



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

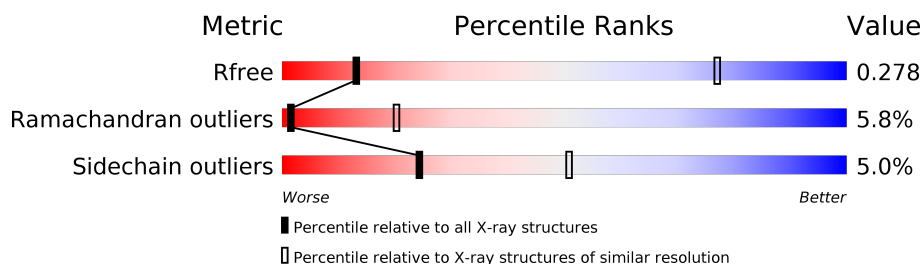
1 Overall quality at a glance ⓘ

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.






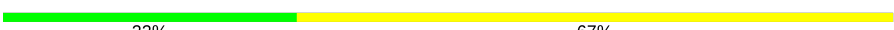
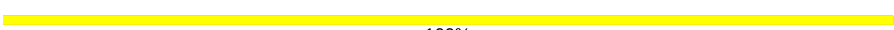
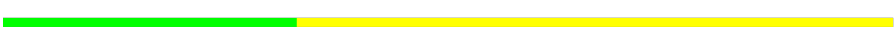













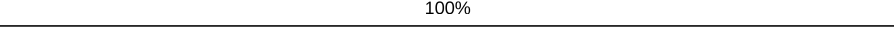



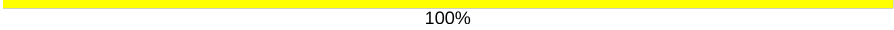
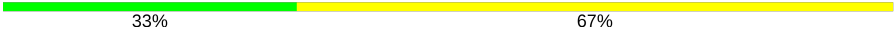
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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% .


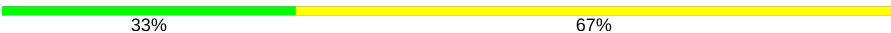
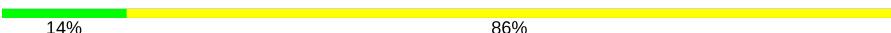


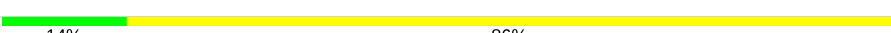
Continued on next page...

Continued from previous page...

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%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

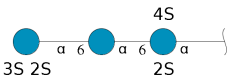
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

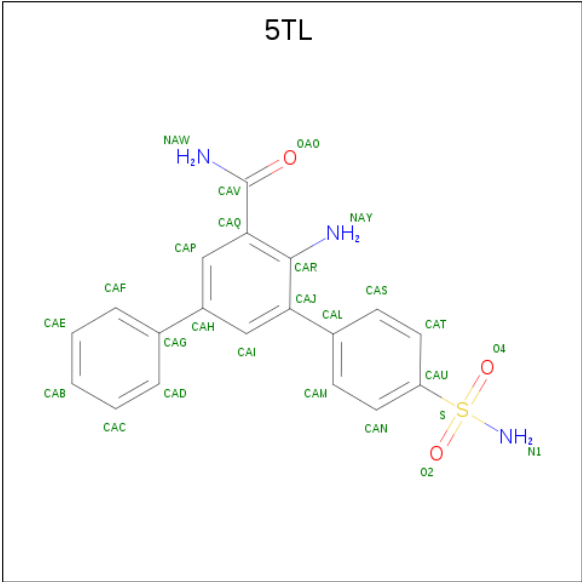
Continued from previous page...

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).

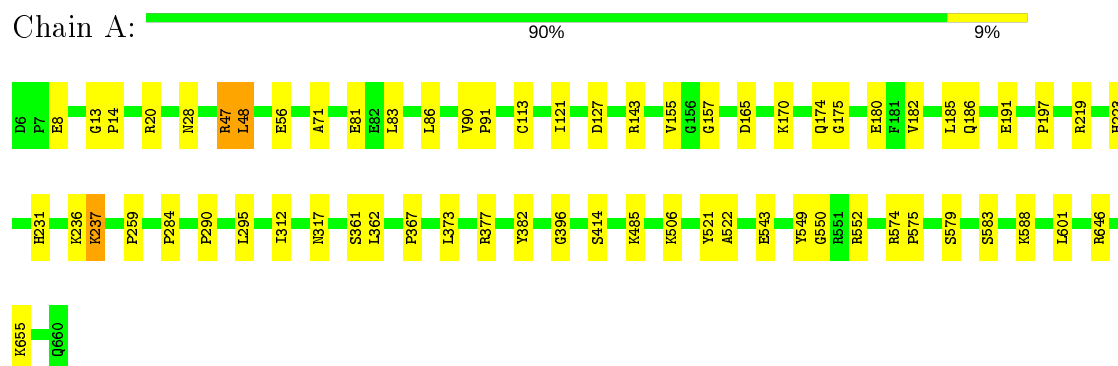


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	C	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	D	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	F	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	G	1	Total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

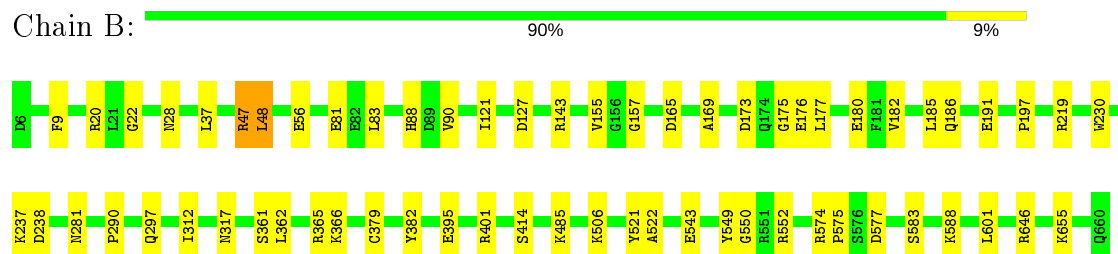
3 Residue-property plots [i](#)

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.

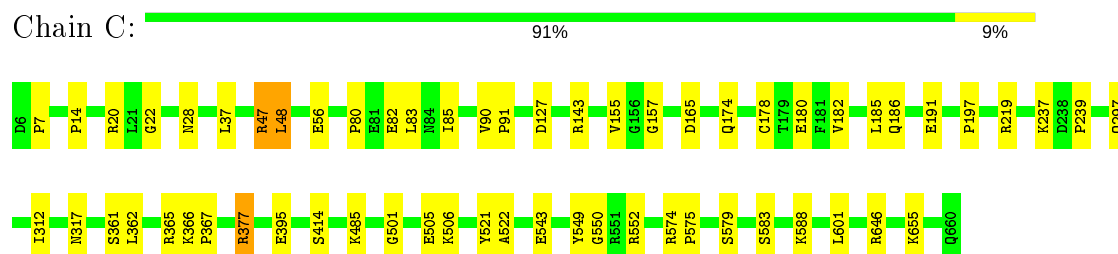
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



