



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 09:34 PM UTC

PDB ID : 5EBZ / pdb_00005ebz
Title : Crystal structure of human IKK1
Authors : Polley, S.; Passos, D.; Huang, D.; Biswas, T.; Verma, I.; Lyumkis, D.; Ghosh, G.
Deposited on : 2015-10-20
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

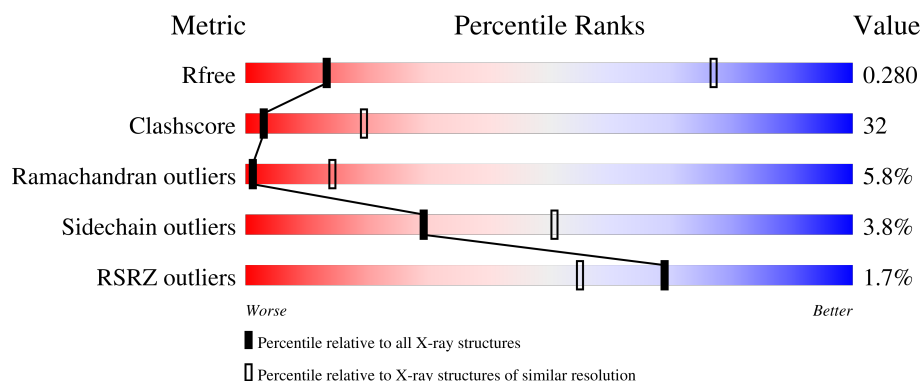
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	2% 44% 50% 6%
1	B	655	2% 43% 51% 6%
1	C	655	2% 43% 52% 5%
1	D	655	3% 42% 54% .
1	E	655	2% 41% 53% 5%

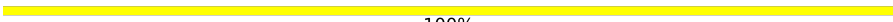
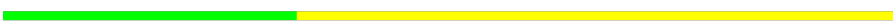
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Mol	Chain	Length	Quality of chain
1	F	655	
1	G	655	
1	H	655	
1	I	655	
1	J	655	
1	K	655	
1	L	655	
2	M	3	
2	N	3	
2	P	3	
2	Q	3	
2	R	3	
2	S	3	
2	U	3	
2	V	3	
2	W	3	
2	X	3	
2	Y	3	
2	Z	3	
2	a	3	
2	b	3	
2	d	3	
2	e	3	
2	f	3	
2	g	3	

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Mol	Chain	Length	Quality of chain
2	h	3	 100%
2	j	3	 100%
2	k	3	 33% 67%
2	l	3	 33% 33% 33%
2	m	3	 67% 33%
2	n	3	 100%
3	O	7	 14% 71% 14%
3	T	7	 43% 57%
3	c	7	 14% 86%
3	i	7	 14% 86%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	j	2	-	-	X	-
4	5TL	A	701	-	X	-	-
4	5TL	B	701	-	X	-	-
4	5TL	C	701	-	X	-	-
4	5TL	D	701	-	X	-	-
4	5TL	E	701	-	X	-	-
4	5TL	F	701	-	X	-	-
4	5TL	G	701	-	X	-	-
4	5TL	H	701	-	X	-	-
4	5TL	I	701	-	X	-	-
4	5TL	J	701	-	X	-	-
4	5TL	K	701	-	X	-	-
4	5TL	L	701	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 65132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Inhibitor of nuclear factor kappa-B kinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	B	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	C	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	D	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	E	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	F	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	G	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	H	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	I	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	J	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	K	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	L	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASP	-	expression tag	UNP O15111
A	7	PRO	-	expression tag	UNP O15111
A	8	GLU	-	expression tag	UNP O15111
A	9	PHE	-	expression tag	UNP O15111
A	176	GLU	SER	engineered mutation	UNP O15111

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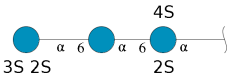
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation	UNP O15111
B	180	GLU	SER	engineered mutation	UNP O15111
B	268	ILE	VAL	variant	UNP O15111
C	6	ASP	-	expression tag	UNP O15111
C	7	PRO	-	expression tag	UNP O15111
C	8	GLU	-	expression tag	UNP O15111
C	9	PHE	-	expression tag	UNP O15111
C	176	GLU	SER	engineered mutation	UNP O15111
C	180	GLU	SER	engineered mutation	UNP O15111
C	268	ILE	VAL	variant	UNP O15111
D	6	ASP	-	expression tag	UNP O15111
D	7	PRO	-	expression tag	UNP O15111
D	8	GLU	-	expression tag	UNP O15111
D	9	PHE	-	expression tag	UNP O15111
D	176	GLU	SER	engineered mutation	UNP O15111
D	180	GLU	SER	engineered mutation	UNP O15111
D	268	ILE	VAL	variant	UNP O15111
E	6	ASP	-	expression tag	UNP O15111
E	7	PRO	-	expression tag	UNP O15111
E	8	GLU	-	expression tag	UNP O15111
E	9	PHE	-	expression tag	UNP O15111
E	176	GLU	SER	engineered mutation	UNP O15111
E	180	GLU	SER	engineered mutation	UNP O15111
E	268	ILE	VAL	variant	UNP O15111
F	6	ASP	-	expression tag	UNP O15111
F	7	PRO	-	expression tag	UNP O15111
F	8	GLU	-	expression tag	UNP O15111
F	9	PHE	-	expression tag	UNP O15111
F	176	GLU	SER	engineered mutation	UNP O15111
F	180	GLU	SER	engineered mutation	UNP O15111
F	268	ILE	VAL	variant	UNP O15111
G	6	ASP	-	expression tag	UNP O15111
G	7	PRO	-	expression tag	UNP O15111
G	8	GLU	-	expression tag	UNP O15111
G	9	PHE	-	expression tag	UNP O15111
G	176	GLU	SER	engineered mutation	UNP O15111

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Chain	Residue	Modelled	Actual	Comment	Reference
G	180	GLU	SER	engineered mutation	UNP O15111
G	268	ILE	VAL	variant	UNP O15111
H	6	ASP	-	expression tag	UNP O15111
H	7	PRO	-	expression tag	UNP O15111
H	8	GLU	-	expression tag	UNP O15111
H	9	PHE	-	expression tag	UNP O15111
H	176	GLU	SER	engineered mutation	UNP O15111
H	180	GLU	SER	engineered mutation	UNP O15111
H	268	ILE	VAL	variant	UNP O15111
I	6	ASP	-	expression tag	UNP O15111
I	7	PRO	-	expression tag	UNP O15111
I	8	GLU	-	expression tag	UNP O15111
I	9	PHE	-	expression tag	UNP O15111
I	176	GLU	SER	engineered mutation	UNP O15111
I	180	GLU	SER	engineered mutation	UNP O15111
I	268	ILE	VAL	variant	UNP O15111
J	6	ASP	-	expression tag	UNP O15111
J	7	PRO	-	expression tag	UNP O15111
J	8	GLU	-	expression tag	UNP O15111
J	9	PHE	-	expression tag	UNP O15111
J	176	GLU	SER	engineered mutation	UNP O15111
J	180	GLU	SER	engineered mutation	UNP O15111
J	268	ILE	VAL	variant	UNP O15111
K	6	ASP	-	expression tag	UNP O15111
K	7	PRO	-	expression tag	UNP O15111
K	8	GLU	-	expression tag	UNP O15111
K	9	PHE	-	expression tag	UNP O15111
K	176	GLU	SER	engineered mutation	UNP O15111
K	180	GLU	SER	engineered mutation	UNP O15111
K	268	ILE	VAL	variant	UNP O15111
L	6	ASP	-	expression tag	UNP O15111
L	7	PRO	-	expression tag	UNP O15111
L	8	GLU	-	expression tag	UNP O15111
L	9	PHE	-	expression tag	UNP O15111
L	176	GLU	SER	engineered mutation	UNP O15111
L	180	GLU	SER	engineered mutation	UNP O15111
L	268	ILE	VAL	variant	UNP O15111

- Molecule 2 is an oligosaccharide called 2,3-di-O-sulfo- α -D-glucopyranose-(1-6)- α -D-glucopyranose-(1-6)-2,4-di-O-sulfo- α -D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	N	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	P	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	Q	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	R	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	S	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	U	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	V	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	W	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	X	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	Y	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	Z	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	a	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	b	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	d	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	e	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	f	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	g	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	h	3	Total	C	O	S	0	0	0
			50	18	28	4			

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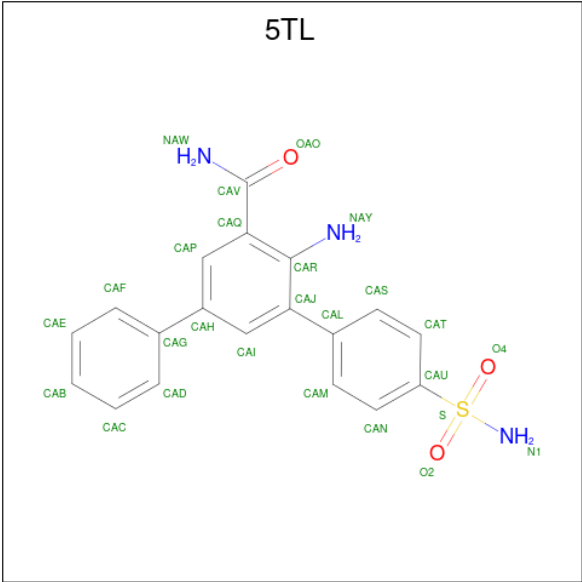
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	j	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	k	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	l	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	m	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	n	3	Total	C	O	S	0	0	0
			50	18	28	4			

- Molecule 3 is an oligosaccharide called [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	O	7	Total	C	O	S	0	0	0
			116	42	62	12			
3	T	7	Total	C	O	S	0	0	0
			116	42	62	12			
3	c	7	Total	C	O	S	0	0	0
			116	42	62	12			
3	i	7	Total	C	O	S	0	0	0
			116	42	62	12			

- Molecule 4 is 2-azanyl-5-phenyl-3-(4-sulfamoylphenyl)benzamide (CCD ID: 5TL) (formula: C₁₉H₁₇N₃O₃S).

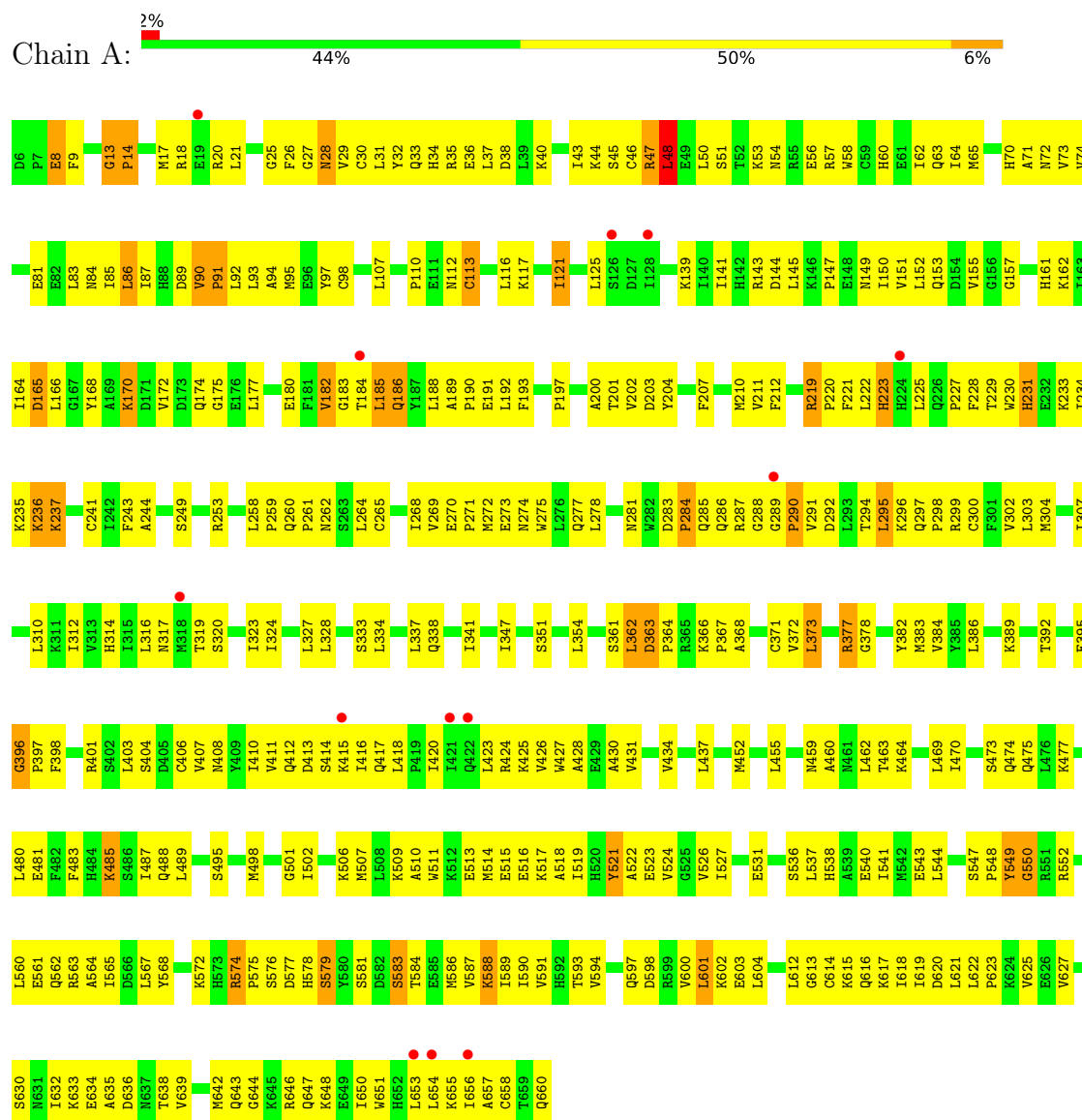


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	C	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	D	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	F	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	G	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	H	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	I	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	J	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	K	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	L	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

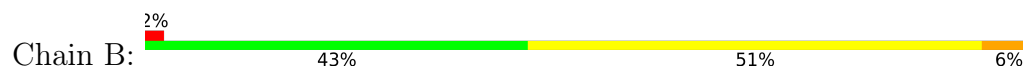
3 Residue-property plots

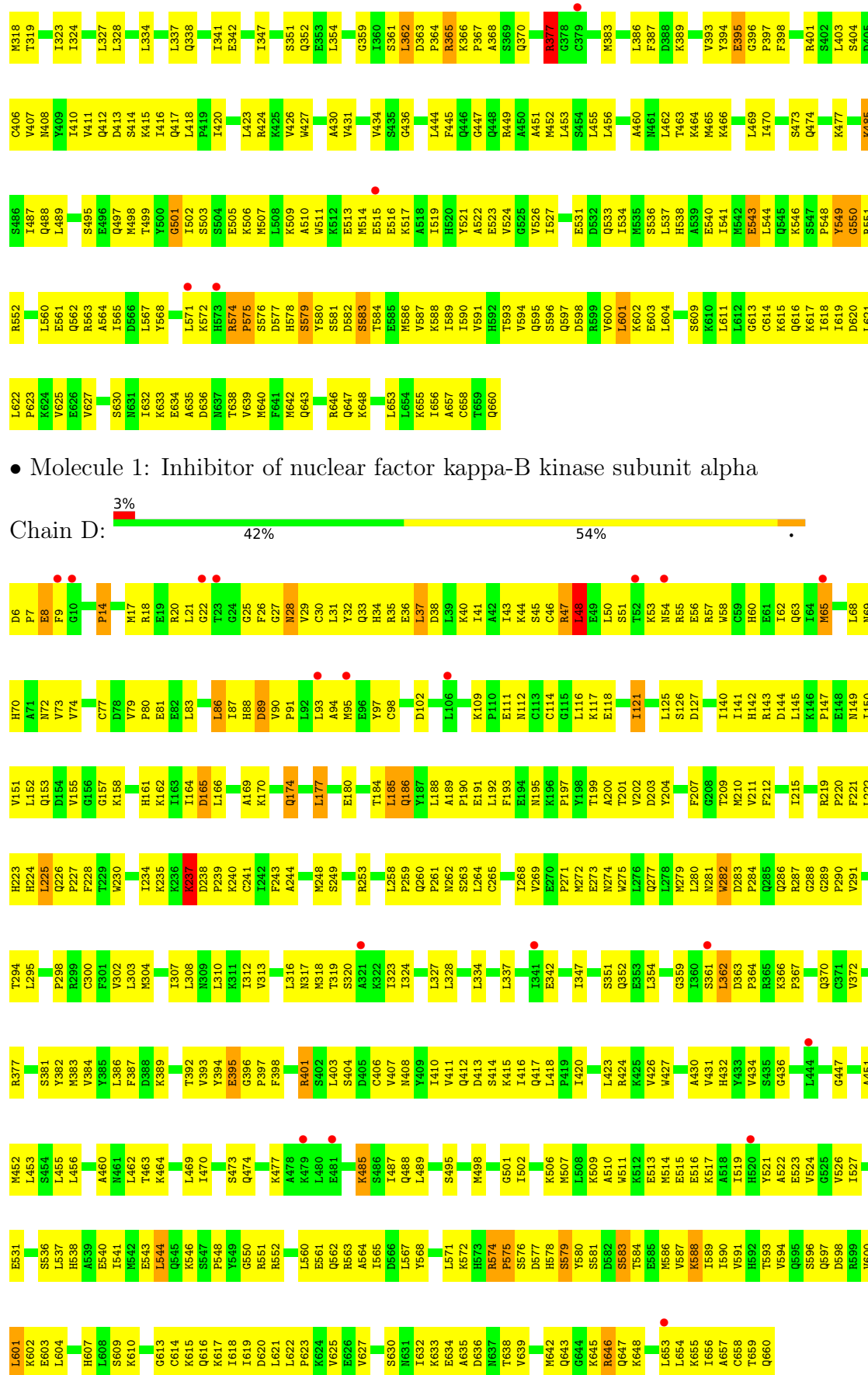
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Inhibitor of nuclear factor kappa-B kinase subunit alpha

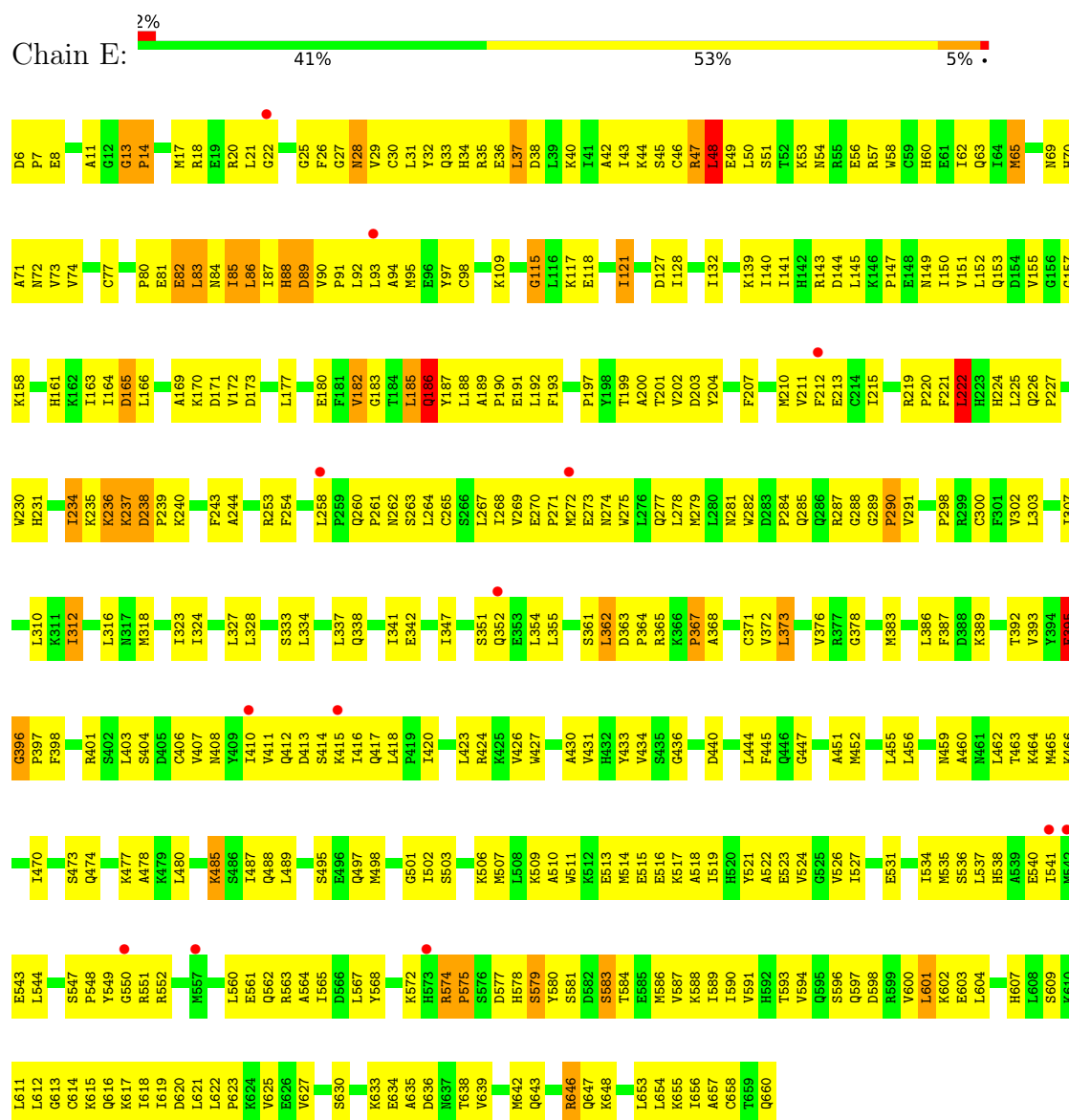


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

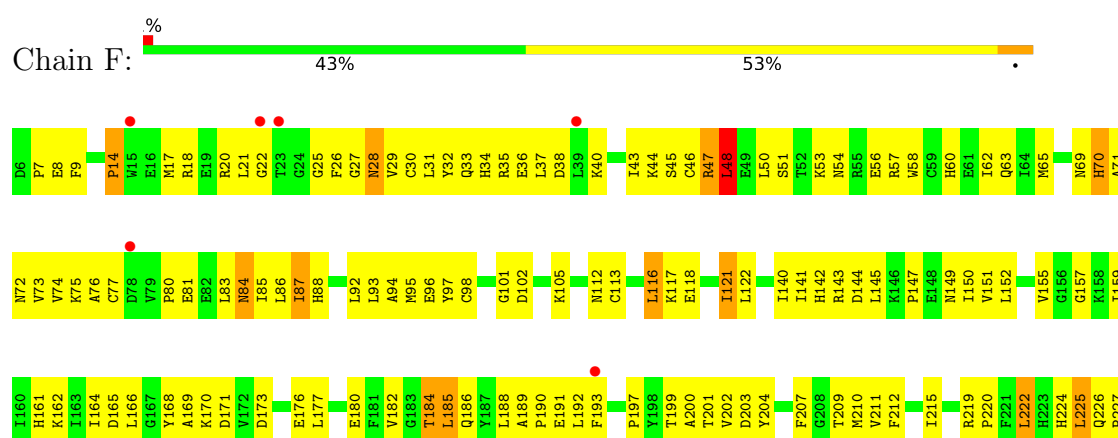


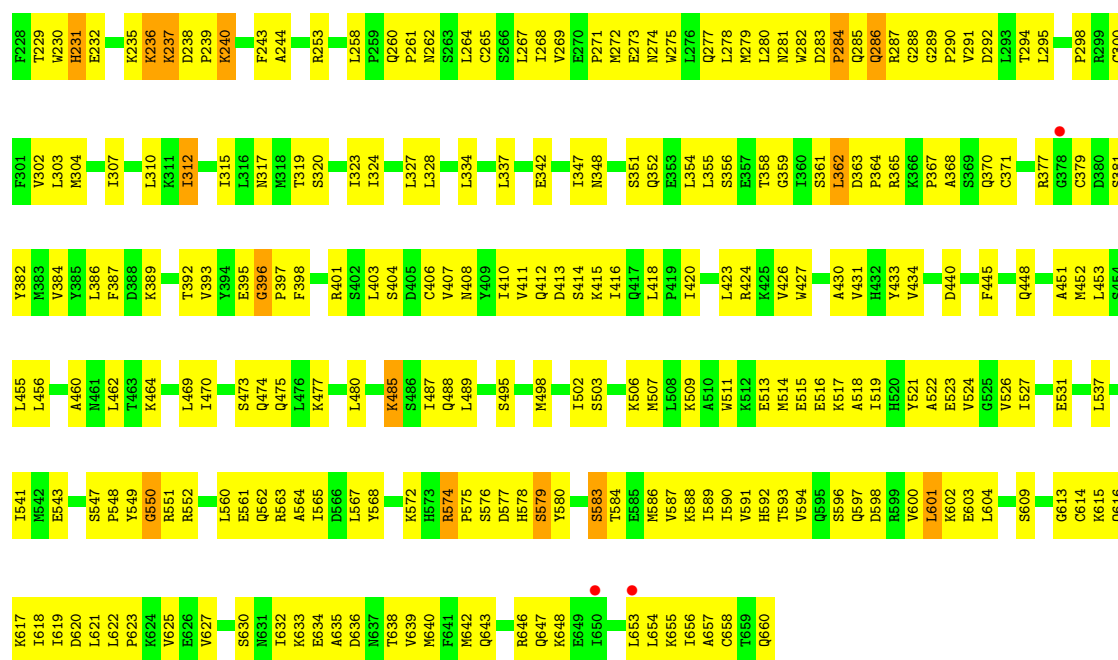


• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

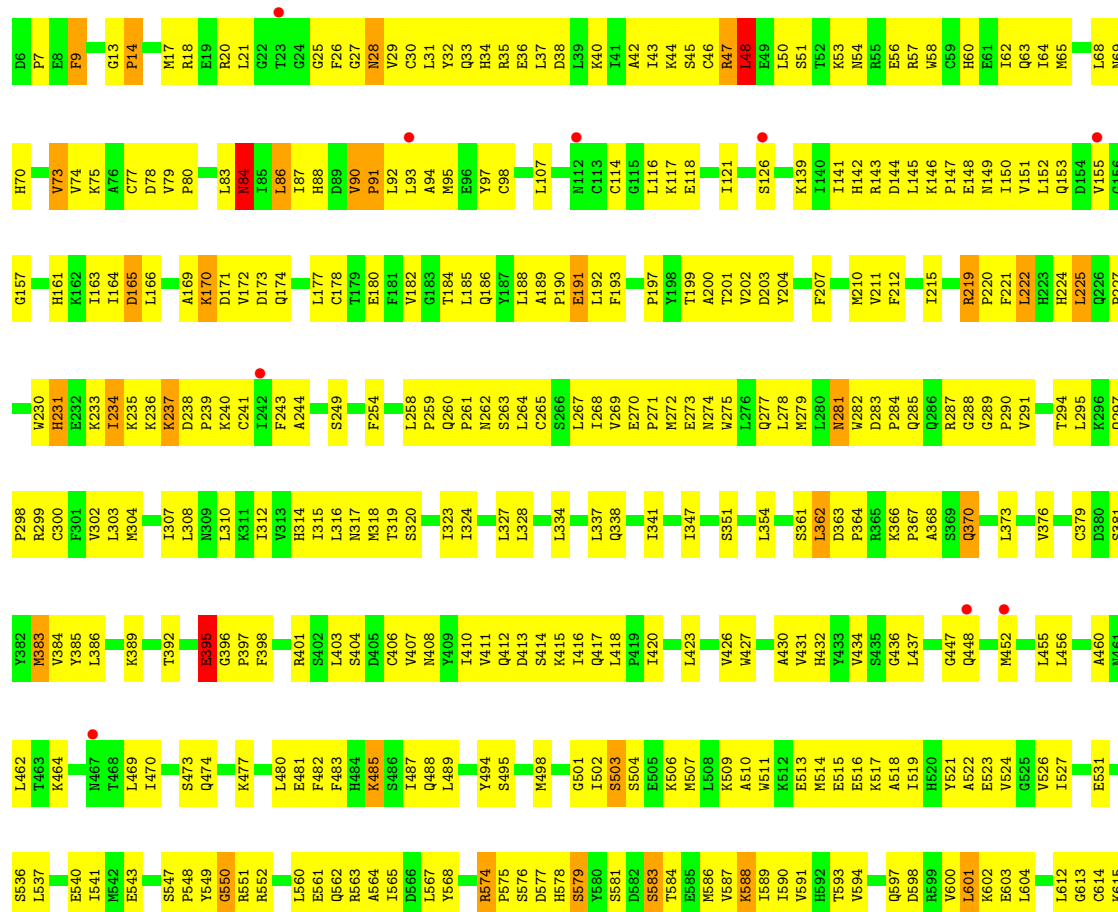
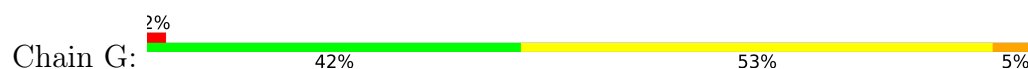


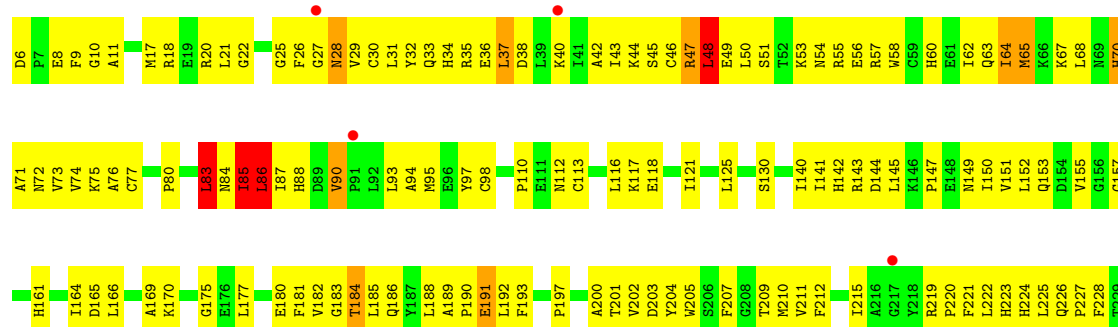
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



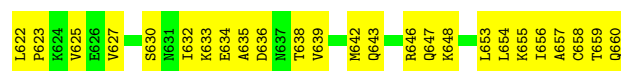


● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

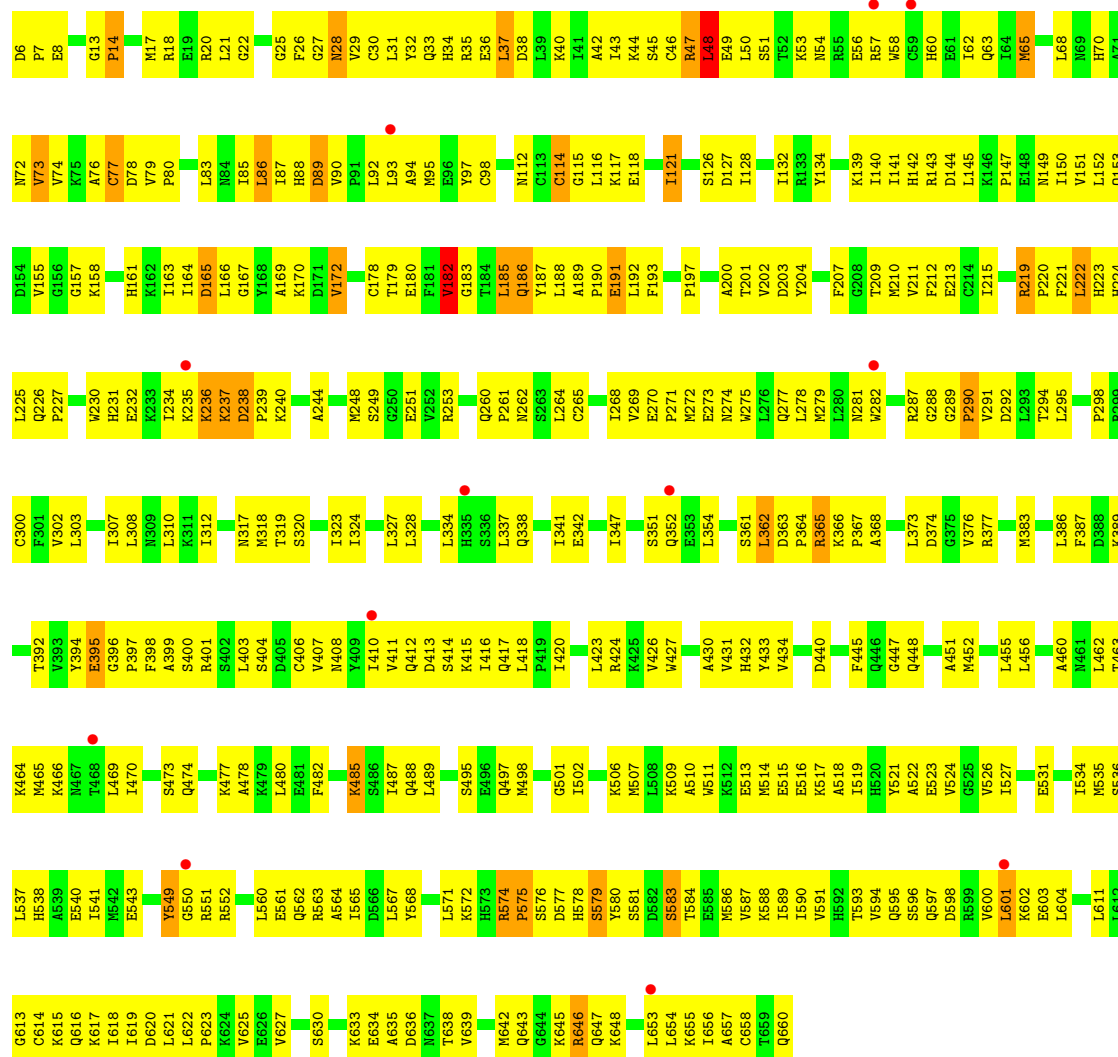




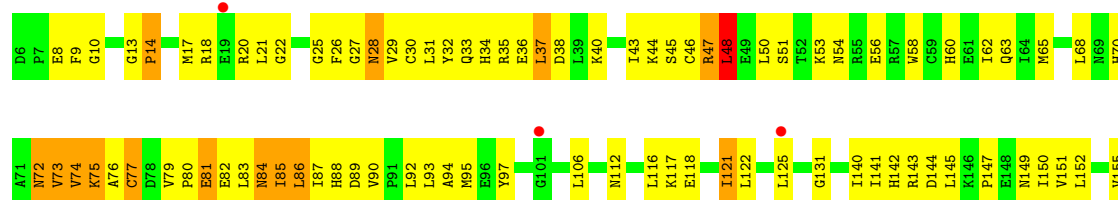


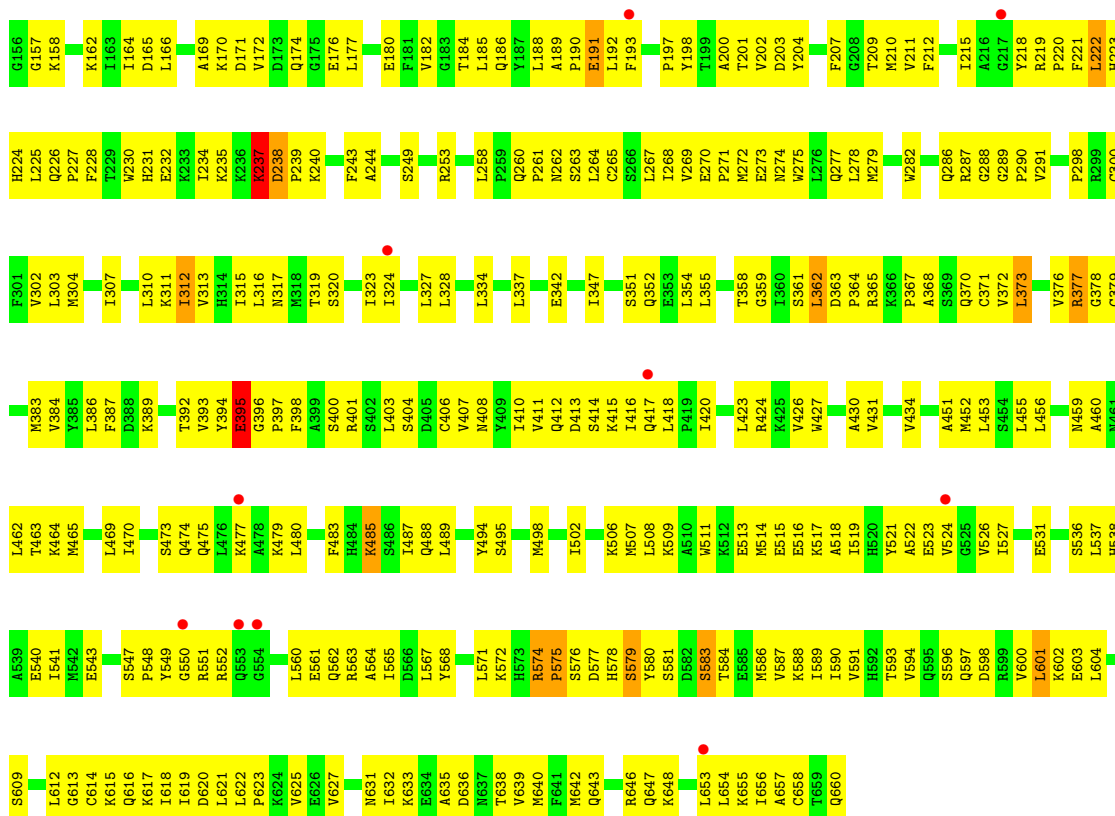


• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha





- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain M:



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain N:

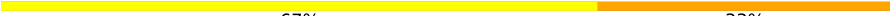


- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain P:



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain Q:  67% 33%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain R:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain S:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain U:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain V:  33% 33% 33%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain W:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain X:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain Y:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain Z:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain a:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain b:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain d:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain e:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain f:  33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain g: 33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain h: 100%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain j: 100%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain k: 33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain l: 33% 33% 33%

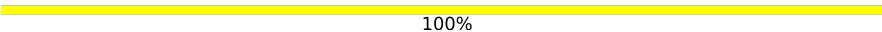


- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain m: 67% 33%

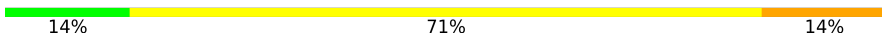


- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain n:  100%

5LS1
GLC2
PDX3

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain O:  14% 71% 14%

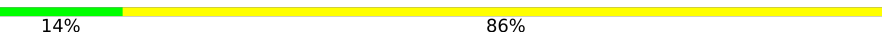
5LS1
5TJ2
5TM3
5TJ4
24K5
5TK6
5TH7

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain T:  43% 57%

5LS1
5TJ2
5TM3
5TJ4
24K5
5TK6
5TH7

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain c:  14% 86%

5LS1
5TJ2
5TM3
5TJ4
24K5
5TK6
5TH7

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-b

is(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain i:

14%

86%

5LS1	5LJ2	5TH3	5LJ4	24K5	5TH6	5TH7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	174.51Å 186.94Å 275.83Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	29.94 – 4.50 29.94 – 4.50	Depositor EDS
% Data completeness (in resolution range)	68.1 (29.94-4.50) 82.6 (29.94-4.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.238 , 0.276 0.241 , 0.280	Depositor DCC
R_{free} test set	4167 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	178.9	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 444.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	65132	wwPDB-VP
Average B, all atoms (Å ²)	267.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5998e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5TJ, Z4K, 5TK, PDX, 5TH, 5TM, 5LS, 5TL, GLC

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	0.34	0/5370	0.73	2/7239 (0.0%)
1	B	0.30	0/5370	0.73	0/7239
1	C	0.31	0/5370	0.72	0/7239
1	D	0.30	0/5370	0.74	0/7239
1	E	0.33	0/5370	0.72	1/7239 (0.0%)
1	F	0.30	0/5370	0.74	1/7239 (0.0%)
1	G	0.35	0/5370	0.72	0/7239
1	H	0.30	0/5370	0.72	0/7239
1	I	0.31	0/5370	0.73	1/7239 (0.0%)
1	J	0.30	0/5370	0.73	1/7239 (0.0%)
1	K	0.32	0/5370	0.72	1/7239 (0.0%)
1	L	0.30	0/5370	0.72	0/7239
All	All	0.31	0/64440	0.73	7/86868 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ASP	CA-C-N	6.10	125.58	119.24
1	A	363	ASP	C-N-CA	6.10	125.58	119.24
1	E	8	GLU	CB-CA-C	-5.85	109.85	116.63
1	I	86	LEU	CB-CA-C	-5.61	109.12	115.79
1	J	234	ILE	N-CA-C	-5.29	107.56	112.43

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	5263	0	5320	370	0
1	B	5263	0	5320	371	0
1	C	5263	0	5320	350	0
1	D	5263	0	5320	360	0
1	E	5263	0	5320	359	0
1	F	5263	0	5320	337	0
1	G	5263	0	5320	389	0
1	H	5263	0	5320	345	0
1	I	5263	0	5320	341	0
1	J	5263	0	5320	343	0
1	K	5263	0	5320	364	0
1	L	5263	0	5320	363	0
2	M	50	0	19	0	0
2	N	50	0	19	1	0
2	P	50	0	19	1	0
2	Q	50	0	19	4	0
2	R	50	0	19	1	0
2	S	50	0	19	3	0
2	U	50	0	19	0	0
2	V	50	0	19	1	0
2	W	50	0	19	1	0
2	X	50	0	19	1	0
2	Y	50	0	19	2	0
2	Z	50	0	19	1	0
2	a	50	0	19	0	0
2	b	50	0	19	1	0
2	d	50	0	19	1	0
2	e	50	0	19	1	0
2	f	50	0	19	0	0
2	g	50	0	19	0	0
2	h	50	0	19	4	0
2	j	50	0	19	6	0
2	k	50	0	19	0	0
2	l	50	0	19	1	0
2	m	50	0	19	2	0
2	n	50	0	19	2	0
3	O	116	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	116	0	0	5	0
3	c	116	0	0	0	0
3	i	116	0	0	0	0
4	A	26	0	0	3	0
4	B	26	0	0	2	0
4	C	26	0	0	4	0
4	D	26	0	0	2	0
4	E	26	0	0	3	0
4	F	26	0	0	6	0
4	G	26	0	0	4	0
4	H	26	0	0	2	0
4	I	26	0	0	6	0
4	J	26	0	0	2	0
4	K	26	0	0	3	0
4	L	26	0	0	2	0
All	All	65132	0	64296	4141	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 32.

