



## Full wwPDB EM Validation Report ⓘ

May 22, 2023 – 03:15 PM EDT

PDB ID : 8SAW  
EMDB ID : EMD-40282  
Title : CryoEM structure of DH270.UCA.G57R-CH848.10.17DT  
Authors : Henderson, R.; Zhou, Y.; Stalls, V.; Bartesaghi, B.; Acharya, P.  
Deposited on : 2023-04-02  
Resolution : 3.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

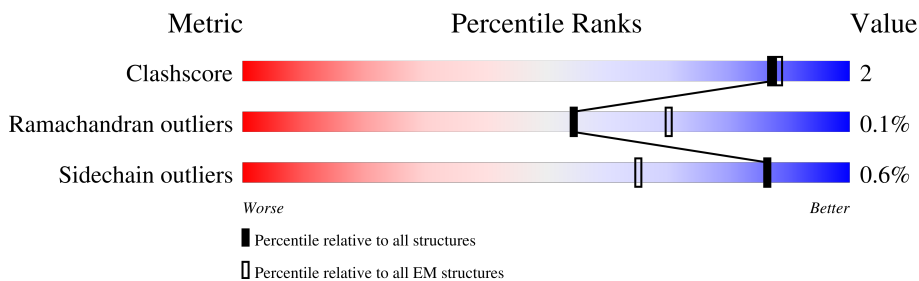
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	471	
1	E	471	
1	K	471	
2	B	132	
2	F	132	
2	L	132	
3	C	127	
3	H	127	
3	M	127	

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Mol	Chain	Length	Quality of chain
4	D	110	 94% 6%
4	I	110	 94% 6%
4	N	110	 95% 5%
5	G	3	 100%
5	Q	3	 100%
5	U	3	 100%
6	J	9	 33% 67%
6	R	9	 33% 67%
6	V	9	 33% 67%
7	O	2	 100%
7	P	2	 100%
7	S	2	 100%
7	T	2	 100%
7	W	2	 100%
7	X	2	 100%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 38848 atoms, of which 19105 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 CH848.3.D0949.10.17chim.6R.SOSIP.664 gp120A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	462	7144	2261	3530	627	697	29	0	0
1	E	462	7144	2261	3530	627	697	29	0	0
1	K	462	7145	2261	3531	627	697	29	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP A0A1W6IPB2
A	32	GLU	-	expression tag	UNP A0A1W6IPB2
A	33	ASN	-	expression tag	UNP A0A1W6IPB2
A	201	CYS	VAL	conflict	UNP A0A1W6IPB2
A	433	CYS	ALA	conflict	UNP A0A1W6IPB2
A	490	LYS	GLU	conflict	UNP A0A1W6IPB2
A	492	GLU	GLN	conflict	UNP A0A1W6IPB2
A	496	VAL	ILE	conflict	UNP A0A1W6IPB2
A	500	ARG	GLY	conflict	UNP A0A1W6IPB2
A	501	CYS	ALA	conflict	UNP A0A1W6IPB2
A	507	GLY	GLU	conflict	UNP A0A1W6IPB2
A	509	ARG	GLU	conflict	UNP A0A1W6IPB2
A	510	ARG	LYS	conflict	UNP A0A1W6IPB2
A	512	ARG	-	expression tag	UNP A0A1W6IPB2
A	513	ARG	-	expression tag	UNP A0A1W6IPB2
E	31	ALA	-	expression tag	UNP A0A1W6IPB2
E	32	GLU	-	expression tag	UNP A0A1W6IPB2
E	33	ASN	-	expression tag	UNP A0A1W6IPB2
E	201	CYS	VAL	conflict	UNP A0A1W6IPB2
E	433	CYS	ALA	conflict	UNP A0A1W6IPB2
E	490	LYS	GLU	conflict	UNP A0A1W6IPB2
E	492	GLU	GLN	conflict	UNP A0A1W6IPB2
E	496	VAL	ILE	conflict	UNP A0A1W6IPB2
E	500	ARG	GLY	conflict	UNP A0A1W6IPB2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	501	CYS	ALA	conflict	UNP A0A1W6IPB2
E	507	GLY	GLU	conflict	UNP A0A1W6IPB2
E	509	ARG	GLU	conflict	UNP A0A1W6IPB2
E	510	ARG	LYS	conflict	UNP A0A1W6IPB2
E	512	ARG	-	expression tag	UNP A0A1W6IPB2
E	513	ARG	-	expression tag	UNP A0A1W6IPB2
K	0	ALA	-	expression tag	UNP A0A1W6IPB2
K	1	GLU	-	expression tag	UNP A0A1W6IPB2
K	2	ASN	-	expression tag	UNP A0A1W6IPB2
K	162	CYS	VAL	conflict	UNP A0A1W6IPB2
K	390	CYS	ALA	conflict	UNP A0A1W6IPB2
K	447	LYS	GLU	conflict	UNP A0A1W6IPB2
K	449	GLU	GLN	conflict	UNP A0A1W6IPB2
K	453	VAL	ILE	conflict	UNP A0A1W6IPB2
K	457	ARG	GLY	conflict	UNP A0A1W6IPB2
K	458	CYS	ALA	conflict	UNP A0A1W6IPB2
K	464	GLY	GLU	conflict	UNP A0A1W6IPB2
K	466	ARG	GLU	conflict	UNP A0A1W6IPB2
K	467	ARG	LYS	conflict	UNP A0A1W6IPB2
K	469	ARG	-	expression tag	UNP A0A1W6IPB2
K	470	ARG	-	expression tag	UNP A0A1W6IPB2

- Molecule 2 is a protein called CH848.3.D0949.10.17chim.6R.SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace	
2	B	123	Total	C	H	N	O	S	0	0
			1925	613	950	169	187	6		
2	F	123	Total	C	H	N	O	S	0	0
			1925	613	950	169	187	6		
2	L	123	Total	C	H	N	O	S	0	0
			1925	613	950	169	187	6		

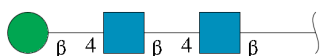
- Molecule 3 is a protein called DH270.UCA. G57R heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
3	C	126	Total	C	H	N	O	S	0	0
			1941	631	945	171	188	6		
3	H	126	Total	C	H	N	O	S	0	0
			1941	631	945	171	188	6		
3	M	126	Total	C	H	N	O	S	0	0
			1941	631	945	171	188	6		

- Molecule 4 is a protein called DH270.UCA. G57R light chain.

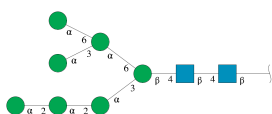
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	110	Total	C	H	N	O	S	0	0
			1568	492	772	133	167	4		
4	I	110	Total	C	H	N	O	S	0	0
			1565	492	769	133	167	4		
4	N	110	Total	C	H	N	O	S	0	0
			1568	492	772	133	167	4		

- Molecule 5 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
			Total	C	H	N	O		
5	G	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
5	Q	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
5	U	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 6 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
			Total	C	H	N	O		
6	J	9	Total	C	H	N	O	0	0
			193	58	88	2	45		
6	R	9	Total	C	H	N	O	0	0
			193	58	88	2	45		
6	V	9	Total	C	H	N	O	0	0
			193	58	88	2	45		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

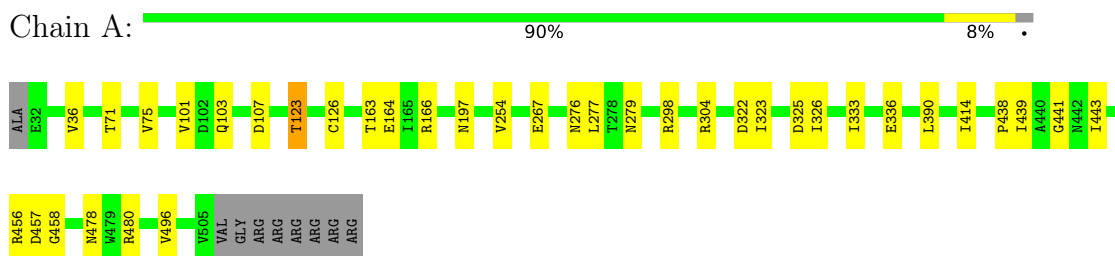


Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
7	P	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
7	S	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
7	T	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
7	W	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
7	X	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

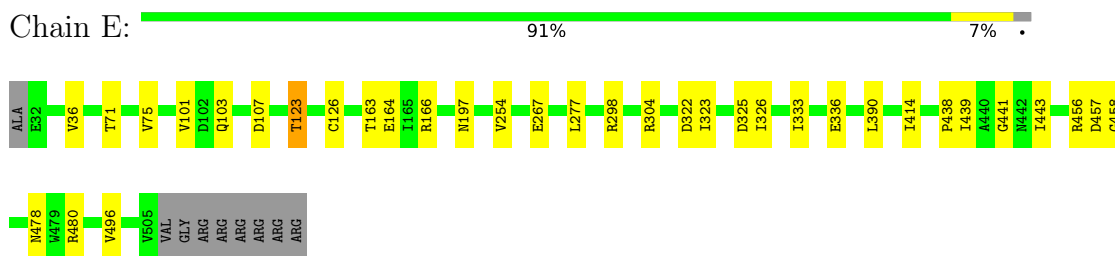
### 3 Residue-property plots

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. 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. 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.