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

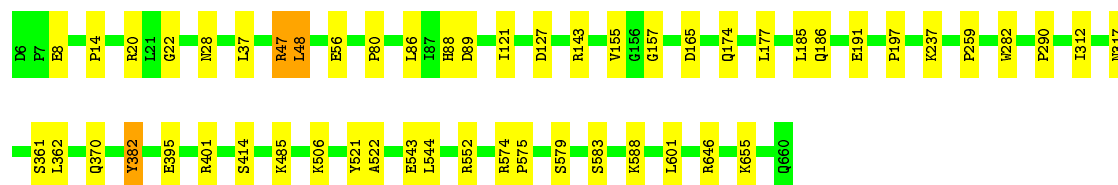


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



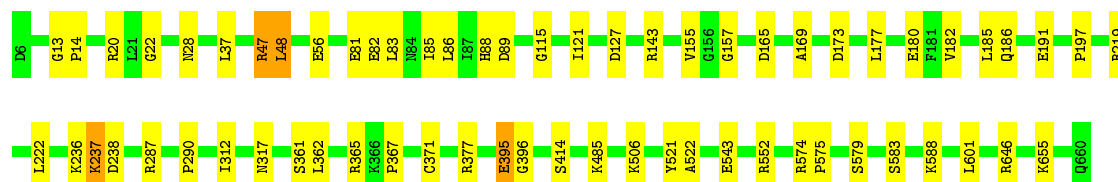
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha





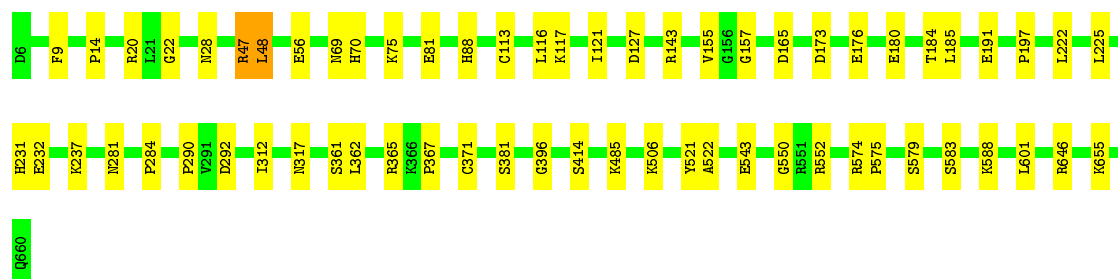
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain E: 90% 9%



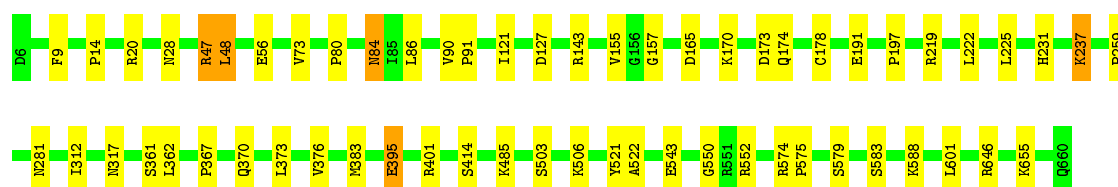
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain F: 90% 9%



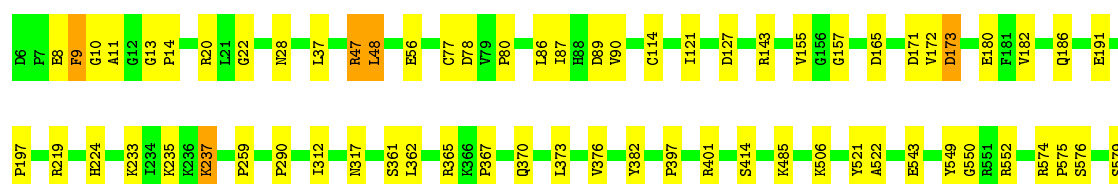
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain G: 91% 8%



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

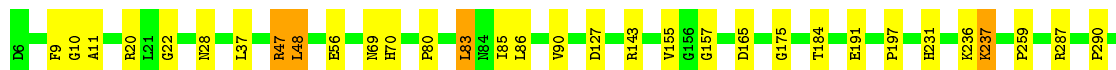
Chain H: 89% 10%





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

Chain I: 90% 9% .



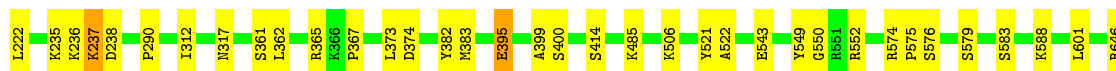
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain J: 90% 9% .



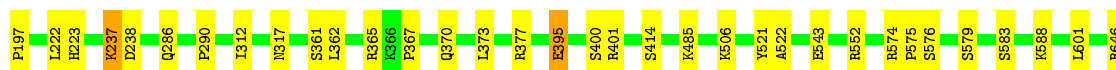
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain K: 90% 10% .



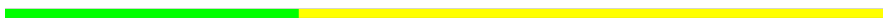
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

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
------	------	------	------	------	------	------

● 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
------	------	------	------	------	------	------

● 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
------	------	------	------	------	------	------

● 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
------	------	------	------	------	------	------

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)	Xtrriage
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	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 311.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

