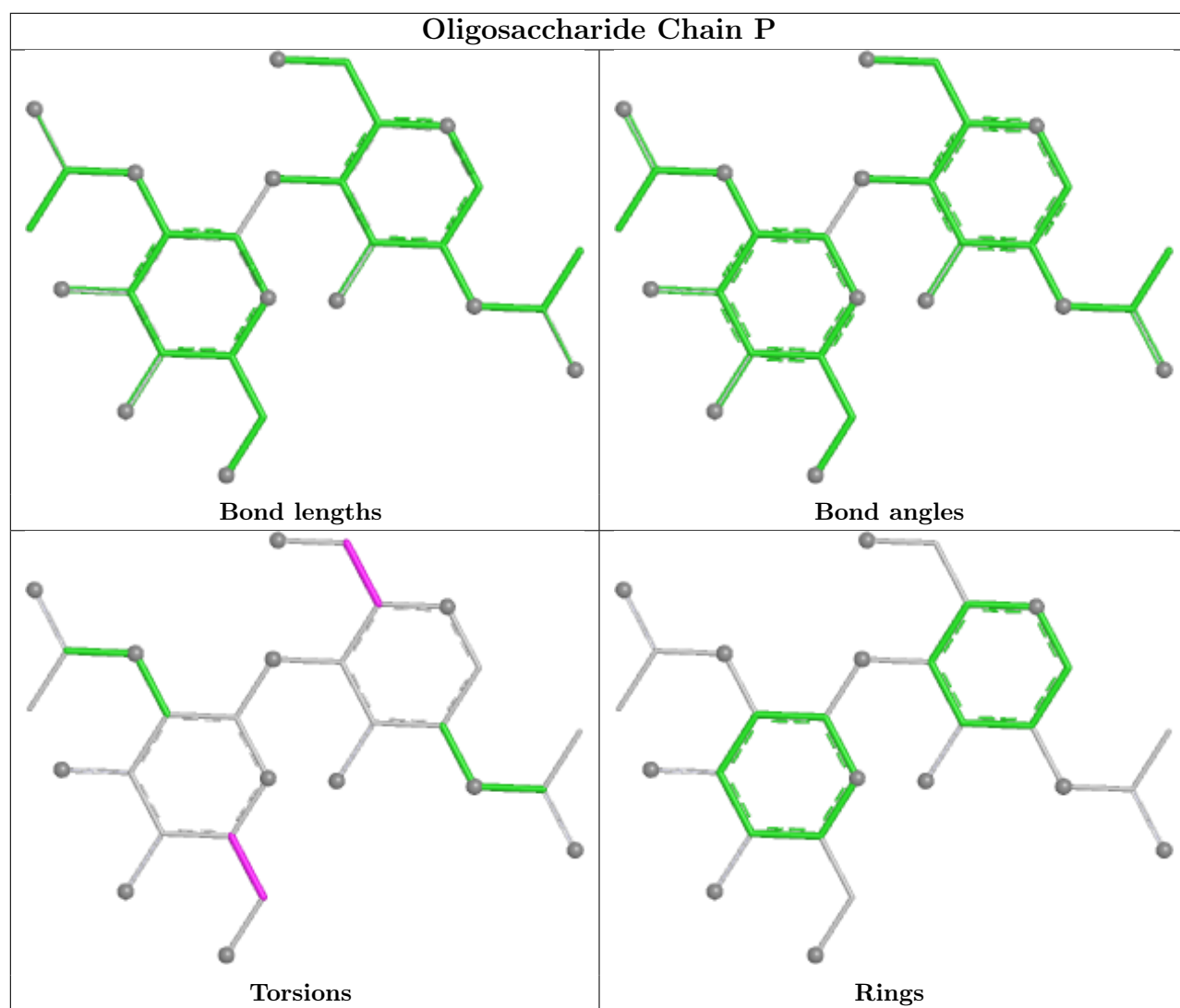
24 monomers are involved in 31 short contacts:

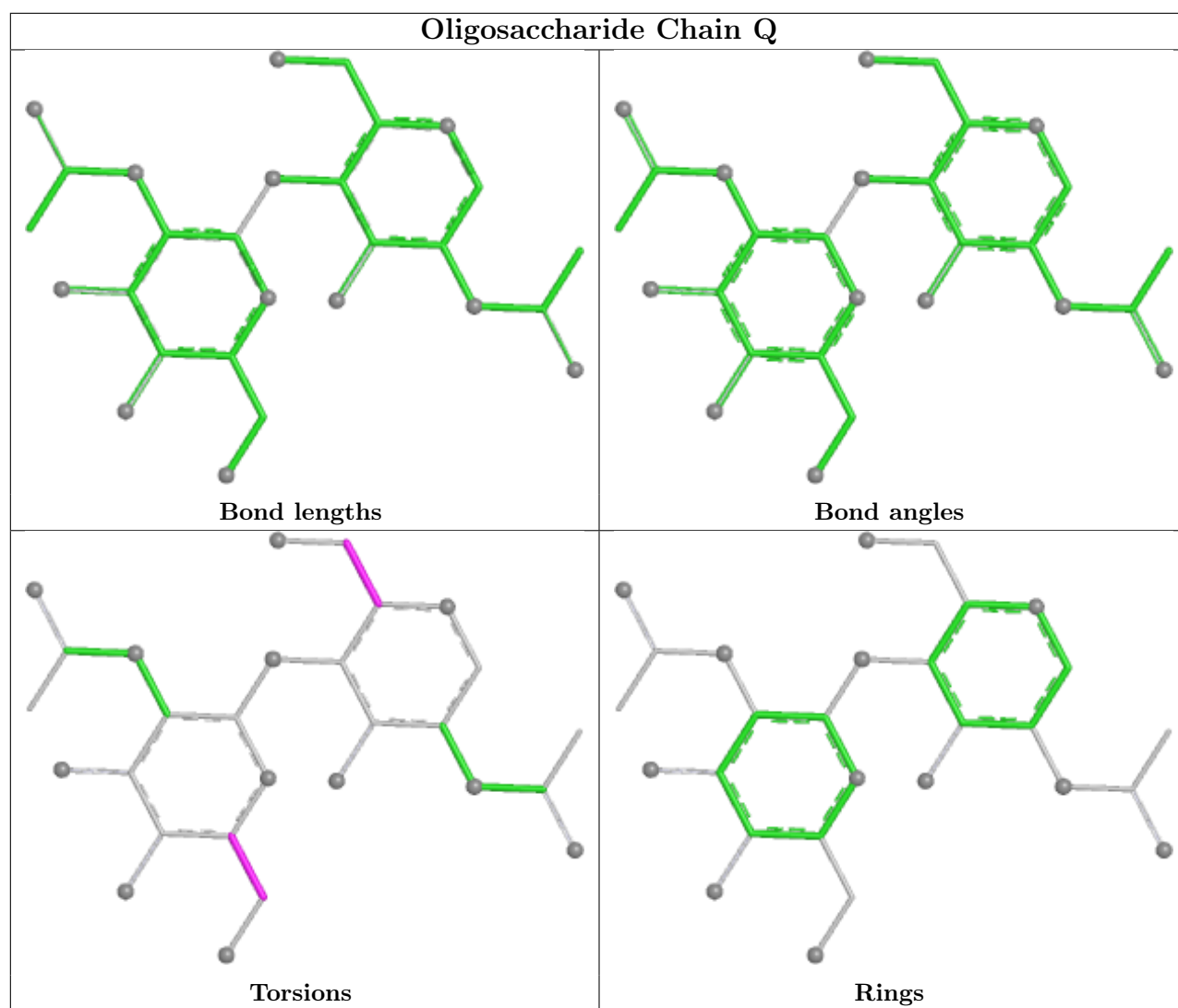
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	n	2	NAG	3	0
7	W	2	NAG	2	0
11	i	4	MAN	1	0
7	v	1	NAG	1	0
7	r	1	NAG	1	0
11	i	7	MAN	1	0
7	y	2	NAG	2	0
11	w	9	MAN	1	0
8	q	1	NAG	2	0
8	q	2	NAG	1	0
7	W	1	NAG	7	0
11	U	3	BMA	1	0
8	O	1	NAG	1	0
7	p	1	NAG	1	0
11	w	4	MAN	1	0
7	y	1	NAG	2	0
9	t	1	NAG	1	0
11	w	7	MAN	1	0
7	r	2	NAG	1	0
7	a	1	NAG	2	0
11	U	1	NAG	1	0
10	u	2	NAG	1	0
11	i	3	BMA	1	0
7	V	1	NAG	1	0

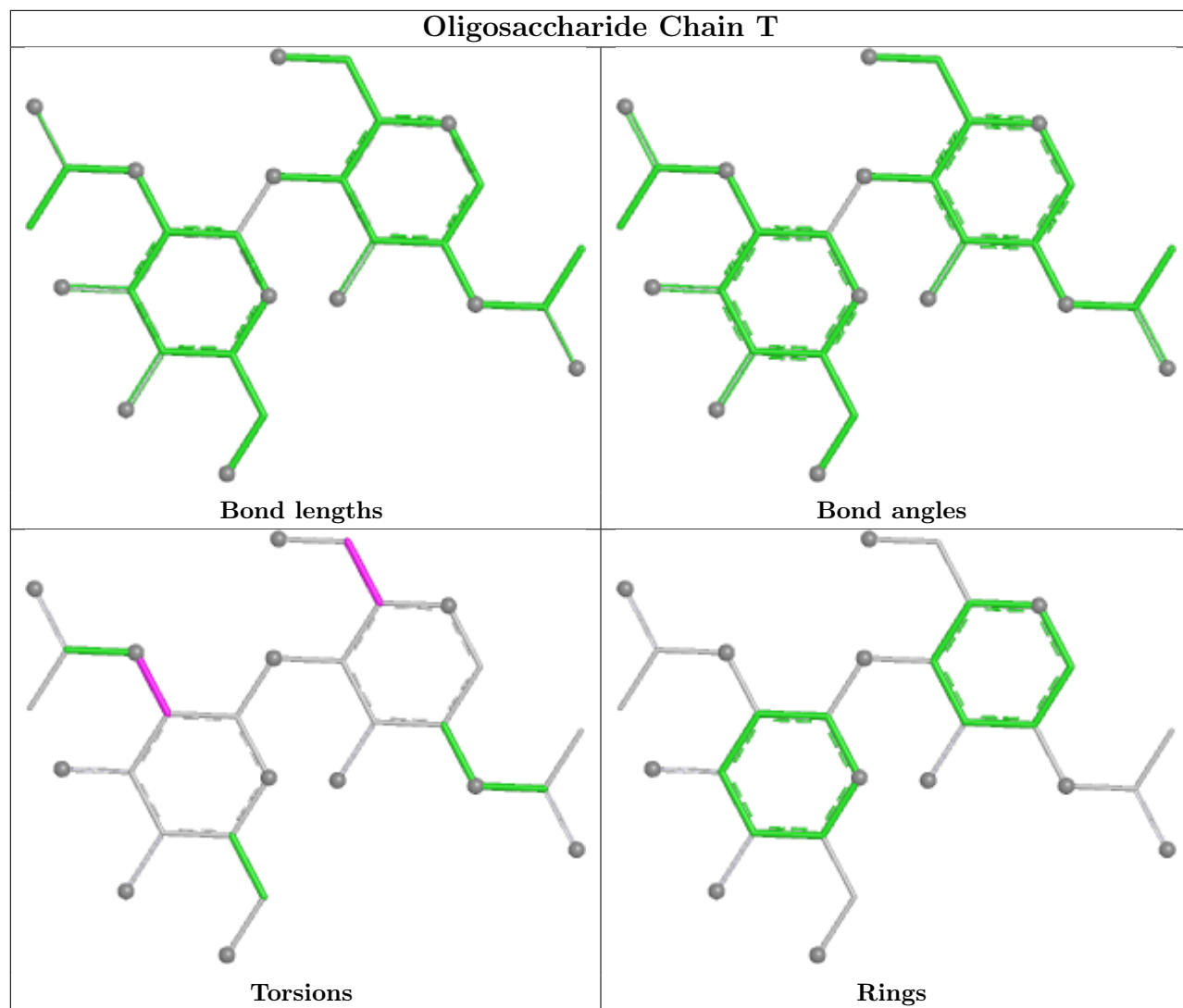
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