The worst 5 of 4141 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)
4:J:701:5TL:NAY	4:J:701:5TL:CAS	1.99	1.20
4:G:701:5TL:NAY	4:G:701:5TL:CAS	2.00	1.18
4:D:701:5TL:NAY	4:D:701:5TL:CAS	1.99	1.17
4:K:701:5TL:CAS	4:K:701:5TL:NAY	2.00	1.17
4:A:701:5TL:NAY	4:A:701:5TL:CAS	2.00	1.16

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 X-ray entries followed by that with respect to entries of similar resolution.

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	653/655 (100%)	504 (77%)	113 (17%)	36 (6%)	1	15
1	B	653/655 (100%)	514 (79%)	106 (16%)	33 (5%)	1	15
1	C	653/655 (100%)	511 (78%)	105 (16%)	37 (6%)	1	14
1	D	653/655 (100%)	515 (79%)	104 (16%)	34 (5%)	1	15
1	E	653/655 (100%)	511 (78%)	104 (16%)	38 (6%)	1	14
1	F	653/655 (100%)	505 (77%)	111 (17%)	37 (6%)	1	14
1	G	653/655 (100%)	508 (78%)	114 (18%)	31 (5%)	2	17
1	H	653/655 (100%)	507 (78%)	99 (15%)	47 (7%)	1	11
1	I	653/655 (100%)	502 (77%)	110 (17%)	41 (6%)	1	13
1	J	653/655 (100%)	515 (79%)	98 (15%)	40 (6%)	1	13
1	K	653/655 (100%)	506 (78%)	105 (16%)	42 (6%)	1	13
1	L	653/655 (100%)	500 (77%)	113 (17%)	40 (6%)	1	13
All	All	7836/7860 (100%)	6098 (78%)	1282 (16%)	456 (6%)	1	14

5 of 456 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	521	TYR
1	A	549	TYR
1	B	48	LEU
1	B	173	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	589/589 (100%)	564 (96%)	25 (4%)	26	48
1	B	589/589 (100%)	562 (95%)	27 (5%)	24	46
1	C	589/589 (100%)	568 (96%)	21 (4%)	31	52
1	D	589/589 (100%)	573 (97%)	16 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	589/589 (100%)	566 (96%)	23 (4%)	28	50
1	F	589/589 (100%)	567 (96%)	22 (4%)	30	51
1	G	589/589 (100%)	561 (95%)	28 (5%)	23	45
1	H	589/589 (100%)	565 (96%)	24 (4%)	27	49
1	I	589/589 (100%)	570 (97%)	19 (3%)	34	55
1	J	589/589 (100%)	569 (97%)	20 (3%)	32	54
1	K	589/589 (100%)	570 (97%)	19 (3%)	34	55
1	L	589/589 (100%)	564 (96%)	25 (4%)	26	48
All	All	7068/7068 (100%)	6799 (96%)	269 (4%)	29	51

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	185	LEU
1	K	395	GLU
1	L	373	LEU
1	E	185	LEU
1	E	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 340 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	262	ASN
1	K	28	ASN
1	I	352	GLN
1	J	112	ASN
1	K	488	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

100 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	5LS	M	1	2	20,20,20	1.34	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	M	2	2	11,11,12	0.58	0	15,15,17	0.37	0
2	PDX	M	3	2	19,19,20	1.36	2 (10%)	22,29,31	1.02	2 (9%)
2	5LS	N	1	2	20,20,20	1.27	1 (5%)	25,31,31	0.96	2 (8%)
2	GLC	N	2	2	11,11,12	0.85	0	15,15,17	0.99	1 (6%)
2	PDX	N	3	2	19,19,20	1.31	2 (10%)	22,29,31	1.02	2 (9%)
3	5LS	O	1	3	20,20,20	1.08	0	25,31,31	1.01	2 (8%)
3	5TJ	O	2	3	14,17,18	0.98	0	19,24,26	0.93	2 (10%)
3	5TM	O	3	3	14,17,18	1.21	1 (7%)	18,24,26	0.88	1 (5%)
3	5TJ	O	4	3	14,17,18	1.00	0	19,24,26	0.75	1 (5%)
3	Z4K	O	5	3	15,15,16	1.20	1 (6%)	17,22,24	0.76	0
3	5TK	O	6	3	10,13,14	0.60	0	15,17,19	0.36	0
3	5TH	O	7	3	14,17,18	1.40	2 (14%)	17,24,26	0.71	1 (5%)
2	5LS	P	1	2	20,20,20	1.22	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	P	2	2	11,11,12	0.67	0	15,15,17	0.40	0
2	PDX	P	3	2	19,19,20	1.25	2 (10%)	22,29,31	0.95	1 (4%)
2	5LS	Q	1	2	20,20,20	1.18	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	Q	2	2	11,11,12	0.58	0	15,15,17	0.34	0
2	PDX	Q	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.06	3 (13%)
2	5LS	R	1	2	20,20,20	1.28	1 (5%)	25,31,31	0.96	2 (8%)
2	GLC	R	2	2	11,11,12	0.54	0	15,15,17	0.34	0
2	PDX	R	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.05	2 (9%)
2	5LS	S	1	2	20,20,20	1.40	1 (5%)	25,31,31	0.85	1 (4%)
2	GLC	S	2	2	11,11,12	0.49	0	15,15,17	0.37	0
2	PDX	S	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.07	2 (9%)
3	5LS	T	1	3	20,20,20	1.30	1 (5%)	25,31,31	0.97	2 (8%)
3	5TJ	T	2	3	14,17,18	0.96	0	19,24,26	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5TM	T	3	3	14,17,18	1.15	1 (7%)	18,24,26	0.93	1 (5%)
3	5TJ	T	4	3	14,17,18	0.95	0	19,24,26	0.80	1 (5%)
3	Z4K	T	5	3	15,15,16	1.13	1 (6%)	17,22,24	0.73	1 (5%)
3	5TK	T	6	3	10,13,14	0.67	0	15,17,19	0.55	0
3	5TH	T	7	3	14,17,18	1.42	2 (14%)	17,24,26	0.84	1 (5%)
2	5LS	U	1	2	20,20,20	1.29	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	U	2	2	11,11,12	0.56	0	15,15,17	0.36	0
2	PDX	U	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.04	2 (9%)
2	5LS	V	1	2	20,20,20	1.16	1 (5%)	25,31,31	1.02	2 (8%)
2	GLC	V	2	2	11,11,12	0.60	0	15,15,17	0.47	0
2	PDX	V	3	2	19,19,20	1.34	2 (10%)	22,29,31	0.99	2 (9%)
2	5LS	W	1	2	20,20,20	1.25	1 (5%)	25,31,31	1.00	2 (8%)
2	GLC	W	2	2	11,11,12	0.62	0	15,15,17	0.50	0
2	PDX	W	3	2	19,19,20	1.44	2 (10%)	22,29,31	1.13	3 (13%)
2	5LS	X	1	2	20,20,20	1.28	1 (5%)	25,31,31	1.00	3 (12%)
2	GLC	X	2	2	11,11,12	0.66	0	15,15,17	0.62	0
2	PDX	X	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.04	2 (9%)
2	5LS	Y	1	2	20,20,20	1.37	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	Y	2	2	11,11,12	0.60	0	15,15,17	0.55	0
2	PDX	Y	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.02	2 (9%)
2	5LS	Z	1	2	20,20,20	1.22	1 (5%)	25,31,31	1.02	2 (8%)
2	GLC	Z	2	2	11,11,12	0.70	0	15,15,17	0.46	0
2	PDX	Z	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.00	2 (9%)
2	5LS	a	1	2	20,20,20	1.37	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	a	2	2	11,11,12	0.58	0	15,15,17	0.32	0
2	PDX	a	3	2	19,19,20	1.35	2 (10%)	22,29,31	1.05	2 (9%)
2	5LS	b	1	2	20,20,20	1.37	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	b	2	2	11,11,12	0.56	0	15,15,17	0.44	0
2	PDX	b	3	2	19,19,20	1.32	2 (10%)	22,29,31	1.03	2 (9%)
3	5LS	c	1	3	20,20,20	1.08	1 (5%)	25,31,31	0.99	2 (8%)
3	5TJ	c	2	3	14,17,18	0.97	0	19,24,26	0.76	1 (5%)
3	5TM	c	3	3	14,17,18	1.26	2 (14%)	18,24,26	0.98	1 (5%)
3	5TJ	c	4	3	14,17,18	1.00	0	19,24,26	0.79	1 (5%)
3	Z4K	c	5	3	15,15,16	1.17	1 (6%)	17,22,24	0.71	1 (5%)
3	5TK	c	6	3	10,13,14	0.66	0	15,17,19	0.36	0
3	5TH	c	7	3	14,17,18	1.29	2 (14%)	17,24,26	0.79	1 (5%)
2	5LS	d	1	2	20,20,20	1.32	1 (5%)	25,31,31	1.00	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	d	2	2	11,11,12	0.79	0	15,15,17	0.42	0
2	PDX	d	3	2	19,19,20	1.39	2 (10%)	22,29,31	1.01	2 (9%)
2	5LS	e	1	2	20,20,20	1.29	1 (5%)	25,31,31	0.97	2 (8%)
2	GLC	e	2	2	11,11,12	0.80	0	15,15,17	1.08	1 (6%)
2	PDX	e	3	2	19,19,20	1.36	2 (10%)	22,29,31	1.03	2 (9%)
2	5LS	f	1	2	20,20,20	1.35	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	f	2	2	11,11,12	0.68	0	15,15,17	0.35	0
2	PDX	f	3	2	19,19,20	1.49	2 (10%)	22,29,31	1.23	3 (13%)
2	5LS	g	1	2	20,20,20	1.06	0	25,31,31	1.01	3 (12%)
2	GLC	g	2	2	11,11,12	0.67	0	15,15,17	0.53	0
2	PDX	g	3	2	19,19,20	1.39	2 (10%)	22,29,31	1.03	3 (13%)
2	5LS	h	1	2	20,20,20	1.28	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	h	2	2	11,11,12	0.61	0	15,15,17	0.47	0
2	PDX	h	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.01	2 (9%)
3	5LS	i	1	3	20,20,20	1.23	1 (5%)	25,31,31	0.97	2 (8%)
3	5TJ	i	2	3	14,17,18	0.97	0	19,24,26	0.83	1 (5%)
3	5TM	i	3	3	14,17,18	1.22	1 (7%)	18,24,26	0.89	1 (5%)
3	5TJ	i	4	3	14,17,18	0.97	0	19,24,26	0.84	1 (5%)
3	Z4K	i	5	3	15,15,16	1.22	1 (6%)	17,22,24	0.67	0
3	5TK	i	6	3	10,13,14	0.56	0	15,17,19	0.34	0
3	5TH	i	7	3	14,17,18	1.36	2 (14%)	17,24,26	0.76	0
2	5LS	j	1	2	20,20,20	1.08	0	25,31,31	1.00	3 (12%)
2	GLC	j	2	2	11,11,12	0.93	0	15,15,17	1.04	2 (13%)
2	PDX	j	3	2	19,19,20	1.41	2 (10%)	22,29,31	1.22	3 (13%)
2	5LS	k	1	2	20,20,20	1.27	1 (5%)	25,31,31	0.97	2 (8%)
2	GLC	k	2	2	11,11,12	0.61	0	15,15,17	0.33	0
2	PDX	k	3	2	19,19,20	1.39	2 (10%)	22,29,31	1.00	2 (9%)
2	5LS	l	1	2	20,20,20	1.14	1 (5%)	25,31,31	0.89	1 (4%)
2	GLC	l	2	2	11,11,12	0.55	0	15,15,17	0.44	0
2	PDX	l	3	2	19,19,20	1.36	2 (10%)	22,29,31	1.03	2 (9%)
2	5LS	m	1	2	20,20,20	1.32	1 (5%)	25,31,31	0.93	2 (8%)
2	GLC	m	2	2	11,11,12	0.64	0	15,15,17	0.43	0
2	PDX	m	3	2	19,19,20	1.43	2 (10%)	22,29,31	1.16	3 (13%)
2	5LS	n	1	2	20,20,20	1.23	1 (5%)	25,31,31	1.52	3 (12%)
2	GLC	n	2	2	11,11,12	0.58	0	15,15,17	0.46	0
2	PDX	n	3	2	19,19,20	1.36	2 (10%)	22,29,31	0.96	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5LS	M	1	2	-	2/12/32/32	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	PDX	M	3	2	-	0/12/29/32	0/1/1/1
2	5LS	N	1	2	-	2/12/32/32	0/1/1/1
2	GLC	N	2	2	-	2/2/19/22	0/1/1/1
2	PDX	N	3	2	-	1/12/29/32	0/1/1/1
3	5LS	O	1	3	-	0/12/32/32	0/1/1/1
3	5TJ	O	2	3	-	1/9/27/30	0/1/1/1
3	5TM	O	3	3	-	2/9/27/30	0/1/1/1
3	5TJ	O	4	3	-	2/9/27/30	0/1/1/1
3	Z4K	O	5	3	-	1/7/24/27	0/1/1/1
3	5TK	O	6	3	-	0/4/22/25	0/1/1/1
3	5TH	O	7	3	-	1/9/27/30	0/1/1/1
2	5LS	P	1	2	-	2/12/32/32	0/1/1/1
2	GLC	P	2	2	-	2/2/19/22	0/1/1/1
2	PDX	P	3	2	-	3/12/29/32	0/1/1/1
2	5LS	Q	1	2	-	2/12/32/32	0/1/1/1
2	GLC	Q	2	2	-	0/2/19/22	0/1/1/1
2	PDX	Q	3	2	-	0/12/29/32	0/1/1/1
2	5LS	R	1	2	-	0/12/32/32	0/1/1/1
2	GLC	R	2	2	-	0/2/19/22	0/1/1/1
2	PDX	R	3	2	-	2/12/29/32	0/1/1/1
2	5LS	S	1	2	-	2/12/32/32	0/1/1/1
2	GLC	S	2	2	-	0/2/19/22	0/1/1/1
2	PDX	S	3	2	-	0/12/29/32	0/1/1/1
3	5LS	T	1	3	-	0/12/32/32	0/1/1/1
3	5TJ	T	2	3	-	1/9/27/30	0/1/1/1
3	5TM	T	3	3	-	0/9/27/30	0/1/1/1
3	5TJ	T	4	3	-	0/9/27/30	0/1/1/1
3	Z4K	T	5	3	-	0/7/24/27	0/1/1/1
3	5TK	T	6	3	-	1/4/22/25	0/1/1/1
3	5TH	T	7	3	-	0/9/27/30	0/1/1/1
2	5LS	U	1	2	-	0/12/32/32	0/1/1/1
2	GLC	U	2	2	-	1/2/19/22	0/1/1/1
2	PDX	U	3	2	-	0/12/29/32	0/1/1/1
2	5LS	V	1	2	-	1/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	V	2	2	-	0/2/19/22	0/1/1/1
2	PDX	V	3	2	-	2/12/29/32	0/1/1/1
2	5LS	W	1	2	-	2/12/32/32	0/1/1/1
2	GLC	W	2	2	-	1/2/19/22	0/1/1/1
2	PDX	W	3	2	-	2/12/29/32	0/1/1/1
2	5LS	X	1	2	-	0/12/32/32	0/1/1/1
2	GLC	X	2	2	-	0/2/19/22	0/1/1/1
2	PDX	X	3	2	-	2/12/29/32	0/1/1/1
2	5LS	Y	1	2	-	0/12/32/32	0/1/1/1
2	GLC	Y	2	2	-	0/2/19/22	0/1/1/1
2	PDX	Y	3	2	-	1/12/29/32	0/1/1/1
2	5LS	Z	1	2	-	0/12/32/32	0/1/1/1
2	GLC	Z	2	2	-	2/2/19/22	0/1/1/1
2	PDX	Z	3	2	-	0/12/29/32	0/1/1/1
2	5LS	a	1	2	-	0/12/32/32	0/1/1/1
2	GLC	a	2	2	-	2/2/19/22	0/1/1/1
2	PDX	a	3	2	-	2/12/29/32	0/1/1/1
2	5LS	b	1	2	-	0/12/32/32	0/1/1/1
2	GLC	b	2	2	-	0/2/19/22	0/1/1/1
2	PDX	b	3	2	-	0/12/29/32	0/1/1/1
3	5LS	c	1	3	-	0/12/32/32	0/1/1/1
3	5TJ	c	2	3	-	3/9/27/30	0/1/1/1
3	5TM	c	3	3	-	2/9/27/30	0/1/1/1
3	5TJ	c	4	3	-	0/9/27/30	0/1/1/1
3	Z4K	c	5	3	-	1/7/24/27	0/1/1/1
3	5TK	c	6	3	-	2/4/22/25	0/1/1/1
3	5TH	c	7	3	-	4/9/27/30	0/1/1/1
2	5LS	d	1	2	-	0/12/32/32	0/1/1/1
2	GLC	d	2	2	-	0/2/19/22	0/1/1/1
2	PDX	d	3	2	-	0/12/29/32	0/1/1/1
2	5LS	e	1	2	-	1/12/32/32	0/1/1/1
2	GLC	e	2	2	-	1/2/19/22	0/1/1/1
2	PDX	e	3	2	-	2/12/29/32	0/1/1/1
2	5LS	f	1	2	-	0/12/32/32	0/1/1/1
2	GLC	f	2	2	-	2/2/19/22	0/1/1/1
2	PDX	f	3	2	-	0/12/29/32	0/1/1/1
2	5LS	g	1	2	-	0/12/32/32	0/1/1/1
2	GLC	g	2	2	-	0/2/19/22	0/1/1/1
2	PDX	g	3	2	-	2/12/29/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5LS	h	1	2	-	0/12/32/32	0/1/1/1
2	GLC	h	2	2	-	2/2/19/22	0/1/1/1
2	PDX	h	3	2	-	0/12/29/32	0/1/1/1
3	5LS	i	1	3	-	2/12/32/32	0/1/1/1
3	5TJ	i	2	3	-	1/9/27/30	0/1/1/1
3	5TM	i	3	3	-	2/9/27/30	0/1/1/1
3	5TJ	i	4	3	-	2/9/27/30	0/1/1/1
3	Z4K	i	5	3	-	2/7/24/27	0/1/1/1
3	5TK	i	6	3	-	0/4/22/25	0/1/1/1
3	5TH	i	7	3	-	2/9/27/30	0/1/1/1
2	5LS	j	1	2	-	2/12/32/32	0/1/1/1
2	GLC	j	2	2	-	2/2/19/22	0/1/1/1
2	PDX	j	3	2	-	1/12/29/32	0/1/1/1
2	5LS	k	1	2	-	2/12/32/32	0/1/1/1
2	GLC	k	2	2	-	0/2/19/22	0/1/1/1
2	PDX	k	3	2	-	0/12/29/32	0/1/1/1
2	5LS	l	1	2	-	3/12/32/32	0/1/1/1
2	GLC	l	2	2	-	0/2/19/22	0/1/1/1
2	PDX	l	3	2	-	0/12/29/32	0/1/1/1
2	5LS	m	1	2	-	1/12/32/32	0/1/1/1
2	GLC	m	2	2	-	2/2/19/22	0/1/1/1
2	PDX	m	3	2	-	0/12/29/32	0/1/1/1
2	5LS	n	1	2	-	2/12/32/32	0/1/1/1
2	GLC	n	2	2	-	2/2/19/22	0/1/1/1
2	PDX	n	3	2	-	2/12/29/32	0/1/1/1

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	5LS	C1-C2	4.65	1.56	1.52
2	b	1	5LS	C1-C2	4.15	1.56	1.52
2	a	1	5LS	C1-C2	4.11	1.56	1.52
2	Y	1	5LS	C1-C2	4.09	1.56	1.52
2	f	1	5LS	C1-C2	4.08	1.56	1.52

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	1	5LS	O2-C2-C1	6.16	115.86	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3	PDX	C1-C2-C3	3.53	114.69	109.40
3	c	3	5TM	O2-C2-C3	3.37	110.38	106.65
2	S	3	PDX	O2-C2-C3	3.33	110.34	106.65
2	U	3	PDX	O2-C2-C3	3.32	110.33	106.65

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	3	PDX	C2-C3-O3-S'
2	P	3	PDX	C4-C3-O3-S'
2	S	1	5LS	C3-C4-O4-S2
2	S	1	5LS	C5-C4-O4-S2
2	l	1	5LS	C3-C4-O4-S2

There are no ring outliers.

31 monomers are involved in 41 short contacts:

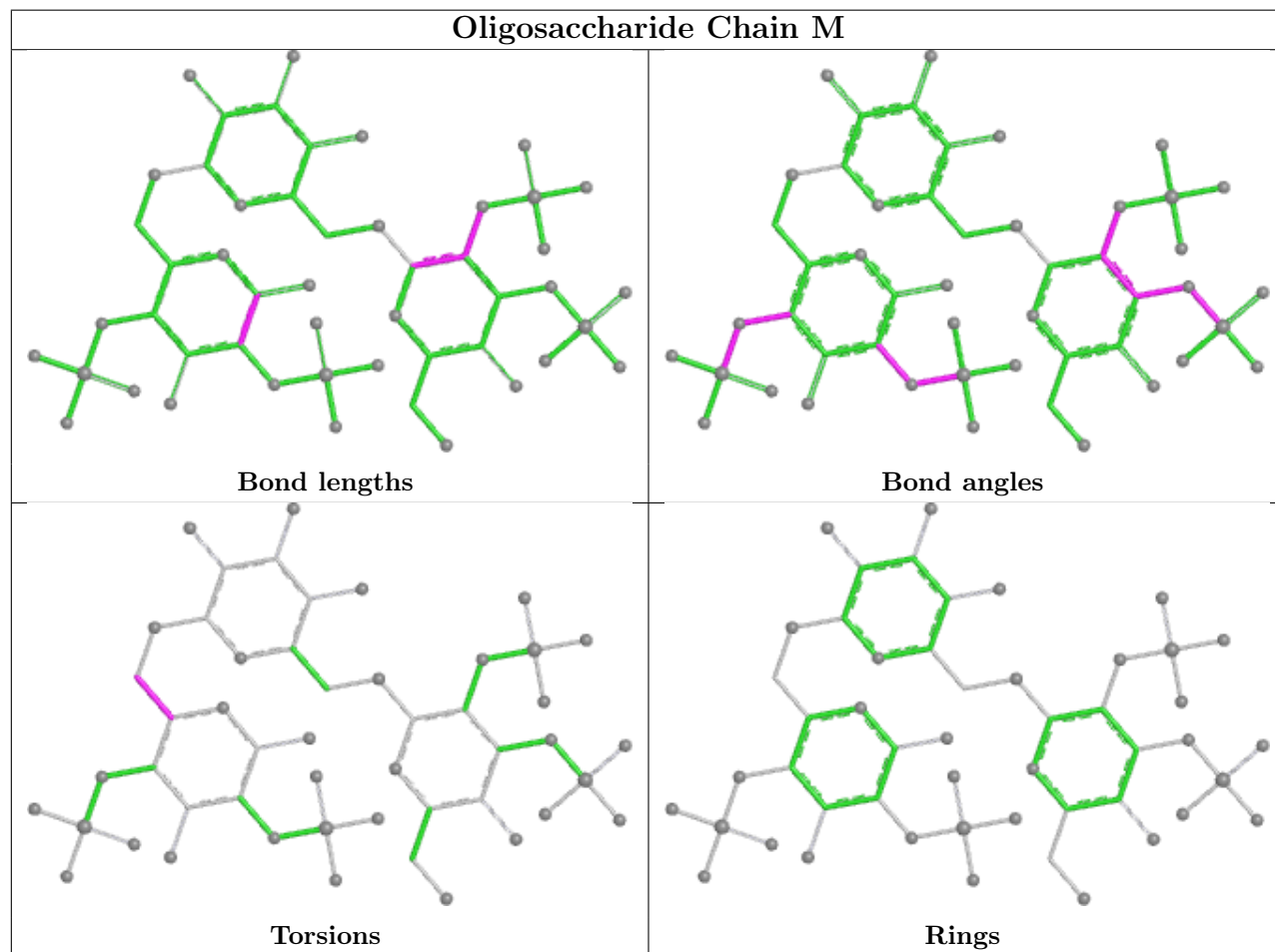
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	3	PDX	1	0
2	l	3	PDX	1	0
2	S	2	GLC	3	0
3	T	5	Z4K	2	0
3	T	6	5TK	1	0
2	Y	2	GLC	2	0
2	N	2	GLC	1	0
2	W	2	GLC	1	0
2	j	2	GLC	6	0
2	e	1	5LS	1	0
2	h	2	GLC	4	0
2	V	1	5LS	1	0
2	m	3	PDX	2	0
3	T	2	5TJ	1	0
2	Q	2	GLC	3	0
2	b	2	GLC	1	0
3	O	1	5LS	2	0
3	T	3	5TM	1	0
2	e	2	GLC	1	0
3	T	7	5TH	1	0
2	R	1	5LS	1	0
2	j	3	PDX	4	0

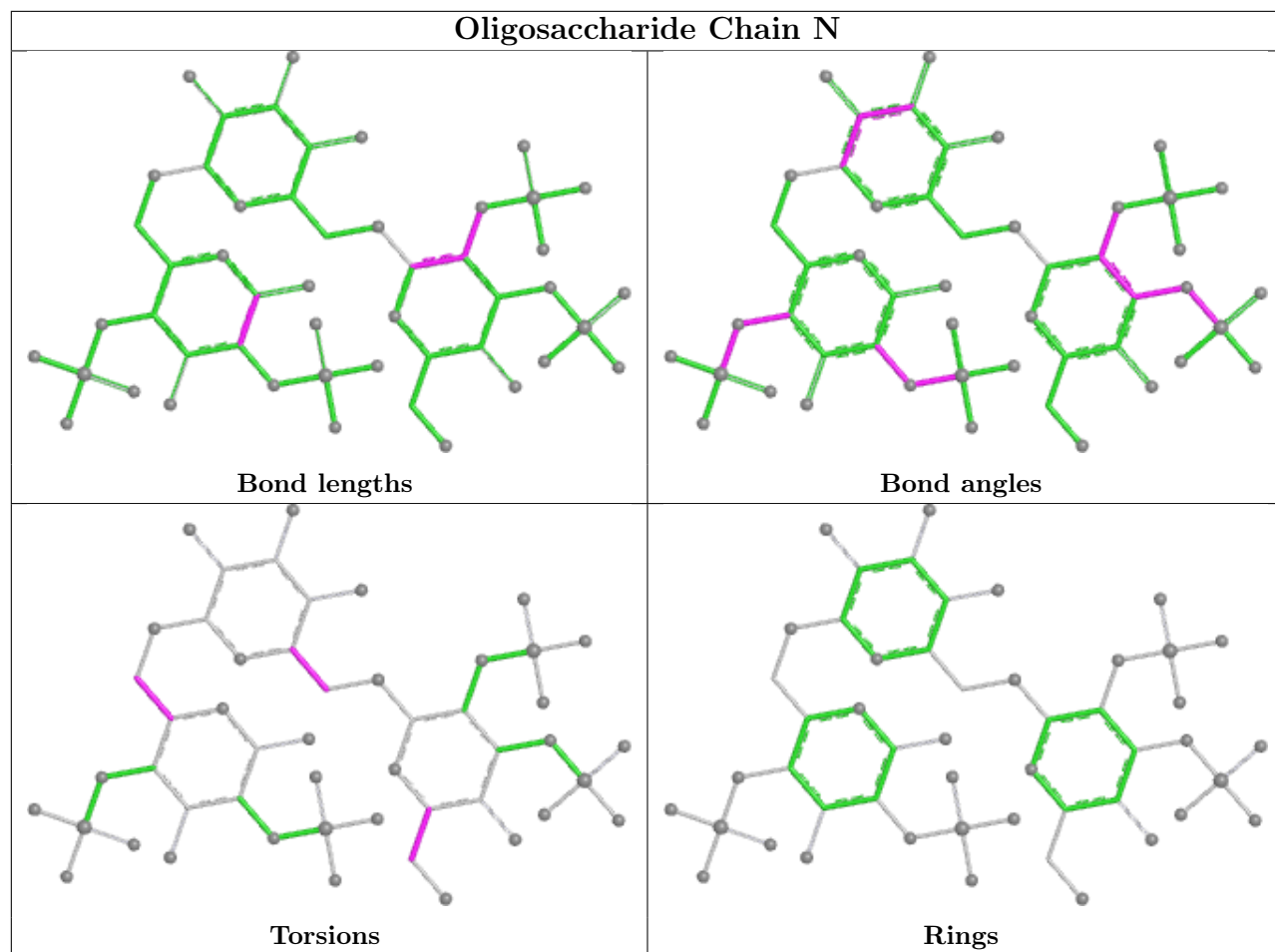
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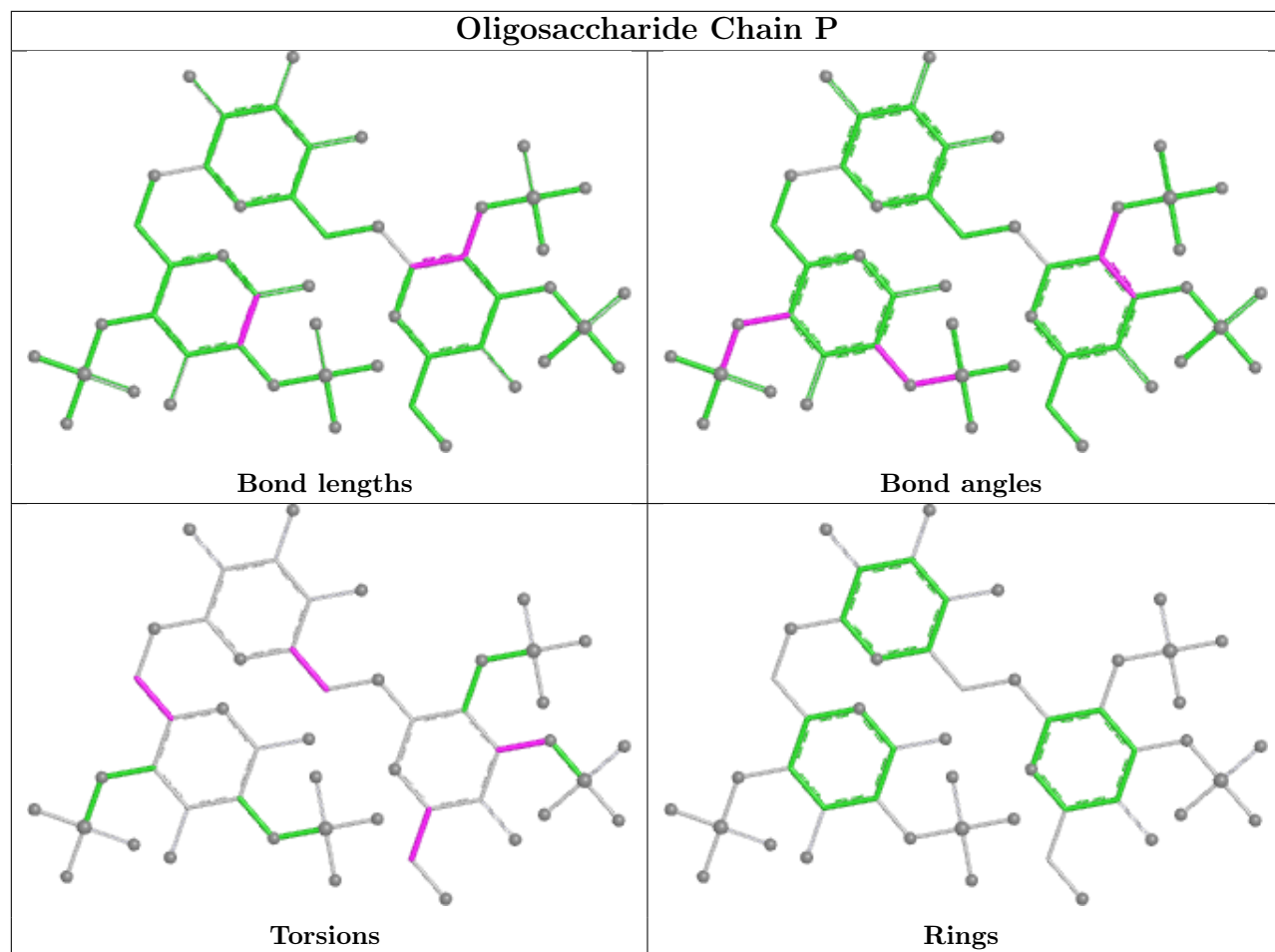
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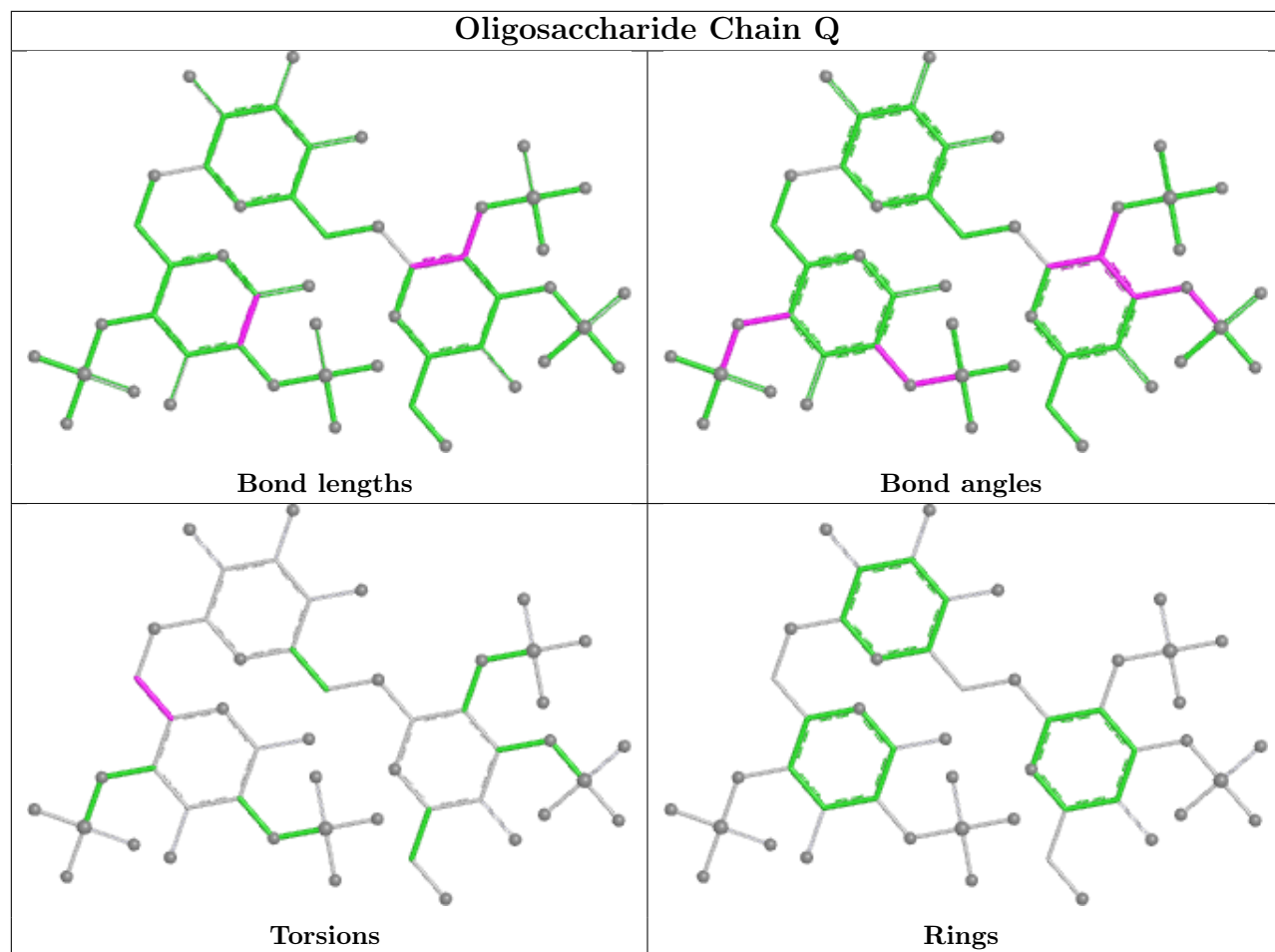
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	2	GLC	1	0
2	X	2	GLC	1	0
2	m	2	GLC	2	0
2	P	3	PDX	1	0
2	n	2	GLC	2	0
2	N	1	5LS	1	0
2	j	1	5LS	2	0
2	R	3	PDX	1	0
2	d	2	GLC	1	0