All (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
1	B	180	GLU
1	B	521	TYR
1	C	7	PRO
1	C	48	LEU
1	C	180	GLU
1	C	186	GLN
1	C	237	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	521	TYR
1	C	549	TYR
1	D	8	GLU
1	D	48	LEU
1	D	282	TRP
1	D	521	TYR
1	E	48	LEU
1	E	89	ASP
1	E	173	ASP
1	E	180	GLU
1	E	186	GLN
1	E	521	TYR
1	F	48	LEU
1	F	70	HIS
1	F	521	TYR
1	F	579	SER
1	G	48	LEU
1	G	395	GLU
1	G	521	TYR
1	H	8	GLU
1	H	14	PRO
1	H	48	LEU
1	H	80	PRO
1	H	87	ILE
1	H	172	VAL
1	H	173	ASP
1	H	180	GLU
1	H	365	ARG
1	H	521	TYR
1	I	48	LEU
1	I	184	THR
1	I	370	GLN
1	I	521	TYR
1	I	549	TYR
1	J	48	LEU
1	J	395	GLU
1	J	521	TYR
1	J	549	TYR
1	K	14	PRO
1	K	48	LEU
1	K	186	GLN
1	K	365	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	521	TYR
1	L	14	PRO
1	L	48	LEU
1	L	80	PRO
1	L	521	TYR
1	A	28	ASN
1	A	47	ARG
1	A	86	LEU
1	A	237	LYS
1	A	583	SER
1	B	28	ASN
1	B	47	ARG
1	B	175	GLY
1	B	549	TYR
1	B	575	PRO
1	B	583	SER
1	C	28	ASN
1	C	47	ARG
1	C	174	GLN
1	C	367	PRO
1	C	377	ARG
1	C	395	GLU
1	C	501	GLY
1	C	583	SER
1	D	28	ASN
1	D	47	ARG
1	D	89	ASP
1	D	186	GLN
1	D	237	LYS
1	D	579	SER
1	D	583	SER
1	E	14	PRO
1	E	28	ASN
1	E	222	LEU
1	E	579	SER
1	E	583	SER
1	F	28	ASN
1	F	47	ARG
1	F	365	ARG
1	F	583	SER
1	G	14	PRO
1	G	28	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	73	VAL
1	G	91	PRO
1	G	367	PRO
1	G	579	SER
1	G	583	SER
1	H	28	ASN
1	H	47	ARG
1	H	78	ASP
1	H	186	GLN
1	H	233	LYS
1	H	575	PRO
1	H	579	SER
1	H	583	SER
1	I	11	ALA
1	I	28	ASN
1	I	47	ARG
1	I	83	LEU
1	I	237	LYS
1	I	365	ARG
1	I	395	GLU
1	I	579	SER
1	I	583	SER
1	J	28	ASN
1	J	87	ILE
1	J	173	ASP
1	J	175	GLY
1	J	186	GLN
1	J	579	SER
1	J	583	SER
1	K	28	ASN
1	K	172	VAL
1	K	222	LEU
1	K	237	LYS
1	K	395	GLU
1	K	549	TYR
1	K	579	SER
1	K	583	SER
1	L	28	ASN
1	L	47	ARG
1	L	73	VAL
1	L	77	CYS
1	L	81	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	174	GLN
1	L	365	ARG
1	L	367	PRO
1	L	400	SER
1	L	579	SER
1	L	583	SER
1	A	13	GLY
1	A	14	PRO
1	A	71	ALA
1	A	165	ASP
1	A	174	GLN
1	A	361	SER
1	A	362	LEU
1	A	550	GLY
1	A	575	PRO
1	A	579	SER
1	A	588	LYS
1	B	165	ASP
1	B	169	ALA
1	B	186	GLN
1	B	361	SER
1	B	362	LEU
1	B	365	ARG
1	B	588	LYS
1	C	14	PRO
1	C	80	PRO
1	C	165	ASP
1	C	361	SER
1	C	362	LEU
1	C	505	GLU
1	C	550	GLY
1	C	588	LYS
1	D	86	LEU
1	D	88	HIS
1	D	165	ASP
1	D	177	LEU
1	D	361	SER
1	D	362	LEU
1	D	382	TYR
1	D	395	GLU
1	D	575	PRO
1	D	588	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	13	GLY
1	E	47	ARG
1	E	165	ASP
1	E	169	ALA
1	E	182	VAL
1	E	237	LYS
1	E	290	PRO
1	E	361	SER
1	E	362	LEU
1	E	365	ARG
1	E	396	GLY
1	E	575	PRO
1	E	588	LYS
1	F	9	PHE
1	F	69	ASN
1	F	88	HIS
1	F	165	ASP
1	F	180	GLU
1	F	237	LYS
1	F	290	PRO
1	F	292	ASP
1	F	361	SER
1	F	362	LEU
1	F	367	PRO
1	F	575	PRO
1	F	588	LYS
1	G	9	PHE
1	G	47	ARG
1	G	80	PRO
1	G	165	ASP
1	G	237	LYS
1	G	361	SER
1	G	362	LEU
1	G	575	PRO
1	G	588	LYS
1	H	11	ALA
1	H	165	ASP
1	H	237	LYS
1	H	290	PRO
1	H	361	SER
1	H	362	LEU
1	H	367	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	549	TYR
1	H	588	LYS
1	I	9	PHE
1	I	80	PRO
1	I	165	ASP
1	I	361	SER
1	I	362	LEU
1	I	505	GLU
1	I	588	LYS
1	J	47	ARG
1	J	88	HIS
1	J	165	ASP
1	J	180	GLU
1	J	224	HIS
1	J	237	LYS
1	J	361	SER
1	J	362	LEU
1	J	400	SER
1	J	550	GLY
1	J	575	PRO
1	J	588	LYS
1	K	47	ARG
1	K	165	ASP
1	K	179	THR
1	K	290	PRO
1	K	361	SER
1	K	362	LEU
1	K	575	PRO
1	K	588	LYS
1	L	8	GLU
1	L	165	ASP
1	L	180	GLU
1	L	361	SER
1	L	362	LEU
1	L	395	GLU
1	L	575	PRO
1	L	588	LYS
1	A	8	GLU
1	A	91	PRO
1	A	157	GLY
1	A	186	GLN
1	A	284	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	414	SER
1	B	237	LYS
1	B	414	SER
1	C	85	ILE
1	C	157	GLY
1	C	365	ARG
1	C	414	SER
1	C	575	PRO
1	D	14	PRO
1	D	157	GLY
1	D	290	PRO
1	D	414	SER
1	E	157	GLY
1	E	414	SER
1	F	113	CYS
1	F	173	ASP
1	F	381	SER
1	F	396	GLY
1	F	414	SER
1	G	157	GLY
1	G	414	SER
1	H	9	PHE
1	H	414	SER
1	H	576	SER
1	I	10	GLY
1	I	70	HIS
1	I	157	GLY
1	I	381	SER
1	I	414	SER
1	J	157	GLY
1	J	284	PRO
1	J	414	SER
1	K	77	CYS
1	K	80	PRO
1	K	89	ASP
1	K	157	GLY
1	K	180	GLU
1	K	367	PRO
1	K	383	MET
1	K	414	SER
1	K	576	SER
1	L	222	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	237	LYS
1	L	290	PRO
1	L	414	SER
1	L	576	SER
1	A	290	PRO
1	A	367	PRO
1	A	396	GLY
1	A	522	ALA
1	B	83	LEU
1	B	157	GLY
1	B	177	LEU
1	B	182	VAL
1	B	312	ILE
1	B	379	CYS
1	B	522	ALA
1	C	182	VAL
1	C	312	ILE
1	C	522	ALA
1	D	37	LEU
1	D	312	ILE
1	D	522	ALA
1	E	88	HIS
1	E	367	PRO
1	E	395	GLU
1	E	522	ALA
1	F	117	LYS
1	F	157	GLY
1	F	312	ILE
1	F	522	ALA
1	G	84	ASN
1	G	178	CYS
1	G	522	ALA
1	H	10	GLY
1	H	77	CYS
1	H	157	GLY
1	H	182	VAL
1	H	312	ILE
1	H	522	ALA
1	I	85	ILE
1	I	290	PRO
1	I	312	ILE
1	I	504	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	522	ALA
1	I	575	PRO
1	I	576	SER
1	J	14	PRO
1	J	37	LEU
1	J	290	PRO
1	J	312	ILE
1	J	379	CYS
1	J	522	ALA
1	K	312	ILE
1	K	400	SER
1	K	522	ALA
1	K	550	GLY
1	L	84	ASN
1	L	85	ILE
1	L	157	GLY
1	L	522	ALA
1	A	312	ILE
1	B	37	LEU
1	C	37	LEU
1	E	37	LEU
1	E	312	ILE
1	F	14	PRO
1	F	284	PRO
1	G	312	ILE
1	H	37	LEU
1	H	89	ASP
1	I	37	LEU
1	I	175	GLY
1	I	377	ARG
1	I	550	GLY
1	J	13	GLY
1	K	37	LEU
1	K	182	VAL
1	K	399	ALA
1	L	37	LEU
1	L	312	ILE
1	A	182	VAL
1	A	197	PRO
1	B	197	PRO
1	B	550	GLY
1	C	197	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	197	PRO
1	E	197	PRO
1	F	197	PRO
1	G	197	PRO
1	H	13	GLY
1	H	197	PRO
1	I	197	PRO
1	J	80	PRO
1	J	197	PRO
1	J	376	VAL
1	K	197	PRO
1	L	10	GLY
1	L	197	PRO
1	B	290	PRO
1	E	85	ILE
1	E	115	GLY
1	H	550	GLY
1	A	155	VAL
1	B	155	VAL
1	C	91	PRO
1	C	155	VAL
1	C	239	PRO
1	D	80	PRO
1	D	155	VAL
1	E	155	VAL
1	G	155	VAL
1	G	376	VAL
1	H	155	VAL
1	I	155	VAL
1	J	10	GLY
1	J	375	GLY
1	K	73	VAL
1	K	155	VAL
1	L	155	VAL
1	A	121	ILE
1	A	175	GLY
1	B	22	GLY
1	B	121	ILE
1	C	22	GLY
1	E	121	ILE
1	F	22	GLY
1	F	121	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	155	VAL
1	F	550	GLY
1	G	259	PRO
1	G	550	GLY
1	H	22	GLY
1	H	121	ILE
1	H	259	PRO
1	H	376	VAL
1	J	22	GLY
1	J	155	VAL
1	K	121	ILE
1	L	22	GLY
1	L	182	VAL
1	A	259	PRO
1	D	22	GLY
1	D	121	ILE
1	D	259	PRO
1	E	22	GLY
1	G	121	ILE
1	H	397	PRO
1	I	22	GLY
1	I	259	PRO
1	K	22	GLY
1	L	121	ILE