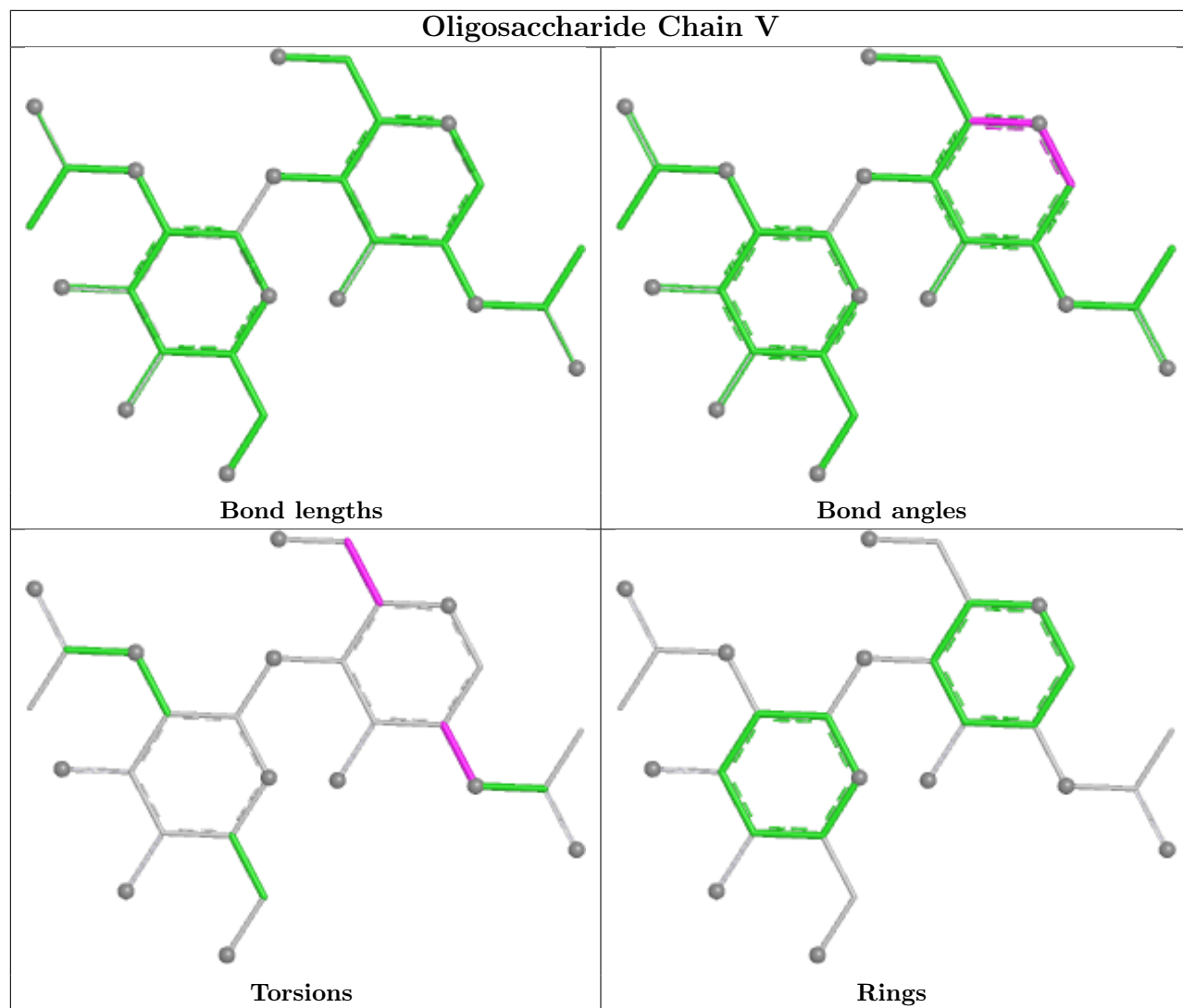


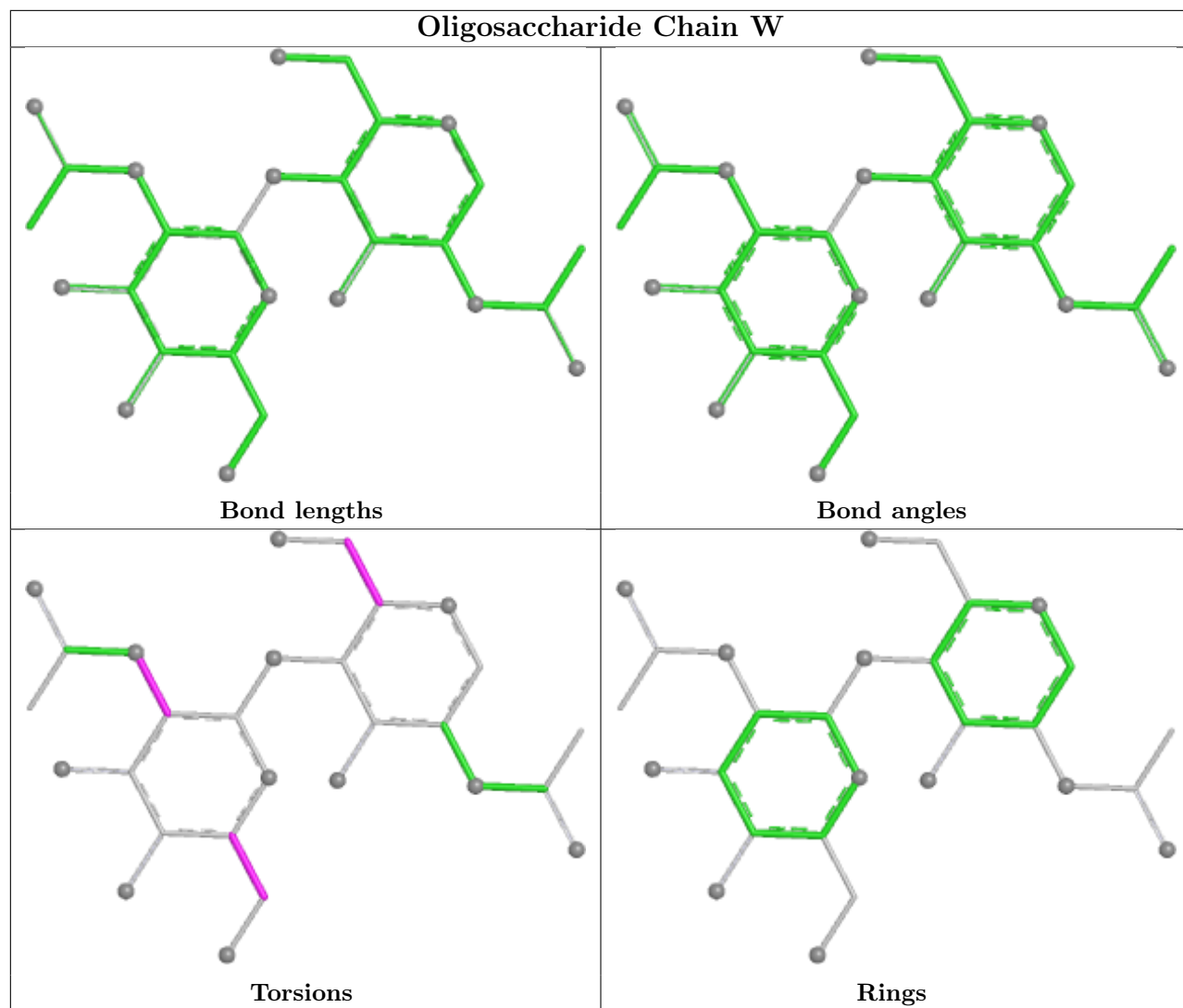


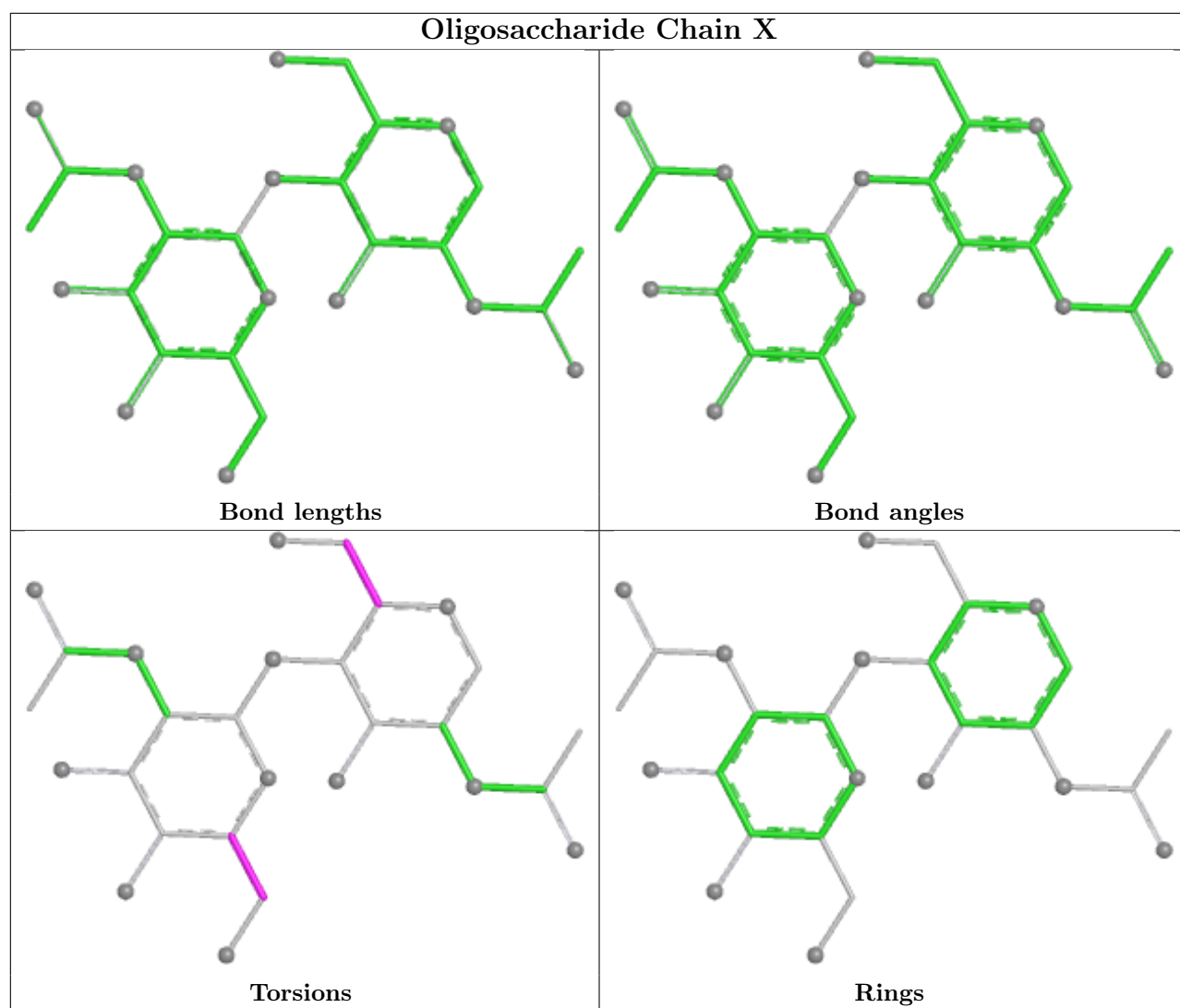


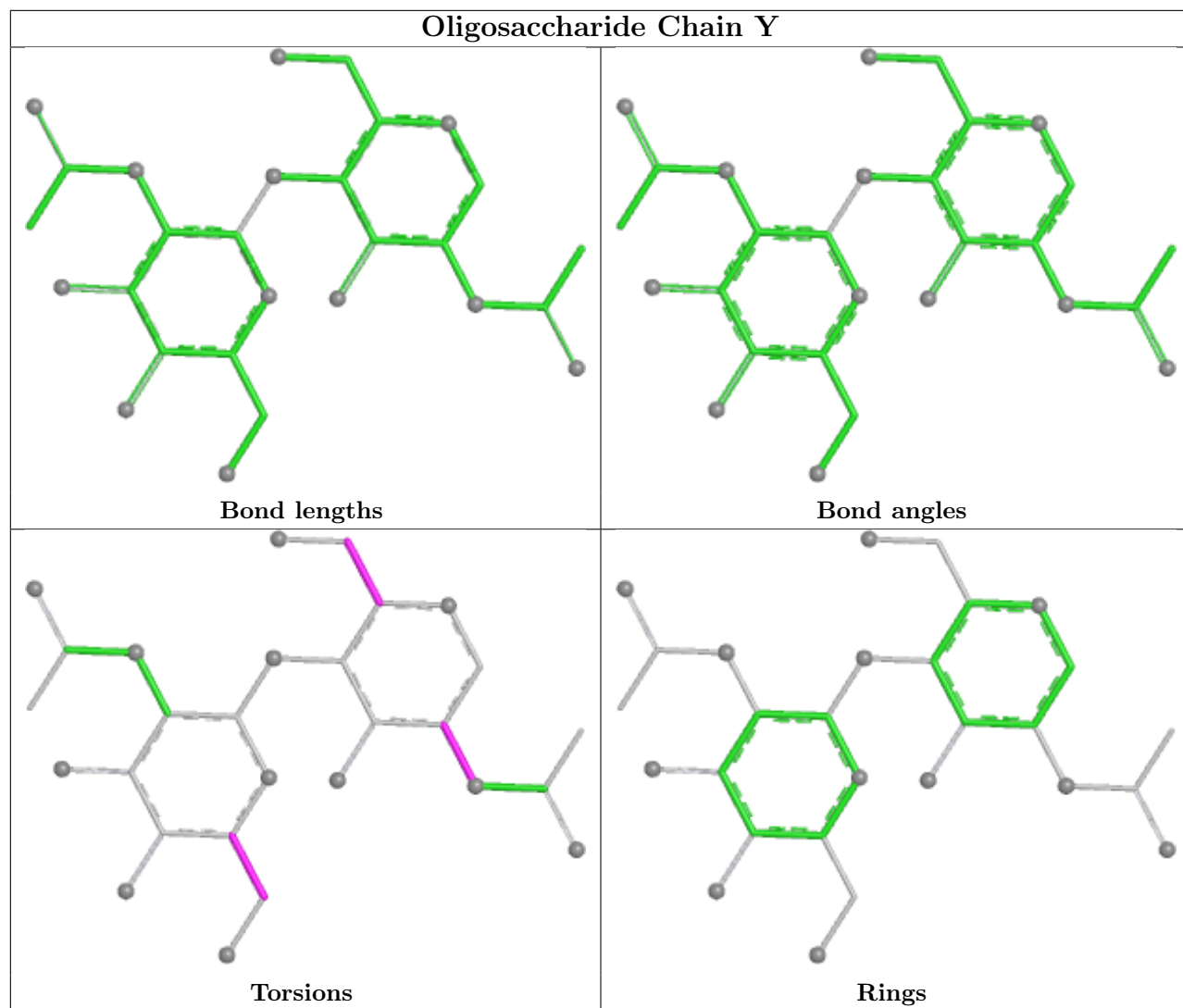


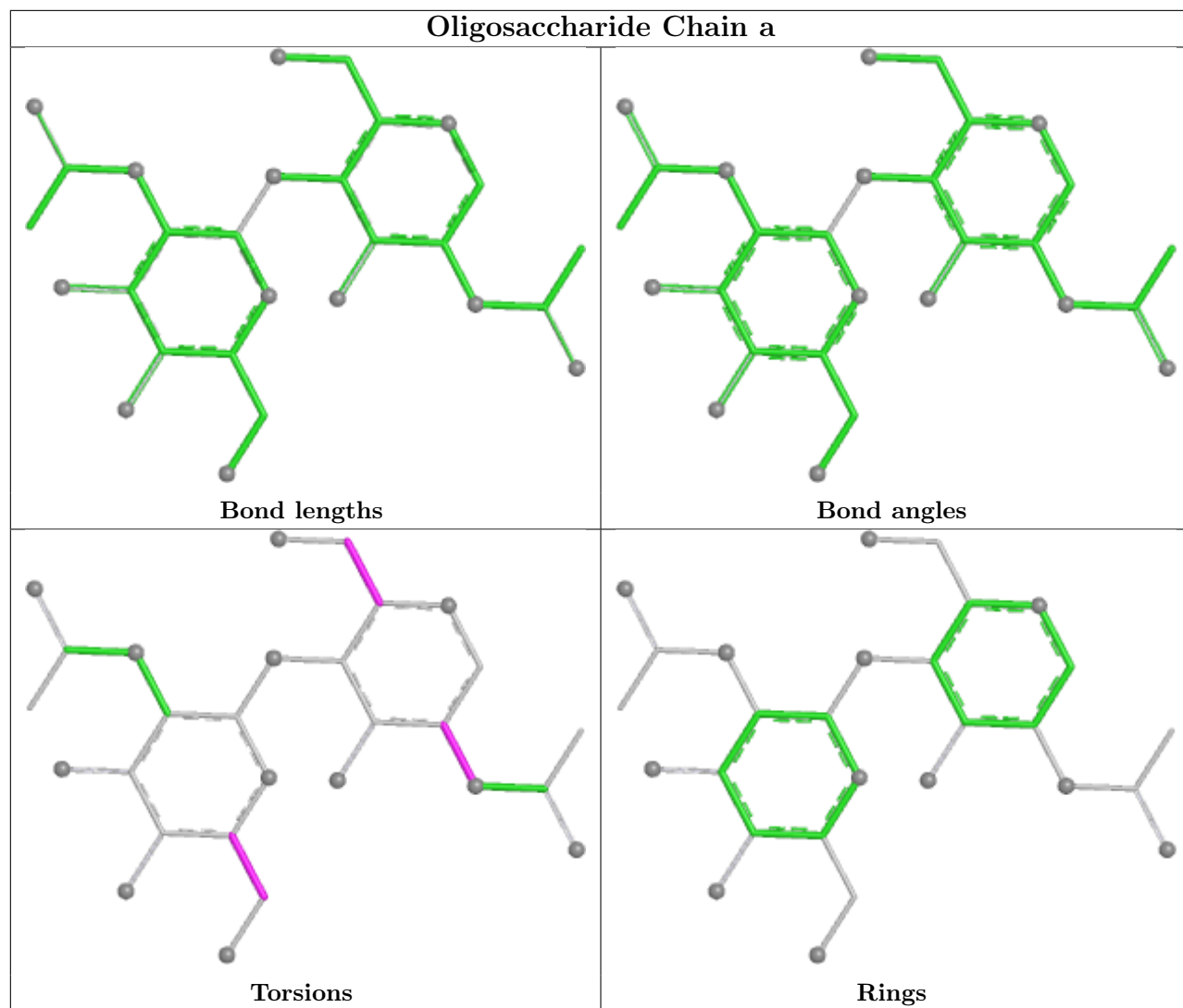


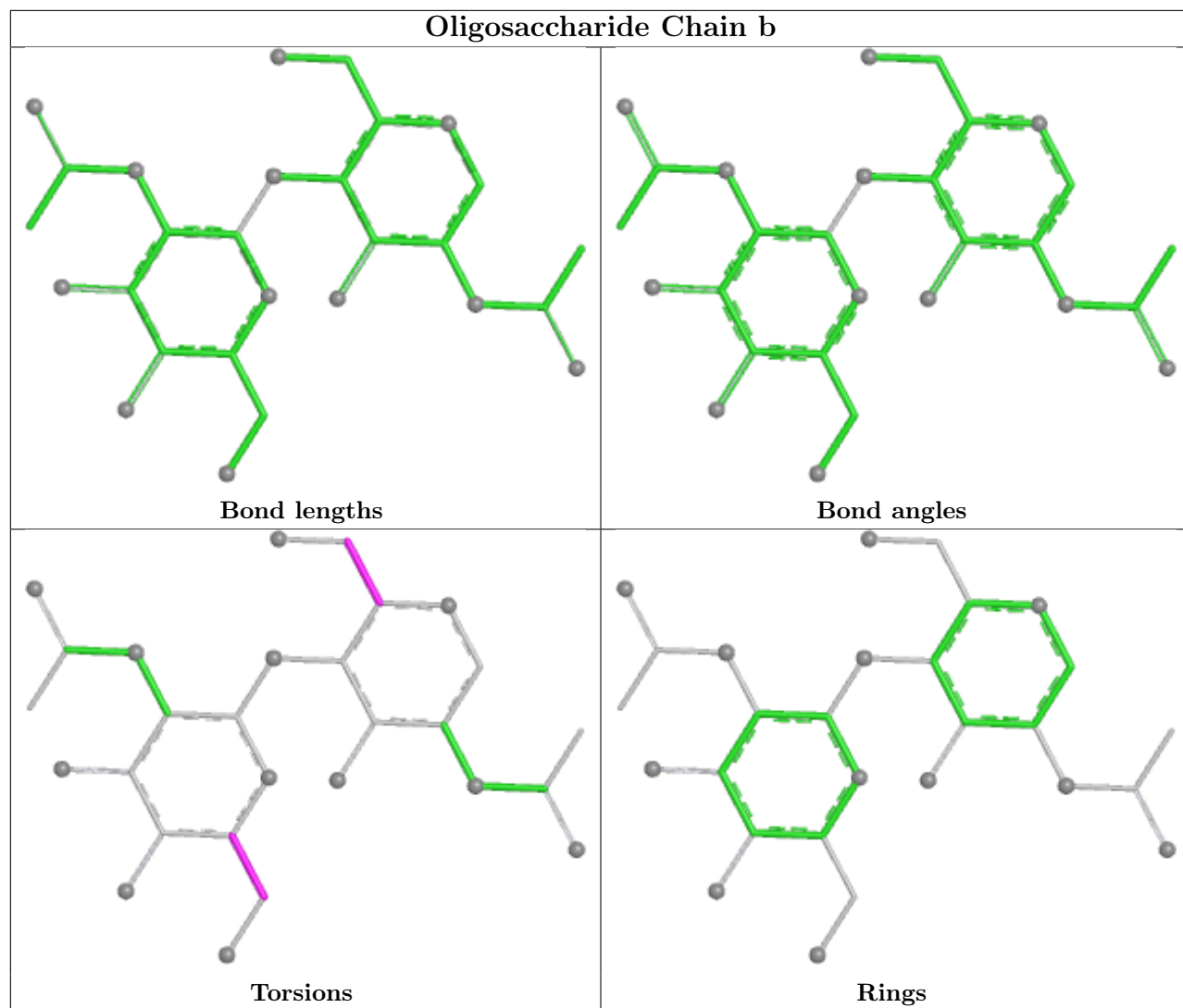