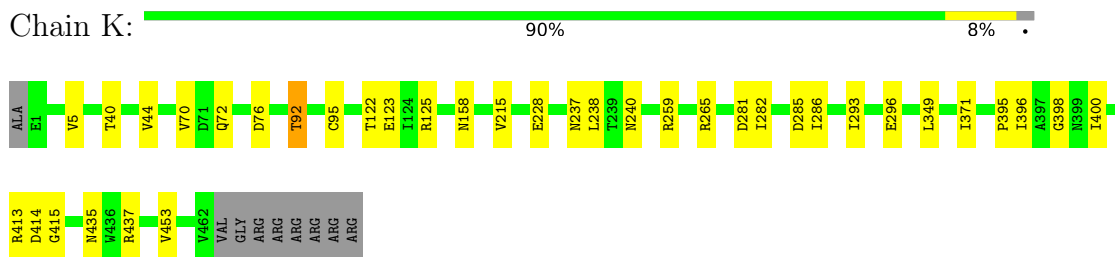
- Molecule 1: CH848.3.D0949.10.17chim.6R.SOSIP.664 gp120A



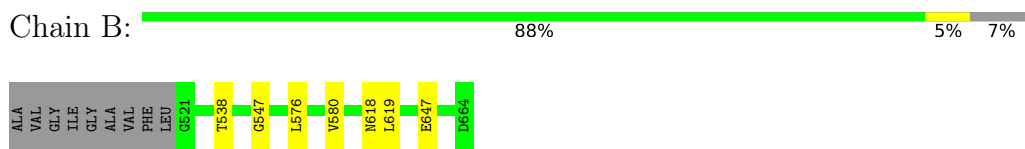
- Molecule 1: CH848.3.D0949.10.17chim.6R.SOSIP.664 gp120A



- Molecule 1: CH848.3.D0949.10.17chim.6R.SOSIP.664 gp120A




- Molecule 2: CH848.3.D0949.10.17chim.6R.SOSIP.664 gp41




- Molecule 2: CH848.3.D0949.10.17chim.6R.SOSIP.664 gp41



Chain F:  88% 5% 7%



- Molecule 2: CH848.3.D0949.10.17chim.6R..SOSIP.664 gp41

Chain L:  88% 5% 7%



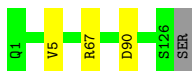
- Molecule 3: DH270.UCA. G57R heavy chain

Chain C:  97% ..



- Molecule 3: DH270.UCA. G57R heavy chain

Chain H:  97% ..



- Molecule 3: DH270.UCA. G57R heavy chain

Chain M:  97% ..



- Molecule 4: DH270.UCA. G57R light chain

Chain D:  94% 6%



- Molecule 4: DH270.UCA. G57R light chain

Chain I:  94% 6%



- Molecule 4: DH270.UCA. G57R light chain

Chain N:  95% 5%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



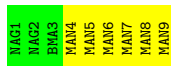
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%



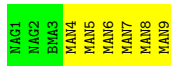
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%



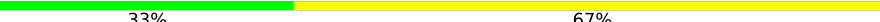
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 67%



- Molecule 6: 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 V:  33% 67%

 MANG1  
MANG2  
MANG3  
MANG4  
MANG5  
MANG6  
MANG7  
MANG8  
MANG9

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

Chain O:  100%

 MANG1  
MANG2

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

Chain P:  100%

 MANG1  
MANG2

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

Chain S:  100%

 MANG1  
MANG2

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

Chain T:  100%

 MANG1  
MANG2

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

Chain W:  100%

 MANG1  
MANG2

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

Chain X:  100%

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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.25	0/3691	0.52	0/5022
1	E	0.25	0/3691	0.52	0/5022
1	K	0.25	0/3691	0.52	0/5022
2	B	0.24	0/993	0.48	0/1348
2	F	0.24	0/993	0.48	0/1348
2	L	0.24	0/993	0.48	0/1348
3	C	0.25	0/1024	0.53	0/1390
3	H	0.25	0/1024	0.53	0/1390
3	M	0.25	0/1024	0.53	0/1390
4	D	0.26	0/811	0.51	0/1100
4	I	0.25	0/811	0.51	0/1100
4	N	0.26	0/811	0.51	0/1100
All	All	0.25	0/19557	0.51	0/26580

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3614	3530	3530	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3614	3530	3530	22	0
1	K	3614	3531	3533	23	0
2	B	975	950	950	6	0
2	F	975	950	950	6	0
2	L	975	950	950	6	0
3	C	996	945	945	1	0
3	H	996	945	945	1	0
3	M	996	945	945	1	0
4	D	796	772	772	3	0
4	I	796	769	769	3	0
4	N	796	772	772	2	0
5	G	39	34	34	0	0
5	Q	39	34	34	0	0
5	U	39	34	34	0	0
6	J	105	88	88	0	0
6	R	105	88	88	0	0
6	V	105	88	88	0	0
7	O	28	25	25	0	0
7	P	28	25	25	0	0
7	S	28	25	25	0	0
7	T	28	25	25	0	0
7	W	28	25	25	0	0
7	X	28	25	25	0	0
All	All	19743	19105	19107	79	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 2.

All (79) 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)
2:B:576:LEU:HD11	2:L:48:VAL:HG21	1.68	0.76
2:B:580:VAL:HG21	2:F:576:LEU:HD11	1.68	0.74
2:F:580:VAL:HG21	2:L:44:LEU:HD11	1.70	0.71
2:B:538:THR:OG1	2:L:115:GLU:OE2	2.12	0.65
2:F:647:GLU:OE2	2:L:27:THR:OG1	2.12	0.63
1:A:304:ARG:NH1	1:A:438:PRO:O	2.32	0.62
1:E:304:ARG:NH1	1:E:438:PRO:O	2.32	0.62
1:K:265:ARG:NH1	1:K:395:PRO:O	2.32	0.62
1:E:123:THR:O	1:K:125:ARG:NH2	2.34	0.60
1:A:166:ARG:NH2	1:K:95:CYS:SG	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:O	1:E:166:ARG:NH2	2.36	0.58
1:A:166:ARG:NH2	1:K:92:THR:O	2.36	0.58
1:A:126:CYS:SG	1:E:166:ARG:NH2	2.78	0.57
1:E:36:VAL:HG23	1:E:496:VAL:HG13	1.87	0.56
1:A:36:VAL:HG23	1:A:496:VAL:HG13	1.88	0.55
1:K:5:VAL:HG23	1:K:453:VAL:HG13	1.88	0.55
1:E:325:ASP:OD1	1:E:326:ILE:N	2.42	0.53
1:E:126:CYS:SG	1:K:125:ARG:NH2	2.82	0.52
1:A:325:ASP:OD1	1:A:326:ILE:N	2.42	0.52
1:K:285:ASP:OD1	1:K:286:ILE:N	2.42	0.52
1:K:396:ILE:HD11	1:K:400:ILE:HD13	1.91	0.52
1:E:277:LEU:O	1:E:456:ARG:NH2	2.43	0.52
1:E:197:ASN:ND2	1:K:123:GLU:OE1	2.43	0.52
1:E:439:ILE:HD11	1:E:443:ILE:HD13	1.91	0.52
1:A:277:LEU:O	1:A:456:ARG:NH2	2.43	0.52
1:A:333:ILE:HD11	1:A:390:LEU:HD22	1.92	0.51
1:A:439:ILE:HD11	1:A:443:ILE:HD13	1.91	0.51
1:K:238:LEU:O	1:K:413:ARG:NH2	2.44	0.51
2:B:647:GLU:OE2	2:F:538:THR:OG1	2.20	0.51
1:A:298:ARG:NH2	1:A:441:GLY:O	2.43	0.51
1:K:259:ARG:NH2	1:K:398:GLY:O	2.44	0.51
1:A:75:VAL:HG11	2:B:547:GLY:HA2	1.93	0.50
1:K:293:ILE:HD11	1:K:349:LEU:HD22	1.92	0.50
1:E:75:VAL:HG11	2:F:547:GLY:HA2	1.94	0.50
1:E:333:ILE:HD11	1:E:390:LEU:HD22	1.92	0.50
1:A:164:GLU:OE1	1:K:158:ASN:ND2	2.45	0.50
1:E:298:ARG:NH2	1:E:441:GLY:O	2.44	0.50
1:K:44:VAL:HG11	2:L:36:GLY:HA2	1.94	0.49
2:L:86:ASN:OD1	2:L:87:LEU:N	2.45	0.49
1:A:197:ASN:ND2	1:E:164:GLU:OE1	2.45	0.49
4:D:63:ARG:NH1	4:D:79:GLY:O	2.46	0.48
4:I:94:ARG:NH1	4:I:110:GLY:O	2.47	0.48
2:B:618:ASN:OD1	2:B:619:LEU:N	2.45	0.48
4:N:63:ARG:NH1	4:N:79:GLY:O	2.46	0.47
2:F:618:ASN:OD1	2:F:619:LEU:N	2.45	0.47
1:A:163:THR:OG1	1:A:164:GLU:N	2.48	0.47
1:K:122:THR:OG1	1:K:123:GLU:N	2.48	0.47
1:E:163:THR:OG1	1:E:164:GLU:N	2.49	0.46
1:E:103:GLN:NE2	1:E:107:ASP:OD2	2.50	0.45
1:A:103:GLN:NE2	1:A:107:ASP:OD2	2.50	0.45
1:K:215:VAL:O	1:K:435:ASN:ND2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:OE1	1:A:336:GLU:N	2.51	0.44
1:K:72:GLN:NE2	1:K:76:ASP:OD2	2.50	0.44
4:D:52:GLU:O	4:D:54:SER:N	2.43	0.44
1:K:296:GLU:N	1:K:296:GLU:OE1	2.51	0.44
1:K:281:ASP:OD1	1:K:282:ILE:N	2.50	0.44
1:E:254:VAL:O	1:E:478:ASN:ND2	2.46	0.44
1:K:228:GLU:N	1:K:228:GLU:OE1	2.51	0.44
1:A:267:GLU:OE1	1:A:267:GLU:N	2.51	0.43
3:C:67:ARG:NH2	3:C:90:ASP:OD2	2.51	0.43
1:A:254:VAL:O	1:A:478:ASN:ND2	2.46	0.43
1:A:457:ASP:OD1	1:A:458:GLY:N	2.51	0.43
1:E:336:GLU:OE1	1:E:336:GLU:N	2.50	0.43
1:A:322:ASP:OD1	1:A:323:ILE:N	2.50	0.43
4:I:83:GLU:O	4:I:85:SER:N	2.43	0.43
1:K:414:ASP:OD1	1:K:415:GLY:N	2.51	0.43
3:M:67:ARG:NH2	3:M:90:ASP:OD2	2.51	0.43
1:E:322:ASP:OD1	1:E:323:ILE:N	2.50	0.42
1:E:267:GLU:OE1	1:E:267:GLU:N	2.51	0.42
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.52	0.42
4:N:3:ALA:HA	4:N:100:ILE:HD11	2.01	0.42
1:E:101:VAL:HG11	1:E:480:ARG:HA	2.01	0.42
1:E:457:ASP:OD1	1:E:458:GLY:N	2.51	0.42
1:A:276:ASN:ND2	1:A:279:ASN:OD1	2.51	0.42
4:D:3:ALA:HA	4:D:100:ILE:HD11	2.02	0.42
1:K:70:VAL:HG11	1:K:437:ARG:HA	2.01	0.41
1:K:237:ASN:ND2	1:K:240:ASN:OD1	2.51	0.41
4:I:34:ALA:HA	4:I:131:ILE:HD11	2.01	0.41
1:A:101:VAL:HG11	1:A:480:ARG:HA	2.01	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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	460/471 (98%)	441 (96%)	18 (4%)	1 (0%)	47	77
1	E	460/471 (98%)	441 (96%)	18 (4%)	1 (0%)	47	77
1	K	460/471 (98%)	441 (96%)	18 (4%)	1 (0%)	47	77
2	B	121/132 (92%)	120 (99%)	1 (1%)	0	100	100
2	F	121/132 (92%)	120 (99%)	1 (1%)	0	100	100
2	L	121/132 (92%)	120 (99%)	1 (1%)	0	100	100
3	C	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
3	H	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
3	M	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
4	D	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
4	I	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
4	N	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
All	All	2439/2520 (97%)	2360 (97%)	76 (3%)	3 (0%)	54	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	THR
1	E	123	THR
1	K	92	THR

