



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:41 AM BST

PDB ID : 5EBZ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

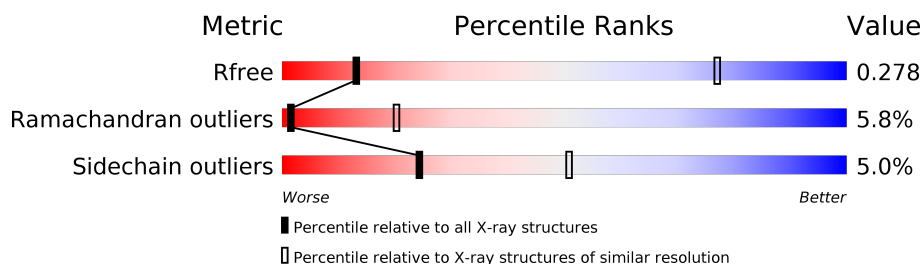
1 Overall quality at a glance

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.






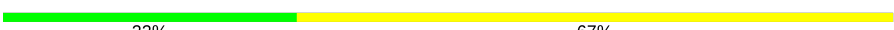
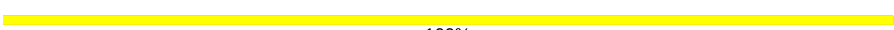
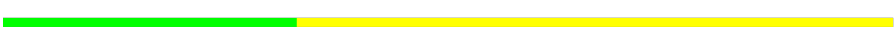













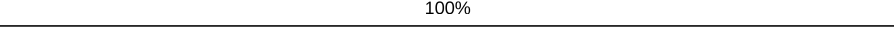



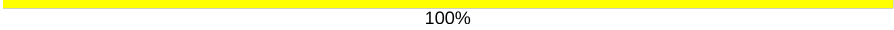
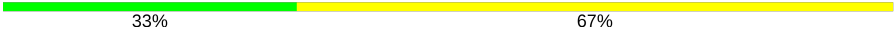
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	655	90% 9%
1	B	655	90% 9%
1	C	655	91% 9%
1	D	655	92% 8%
1	E	655	90% 9% .
1	F	655	90% 9%
1	G	655	91% 8% .
1	H	655	89% 10% .
1	I	655	90% 9% .


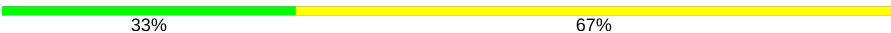
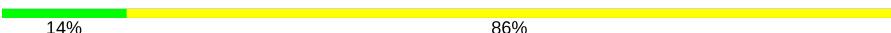


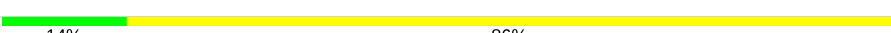
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Mol	Chain	Length	Quality of chain
1	J	655	 90% 9%
1	K	655	 90% 10%
1	L	655	 90% 9%
2	M	3	 33% 67%
2	N	3	 100%
2	P	3	 33% 67%
2	Q	3	 33% 67%
2	R	3	 33% 67%
2	S	3	 33% 67%
2	U	3	 33% 67%
2	V	3	 33% 67%
2	W	3	 33% 67%
2	X	3	 100%
2	Y	3	 33% 67%
2	Z	3	 33% 67%
2	a	3	 33% 67%
2	b	3	 33% 67%
2	d	3	 33% 67%
2	e	3	 100%
2	f	3	 33% 67%
2	g	3	 33% 67%
2	h	3	 33% 67%
2	j	3	 100%
2	k	3	 33% 67%
2	l	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	m	3	 33% 67%
2	n	3	 33% 67%
3	O	7	 14% 86%
3	T	7	 14% 86%
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
4	5TL	A	701	-	X	-	-
4	5TL	B	701	-	X	-	-
4	5TL	C	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	-	-

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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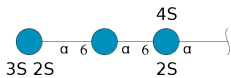
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation	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-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-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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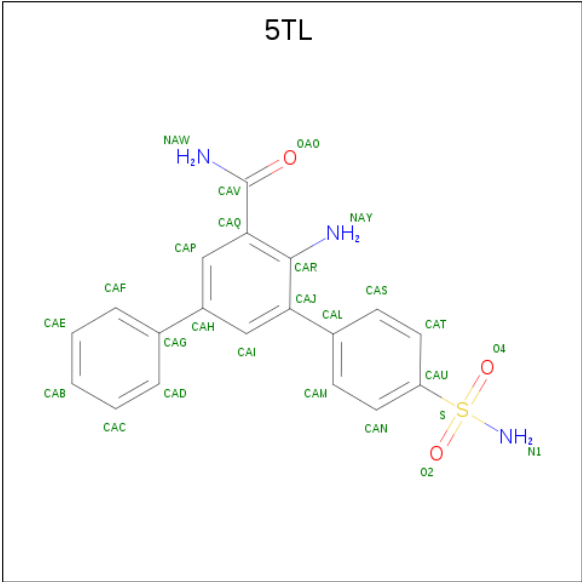
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	j	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	k	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	l	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	m	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	n	3	Total	C	O	S	0	0	0
			50	18	28	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 (three-letter code: 5TL) (formula: C₁₉H₁₇N₃O₃S).

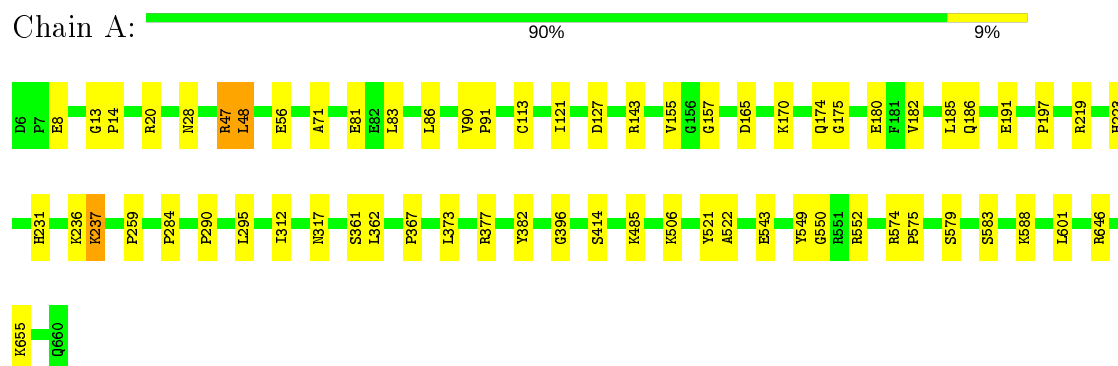


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	C	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	D	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	F	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	G	1	Total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

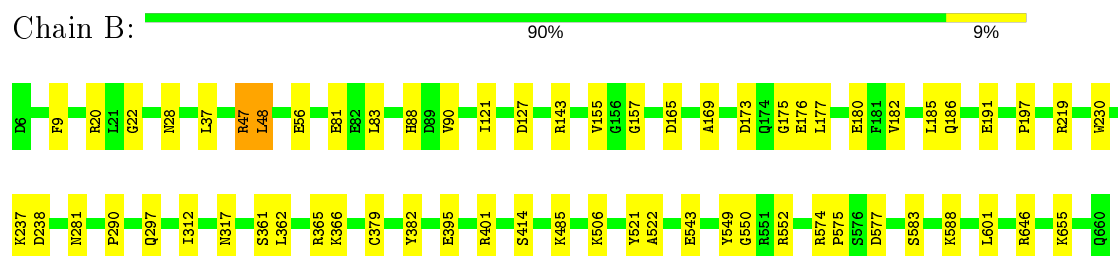
3 Residue-property plots

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. 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.

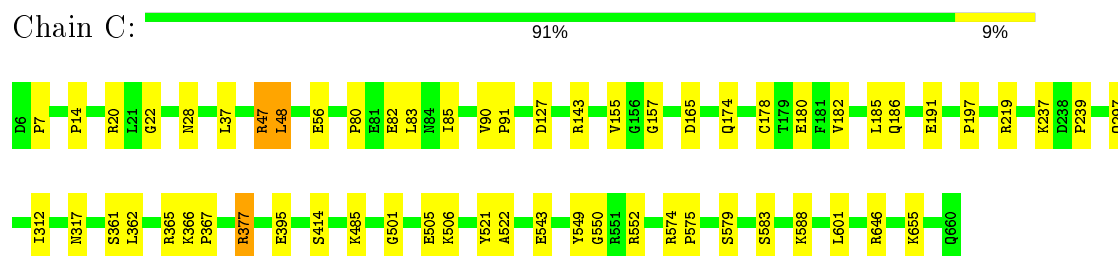
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



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

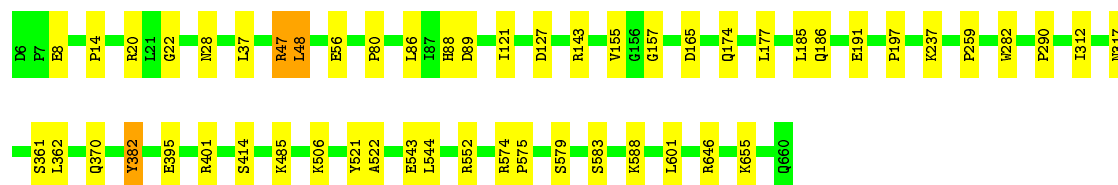


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



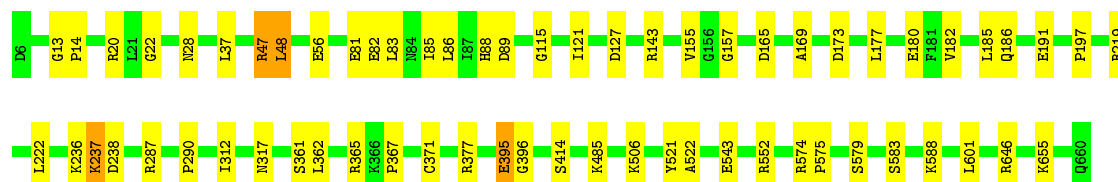
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha





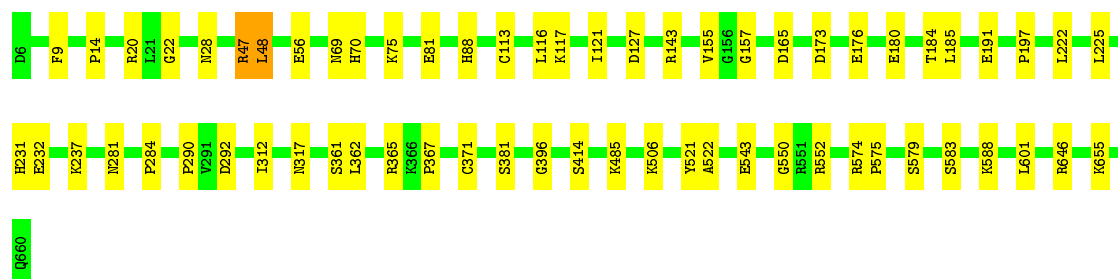
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain E: 90% 9%



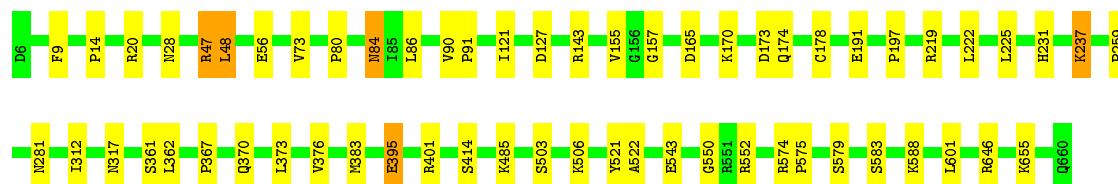
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain F: 90% 9%



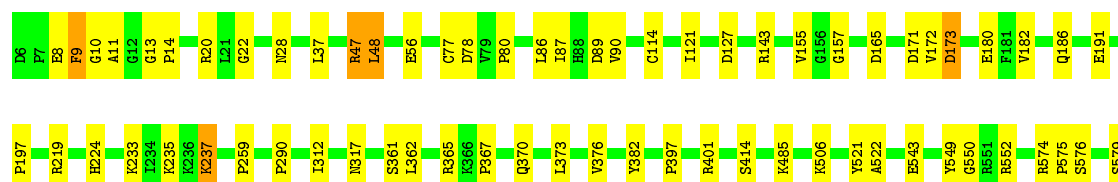
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain G: 91% 8%



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

Chain H: 89% 10%





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

Chain I: 90% 9%



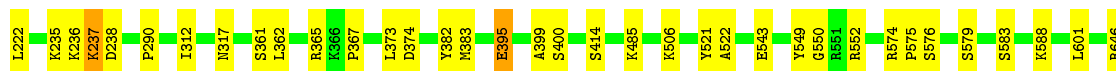
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain J: 90% 9%



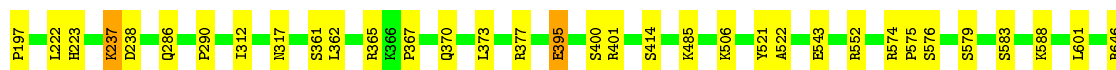
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain K: 90% 10%



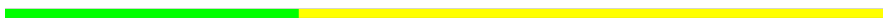
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain L: 90% 9%






- 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:  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 N:  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 P:  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 Q:  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 R:  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 S:  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 U:  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 V:  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 W:  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 X:  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 Y:  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 Z:  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 a:  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 b:



- 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:



- 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:



- 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:



- 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:



- 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:



- 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%

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 k:  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 l:  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 m:  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 n:  33% 67%

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% 86%

5LS1	5LJ2	5TN3	5TJ4	24K5	5TK6	5TH7
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● 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:

14%

86%

5LS1	5LJ2	5TN3	5TJ4	24K5	5TK6	5TH7
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● 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	5LJ2	5TN3	5TJ4	24K5	5TK6	5TH7
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● 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 i:

14%

86%

5LS1	5LJ2	5TN3	5TJ4	24K5	5TK6	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 44.79 – 4.44	Depositor EDS
% Data completeness (in resolution range)	68.1 (29.94-4.50) 80.6 (44.79-4.44)	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 0.243 , 0.278	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)	0.27 , 311.6	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	0.89	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/5370	0.43	0/7239
1	B	0.27	0/5370	0.42	0/7239
1	C	0.27	0/5370	0.43	0/7239
1	D	0.27	0/5370	0.43	0/7239
1	E	0.28	0/5370	0.43	0/7239
1	F	0.27	0/5370	0.43	0/7239
1	G	0.31	0/5370	0.44	0/7239
1	H	0.27	0/5370	0.42	0/7239
1	I	0.27	0/5370	0.43	0/7239
1	J	0.27	0/5370	0.43	0/7239
1	K	0.28	0/5370	0.43	0/7239
1	L	0.26	0/5370	0.42	0/7239
All	All	0.28	0/64440	0.43	0/86868

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	2	21
1	B	653/655 (100%)	514 (79%)	106 (16%)	33 (5%)	2	22
1	C	653/655 (100%)	511 (78%)	105 (16%)	37 (6%)	1	20
1	D	653/655 (100%)	515 (79%)	104 (16%)	34 (5%)	2	22
1	E	653/655 (100%)	511 (78%)	104 (16%)	38 (6%)	1	20
1	F	653/655 (100%)	505 (77%)	111 (17%)	37 (6%)	1	20
1	G	653/655 (100%)	508 (78%)	114 (18%)	31 (5%)	2	24
1	H	653/655 (100%)	507 (78%)	99 (15%)	47 (7%)	1	16
1	I	653/655 (100%)	502 (77%)	110 (17%)	41 (6%)	1	19
1	J	653/655 (100%)	515 (79%)	98 (15%)	40 (6%)	1	19
1	K	653/655 (100%)	506 (78%)	105 (16%)	42 (6%)	1	19
1	L	653/655 (100%)	500 (77%)	113 (17%)	40 (6%)	1	19
All	All	7836/7860 (100%)	6098 (78%)	1282 (16%)	456 (6%)	1	20

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 [i](#)

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%)	557 (95%)	32 (5%)	22	49	
1	B	589/589 (100%)	557 (95%)	32 (5%)	22	49	
1	C	589/589 (100%)	563 (96%)	26 (4%)	28	54	
1	D	589/589 (100%)	567 (96%)	22 (4%)	34	59	
1	E	589/589 (100%)	559 (95%)	30 (5%)	24	50	
1	F	589/589 (100%)	561 (95%)	28 (5%)	25	52	
1	G	589/589 (100%)	555 (94%)	34 (6%)	20	47	
1	H	589/589 (100%)	559 (95%)	30 (5%)	24	50	
1	I	589/589 (100%)	561 (95%)	28 (5%)	25	52	
1	J	589/589 (100%)	560 (95%)	29 (5%)	25	51	
1	K	589/589 (100%)	559 (95%)	30 (5%)	24	50	
1	L	589/589 (100%)	557 (95%)	32 (5%)	22	49	
All	All	7068/7068 (100%)	6715 (95%)	353 (5%)	24	51	

5 of 353 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	281	ASN
1	G	506	LYS
1	L	72	ASN
1	F	543	GLU
1	G	170	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 276 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	317	ASN
1	G	475	GLN
1	L	72	ASN
1	F	459	ASN
1	G	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1.35	1 (5%)	21,31,31	1.10	2 (9%)
2	GLC	M	2	2	11,11,12	0.59	0	15,15,17	0.41	0
2	PDX	M	3	2	19,19,20	1.36	2 (10%)	20,29,31	1.34	3 (15%)
2	5LS	N	1	2	20,20,20	1.29	1 (5%)	21,31,31	1.10	2 (9%)
2	GLC	N	2	2	11,11,12	0.87	0	15,15,17	1.14	1 (6%)
2	PDX	N	3	2	19,19,20	1.31	2 (10%)	20,29,31	1.38	3 (15%)
3	5LS	O	1	3	20,20,20	1.11	0	21,31,31	1.13	2 (9%)
3	5TJ	O	2	3	14,17,18	1.01	0	17,24,26	0.93	1 (5%)
3	5TM	O	3	3	14,17,18	1.19	1 (7%)	16,24,26	1.32	2 (12%)
3	5TJ	O	4	3	14,17,18	1.02	0	17,24,26	0.84	1 (5%)
3	Z4K	O	5	3	15,15,16	1.18	1 (6%)	18,22,24	1.18	1 (5%)
3	5TK	O	6	3	10,13,14	0.59	0	13,17,19	0.41	0
3	5TH	O	7	3	14,17,18	1.38	2 (14%)	16,24,26	1.19	2 (12%)
2	5LS	P	1	2	20,20,20	1.25	2 (10%)	21,31,31	1.12	2 (9%)
2	GLC	P	2	2	11,11,12	0.69	0	15,15,17	0.44	0
2	PDX	P	3	2	19,19,20	1.25	2 (10%)	20,29,31	1.21	2 (10%)
2	5LS	Q	1	2	20,20,20	1.22	2 (10%)	21,31,31	1.13	2 (9%)
2	GLC	Q	2	2	11,11,12	0.59	0	15,15,17	0.37	0
2	PDX	Q	3	2	19,19,20	1.38	2 (10%)	20,29,31	1.37	4 (20%)
2	5LS	R	1	2	20,20,20	1.30	1 (5%)	21,31,31	1.08	2 (9%)
2	GLC	R	2	2	11,11,12	0.55	0	15,15,17	0.37	0
2	PDX	R	3	2	19,19,20	1.37	2 (10%)	20,29,31	1.36	3 (15%)
2	5LS	S	1	2	20,20,20	1.40	1 (5%)	21,31,31	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	S	2	2	11,11,12	0.49	0	15,15,17	0.41	0
2	PDX	S	3	2	19,19,20	1.38	2 (10%)	20,29,31	1.41	3 (15%)
3	5LS	T	1	3	20,20,20	1.32	1 (5%)	21,31,31	1.10	2 (9%)
3	5TJ	T	2	3	14,17,18	0.99	0	17,24,26	0.88	1 (5%)
3	5TM	T	3	3	14,17,18	1.14	1 (7%)	16,24,26	1.37	2 (12%)
3	5TJ	T	4	3	14,17,18	0.98	0	17,24,26	0.89	1 (5%)
3	Z4K	T	5	3	15,15,16	1.12	1 (6%)	18,22,24	1.14	2 (11%)
3	5TK	T	6	3	10,13,14	0.66	0	13,17,19	0.64	0
3	5TH	T	7	3	14,17,18	1.41	2 (14%)	16,24,26	1.33	2 (12%)
2	5LS	U	1	2	20,20,20	1.31	1 (5%)	21,31,31	1.10	2 (9%)
2	GLC	U	2	2	11,11,12	0.57	0	15,15,17	0.38	0
2	PDX	U	3	2	19,19,20	1.34	2 (10%)	20,29,31	1.39	3 (15%)
2	5LS	V	1	2	20,20,20	1.19	1 (5%)	21,31,31	1.14	2 (9%)
2	GLC	V	2	2	11,11,12	0.62	0	15,15,17	0.50	0
2	PDX	V	3	2	19,19,20	1.34	2 (10%)	20,29,31	1.28	3 (15%)
2	5LS	W	1	2	20,20,20	1.28	2 (10%)	21,31,31	1.13	2 (9%)
2	GLC	W	2	2	11,11,12	0.63	0	15,15,17	0.54	0
2	PDX	W	3	2	19,19,20	1.44	2 (10%)	20,29,31	1.40	4 (20%)
2	5LS	X	1	2	20,20,20	1.30	1 (5%)	21,31,31	1.11	3 (14%)
2	GLC	X	2	2	11,11,12	0.67	0	15,15,17	0.69	1 (6%)
2	PDX	X	3	2	19,19,20	1.38	2 (10%)	20,29,31	1.35	3 (15%)
2	5LS	Y	1	2	20,20,20	1.38	1 (5%)	21,31,31	1.13	2 (9%)
2	GLC	Y	2	2	11,11,12	0.60	0	15,15,17	0.58	0
2	PDX	Y	3	2	19,19,20	1.34	2 (10%)	20,29,31	1.33	3 (15%)
2	5LS	Z	1	2	20,20,20	1.24	1 (5%)	21,31,31	1.13	2 (9%)
2	GLC	Z	2	2	11,11,12	0.70	0	15,15,17	0.50	0
2	PDX	Z	3	2	19,19,20	1.34	2 (10%)	20,29,31	1.36	3 (15%)
2	5LS	a	1	2	20,20,20	1.39	1 (5%)	21,31,31	1.12	2 (9%)
2	GLC	a	2	2	11,11,12	0.59	0	15,15,17	0.33	0
2	PDX	a	3	2	19,19,20	1.36	2 (10%)	20,29,31	1.44	3 (15%)
2	5LS	b	1	2	20,20,20	1.38	1 (5%)	21,31,31	1.12	2 (9%)
2	GLC	b	2	2	11,11,12	0.56	0	15,15,17	0.48	0
2	PDX	b	3	2	19,19,20	1.32	2 (10%)	20,29,31	1.39	3 (15%)
3	5LS	c	1	3	20,20,20	1.11	1 (5%)	21,31,31	1.08	2 (9%)
3	5TJ	c	2	3	14,17,18	1.00	0	17,24,26	0.85	1 (5%)
3	5TM	c	3	3	14,17,18	1.24	2 (14%)	16,24,26	1.39	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5TJ	c	4	3	14,17,18	1.02	0	17,24,26	0.90	1 (5%)
3	Z4K	c	5	3	15,15,16	1.16	1 (6%)	18,22,24	1.19	2 (11%)
3	5TK	c	6	3	10,13,14	0.66	0	13,17,19	0.44	0
3	5TH	c	7	3	14,17,18	1.27	2 (14%)	16,24,26	1.24	2 (12%)
2	5LS	d	1	2	20,20,20	1.33	1 (5%)	21,31,31	1.12	2 (9%)
2	GLC	d	2	2	11,11,12	0.80	0	15,15,17	0.46	0
2	PDX	d	3	2	19,19,20	1.39	2 (10%)	20,29,31	1.32	3 (15%)
2	5LS	e	1	2	20,20,20	1.31	1 (5%)	21,31,31	1.11	2 (9%)
2	GLC	e	2	2	11,11,12	0.82	0	15,15,17	1.23	1 (6%)
2	PDX	e	3	2	19,19,20	1.36	2 (10%)	20,29,31	1.37	3 (15%)
2	5LS	f	1	2	20,20,20	1.36	1 (5%)	21,31,31	1.12	2 (9%)
2	GLC	f	2	2	11,11,12	0.69	0	15,15,17	0.39	0
2	PDX	f	3	2	19,19,20	1.49	2 (10%)	20,29,31	1.46	4 (20%)
2	5LS	g	1	2	20,20,20	1.09	0	21,31,31	1.15	3 (14%)
2	GLC	g	2	2	11,11,12	0.68	0	15,15,17	0.59	0
2	PDX	g	3	2	19,19,20	1.40	2 (10%)	20,29,31	1.32	4 (20%)
2	5LS	h	1	2	20,20,20	1.30	1 (5%)	21,31,31	1.12	2 (9%)
2	GLC	h	2	2	11,11,12	0.60	0	15,15,17	0.51	0
2	PDX	h	3	2	19,19,20	1.34	2 (10%)	20,29,31	1.37	3 (15%)
3	5LS	i	1	3	20,20,20	1.25	2 (10%)	21,31,31	1.13	2 (9%)
3	5TJ	i	2	3	14,17,18	1.00	0	17,24,26	0.94	1 (5%)
3	5TM	i	3	3	14,17,18	1.21	1 (7%)	16,24,26	1.39	2 (12%)
3	5TJ	i	4	3	14,17,18	0.99	0	17,24,26	0.95	1 (5%)
3	Z4K	i	5	3	15,15,16	1.21	1 (6%)	18,22,24	1.11	1 (5%)
3	5TK	i	6	3	10,13,14	0.56	0	13,17,19	0.38	0
3	5TH	i	7	3	14,17,18	1.35	2 (14%)	16,24,26	1.22	1 (6%)
2	5LS	j	1	2	20,20,20	1.12	0	21,31,31	1.14	3 (14%)
2	GLC	j	2	2	11,11,12	0.94	0	15,15,17	1.15	2 (13%)
2	PDX	j	3	2	19,19,20	1.41	2 (10%)	20,29,31	1.50	5 (25%)
2	5LS	k	1	2	20,20,20	1.29	1 (5%)	21,31,31	1.08	2 (9%)
2	GLC	k	2	2	11,11,12	0.62	0	15,15,17	0.32	0
2	PDX	k	3	2	19,19,20	1.39	2 (10%)	20,29,31	1.32	3 (15%)
2	5LS	l	1	2	20,20,20	1.16	2 (10%)	21,31,31	0.96	1 (4%)
2	GLC	l	2	2	11,11,12	0.55	0	15,15,17	0.48	0
2	PDX	l	3	2	19,19,20	1.36	2 (10%)	20,29,31	1.41	3 (15%)
2	5LS	m	1	2	20,20,20	1.34	1 (5%)	21,31,31	1.08	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	m	2	2	11,11,12	0.64	0	15,15,17	0.49	0
2	PDX	m	3	2	19,19,20	1.43	2 (10%)	20,29,31	1.49	4 (20%)
2	5LS	n	1	2	20,20,20	1.25	1 (5%)	21,31,31	1.59	2 (9%)
2	GLC	n	2	2	11,11,12	0.58	0	15,15,17	0.47	0
2	PDX	n	3	2	19,19,20	1.36	2 (10%)	20,29,31	1.32	3 (15%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/2/19/22	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
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	-	2/9/27/30	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	5LS	C1-C2	4.55	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	1	5LS	C1-C2	4.06	1.56	1.52
2	a	1	5LS	C1-C2	4.02	1.56	1.52
2	f	3	PDX	C1-C2	4.00	1.58	1.51
2	Y	1	5LS	C1-C2	4.00	1.56	1.52