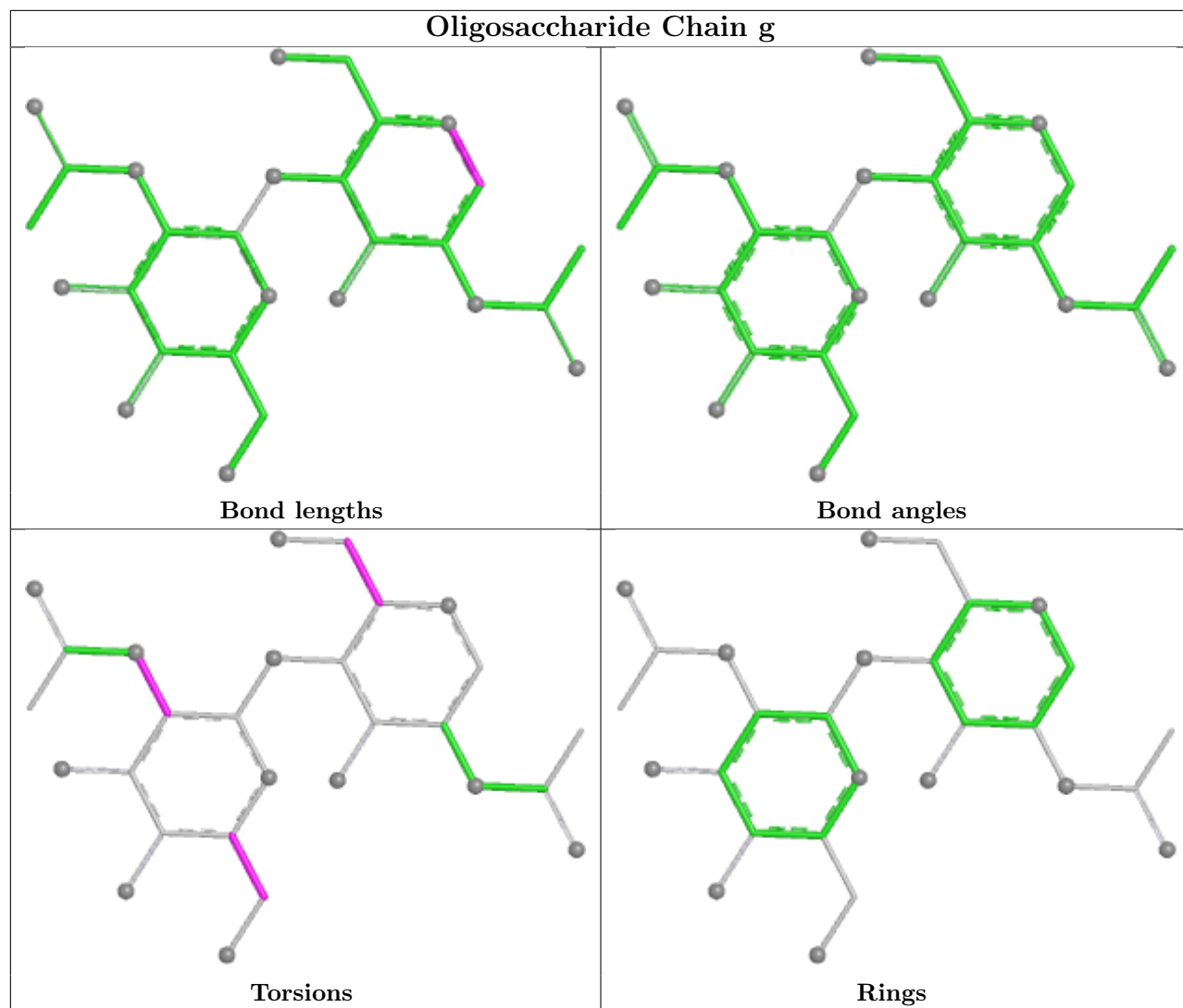


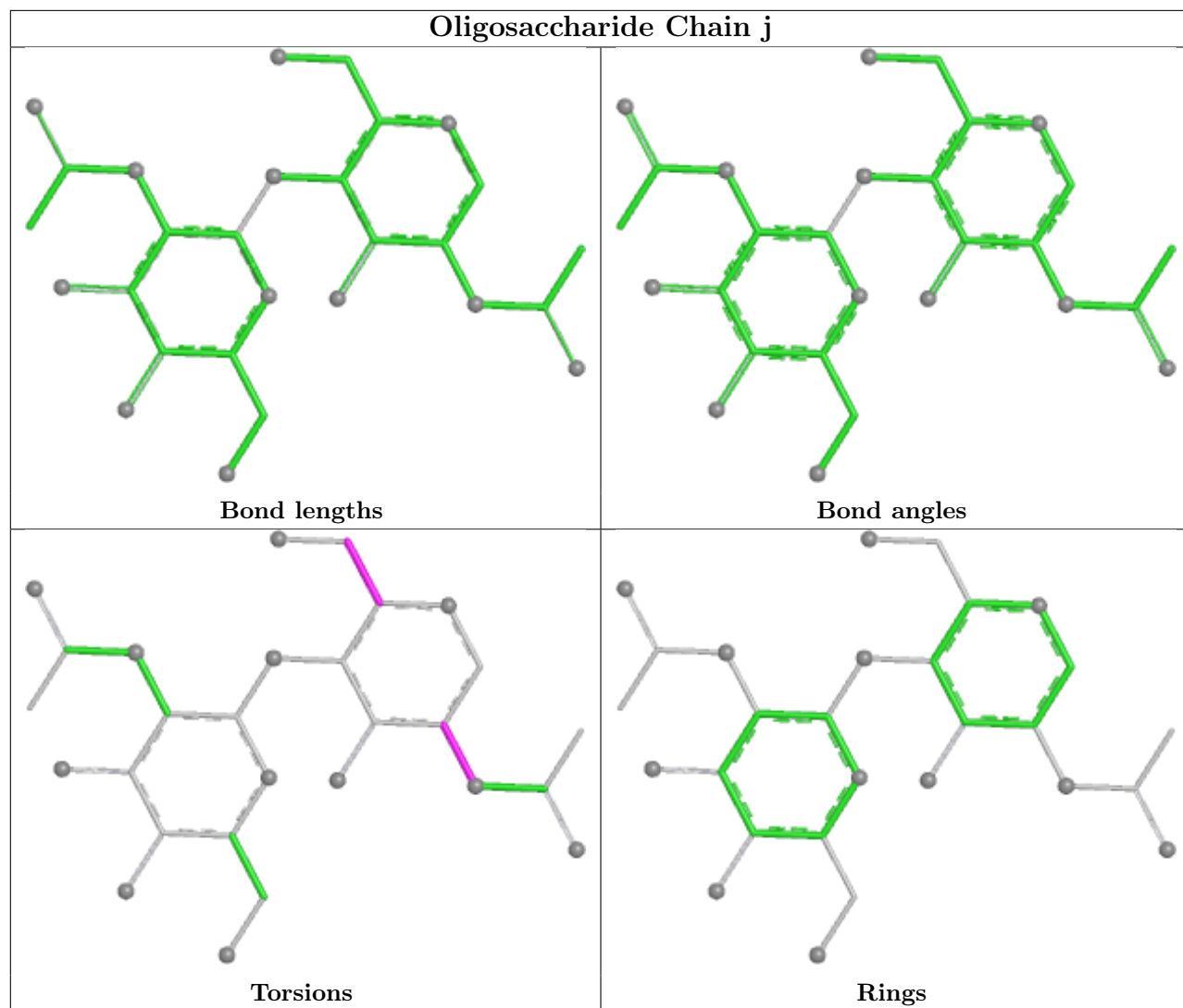


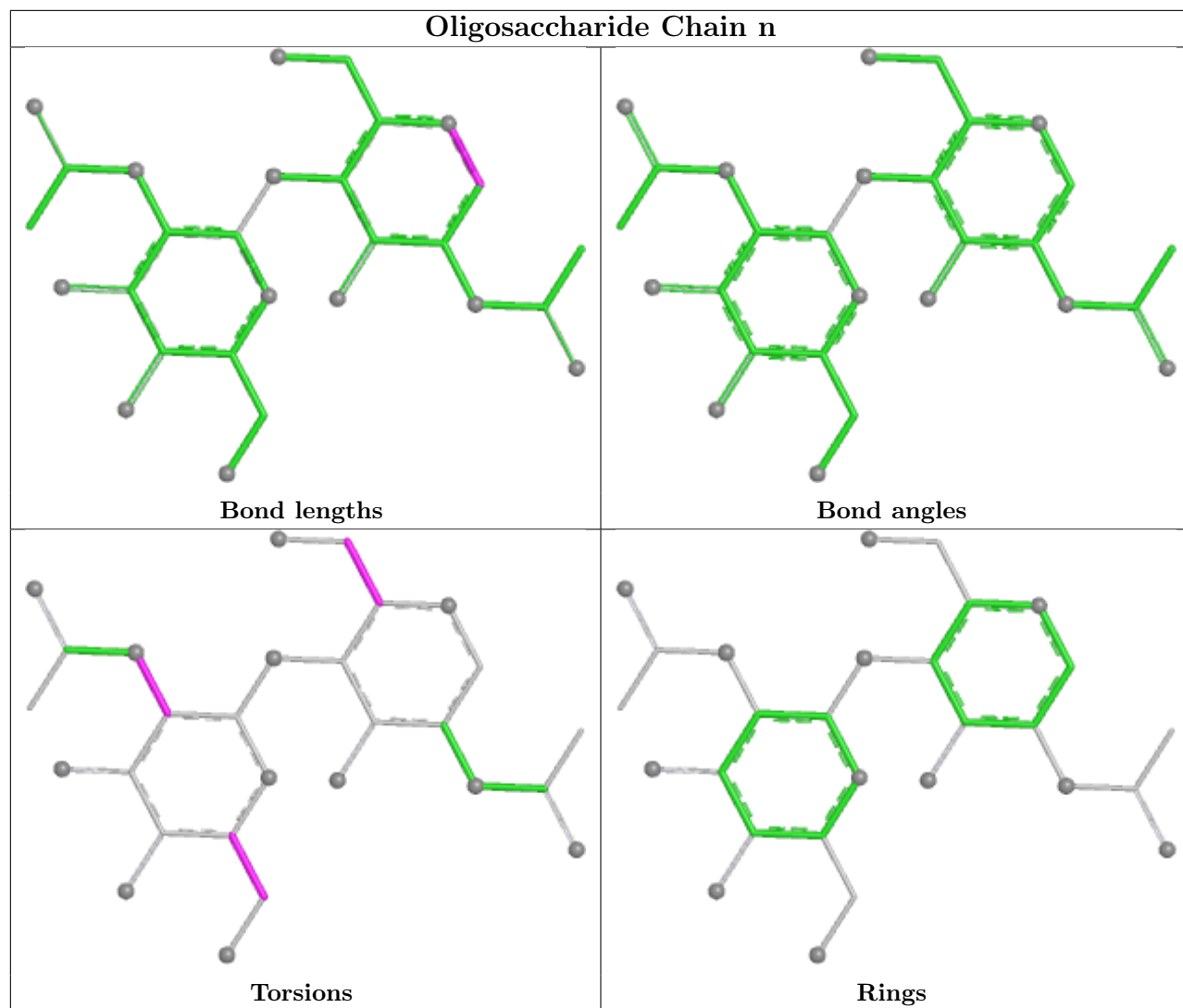


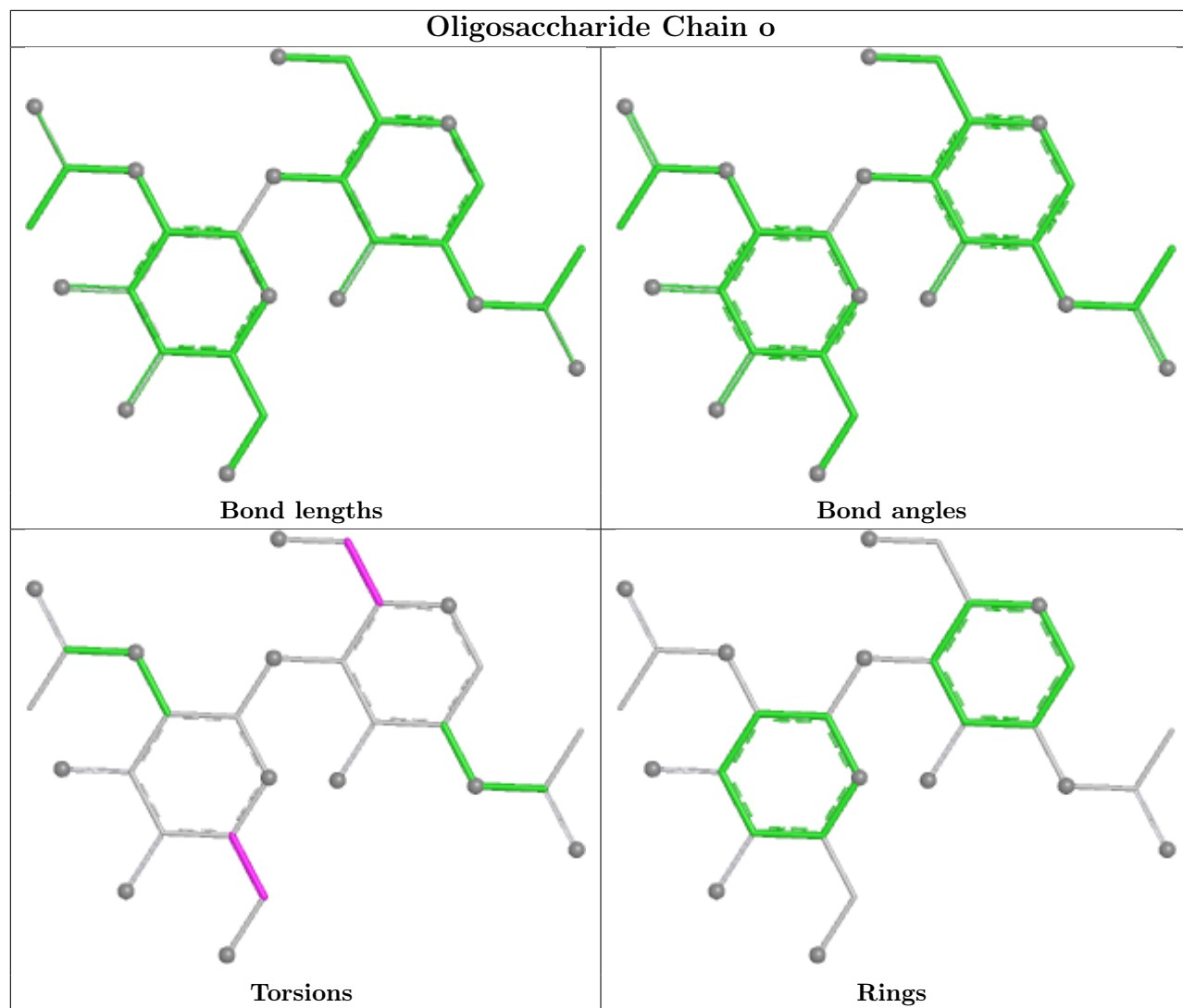


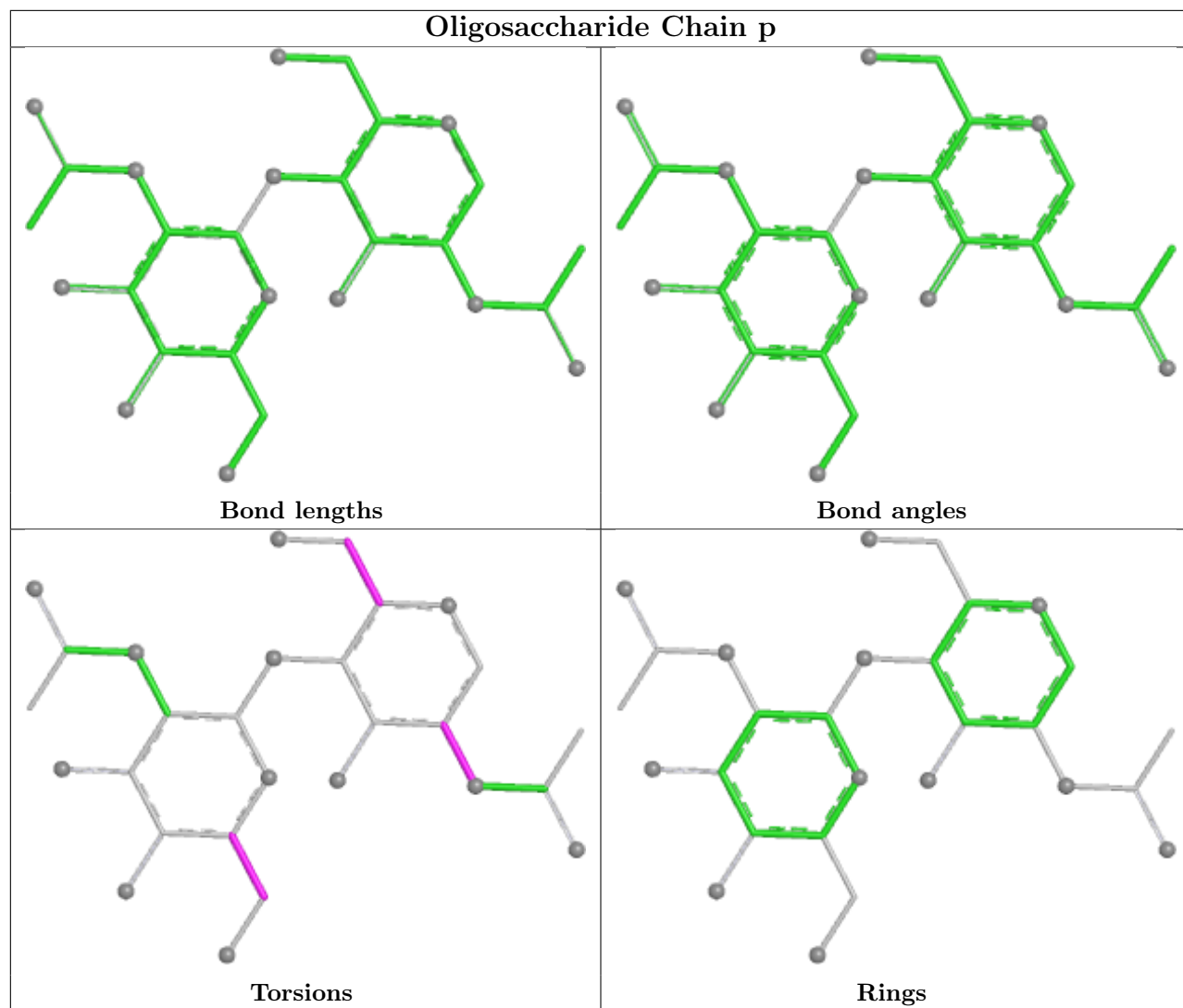


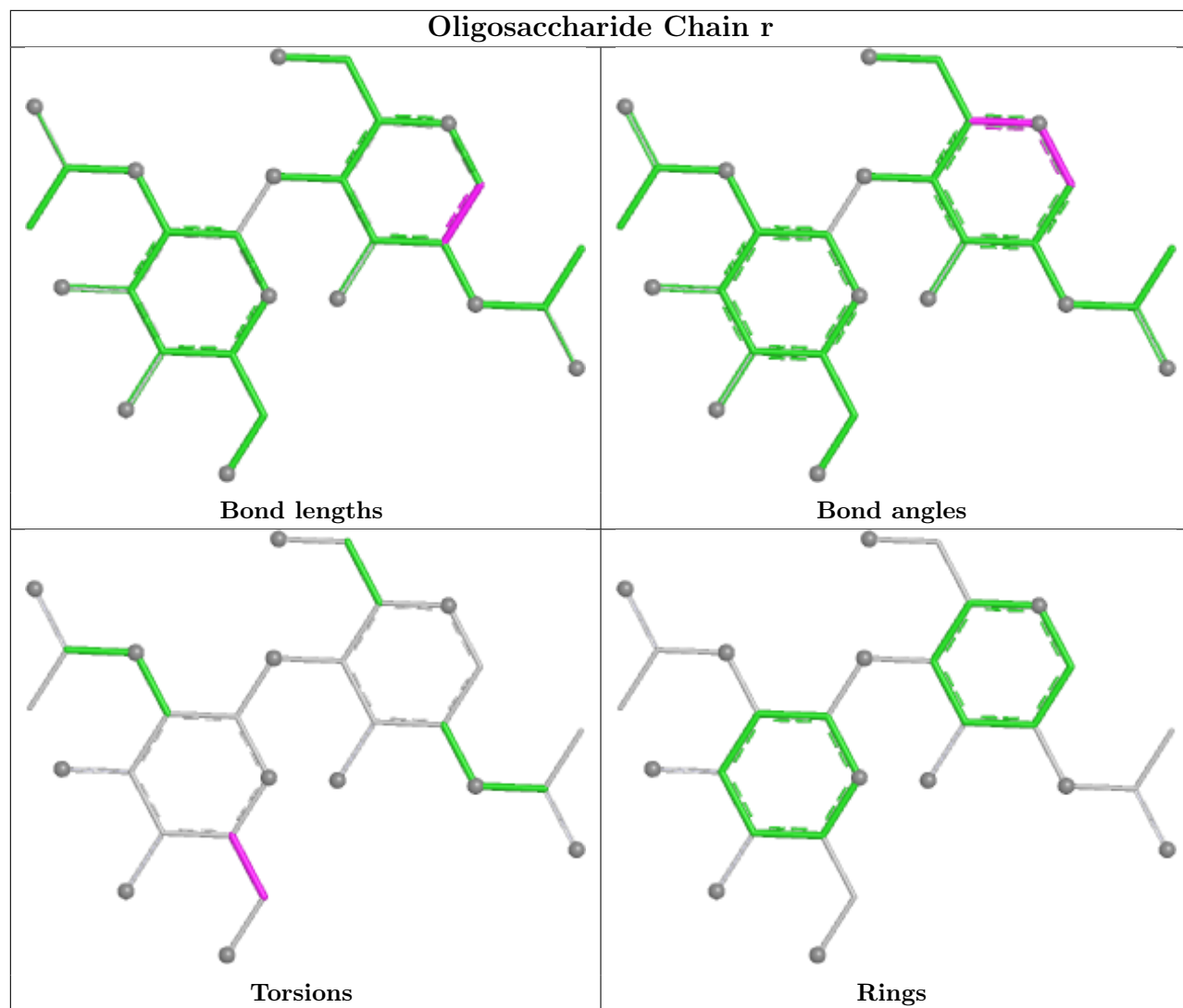