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%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	47	ARG
1	A	48	LEU
1	A	56	GLU
1	A	81	GLU
1	A	83	LEU
1	A	90	VAL
1	A	113	CYS
1	A	127	ASP
1	A	143	ARG
1	A	170	LYS
1	A	180	GLU
1	A	185	LEU
1	A	191	GLU
1	A	219	ARG
1	A	223	HIS
1	A	231	HIS
1	A	236	LYS
1	A	237	LYS
1	A	295	LEU
1	A	317	ASN
1	A	373	LEU
1	A	377	ARG
1	A	382	TYR
1	A	485	LYS
1	A	506	LYS
1	A	543	GLU
1	A	552	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	574	ARG
1	A	601	LEU
1	A	646	ARG
1	A	655	LYS
1	B	9	PHE
1	B	20	ARG
1	B	47	ARG
1	B	48	LEU
1	B	56	GLU
1	B	81	GLU
1	B	88	HIS
1	B	90	VAL
1	B	127	ASP
1	B	143	ARG
1	B	176	GLU
1	B	185	LEU
1	B	191	GLU
1	B	219	ARG
1	B	230	TRP
1	B	238	ASP
1	B	281	ASN
1	B	297	GLN
1	B	317	ASN
1	B	366	LYS
1	B	382	TYR
1	B	395	GLU
1	B	401	ARG
1	B	485	LYS
1	B	506	LYS
1	B	543	GLU
1	B	552	ARG
1	B	574	ARG
1	B	577	ASP
1	B	601	LEU
1	B	646	ARG
1	B	655	LYS
1	C	20	ARG
1	C	47	ARG
1	C	48	LEU
1	C	56	GLU
1	C	82	GLU
1	C	83	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	90	VAL
1	C	127	ASP
1	C	143	ARG
1	C	178	CYS
1	C	185	LEU
1	C	191	GLU
1	C	219	ARG
1	C	297	GLN
1	C	317	ASN
1	C	366	LYS
1	C	377	ARG
1	C	485	LYS
1	C	506	LYS
1	C	543	GLU
1	C	552	ARG
1	C	574	ARG
1	C	579	SER
1	C	601	LEU
1	C	646	ARG
1	C	655	LYS
1	D	20	ARG
1	D	47	ARG
1	D	48	LEU
1	D	56	GLU
1	D	127	ASP
1	D	143	ARG
1	D	174	GLN
1	D	185	LEU
1	D	191	GLU
1	D	317	ASN
1	D	370	GLN
1	D	382	TYR
1	D	401	ARG
1	D	485	LYS
1	D	506	LYS
1	D	543	GLU
1	D	544	LEU
1	D	552	ARG
1	D	574	ARG
1	D	601	LEU
1	D	646	ARG
1	D	655	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	20	ARG
1	E	47	ARG
1	E	48	LEU
1	E	56	GLU
1	E	81	GLU
1	E	82	GLU
1	E	83	LEU
1	E	86	LEU
1	E	127	ASP
1	E	143	ARG
1	E	177	LEU
1	E	185	LEU
1	E	191	GLU
1	E	219	ARG
1	E	236	LYS
1	E	237	LYS
1	E	238	ASP
1	E	287	ARG
1	E	317	ASN
1	E	371	CYS
1	E	377	ARG
1	E	395	GLU
1	E	485	LYS
1	E	506	LYS
1	E	543	GLU
1	E	552	ARG
1	E	574	ARG
1	E	601	LEU
1	E	646	ARG
1	E	655	LYS
1	F	20	ARG
1	F	47	ARG
1	F	48	LEU
1	F	56	GLU
1	F	75	LYS
1	F	81	GLU
1	F	116	LEU
1	F	127	ASP
1	F	143	ARG
1	F	176	GLU
1	F	184	THR
1	F	185	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	191	GLU
1	F	222	LEU
1	F	225	LEU
1	F	231	HIS
1	F	232	GLU
1	F	281	ASN
1	F	317	ASN
1	F	371	CYS
1	F	485	LYS
1	F	506	LYS
1	F	543	GLU
1	F	552	ARG
1	F	574	ARG
1	F	601	LEU
1	F	646	ARG
1	F	655	LYS
1	G	20	ARG
1	G	47	ARG
1	G	48	LEU
1	G	56	GLU
1	G	84	ASN
1	G	86	LEU
1	G	90	VAL
1	G	127	ASP
1	G	143	ARG
1	G	170	LYS
1	G	173	ASP
1	G	174	GLN
1	G	191	GLU
1	G	219	ARG
1	G	222	LEU
1	G	225	LEU
1	G	231	HIS
1	G	237	LYS
1	G	281	ASN
1	G	317	ASN
1	G	370	GLN
1	G	373	LEU
1	G	383	MET
1	G	395	GLU
1	G	401	ARG
1	G	485	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	503	SER
1	G	506	LYS
1	G	543	GLU
1	G	552	ARG
1	G	574	ARG
1	G	601	LEU
1	G	646	ARG
1	G	655	LYS
1	H	9	PHE
1	H	20	ARG
1	H	47	ARG
1	H	48	LEU
1	H	56	GLU
1	H	86	LEU
1	H	90	VAL
1	H	114	CYS
1	H	127	ASP
1	H	143	ARG
1	H	171	ASP
1	H	173	ASP
1	H	191	GLU
1	H	219	ARG
1	H	224	HIS
1	H	235	LYS
1	H	237	LYS
1	H	317	ASN
1	H	370	GLN
1	H	373	LEU
1	H	382	TYR
1	H	401	ARG
1	H	485	LYS
1	H	506	LYS
1	H	543	GLU
1	H	552	ARG
1	H	574	ARG
1	H	601	LEU
1	H	646	ARG
1	H	655	LYS
1	I	20	ARG
1	I	47	ARG
1	I	48	LEU
1	I	56	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	69	ASN
1	I	83	LEU
1	I	86	LEU
1	I	90	VAL
1	I	127	ASP
1	I	143	ARG
1	I	191	GLU
1	I	231	HIS
1	I	236	LYS
1	I	237	LYS
1	I	287	ARG
1	I	317	ASN
1	I	366	LYS
1	I	370	GLN
1	I	377	ARG
1	I	401	ARG
1	I	485	LYS
1	I	506	LYS
1	I	543	GLU
1	I	552	ARG
1	I	574	ARG
1	I	601	LEU
1	I	646	ARG
1	I	655	LYS
1	J	20	ARG
1	J	47	ARG
1	J	48	LEU
1	J	56	GLU
1	J	73	VAL
1	J	114	CYS
1	J	127	ASP
1	J	143	ARG
1	J	178	CYS
1	J	191	GLU
1	J	219	ARG
1	J	223	HIS
1	J	225	LEU
1	J	230	TRP
1	J	236	LYS
1	J	237	LYS
1	J	283	ASP
1	J	317	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	370	GLN
1	J	379	CYS
1	J	485	LYS
1	J	499	THR
1	J	506	LYS
1	J	543	GLU
1	J	552	ARG
1	J	574	ARG
1	J	601	LEU
1	J	646	ARG
1	J	655	LYS