### 5.3.2 Protein sidechains [i](#)

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	411/418 (98%)	409 (100%)	2 (0%)	88	93
1	E	411/418 (98%)	409 (100%)	2 (0%)	88	93
1	K	411/418 (98%)	409 (100%)	2 (0%)	88	93
2	B	105/110 (96%)	105 (100%)	0	100	100
2	F	105/110 (96%)	105 (100%)	0	100	100
2	L	105/110 (96%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	104/105 (99%)	103 (99%)	1 (1%)	76	86
3	H	104/105 (99%)	103 (99%)	1 (1%)	76	86
3	M	104/105 (99%)	103 (99%)	1 (1%)	76	86
4	D	90/90 (100%)	89 (99%)	1 (1%)	73	85
4	I	90/90 (100%)	89 (99%)	1 (1%)	73	85
4	N	90/90 (100%)	89 (99%)	1 (1%)	73	85
All	All	2130/2169 (98%)	2118 (99%)	12 (1%)	86	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	414	ILE
3	C	5	VAL
4	D	90	CYS
1	E	71	THR
1	E	414	ILE
3	H	5	VAL
4	I	121	CYS
1	K	40	THR
1	K	371	ILE
3	M	5	VAL
4	N	90	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

48 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	G	1	5,1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.46	0
5	BMA	G	3	5	11,11,12	0.54	0	15,15,17	0.78	0
6	NAG	J	1	6,1	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	J	2	6	14,14,15	0.20	0	17,19,21	0.39	0
6	BMA	J	3	6	11,11,12	0.55	0	15,15,17	0.79	0
6	MAN	J	4	6	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
6	MAN	J	5	6	11,11,12	0.64	0	15,15,17	1.10	2 (13%)
6	MAN	J	6	6	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
6	MAN	J	7	6	11,11,12	0.59	0	15,15,17	0.93	2 (13%)
6	MAN	J	8	6	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
6	MAN	J	9	6	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
7	NAG	O	1	7,1	14,14,15	0.18	0	17,19,21	0.41	0
7	NAG	O	2	7	14,14,15	0.23	0	17,19,21	0.40	0
7	NAG	P	1	7,1	14,14,15	0.36	0	17,19,21	0.54	0
7	NAG	P	2	7	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	Q	1	5,1	14,14,15	0.21	0	17,19,21	0.38	0
5	NAG	Q	2	5	14,14,15	0.23	0	17,19,21	0.47	0
5	BMA	Q	3	5	11,11,12	0.55	0	15,15,17	0.77	0
6	NAG	R	1	6,1	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	R	2	6	14,14,15	0.19	0	17,19,21	0.39	0
6	BMA	R	3	6	11,11,12	0.55	0	15,15,17	0.79	0
6	MAN	R	4	6	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
6	MAN	R	5	6	11,11,12	0.64	0	15,15,17	1.09	2 (13%)
6	MAN	R	6	6	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
6	MAN	R	7	6	11,11,12	0.58	0	15,15,17	0.94	2 (13%)
6	MAN	R	8	6	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
6	MAN	R	9	6	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
7	NAG	S	1	7,1	14,14,15	0.18	0	17,19,21	0.42	0
7	NAG	S	2	7	14,14,15	0.21	0	17,19,21	0.41	0
7	NAG	T	1	7,1	14,14,15	0.36	0	17,19,21	0.53	0
7	NAG	T	2	7	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	U	1	5,1	14,14,15	0.21	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	U	2	5	14,14,15	0.23	0	17,19,21	0.46	0
5	BMA	U	3	5	11,11,12	0.54	0	15,15,17	0.77	0
6	NAG	V	1	6,1	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	V	2	6	14,14,15	0.20	0	17,19,21	0.39	0
6	BMA	V	3	6	11,11,12	0.56	0	15,15,17	0.79	0
6	MAN	V	4	6	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
6	MAN	V	5	6	11,11,12	0.63	0	15,15,17	1.09	2 (13%)
6	MAN	V	6	6	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
6	MAN	V	7	6	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
6	MAN	V	8	6	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
6	MAN	V	9	6	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
7	NAG	W	1	7,1	14,14,15	0.18	0	17,19,21	0.41	0
7	NAG	W	2	7	14,14,15	0.22	0	17,19,21	0.41	0
7	NAG	X	1	7,1	14,14,15	0.36	0	17,19,21	0.52	0
7	NAG	X	2	7	14,14,15	0.23	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	1/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
6	MAN	J	7	6	-	0/2/19/22	0/1/1/1
6	MAN	J	8	6	-	0/2/19/22	0/1/1/1
6	MAN	J	9	6	-	0/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	NAG	P	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	P	2	7	-	4/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1
6	MAN	R	6	6	-	0/2/19/22	0/1/1/1
6	MAN	R	7	6	-	0/2/19/22	0/1/1/1
6	MAN	R	8	6	-	0/2/19/22	0/1/1/1
6	MAN	R	9	6	-	0/2/19/22	0/1/1/1
7	NAG	S	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	NAG	T	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	T	2	7	-	4/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	MAN	V	4	6	-	1/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
6	MAN	V	6	6	-	0/2/19/22	0/1/1/1
6	MAN	V	7	6	-	0/2/19/22	0/1/1/1
6	MAN	V	8	6	-	0/2/19/22	0/1/1/1
6	MAN	V	9	6	-	0/2/19/22	0/1/1/1
7	NAG	W	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	X	2	7	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	4	MAN	C1-O5-C5	2.55	115.65	112.19
6	V	4	MAN	C1-O5-C5	2.49	115.57	112.19
6	V	5	MAN	O2-C2-C3	-2.49	105.16	110.14
6	R	5	MAN	O2-C2-C3	-2.47	105.20	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	5	MAN	O2-C2-C3	-2.45	105.22	110.14
6	J	4	MAN	C1-O5-C5	2.44	115.50	112.19
6	J	5	MAN	C1-O5-C5	2.31	115.33	112.19
6	R	6	MAN	O2-C2-C3	-2.31	105.51	110.14
6	V	6	MAN	O2-C2-C3	-2.30	105.52	110.14
6	J	6	MAN	O2-C2-C3	-2.30	105.54	110.14
6	R	5	MAN	C1-O5-C5	2.29	115.29	112.19
6	J	4	MAN	O2-C2-C3	-2.26	105.61	110.14
6	J	7	MAN	O2-C2-C3	-2.26	105.62	110.14
6	J	9	MAN	C1-O5-C5	2.25	115.25	112.19
6	V	7	MAN	O2-C2-C3	-2.24	105.66	110.14
6	R	7	MAN	O2-C2-C3	-2.23	105.66	110.14
6	J	9	MAN	O2-C2-C3	-2.23	105.67	110.14
6	R	7	MAN	C1-O5-C5	2.23	115.21	112.19
6	V	9	MAN	O2-C2-C3	-2.23	105.68	110.14
6	R	9	MAN	O2-C2-C3	-2.22	105.68	110.14
6	R	9	MAN	C1-O5-C5	2.22	115.20	112.19
6	V	5	MAN	C1-O5-C5	2.22	115.20	112.19
6	R	4	MAN	O2-C2-C3	-2.22	105.69	110.14
6	V	4	MAN	O2-C2-C3	-2.21	105.70	110.14
6	V	6	MAN	C1-O5-C5	2.21	115.18	112.19
6	V	7	MAN	C1-O5-C5	2.20	115.18	112.19
6	V	9	MAN	C1-O5-C5	2.19	115.15	112.19
6	R	6	MAN	C1-O5-C5	2.18	115.15	112.19
6	J	8	MAN	O2-C2-C3	-2.16	105.82	110.14
6	V	8	MAN	O2-C2-C3	-2.15	105.84	110.14
6	J	7	MAN	C1-O5-C5	2.14	115.09	112.19
6	J	8	MAN	C1-O5-C5	2.14	115.09	112.19
6	R	8	MAN	O2-C2-C3	-2.14	105.86	110.14
6	V	8	MAN	C1-O5-C5	2.13	115.08	112.19
6	J	6	MAN	C1-O5-C5	2.11	115.06	112.19
6	R	8	MAN	C1-O5-C5	2.11	115.06	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	3	BMA	C4-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	V	3	BMA	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C3-C2-N2-C7
7	T	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	O	1	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	P	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
7	P	1	NAG	C1-C2-N2-C7
7	T	1	NAG	C1-C2-N2-C7
7	X	1	NAG	C1-C2-N2-C7
6	R	4	MAN	O5-C5-C6-O6
6	V	4	MAN	O5-C5-C6-O6