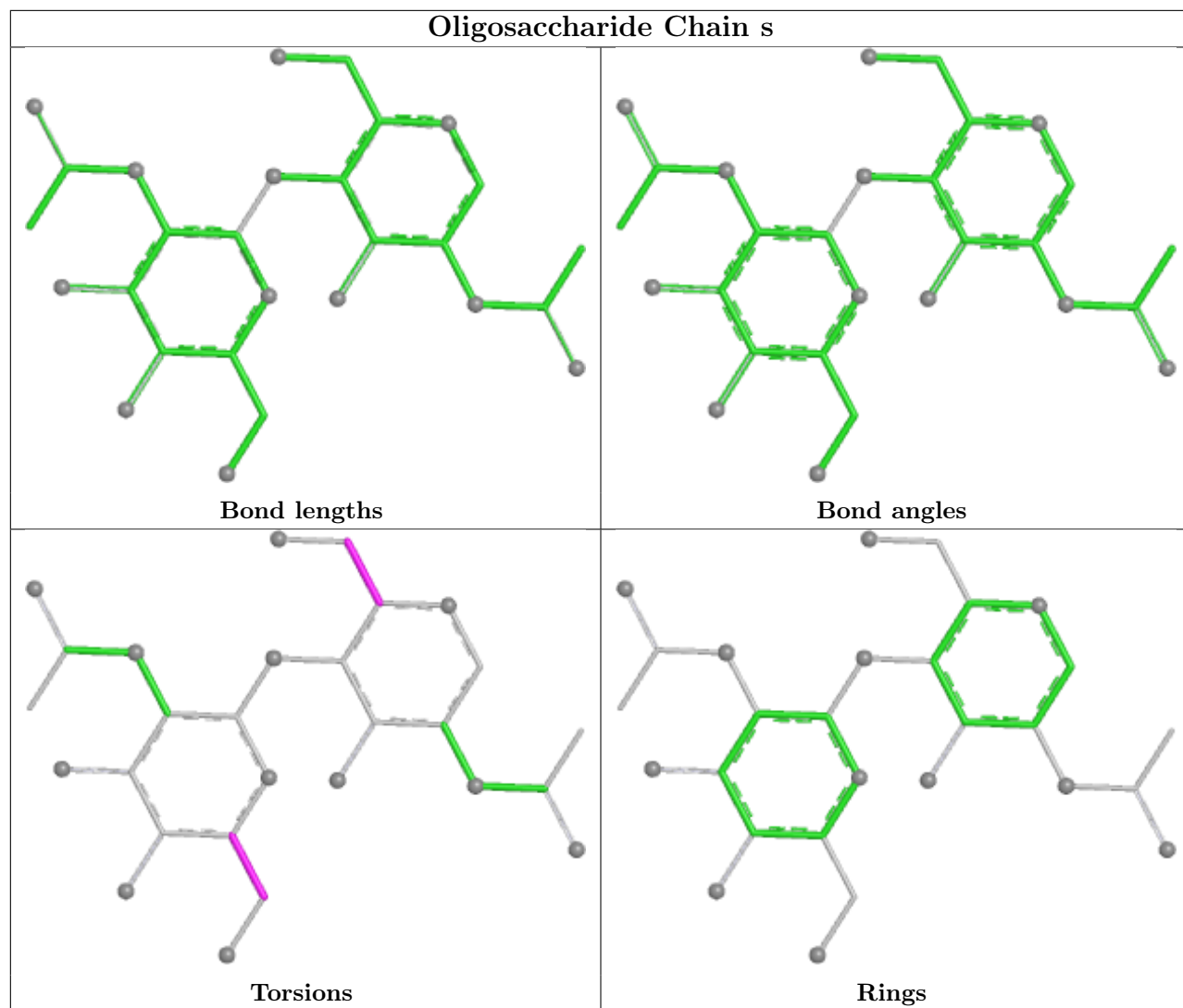


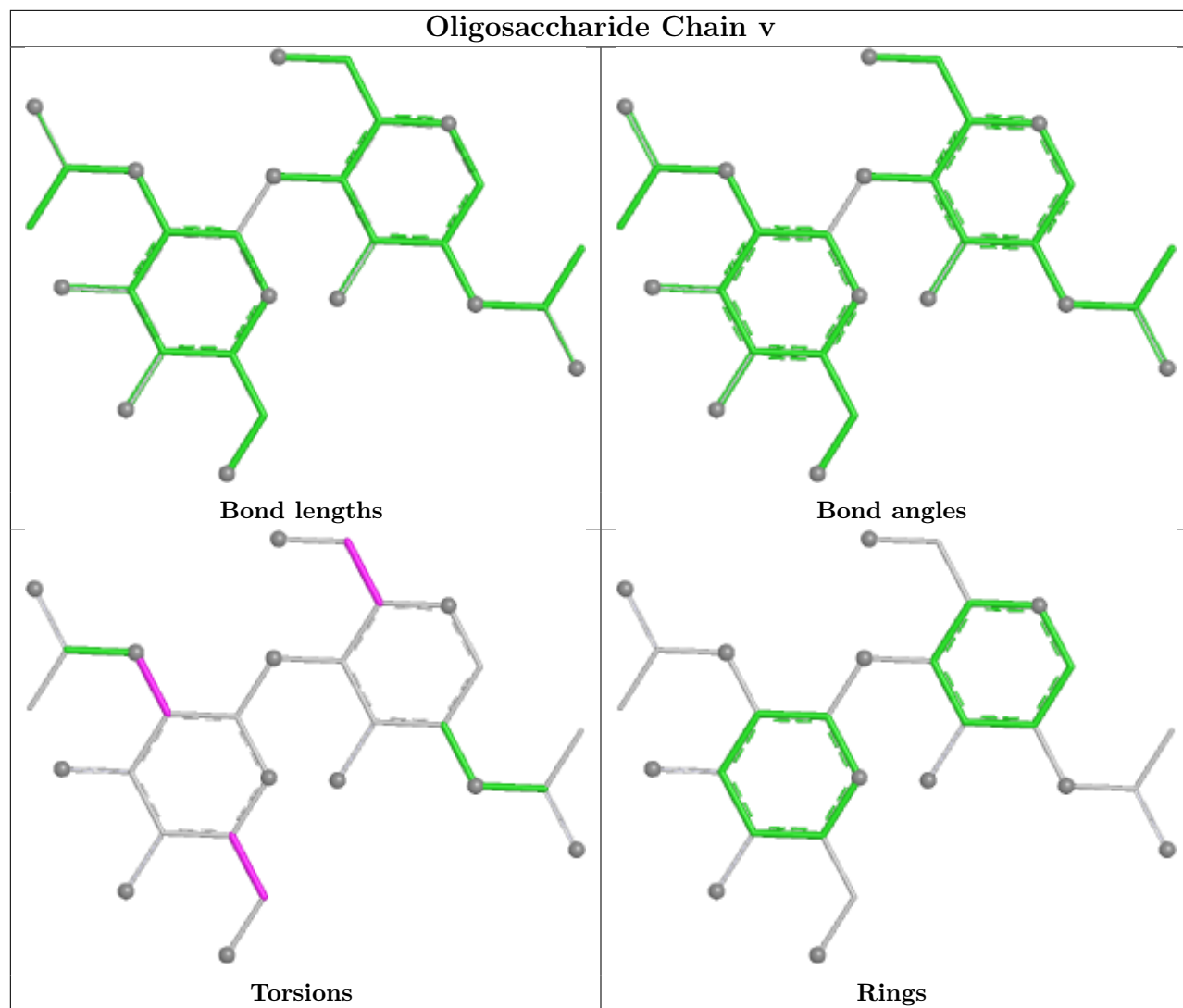


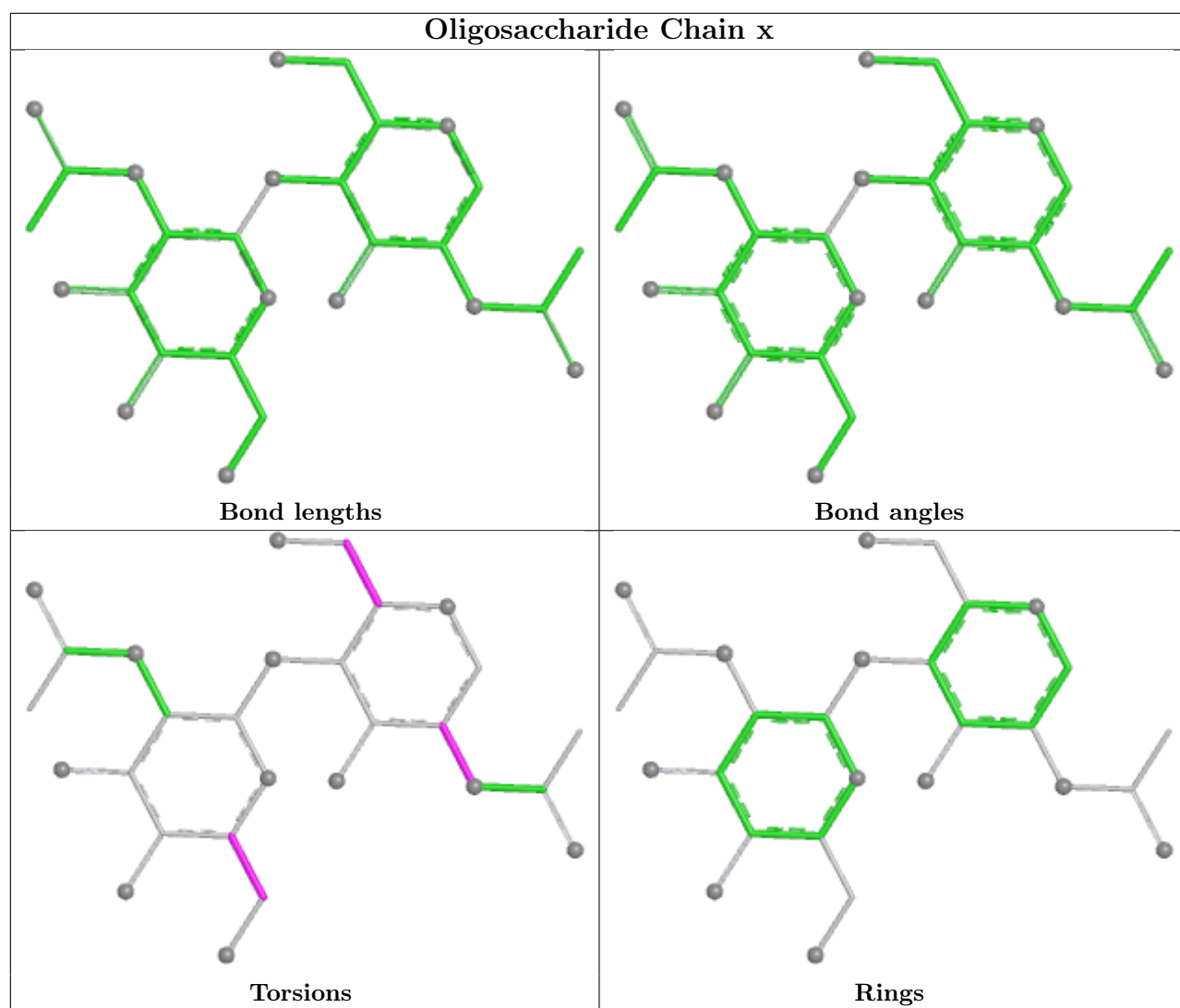


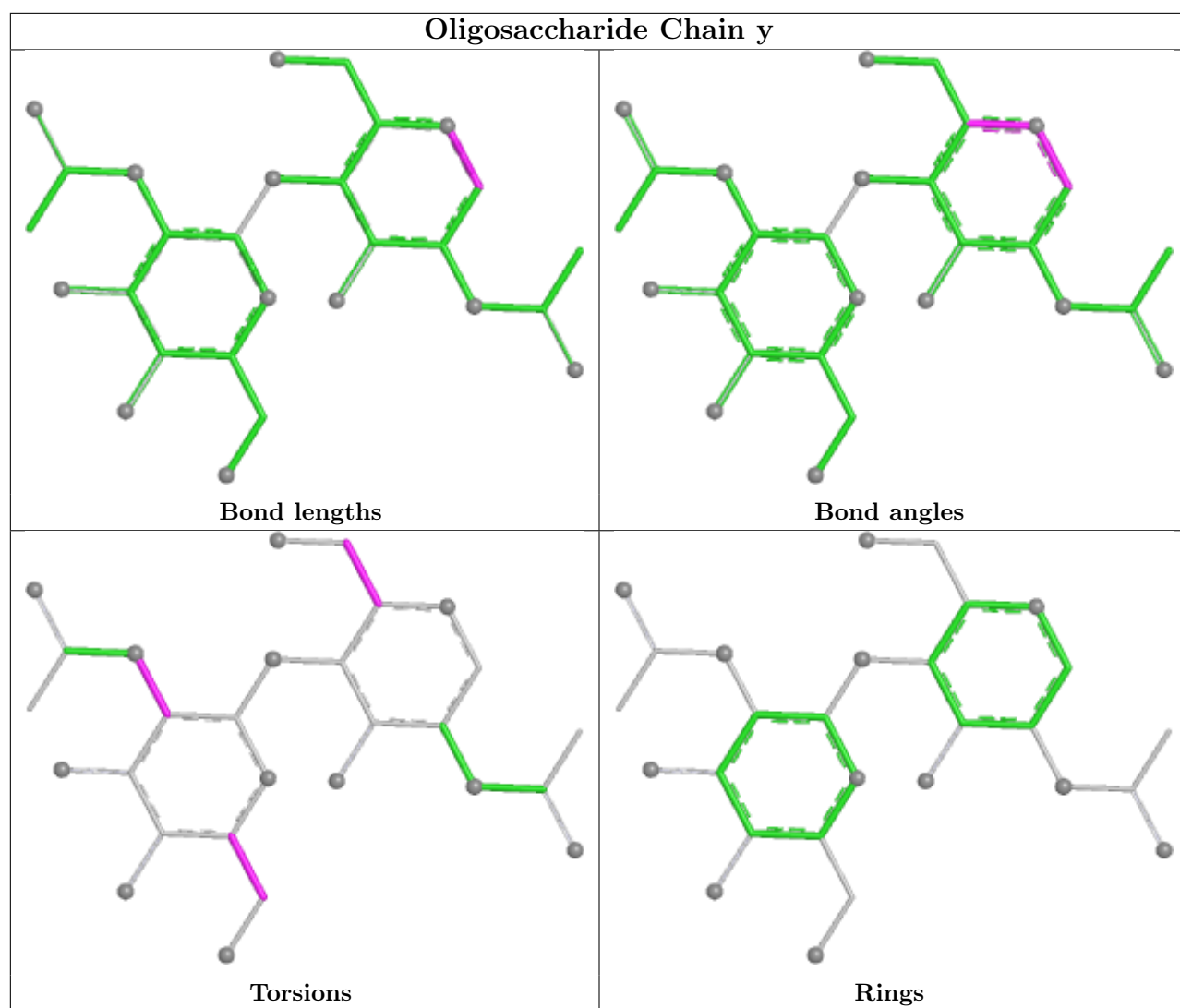


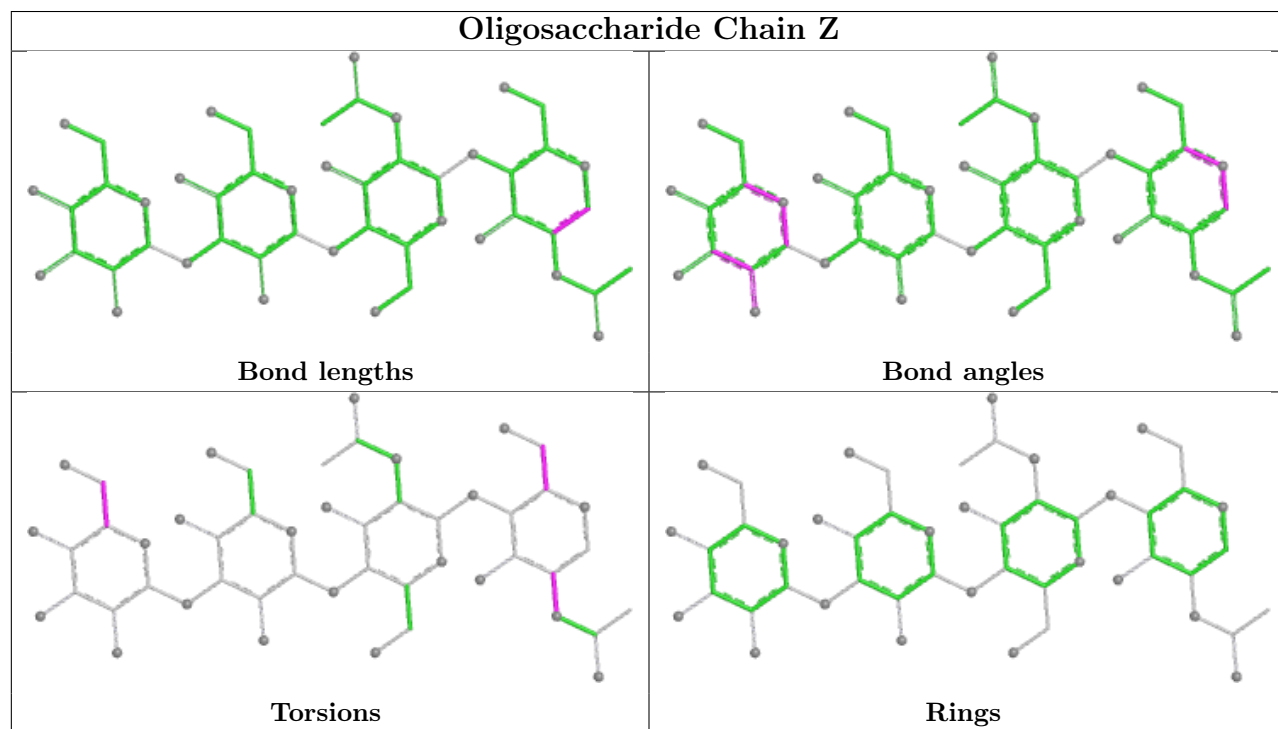
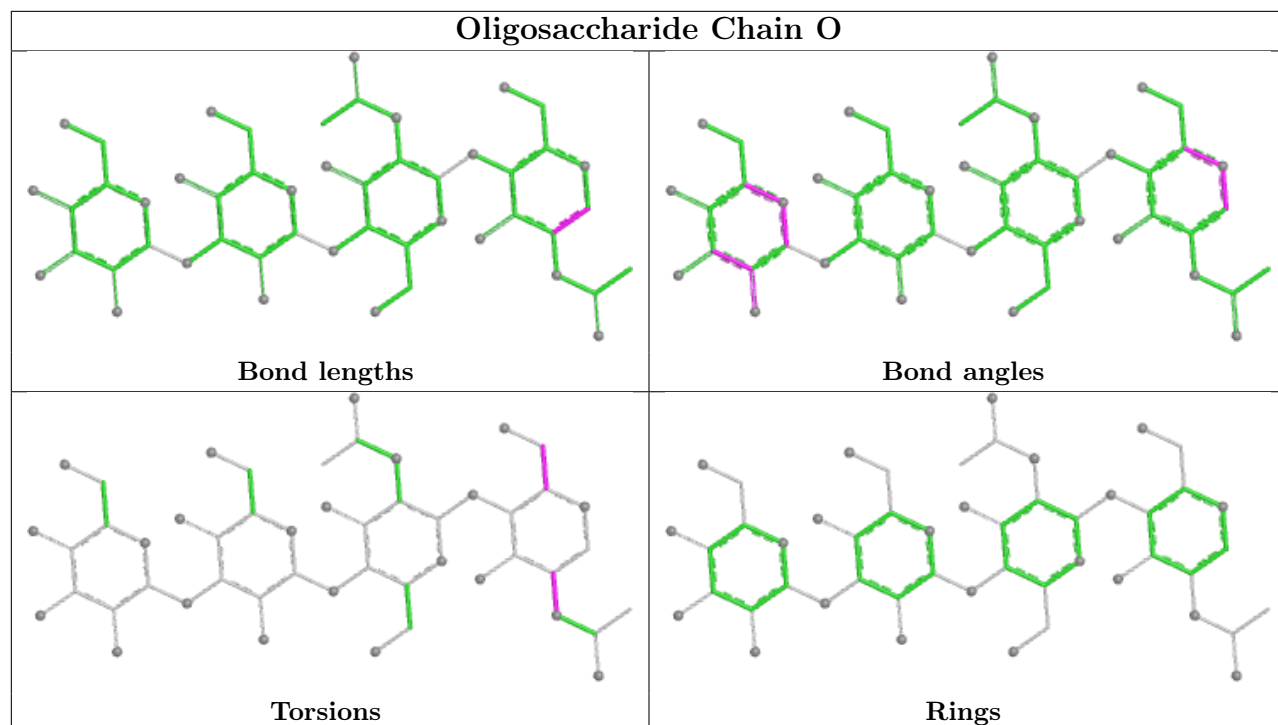