The worst 5 of 169 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
3	T	7	5TH	C2-O2-S1	-4.34	112.25	117.91
3	i	3	5TM	C2-O2-S	-4.33	112.27	117.91
2	a	3	PDX	C2-O2-S	-4.22	112.41	117.91
2	l	3	PDX	C2-O2-S	-4.17	112.48	117.91

There are no chirality outliers.

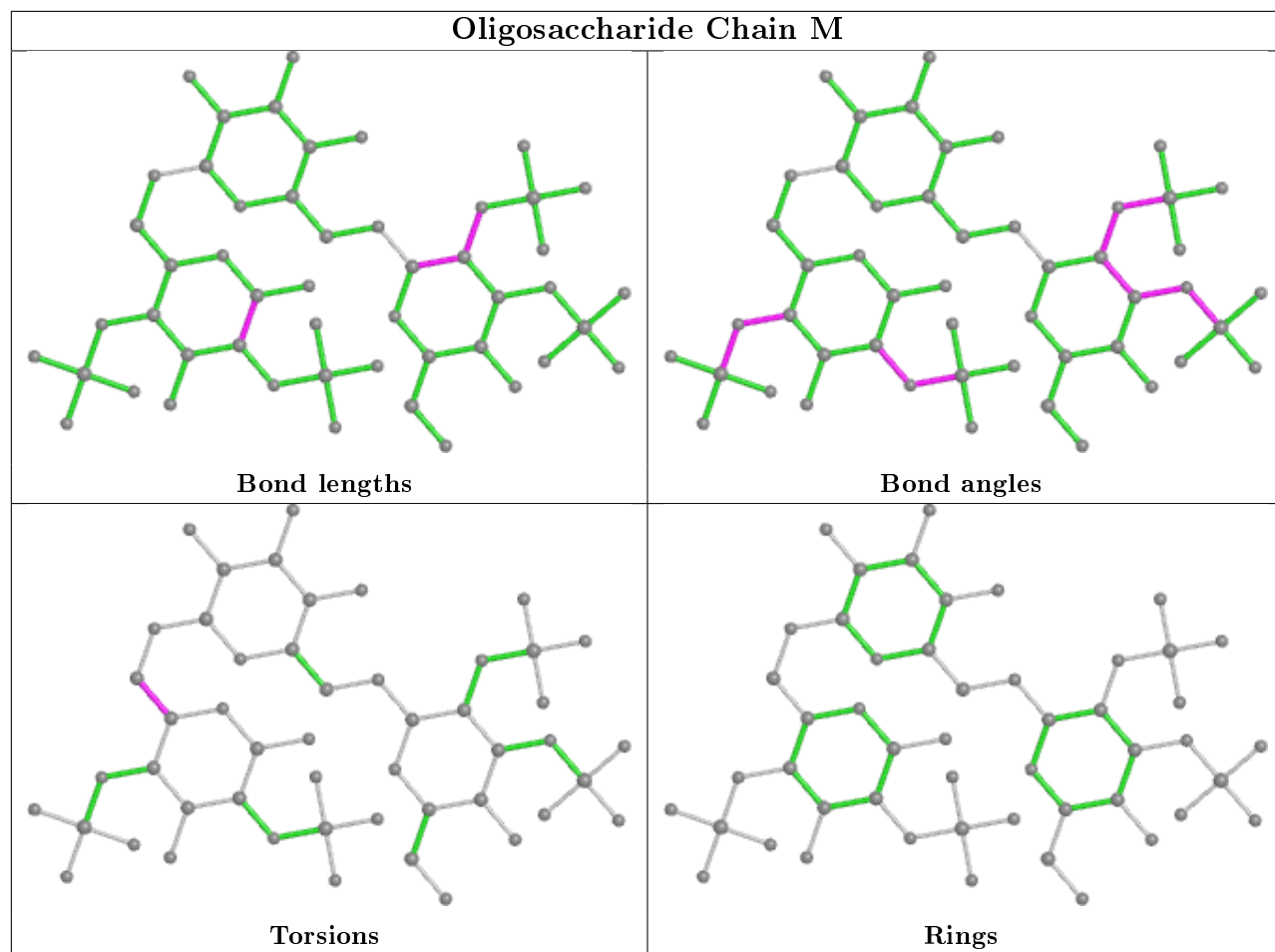
5 of 97 torsion outliers are listed below:

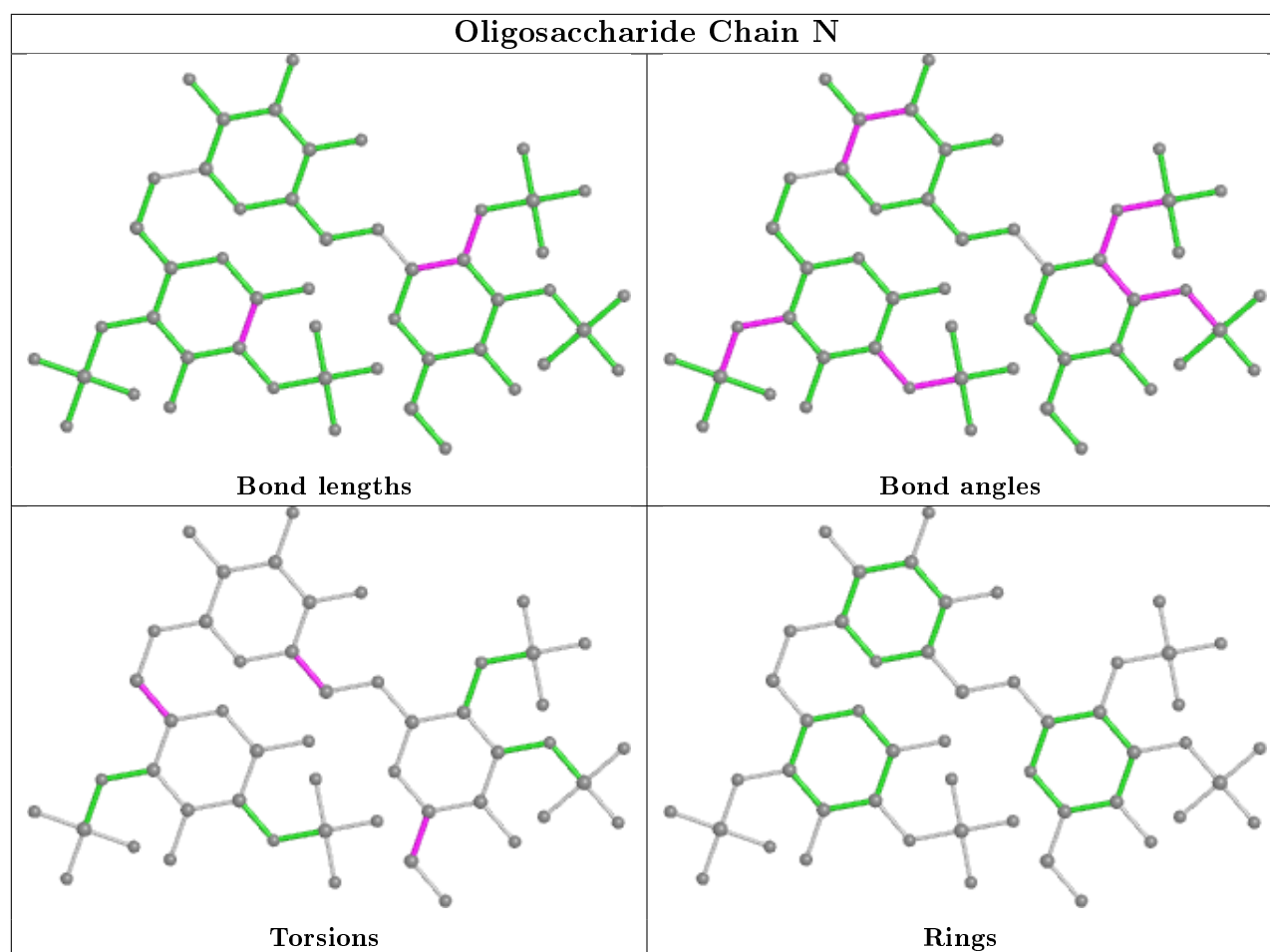
Mol	Chain	Res	Type	Atoms
2	n	1	5LS	C1-C2-O2-S1
2	n	1	5LS	C3-C2-O2-S1
2	S	1	5LS	C3-C4-O4-S2
2	S	1	5LS	C5-C4-O4-S2
2	l	1	5LS	C3-C4-O4-S2

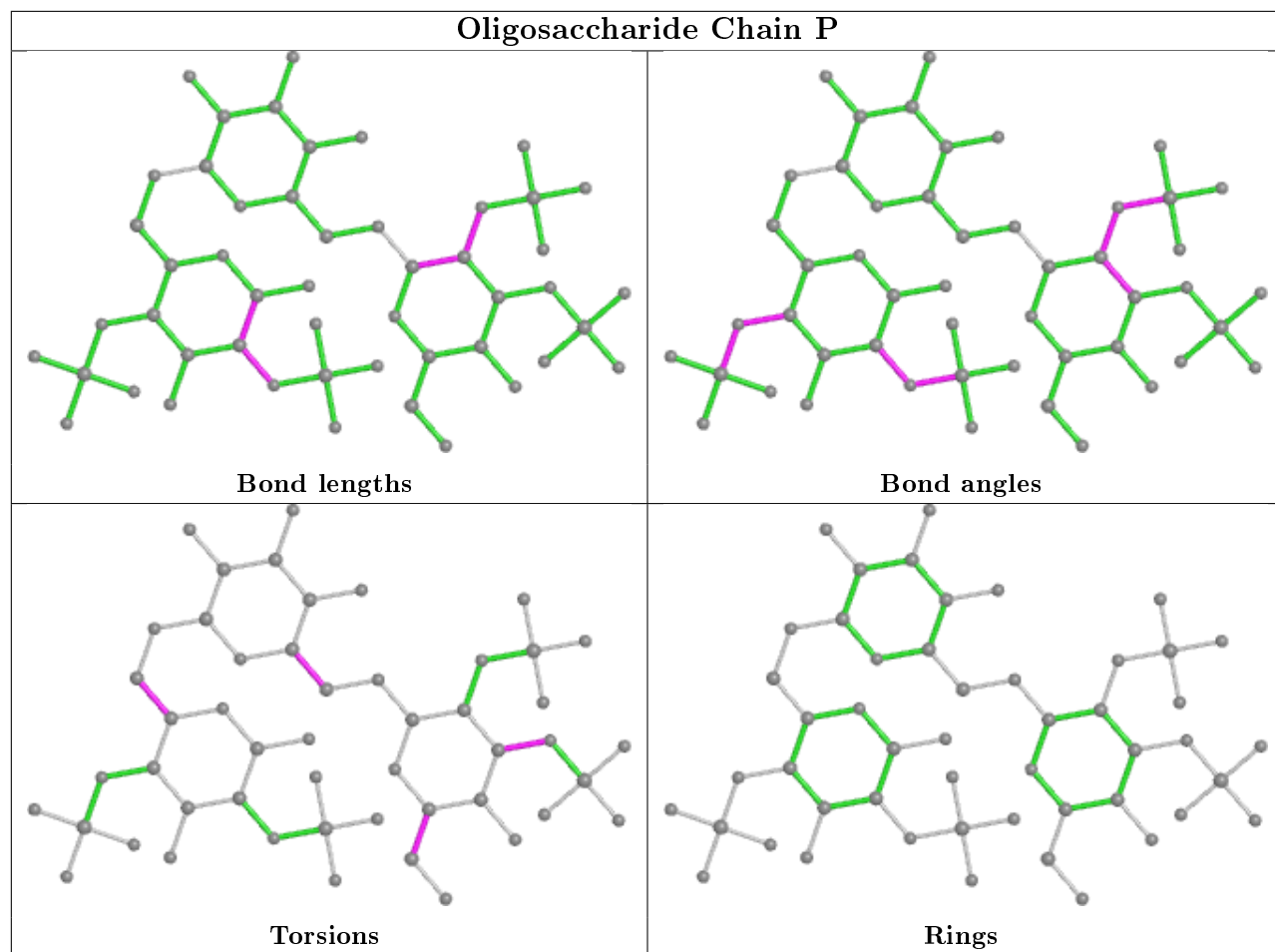
There are no ring outliers.

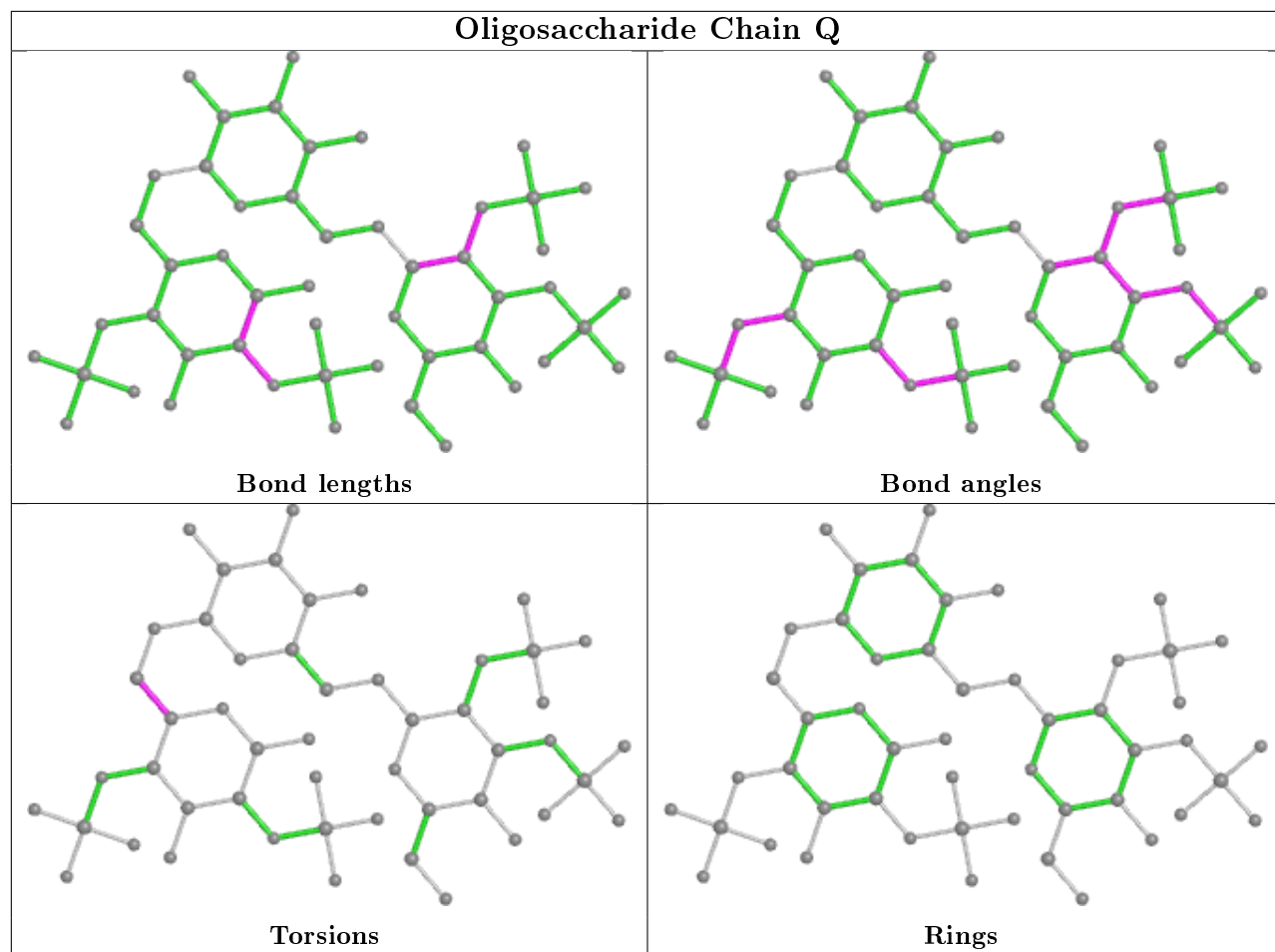
No monomer is involved in short contacts.