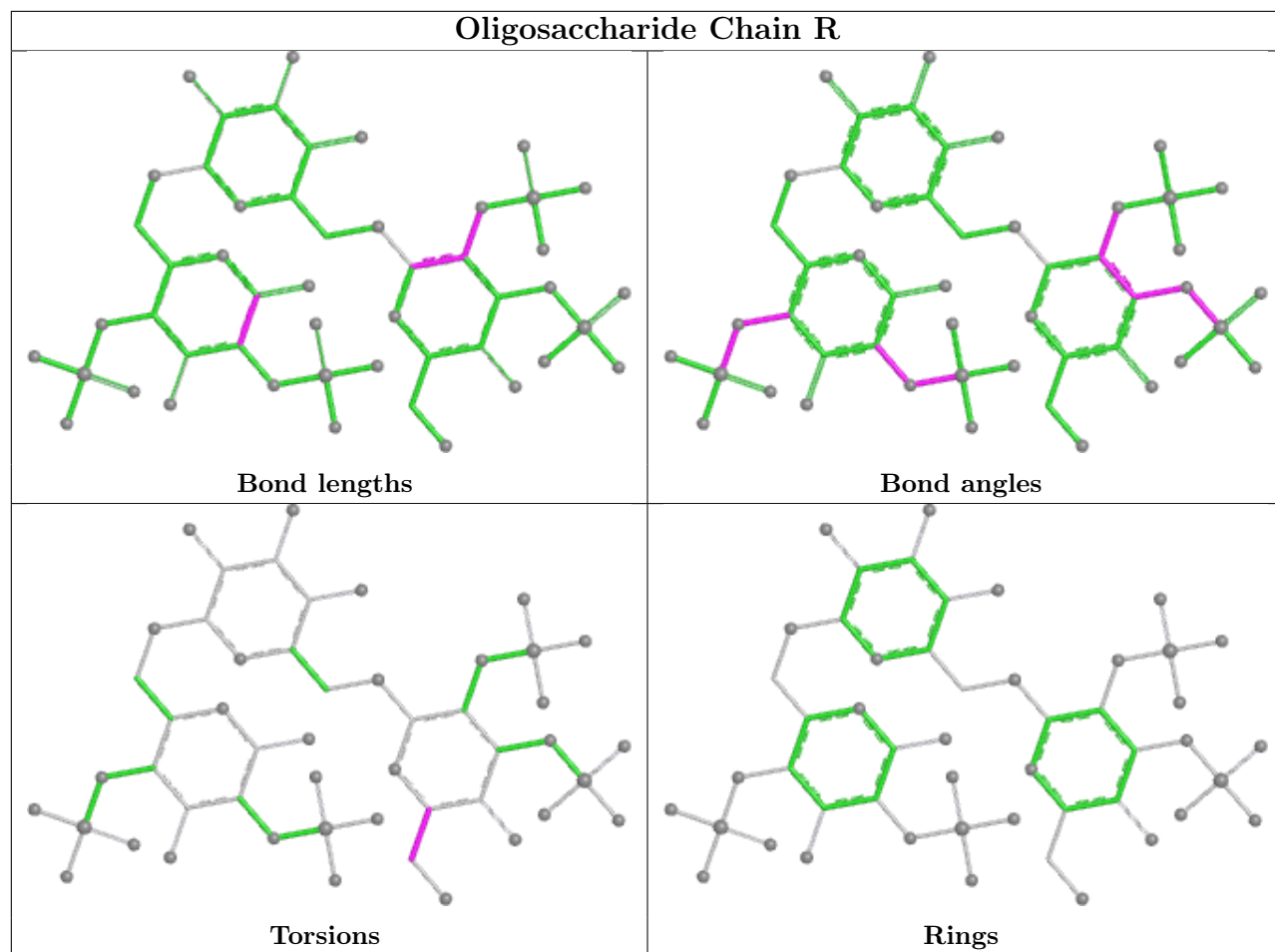
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