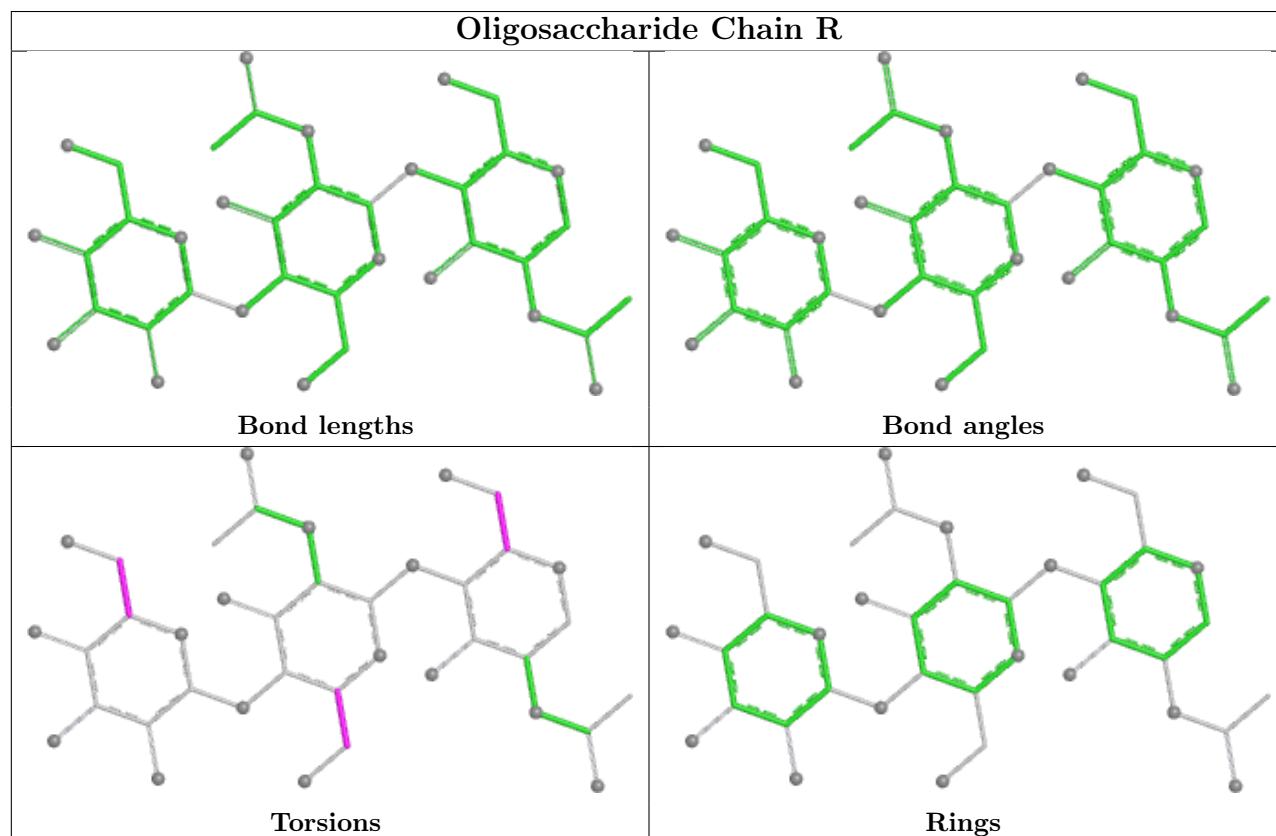
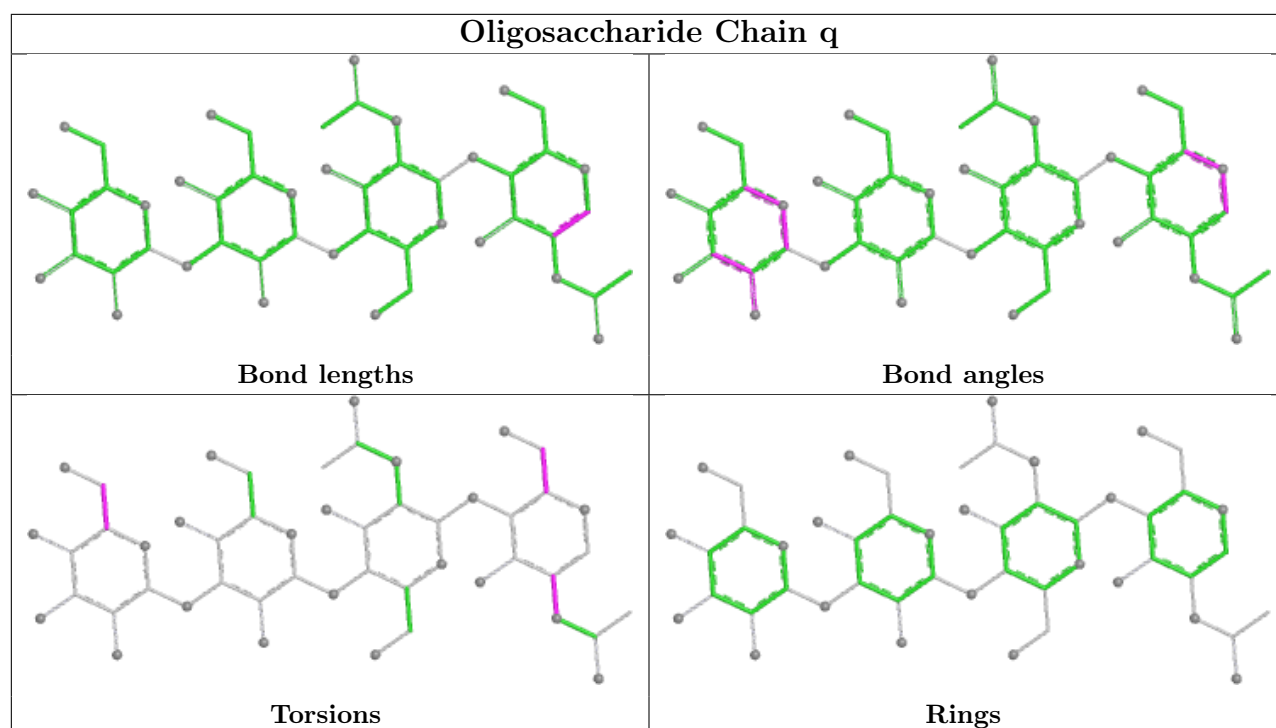


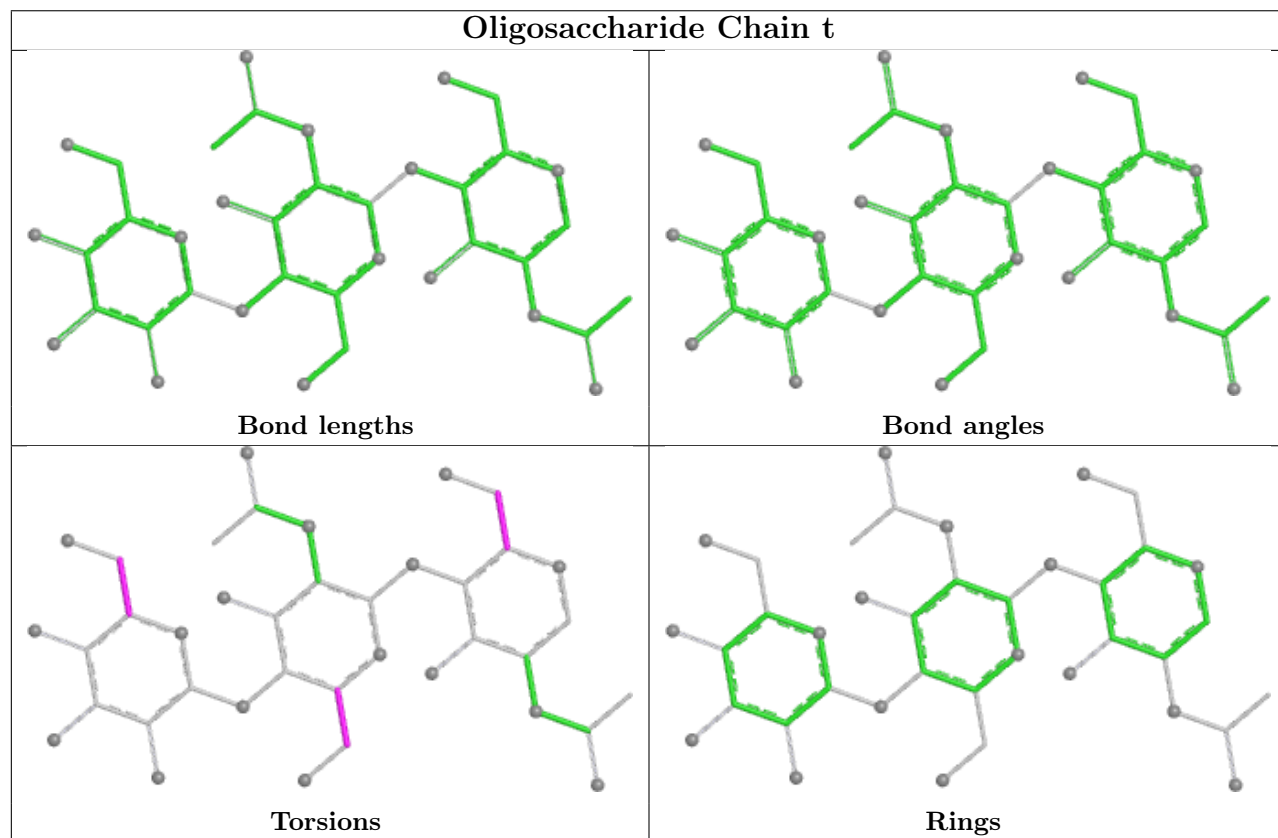
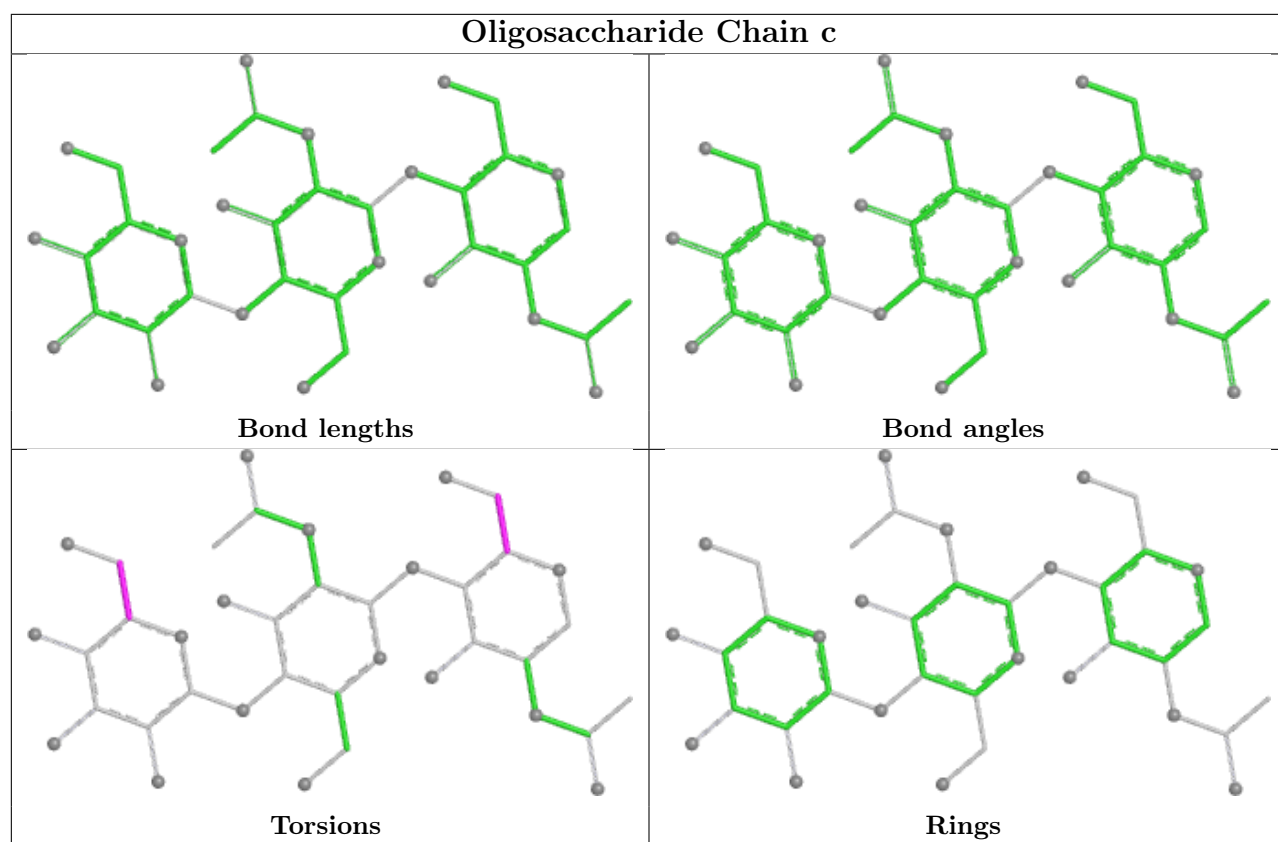