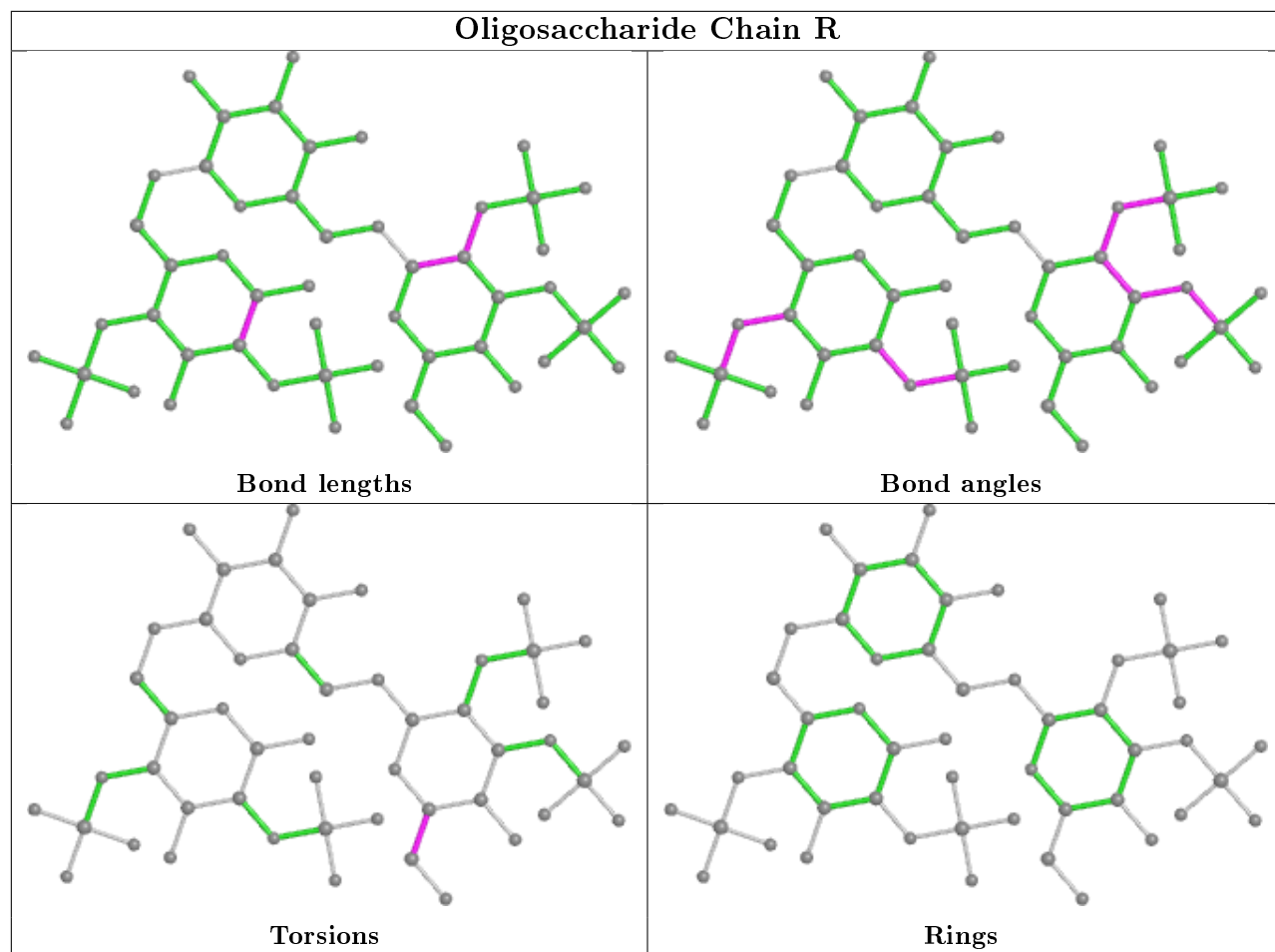
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