1	K	20	ARG
1	K	47	ARG
1	K	48	LEU
1	K	56	GLU
1	K	78	ASP
1	K	114	CYS
1	K	127	ASP
1	K	143	ARG
1	K	168	TYR
1	K	174	GLN
1	K	185	LEU
1	K	191	GLU
1	K	219	ARG
1	K	235	LYS
1	K	236	LYS
1	K	237	LYS
1	K	238	ASP
1	K	317	ASN
1	K	373	LEU
1	K	374	ASP
1	K	382	TYR
1	K	395	GLU
1	K	485	LYS
1	K	506	LYS
1	K	543	GLU
1	K	552	ARG
1	K	574	ARG
1	K	601	LEU
1	K	646	ARG
1	K	655	LYS
1	L	20	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	47	ARG
1	L	48	LEU
1	L	56	GLU
1	L	70	HIS
1	L	72	ASN
1	L	84	ASN
1	L	86	LEU
1	L	88	HIS
1	L	127	ASP
1	L	143	ARG
1	L	173	ASP
1	L	184	THR
1	L	191	GLU
1	L	223	HIS
1	L	237	LYS
1	L	238	ASP
1	L	286	GLN
1	L	317	ASN
1	L	370	GLN
1	L	373	LEU
1	L	377	ARG
1	L	395	GLU
1	L	401	ARG
1	L	485	LYS
1	L	506	LYS
1	L	543	GLU
1	L	552	ARG
1	L	574	ARG
1	L	601	LEU
1	L	646	ARG
1	L	655	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (276) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	84	ASN
1	A	112	ASN
1	A	195	ASN
1	A	260	GLN
1	A	262	ASN
1	A	309	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	ASN
1	A	370	GLN
1	A	408	ASN
1	A	422	GLN
1	A	459	ASN
1	A	475	GLN
1	A	488	GLN
1	A	538	HIS
1	A	573	HIS
1	A	597	GLN
1	A	616	GLN
1	A	631	ASN
1	A	643	GLN
1	B	28	ASN
1	B	33	GLN
1	B	72	ASN
1	B	84	ASN
1	B	112	ASN
1	B	195	ASN
1	B	226	GLN
1	B	260	GLN
1	B	262	ASN
1	B	281	ASN
1	B	286	GLN
1	B	309	ASN
1	B	317	ASN
1	B	370	GLN
1	B	408	ASN
1	B	422	GLN
1	B	475	GLN
1	B	488	GLN
1	B	538	HIS
1	B	545	GLN
1	B	573	HIS
1	B	595	GLN
1	B	597	GLN
1	B	616	GLN
1	B	631	ASN
1	B	643	GLN
1	C	28	ASN
1	C	33	GLN
1	C	63	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	72	ASN
1	C	195	ASN
1	C	260	GLN
1	C	262	ASN
1	C	281	ASN
1	C	297	GLN
1	C	309	ASN
1	C	317	ASN
1	C	370	GLN
1	C	412	GLN
1	C	422	GLN
1	C	475	GLN
1	C	488	GLN
1	C	533	GLN
1	C	538	HIS
1	C	573	HIS
1	C	597	GLN
1	C	616	GLN
1	C	631	ASN
1	C	643	GLN
1	D	28	ASN
1	D	33	GLN
1	D	69	ASN
1	D	84	ASN
1	D	88	HIS
1	D	174	GLN
1	D	186	GLN
1	D	195	ASN
1	D	260	GLN
1	D	262	ASN
1	D	309	ASN
1	D	317	ASN
1	D	408	ASN
1	D	412	GLN
1	D	422	GLN
1	D	459	ASN
1	D	475	GLN
1	D	488	GLN
1	D	538	HIS
1	D	573	HIS
1	D	597	GLN
1	D	616	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	631	ASN
1	D	643	GLN
1	E	28	ASN
1	E	33	GLN
1	E	70	HIS
1	E	84	ASN
1	E	195	ASN
1	E	260	GLN
1	E	262	ASN
1	E	285	GLN
1	E	297	GLN
1	E	309	ASN
1	E	408	ASN
1	E	422	GLN
1	E	475	GLN
1	E	488	GLN
1	E	533	GLN
1	E	538	HIS
1	E	573	HIS
1	E	597	GLN
1	E	616	GLN
1	E	631	ASN
1	E	643	GLN
1	F	28	ASN
1	F	33	GLN
1	F	84	ASN
1	F	186	GLN
1	F	195	ASN
1	F	226	GLN
1	F	260	GLN
1	F	262	ASN
1	F	281	ASN
1	F	309	ASN
1	F	317	ASN
1	F	370	GLN
1	F	408	ASN
1	F	422	GLN
1	F	459	ASN
1	F	475	GLN
1	F	488	GLN
1	F	545	GLN
1	F	573	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	597	GLN
1	F	616	GLN
1	F	631	ASN
1	F	643	GLN
1	G	33	GLN
1	G	69	ASN
1	G	84	ASN
1	G	112	ASN
1	G	186	GLN
1	G	195	ASN
1	G	260	GLN
1	G	262	ASN
1	G	281	ASN
1	G	285	GLN
1	G	286	GLN
1	G	309	ASN
1	G	317	ASN
1	G	370	GLN
1	G	408	ASN
1	G	422	GLN
1	G	459	ASN
1	G	475	GLN
1	G	488	GLN
1	G	538	HIS
1	G	573	HIS
1	G	597	GLN
1	G	616	GLN
1	G	631	ASN
1	G	643	GLN
1	H	28	ASN
1	H	33	GLN
1	H	69	ASN
1	H	72	ASN
1	H	84	ASN
1	H	186	GLN
1	H	195	ASN
1	H	260	GLN
1	H	262	ASN
1	H	297	GLN
1	H	309	ASN
1	H	317	ASN
1	H	370	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	422	GLN
1	H	475	GLN
1	H	488	GLN
1	H	533	GLN
1	H	538	HIS
1	H	545	GLN
1	H	573	HIS
1	H	597	GLN
1	H	616	GLN
1	H	631	ASN
1	H	643	GLN
1	I	28	ASN
1	I	33	GLN
1	I	60	HIS
1	I	69	ASN
1	I	195	ASN
1	I	260	GLN
1	I	262	ASN
1	I	281	ASN
1	I	309	ASN
1	I	317	ASN
1	I	370	GLN
1	I	412	GLN
1	I	422	GLN
1	I	475	GLN
1	I	488	GLN
1	I	533	GLN
1	I	545	GLN
1	I	573	HIS
1	I	597	GLN
1	I	616	GLN
1	I	631	ASN
1	I	643	GLN
1	J	28	ASN
1	J	33	GLN
1	J	63	GLN
1	J	88	HIS
1	J	112	ASN
1	J	186	GLN
1	J	195	ASN
1	J	260	GLN
1	J	262	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	297	GLN
1	J	309	ASN
1	J	370	GLN
1	J	408	ASN
1	J	422	GLN
1	J	459	ASN
1	J	475	GLN
1	J	488	GLN
1	J	533	GLN
1	J	538	HIS