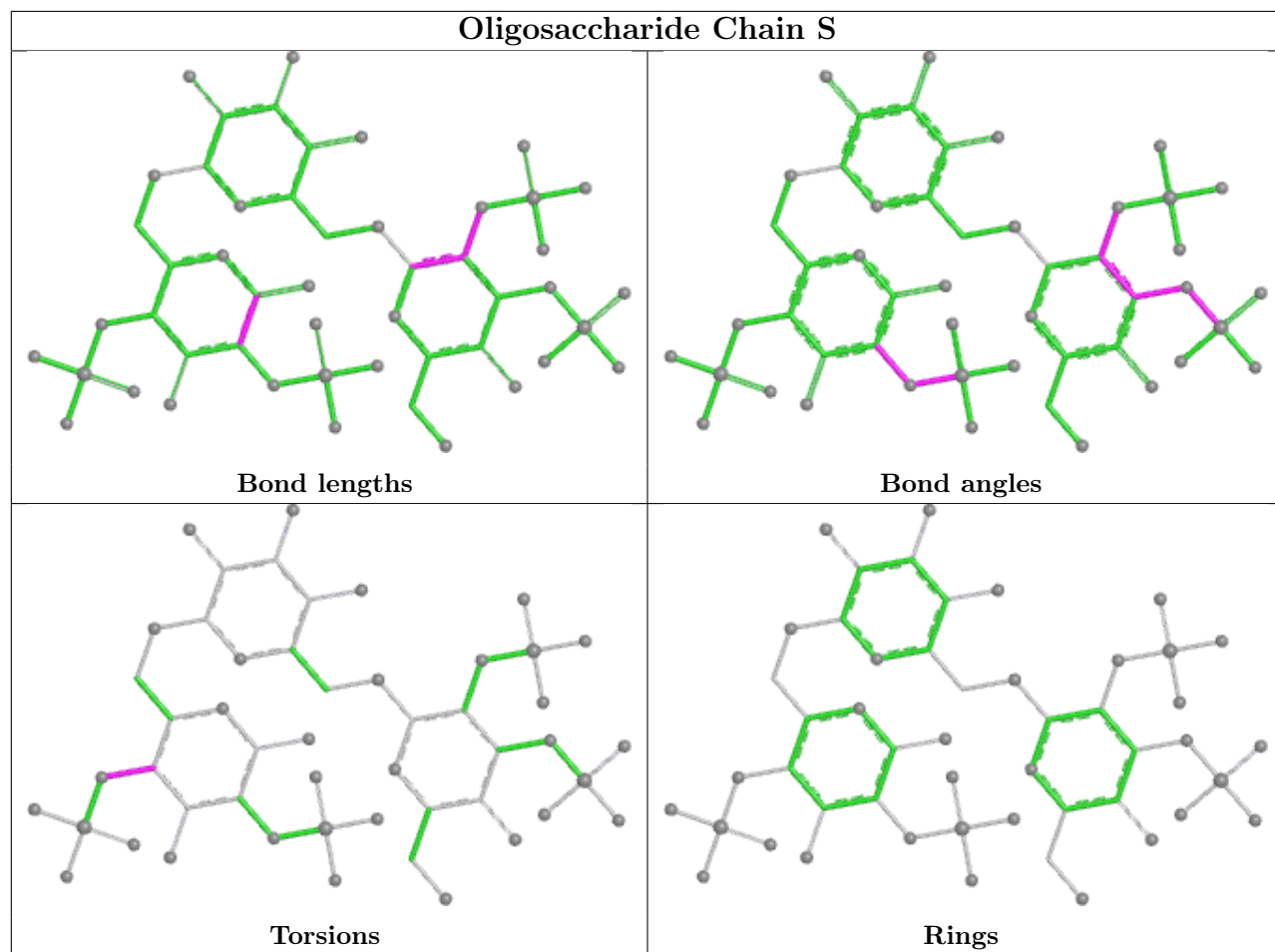


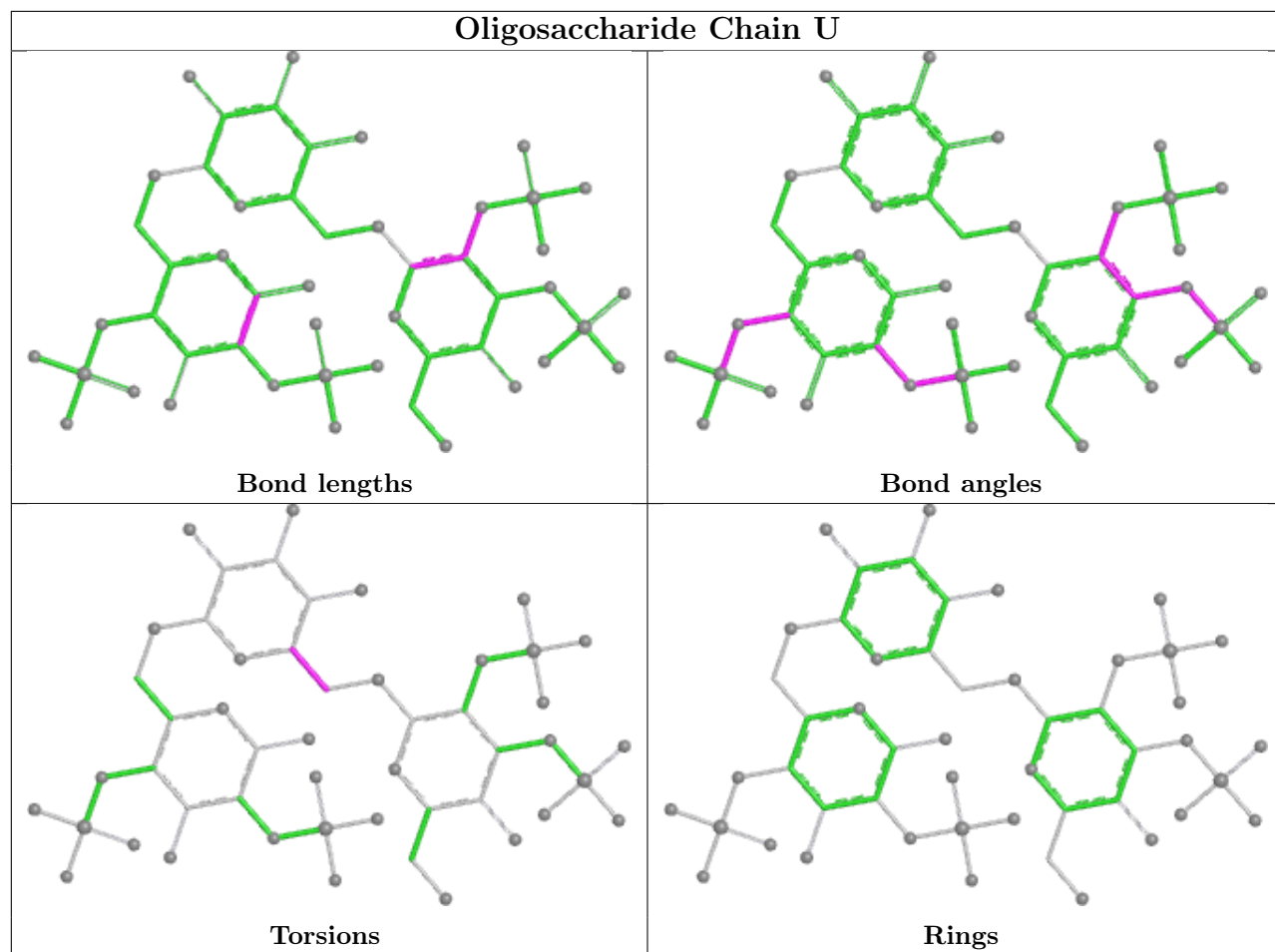


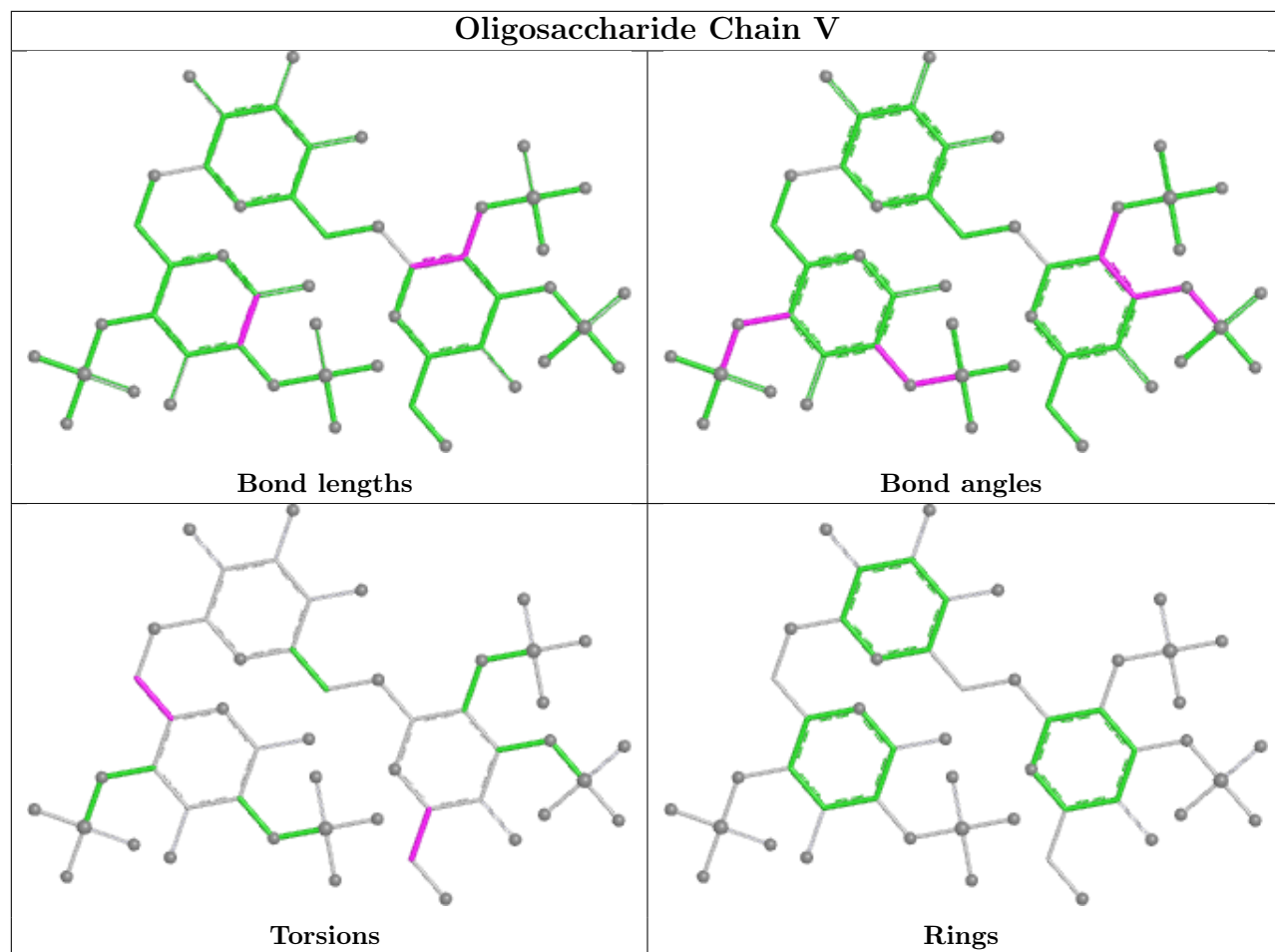


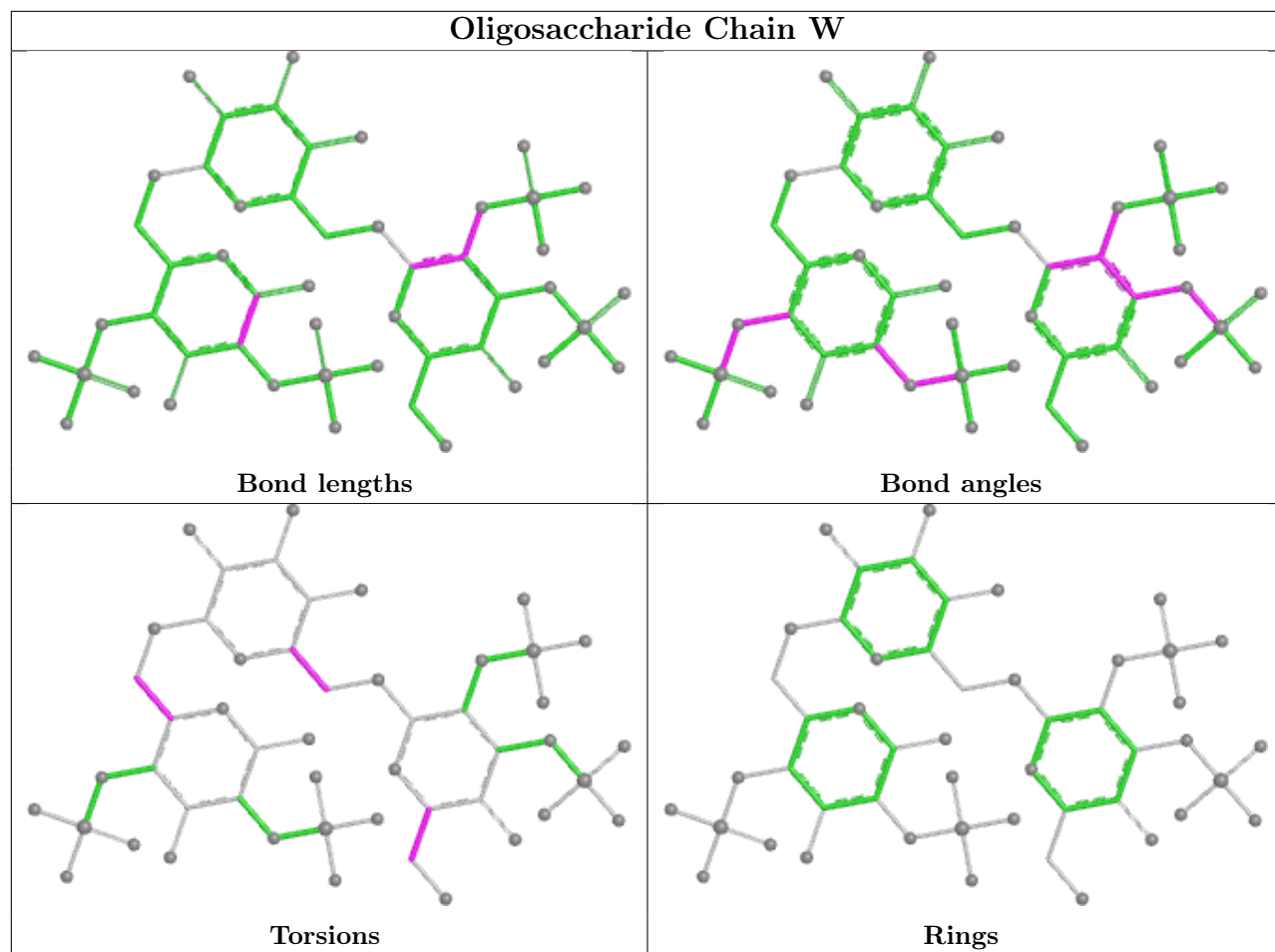


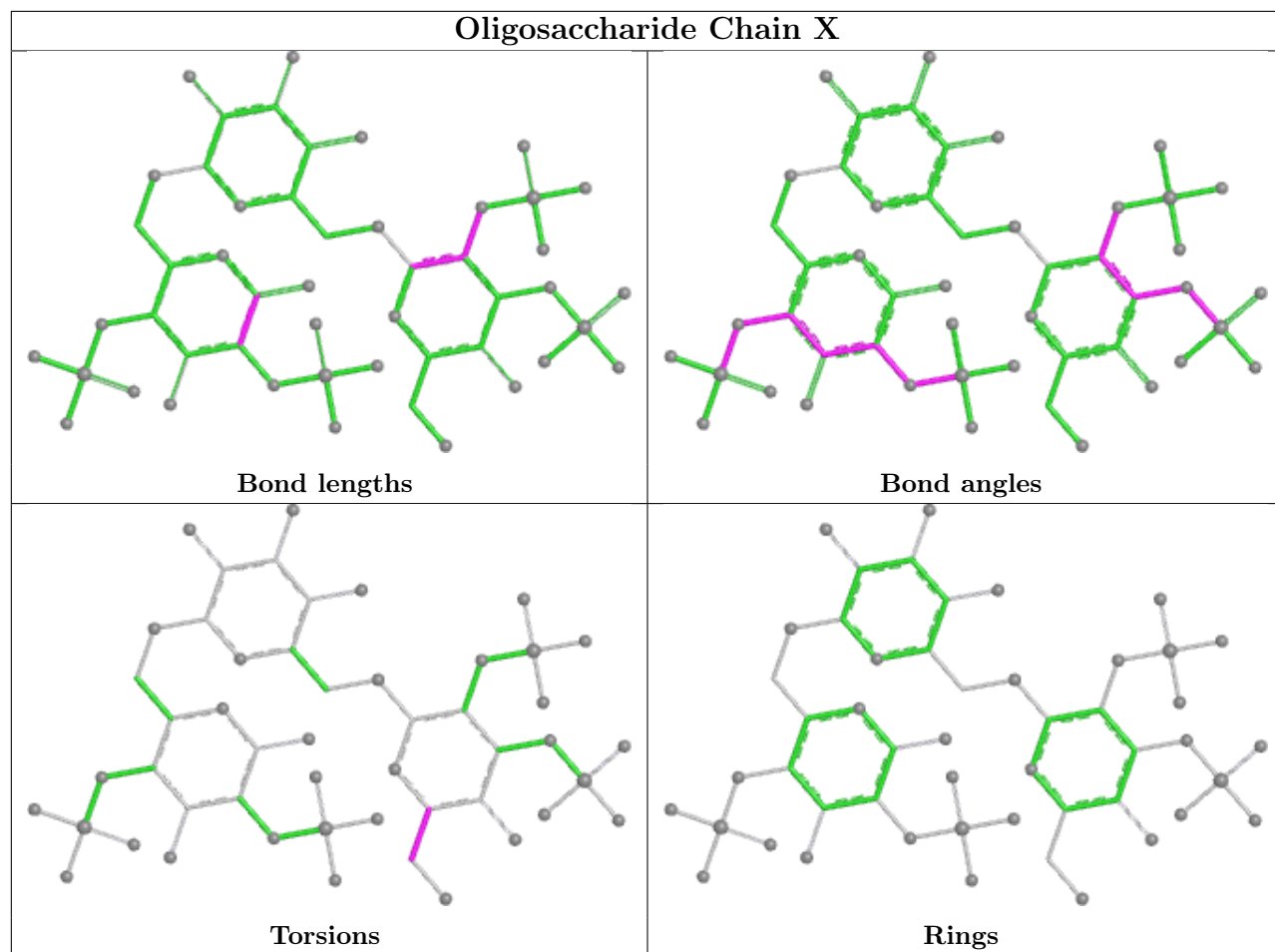


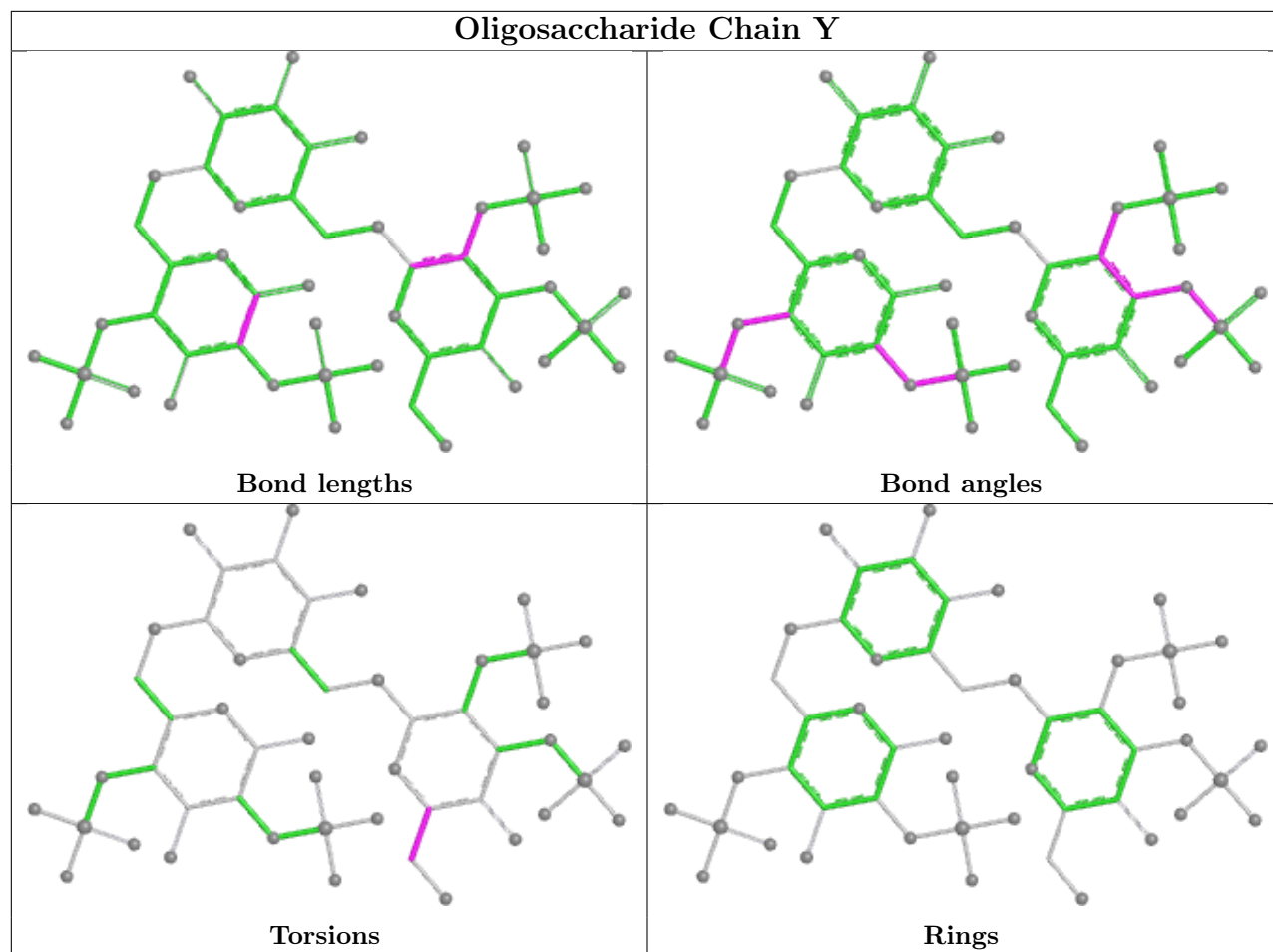


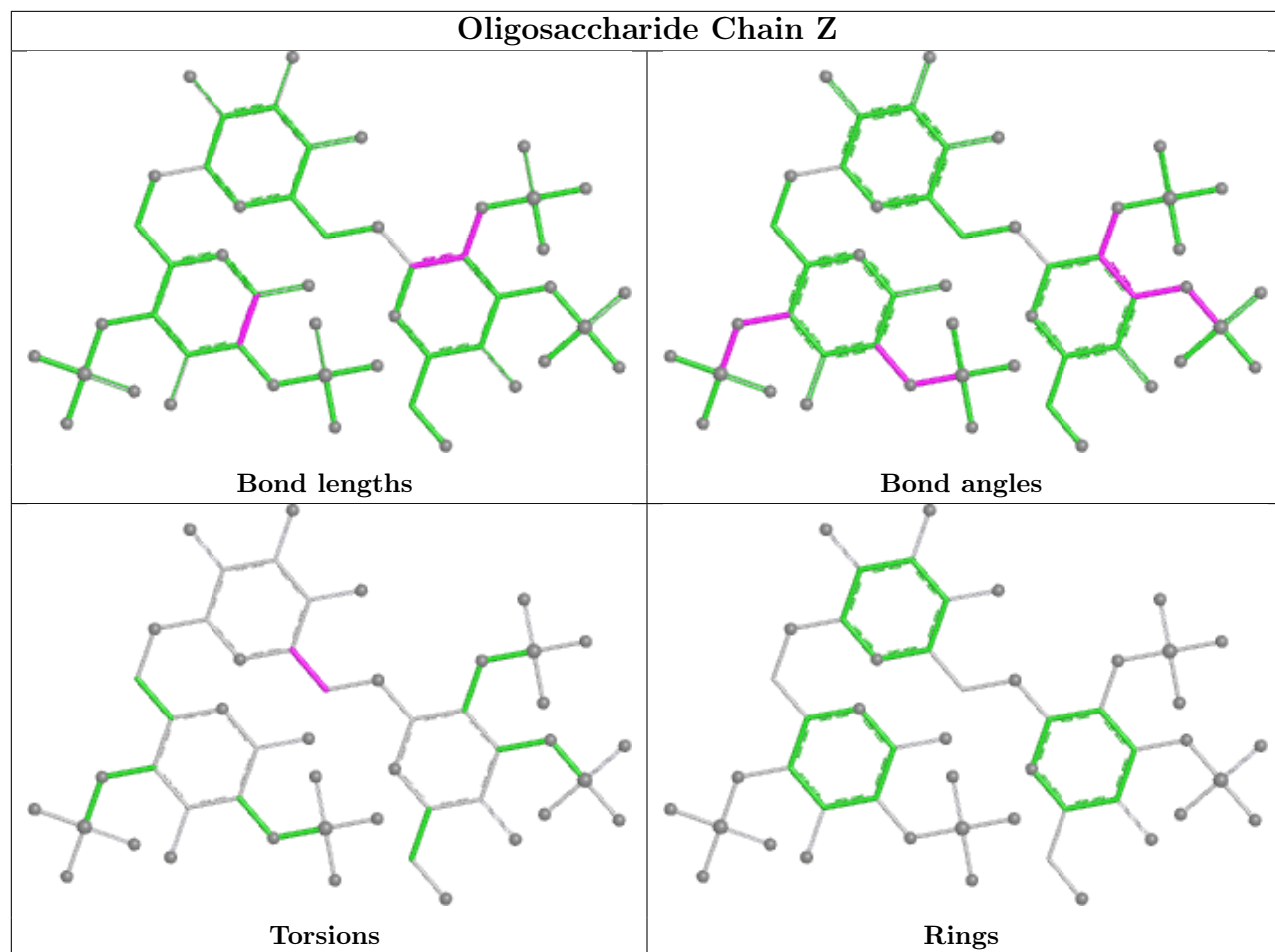


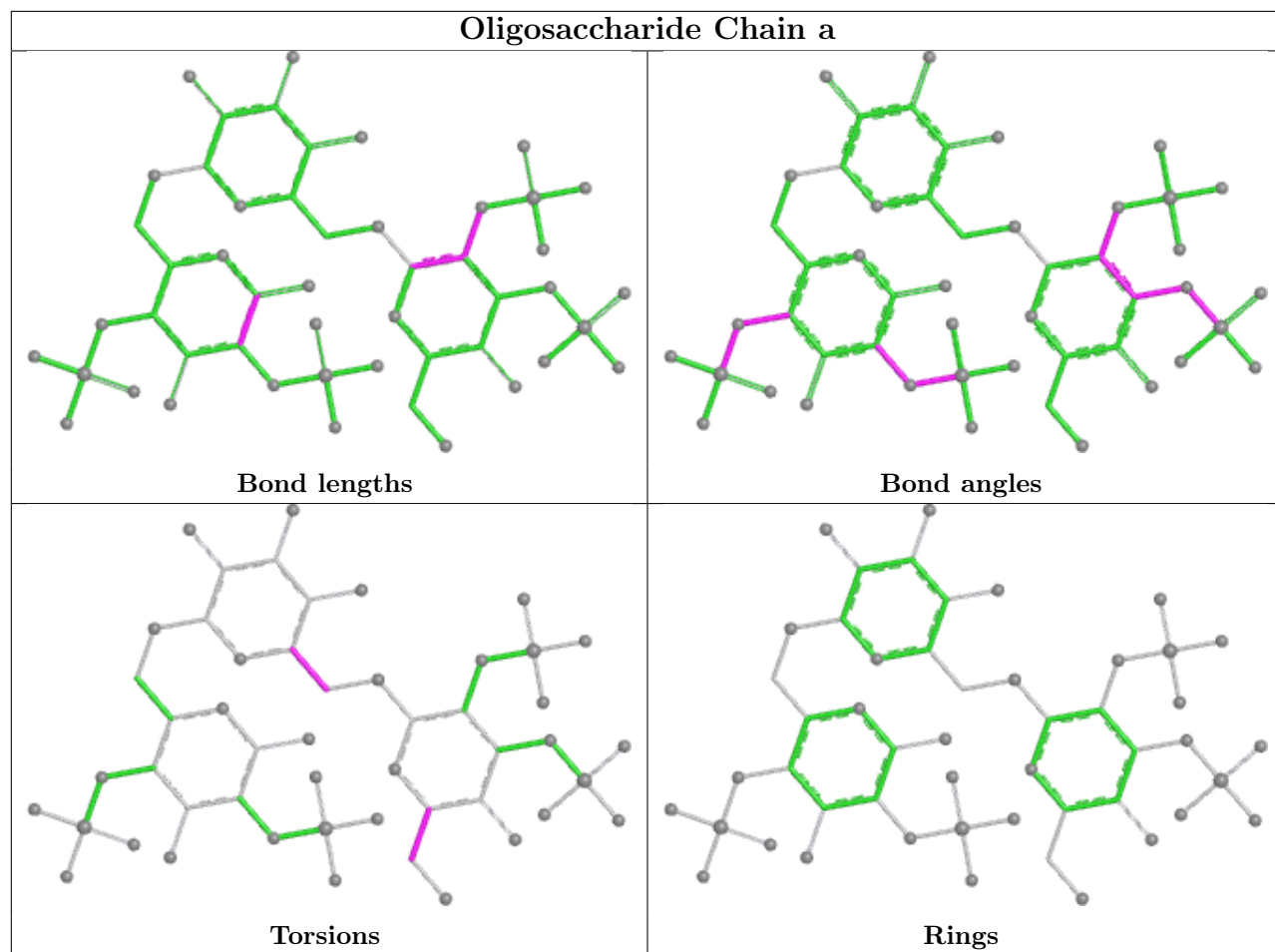


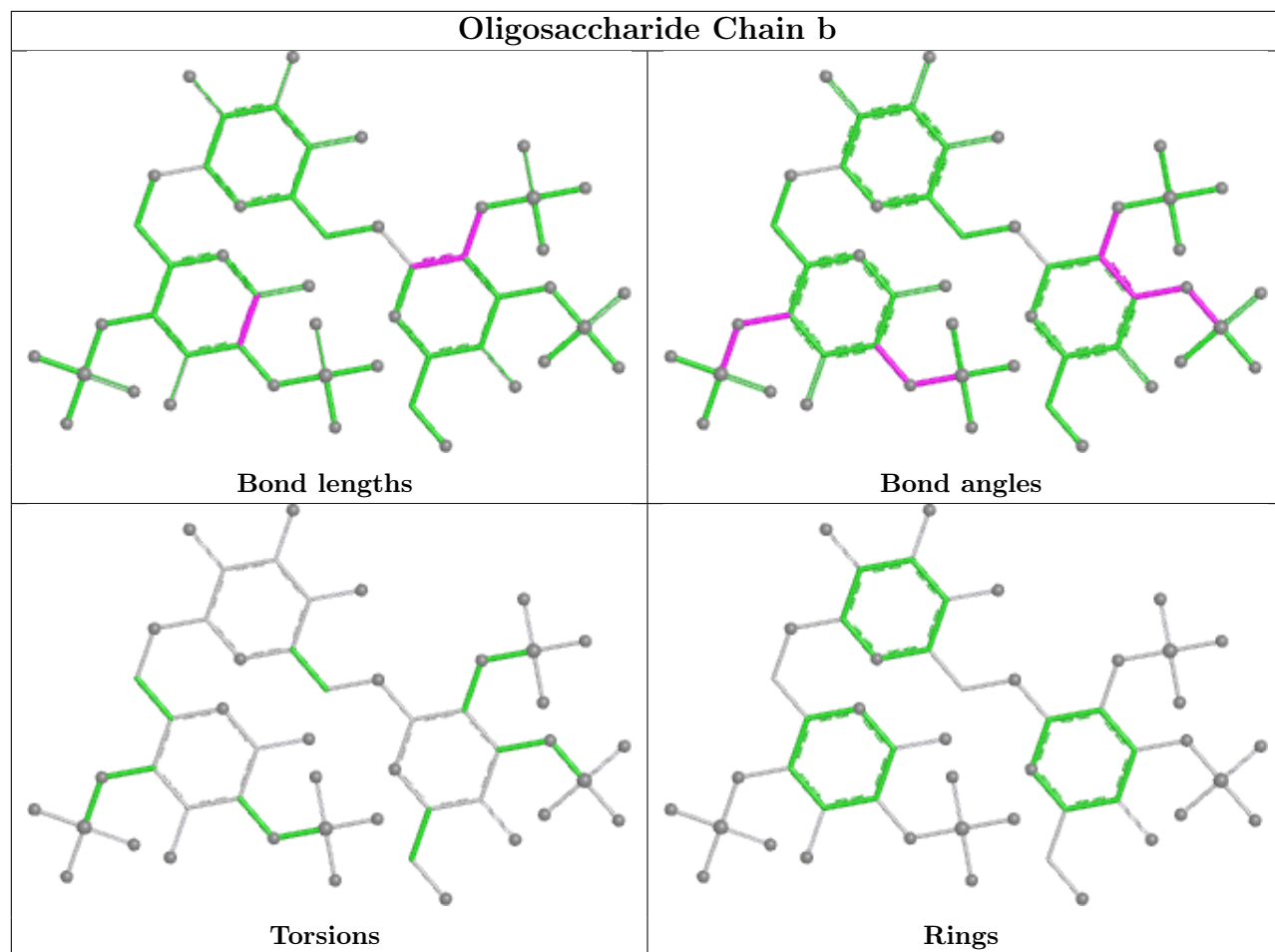


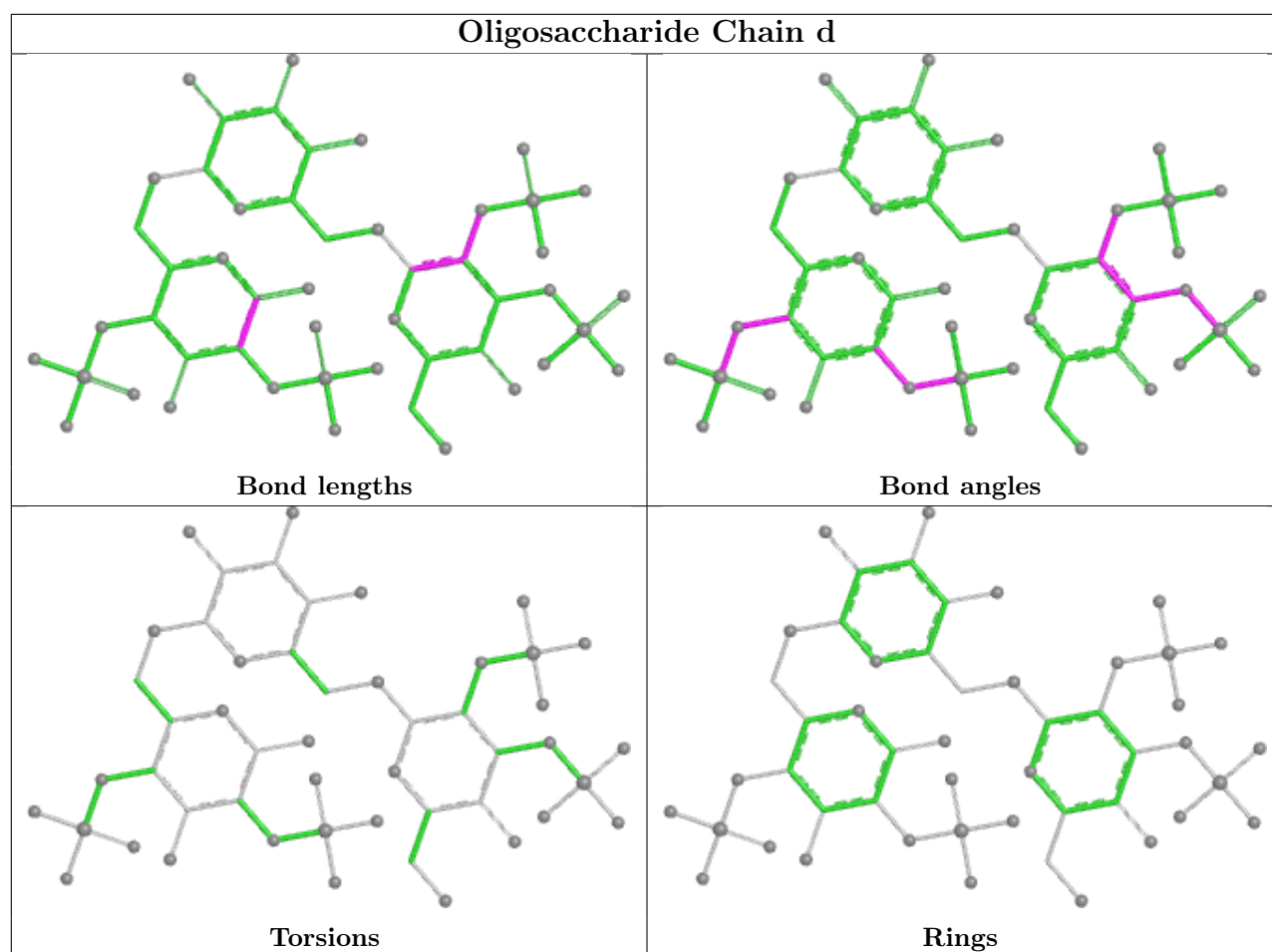


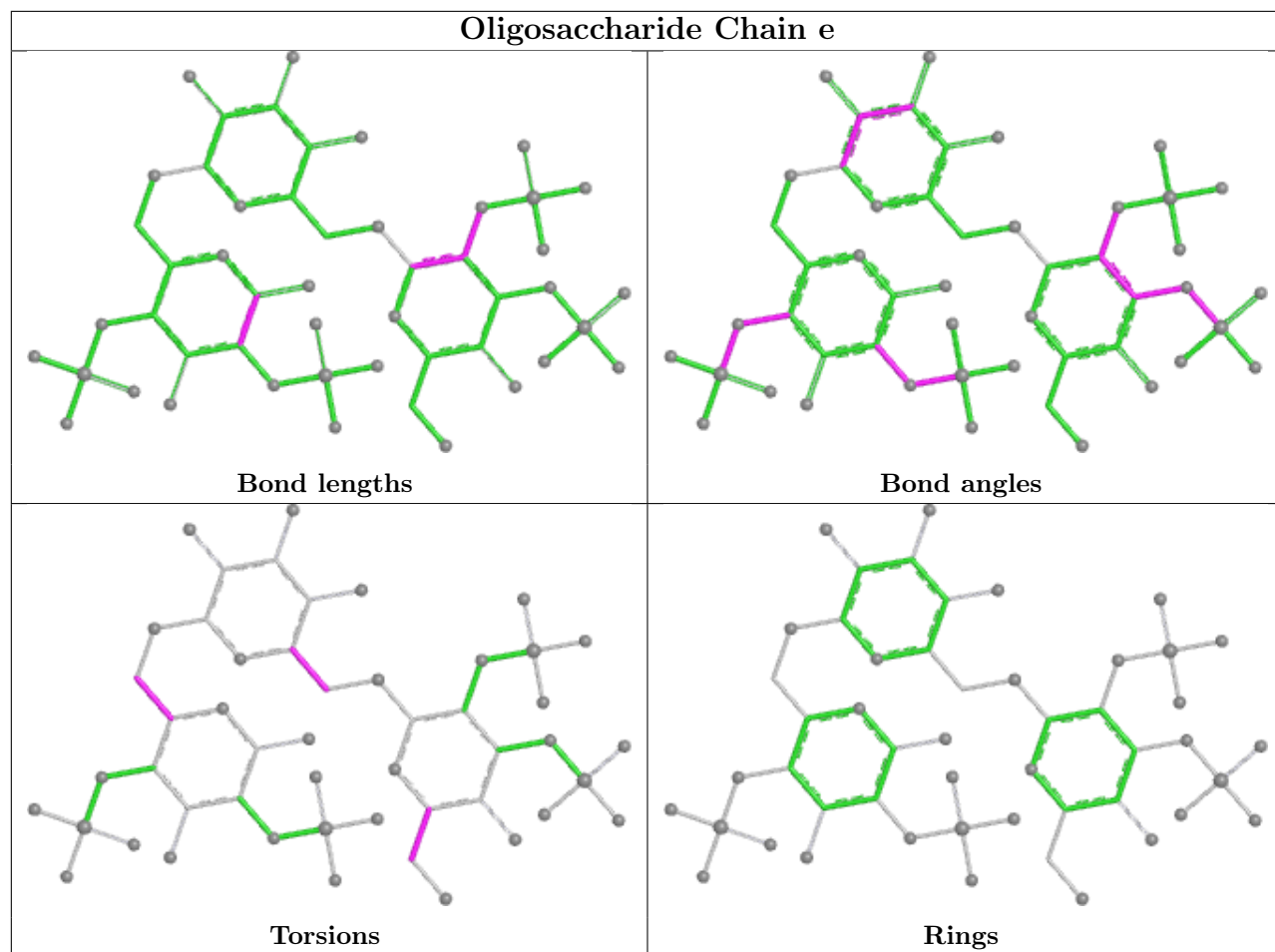


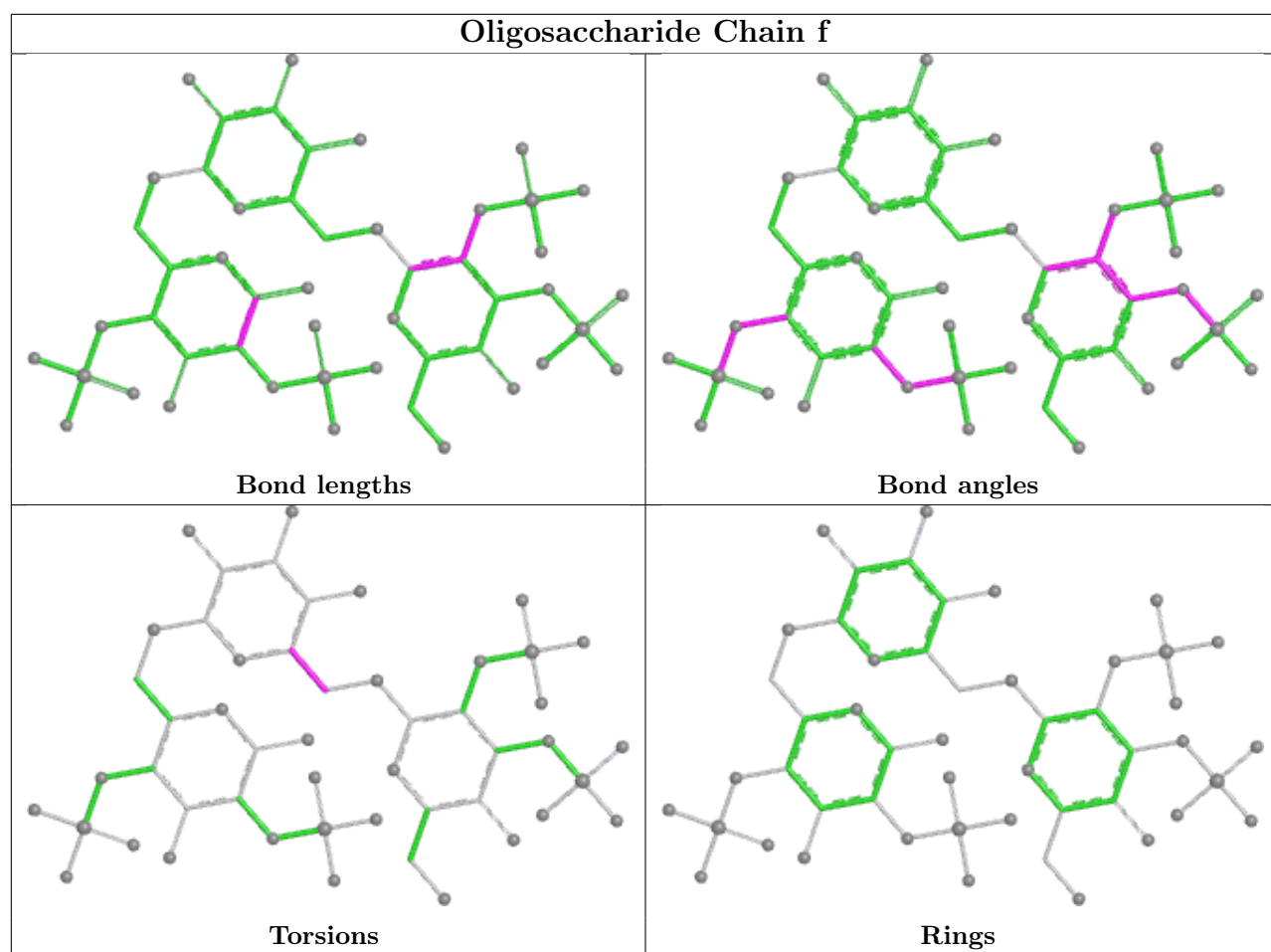


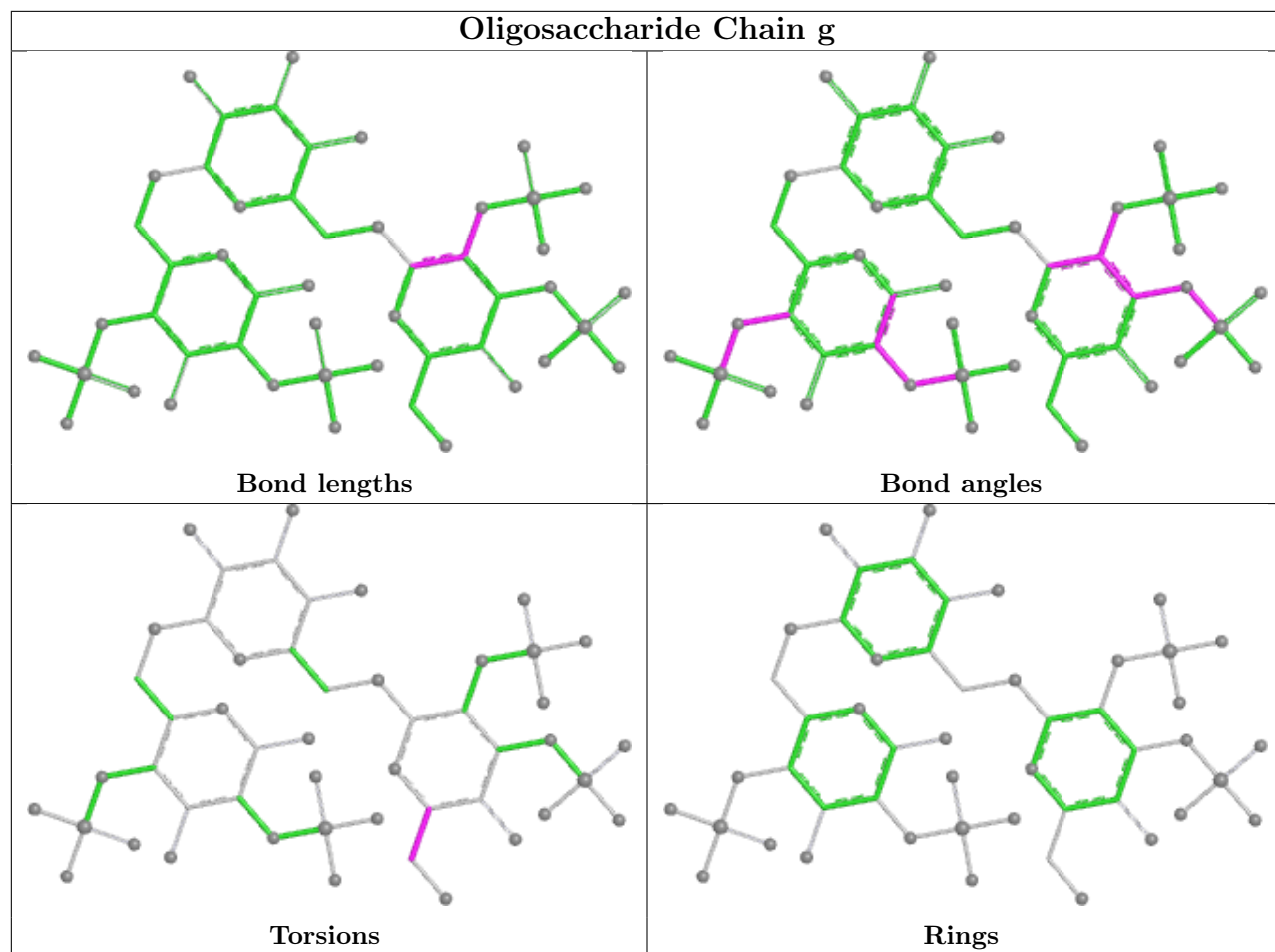


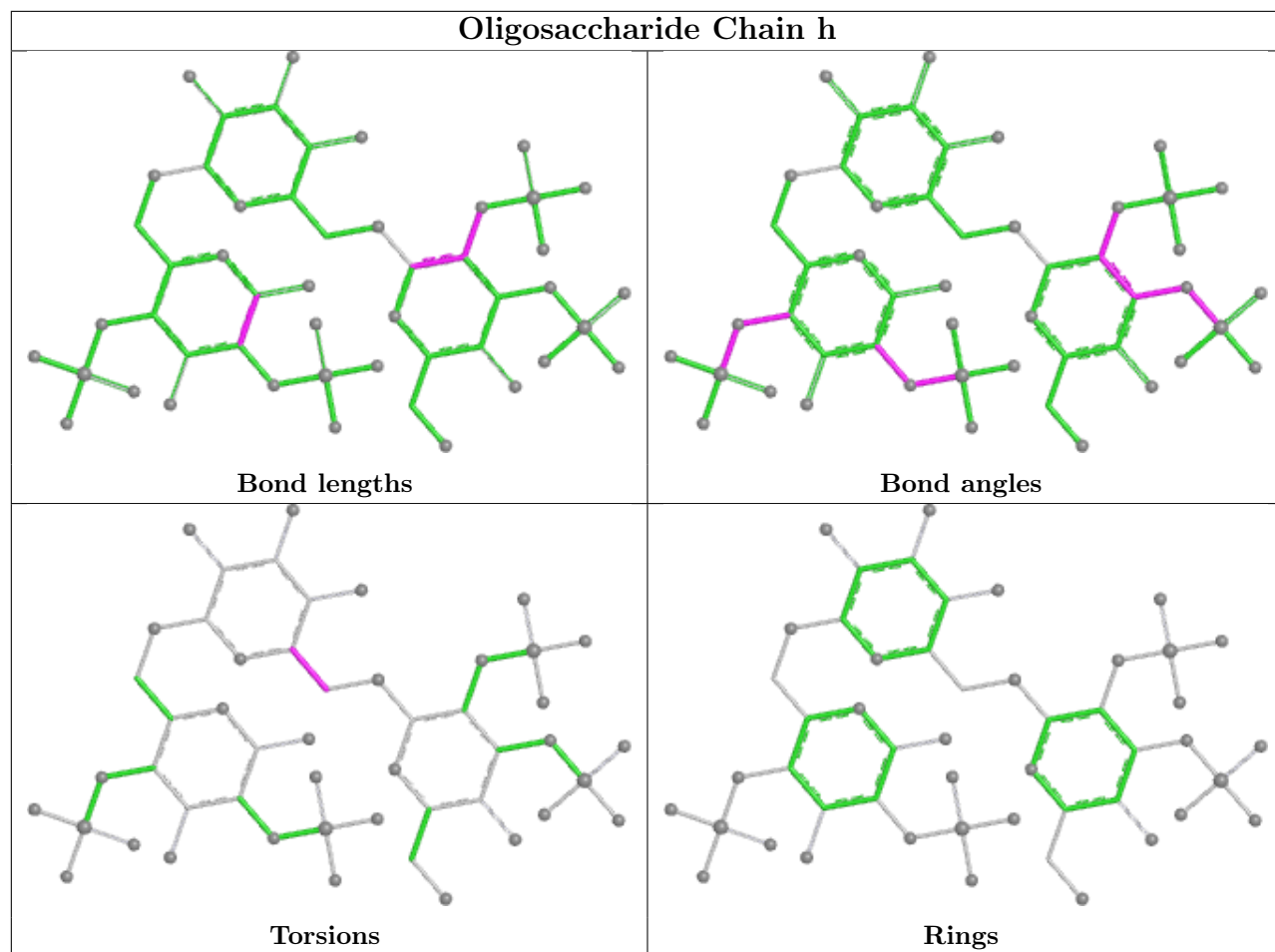


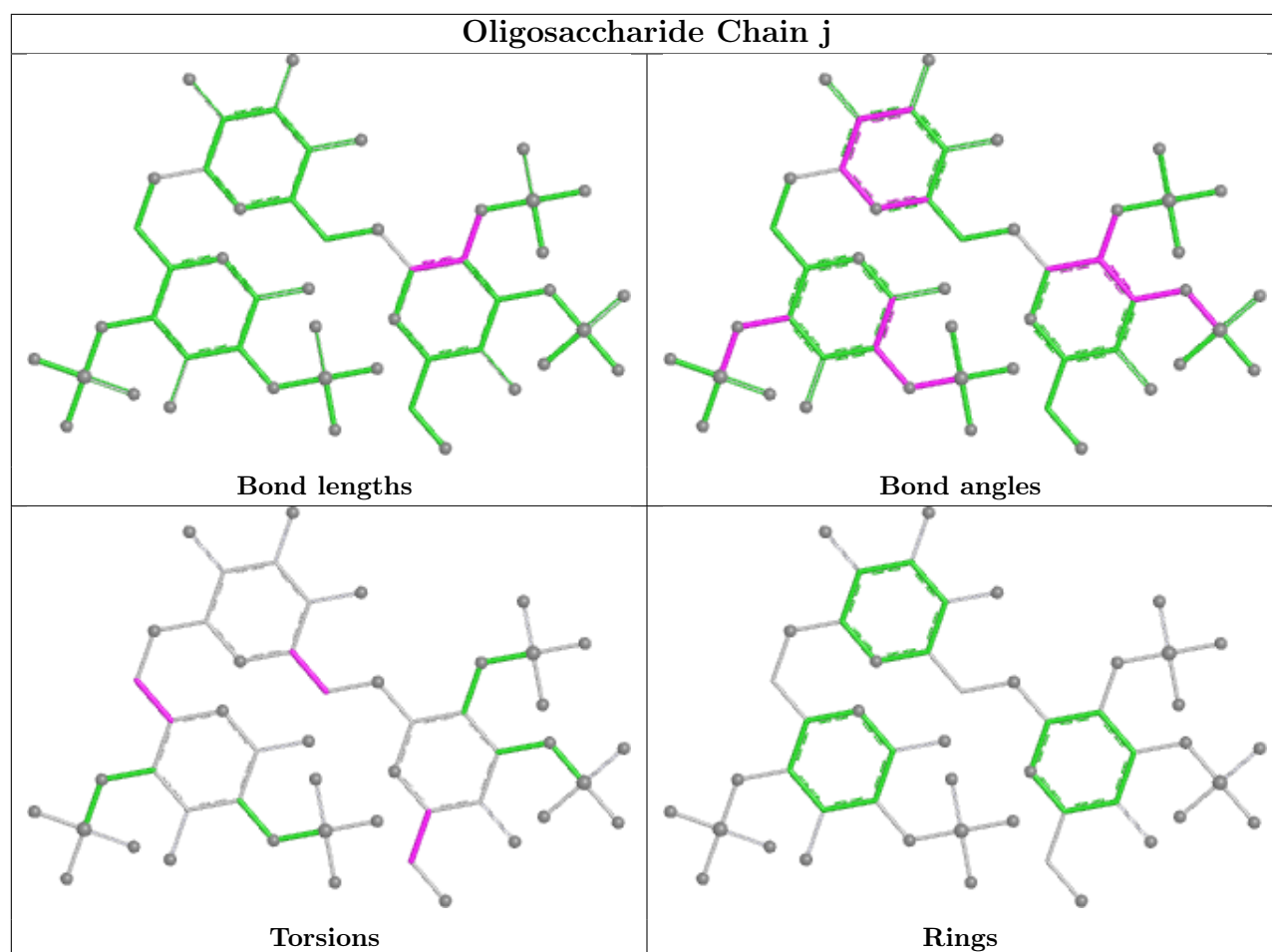


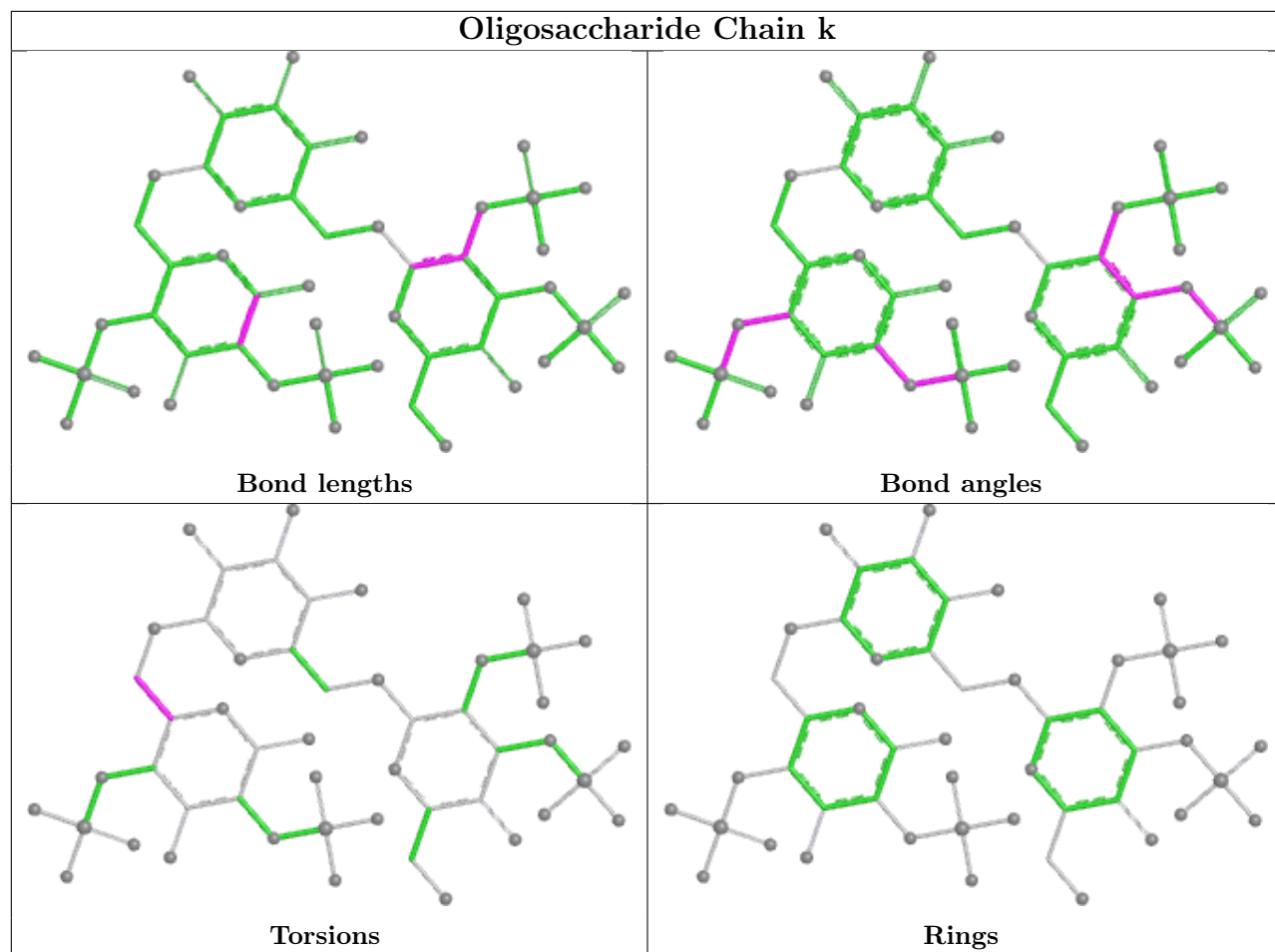


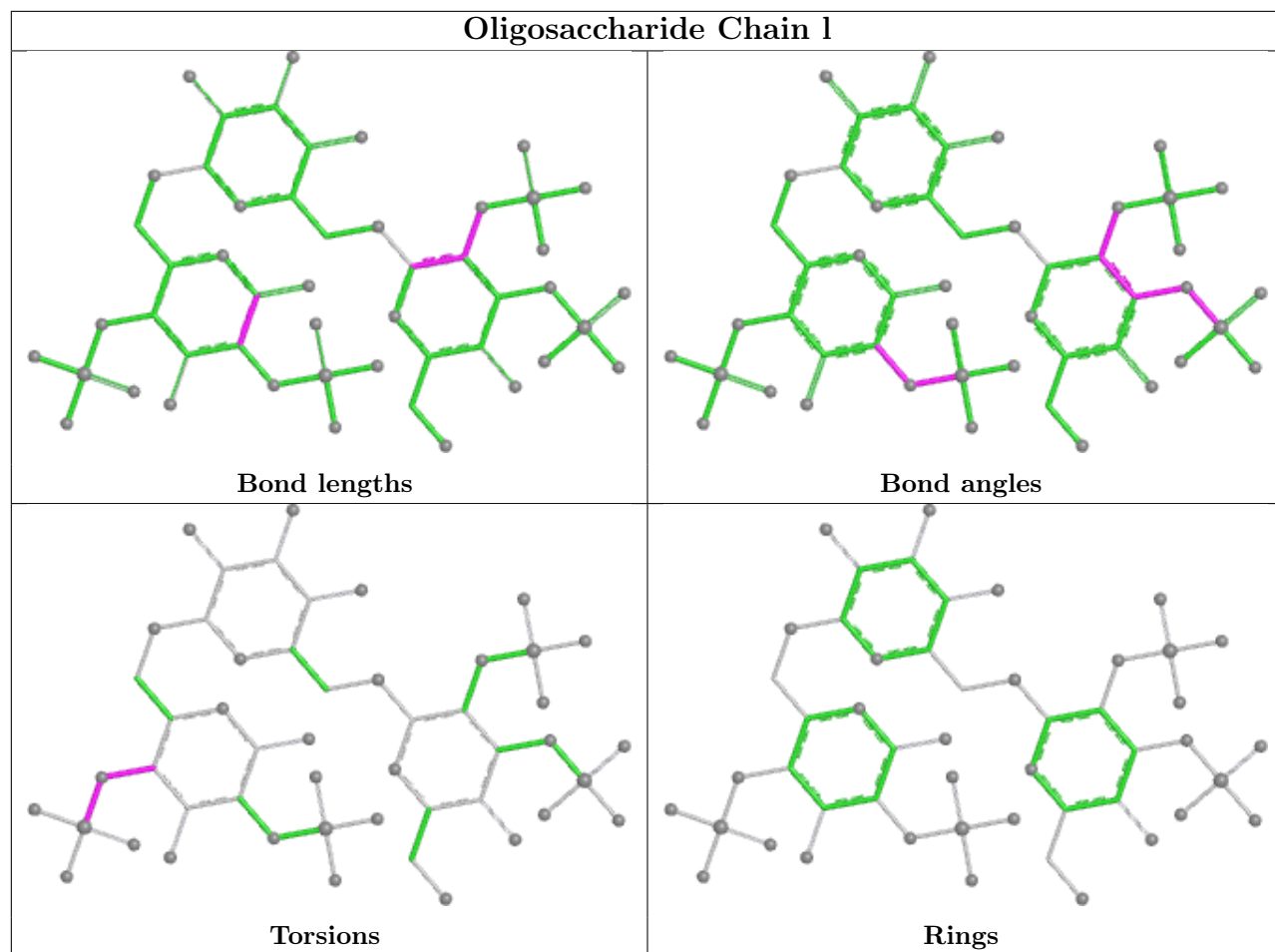


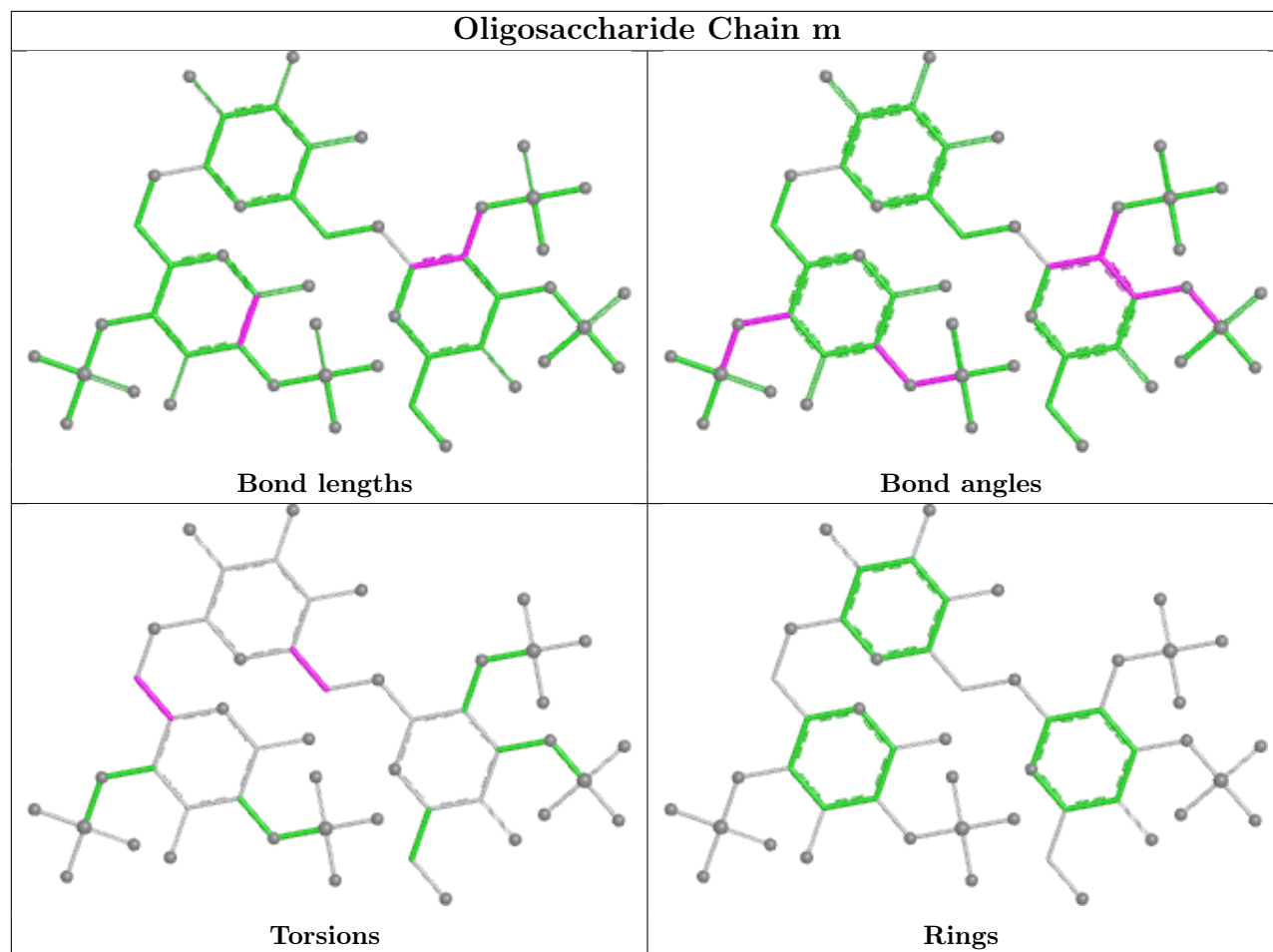


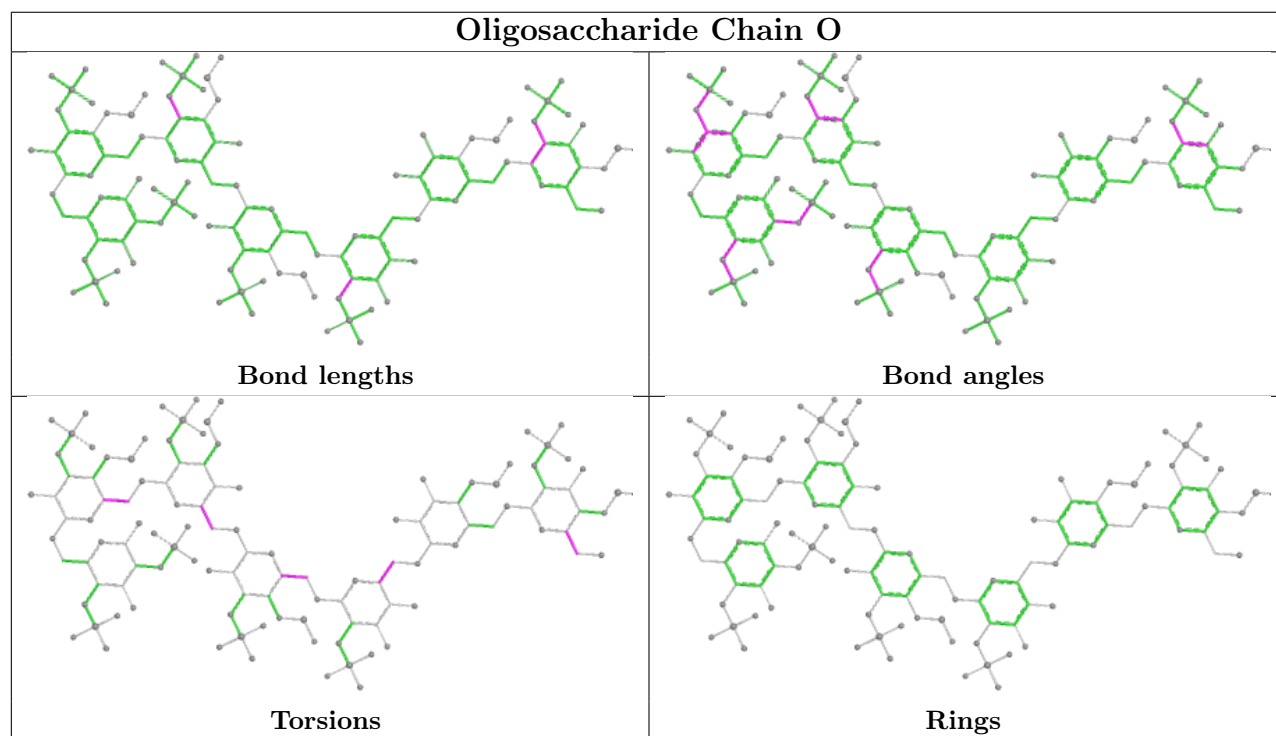
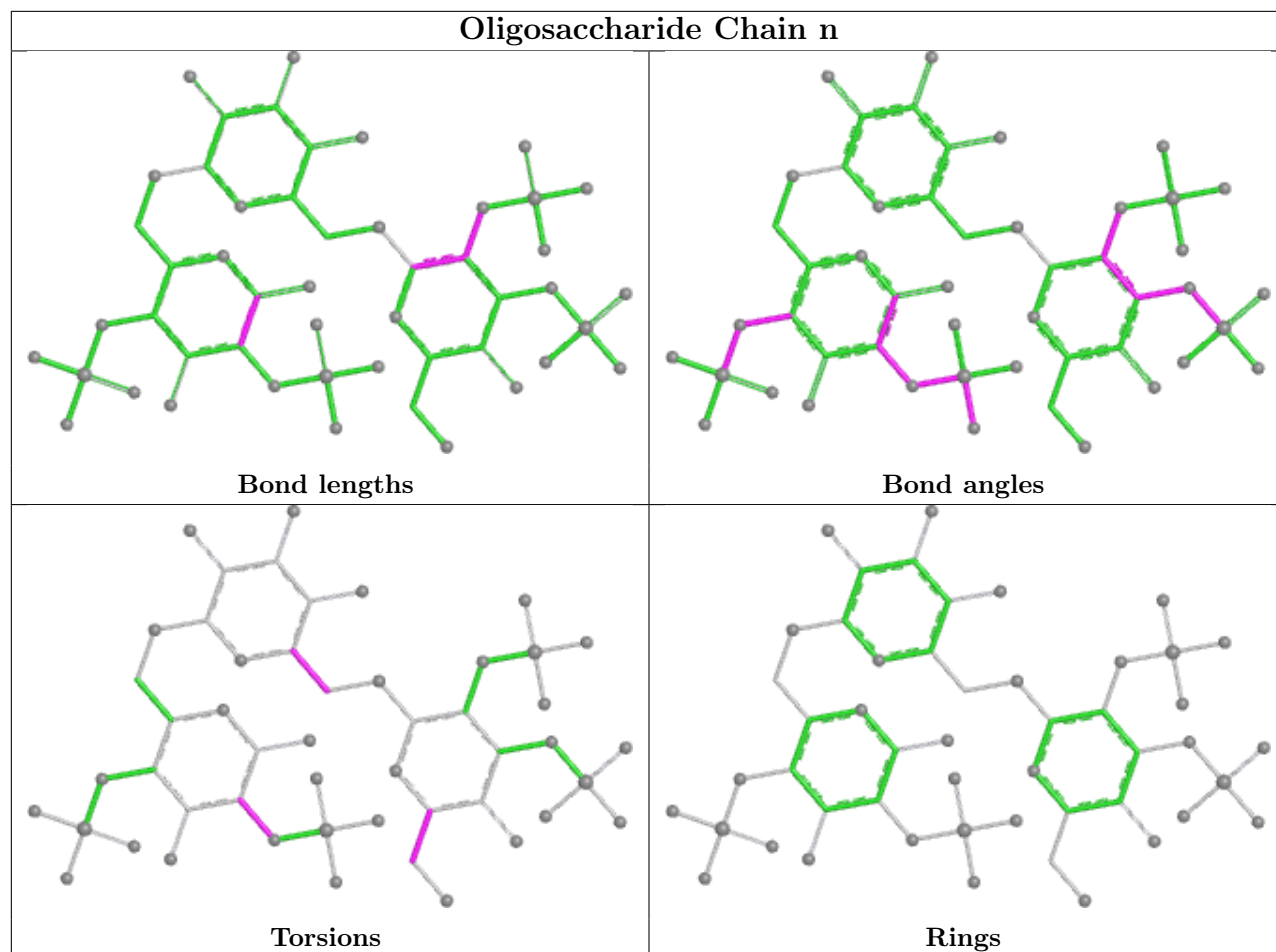


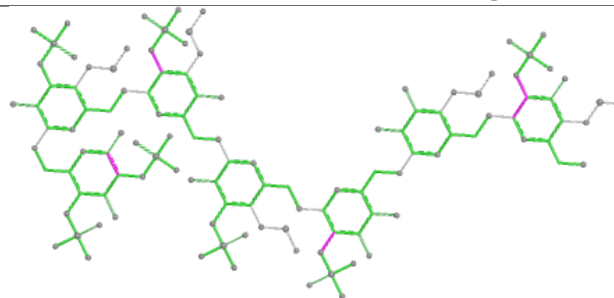
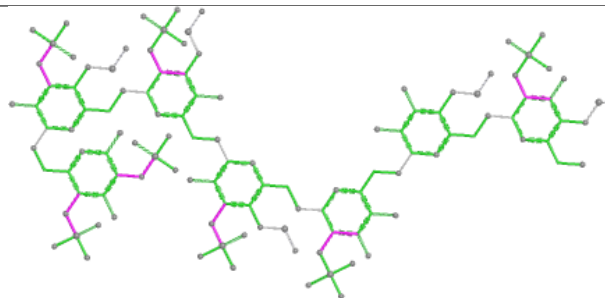
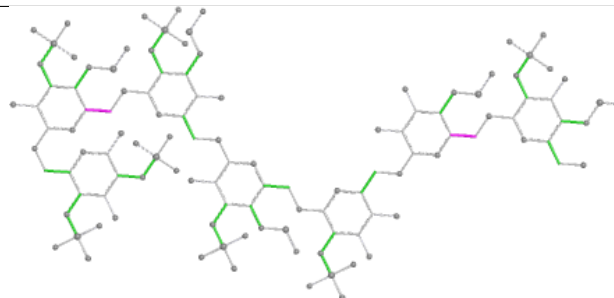
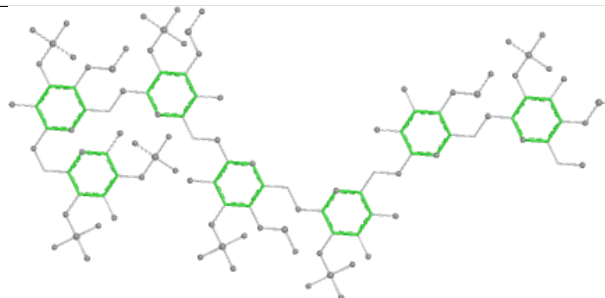
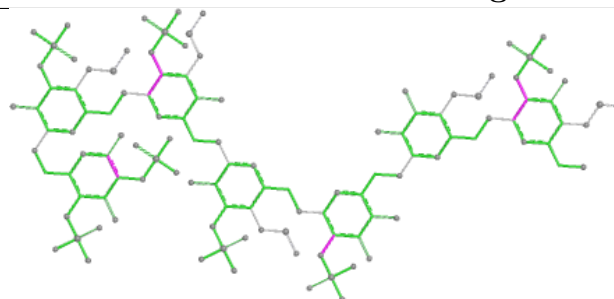
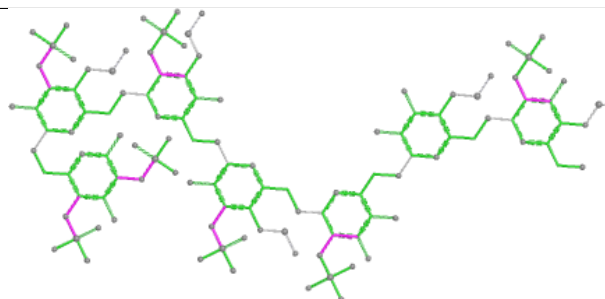
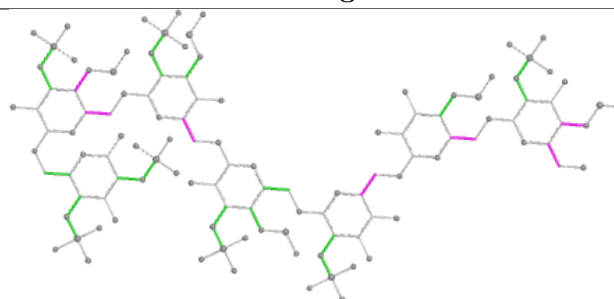
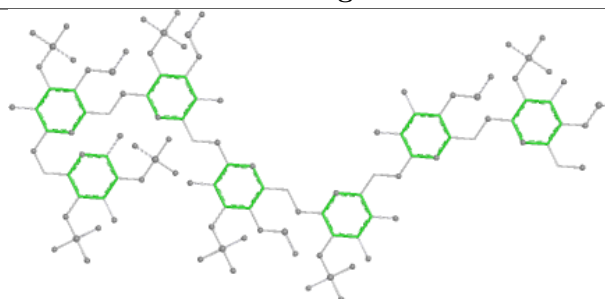


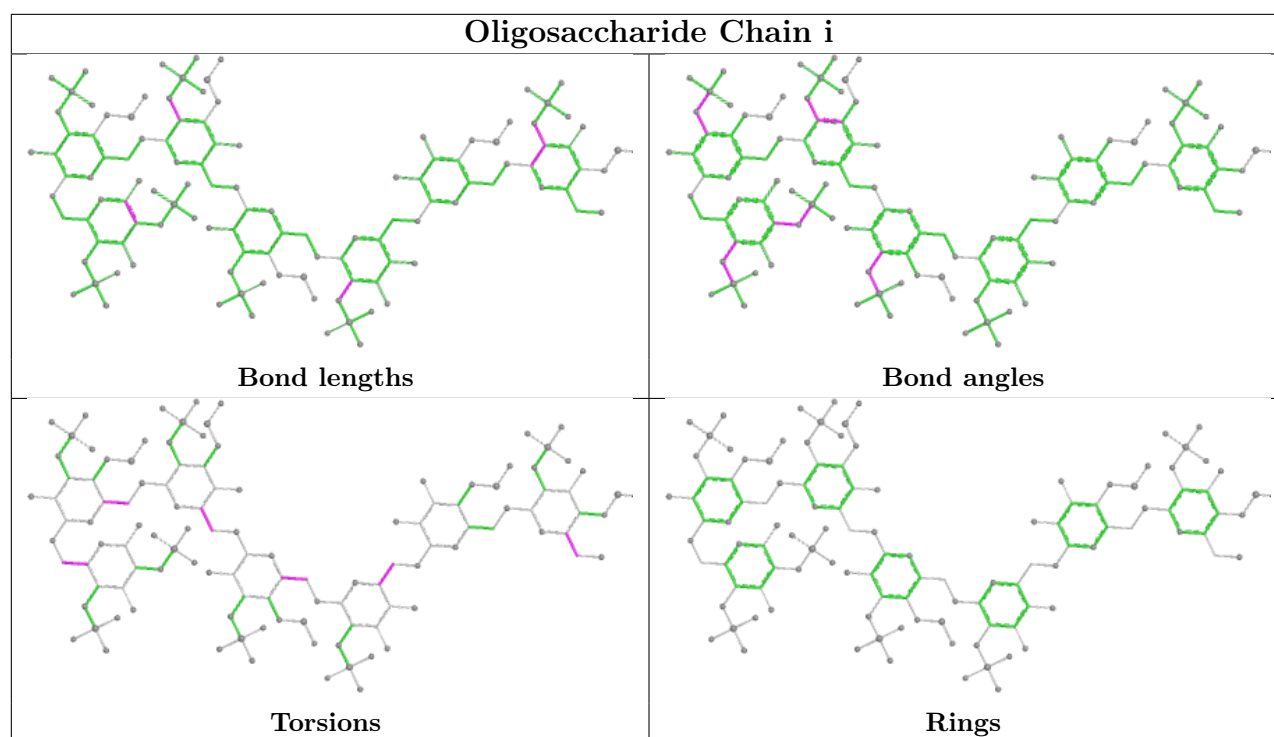








Oligosaccharide Chain T**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain c****Bond lengths****Bond angles****Torsions****Rings**



5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
4	5TL	D	701	-	28,28,28	2.74	10 (35%)	41,41,41	5.01	20 (48%)
4	5TL	C	701	-	28,28,28	2.70	11 (39%)	41,41,41	4.97	22 (53%)
4	5TL	G	701	-	28,28,28	2.69	11 (39%)	41,41,41	4.99	25 (60%)
4	5TL	J	701	-	28,28,28	2.74	12 (42%)	41,41,41	5.02	23 (56%)
4	5TL	A	701	-	28,28,28	2.71	13 (46%)	41,41,41	4.95	23 (56%)
4	5TL	I	701	-	28,28,28	2.71	10 (35%)	41,41,41	4.92	22 (53%)
4	5TL	B	701	-	28,28,28	2.75	12 (42%)	41,41,41	4.89	24 (58%)
4	5TL	K	701	-	28,28,28	2.67	11 (39%)	41,41,41	5.05	21 (51%)
4	5TL	F	701	-	28,28,28	2.73	10 (35%)	41,41,41	4.93	19 (46%)