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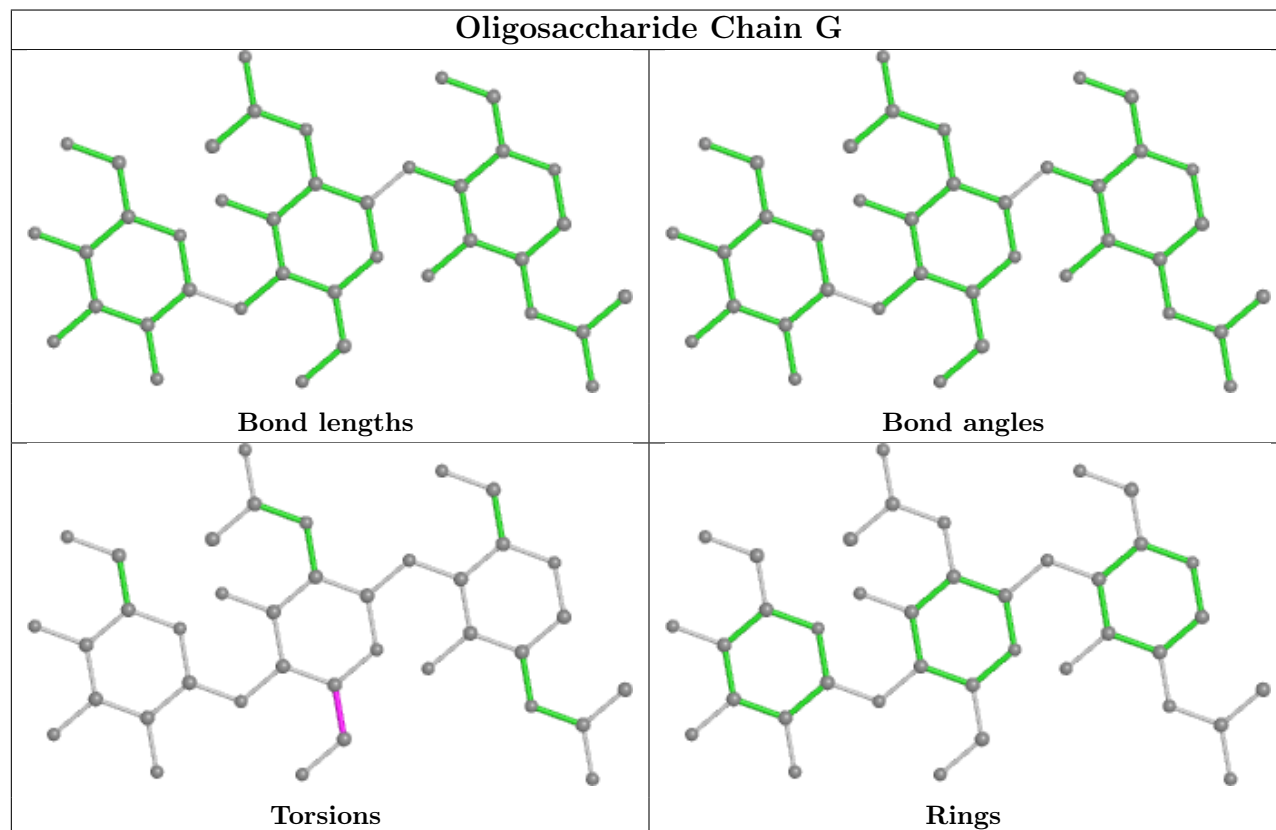
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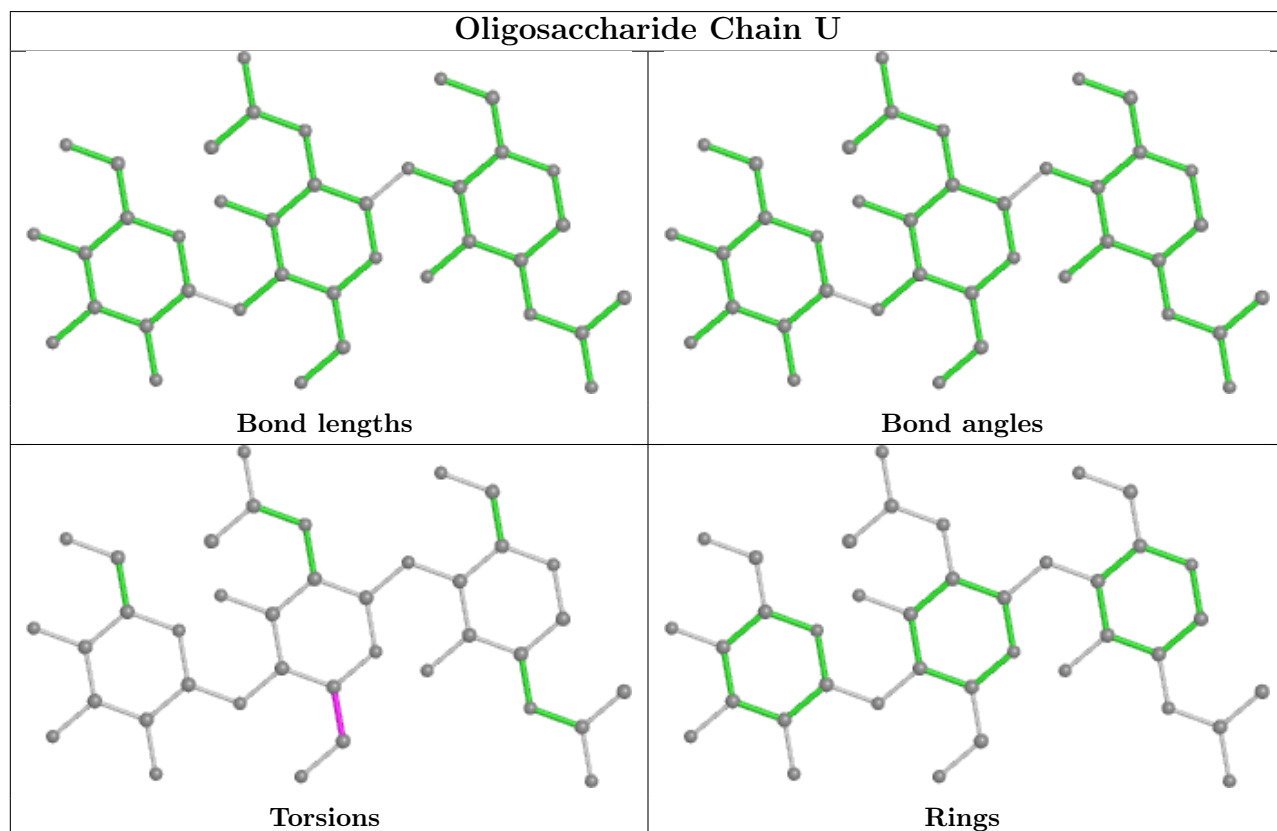
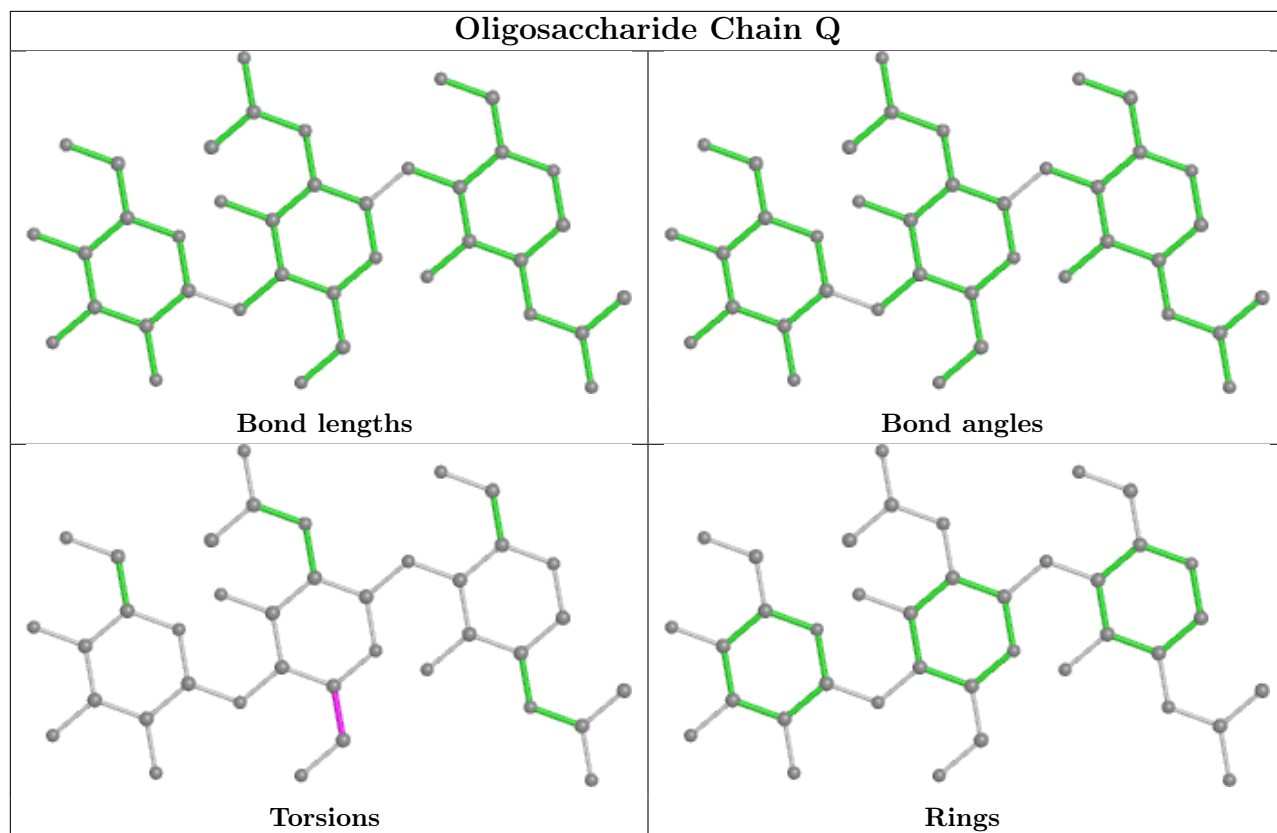
Mol	Chain	Res	Type	Atoms
6	J	4	MAN	O5-C5-C6-O6