1	J	573	HIS
1	J	597	GLN
1	J	616	GLN
1	J	631	ASN
1	J	643	GLN
1	K	28	ASN
1	K	33	GLN
1	K	72	ASN
1	K	195	ASN
1	K	260	GLN
1	K	262	ASN
1	K	309	ASN
1	K	317	ASN
1	K	408	ASN
1	K	422	GLN
1	K	475	GLN
1	K	488	GLN
1	K	497	GLN
1	K	533	GLN
1	K	538	HIS
1	K	573	HIS
1	K	595	GLN
1	K	597	GLN
1	K	616	GLN
1	K	631	ASN
1	K	643	GLN
1	L	28	ASN
1	L	33	GLN
1	L	72	ASN
1	L	186	GLN
1	L	195	ASN
1	L	231	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	260	GLN
1	L	262	ASN
1	L	297	GLN
1	L	309	ASN
1	L	317	ASN
1	L	408	ASN
1	L	422	GLN
1	L	459	ASN
1	L	475	GLN
1	L	484	HIS
1	L	488	GLN
1	L	538	HIS
1	L	573	HIS
1	L	597	GLN
1	L	616	GLN
1	L	631	ASN
1	L	643	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	1.35	1 (5%)	21,31,31	1.10	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	0.59	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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
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
2	f	1	5LS	C1-C2	4.00	1.56	1.52
2	M	1	5LS	C1-C2	3.86	1.56	1.52
2	m	1	5LS	C1-C2	3.82	1.56	1.52
2	d	1	5LS	C1-C2	3.75	1.56	1.52
2	W	3	PDX	C1-C2	3.64	1.57	1.51
2	U	1	5LS	C1-C2	3.63	1.55	1.52
2	R	1	5LS	C1-C2	3.61	1.55	1.52
2	n	1	5LS	C1-C2	3.58	1.55	1.52
3	T	1	5LS	C1-C2	3.58	1.55	1.52
2	m	3	PDX	C1-C2	3.56	1.57	1.51
2	h	1	5LS	C1-C2	3.54	1.55	1.52
2	e	1	5LS	C1-C2	3.46	1.55	1.52
2	j	3	PDX	C1-C2	3.46	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	g	3	PDX	C1-C2	3.39	1.57	1.51
2	k	1	5LS	C1-C2	3.37	1.55	1.52
2	X	1	5LS	C1-C2	3.36	1.55	1.52
2	d	3	PDX	C1-C2	3.35	1.57	1.51
3	T	7	5TH	C1-C2	3.32	1.57	1.51
2	N	1	5LS	C1-C2	3.29	1.55	1.52
2	b	3	PDX	O2-C2	-3.27	1.42	1.47
2	h	3	PDX	O2-C2	-3.21	1.42	1.47
2	N	3	PDX	O2-C2	-3.18	1.42	1.47
2	l	3	PDX	O2-C2	-3.17	1.42	1.47
2	R	3	PDX	O2-C2	-3.17	1.42	1.47
3	O	7	5TH	C1-C2	3.17	1.56	1.51
2	a	3	PDX	O2-C2	-3.15	1.42	1.47
2	W	1	5LS	C1-C2	3.13	1.55	1.52
3	i	7	5TH	O2-C2	-3.13	1.42	1.47
2	k	3	PDX	C1-C2	3.12	1.56	1.51
2	Q	3	PDX	O2-C2	-3.12	1.42	1.47
2	M	3	PDX	O2-C2	-3.11	1.42	1.47
2	Z	3	PDX	O2-C2	-3.10	1.42	1.47
2	X	3	PDX	C1-C2	3.07	1.56	1.51
2	n	3	PDX	O2-C2	-3.07	1.42	1.47
3	i	3	5TM	O2-C2	-3.06	1.42	1.47
2	S	3	PDX	C1-C2	3.05	1.56	1.51
3	i	5	Z4K	O2-C2	-3.05	1.42	1.47
3	O	7	5TH	O2-C2	-3.01	1.42	1.47
3	O	5	Z4K	O2-C2	-3.01	1.42	1.47
2	e	3	PDX	O2-C2	-3.01	1.42	1.47
3	i	1	5LS	C1-C2	3.00	1.55	1.52
2	Z	1	5LS	C1-C2	3.00	1.55	1.52
2	f	3	PDX	O2-C2	-3.00	1.42	1.47
2	V	3	PDX	O2-C2	-3.00	1.42	1.47
2	Y	3	PDX	O2-C2	-2.99	1.42	1.47
2	U	3	PDX	O2-C2	-2.99	1.42	1.47
2	W	3	PDX	O2-C2	-2.98	1.42	1.47
2	S	3	PDX	O2-C2	-2.98	1.42	1.47
2	k	3	PDX	O2-C2	-2.97	1.42	1.47
2	X	3	PDX	O2-C2	-2.97	1.42	1.47
3	c	3	5TM	O2-C2	-2.96	1.42	1.47
2	m	3	PDX	O2-C2	-2.94	1.42	1.47
3	T	5	Z4K	O2-C2	-2.93	1.42	1.47
3	T	3	5TM	O2-C2	-2.93	1.42	1.47
2	P	1	5LS	C1-C2	2.92	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	3	PDX	O2-C2	-2.92	1.42	1.47
2	n	3	PDX	C1-C2	2.92	1.56	1.51
2	V	3	PDX	C1-C2	2.91	1.56	1.51
2	Q	3	PDX	C1-C2	2.89	1.56	1.51
2	P	3	PDX	O2-C2	-2.89	1.42	1.47
2	Y	3	PDX	C1-C2	2.88	1.56	1.51
2	R	3	PDX	C1-C2	2.87	1.56	1.51
2	j	3	PDX	O2-C2	-2.87	1.42	1.47
2	M	3	PDX	C1-C2	2.87	1.56	1.51
3	c	5	Z4K	O2-C2	-2.86	1.42	1.47
2	U	3	PDX	C1-C2	2.84	1.56	1.51
2	g	3	PDX	O2-C2	-2.81	1.43	1.47
3	O	3	5TM	O2-C2	-2.81	1.43	1.47
3	T	7	5TH	O2-C2	-2.81	1.43	1.47
3	i	7	5TH	C1-C2	2.80	1.56	1.51
2	e	3	PDX	C1-C2	2.80	1.56	1.51
2	l	1	5LS	C1-C2	2.74	1.55	1.52
2	Z	3	PDX	C1-C2	2.67	1.56	1.51
2	a	3	PDX	C1-C2	2.66	1.56	1.51
3	c	7	5TH	O2-C2	-2.61	1.43	1.47
2	l	3	PDX	C1-C2	2.60	1.55	1.51
2	h	3	PDX	C1-C2	2.56	1.55	1.51
3	c	7	5TH	C1-C2	2.55	1.55	1.51
2	P	3	PDX	C1-C2	2.49	1.55	1.51
2	V	1	5LS	C1-C2	2.42	1.54	1.52
2	Q	1	5LS	C1-C2	2.41	1.54	1.52
3	c	3	5TM	C1-C2	2.40	1.55	1.51
2	b	3	PDX	C1-C2	2.26	1.55	1.51
2	N	3	PDX	C1-C2	2.12	1.55	1.51
2	Q	1	5LS	O2-C2	-2.01	1.42	1.46
2	l	1	5LS	O2-C2	-2.01	1.42	1.46
3	i	1	5LS	O2-C2	-2.01	1.42	1.46
3	c	1	5LS	C1-C2	2.00	1.54	1.52
2	P	1	5LS	O2-C2	-2.00	1.42	1.46
2	W	1	5LS	O2-C2	-2.00	1.42	1.46