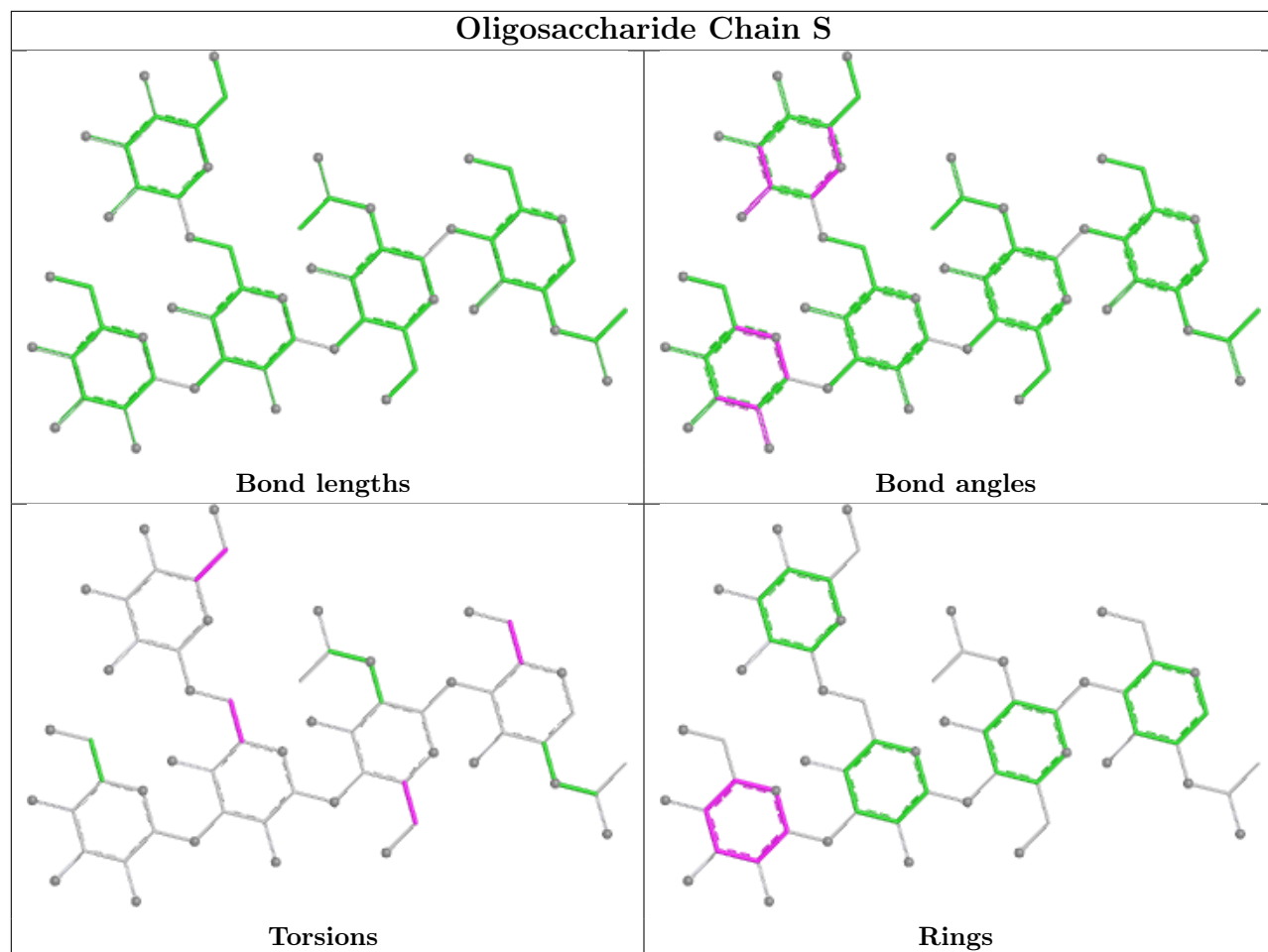


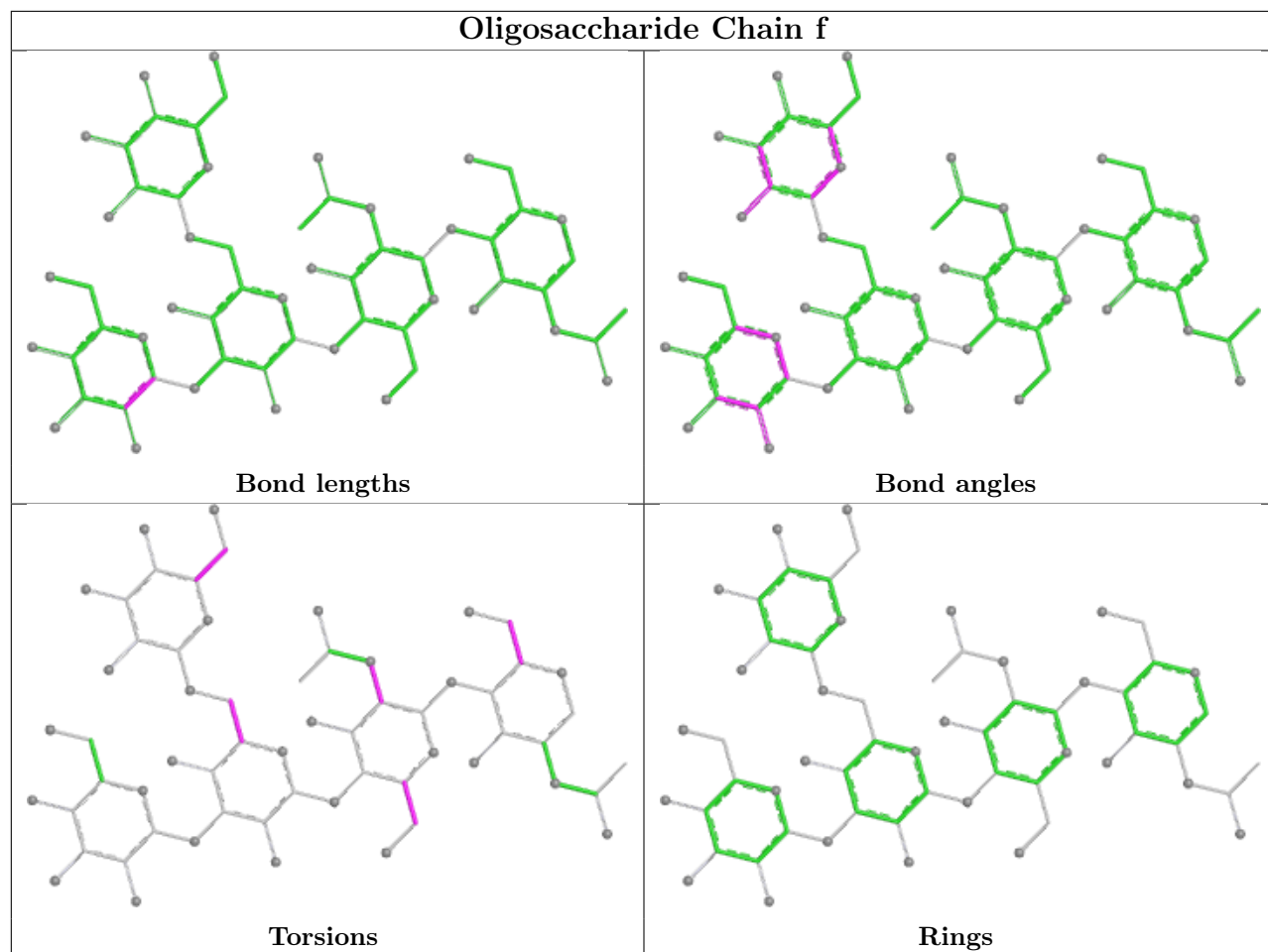


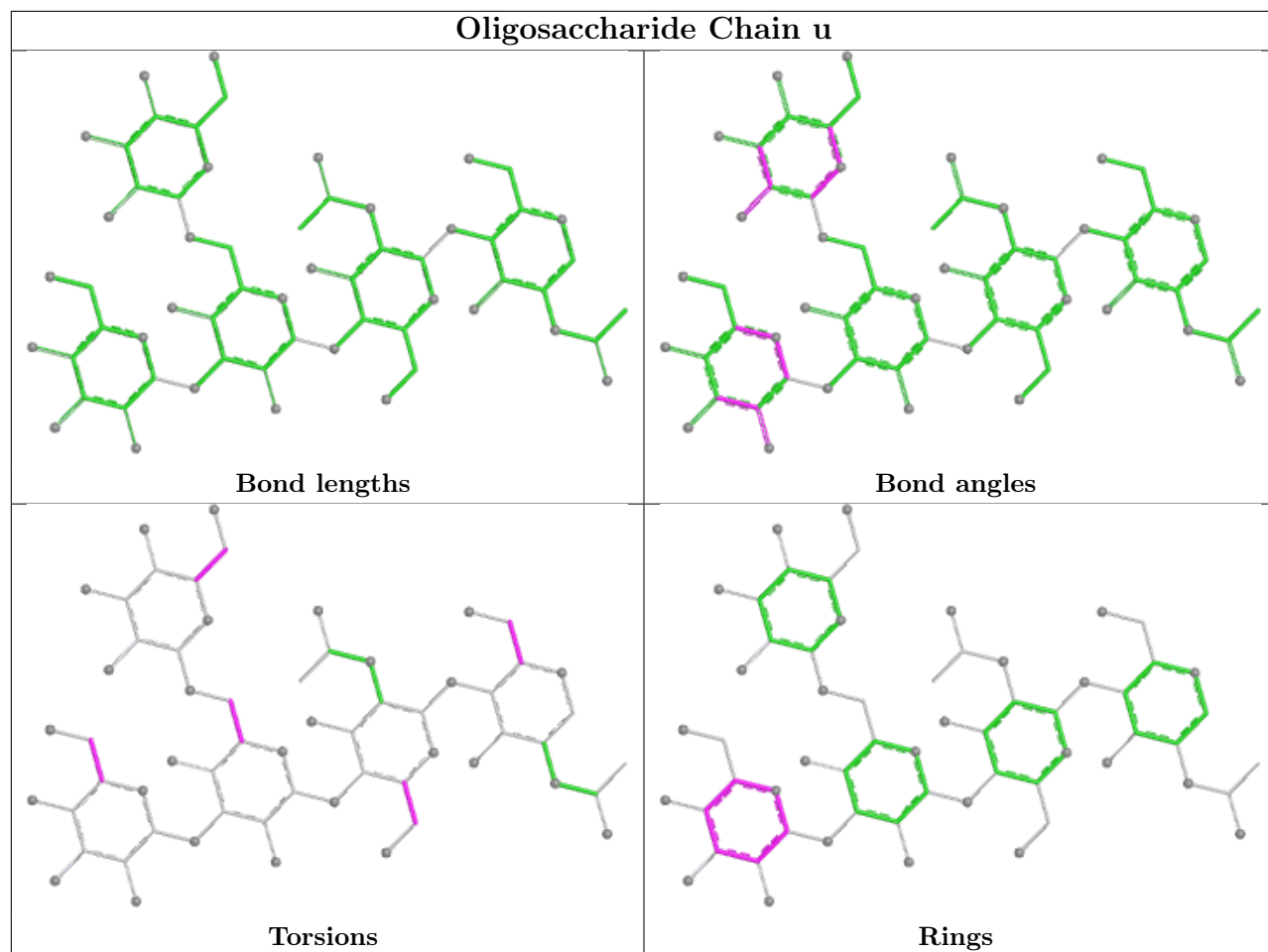


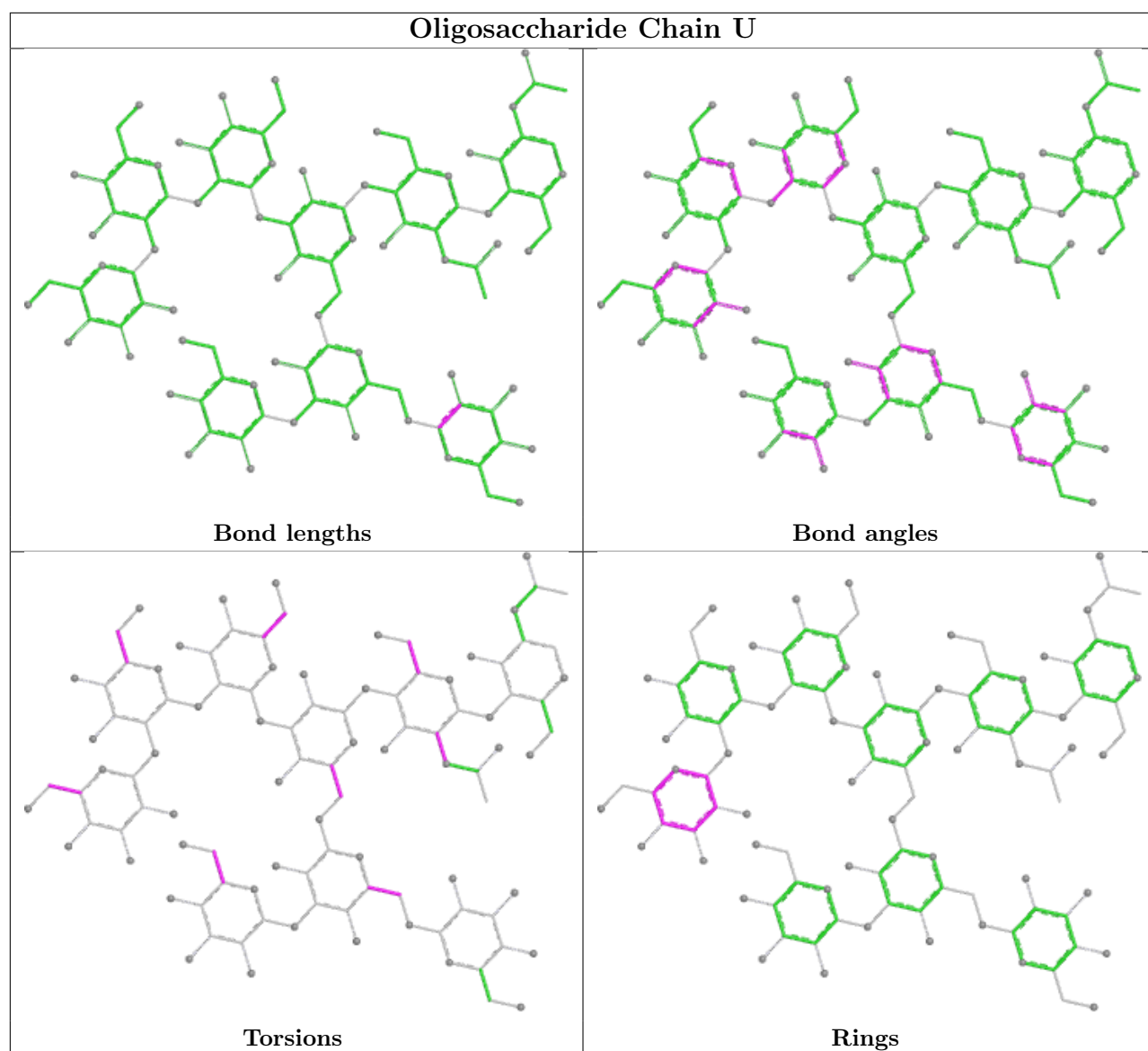


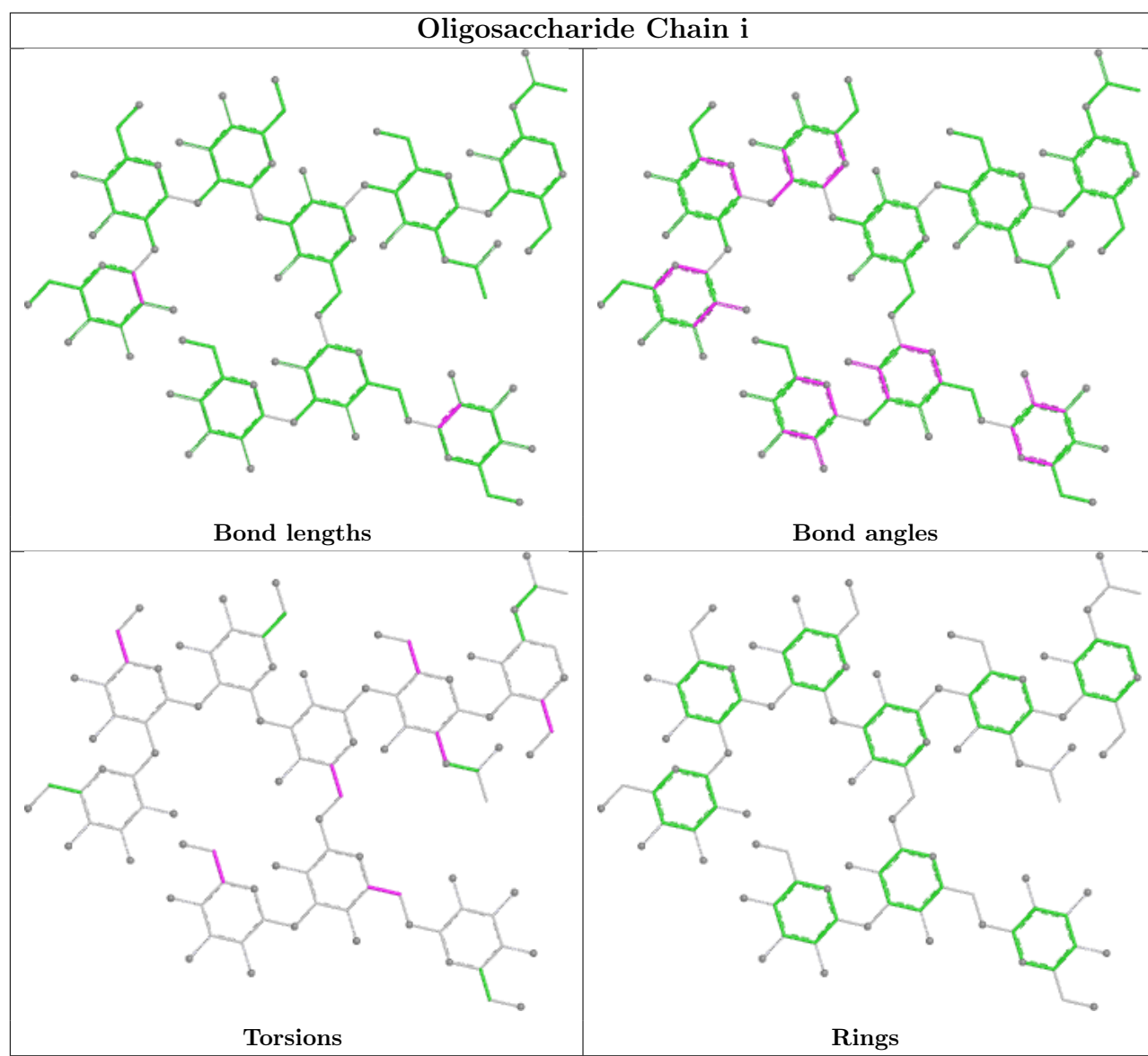


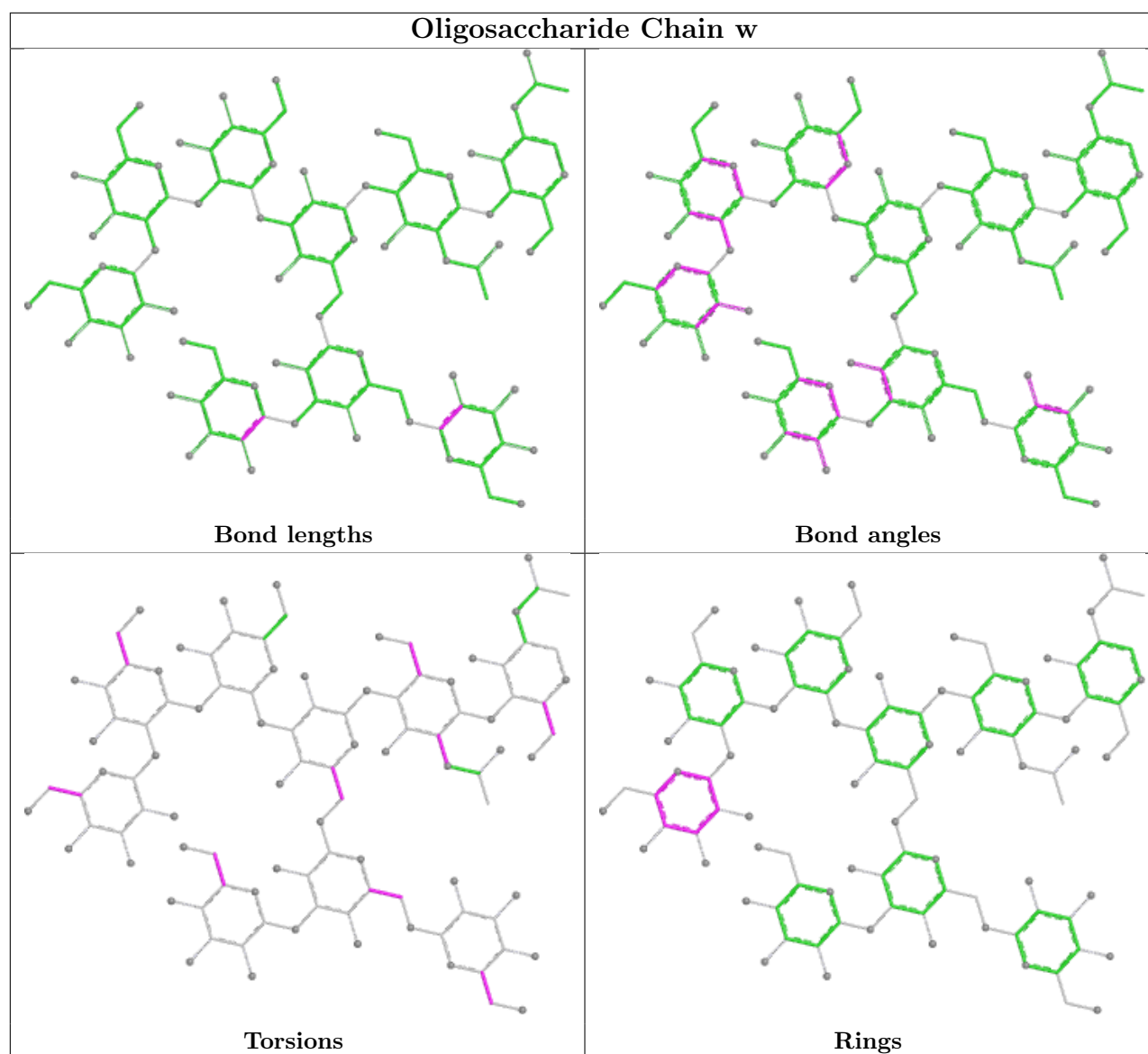












5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	NAG	G	604	1	14,14,15	0.38	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.41	0
12	NAG	A	604	1	14,14,15	0.41	0	17,19,21	0.61	1 (5%)
12	NAG	I	604	1	14,14,15	0.27	0	17,19,21	0.38	0
12	NAG	I	602	1	14,14,15	0.44	0	17,19,21	0.63	0
12	NAG	G	605	1	14,14,15	0.23	0	17,19,21	0.45	0
12	NAG	G	601	1	14,14,15	0.24	0	17,19,21	0.42	0
12	NAG	A	605	1	14,14,15	0.37	0	17,19,21	0.54	0
12	NAG	I	605	1	14,14,15	0.27	0	17,19,21	0.46	0
12	NAG	I	601	1	14,14,15	0.30	0	17,19,21	0.40	0
12	NAG	G	602	1	14,14,15	0.42	0	17,19,21	0.59	0
12	NAG	I	603	1	14,14,15	0.35	0	17,19,21	0.59	0
12	NAG	A	602	1	14,14,15	0.44	0	17,19,21	0.62	0
12	NAG	G	603	1	14,14,15	0.33	0	17,19,21	0.59	0
12	NAG	A	603	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)

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
12	NAG	G	604	1	-	0/6/23/26	0/1/1/1
12	NAG	A	601	1	-	1/6/23/26	0/1/1/1
12	NAG	A	604	1	-	0/6/23/26	0/1/1/1
12	NAG	I	604	1	-	2/6/23/26	0/1/1/1
12	NAG	I	602	1	-	3/6/23/26	0/1/1/1
12	NAG	G	605	1	-	2/6/23/26	0/1/1/1
12	NAG	G	601	1	-	2/6/23/26	0/1/1/1
12	NAG	A	605	1	-	3/6/23/26	0/1/1/1
12	NAG	I	605	1	-	1/6/23/26	0/1/1/1
12	NAG	I	601	1	-	1/6/23/26	0/1/1/1
12	NAG	G	602	1	-	4/6/23/26	0/1/1/1
12	NAG	I	603	1	-	1/6/23/26	0/1/1/1
12	NAG	A	602	1	-	4/6/23/26	0/1/1/1
12	NAG	G	603	1	-	1/6/23/26	0/1/1/1
12	NAG	A	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	A	603	NAG	C1-O5-C5	2.26	115.21	112.19
12	A	604	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	NAG	C4-C5-C6-O6
12	G	602	NAG	C4-C5-C6-O6
12	G	605	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	G	601	NAG	O5-C5-C6-O6
12	G	602	NAG	O5-C5-C6-O6
12	G	605	NAG	C4-C5-C6-O6
12	A	602	NAG	C4-C5-C6-O6
12	I	604	NAG	C4-C5-C6-O6
12	I	604	NAG	O5-C5-C6-O6
12	A	605	NAG	O5-C5-C6-O6
12	I	602	NAG	O5-C5-C6-O6
12	I	603	NAG	O5-C5-C6-O6
12	A	601	NAG	O5-C5-C6-O6
12	I	605	NAG	O5-C5-C6-O6
12	I	601	NAG	O5-C5-C6-O6
12	G	602	NAG	C3-C2-N2-C7
12	A	602	NAG	C3-C2-N2-C7
12	I	602	NAG	C3-C2-N2-C7
12	A	605	NAG	C4-C5-C6-O6
12	G	603	NAG	C4-C5-C6-O6
12	G	602	NAG	C1-C2-N2-C7
12	A	602	NAG	C1-C2-N2-C7
12	I	602	NAG	C1-C2-N2-C7
12	A	605	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	604	NAG	1	0
12	A	604	NAG	1	0
12	I	604	NAG	1	0
12	A	605	NAG	1	0
12	A	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

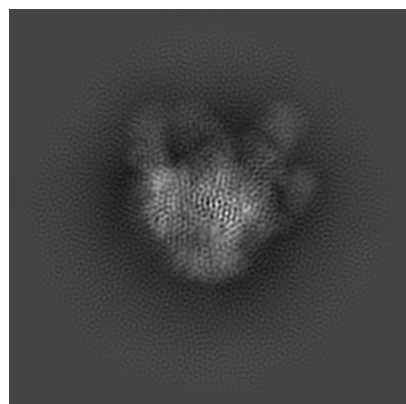
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26648. These allow visual inspection of the internal detail of the map and identification of artifacts.