4	5TL	E	701	-	28,28,28	2.70	10 (35%)	41,41,41	4.95	21 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5TL	L	701	-	28,28,28	2.73	12 (42%)	41,41,41	4.95	21 (51%)
4	5TL	H	701	-	28,28,28	2.74	12 (42%)	41,41,41	4.92	22 (53%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5TL	D	701	-	-	7/18/18/18	0/3/3/3
4	5TL	C	701	-	-	8/18/18/18	0/3/3/3
4	5TL	G	701	-	-	5/18/18/18	0/3/3/3
4	5TL	J	701	-	-	8/18/18/18	0/3/3/3
4	5TL	A	701	-	-	8/18/18/18	0/3/3/3
4	5TL	I	701	-	-	8/18/18/18	0/3/3/3
4	5TL	B	701	-	-	6/18/18/18	0/3/3/3
4	5TL	K	701	-	-	8/18/18/18	0/3/3/3
4	5TL	F	701	-	-	8/18/18/18	0/3/3/3
4	5TL	E	701	-	-	8/18/18/18	0/3/3/3
4	5TL	L	701	-	-	6/18/18/18	0/3/3/3
4	5TL	H	701	-	-	6/18/18/18	0/3/3/3

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	701	5TL	S-N1	-6.33	1.48	1.60
4	H	701	5TL	S-N1	-6.29	1.48	1.60
4	F	701	5TL	S-N1	-6.26	1.48	1.60
4	B	701	5TL	S-N1	-6.20	1.48	1.60
4	L	701	5TL	S-N1	-6.11	1.48	1.60

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	5TL	CAT-CAS-CAL	-14.75	102.19	121.12
4	D	701	5TL	CAS-CAL-CAM	14.71	144.01	117.68
4	J	701	5TL	CAT-CAS-CAL	-14.71	102.24	121.12
4	L	701	5TL	CAT-CAS-CAL	-14.67	102.29	121.12
4	J	701	5TL	CAS-CAL-CAM	14.65	143.88	117.68

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

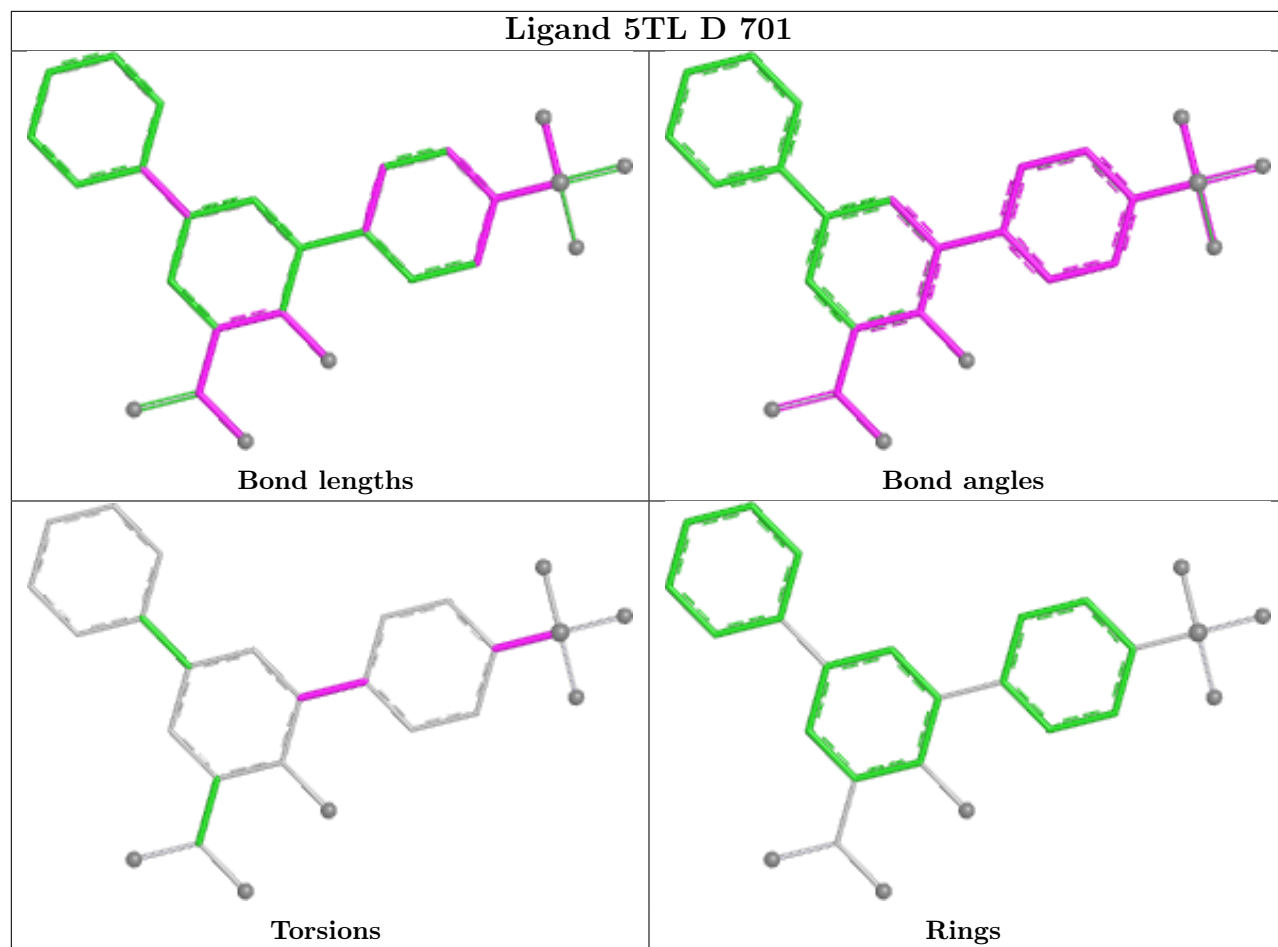
Mol	Chain	Res	Type	Atoms
4	A	701	5TL	CAR-CAJ-CAL-CAM
4	A	701	5TL	CAR-CAJ-CAL-CAS
4	B	701	5TL	CAR-CAJ-CAL-CAM
4	C	701	5TL	CAR-CAJ-CAL-CAM
4	C	701	5TL	CAR-CAJ-CAL-CAS

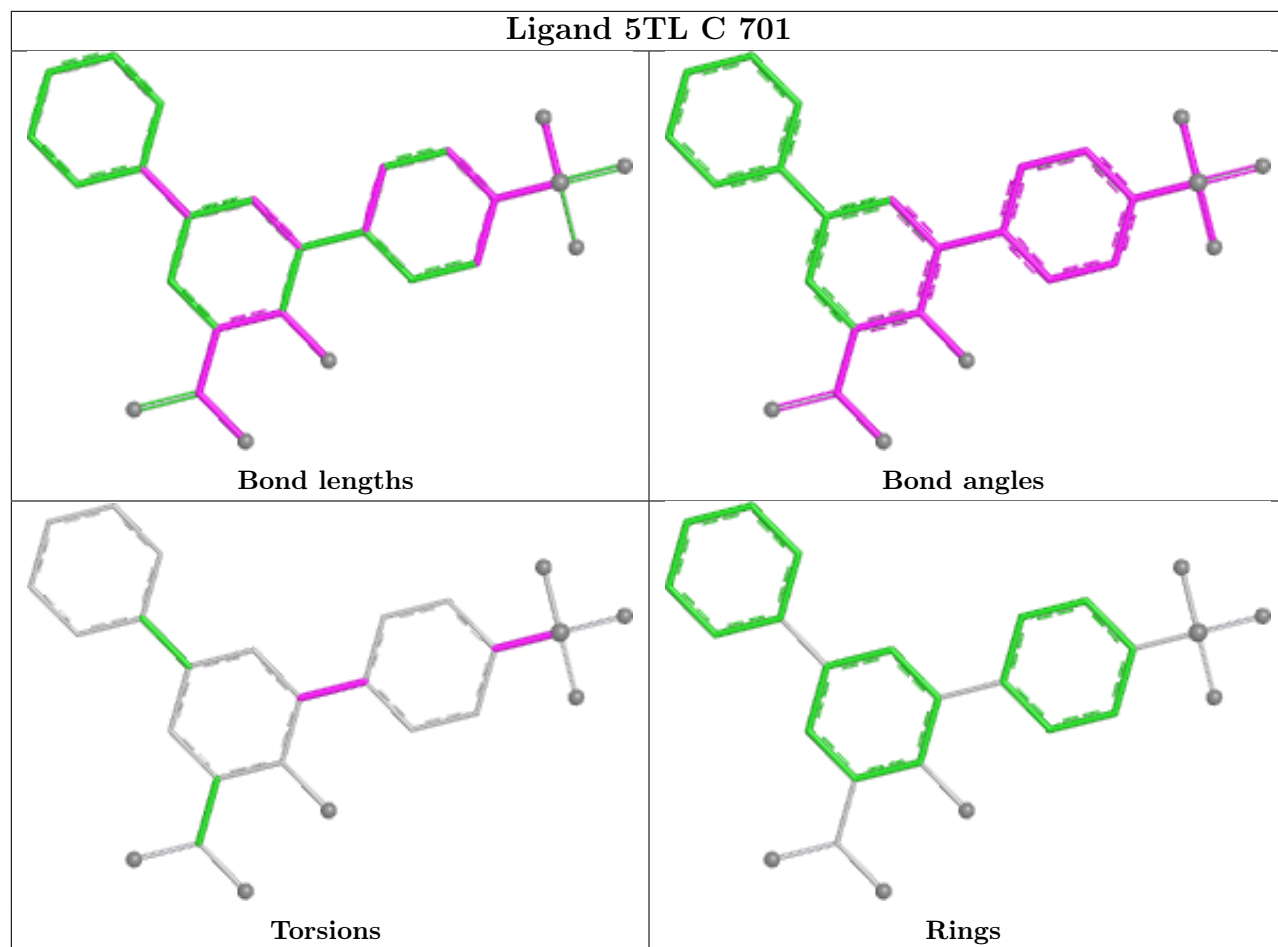
There are no ring outliers.

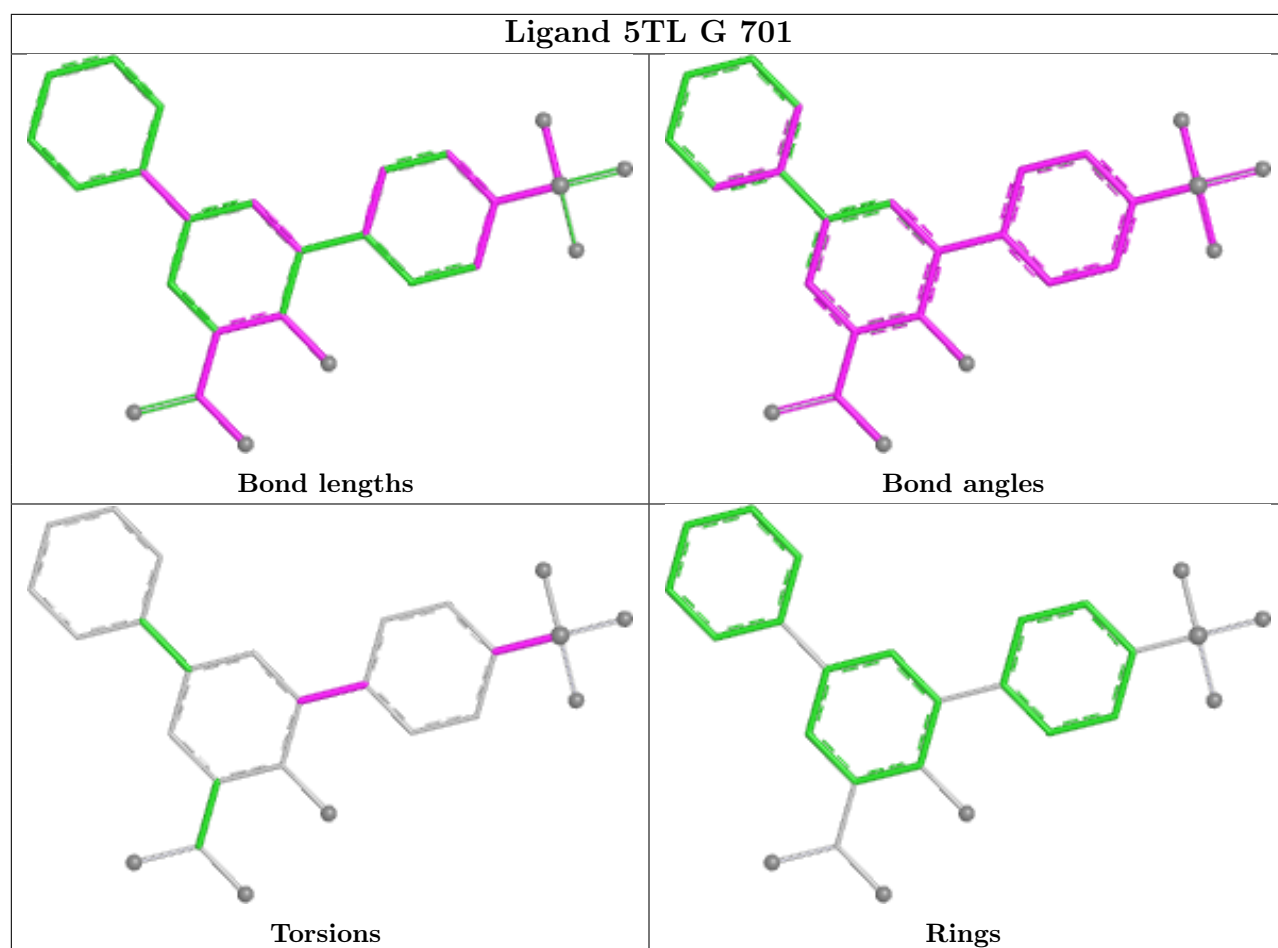
12 monomers are involved in 39 short contacts:

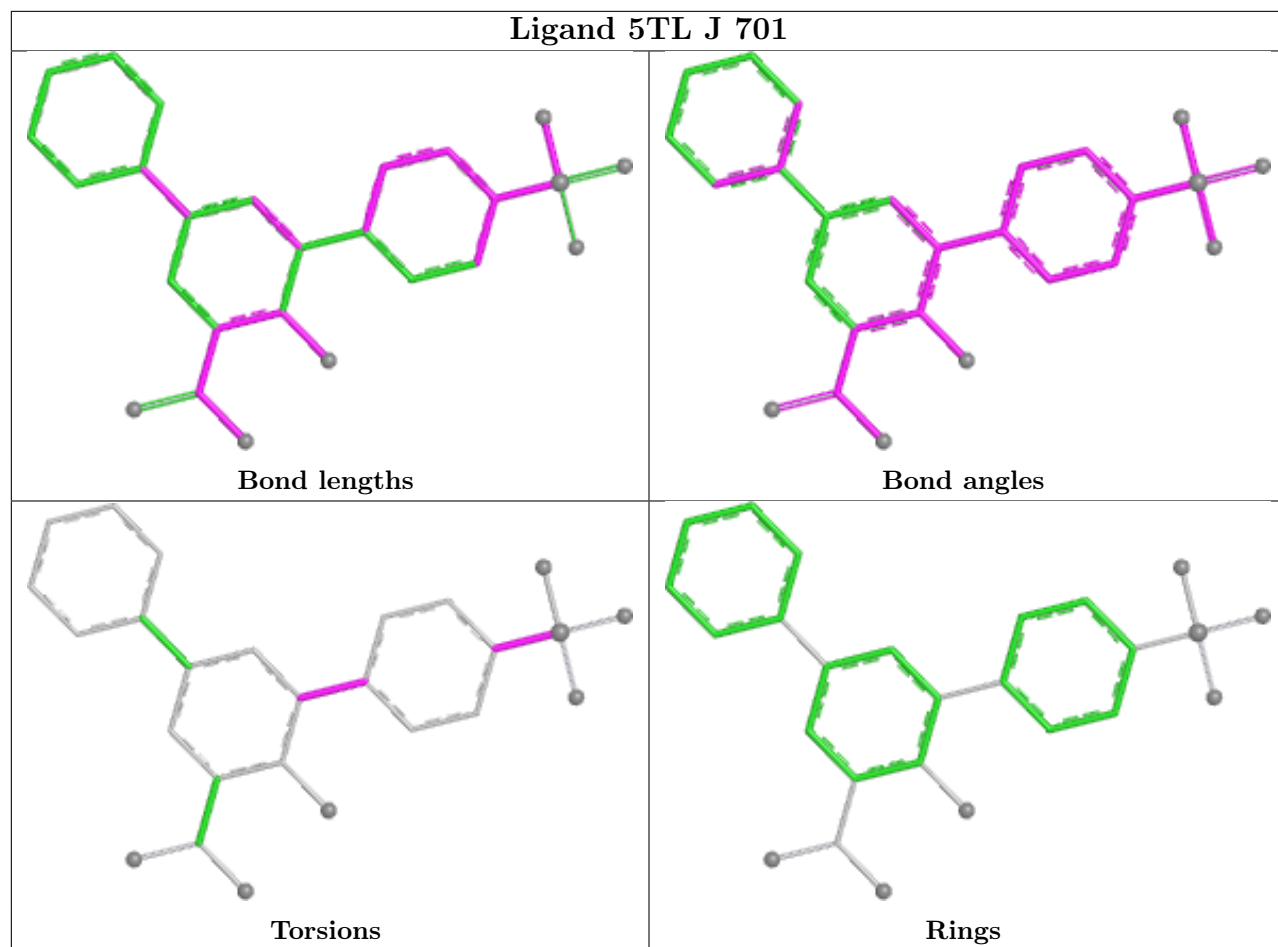
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	701	5TL	2	0
4	C	701	5TL	4	0
4	G	701	5TL	4	0
4	J	701	5TL	2	0
4	A	701	5TL	3	0
4	I	701	5TL	6	0
4	B	701	5TL	2	0
4	K	701	5TL	3	0
4	F	701	5TL	6	0
4	E	701	5TL	3	0
4	L	701	5TL	2	0
4	H	701	5TL	2	0

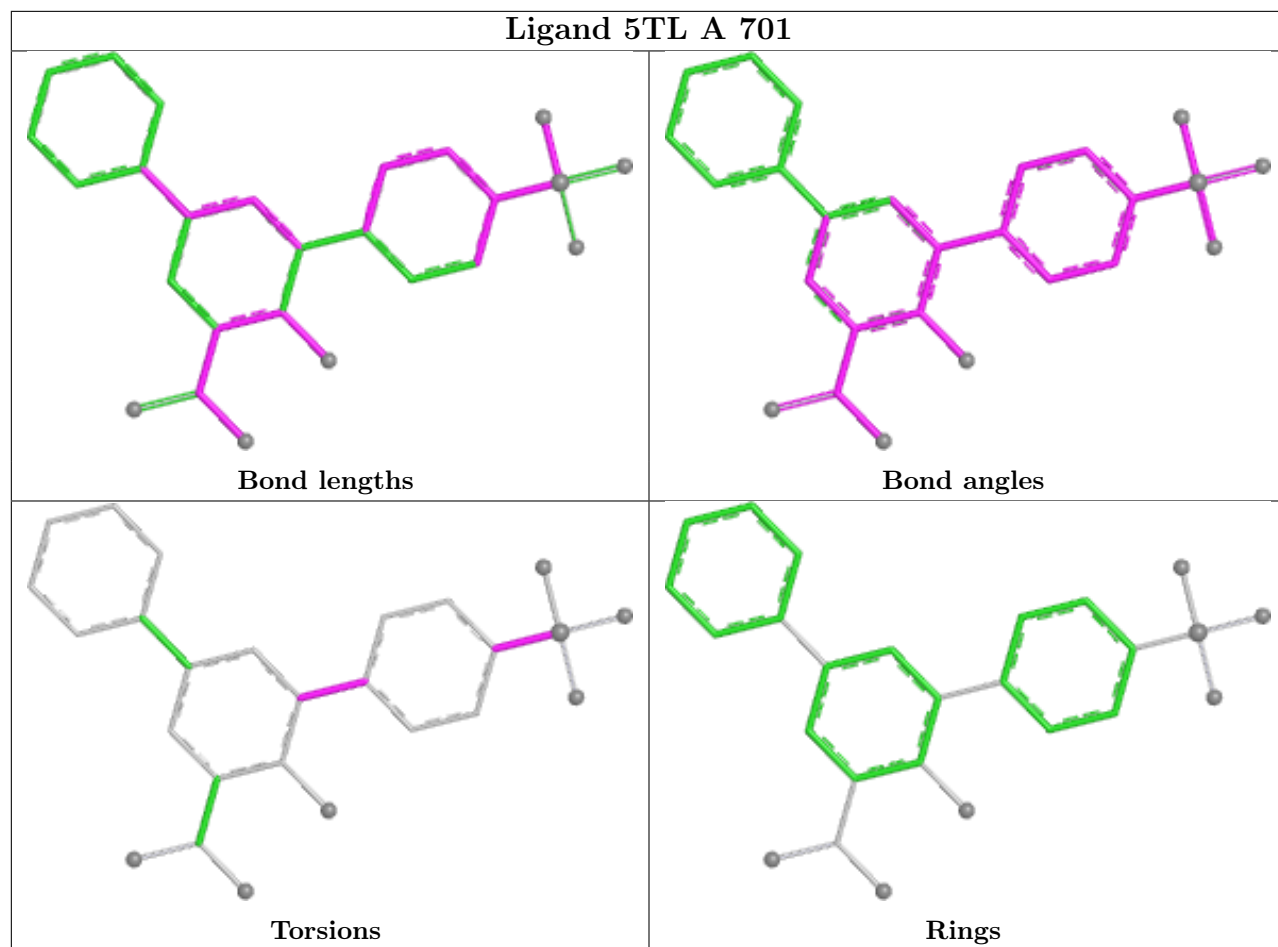
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