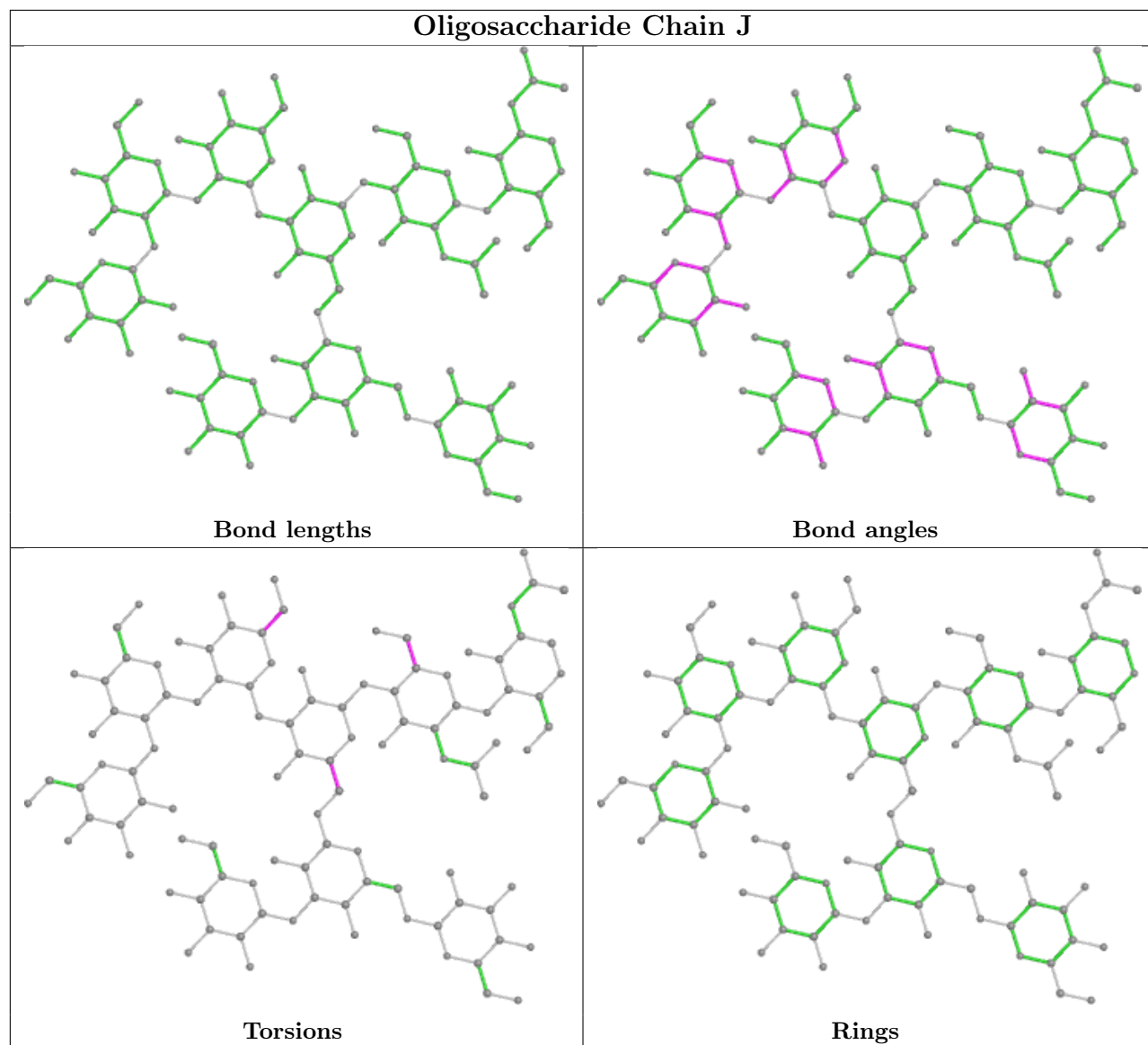
There are no ring outliers.

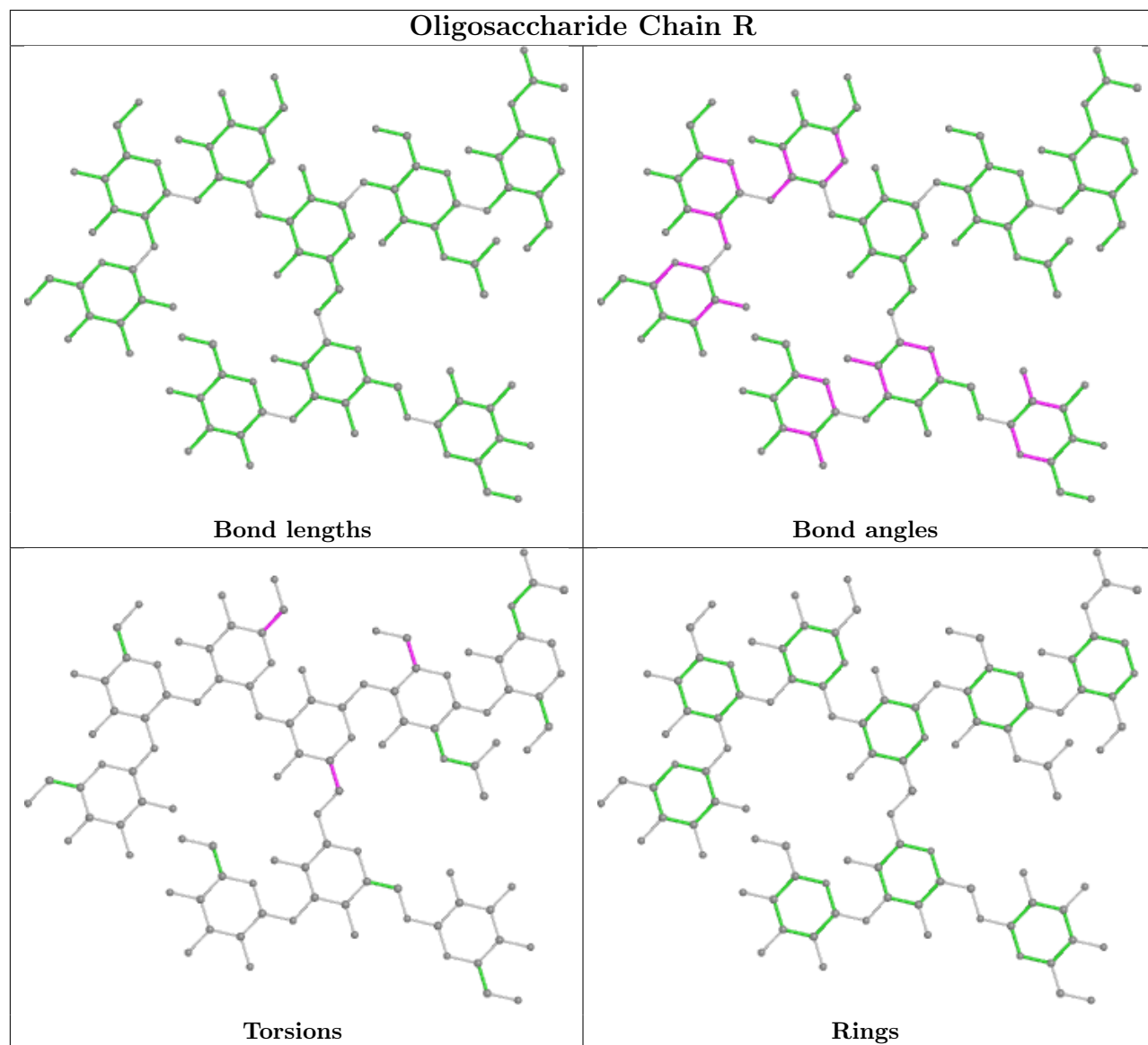
No monomer is involved in short contacts.