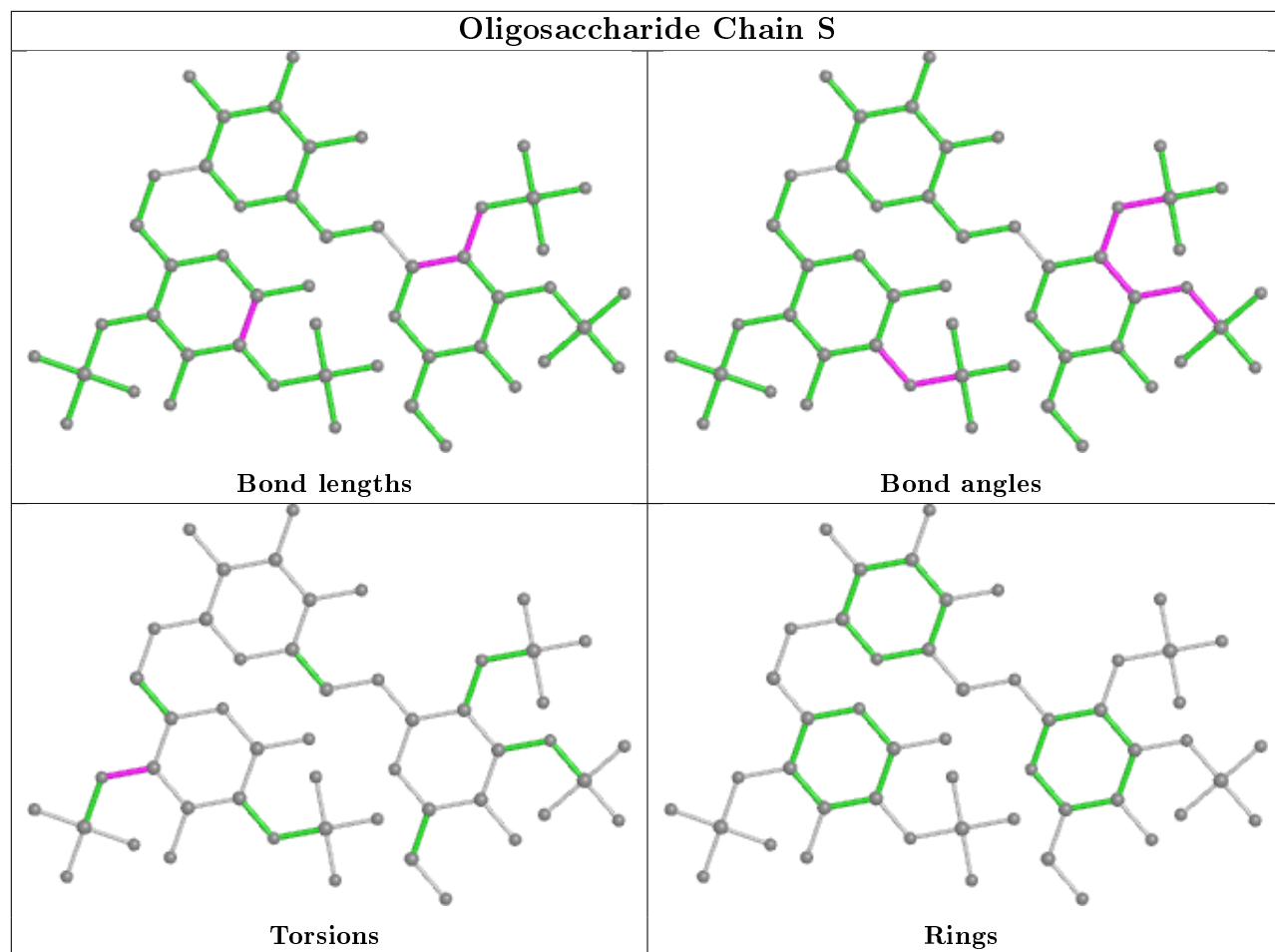


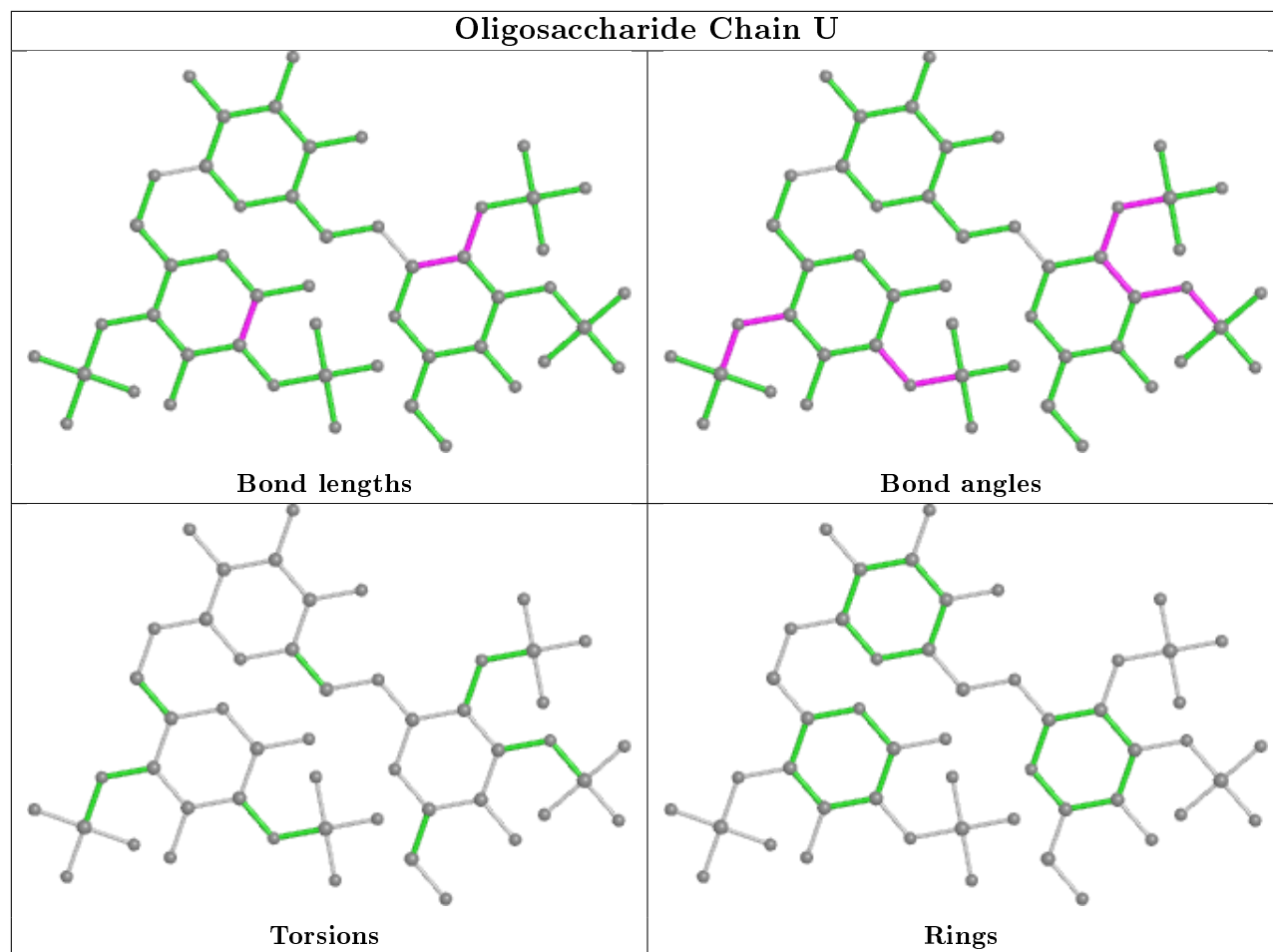


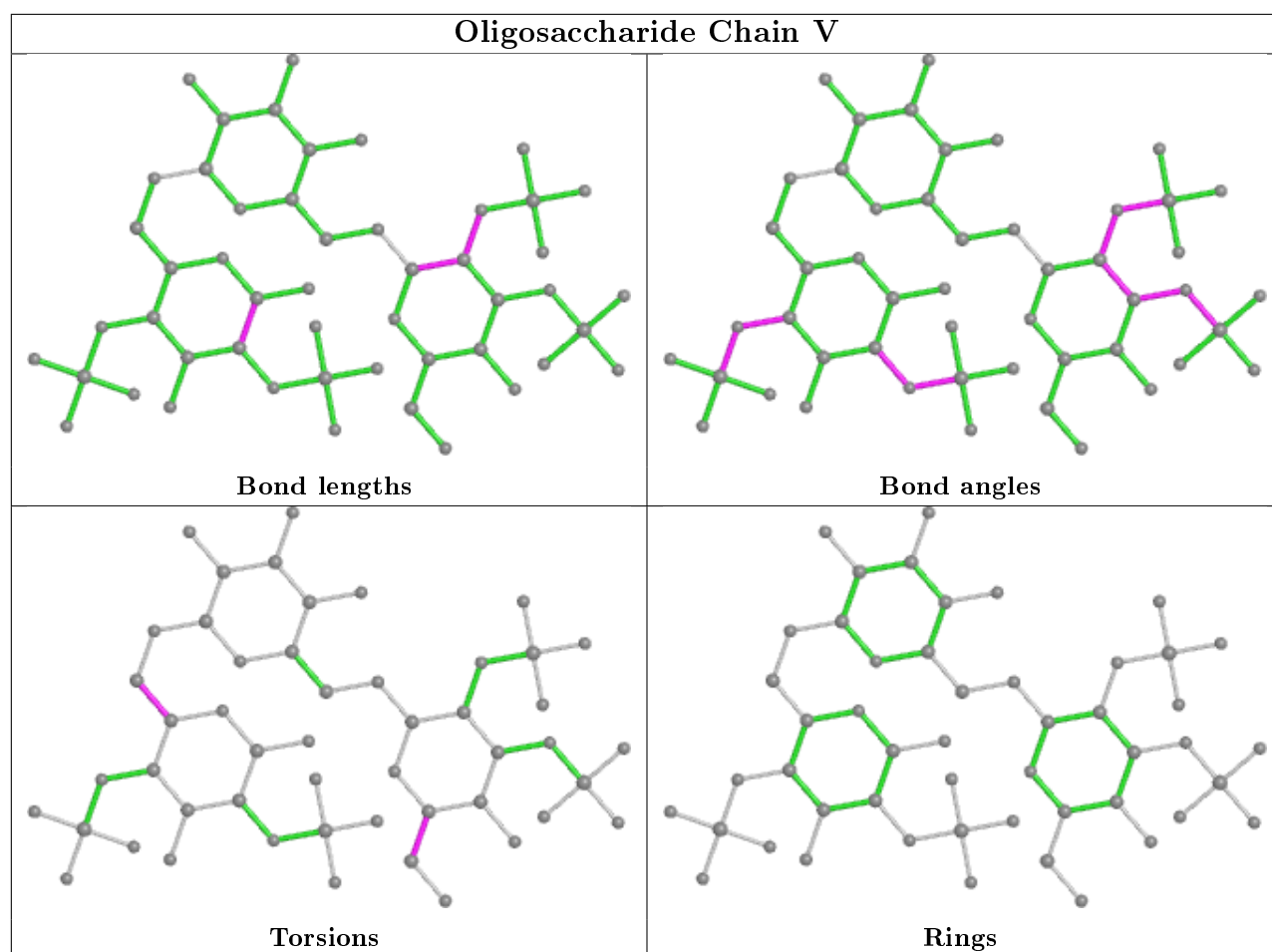


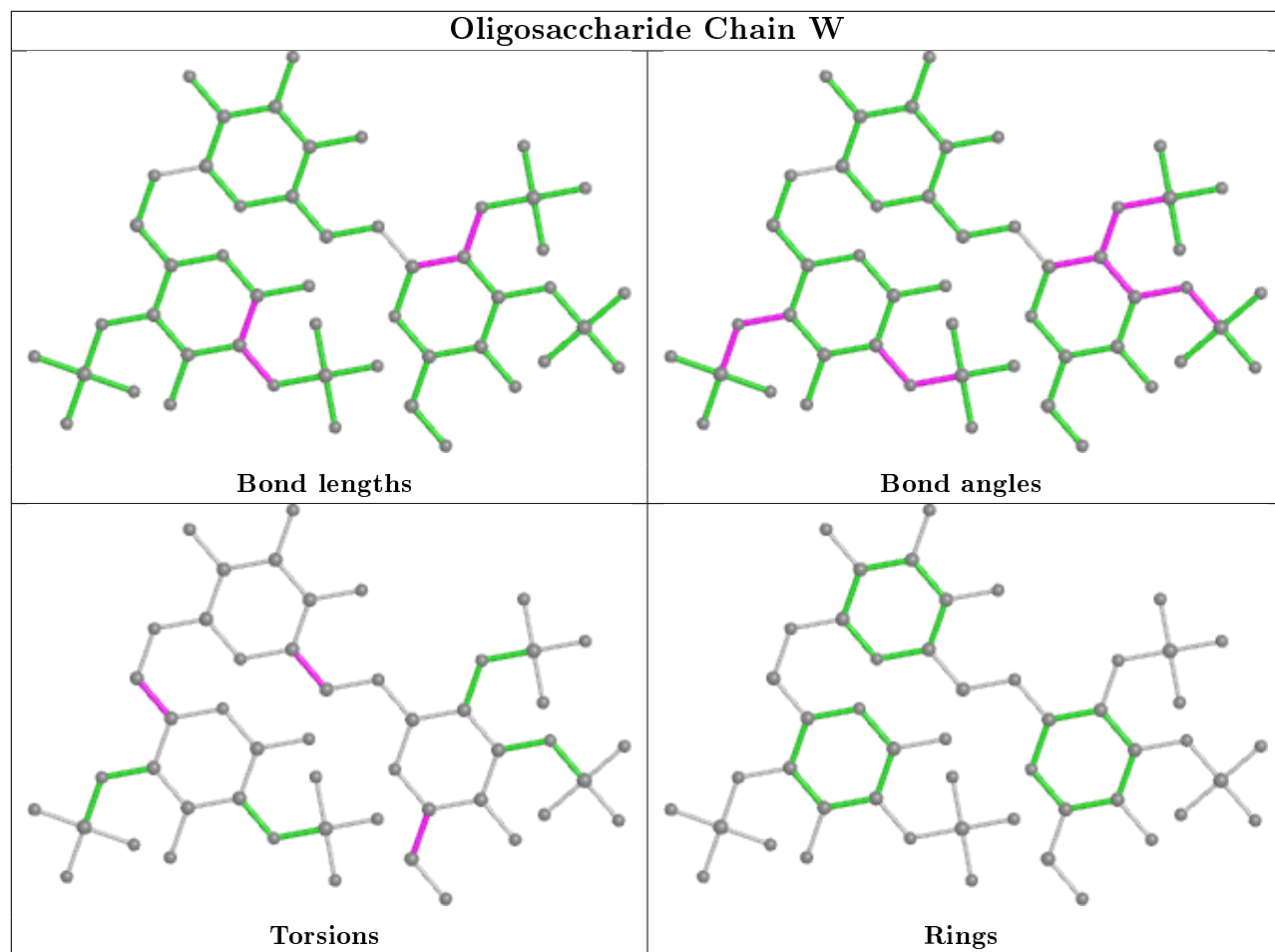


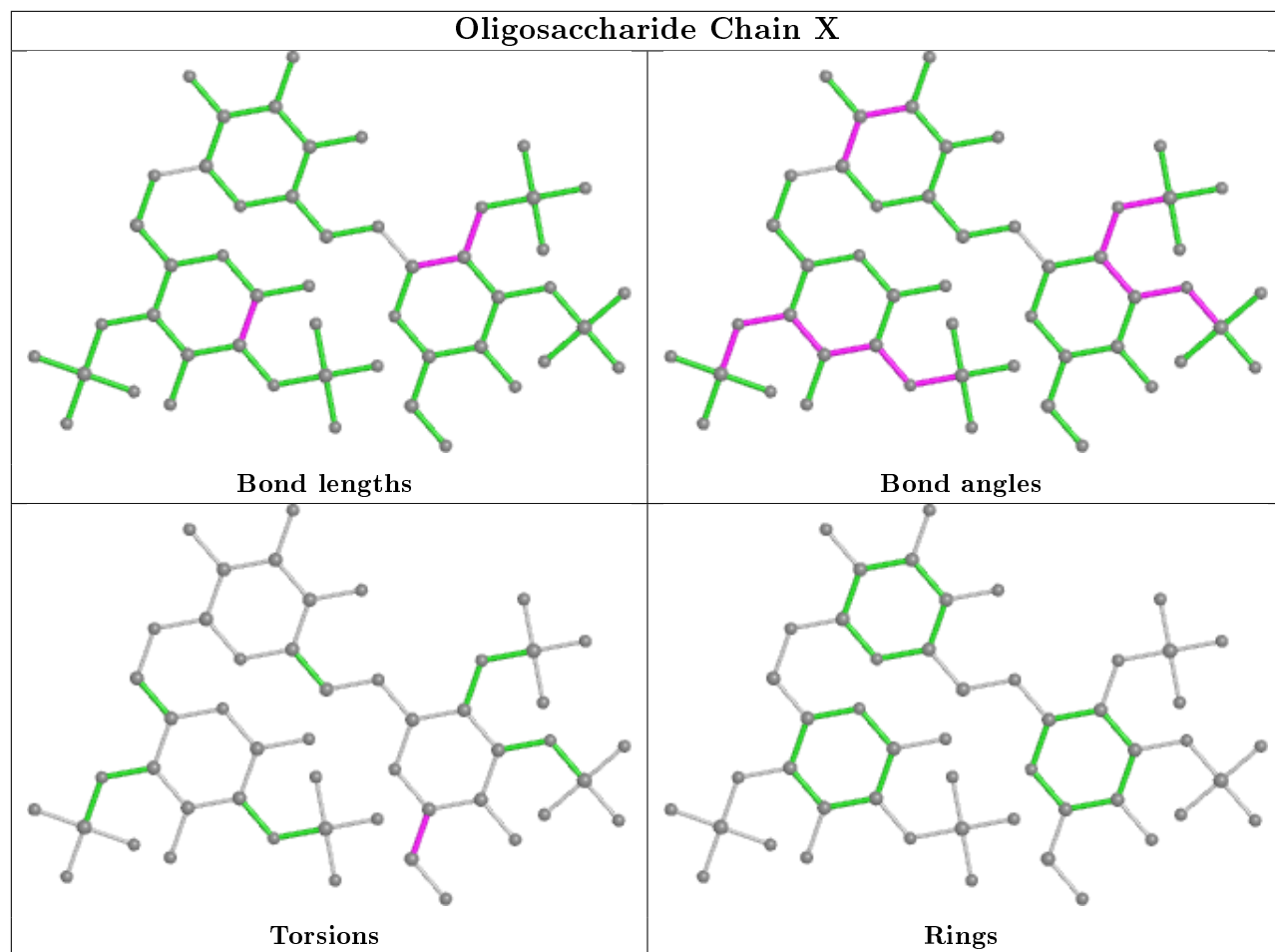


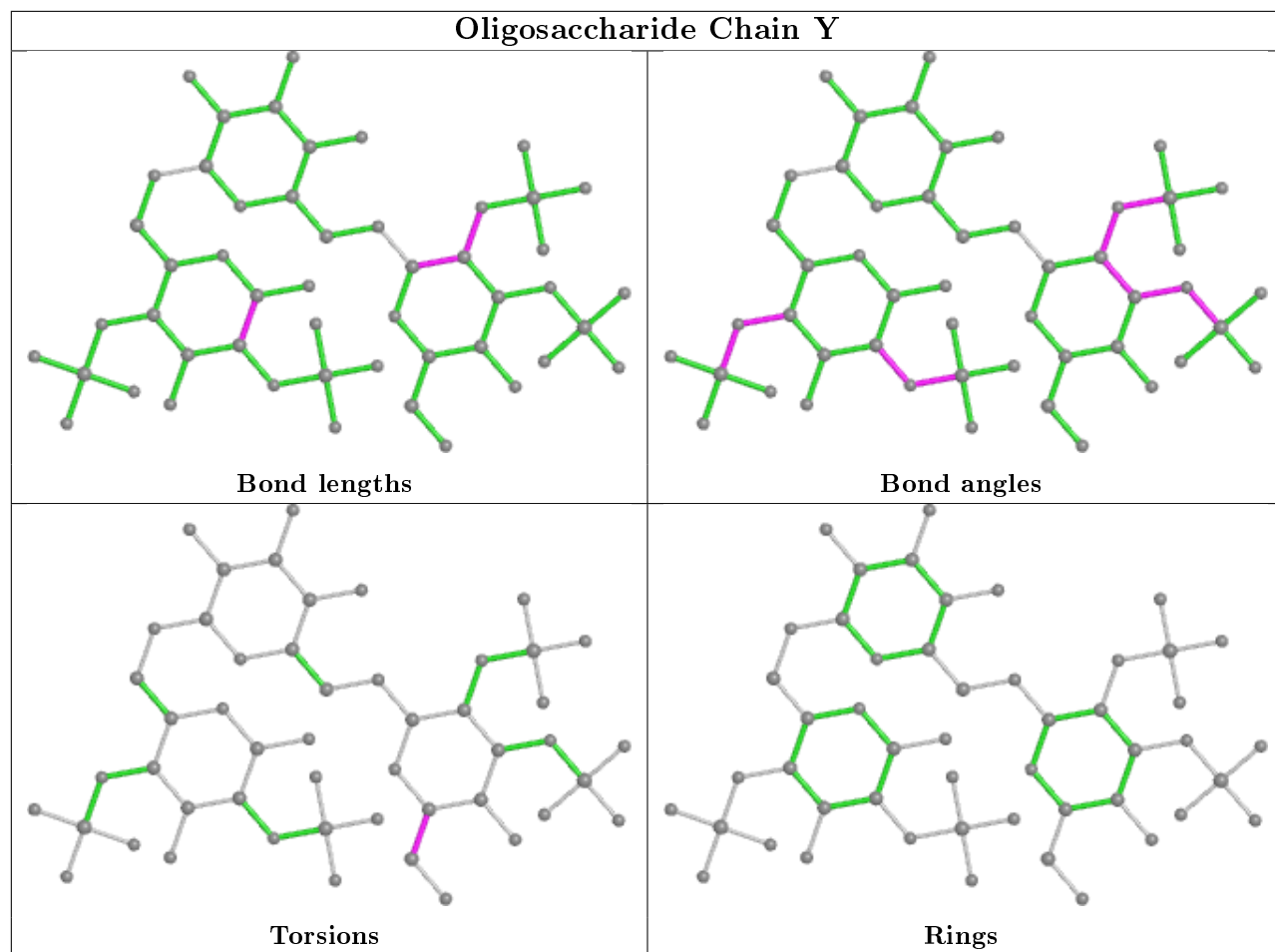




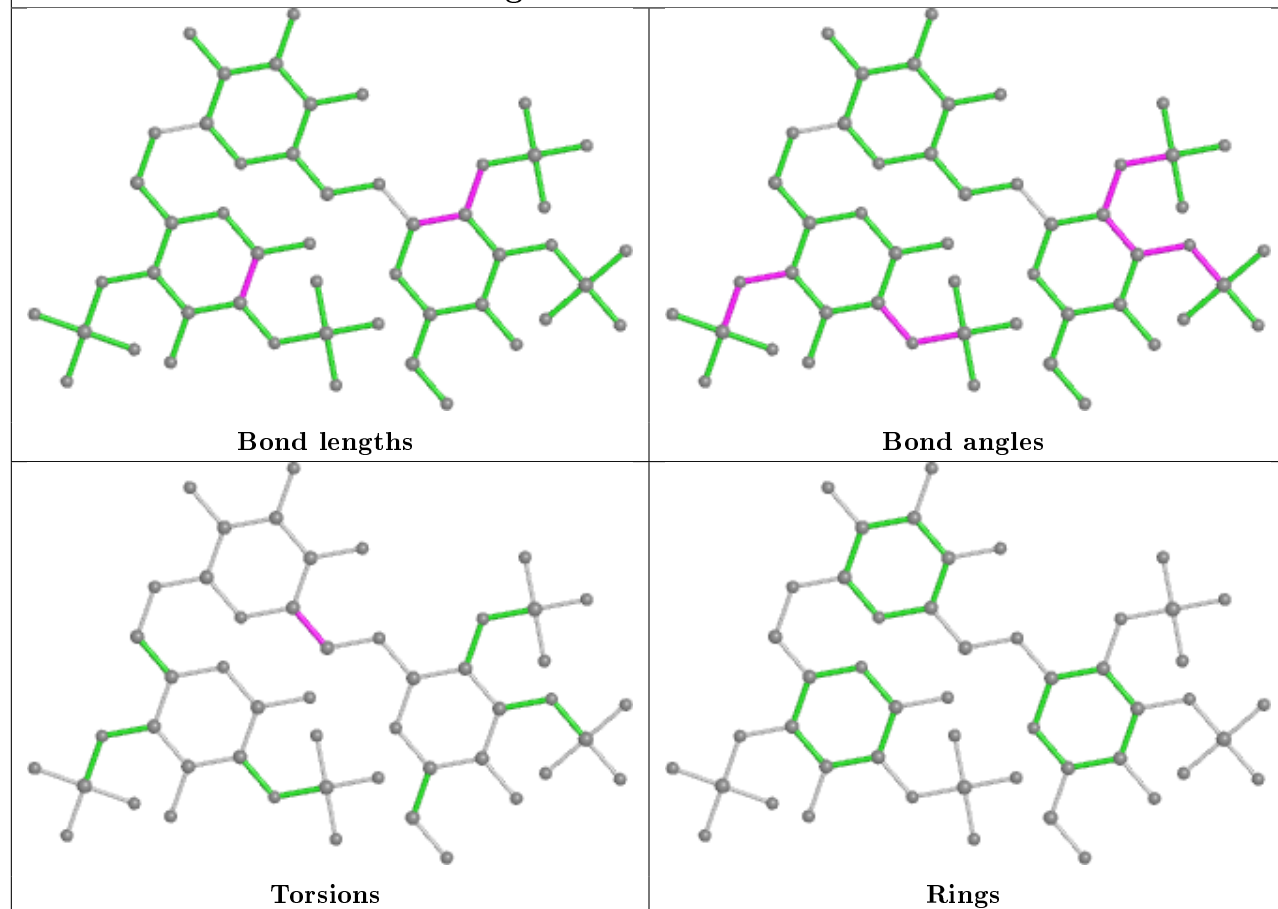




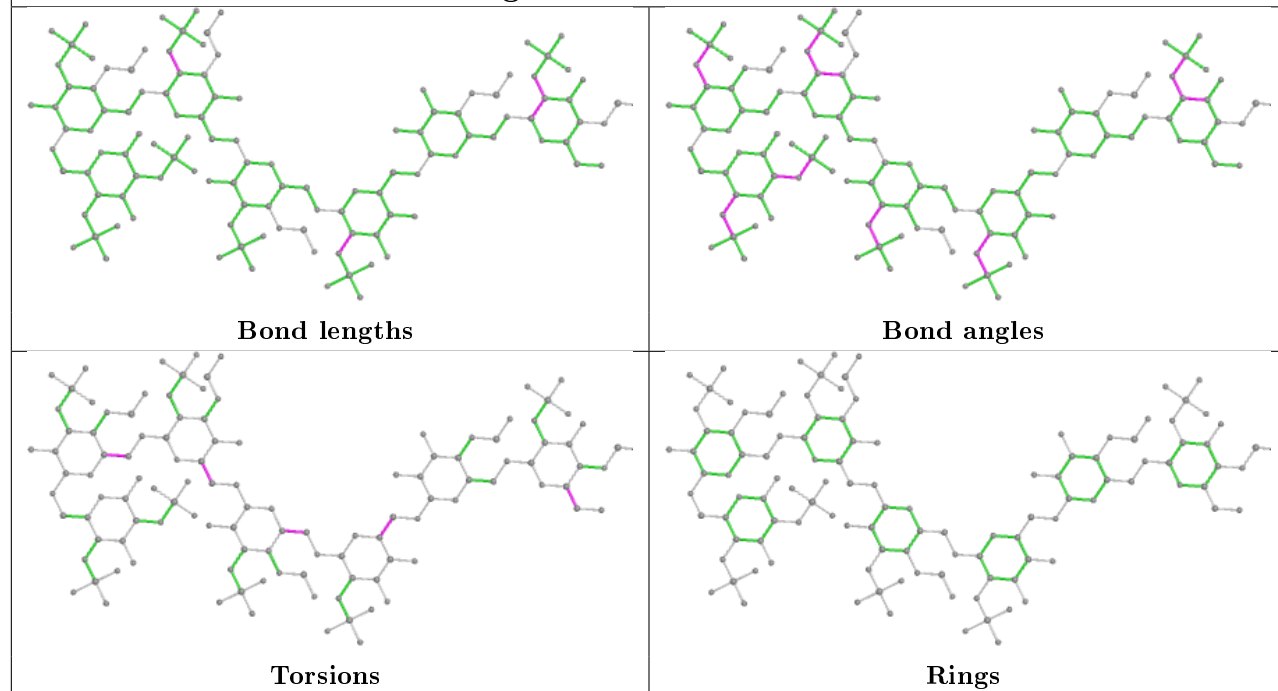


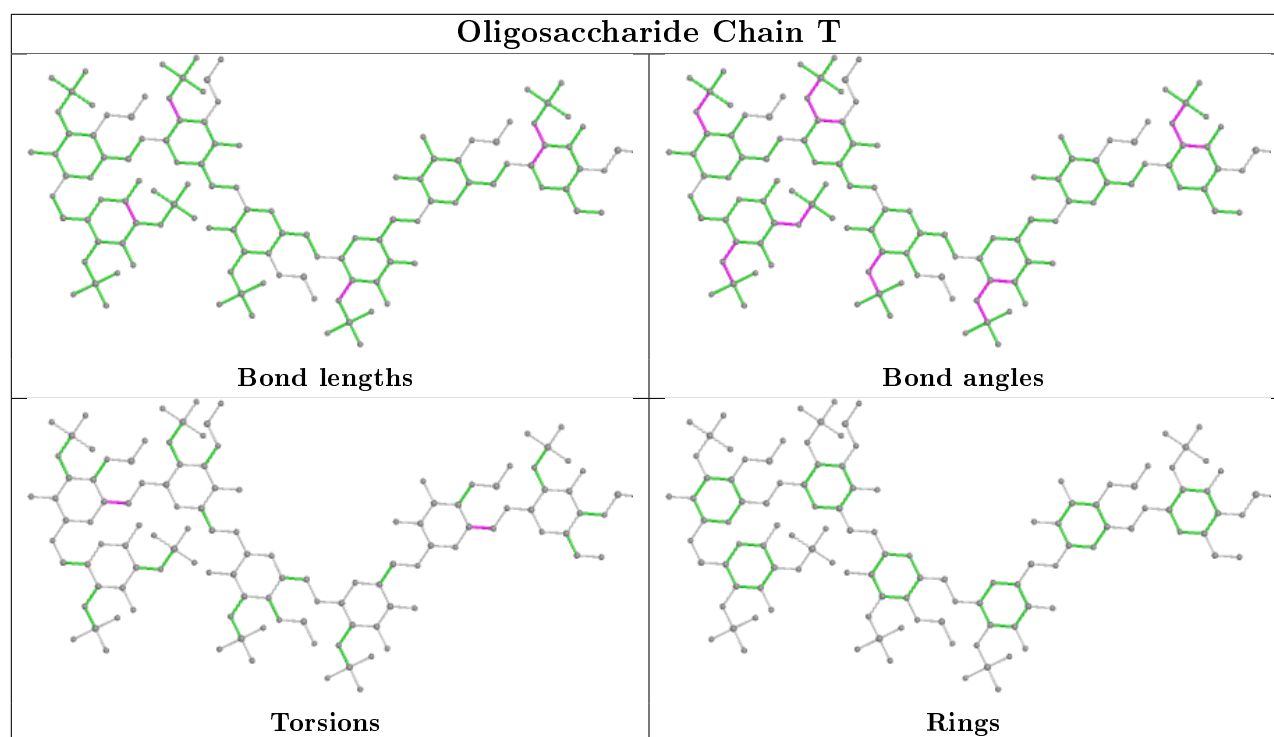


Oligosaccharide Chain Z



Oligosaccharide Chain O





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	2.65	10 (35%)	40,41,41	4.75	18 (45%)
4	5TL	C	701	-	28,28,28	2.61	11 (39%)	40,41,41	4.71	22 (55%)
4	5TL	F	701	-	28,28,28	2.64	10 (35%)	40,41,41	4.67	18 (45%)
4	5TL	E	701	-	28,28,28	2.60	10 (35%)	40,41,41	4.69	20 (50%)
4	5TL	G	701	-	28,28,28	2.60	11 (39%)	40,41,41	4.73	24 (60%)
4	5TL	H	701	-	28,28,28	2.65	11 (39%)	40,41,41	4.66	21 (52%)
4	5TL	J	701	-	28,28,28	2.65	10 (35%)	40,41,41	4.76	19 (47%)
4	5TL	I	701	-	28,28,28	2.63	10 (35%)	40,41,41	4.67	21 (52%)
4	5TL	L	701	-	28,28,28	2.64	10 (35%)	40,41,41	4.69	20 (50%)
4	5TL	K	701	-	28,28,28	2.58	10 (35%)	40,41,41	4.78	21 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5TL	B	701	-	28,28,28	2.66	12 (42%)	40,41,41	4.64	21 (52%)
4	5TL	A	701	-	28,28,28	2.62	12 (42%)	40,41,41	4.70	23 (57%)

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	-	-	6/18/18/18	0/3/3/3
4	5TL	C	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	G	701	-	-	5/18/18/18	0/3/3/3
4	5TL	H	701	-	-	6/18/18/18	0/3/3/3
4	5TL	J	701	-	-	8/18/18/18	0/3/3/3
4	5TL	I	701	-	-	8/18/18/18	0/3/3/3
4	5TL	L	701	-	-	5/18/18/18	0/3/3/3
4	5TL	K	701	-	-	8/18/18/18	0/3/3/3
4	5TL	B	701	-	-	6/18/18/18	0/3/3/3
4	5TL	A	701	-	-	8/18/18/18	0/3/3/3

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	701	5TL	S-N1	-6.22	1.48	1.60
4	H	701	5TL	S-N1	-6.18	1.48	1.60
4	F	701	5TL	S-N1	-6.15	1.48	1.60
4	B	701	5TL	S-N1	-6.09	1.48	1.60
4	L	701	5TL	S-N1	-6.00	1.48	1.60

The worst 5 of 248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	5TL	CAS-CAL-CAM	13.25	144.01	117.59
4	J	701	5TL	CAS-CAL-CAM	13.19	143.88	117.59
4	D	701	5TL	CAT-CAS-CAL	-13.16	102.19	121.13
4	L	701	5TL	CAS-CAL-CAM	13.13	143.76	117.59
4	J	701	5TL	CAT-CAS-CAL	-13.12	102.24	121.13

There are no chirality outliers.

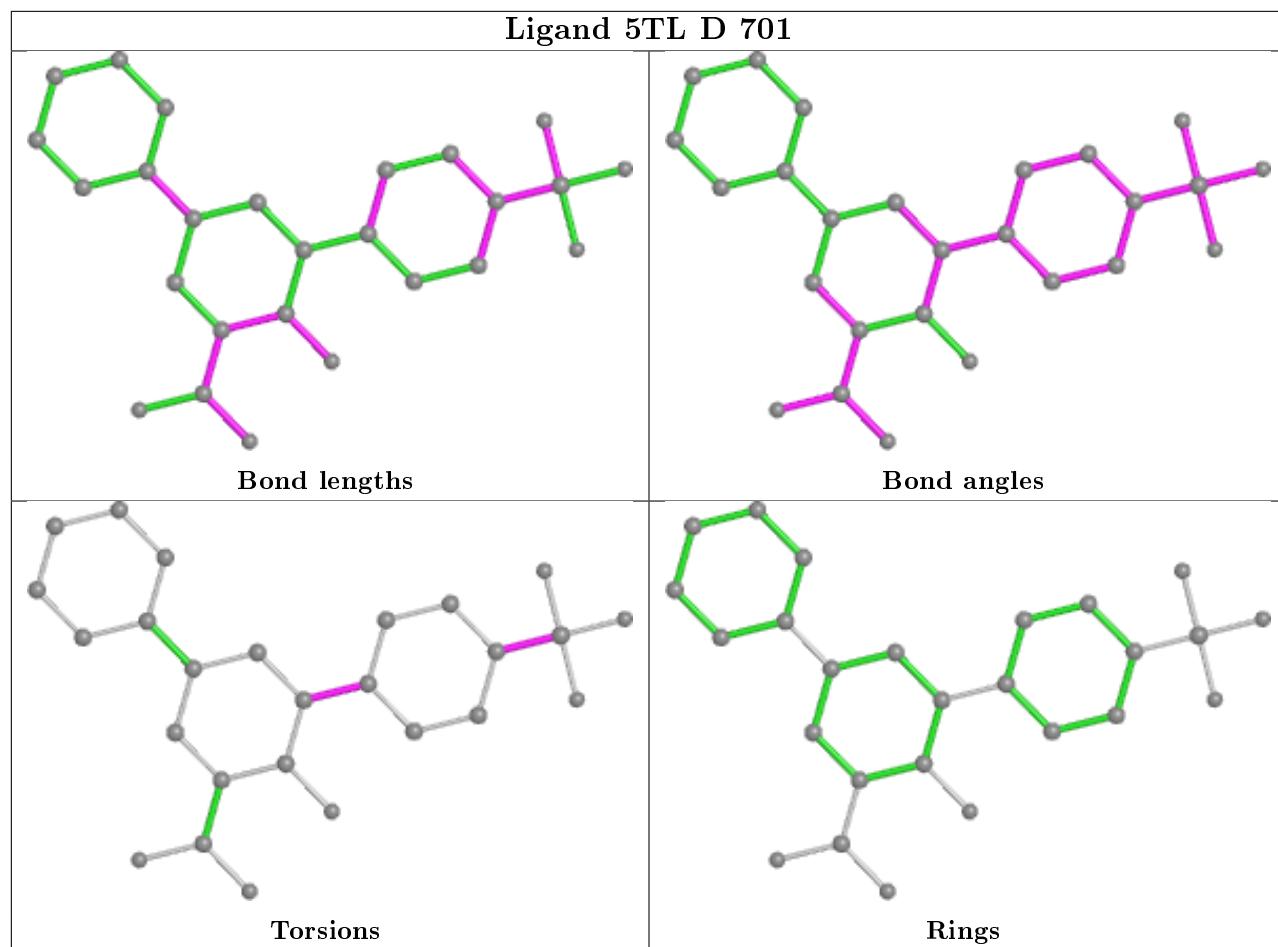
5 of 84 torsion outliers are listed below:

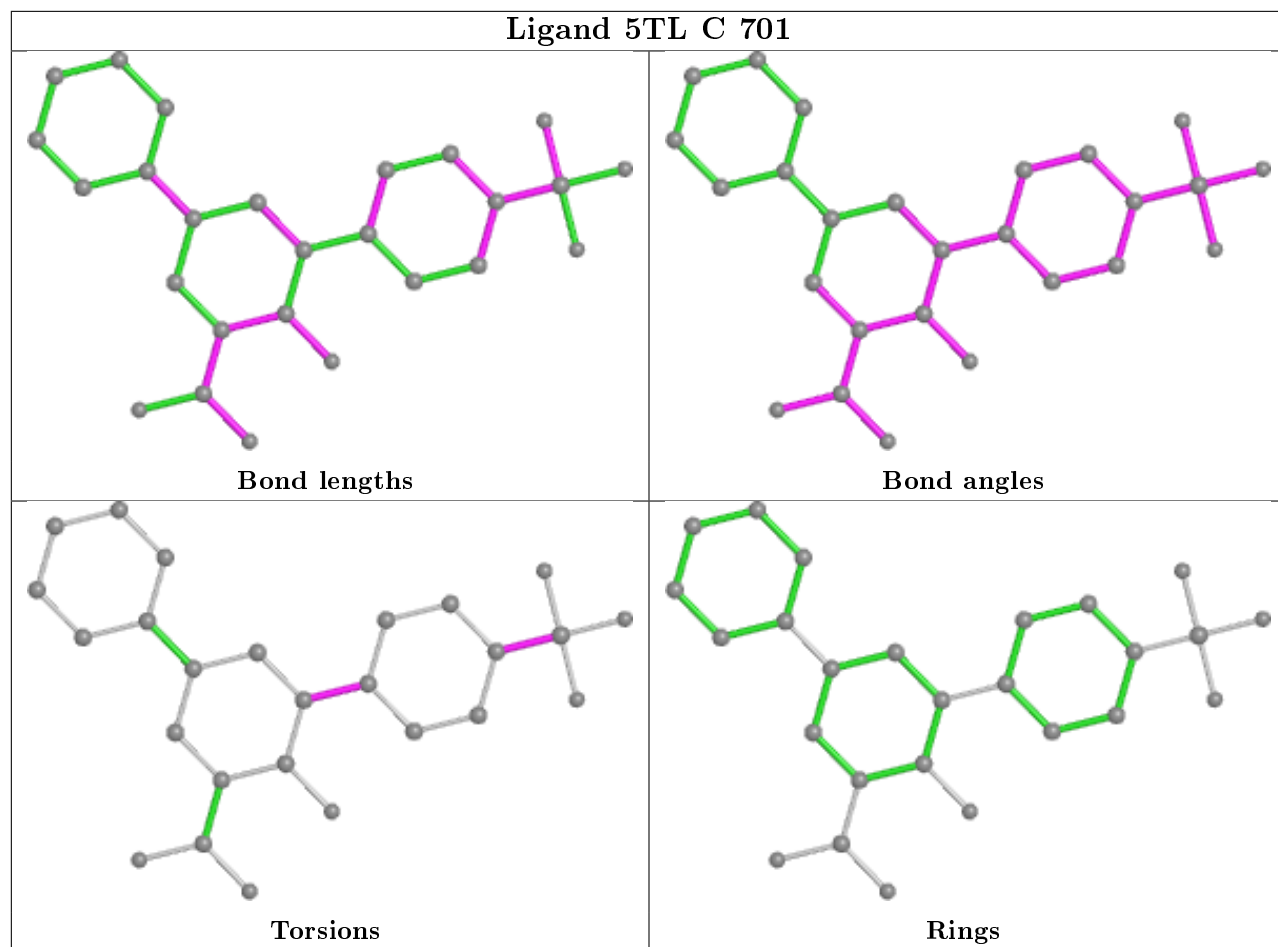
Mol	Chain	Res	Type	Atoms
4	D	701	5TL	CAR-CAJ-CAL-CAM
4	D	701	5TL	CAR-CAJ-CAL-CAS
4	C	701	5TL	CAR-CAJ-CAL-CAM
4	C	701	5TL	CAR-CAJ-CAL-CAS
4	F	701	5TL	CAR-CAJ-CAL-CAM