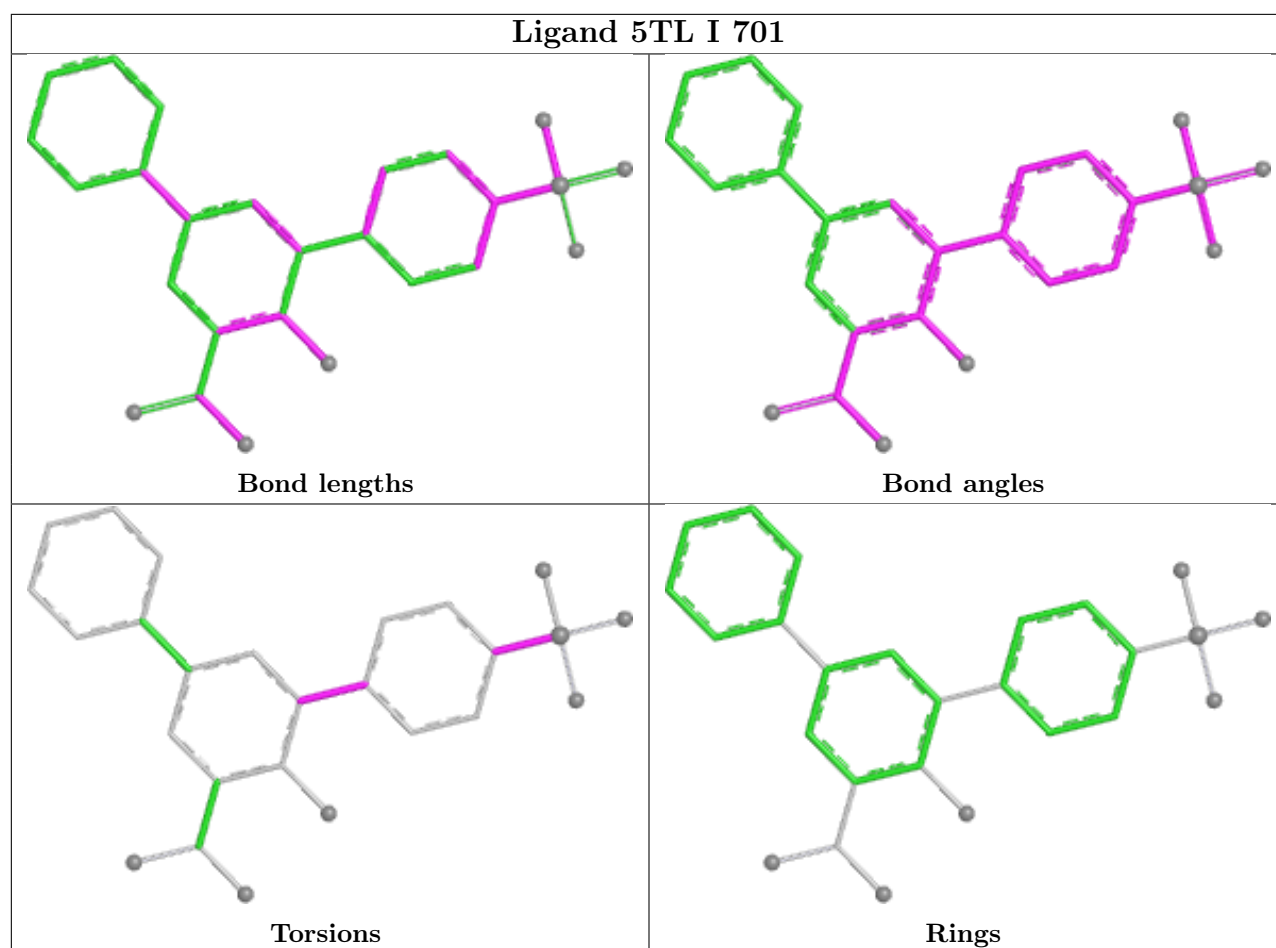


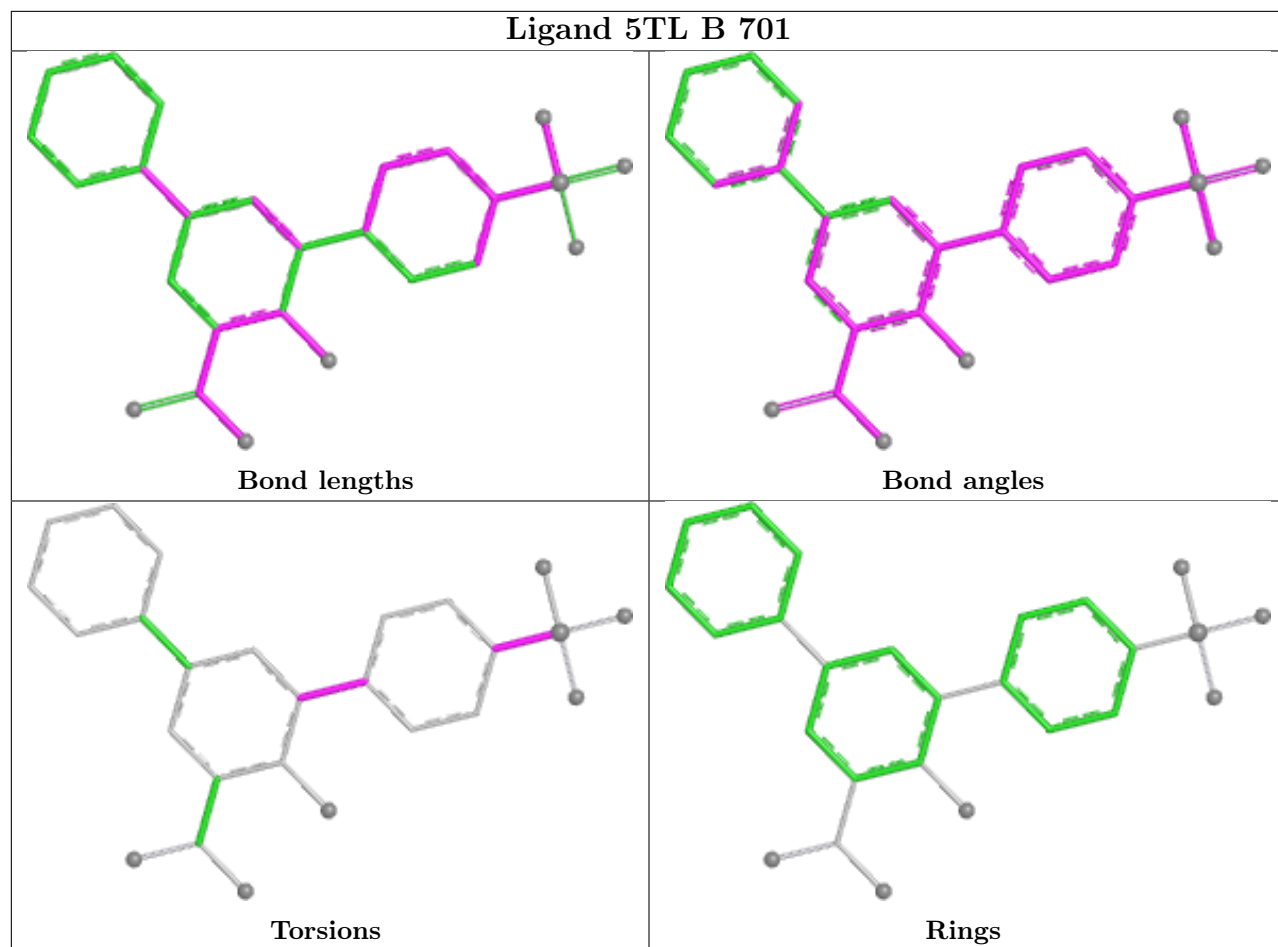


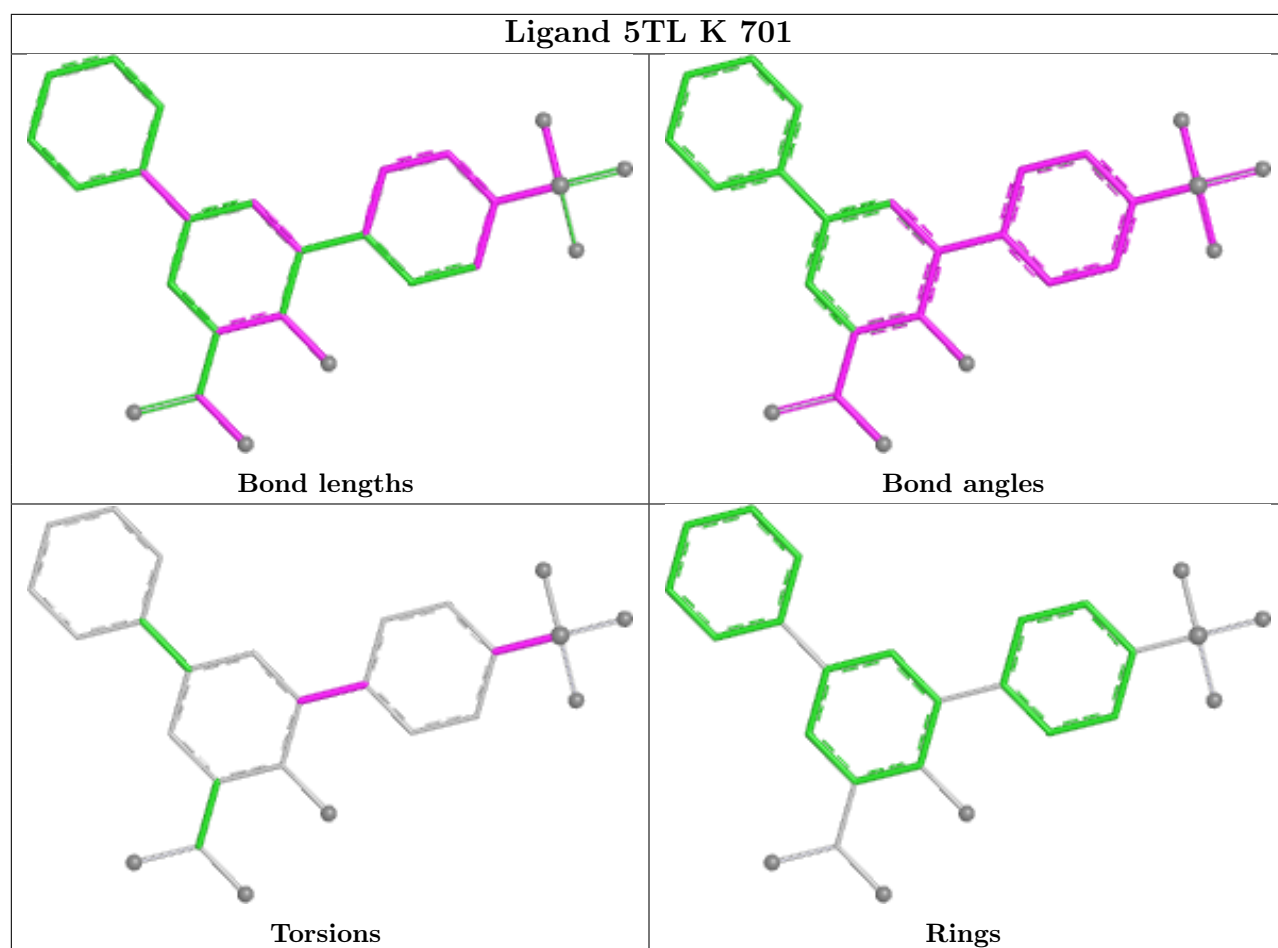


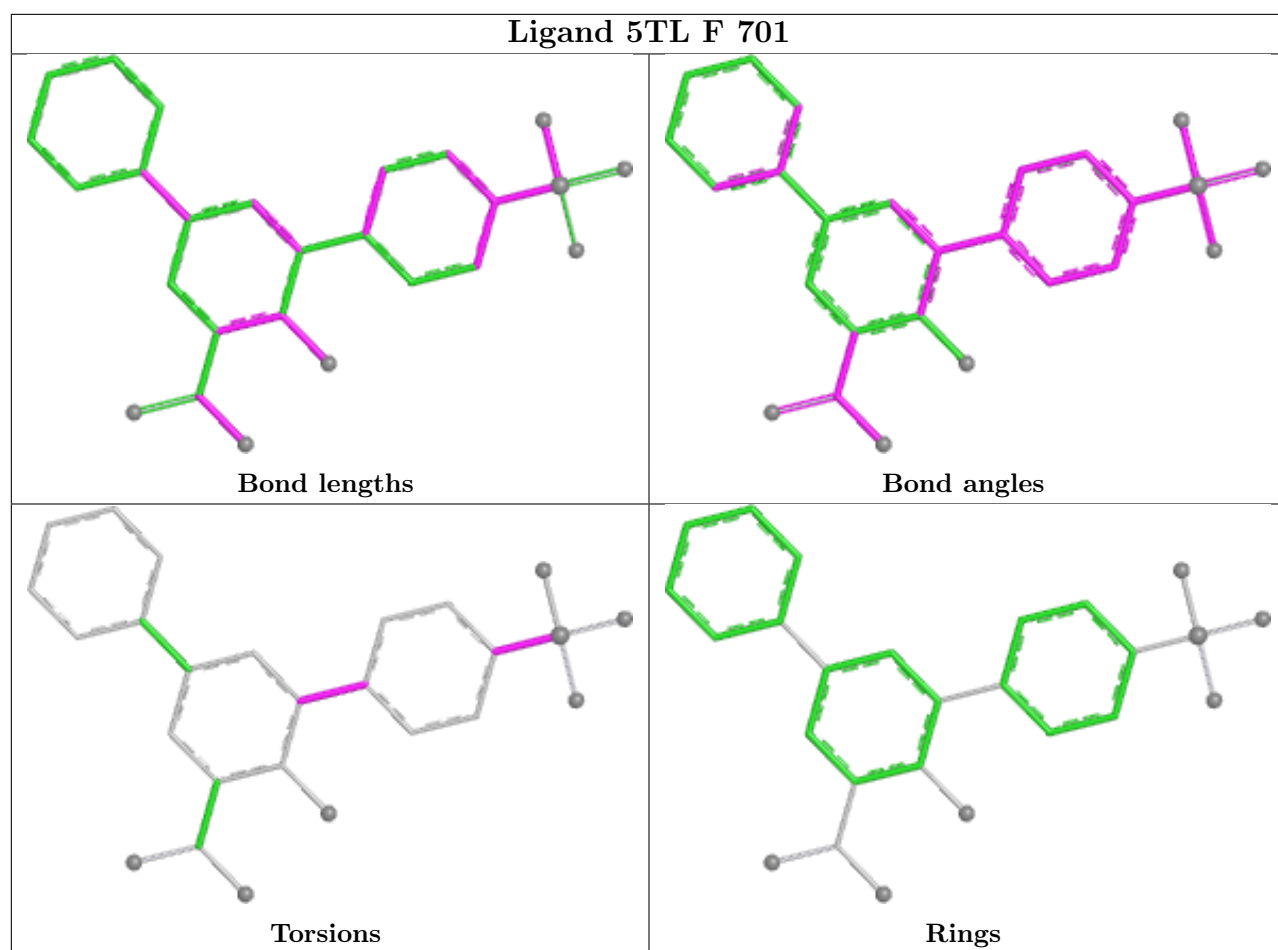


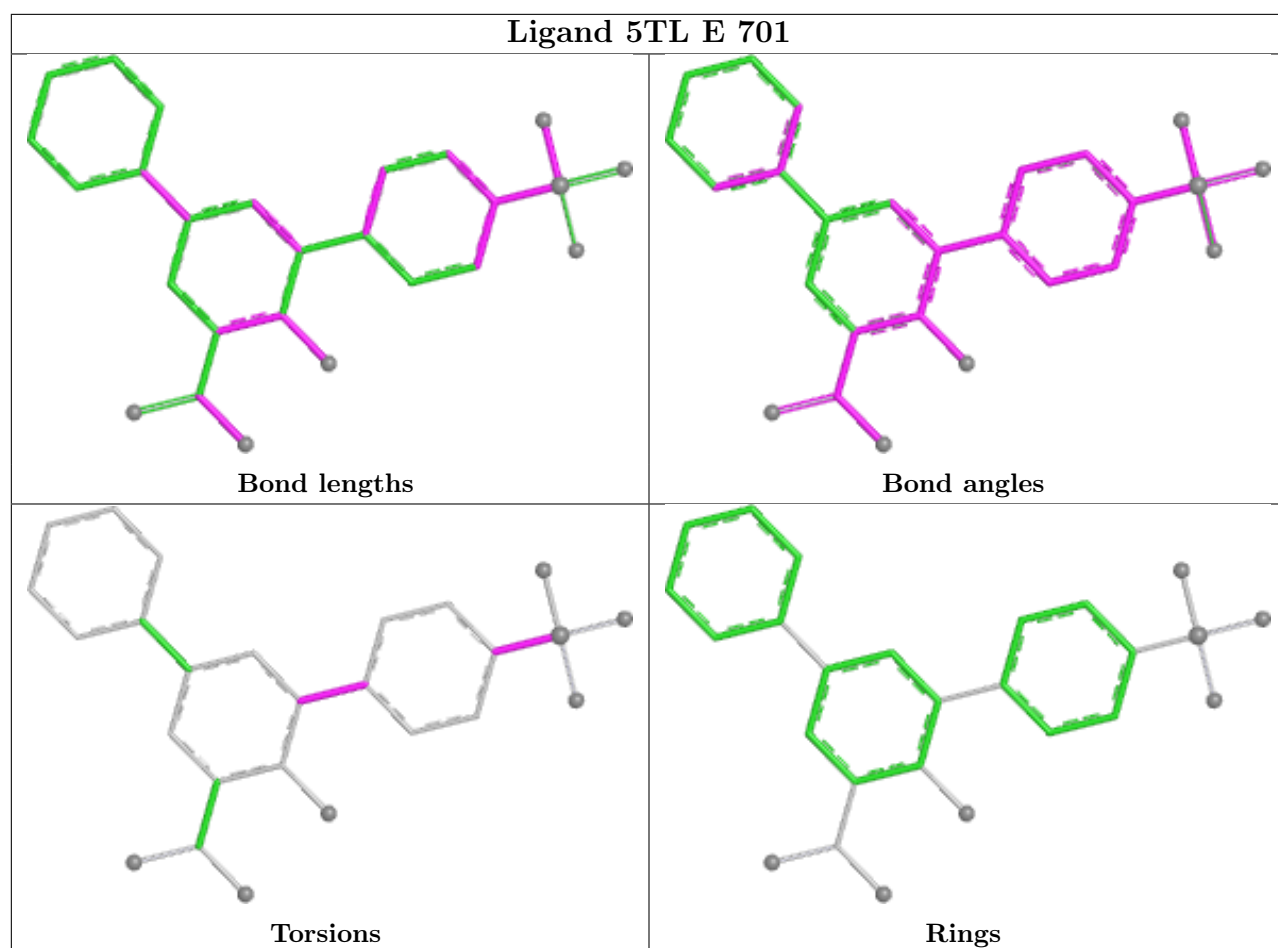


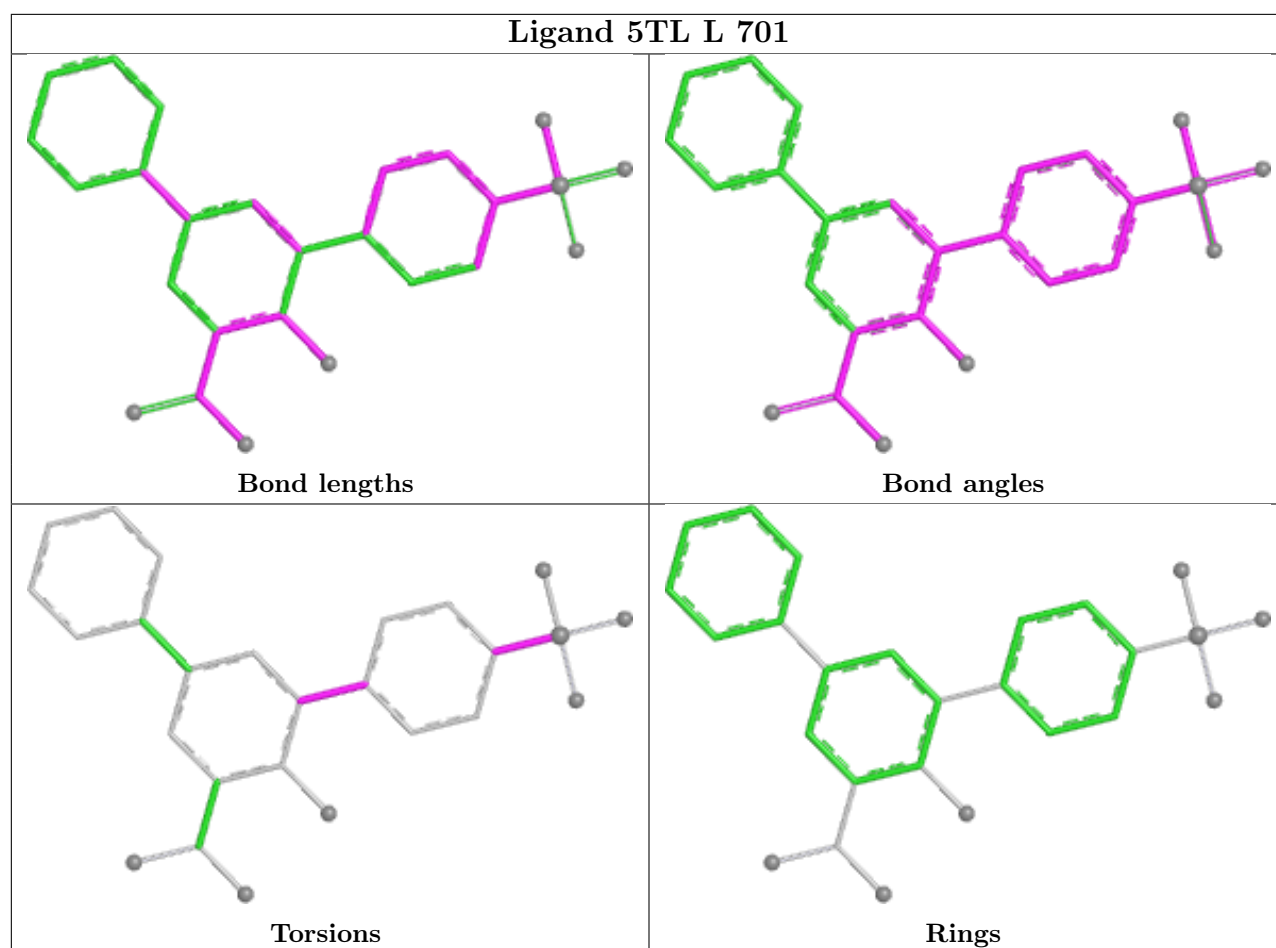


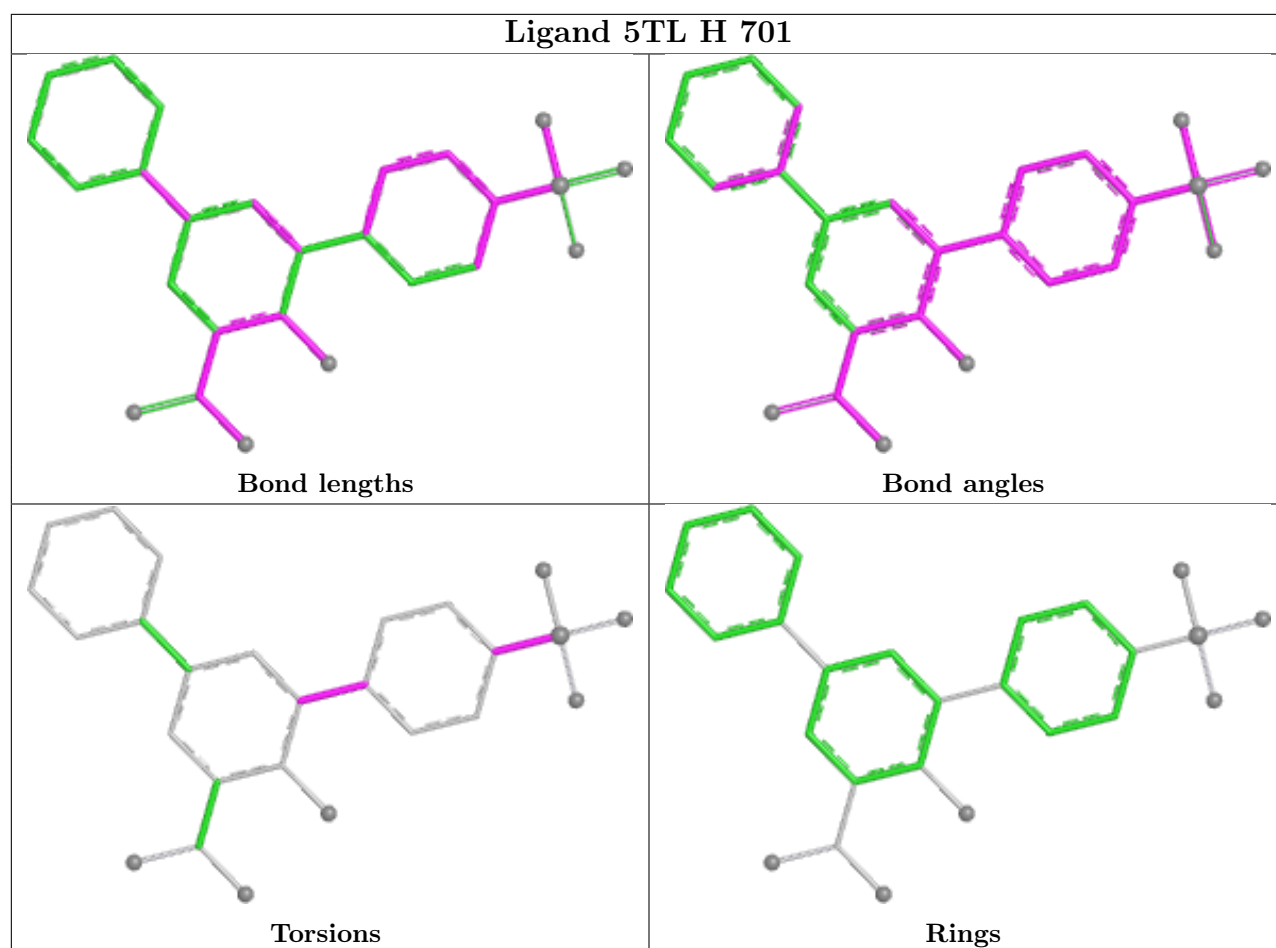












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	655/655 (100%)	-0.00	13 (1%) 65 51	124, 249, 346, 440	0
1	B	655/655 (100%)	-0.11	11 (1%) 69 55	166, 260, 355, 433	0
1	C	655/655 (100%)	-0.05	11 (1%) 69 55	148, 254, 349, 435	0
1	D	655/655 (100%)	-0.05	18 (2%) 56 44	164, 262, 366, 442	0
1	E	655/655 (100%)	0.01	13 (1%) 65 51	132, 252, 350, 465	0
1	F	655/655 (100%)	-0.11	9 (1%) 73 58	164, 262, 370, 469	0
1	G	655/655 (100%)	0.04	10 (1%) 72 57	67, 249, 345, 479	0
1	H	655/655 (100%)	-0.13	6 (0%) 81 67	149, 261, 356, 419	0
1	I	655/655 (100%)	-0.12	8 (1%) 76 62	130, 257, 355, 440	0
1	J	655/655 (100%)	-0.02	12 (1%) 67 53	162, 264, 366, 440	0
1	K	655/655 (100%)	0.05	12 (1%) 67 53	128, 252, 347, 450	0
1	L	655/655 (100%)	0.01	13 (1%) 65 51	165, 263, 370, 484	0
All	All	7860/7860 (100%)	-0.04	136 (1%) 69 55	67, 257, 357, 484	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	LYS	6.0
1	L	653	LEU	4.8
1	K	93	LEU	4.6
1	A	656	ILE	4.5
1	D	65	MET	4.3

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5TH	T	7	17/18	0.01	0.11	286,465,514,523	0
3	5TK	T	6	13/14	0.18	0.11	498,545,563,567	0
2	5LS	Z	1	20/20	0.18	0.09	404,467,489,501	0
2	GLC	U	2	11/12	0.22	0.14	419,441,472,478	0
3	Z4K	O	5	15/16	0.23	0.10	441,493,519,523	0
2	GLC	W	2	11/12	0.25	0.12	347,378,409,472	0
2	PDX	S	3	19/20	0.31	0.10	242,541,570,575	0
2	GLC	R	2	11/12	0.35	0.14	358,404,431,439	0
3	5TH	O	7	17/18	0.35	0.08	382,454,506,522	0
3	5TJ	O	2	17/18	0.36	0.09	520,543,568,570	0
3	5TM	T	3	17/18	0.36	0.12	479,506,524,529	0
3	5LS	T	1	20/20	0.38	0.11	390,510,562,568	0
2	PDX	X	3	19/20	0.40	0.14	120,485,579,583	0
2	PDX	P	3	19/20	0.42	0.11	246,460,539,547	0
2	5LS	Y	1	20/20	0.44	0.08	275,459,474,500	0
3	5TM	O	3	17/18	0.44	0.11	442,503,540,543	0
2	PDX	W	3	19/20	0.50	0.14	366,456,485,489	0
2	PDX	M	3	19/20	0.54	0.06	294,542,568,576	0
3	5TJ	T	4	17/18	0.55	0.09	291,502,575,583	0
3	5TJ	O	4	17/18	0.60	0.08	394,528,538,539	0
2	GLC	X	2	11/12	0.62	0.09	335,392,442,495	0
3	5LS	O	1	20/20	0.62	0.12	410,470,536,552	0
2	5LS	V	1	20/20	0.63	0.08	368,431,456,471	0
2	GLC	P	2	11/12	0.64	0.13	259,379,417,450	0
3	5TK	O	6	13/14	0.66	0.07	377,494,522,528	0
2	5LS	S	1	20/20	0.67	0.11	318,398,444,472	0
2	5LS	U	1	20/20	0.70	0.09	340,440,517,518	0
2	5LS	N	1	20/20	0.72	0.07	320,445,483,493	0
2	PDX	V	3	19/20	0.72	0.08	373,430,480,492	0
2	PDX	R	3	19/20	0.73	0.11	382,434,463,471	0
2	5LS	Q	1	20/20	0.74	0.07	356,421,481,498	0
2	5LS	M	1	20/20	0.77	0.10	337,376,407,435	0
2	PDX	Q	3	19/20	0.77	0.07	309,489,529,530	0
2	GLC	V	2	11/12	0.78	0.12	380,397,417,446	0
2	5LS	W	1	20/20	0.79	0.11	406,436,450,462	0
2	5LS	X	1	20/20	0.79	0.08	384,414,438,442	0
2	5LS	a	1	20/20	-	-	282,367,436,438	0

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Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	a	2	11/12	-	-	370,394,435,475	0
2	PDX	a	3	19/20	-	-	394,475,502,529	0
2	5LS	b	1	20/20	-	-	361,462,493,495	0
2	GLC	b	2	11/12	-	-	263,307,356,360	0
2	PDX	b	3	19/20	-	-	241,384,434,436	0
2	5LS	d	1	20/20	-	-	291,429,473,484	0
2	GLC	d	2	11/12	-	-	220,288,388,445	0
2	PDX	d	3	19/20	-	-	266,436,468,474	0
2	5LS	e	1	20/20	-	-	402,453,485,501	0
2	GLC	e	2	11/12	-	-	394,429,498,537	0
2	PDX	e	3	19/20	-	-	404,488,531,532	0
2	5LS	f	1	20/20	-	-	414,473,550,553	0
2	GLC	f	2	11/12	-	-	361,408,422,461	0
2	PDX	f	3	19/20	-	-	291,428,471,474	0
2	5LS	g	1	20/20	-	-	388,452,499,510	0
2	GLC	g	2	11/12	-	-	216,358,388,409	0
2	PDX	g	3	19/20	-	-	247,401,449,453	0
2	5LS	h	1	20/20	-	-	255,515,567,577	0
2	GLC	h	2	11/12	-	-	197,292,365,403	0
2	PDX	h	3	19/20	-	-	270,404,472,478	0
2	5LS	j	1	20/20	-	-	308,429,475,496	0
2	GLC	j	2	11/12	-	-	329,361,377,405	0
2	PDX	j	3	19/20	-	-	321,419,508,517	0
2	5LS	k	1	20/20	-	-	363,425,467,471	0
2	GLC	k	2	11/12	-	-	360,413,466,537	0
2	PDX	k	3	19/20	-	-	442,555,569,571	0
2	5LS	l	1	20/20	-	-	347,522,574,579	0
2	GLC	l	2	11/12	-	-	321,350,440,452	0
2	PDX	l	3	19/20	-	-	257,458,487,488	0
2	5LS	m	1	20/20	-	-	358,404,444,460	0
2	GLC	m	2	11/12	-	-	330,367,393,433	0
2	PDX	m	3	19/20	-	-	373,474,502,503	0
2	5LS	n	1	20/20	-	-	442,520,539,550	0
2	GLC	n	2	11/12	-	-	315,385,428,432	0
2	PDX	n	3	19/20	-	-	302,421,476,480	0
2	PDX	U	3	19/20	0.80	0.12	395,433,465,466	0
2	GLC	N	2	11/12	0.80	0.08	357,383,424,432	0
2	PDX	Y	3	19/20	0.80	0.08	330,398,456,471	0
2	5LS	P	1	20/20	0.80	0.07	348,474,507,510	0
2	PDX	Z	3	19/20	0.81	0.09	366,469,493,510	0
2	5LS	R	1	20/20	0.84	0.11	412,438,452,452	0
2	GLC	S	2	11/12	0.84	0.07	287,335,428,484	0

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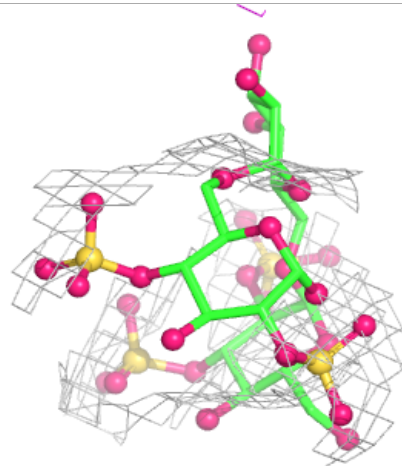
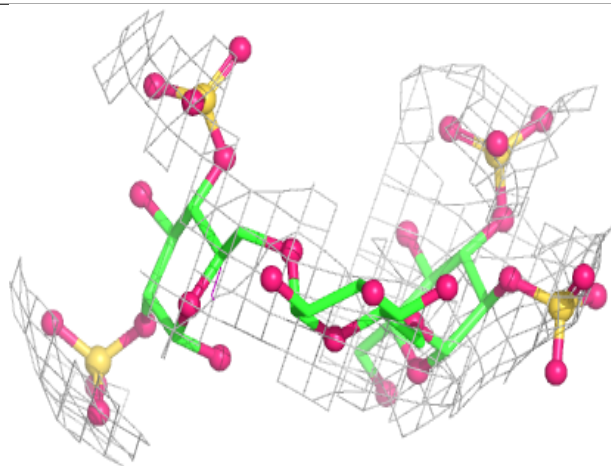
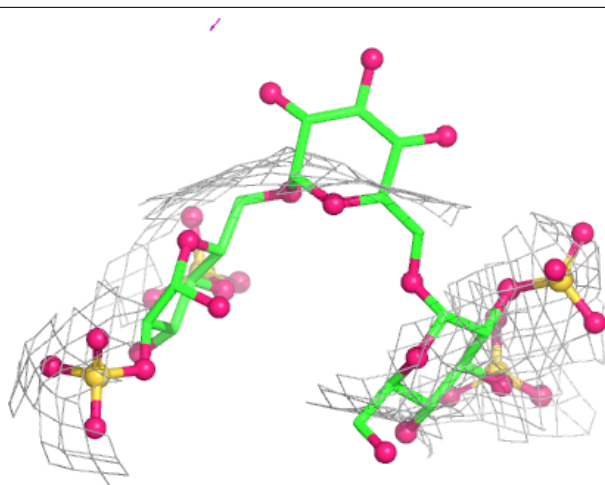
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	Y	2	11/12	0.84	0.06	275,289,341,375	0
3	5TJ	T	2	17/18	0.85	0.07	487,535,554,557	0
2	GLC	Z	2	11/12	0.86	0.10	267,377,431,435	0
2	PDX	N	3	19/20	0.87	0.06	218,410,475,496	0
2	GLC	M	2	11/12	0.88	0.08	366,443,481,495	0
3	Z4K	T	5	15/16	0.89	0.08	512,546,562,567	0
2	GLC	Q	2	11/12	0.96	0.07	333,423,476,483	0
3	5LS	c	1	20/20	-	-	430,502,561,583	0
3	5TJ	c	2	17/18	-	-	305,465,516,533	0
3	5TM	c	3	17/18	-	-	462,507,517,524	0
3	5TJ	c	4	17/18	-	-	452,494,530,541	0
3	Z4K	c	5	15/16	-	-	442,503,528,534	0
3	5TK	c	6	13/14	-	-	431,547,571,574	0
3	5TH	c	7	17/18	-	-	386,527,562,566	0
3	5LS	i	1	20/20	-	-	472,553,561,566	0
3	5TJ	i	2	17/18	-	-	468,554,566,566	0
3	5TM	i	3	17/18	-	-	429,491,543,555	0
3	5TJ	i	4	17/18	-	-	385,519,554,575	0
3	Z4K	i	5	15/16	-	-	437,501,519,520	0
3	5TK	i	6	13/14	-	-	409,452,467,476	0
3	5TH	i	7	17/18	-	-	384,477,520,526	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

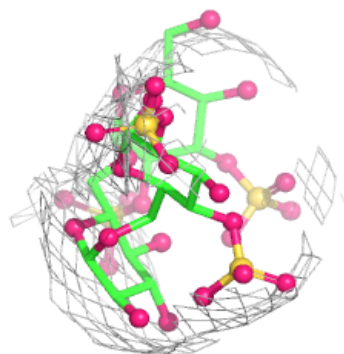
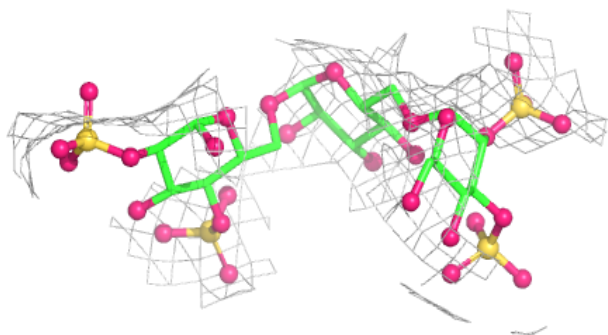
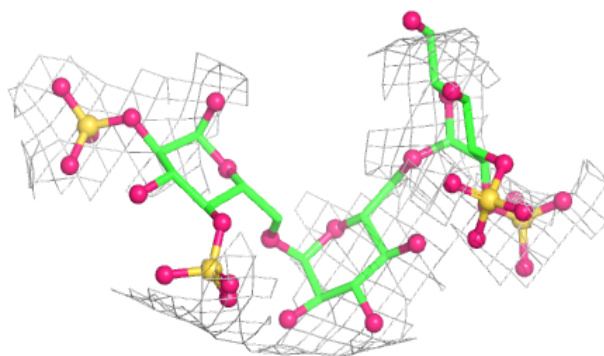
Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