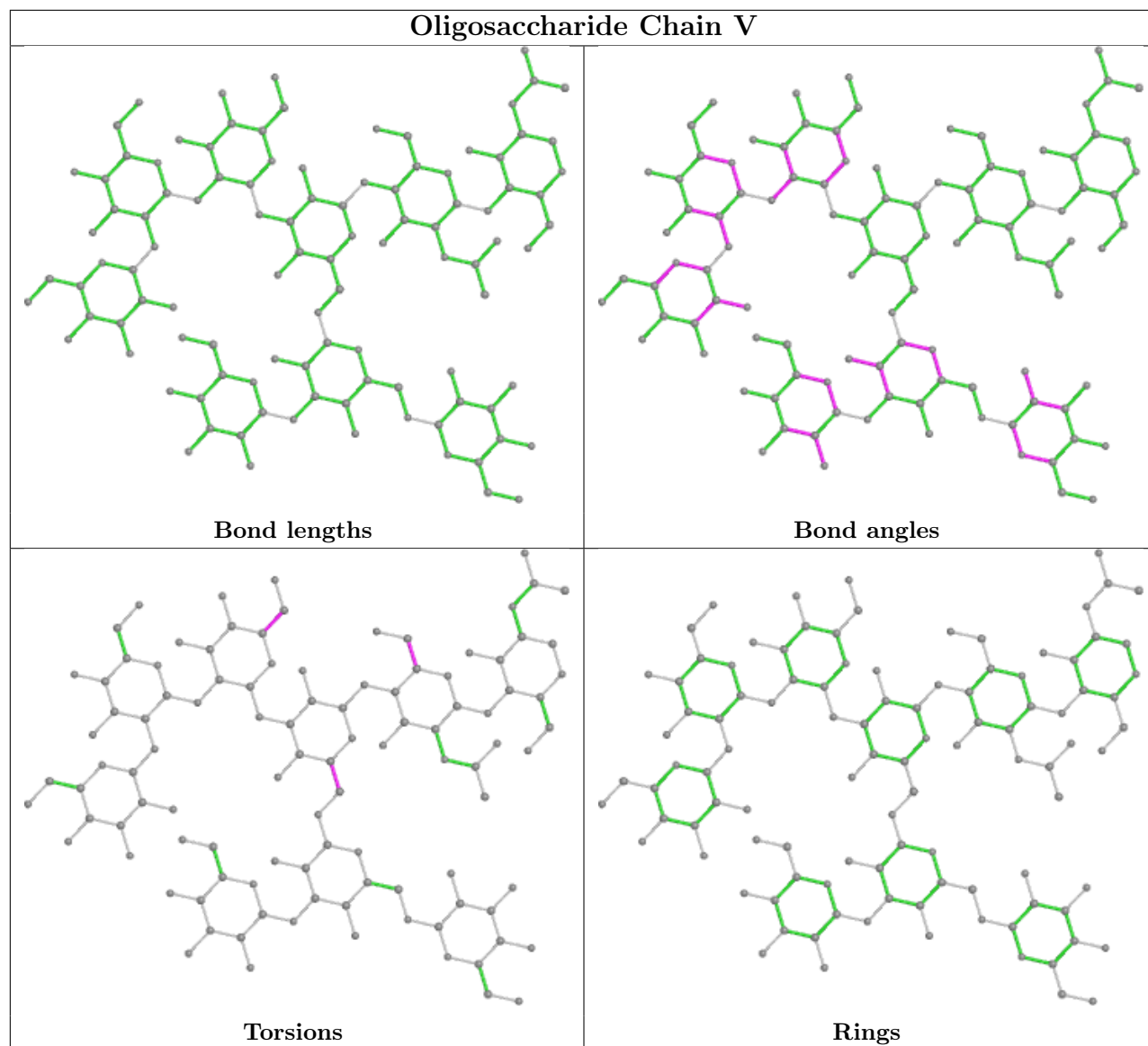
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