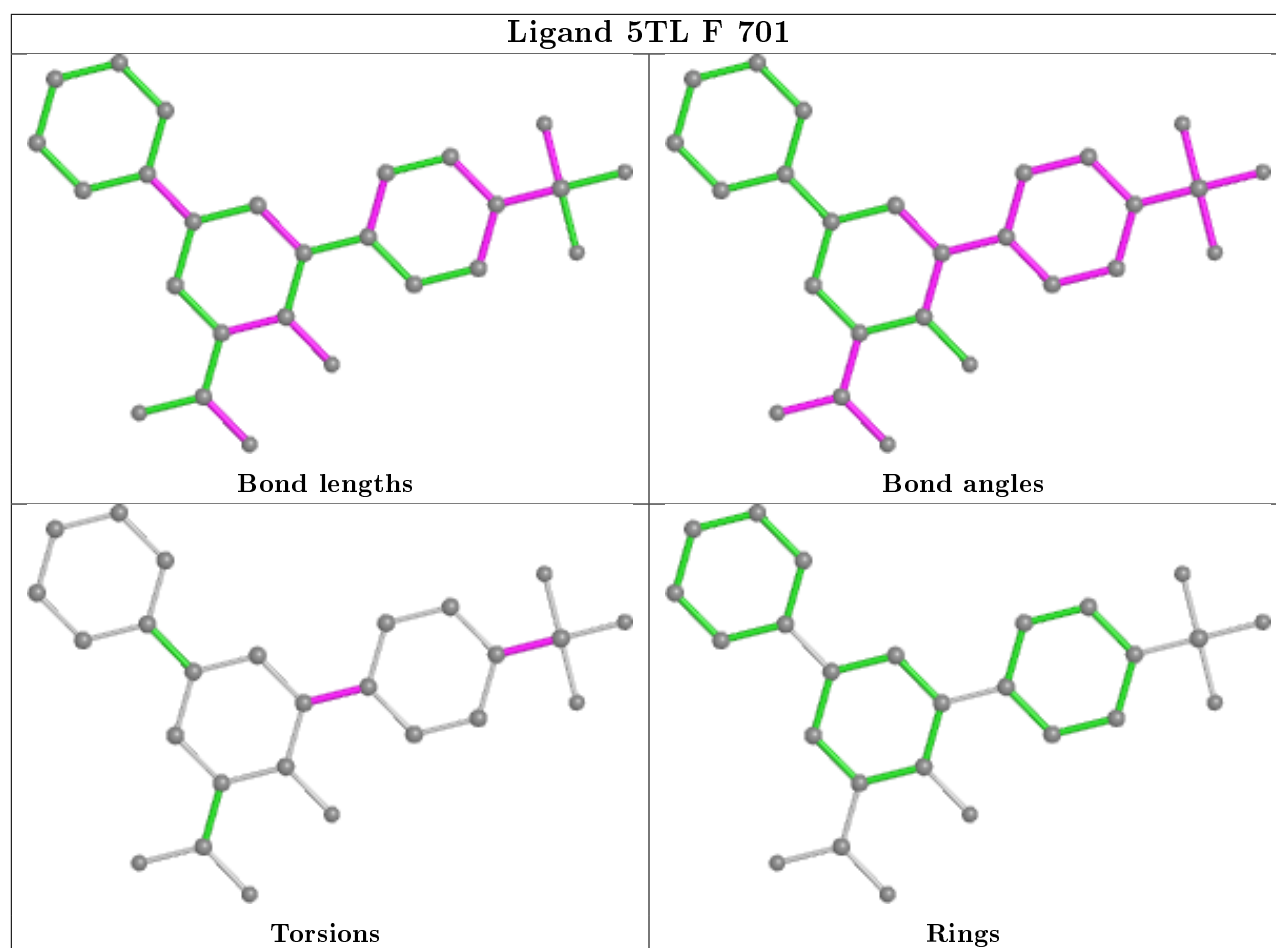
There are no ring outliers.

No monomer is involved in short contacts.

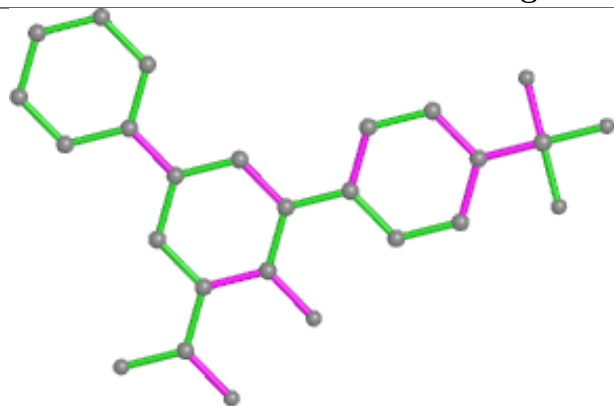
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