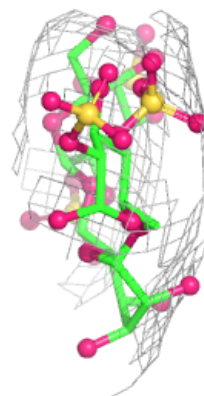
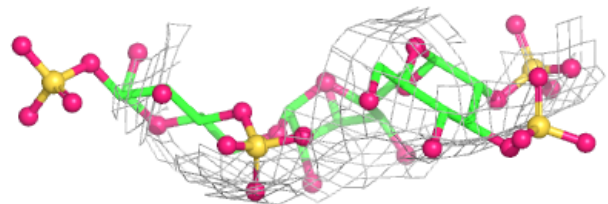
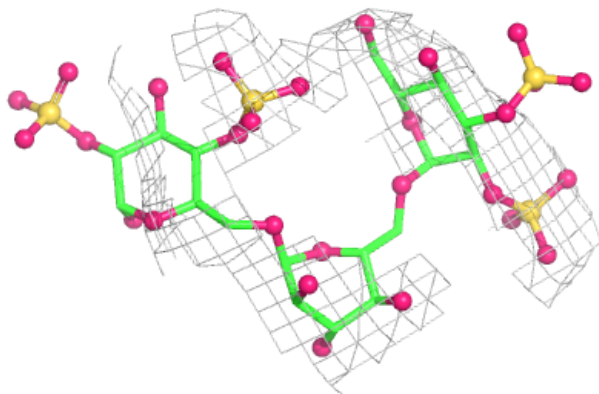


Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

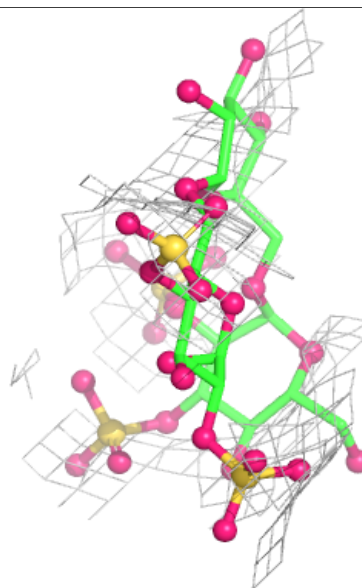
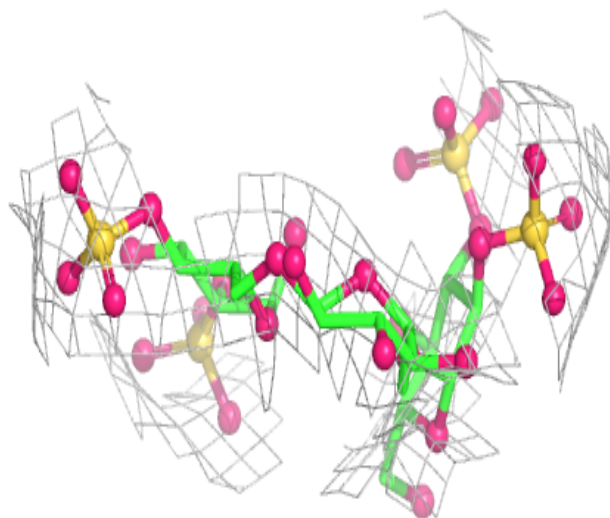
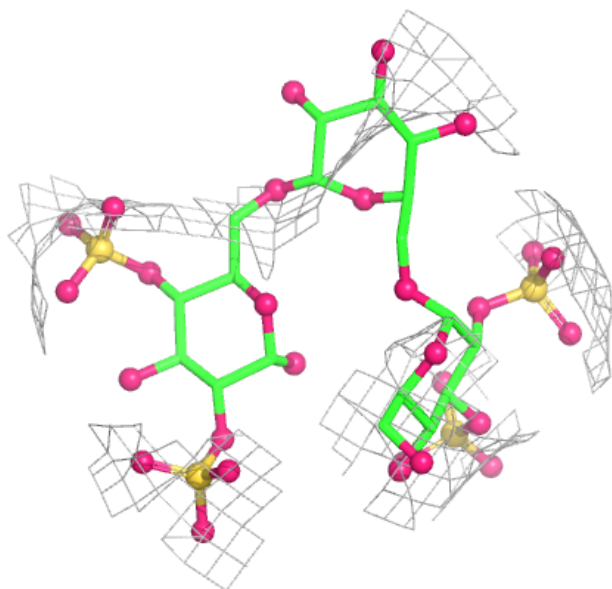
**Electron density around Chain P:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



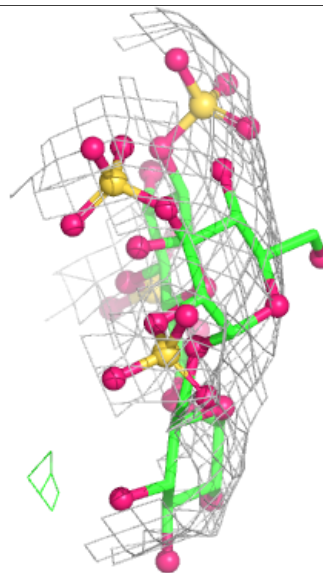
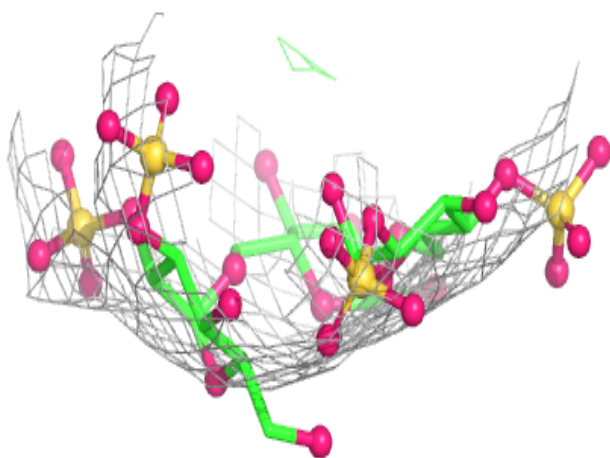
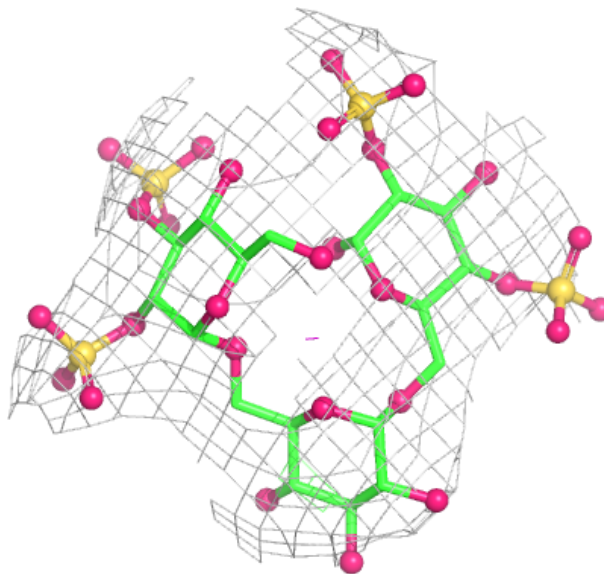
Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



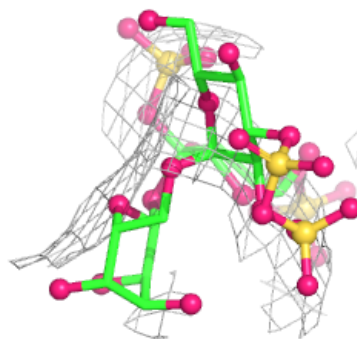
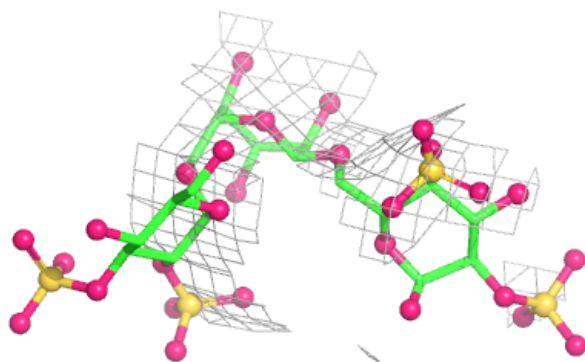
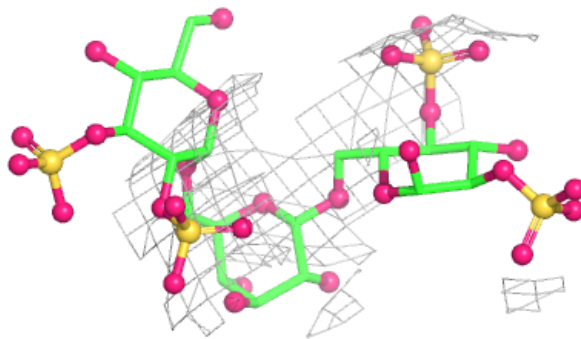
Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



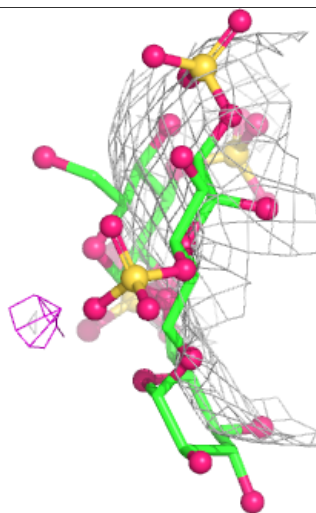
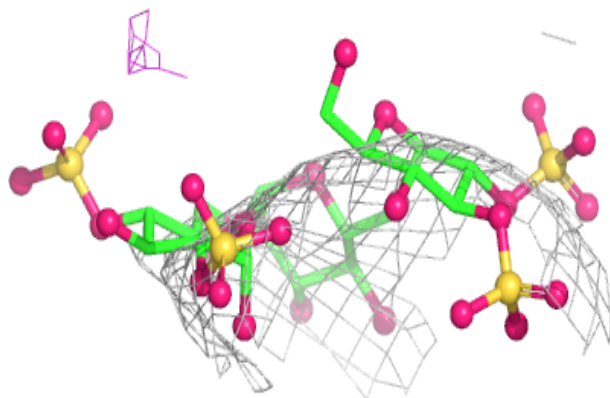
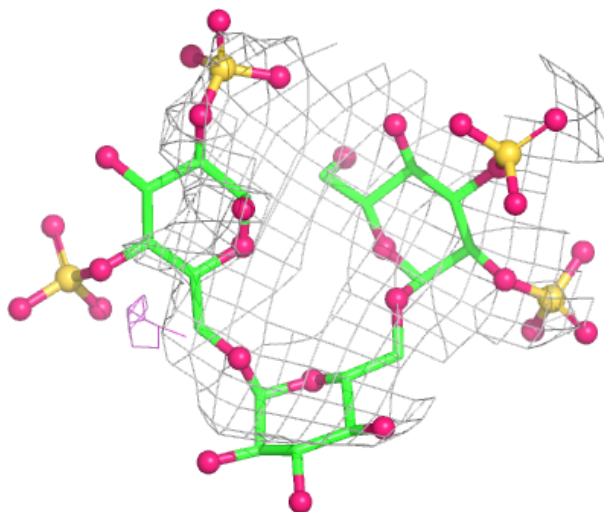
Electron density around Chain S:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



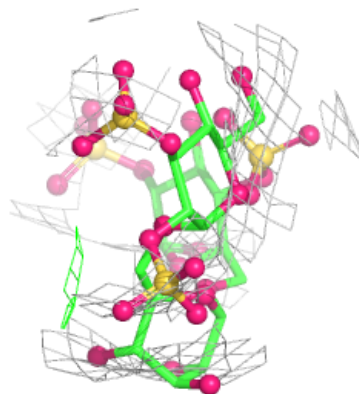
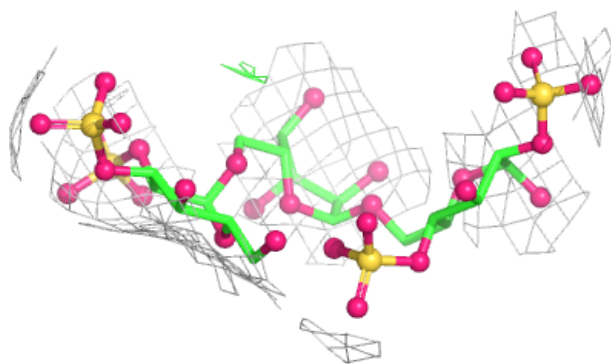
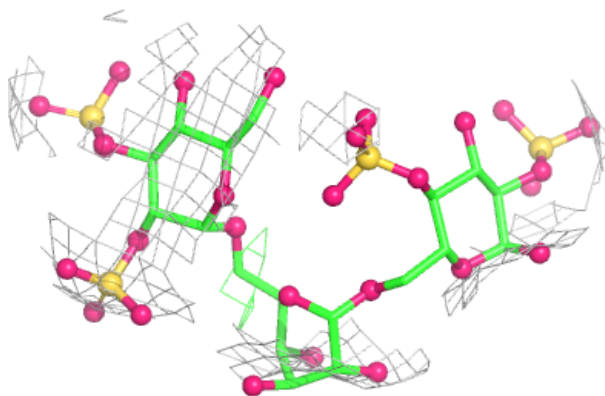
Electron density around Chain U:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



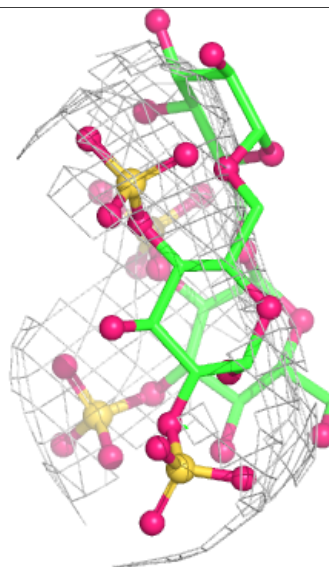
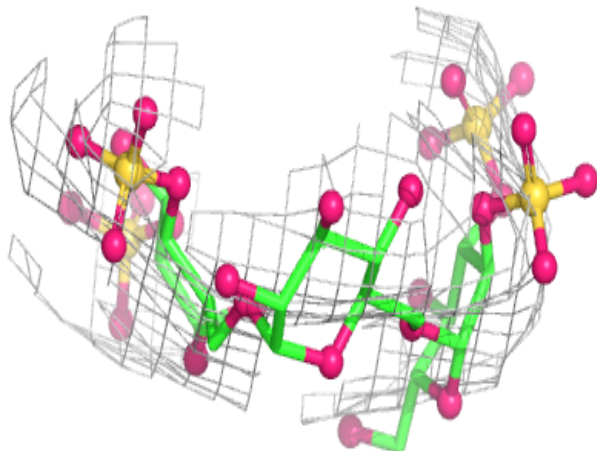
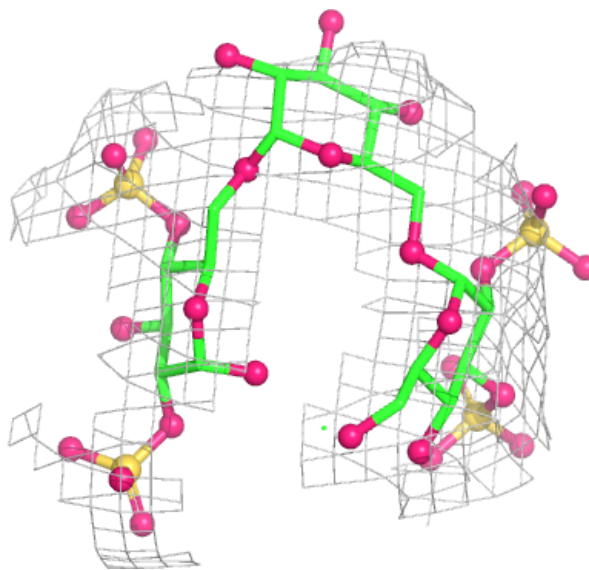
Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



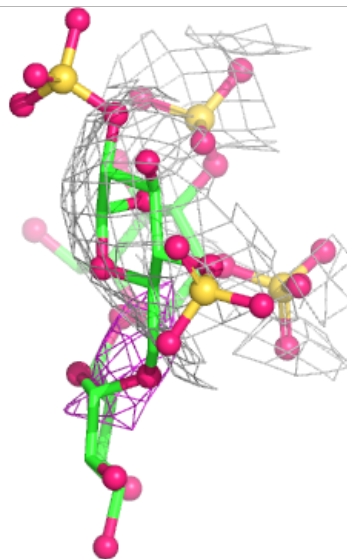
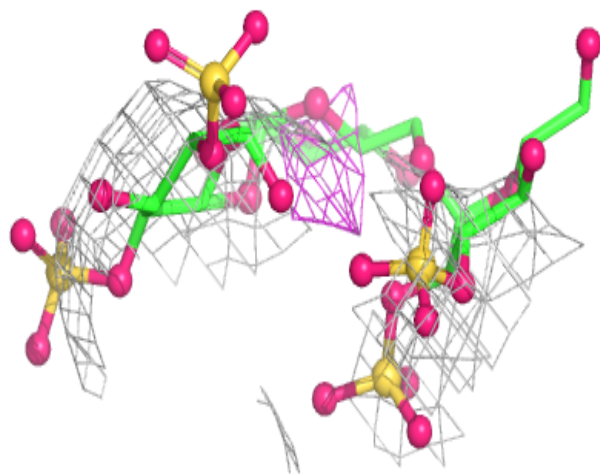
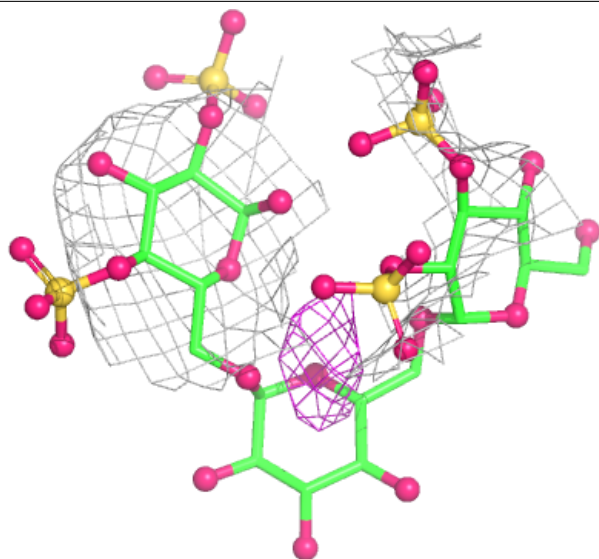
Electron density around Chain W:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



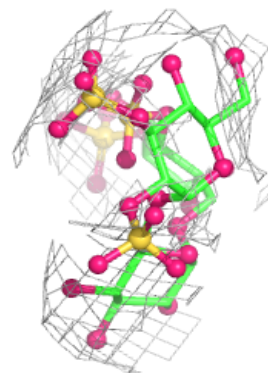
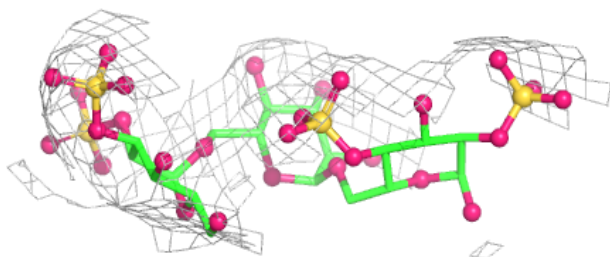
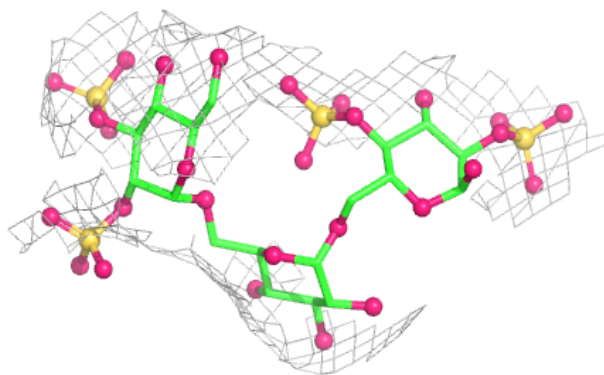
Electron density around Chain X:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

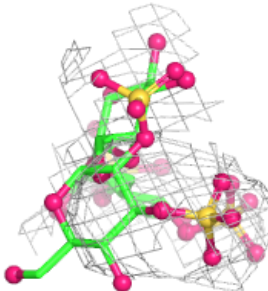
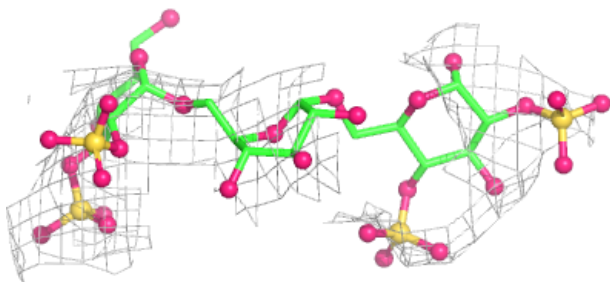
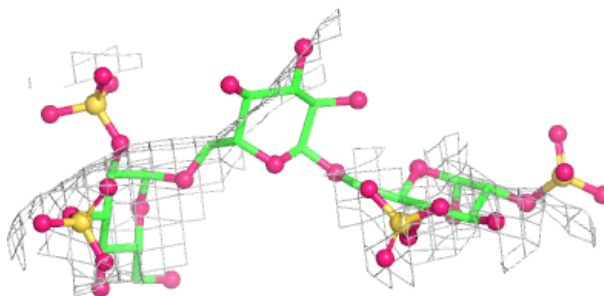


Electron density around Chain Y:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

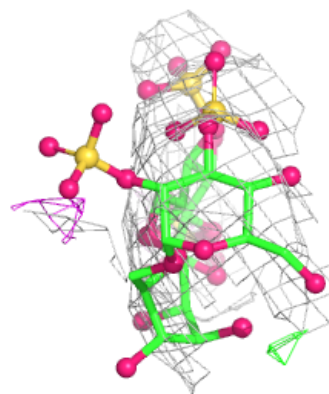
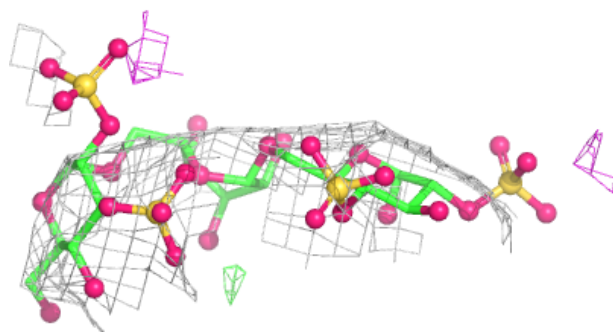
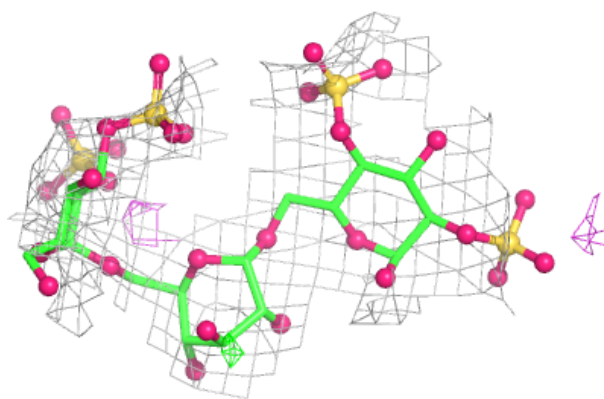
**Electron density around Chain Z:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

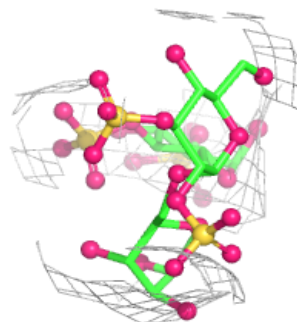
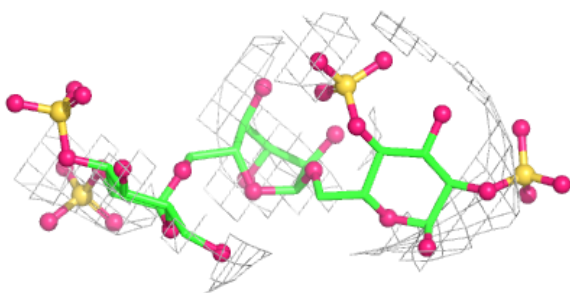
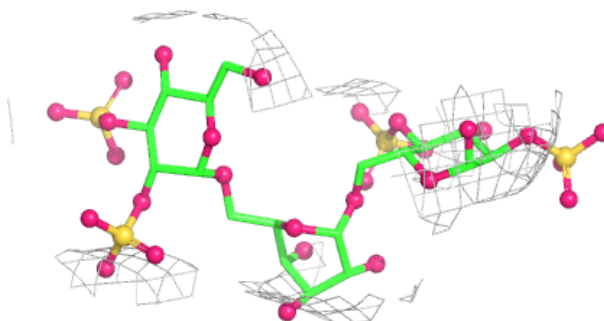


Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

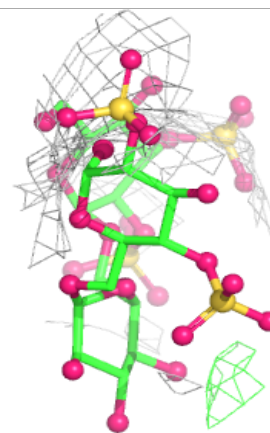
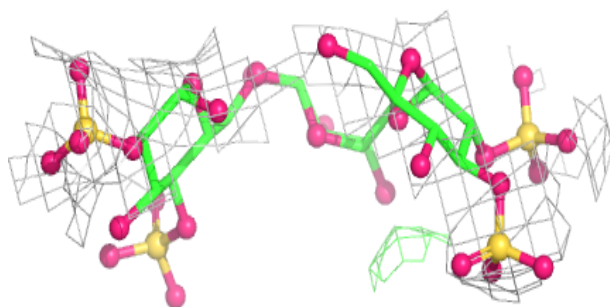
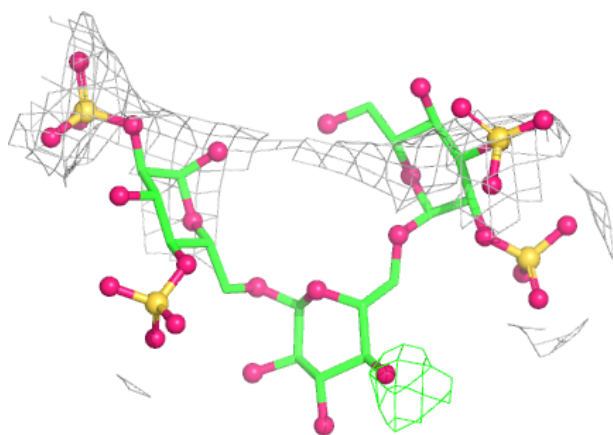
**Electron density around Chain b:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



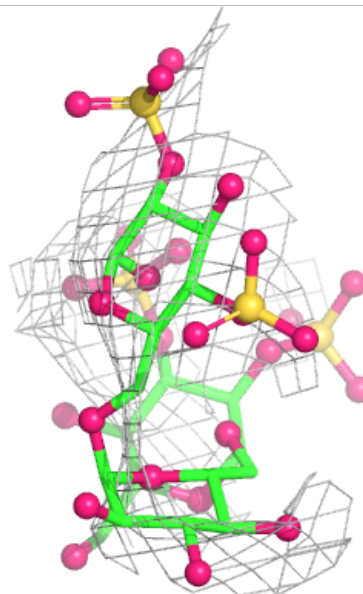
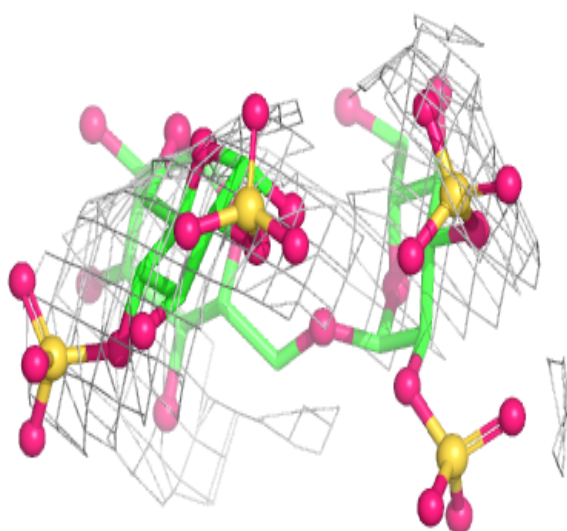
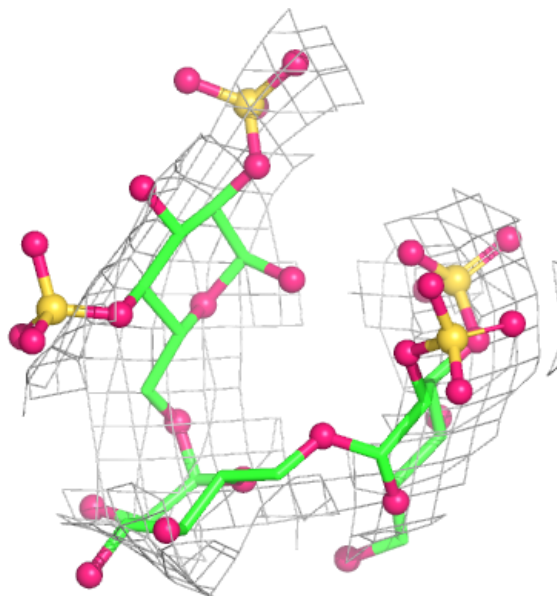
Electron density around Chain d:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



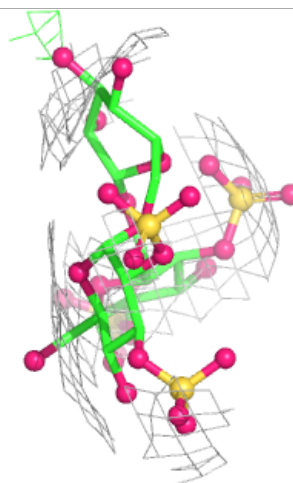
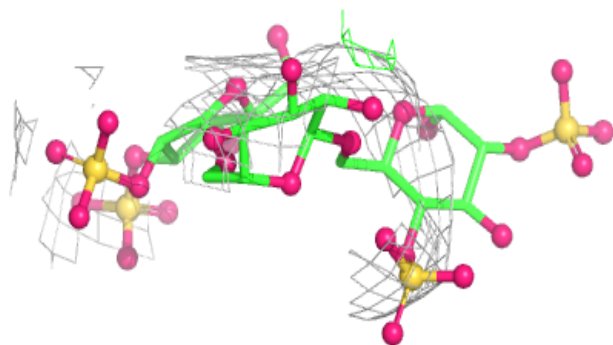
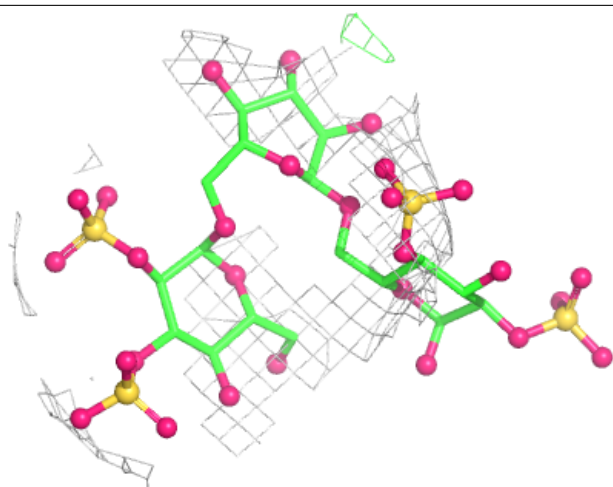
Electron density around Chain e:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



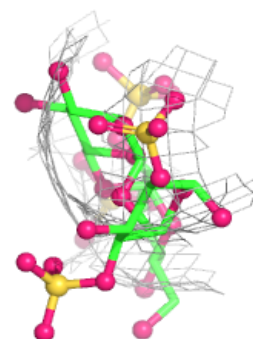
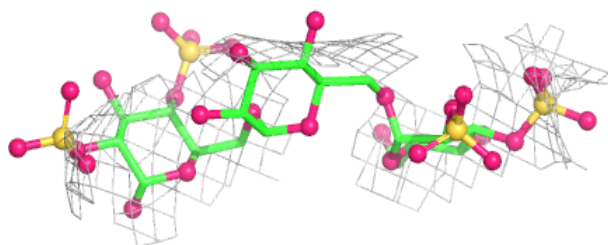
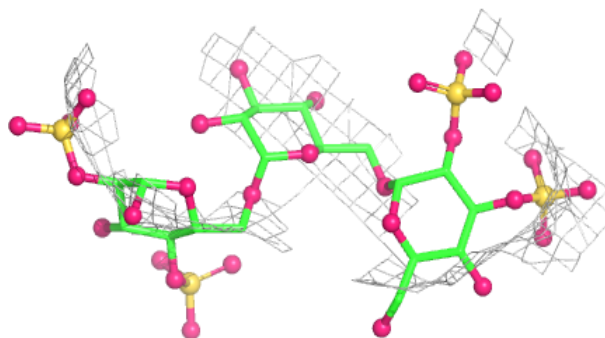
Electron density around Chain f:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

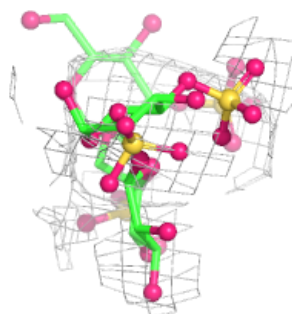
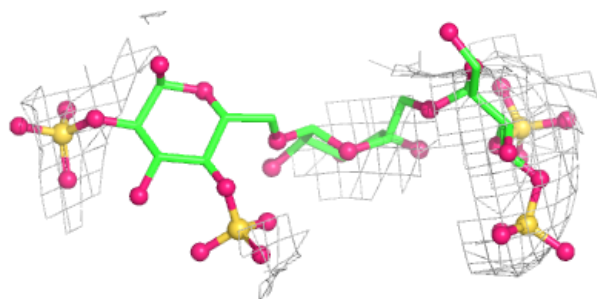
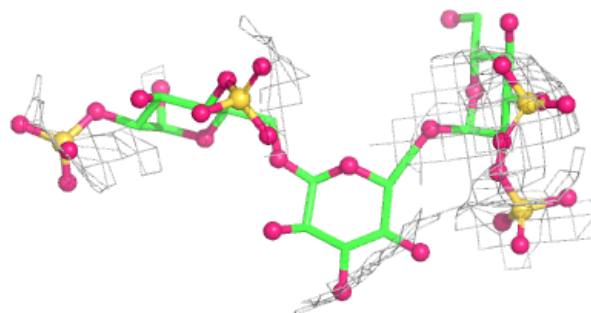


Electron density around Chain g:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

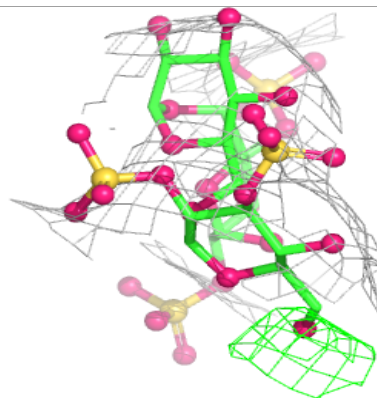
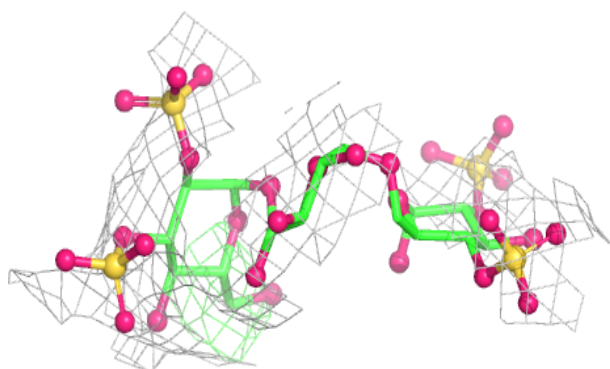
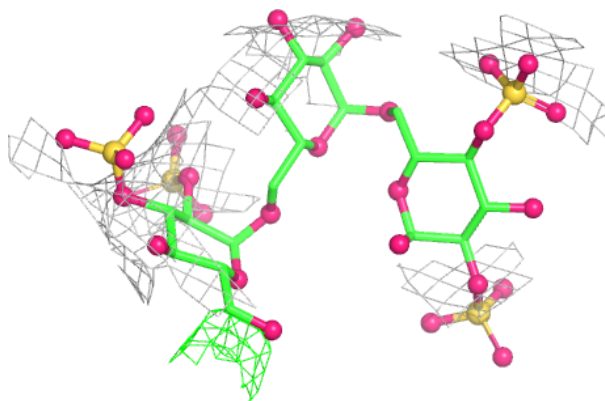
**Electron density around Chain h:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