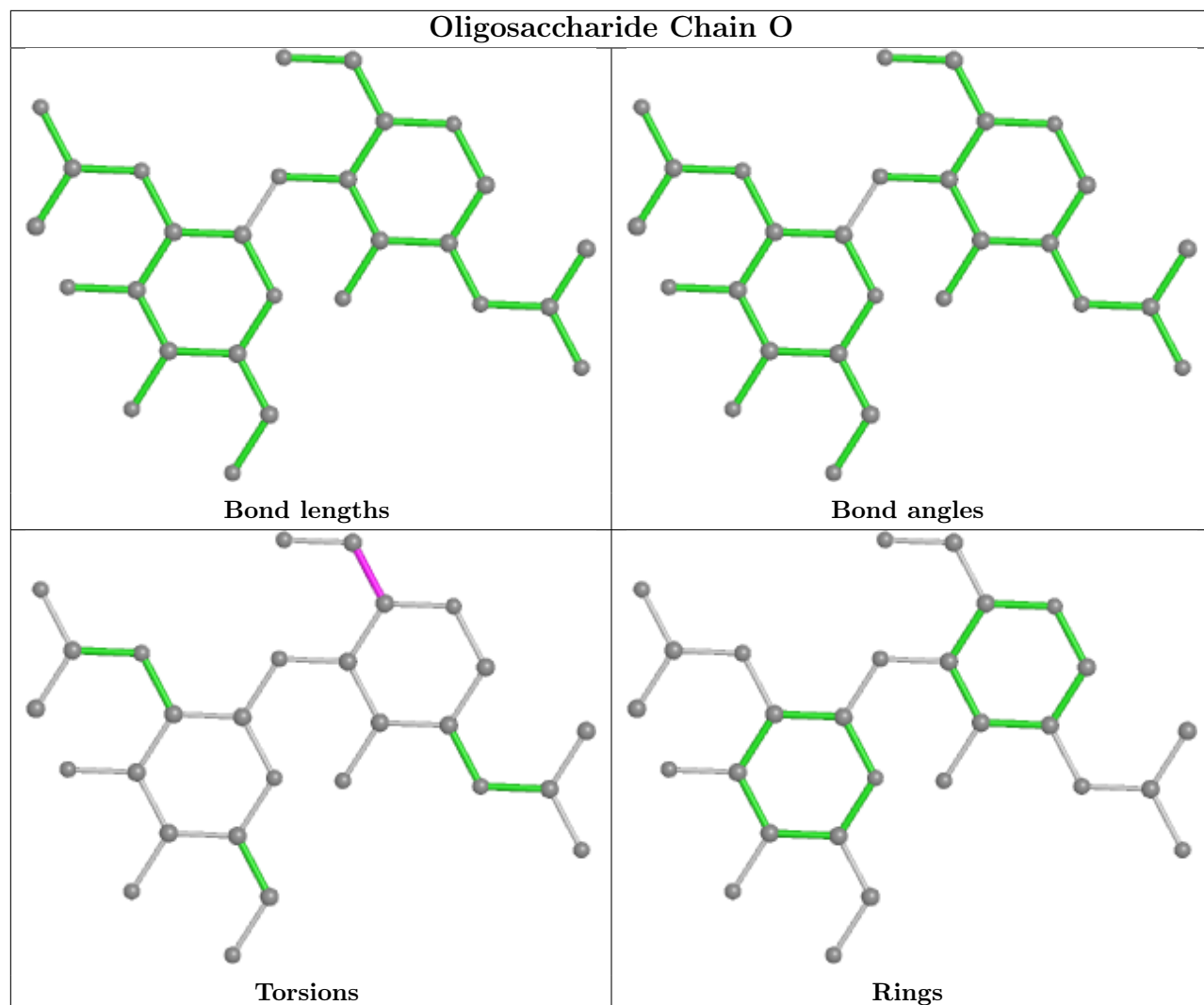


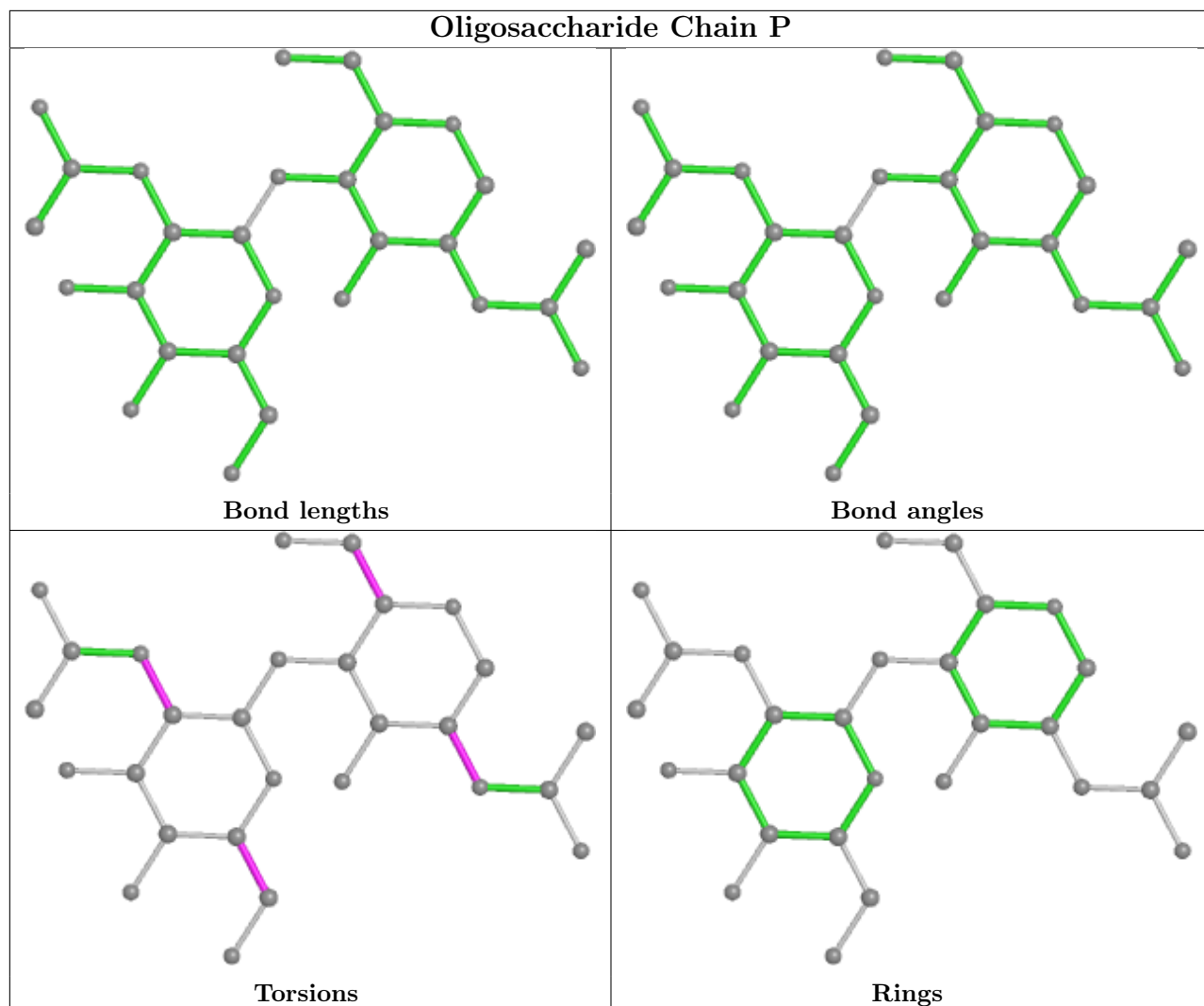


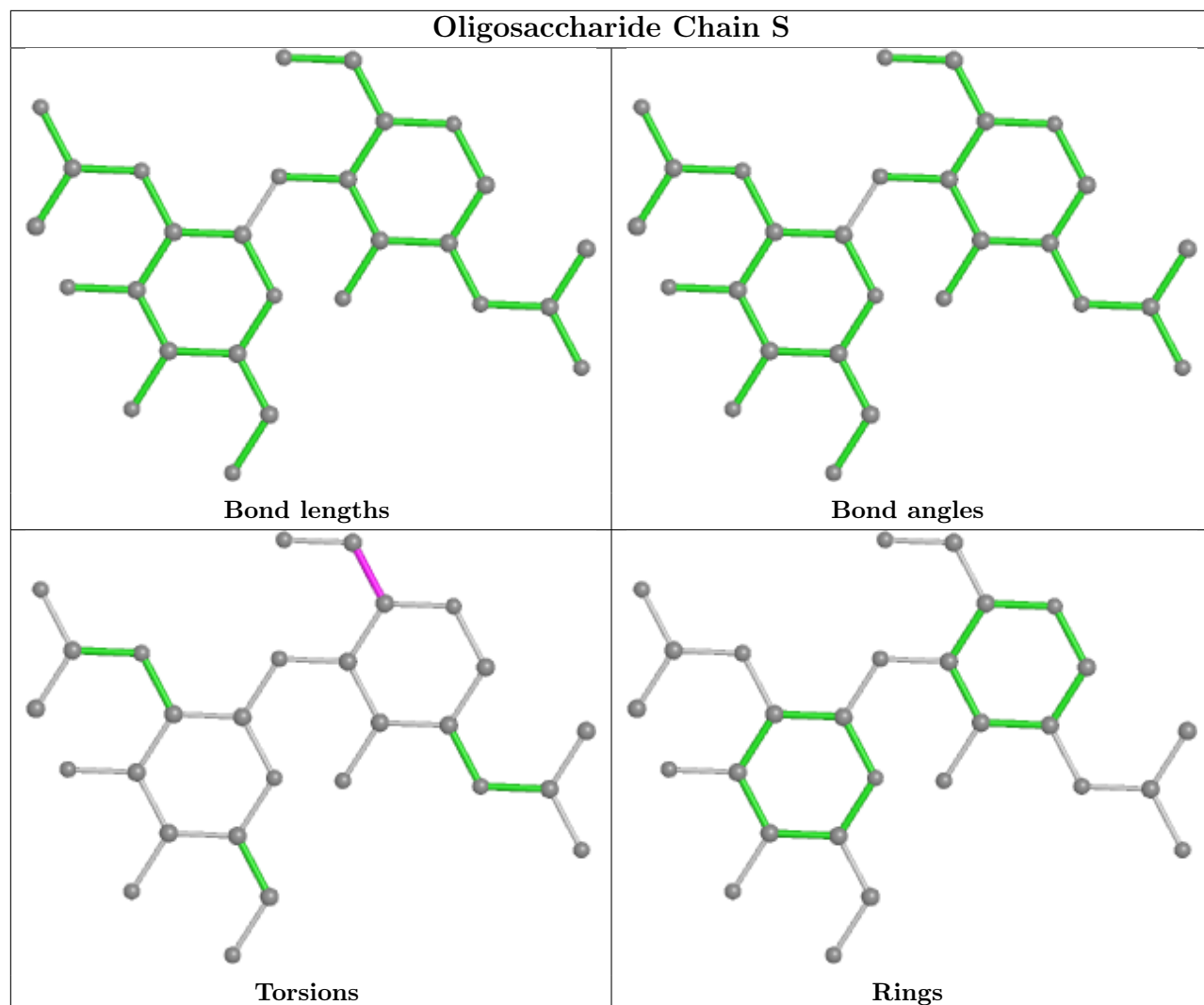




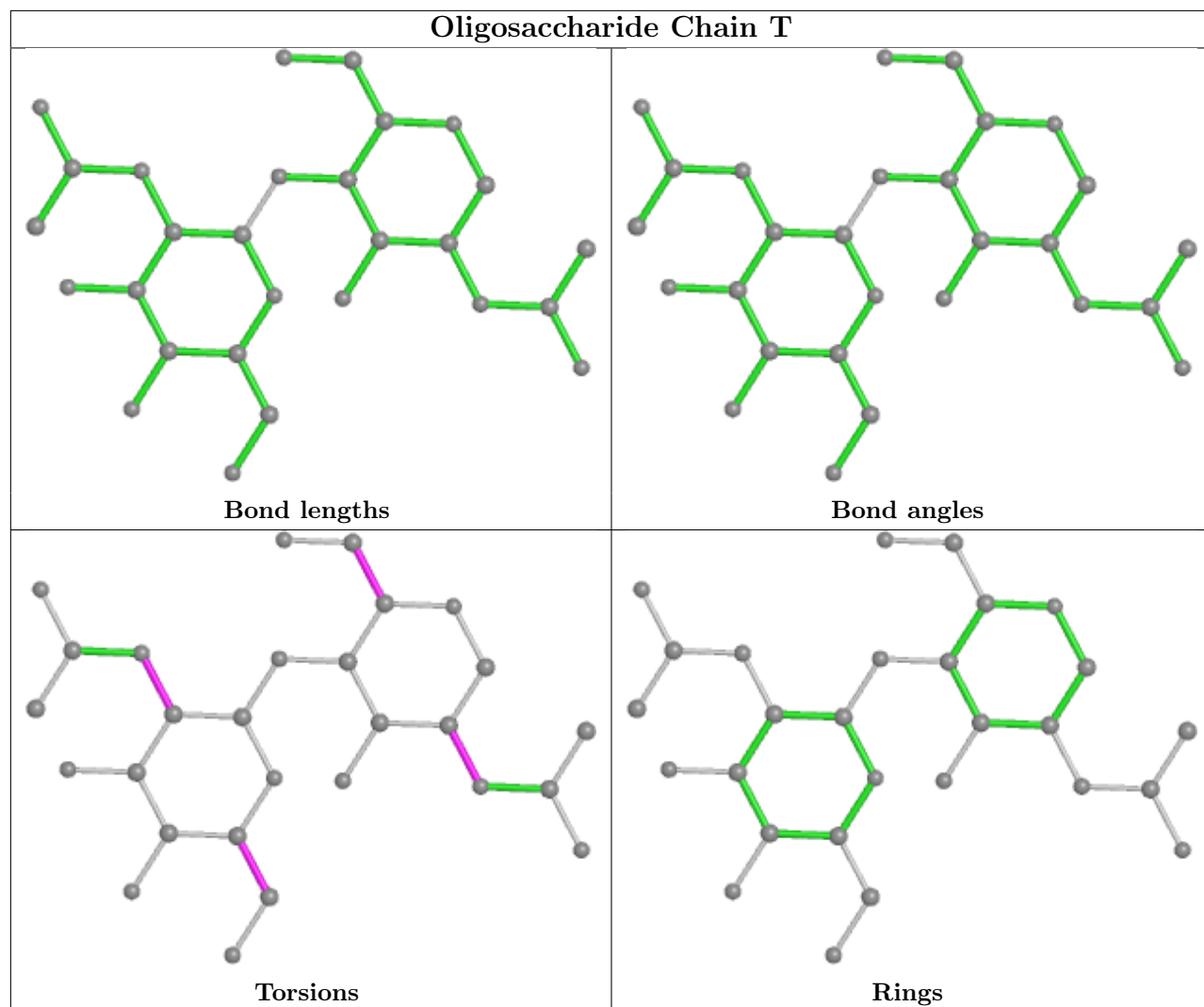


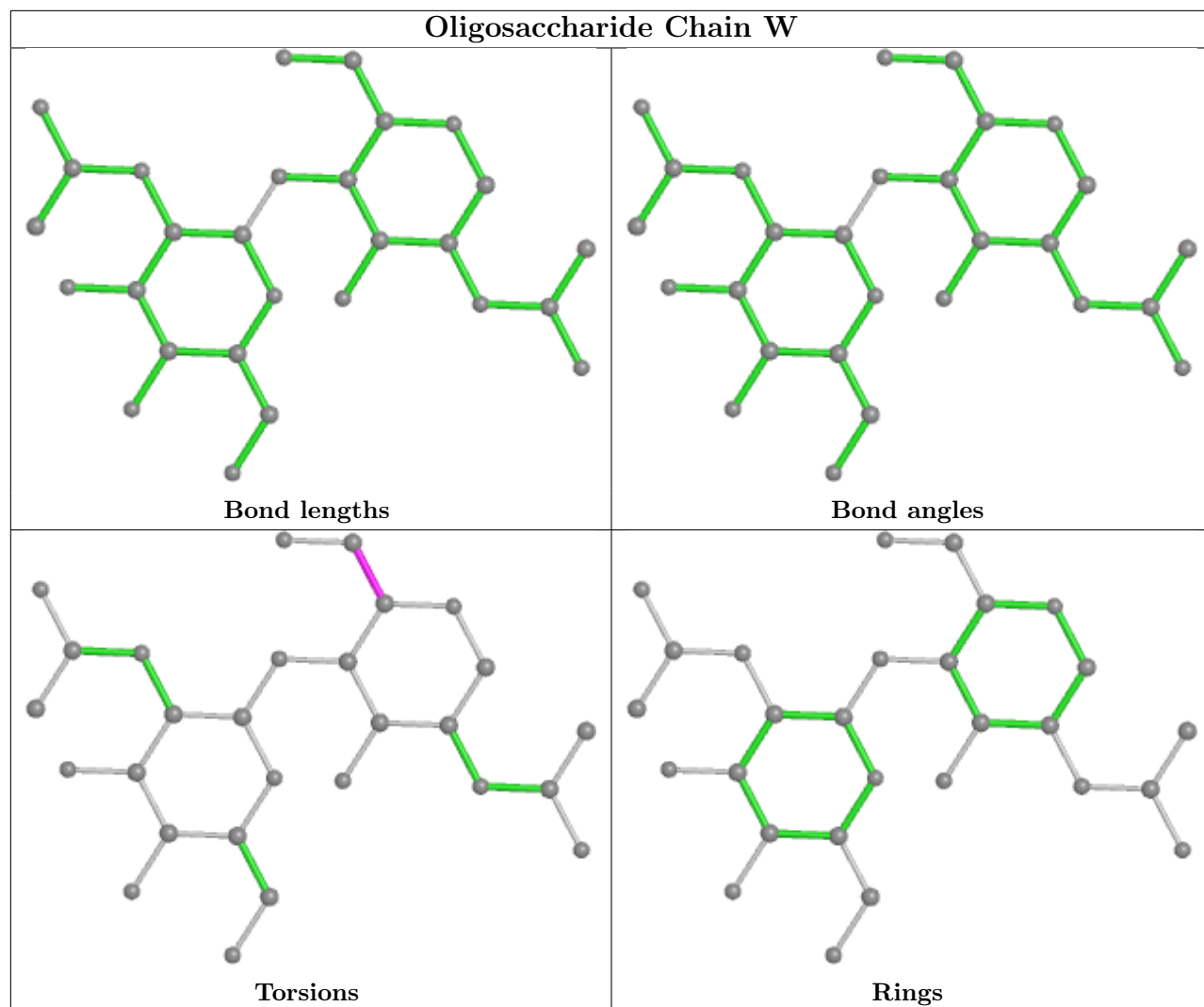


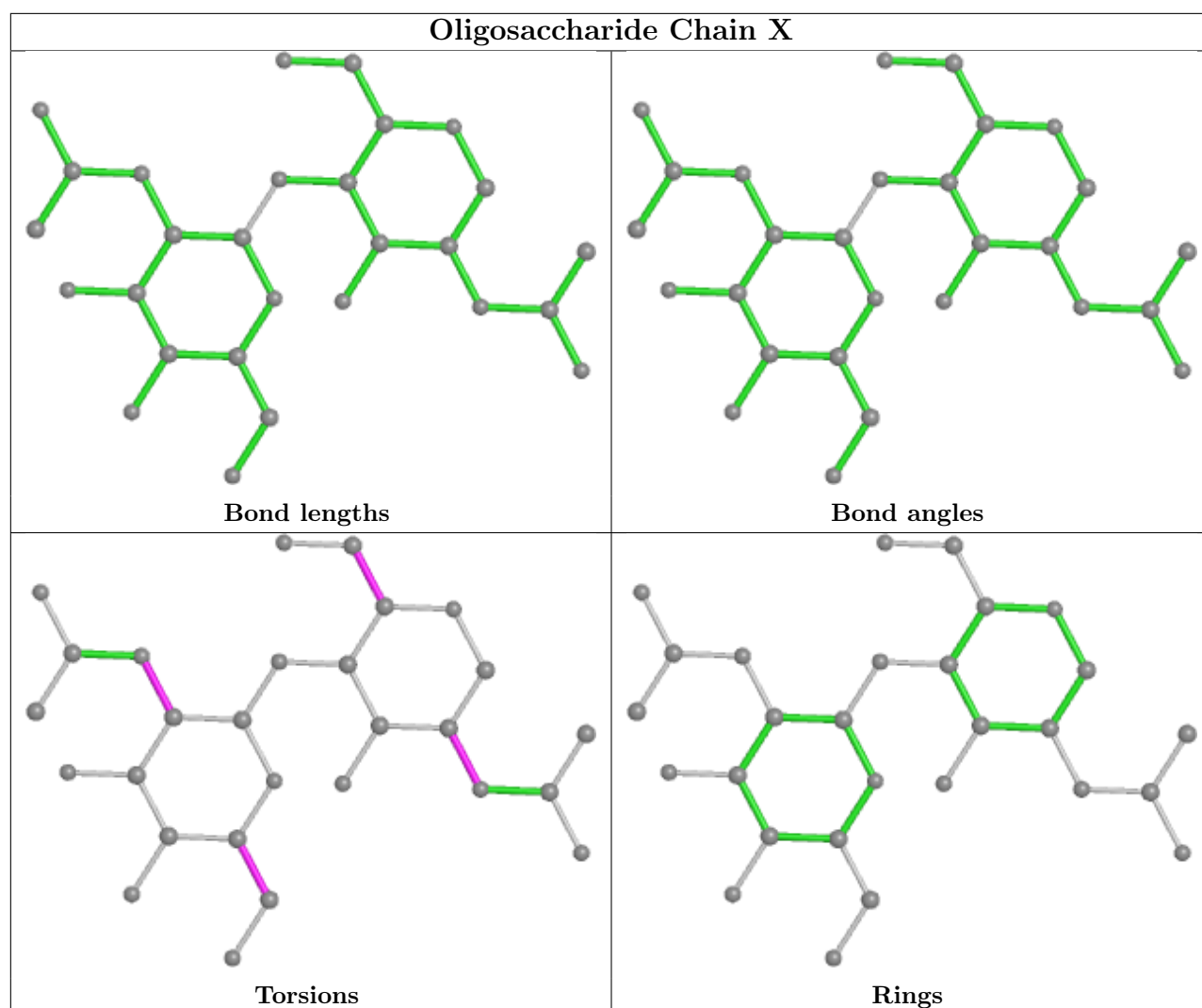












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40282. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis

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

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.