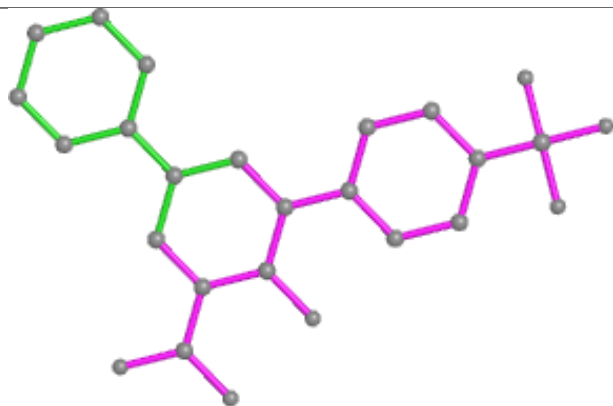




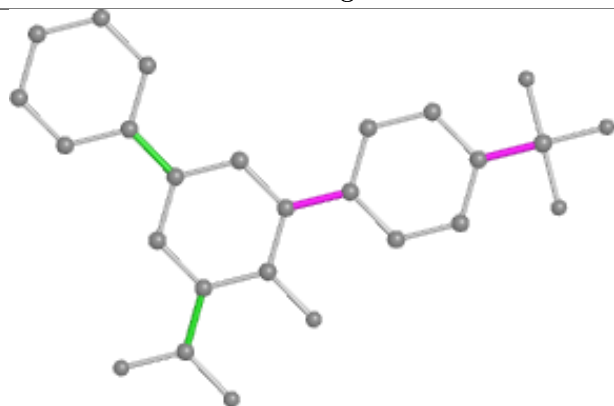
Ligand 5TL E 701



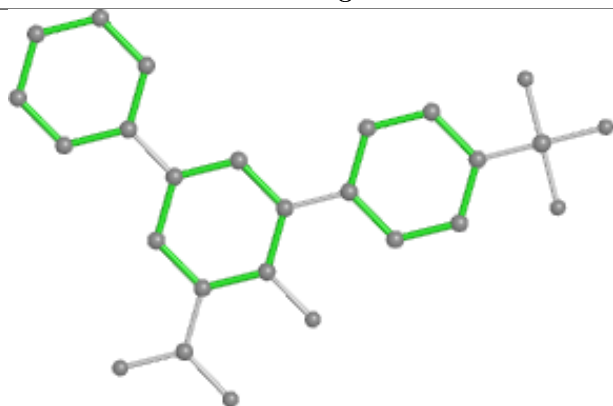
Bond lengths



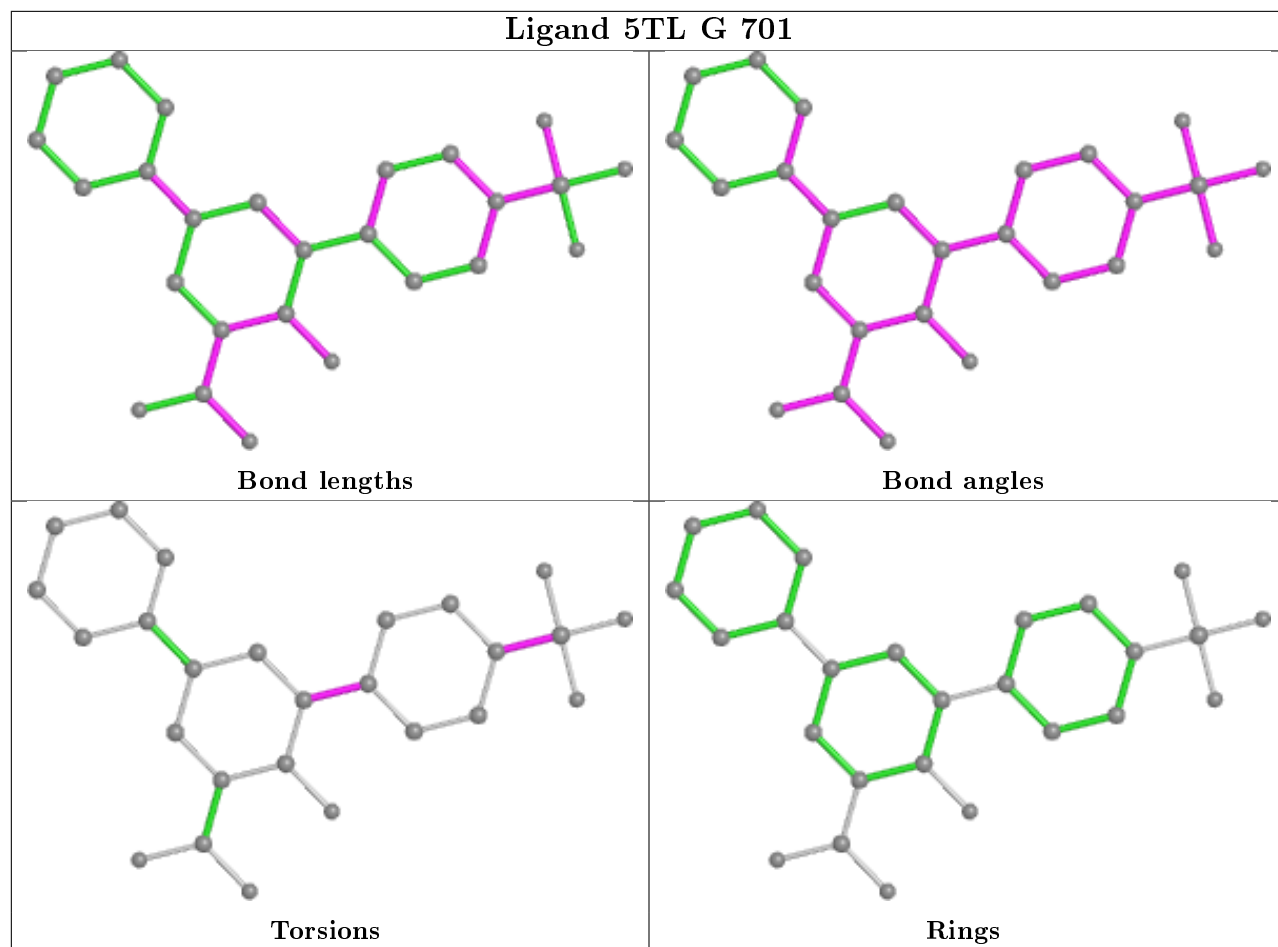
Bond angles

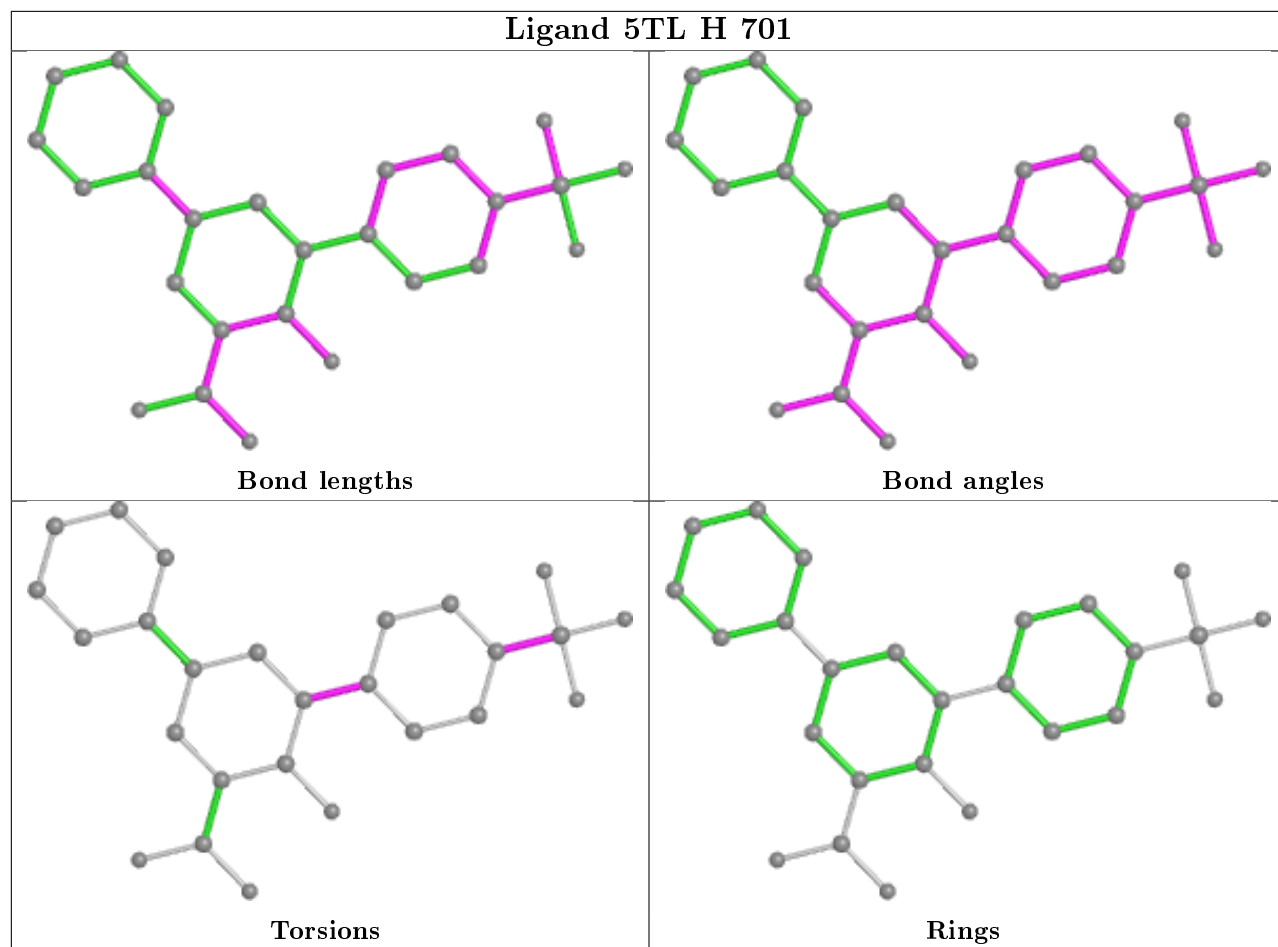


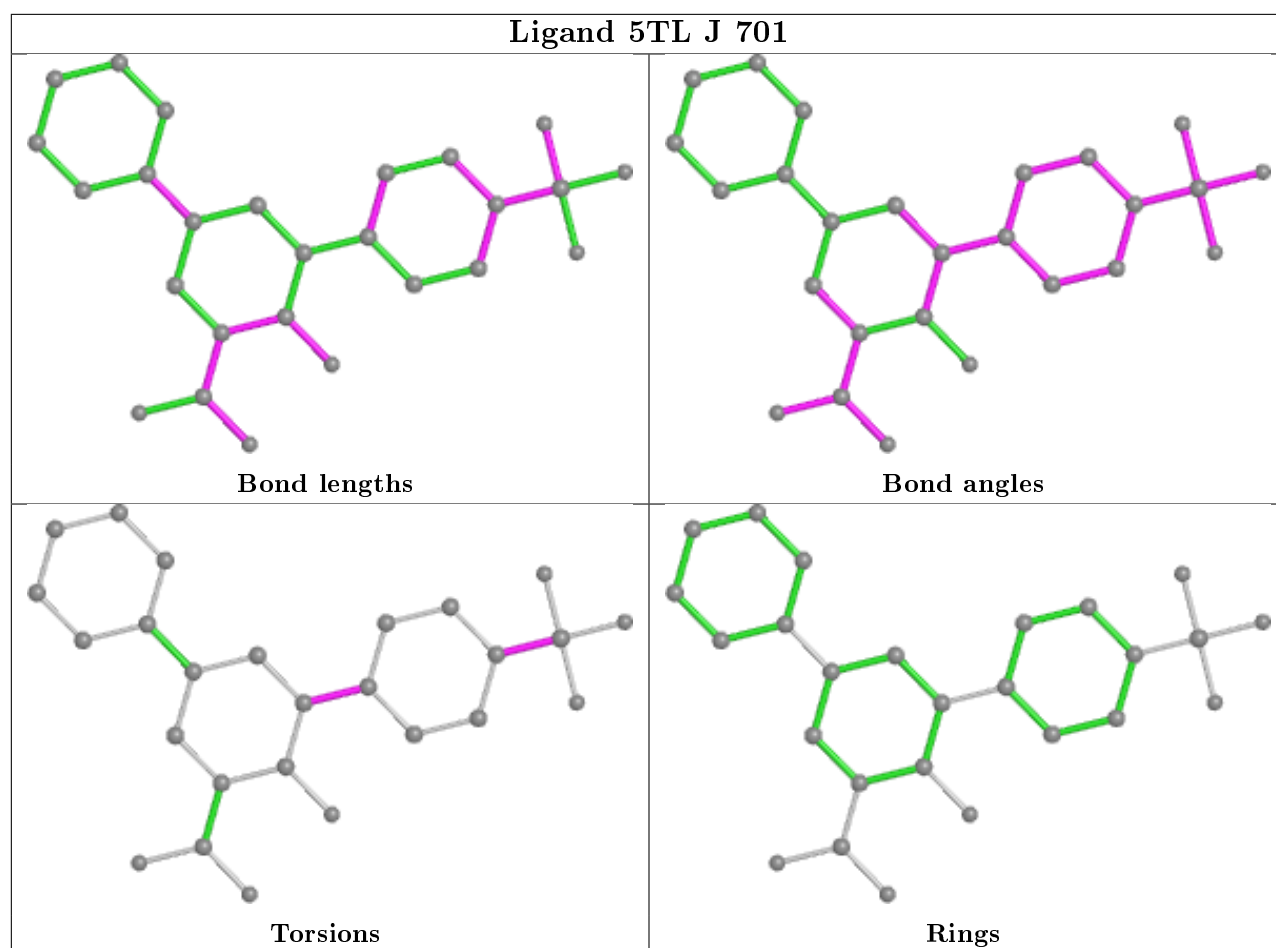
Torsions

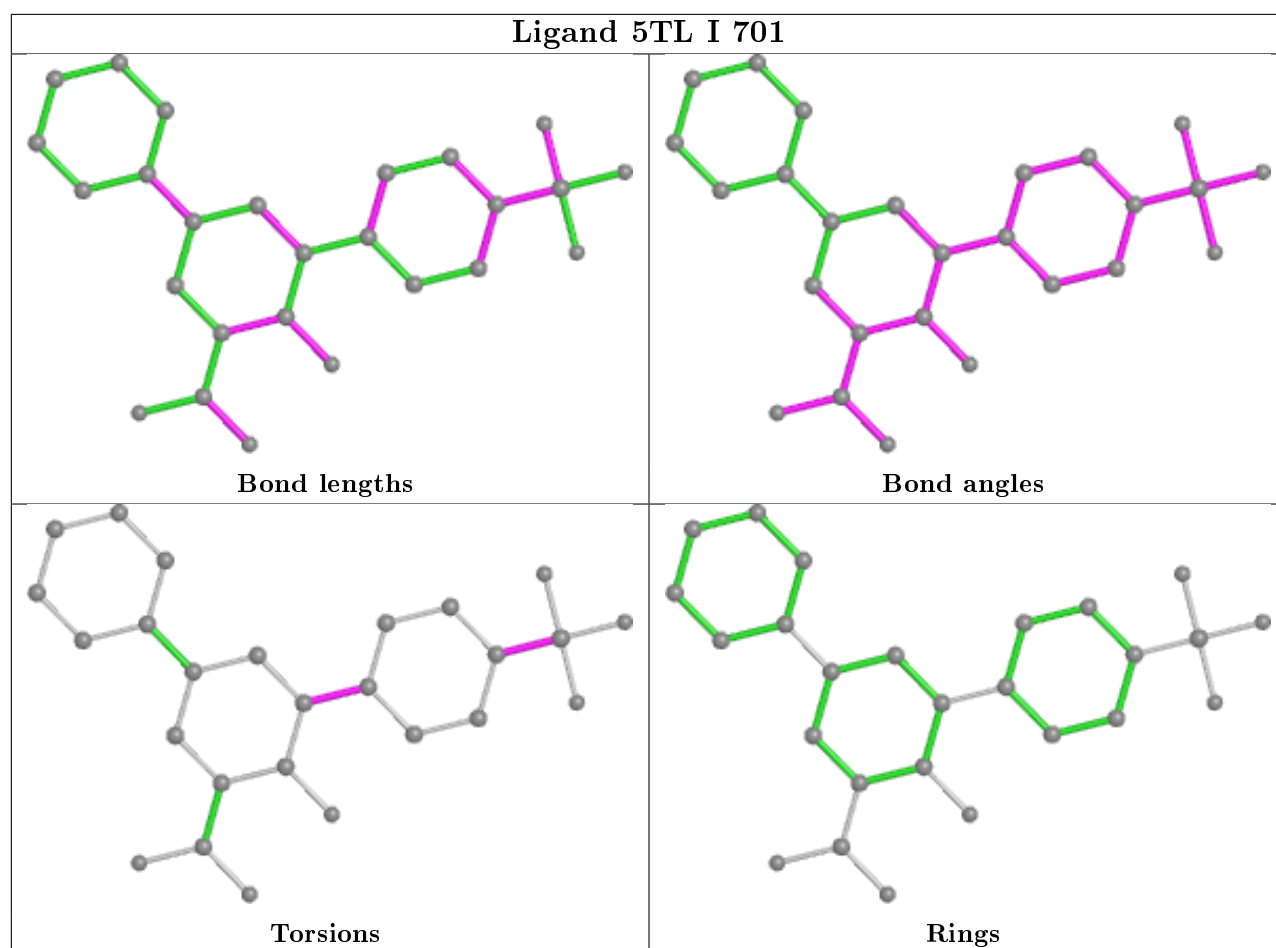


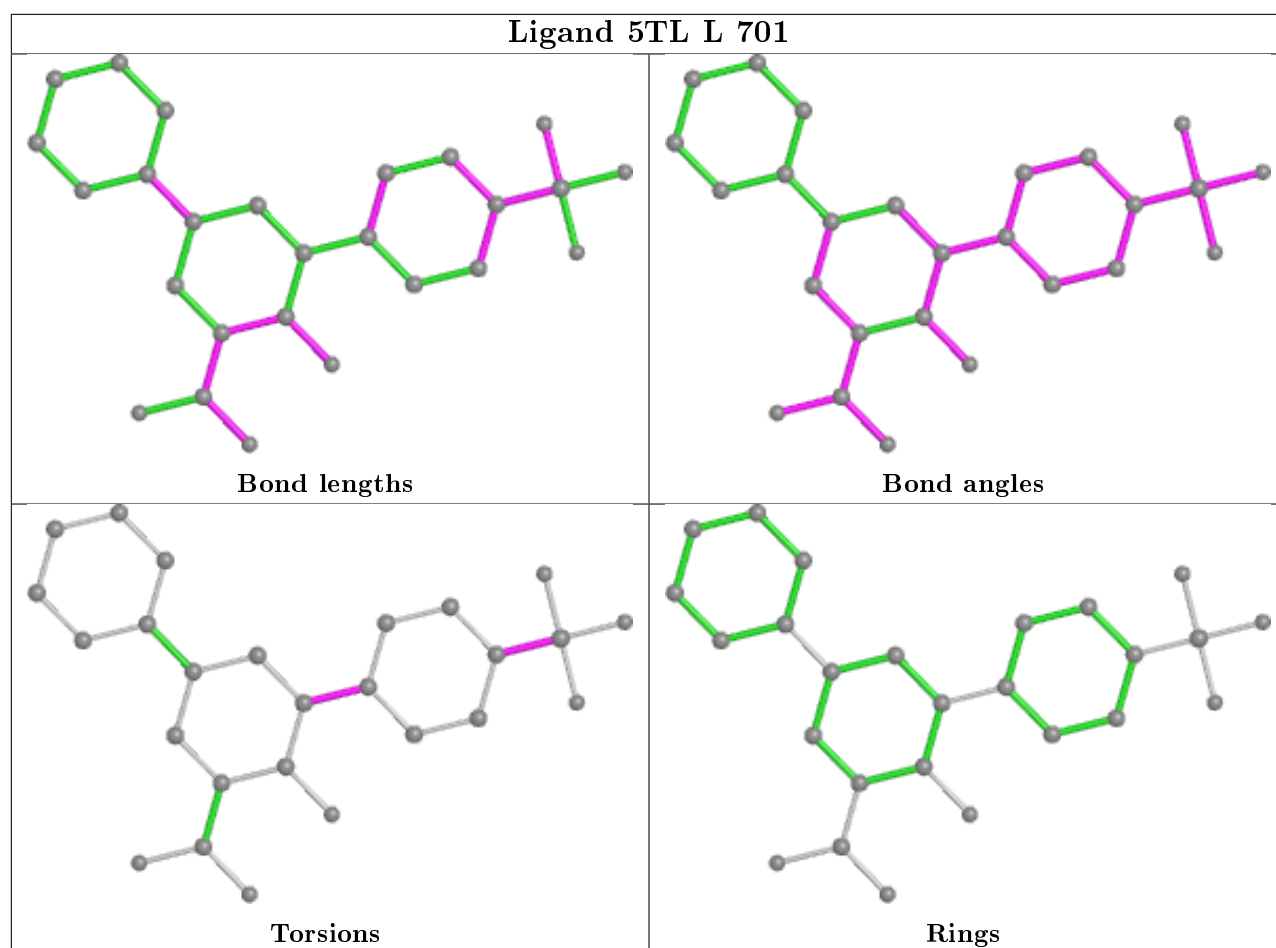
Rings

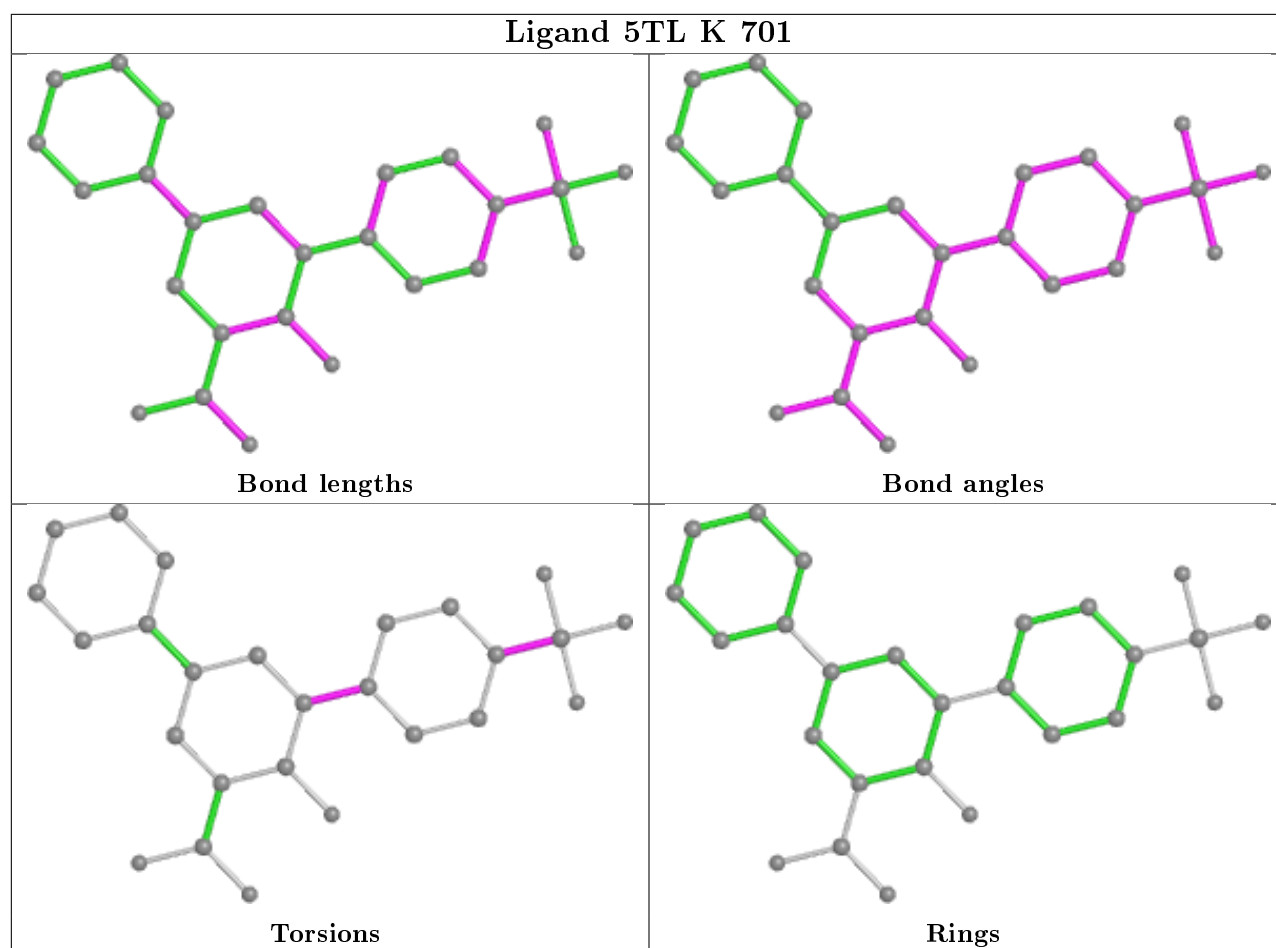


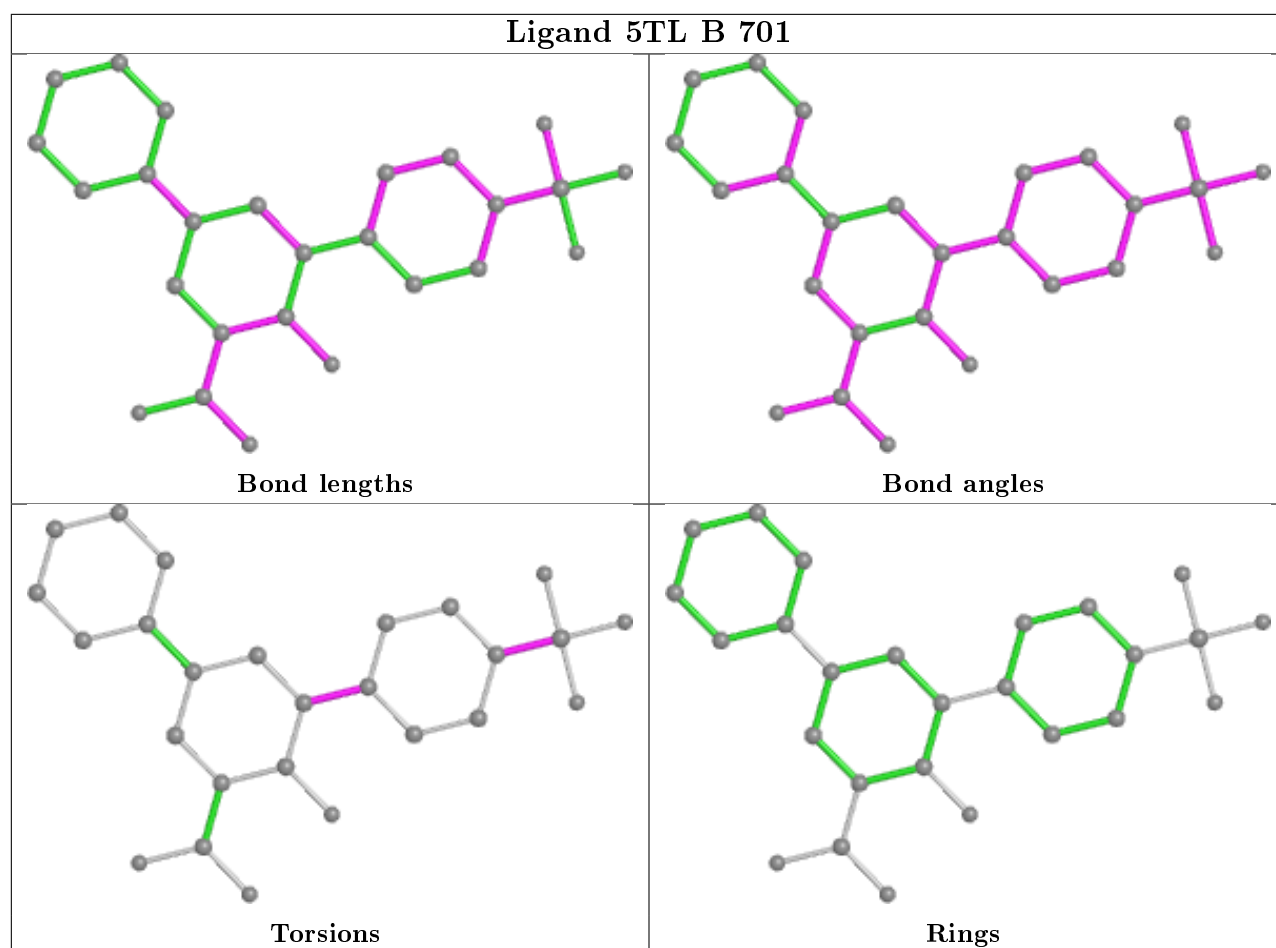


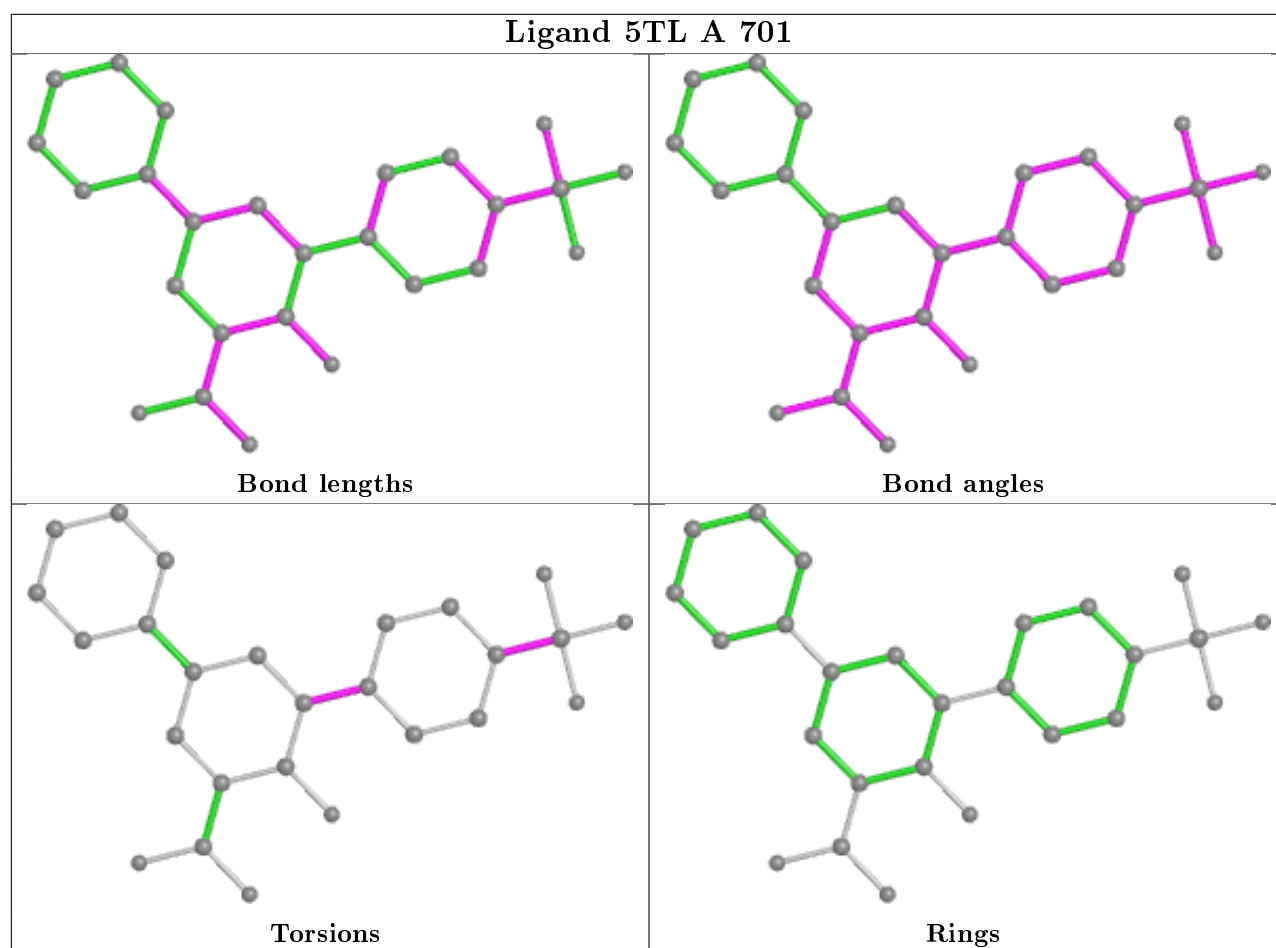












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

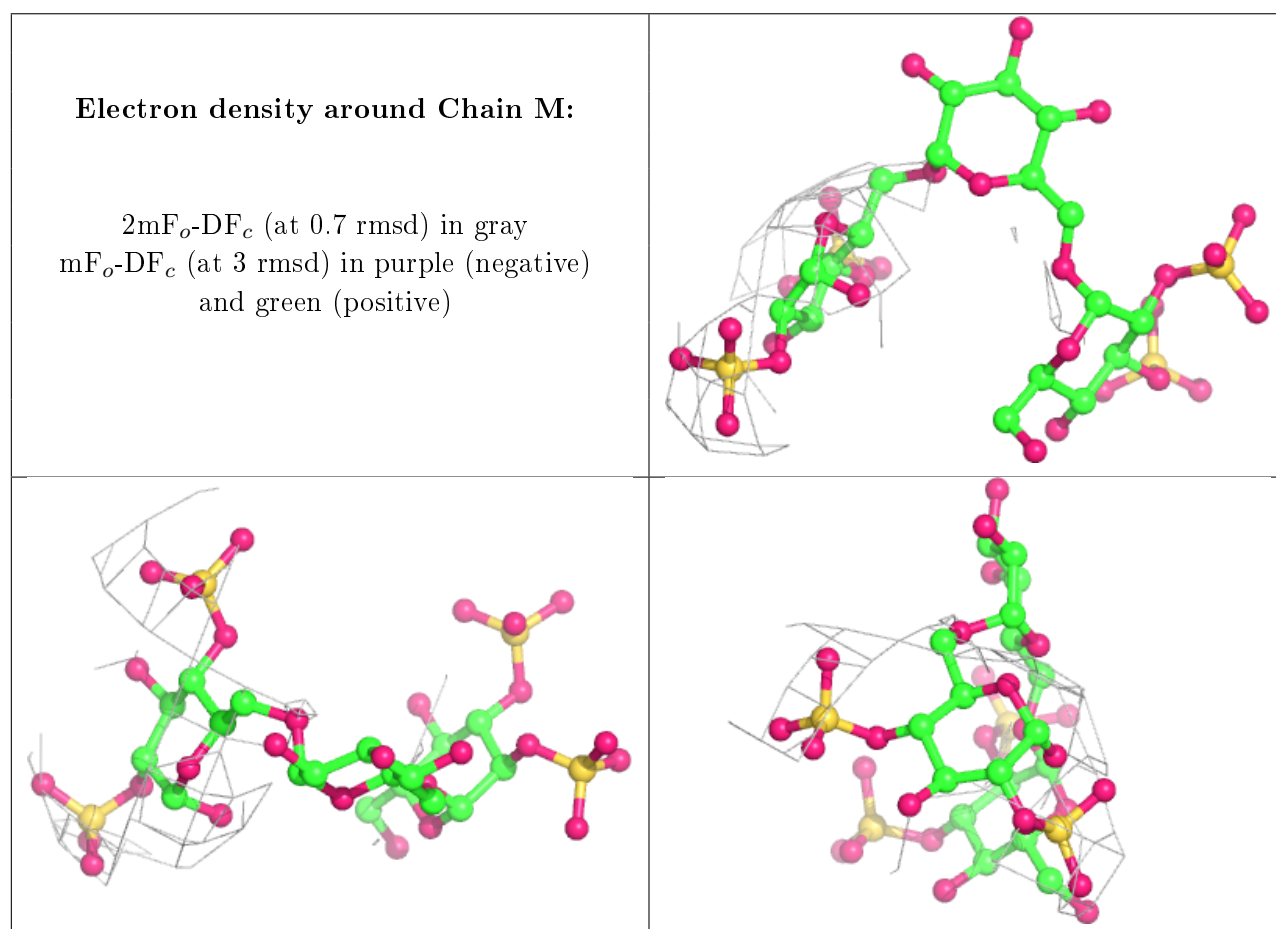
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

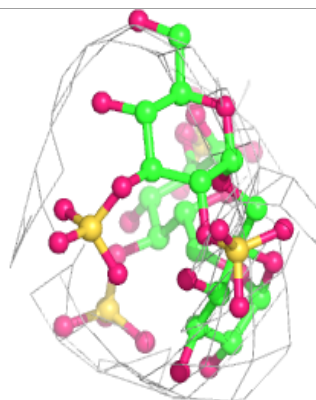
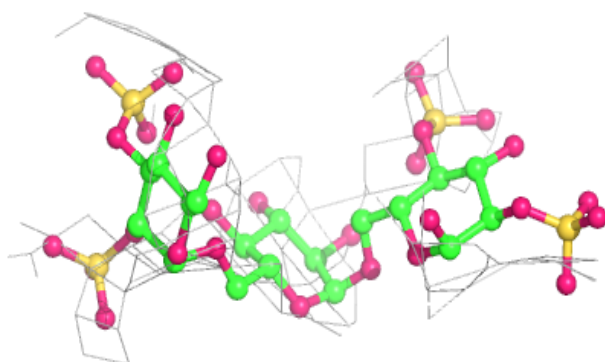
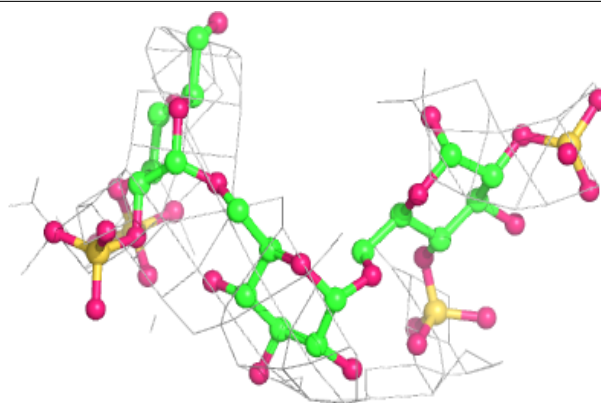
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

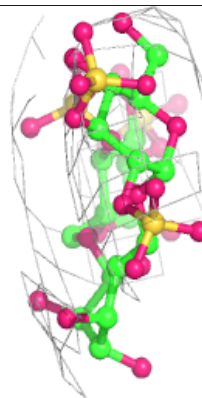
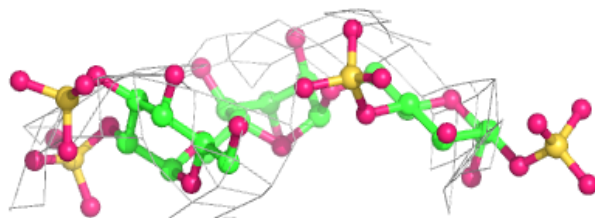
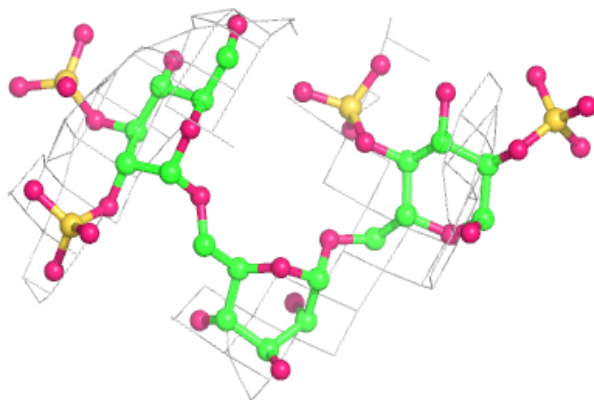