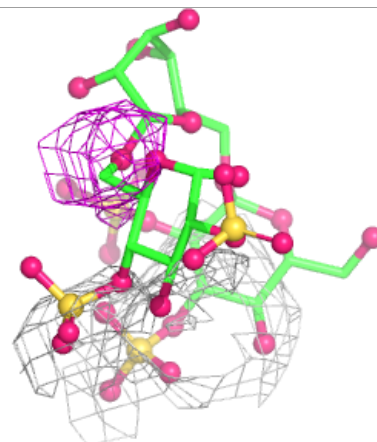
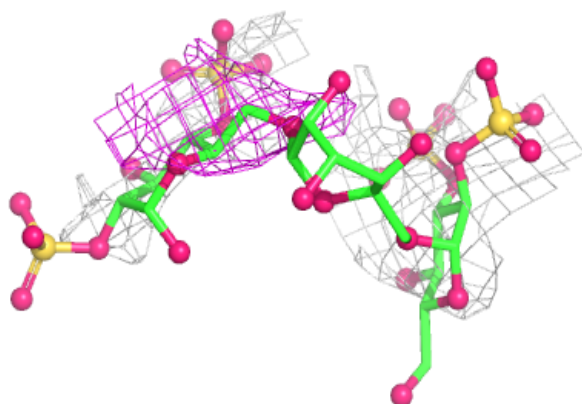
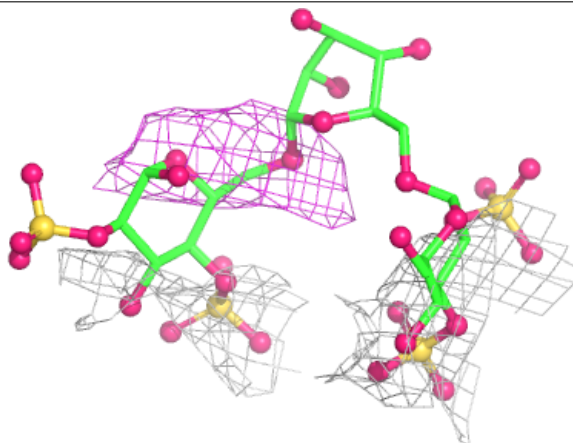


Electron density around Chain j:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

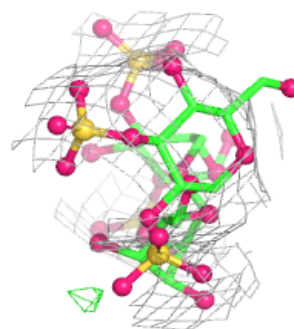
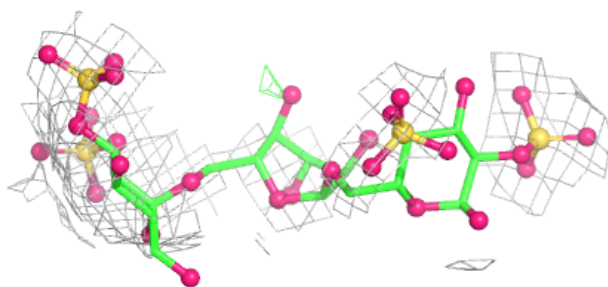
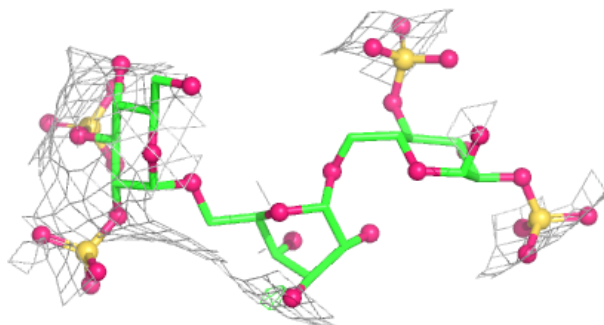
**Electron density around Chain k:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

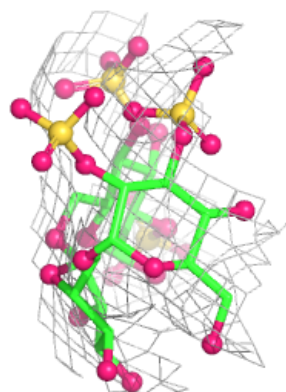
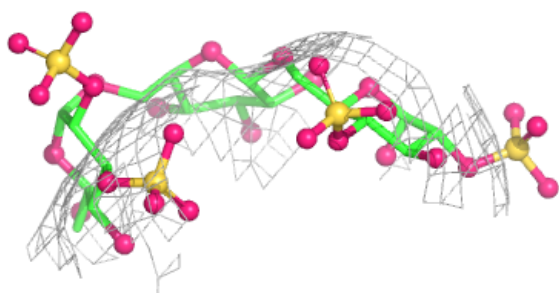
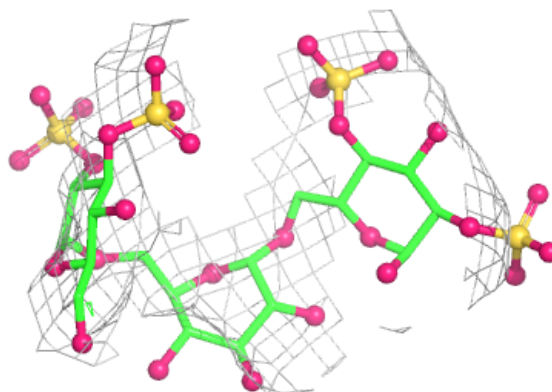


Electron density around Chain l:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

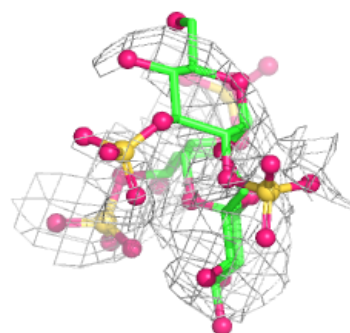
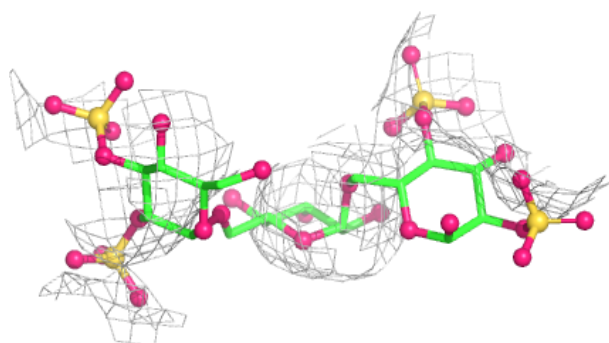
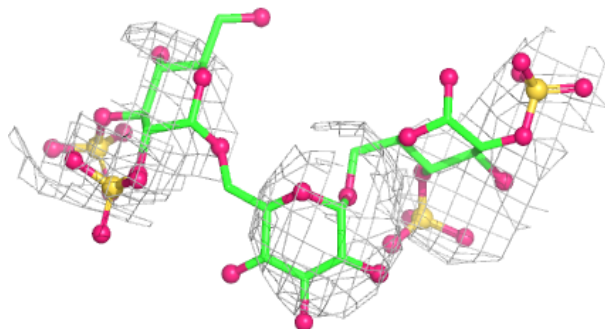
**Electron density around Chain m:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

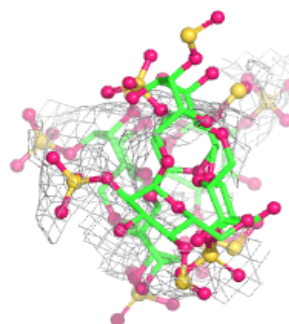
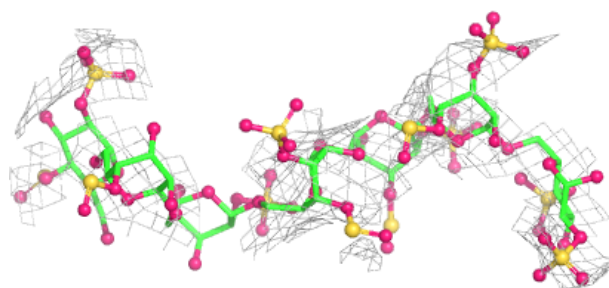
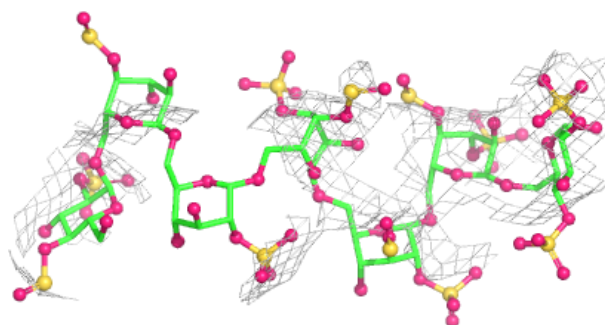


Electron density around Chain n:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

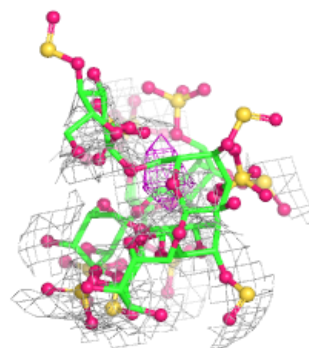
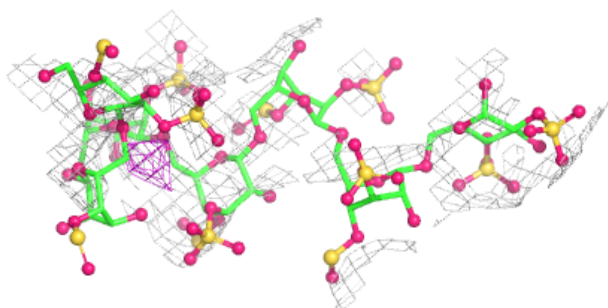
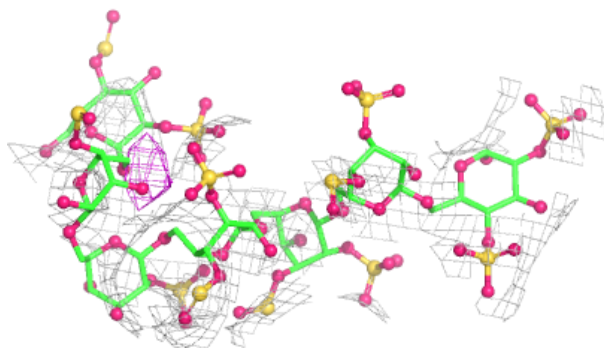
**Electron density around Chain O:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

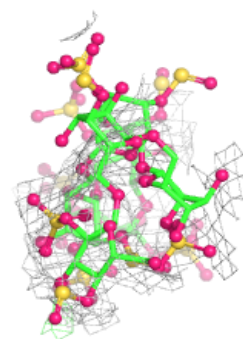
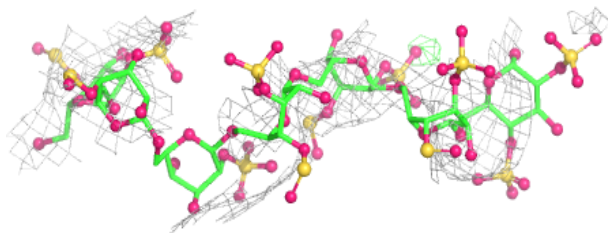
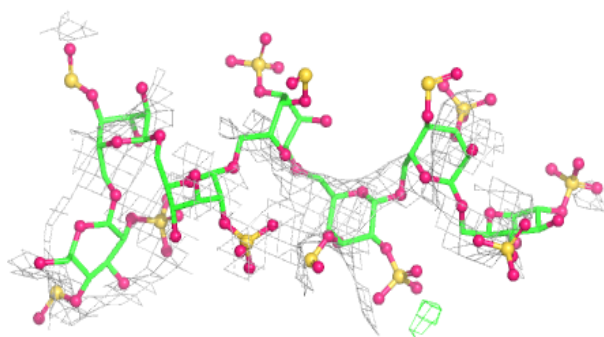


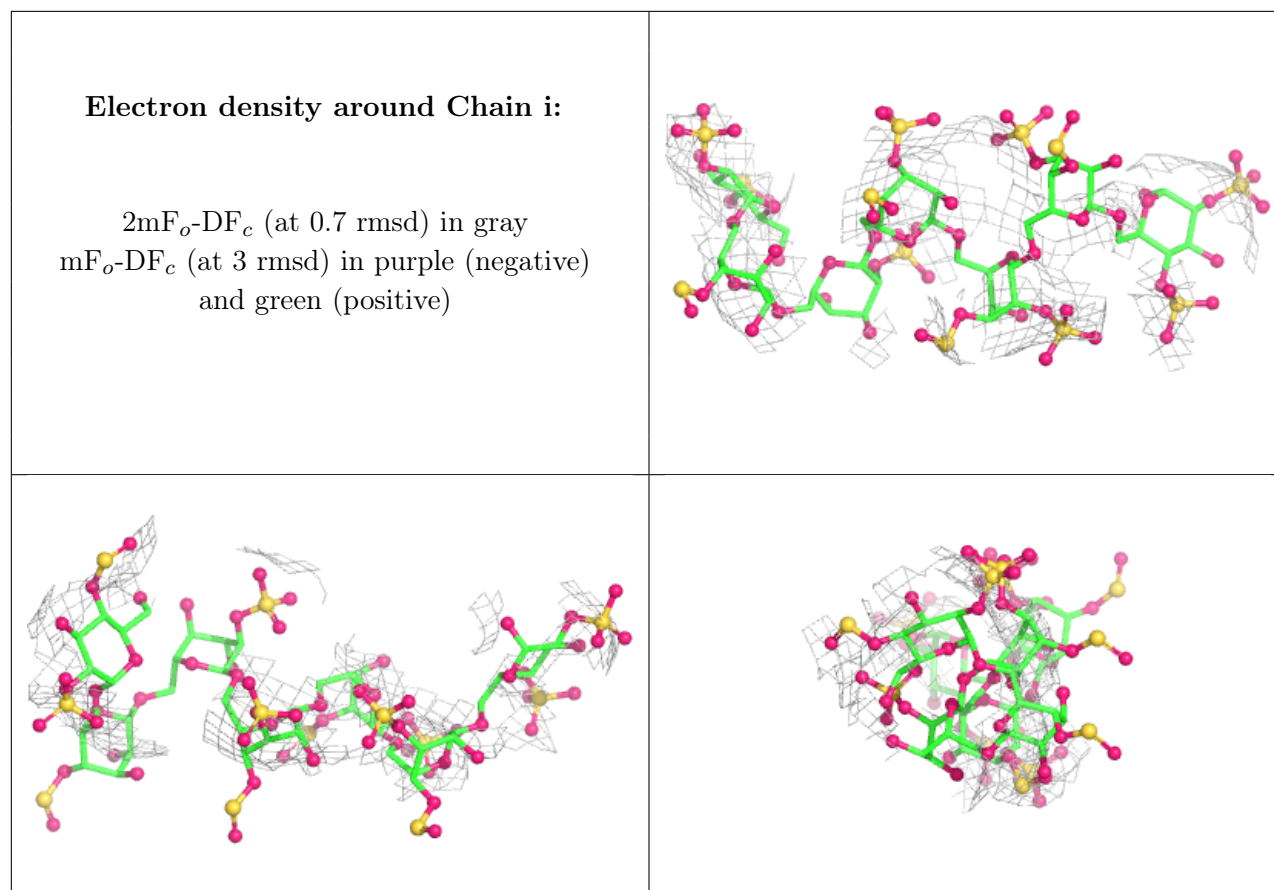
Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain c:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

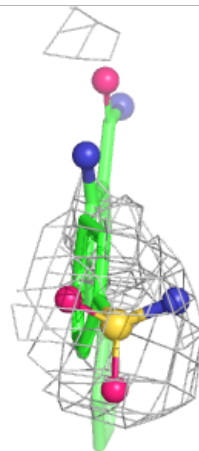
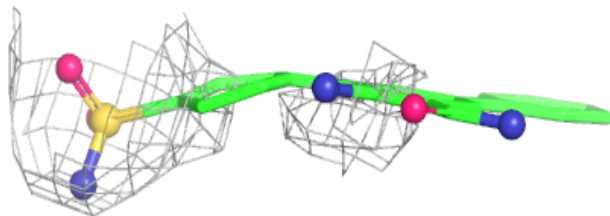
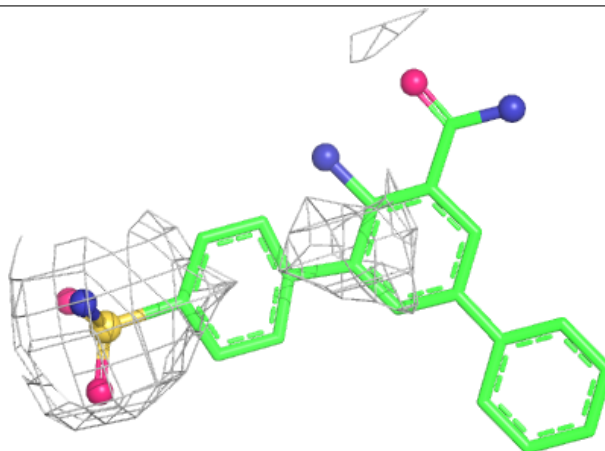
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5TL	B	701	26/26	0.74	0.15	149,237,280,287	0
4	5TL	F	701	26/26	0.75	0.24	157,307,408,431	0
4	5TL	H	701	26/26	0.76	0.17	226,257,279,282	0
4	5TL	L	701	26/26	0.76	0.18	158,266,335,350	0
4	5TL	D	701	26/26	0.81	0.19	197,297,320,332	0
4	5TL	E	701	26/26	0.83	0.17	127,197,233,277	0
4	5TL	J	701	26/26	0.83	0.18	179,264,307,319	0
4	5TL	A	701	26/26	0.83	0.16	121,206,278,306	0
4	5TL	G	701	26/26	0.86	0.14	108,200,280,288	0
4	5TL	I	701	26/26	0.87	0.14	152,242,284,323	0
4	5TL	K	701	26/26	0.89	0.13	131,202,237,288	0
4	5TL	C	701	26/26	0.89	0.14	150,234,279,291	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

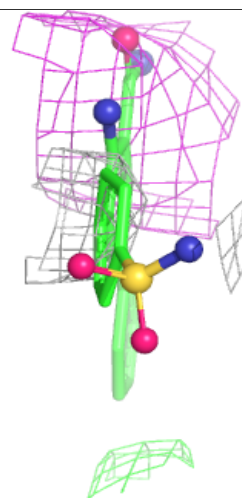
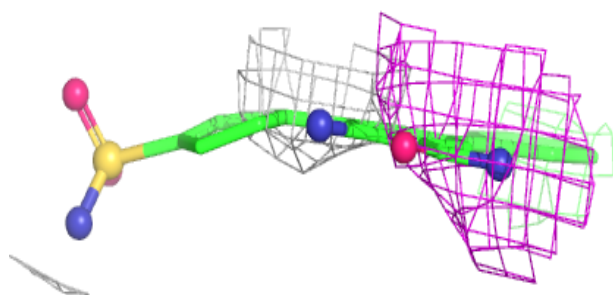
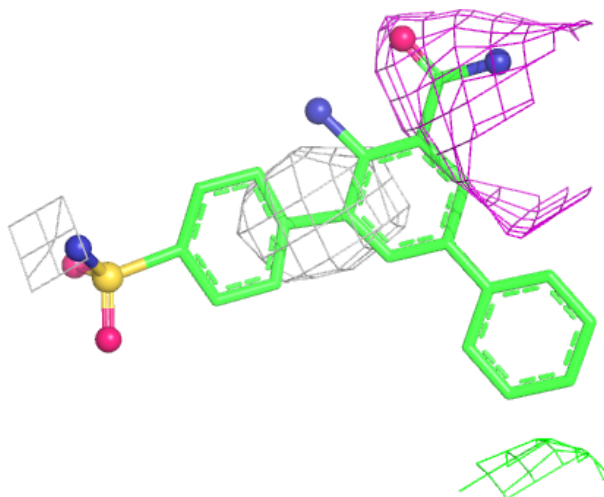
Electron density around 5TL B 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



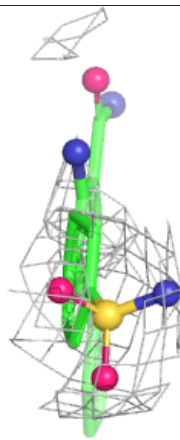
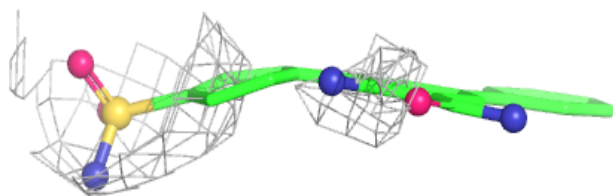
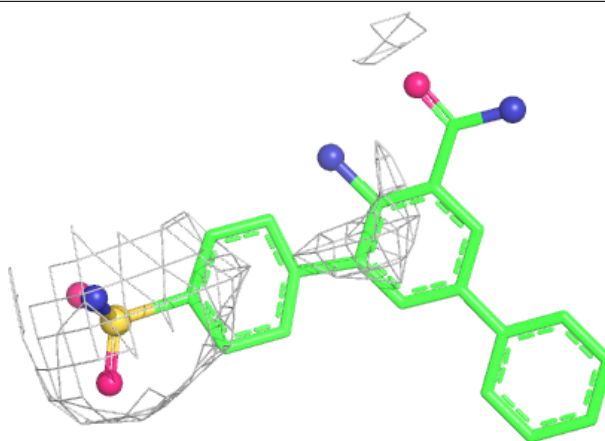
Electron density around 5TL F 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



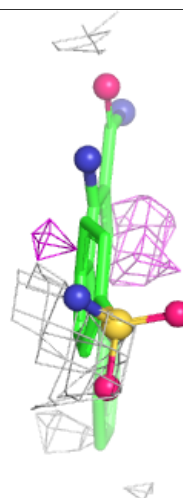
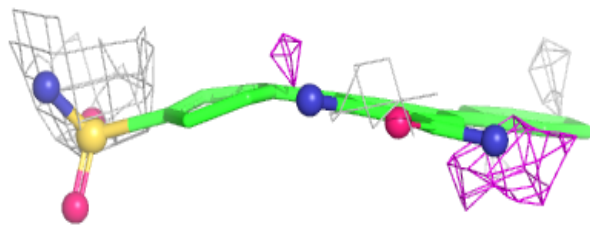
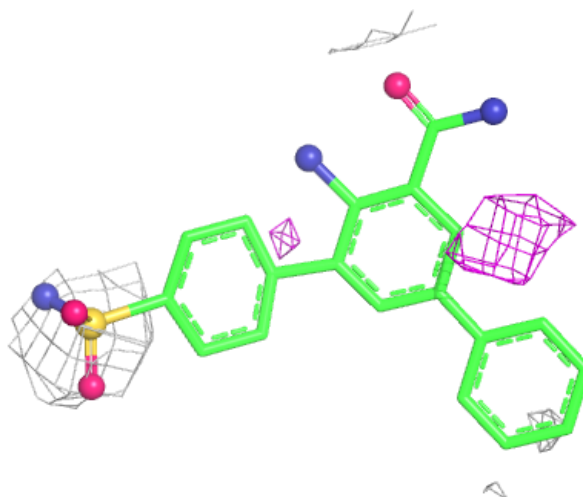
Electron density around 5TL H 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



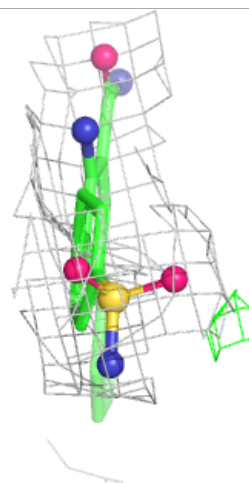
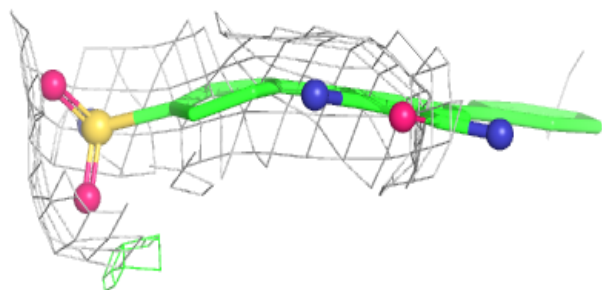
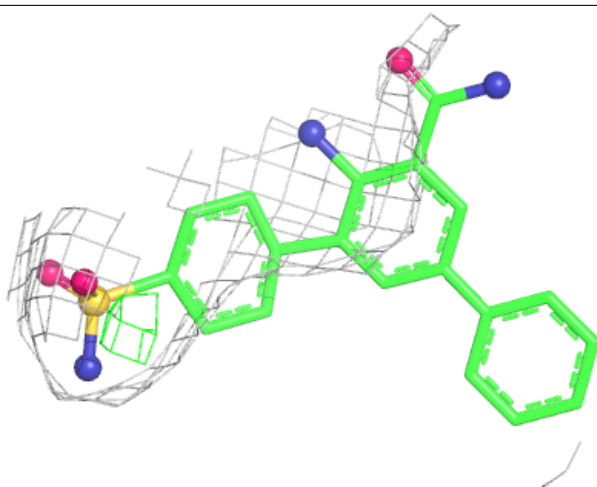
Electron density around 5TL L 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



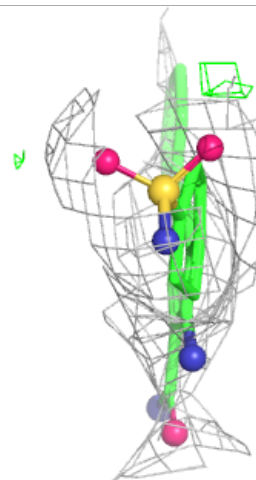
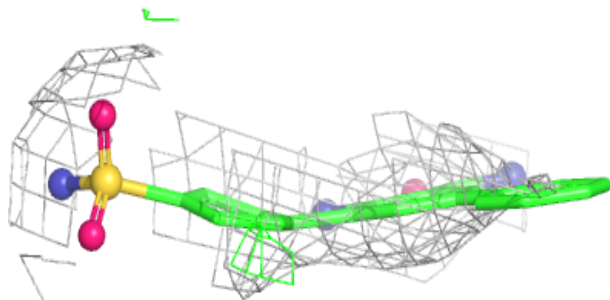
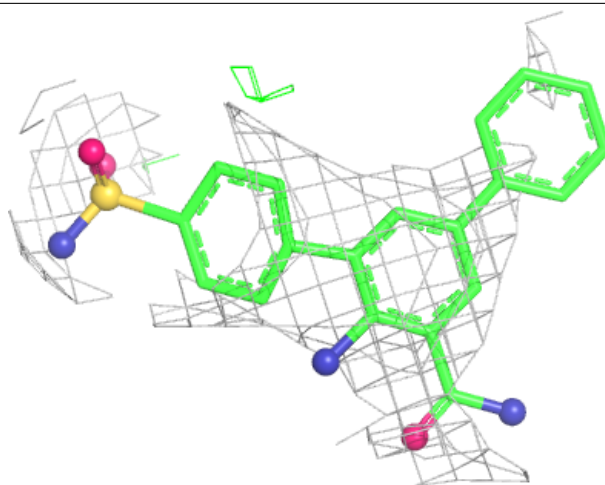
Electron density around 5TL D 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



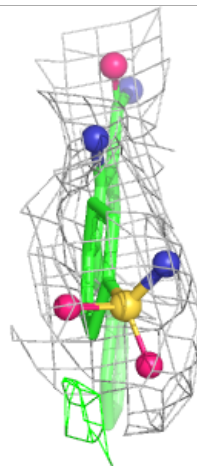
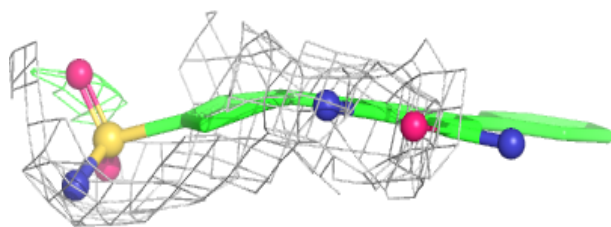
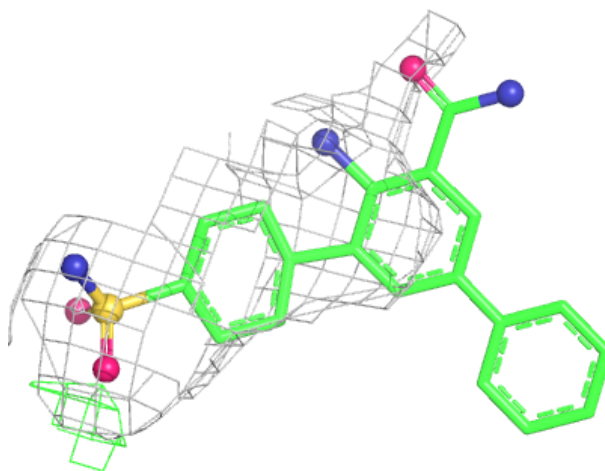
Electron density around 5TL E 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



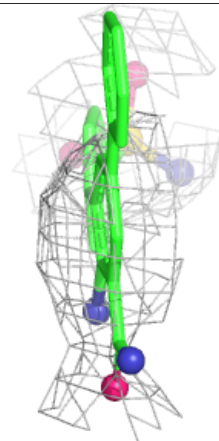
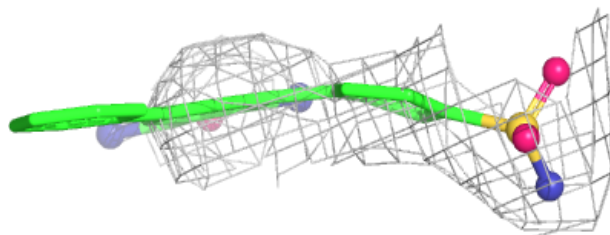
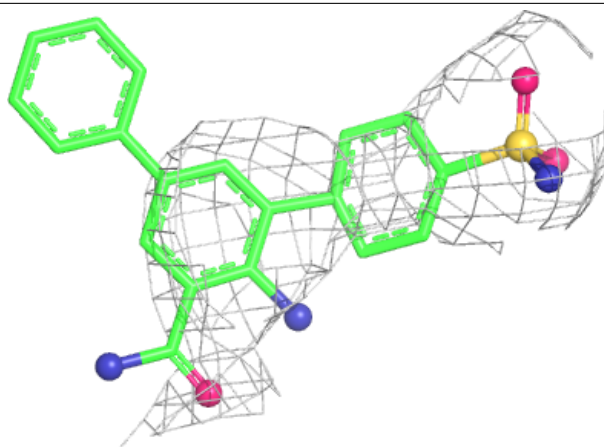
Electron density around 5TL J 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



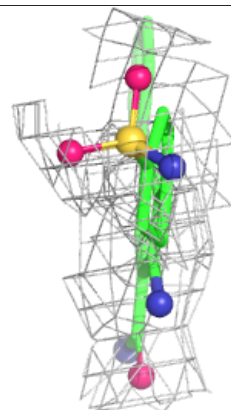
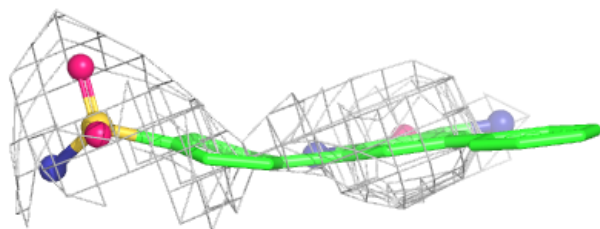
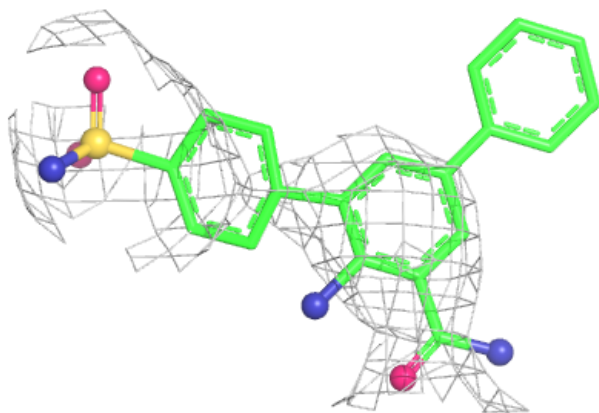
Electron density around 5TL A 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



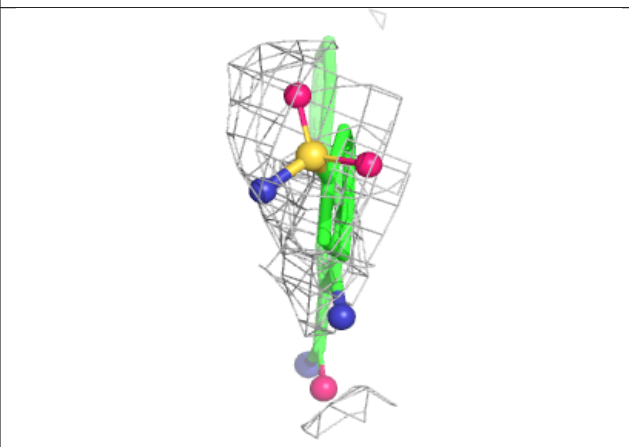
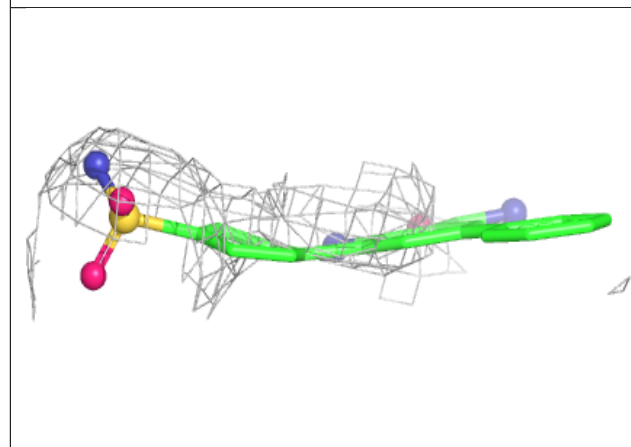
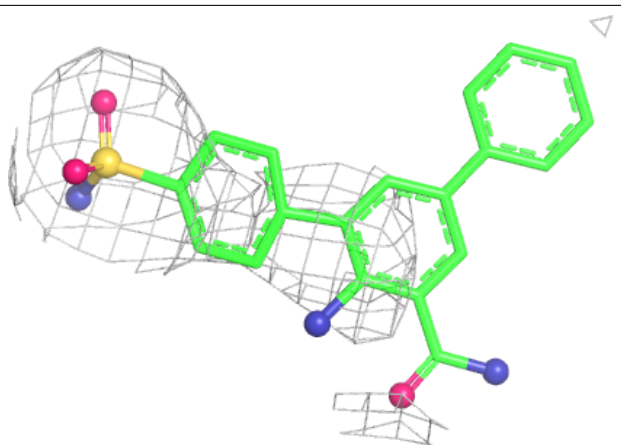
Electron density around 5TL G 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



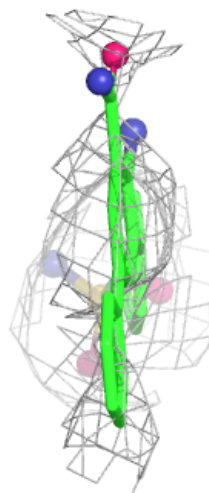
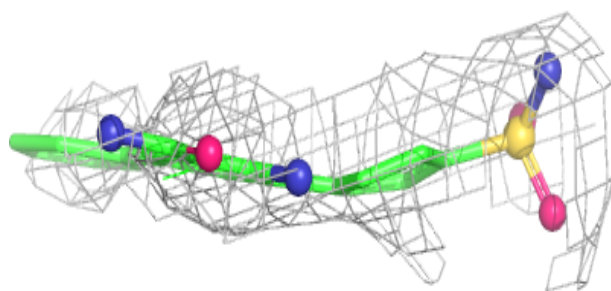
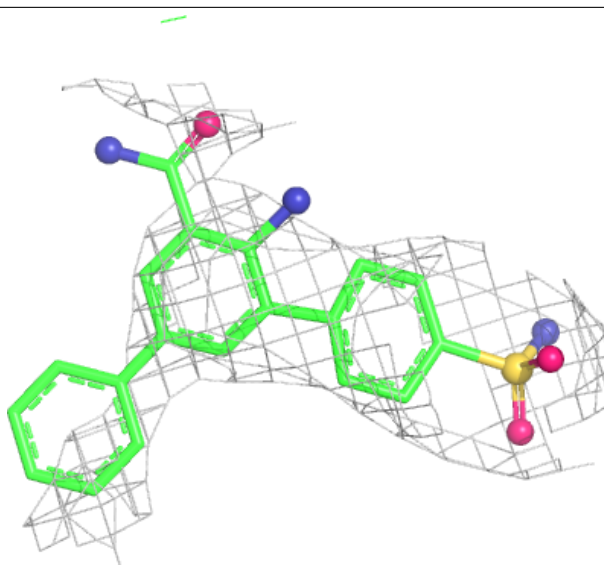
Electron density around 5TL I 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



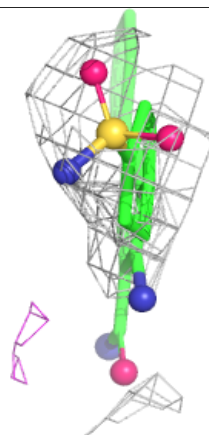
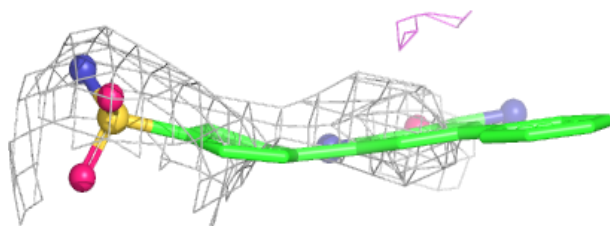
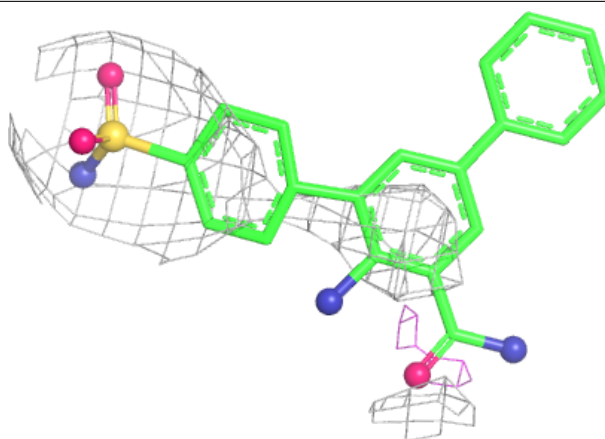
Electron density around 5TL K 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 5TL C 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.