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	c	7	5TH	C2-O2-S1	-4.14	112.51	117.91
3	O	5	Z4K	C2-O2-S1	-4.12	112.54	117.91
3	T	3	5TM	C2-O2-S	-4.08	112.58	117.91
2	b	3	PDX	C2-O2-S	-4.06	112.61	117.91
2	N	3	PDX	C2-O2-S	-4.05	112.64	117.91
3	c	3	5TM	C2-O2-S	-4.03	112.65	117.91
2	e	3	PDX	C2-O2-S	-4.02	112.67	117.91
2	h	3	PDX	C2-O2-S	-4.02	112.67	117.91
3	O	3	5TM	C2-O2-S	-4.01	112.68	117.91
2	S	3	PDX	C2-O2-S	-4.00	112.70	117.91
2	m	3	PDX	C2-O2-S	-3.99	112.71	117.91
2	U	3	PDX	C2-O2-S	-3.98	112.72	117.91
2	Z	3	PDX	C2-O2-S	-3.98	112.72	117.91
3	i	7	5TH	C2-O2-S1	-3.97	112.73	117.91
3	T	5	Z4K	C2-O2-S1	-3.95	112.77	117.91
3	O	7	5TH	C2-O2-S1	-3.94	112.77	117.91
3	c	5	Z4K	C2-O2-S1	-3.93	112.78	117.91
2	n	3	PDX	C2-O2-S	-3.91	112.81	117.91
3	i	5	Z4K	C2-O2-S1	-3.86	112.87	117.91
2	j	3	PDX	C2-O2-S	-3.85	112.89	117.91
2	Y	3	PDX	C2-O2-S	-3.85	112.89	117.91
2	Q	3	PDX	C2-O2-S	-3.85	112.90	117.91
2	P	3	PDX	C2-O2-S	-3.83	112.91	117.91
2	X	3	PDX	C2-O2-S	-3.81	112.94	117.91
2	R	3	PDX	C2-O2-S	-3.81	112.95	117.91
2	M	3	PDX	C2-O2-S	-3.80	112.96	117.91
2	k	3	PDX	C2-O2-S	-3.78	112.98	117.91
2	d	3	PDX	C2-O2-S	-3.66	113.14	117.91
2	e	2	GLC	C1-C2-C3	3.60	114.09	109.67
2	g	3	PDX	C2-O2-S	-3.59	113.22	117.91
2	V	3	PDX	C2-O2-S	-3.59	113.23	117.91
2	f	3	PDX	C2-O2-S	-3.57	113.25	117.91
2	f	3	PDX	C1-C2-C3	3.54	114.69	109.40
2	W	3	PDX	C2-O2-S	-3.52	113.31	117.91
2	Q	1	5LS	C2-O2-S1	-3.42	112.26	118.88
2	g	1	5LS	C2-O2-S1	-3.38	112.35	118.88
3	c	3	5TM	O2-C2-C3	3.37	110.38	106.65
2	a	3	PDX	C3-O3-S'	-3.36	112.37	118.88
2	Y	1	5LS	C4-O4-S2	-3.36	112.38	118.88
3	i	1	5LS	C2-O2-S1	-3.35	112.40	118.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	1	5LS	C2-O2-S1	-3.34	112.42	118.88
2	P	1	5LS	C2-O2-S1	-3.34	112.42	118.88
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
2	N	3	PDX	C3-O3-S'	-3.32	112.47	118.88
2	N	2	GLC	C1-C2-C3	3.32	113.74	109.67
2	Z	1	5LS	C2-O2-S1	-3.31	112.47	118.88
2	a	1	5LS	C4-O4-S2	-3.31	112.48	118.88
2	l	3	PDX	C3-O3-S'	-3.31	112.49	118.88
2	f	1	5LS	C4-O4-S2	-3.29	112.52	118.88
2	S	3	PDX	C3-O3-S'	-3.29	112.52	118.88
2	b	3	PDX	C3-O3-S'	-3.28	112.53	118.88
3	i	2	5TJ	C3-O3-S3	-3.28	112.54	118.88
2	m	3	PDX	C3-O3-S'	-3.28	112.54	118.88
2	h	1	5LS	C2-O2-S1	-3.28	112.55	118.88
2	W	1	5LS	C4-O4-S2	-3.27	112.55	118.88
3	i	1	5LS	C4-O4-S2	-3.26	112.57	118.88
2	N	1	5LS	C2-O2-S1	-3.26	112.58	118.88
3	i	4	5TJ	C3-O3-S3	-3.25	112.59	118.88
2	k	1	5LS	C2-O2-S1	-3.24	112.61	118.88
2	b	1	5LS	C4-O4-S2	-3.24	112.62	118.88
2	Q	1	5LS	C4-O4-S2	-3.24	112.62	118.88
2	a	1	5LS	C2-O2-S1	-3.24	112.62	118.88
2	R	3	PDX	O2-C2-C3	3.24	110.23	106.65
2	j	1	5LS	C2-O2-S1	-3.23	112.63	118.88
2	n	1	5LS	C4-O4-S2	-3.23	112.64	118.88
2	f	1	5LS	C2-O2-S1	-3.22	112.65	118.88
2	V	1	5LS	C4-O4-S2	-3.22	112.66	118.88
2	V	1	5LS	C2-O2-S1	-3.21	112.67	118.88
2	m	1	5LS	C4-O4-S2	-3.21	112.68	118.88
3	O	1	5LS	C2-O2-S1	-3.21	112.68	118.88
2	d	1	5LS	C4-O4-S2	-3.21	112.68	118.88
2	d	1	5LS	C2-O2-S1	-3.20	112.70	118.88
2	R	1	5LS	C4-O4-S2	-3.20	112.70	118.88
3	T	1	5LS	C4-O4-S2	-3.20	112.70	118.88
2	a	3	PDX	O2-C2-C3	3.19	110.19	106.65
2	W	1	5LS	C2-O2-S1	-3.18	112.72	118.88
2	P	3	PDX	O2-C2-C3	3.18	110.17	106.65
2	U	1	5LS	C4-O4-S2	-3.17	112.74	118.88
2	n	3	PDX	C3-O3-S'	-3.17	112.74	118.88
2	P	1	5LS	C4-O4-S2	-3.17	112.75	118.88
2	j	3	PDX	C3-O3-S'	-3.17	112.76	118.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2	5TJ	C3-O3-S3	-3.16	112.77	118.88
3	c	2	5TJ	C3-O3-S3	-3.16	112.77	118.88
2	b	1	5LS	C2-O2-S1	-3.16	112.78	118.88
2	Y	1	5LS	C2-O2-S1	-3.16	112.78	118.88
2	h	1	5LS	C4-O4-S2	-3.15	112.79	118.88
2	h	3	PDX	C3-O3-S'	-3.15	112.79	118.88
2	Z	1	5LS	C4-O4-S2	-3.14	112.81	118.88
2	j	1	5LS	C4-O4-S2	-3.14	112.81	118.88
2	N	1	5LS	C4-O4-S2	-3.13	112.82	118.88
2	R	1	5LS	C2-O2-S1	-3.13	112.83	118.88
3	T	1	5LS	C2-O2-S1	-3.13	112.83	118.88
3	T	4	5TJ	C3-O3-S3	-3.11	112.87	118.88
2	j	2	GLC	C1-C2-C3	3.11	113.48	109.67
3	c	4	5TJ	C3-O3-S3	-3.10	112.88	118.88
2	Z	3	PDX	C3-O3-S'	-3.10	112.89	118.88
2	U	1	5LS	C2-O2-S1	-3.09	112.90	118.88
2	e	3	PDX	O2-C2-C3	3.09	110.07	106.65
2	X	3	PDX	C3-O3-S'	-3.09	112.91	118.88
2	l	3	PDX	O2-C2-C3	3.08	110.07	106.65
2	m	1	5LS	C2-O2-S1	-3.08	112.92	118.88
2	e	1	5LS	C4-O4-S2	-3.08	112.93	118.88
2	X	3	PDX	O2-C2-C3	3.07	110.05	106.65
2	U	3	PDX	C3-O3-S'	-3.07	112.94	118.88
2	e	3	PDX	C3-O3-S'	-3.07	112.95	118.88
2	X	1	5LS	C4-O4-S2	-3.06	112.96	118.88
2	R	3	PDX	C3-O3-S'	-3.05	112.97	118.88
2	M	1	5LS	C4-O4-S2	-3.05	112.98	118.88
2	Q	3	PDX	C3-O3-S'	-3.05	112.98	118.88
2	b	3	PDX	O2-C2-C3	3.05	110.03	106.65
2	W	3	PDX	C1-C2-C3	3.04	113.94	109.40
2	S	1	5LS	C2-O2-S1	-3.03	113.02	118.88
3	O	1	5LS	C4-O4-S2	-3.02	113.04	118.88
2	k	3	PDX	C3-O3-S'	-3.00	113.08	118.88
3	O	4	5TJ	C3-O3-S3	-3.00	113.08	118.88
2	e	1	5LS	C2-O2-S1	-3.00	113.08	118.88
2	g	3	PDX	C3-O3-S'	-3.00	113.09	118.88
2	M	3	PDX	O2-C2-C3	2.99	109.96	106.65
2	k	1	5LS	C4-O4-S2	-2.98	113.11	118.88
2	d	3	PDX	C3-O3-S'	-2.98	113.12	118.88
2	g	1	5LS	C4-O4-S2	-2.98	113.12	118.88
3	c	1	5LS	C2-O2-S1	-2.98	113.12	118.88
2	h	3	PDX	O2-C2-C3	2.97	109.94	106.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	PDX	C3-O3-S'	-2.96	113.16	118.88
2	M	1	5LS	C2-O2-S1	-2.95	113.17	118.88
3	O	3	5TM	O2-C2-C3	2.95	109.92	106.65
2	Y	3	PDX	O2-C2-C3	2.94	109.91	106.65
2	Y	3	PDX	C3-O3-S'	-2.93	113.21	118.88
3	O	2	5TJ	C3-O3-S3	-2.92	113.23	118.88
3	T	3	5TM	O2-C2-C3	2.89	109.85	106.65
2	N	3	PDX	O2-C2-C3	2.88	109.84	106.65
2	X	1	5LS	C2-O2-S1	-2.83	113.41	118.88
2	V	3	PDX	O2-C2-C3	2.80	109.75	106.65
2	Z	3	PDX	O2-C2-C3	2.80	109.75	106.65
2	V	3	PDX	C3-O3-S'	-2.79	113.49	118.88
2	W	3	PDX	C3-O3-S'	-2.77	113.53	118.88
3	i	3	5TM	O2-C2-C3	2.75	109.70	106.65
3	c	1	5LS	C4-O4-S2	-2.70	113.65	118.88
2	d	3	PDX	O2-C2-C3	2.65	109.59	106.65
3	T	7	5TH	O2-C2-C3	2.65	110.65	106.95
2	n	3	PDX	O2-C2-C3	2.61	109.54	106.65
2	f	3	PDX	O2-C2-C3	2.59	109.52	106.65
2	m	3	PDX	O2-C2-C3	2.53	109.46	106.65
2	j	2	GLC	C1-O5-C5	2.49	115.56	112.19
2	f	3	PDX	C3-O3-S'	-2.48	114.08	118.88
2	j	3	PDX	O2-C2-C3	2.48	109.40	106.65
2	k	3	PDX	O2-C2-C3	2.47	109.38	106.65
3	c	7	5TH	O2-C2-C3	2.37	110.26	106.95
2	Q	3	PDX	O2-C2-C3	2.26	109.16	106.65
2	W	3	PDX	O2-C2-C3	2.26	109.16	106.65
2	g	3	PDX	C1-C2-C3	2.23	112.73	109.40
2	X	2	GLC	C1-C2-C3	2.19	112.36	109.67
2	Q	3	PDX	C1-C2-C3	2.19	112.67	109.40
2	X	1	5LS	C4-C3-C2	2.17	113.46	108.96
2	m	3	PDX	C1-C2-C3	2.16	112.63	109.40
2	j	3	PDX	C1-C2-C3	2.13	112.58	109.40
3	T	5	Z4K	O2-C2-C3	2.11	109.90	106.95
3	c	5	Z4K	O2-C2-C3	2.11	109.89	106.95
3	O	7	5TH	O2-C2-C3	2.11	109.89	106.95
2	g	3	PDX	O2-C2-C3	2.10	108.98	106.65
2	g	1	5LS	O2-C2-C1	2.07	110.37	107.58
2	j	1	5LS	O2-C2-C1	2.06	110.35	107.58
2	j	3	PDX	O5-C1-C2	2.01	113.47	109.41