Electron density around Chain N:

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

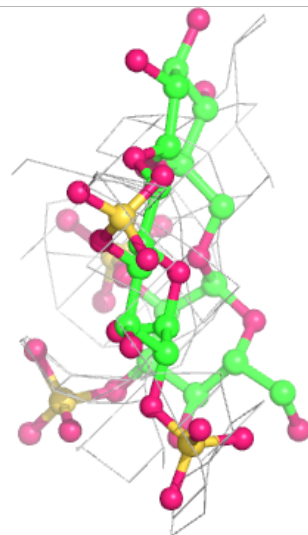
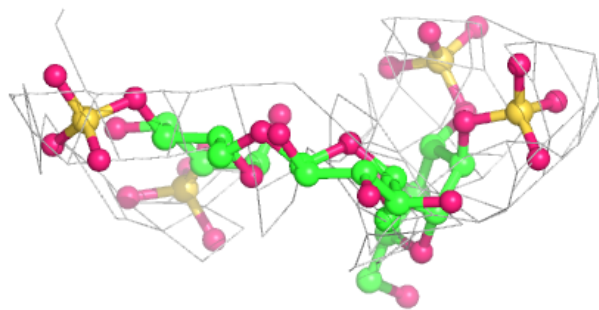
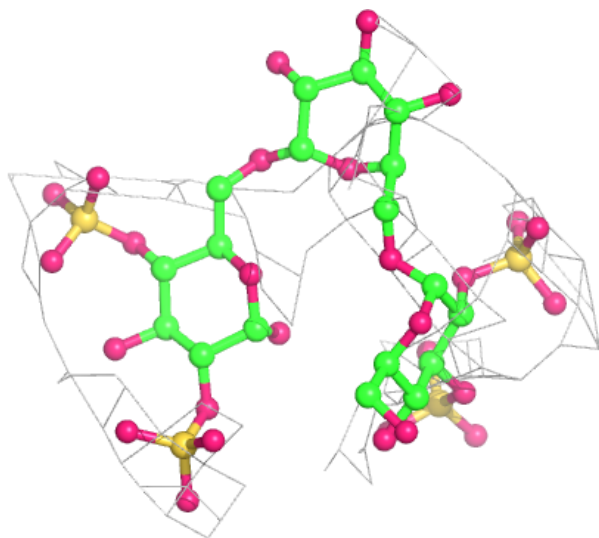
**Electron density around Chain P:**

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



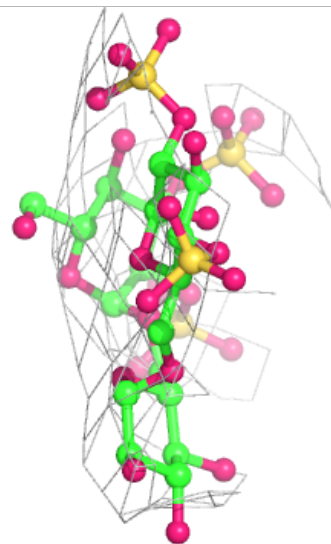
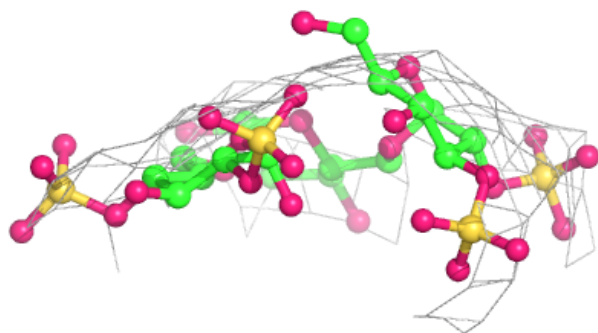
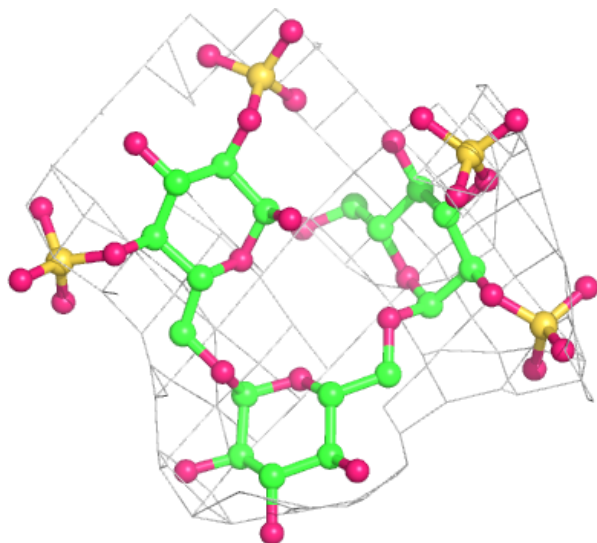
Electron density around Chain Q:

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



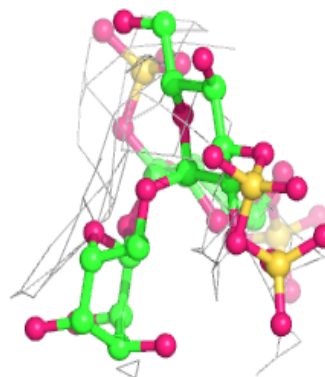
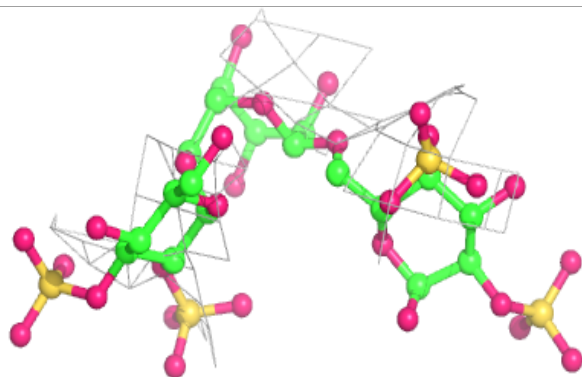
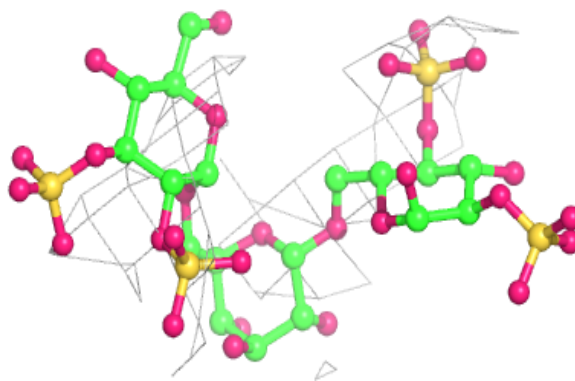
Electron density around Chain R:

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



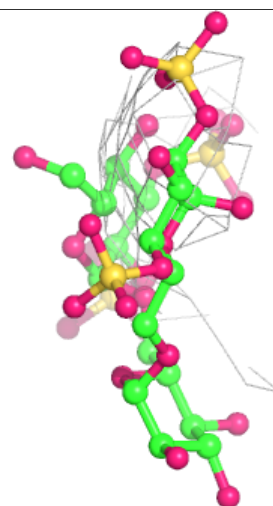
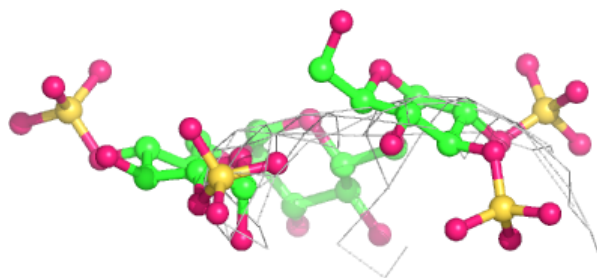
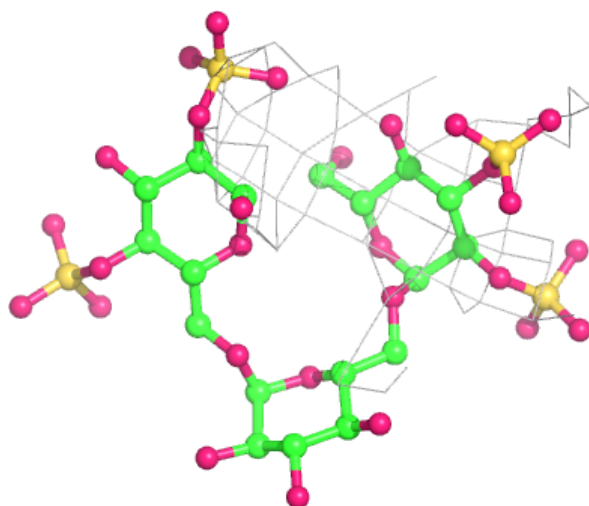
Electron density around Chain S:

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



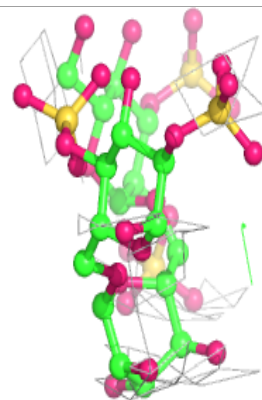
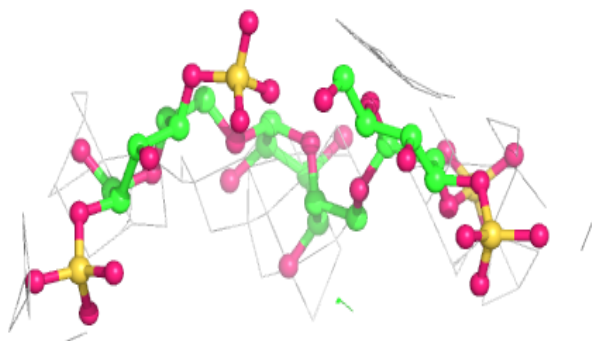
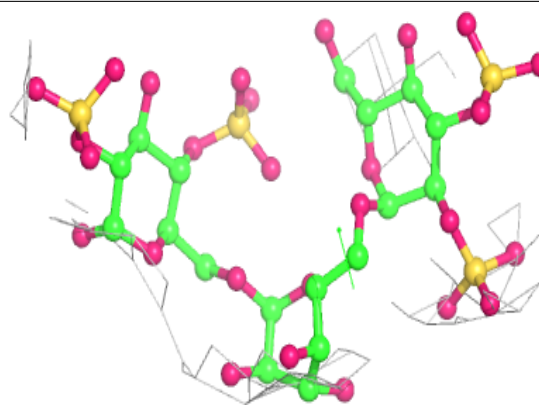
Electron density around Chain U:

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



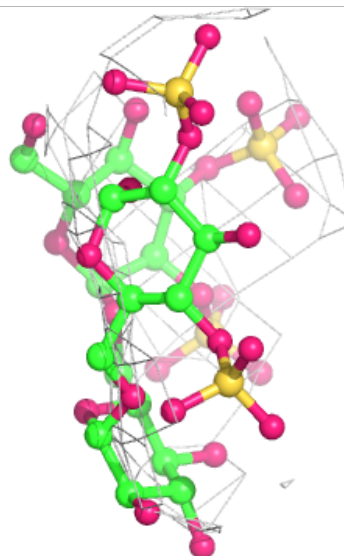
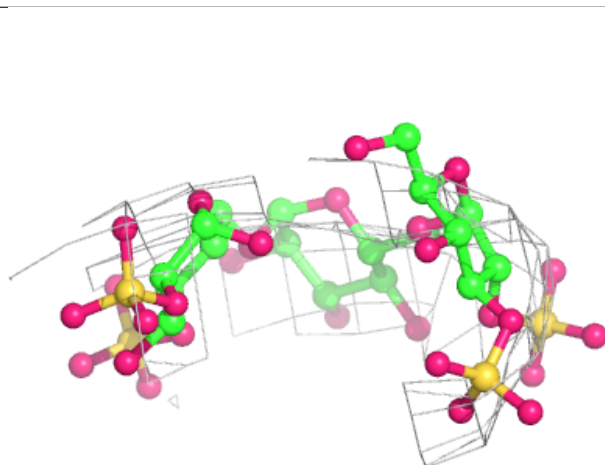
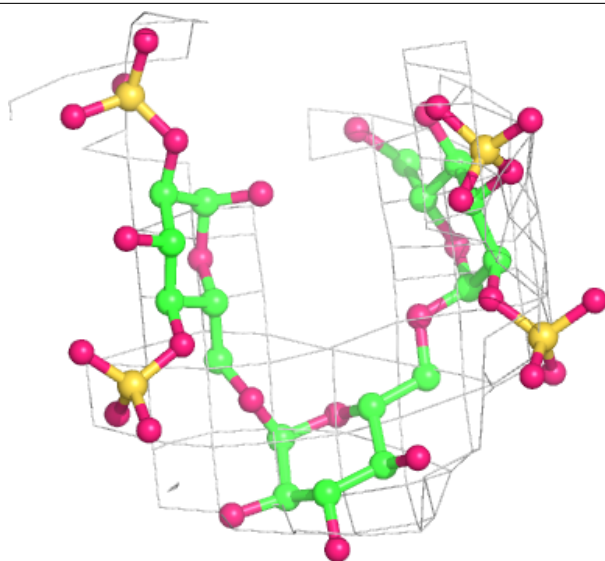
Electron density around Chain V:

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



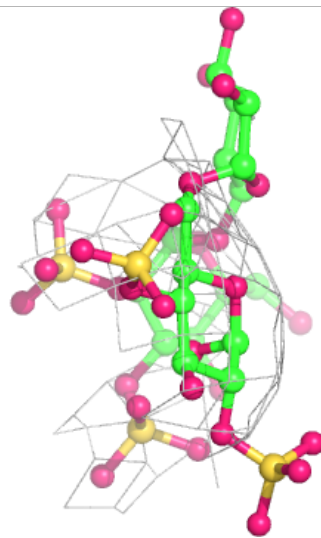
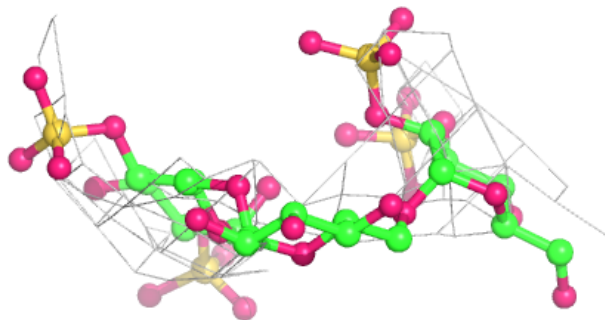
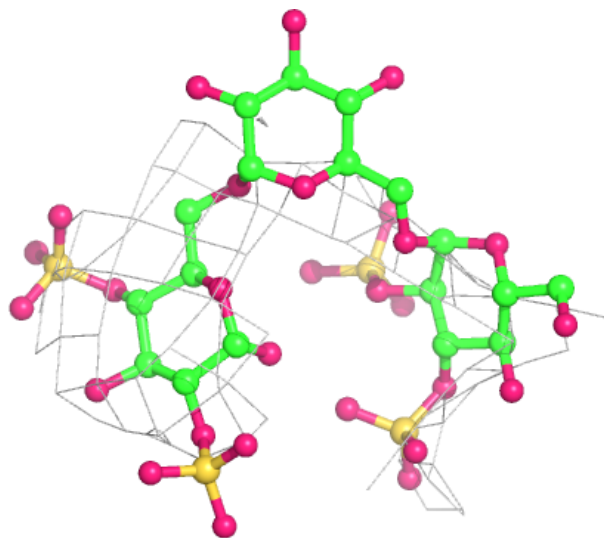
Electron density around Chain W:

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



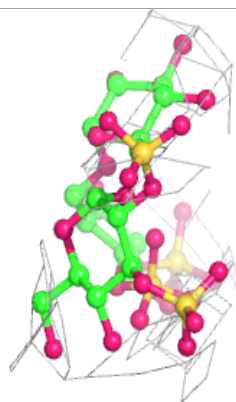
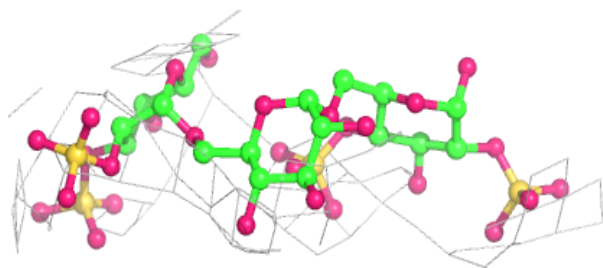
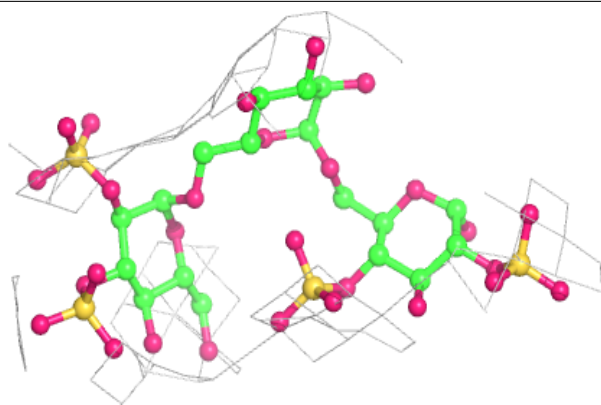
Electron density around Chain X:

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

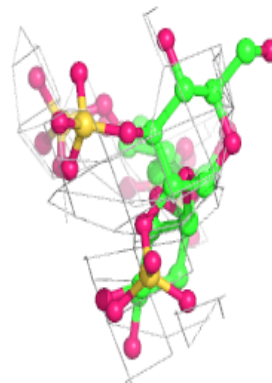
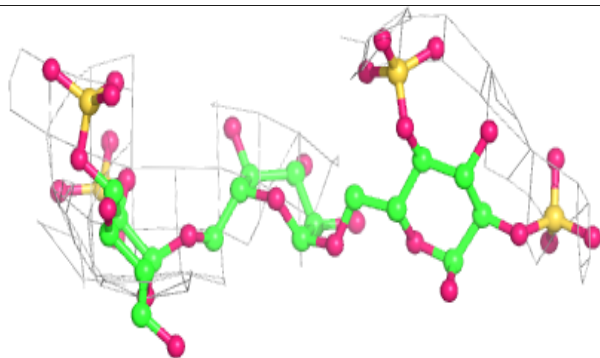
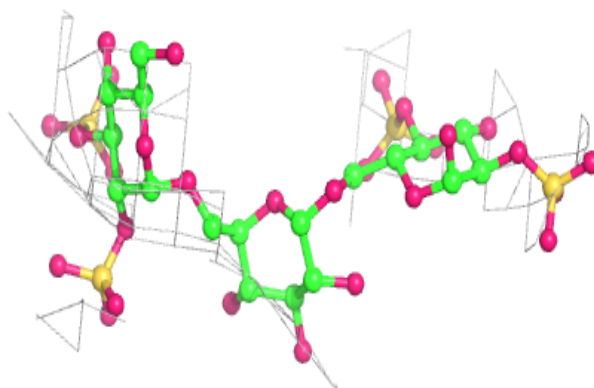


Electron density around Chain Y:

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

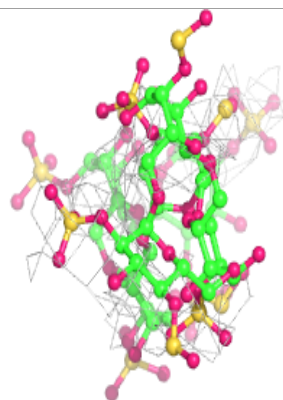
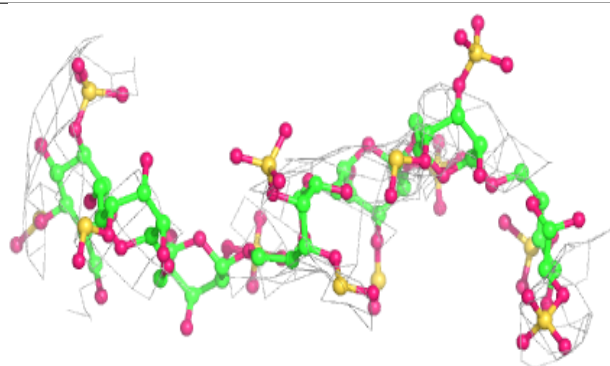
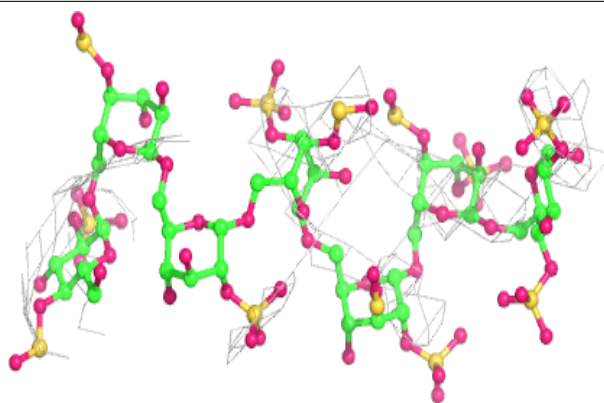
**Electron density around Chain Z:**

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

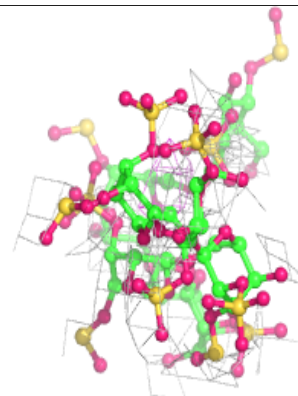
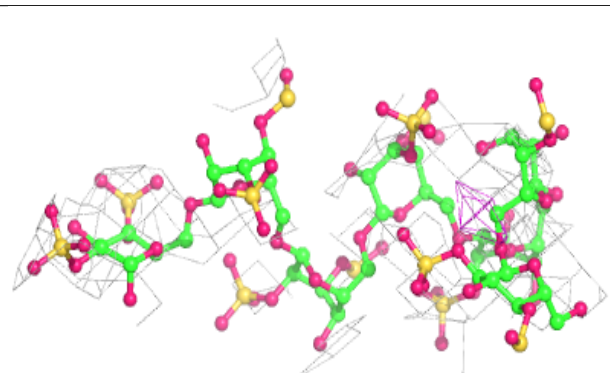
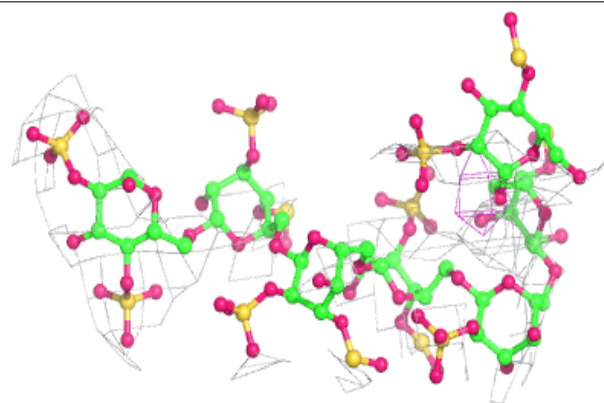