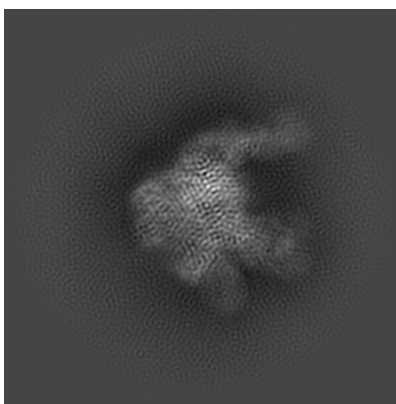
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

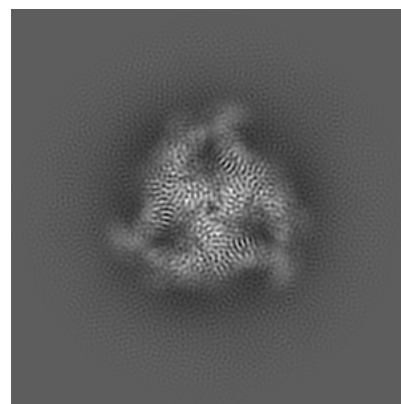
6.1.1 Primary map



X

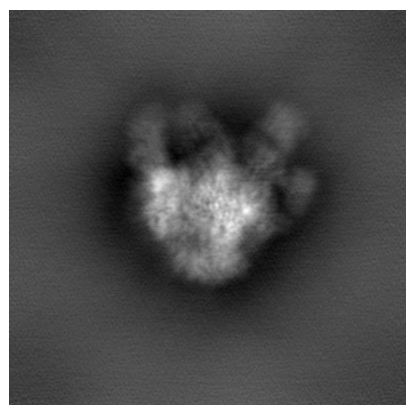


Y

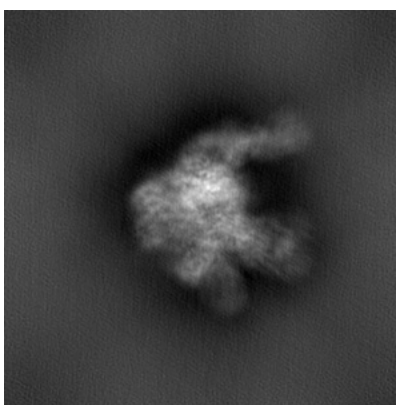


Z

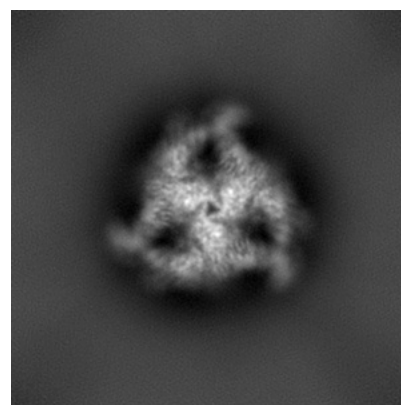
6.1.2 Raw map



X



Y

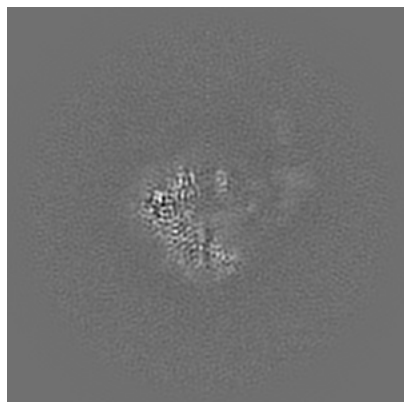


Z

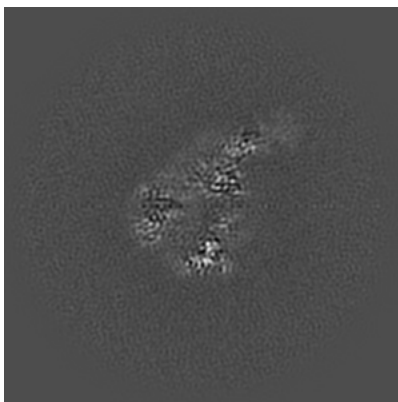
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

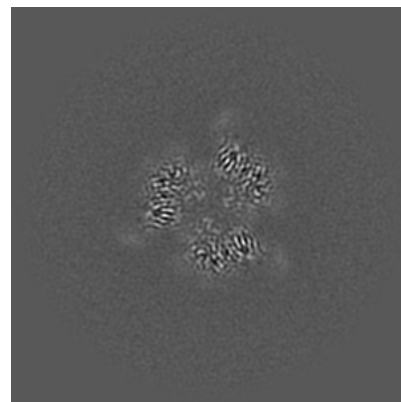
6.2.1 Primary map



X Index: 128

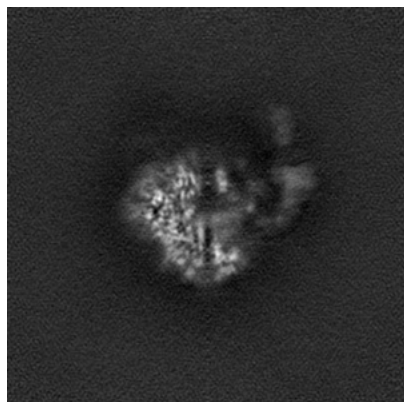


Y Index: 128

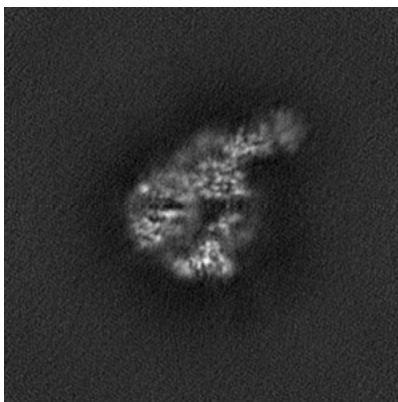


Z Index: 128

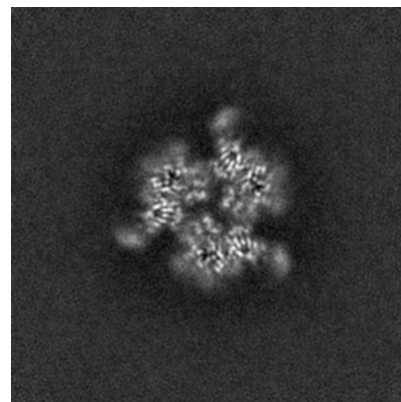
6.2.2 Raw map



X Index: 128



Y Index: 128

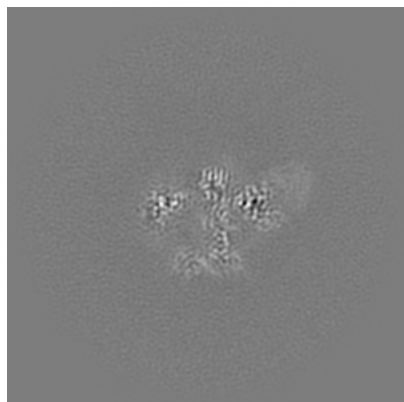


Z Index: 128

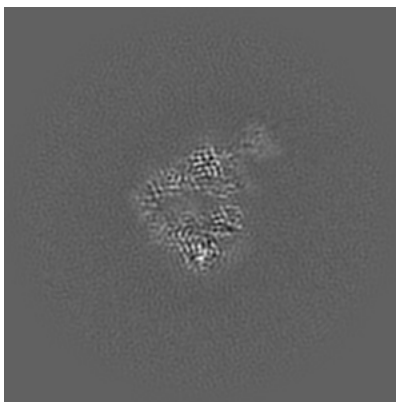
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

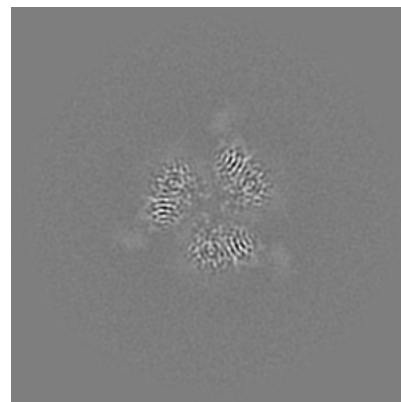
6.3.1 Primary map



X Index: 140

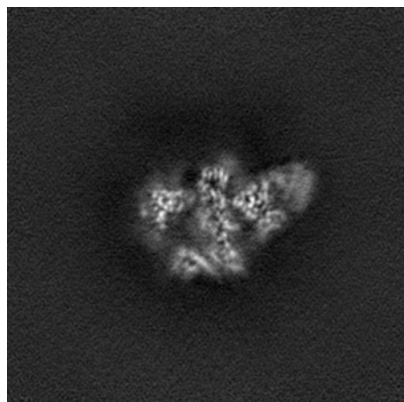


Y Index: 139

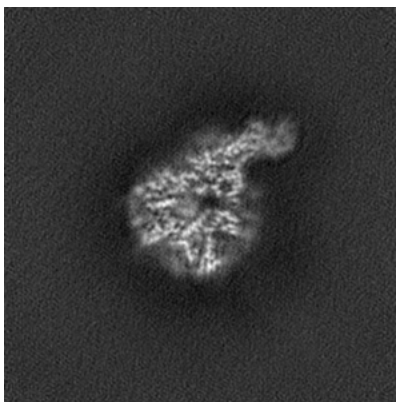


Z Index: 131

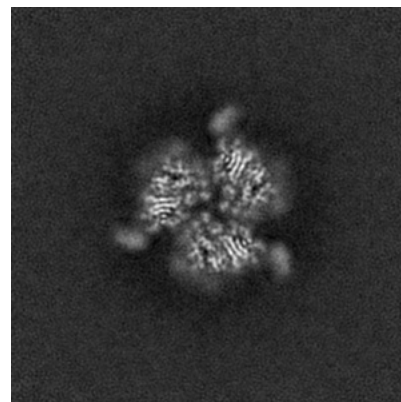
6.3.2 Raw map



X Index: 141



Y Index: 133

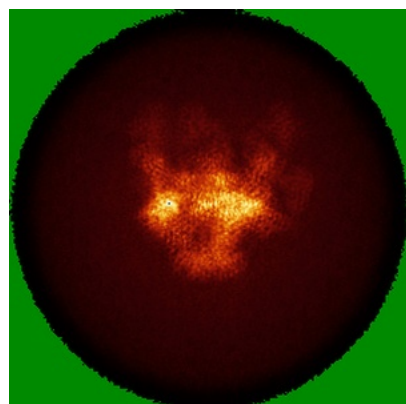


Z Index: 130

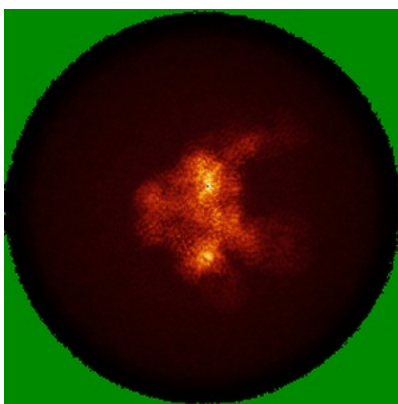
The images above show the largest variance slices of the map in three orthogonal directions.

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

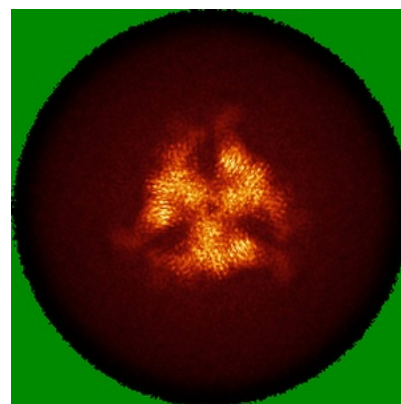
6.4.1 Primary map



X



Y

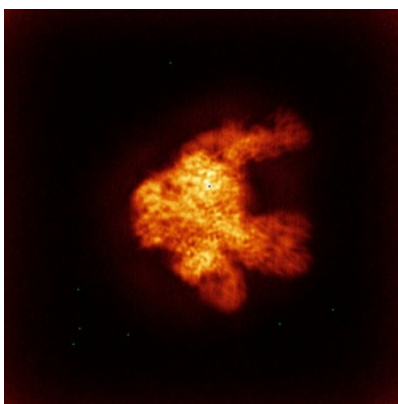


Z

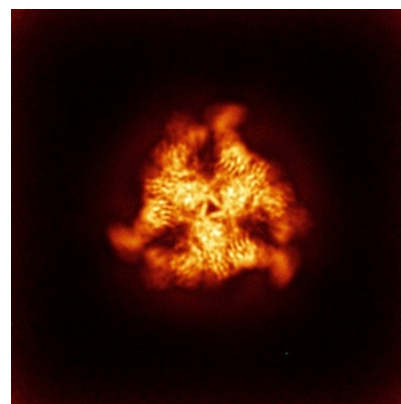
6.4.2 Raw map



X



Y

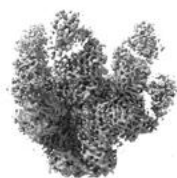


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

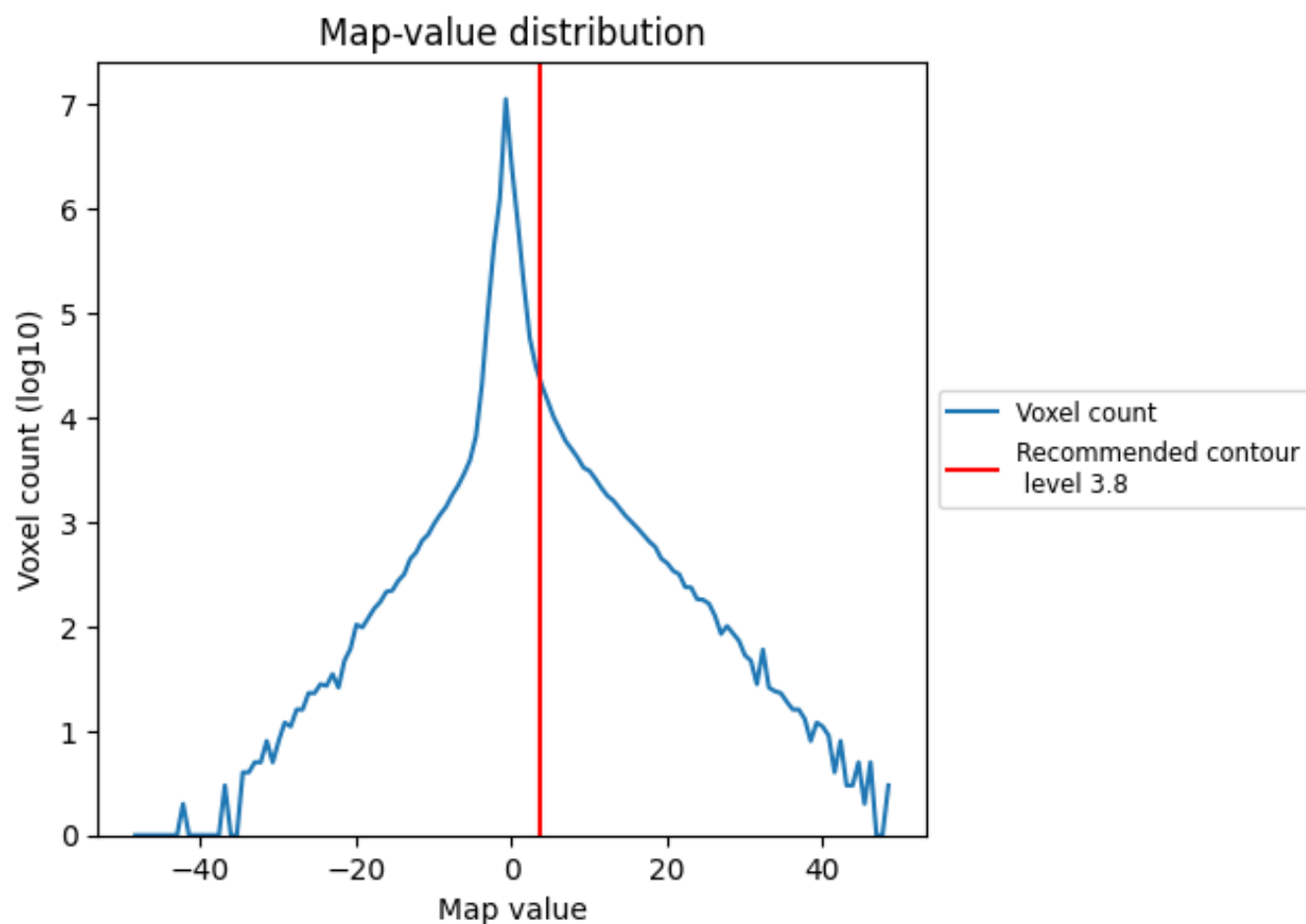
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

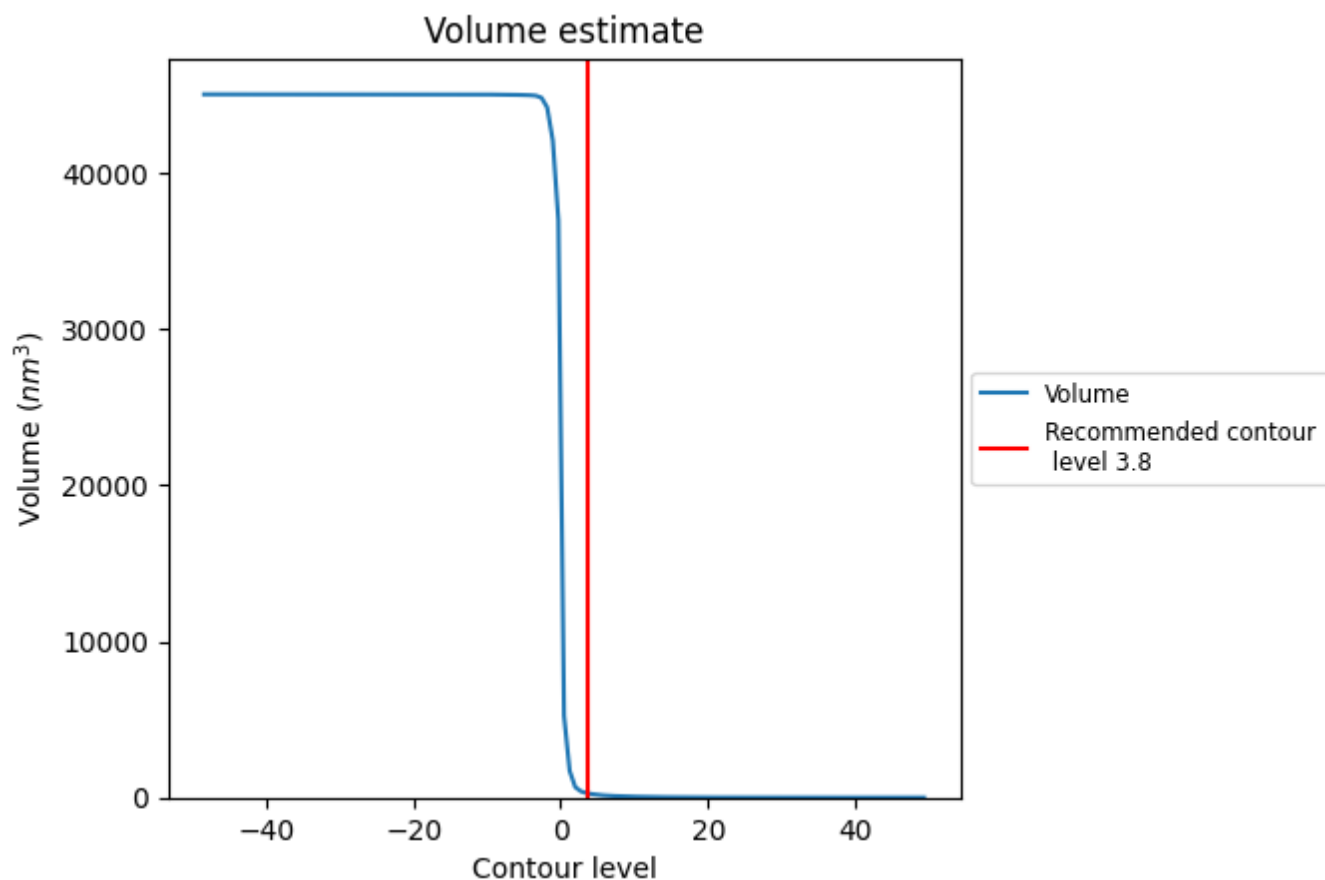
This section contains the results of statistical analysis of the map.