Electron density around Chain O:

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

**Electron density around Chain T:**

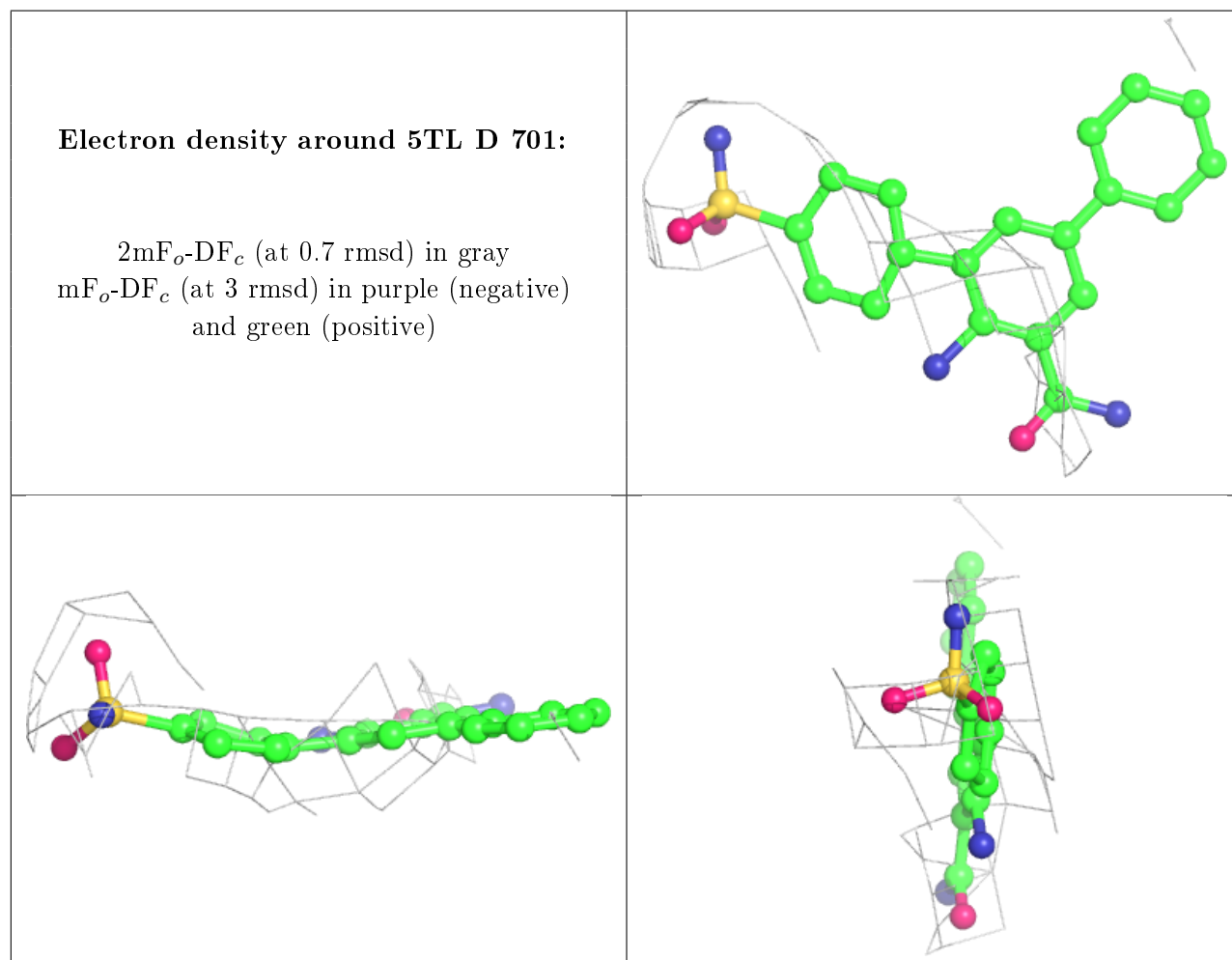
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands ⓘ

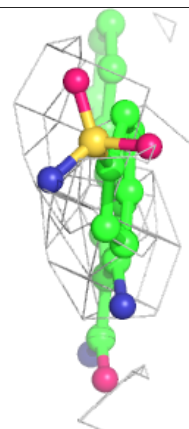
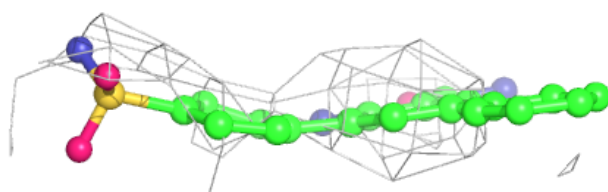
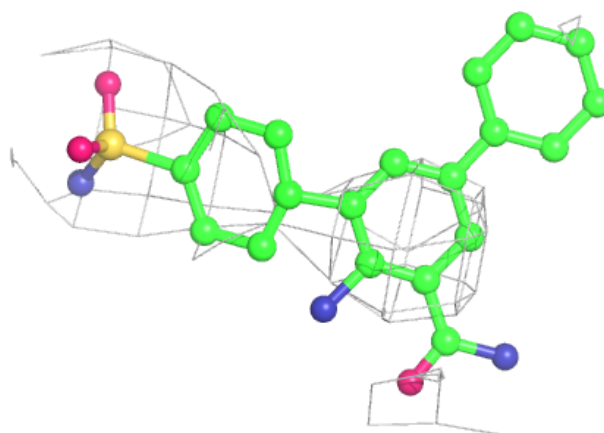
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

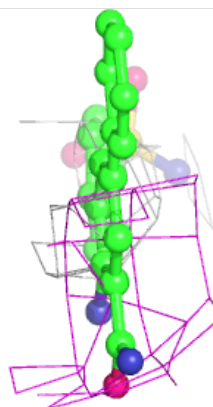
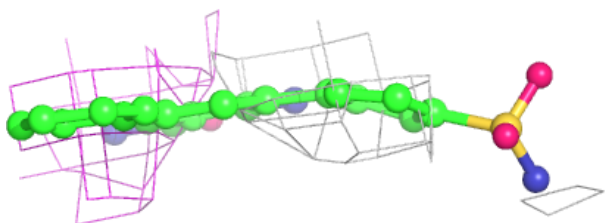
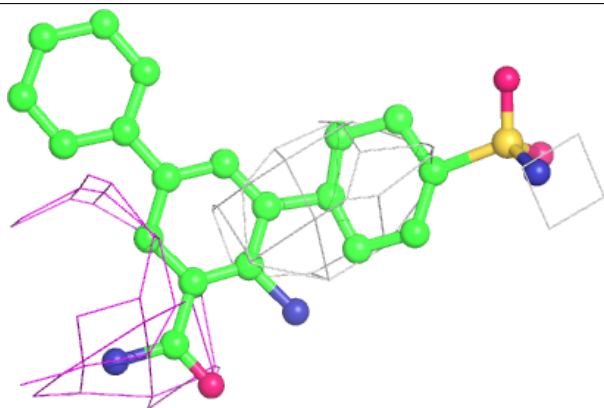


Electron density around 5TL C 701:

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

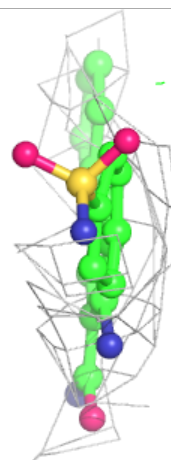
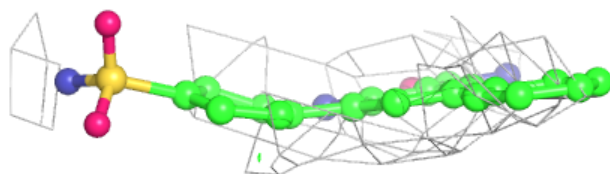
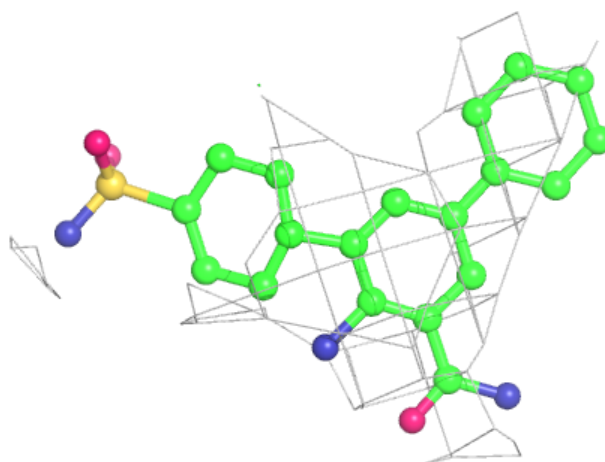
**Electron density around 5TL F 701:**

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



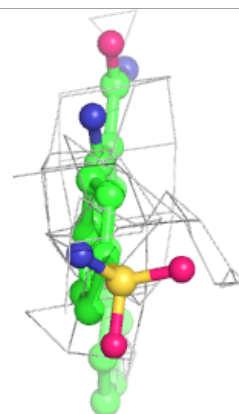
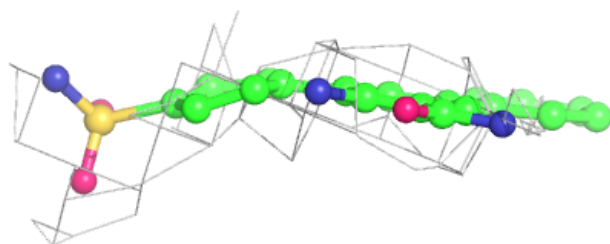
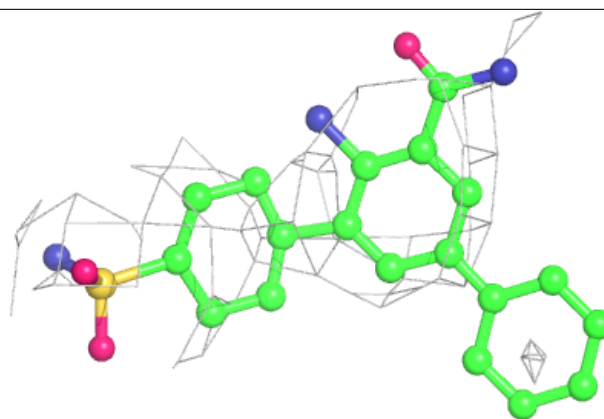
Electron density around 5TL E 701:

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and green (positive)

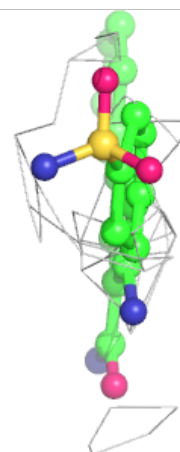
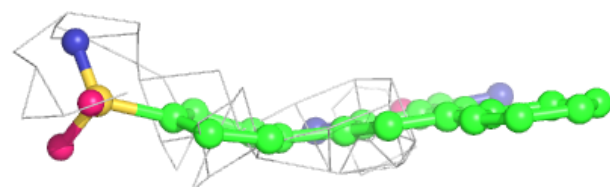
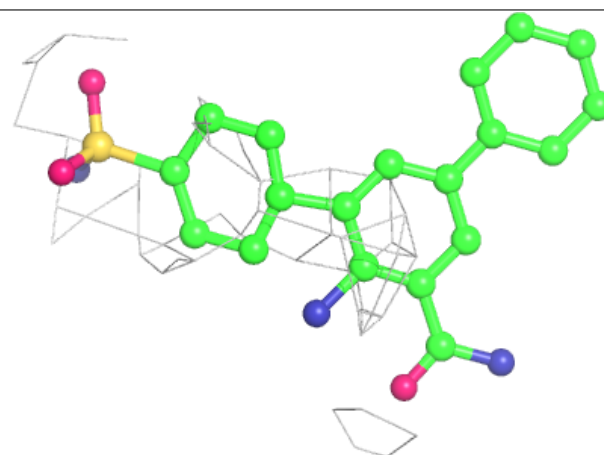


Electron density around 5TL G 701:

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and green (positive)

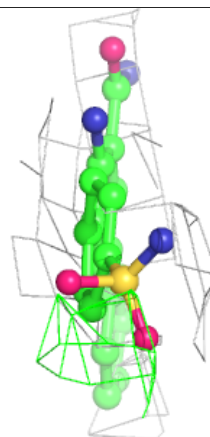
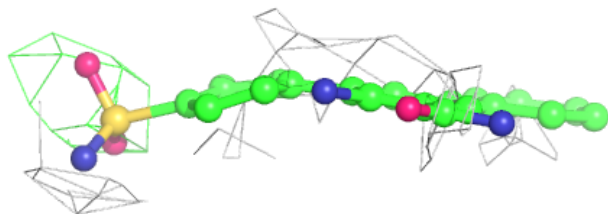
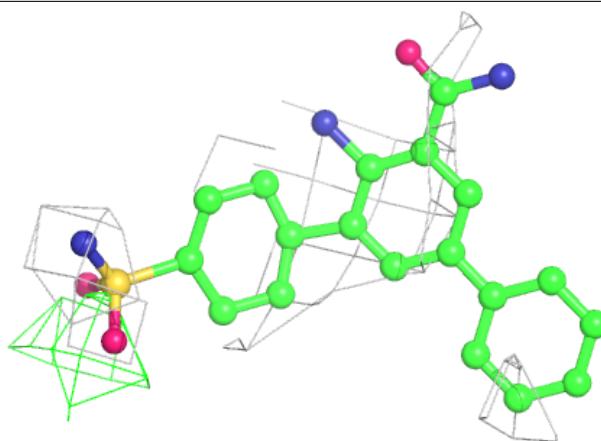
**Electron density around 5TL H 701:**

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



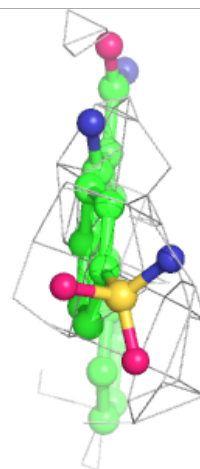
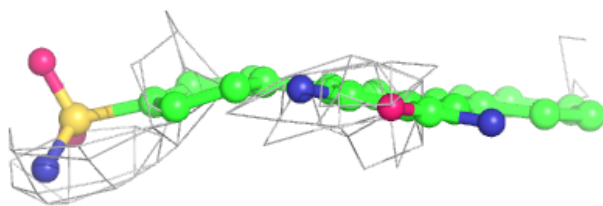
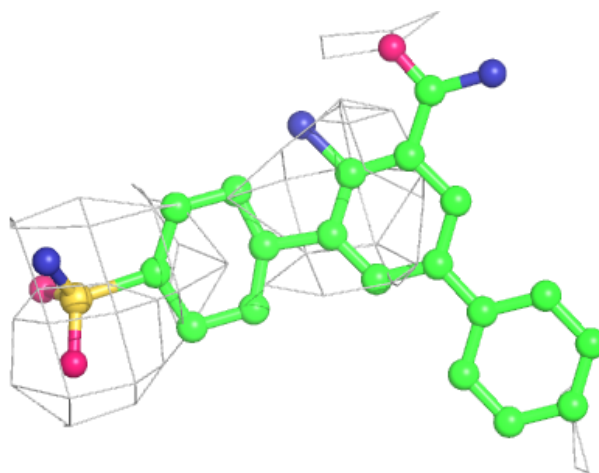
Electron density around 5TL J 701:

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



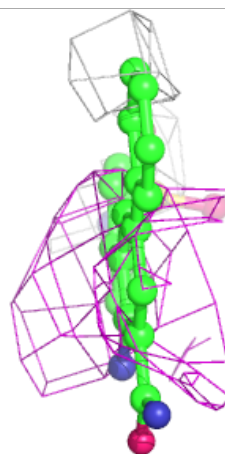
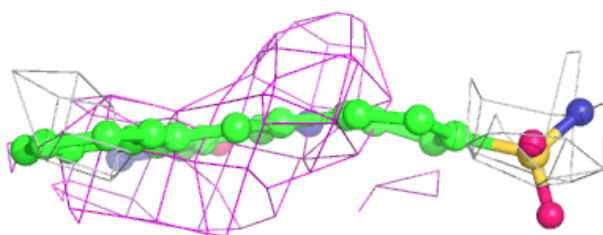
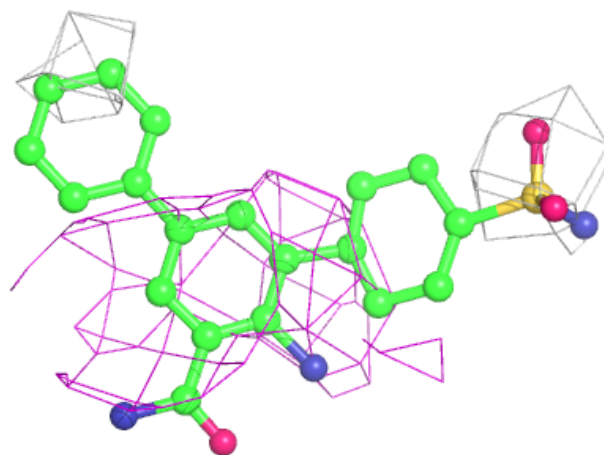
Electron density around 5TL I 701:

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



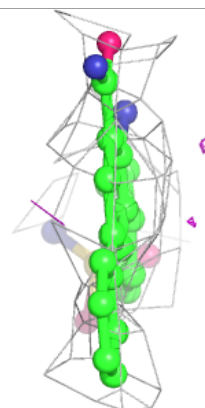
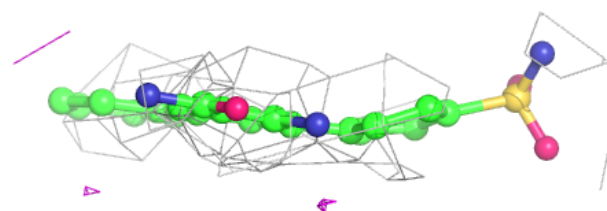
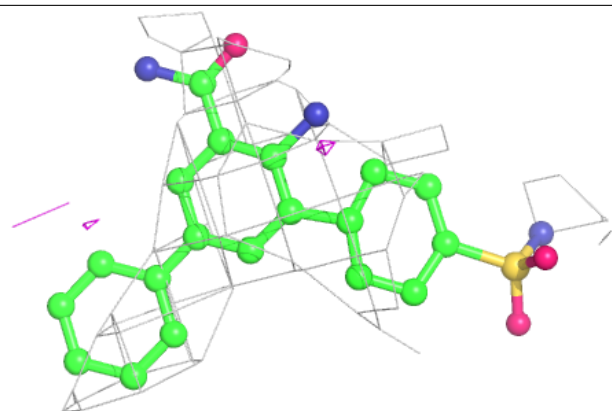
Electron density around 5TL L 701:

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

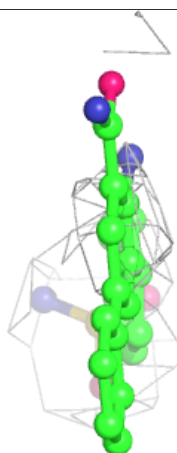
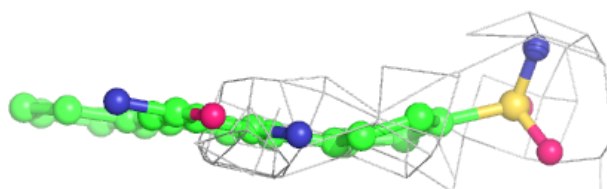
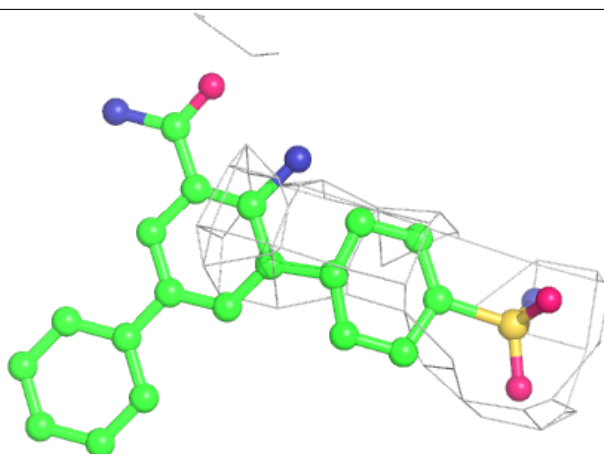


Electron density around 5TL K 701:

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

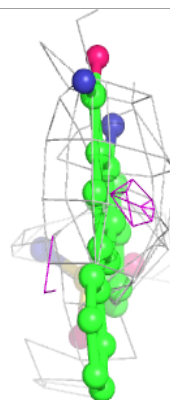
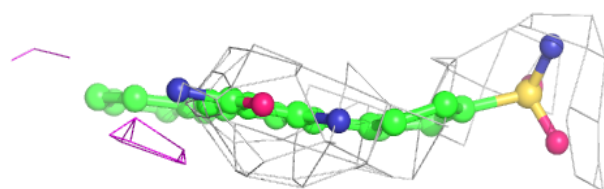
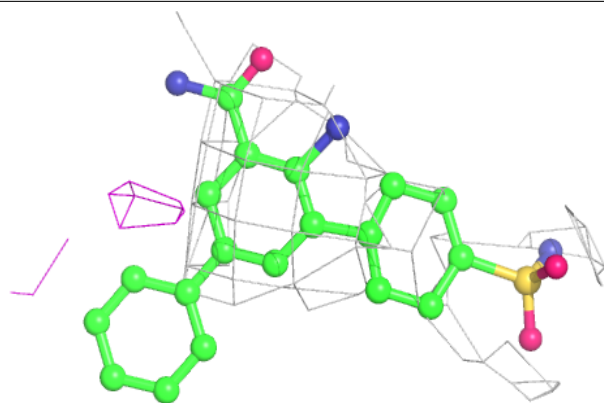
**Electron density around 5TL B 701:**

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



Electron density around 5TL 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)



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.