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.

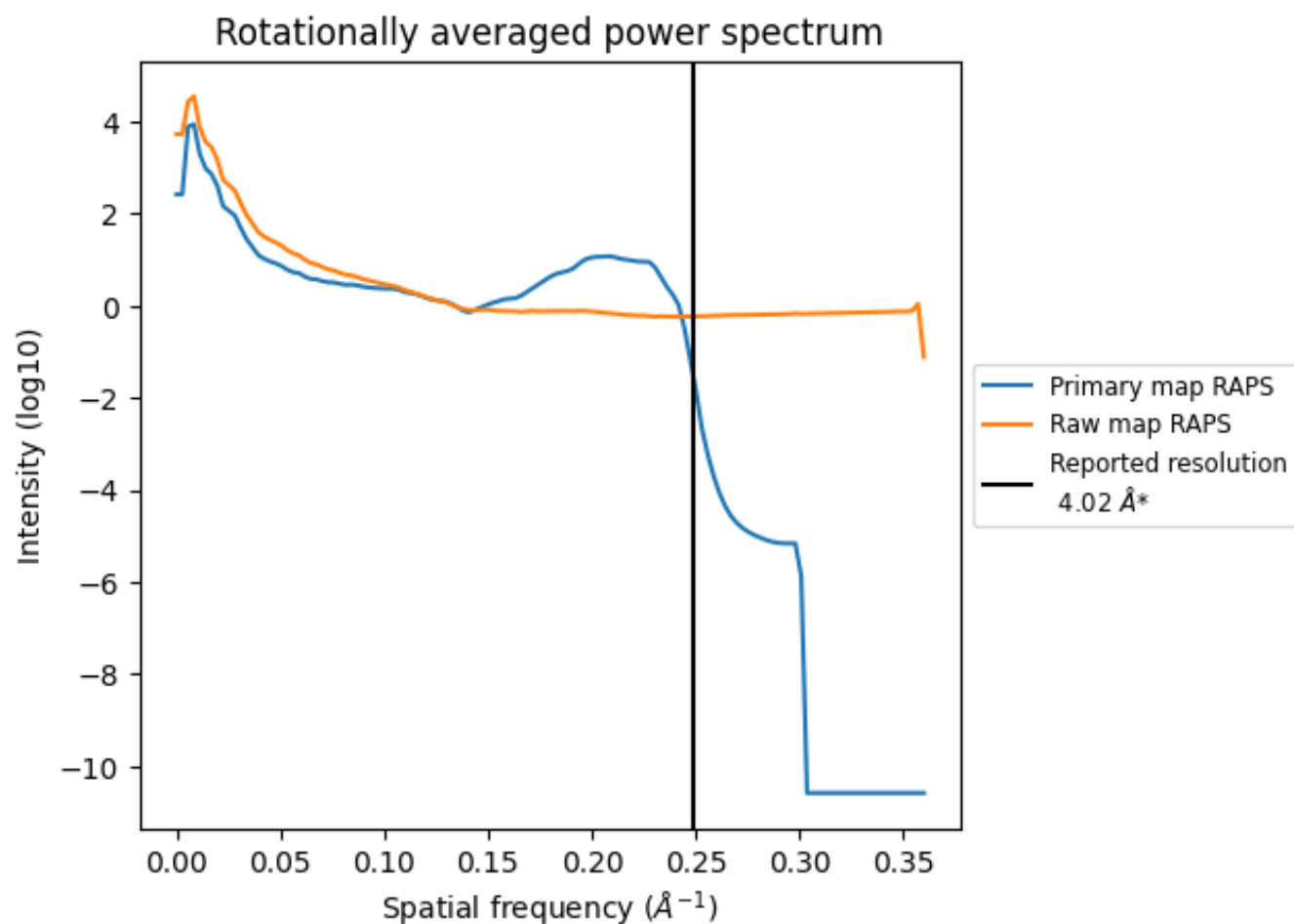
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 237 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 ⓘ

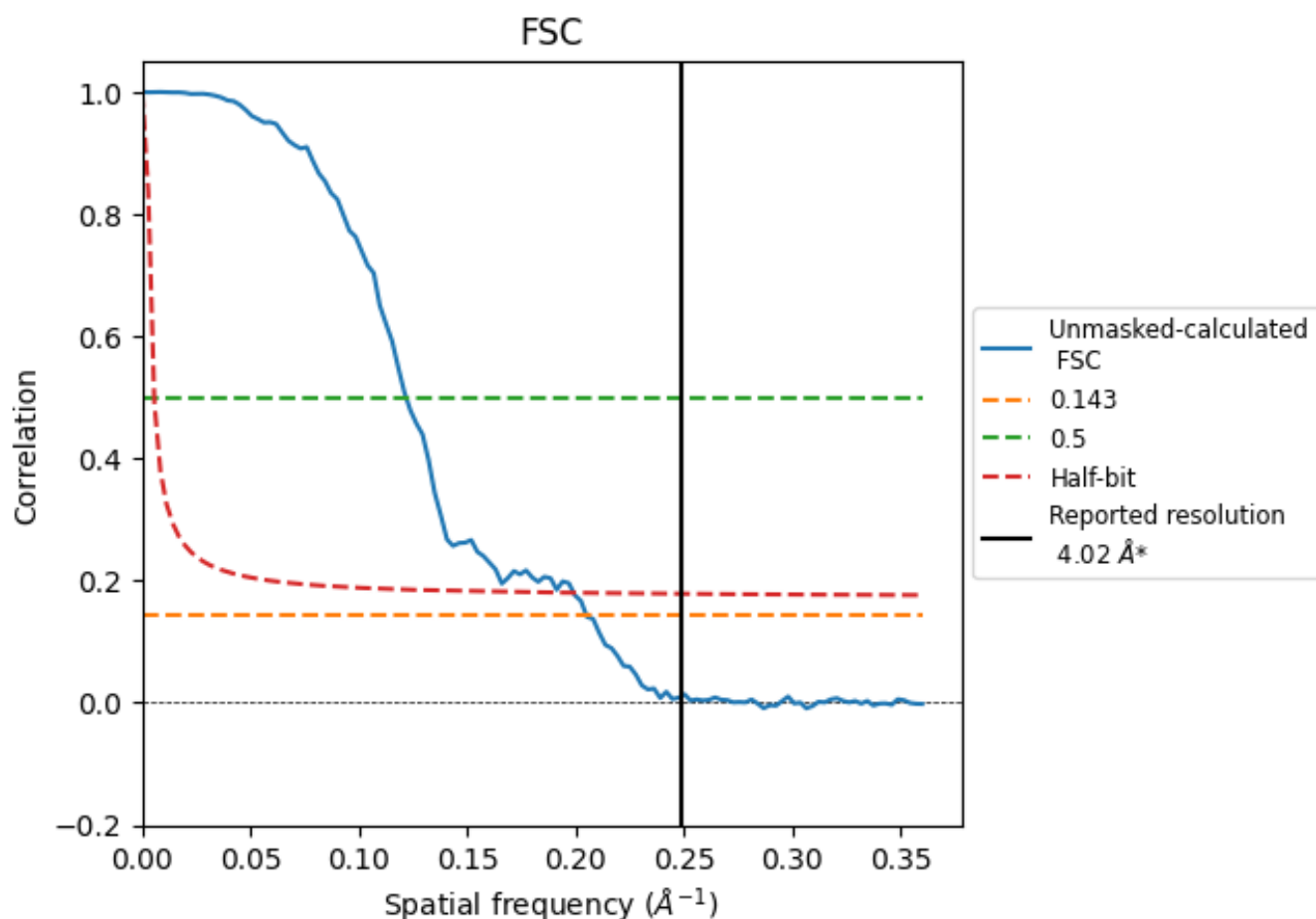


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.249 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

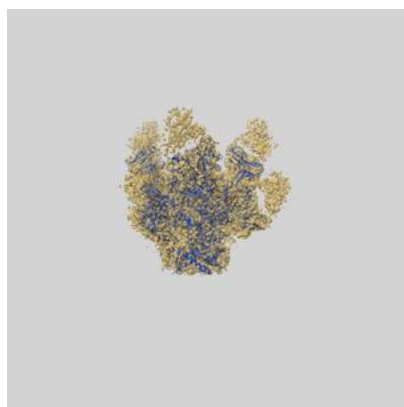
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.88	8.22	5.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.88 differs from the reported value 4.02 by more than 10 %

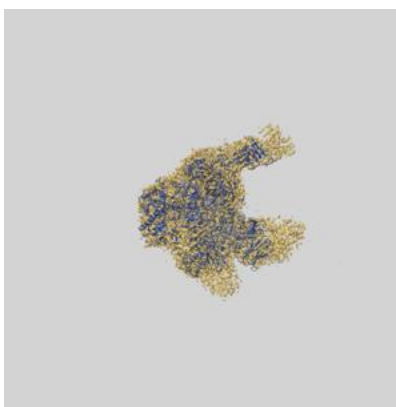
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26648 and PDB model 7UOJ. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

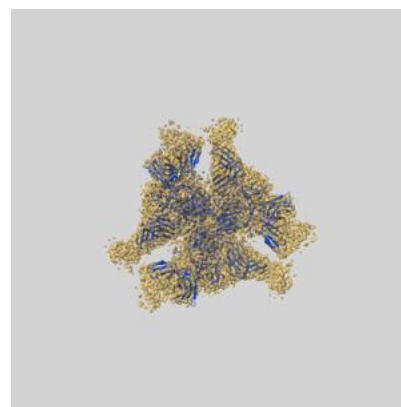
9.1 Map-model overlay [i](#)



X



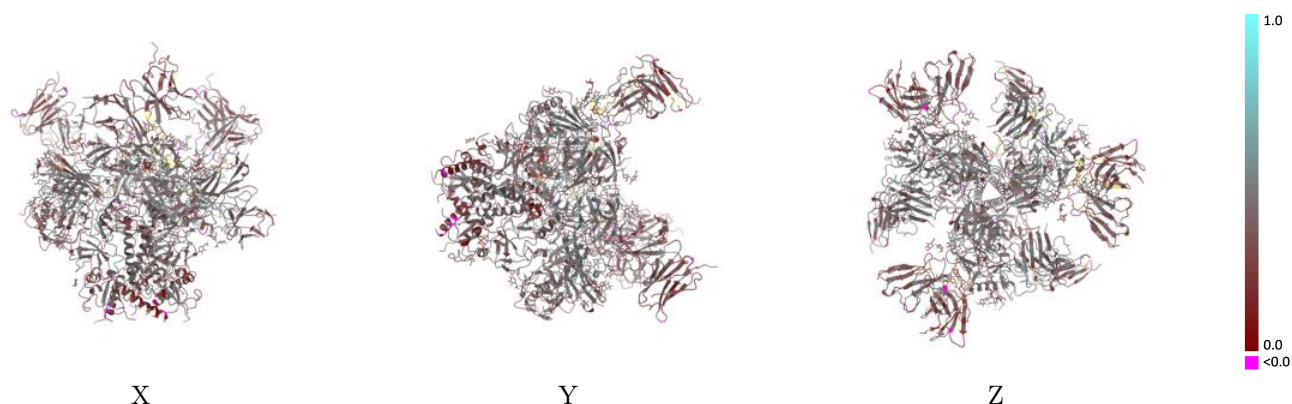
Y



Z

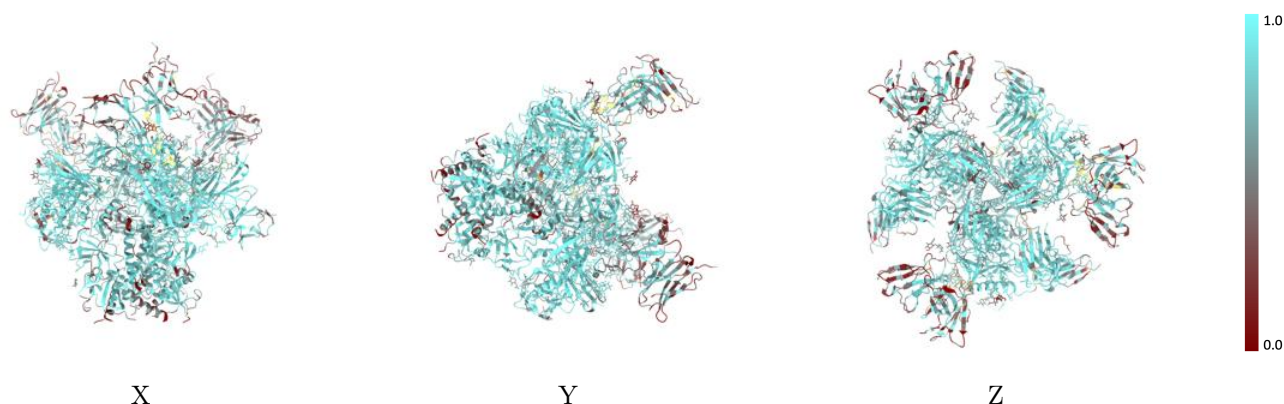
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



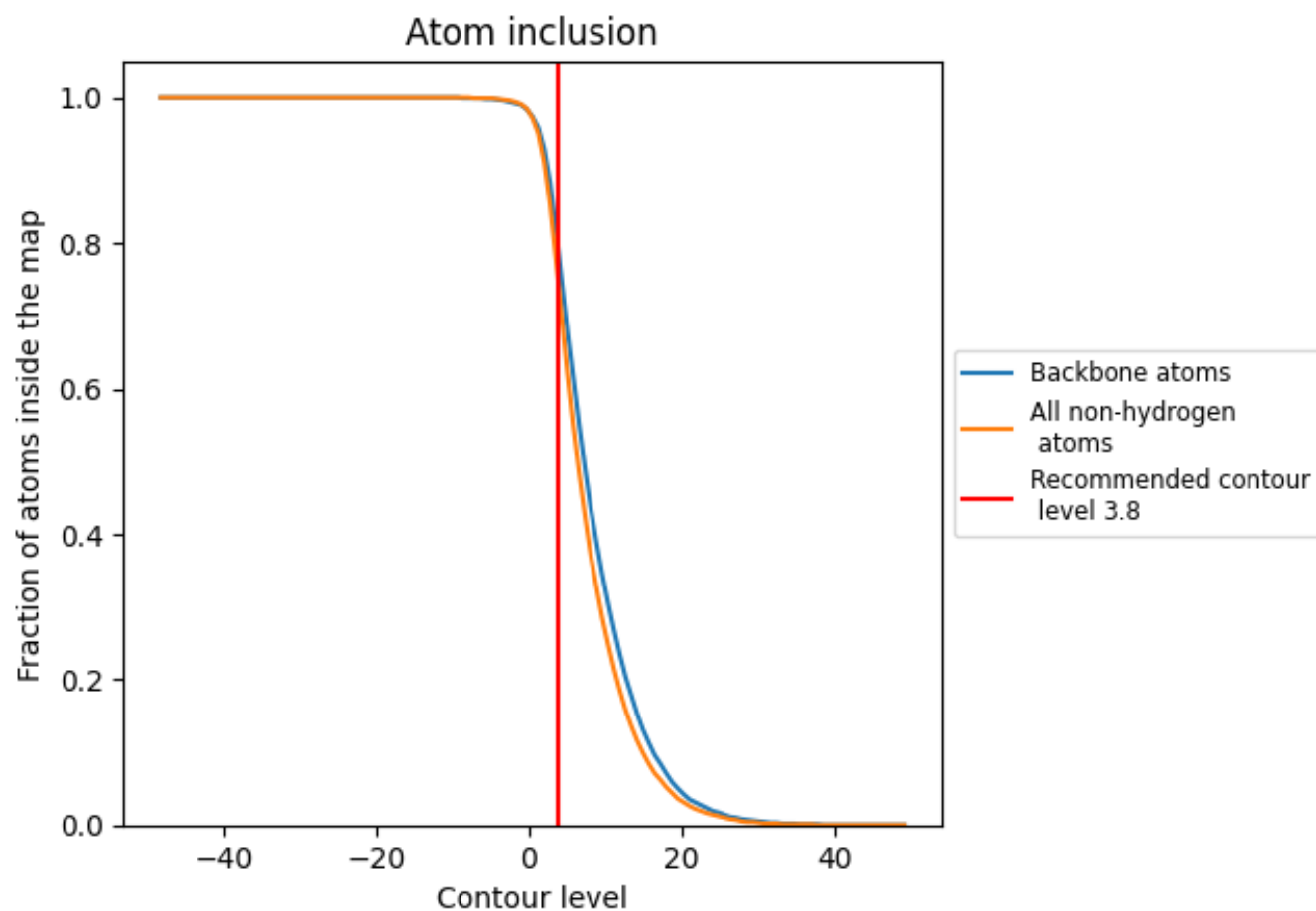
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7500	 0.3900
A	 0.8320	 0.4230
B	 0.7240	 0.3320
C	 0.7080	 0.3290
D	 0.8550	 0.4290
E	 0.7260	 0.3730
F	 0.7140	 0.4710
G	 0.8340	 0.4260
H	 0.8580	 0.4310
I	 0.8380	 0.4260
J	 0.7070	 0.3250
K	 0.8580	 0.4310
L	 0.7350	 0.3820
M	 0.7380	 0.3840
N	 0.3570	 0.3610
O	 0.7800	 0.3940
P	 0.6430	 0.3130
Q	 0.5710	 0.3670
R	 0.8970	 0.4820
S	 0.6890	 0.3280
T	 0.6790	 0.4100
U	 0.7620	 0.4210
V	 0.7500	 0.3900
W	 0.7500	 0.3420
X	 0.7140	 0.4900
Y	 0.4640	 0.3580
Z	 0.7600	 0.4300
a	 0.6430	 0.3070
b	 0.4640	 0.3260
c	 0.8460	 0.4520
d	 0.5710	 0.3290
e	 0.5560	 0.3490
f	 0.6560	 0.3470
g	 0.5000	 0.3970
h	 0.5600	 0.3300



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.8190	 0.4370
j	 0.7500	 0.4280
k	 0.5650	 0.3310
l	 0.5750	 0.3520
m	 0.5650	 0.3470
n	 0.7140	 0.3230
o	 0.6790	 0.4710
p	 0.3930	 0.3410
q	 0.7800	 0.4090
r	 0.7860	 0.3730
s	 0.5360	 0.2630
t	 0.9230	 0.4750
u	 0.5740	 0.3110
v	 0.7500	 0.3810
w	 0.6670	 0.3810
x	 0.7500	 0.4480
y	 0.6790	 0.2990