There are no chirality outliers.

All (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
2	l	1	5LS	C5-C4-O4-S2
3	c	7	5TH	C3-C4-O4-S2
3	c	7	5TH	C5-C4-O4-S2
2	P	3	PDX	C2-C3-O3-S'
2	P	3	PDX	C4-C3-O3-S'
2	j	2	GLC	O5-C5-C6-O6
2	a	3	PDX	O5-C5-C6-O6
3	i	5	Z4K	O5-C5-C6-O6
3	O	3	5TM	O5-C5-C6-O6
2	g	3	PDX	O5-C5-C6-O6
3	i	3	5TM	O5-C5-C6-O6
3	i	1	5LS	O5-C5-C6-O6
3	c	7	5TH	O5-C5-C6-O6
3	c	7	5TH	C4-C5-C6-O6
2	P	1	5LS	O5-C5-C6-O6
3	i	4	5TJ	O5-C5-C6-O6
2	m	2	GLC	O5-C5-C6-O6
3	c	3	5TM	O5-C5-C6-O6
3	i	3	5TM	C4-C5-C6-O6
3	O	3	5TM	C4-C5-C6-O6
2	k	1	5LS	C4-C5-C6-O6
2	g	3	PDX	C4-C5-C6-O6
2	a	3	PDX	C4-C5-C6-O6
3	i	5	Z4K	C4-C5-C6-O6
2	e	3	PDX	C4-C5-C6-O6
2	n	3	PDX	C4-C5-C6-O6
2	f	2	GLC	O5-C5-C6-O6
3	i	7	5TH	O5-C5-C6-O6
2	j	2	GLC	C4-C5-C6-O6
2	M	1	5LS	C4-C5-C6-O6
2	W	3	PDX	O5-C5-C6-O6
3	c	6	5TK	O5-C5-C6-O6
3	i	7	5TH	C4-C5-C6-O6
3	O	4	5TJ	O5-C5-C6-O6
3	i	1	5LS	C4-C5-C6-O6
2	m	2	GLC	C4-C5-C6-O6
2	e	3	PDX	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	n	3	PDX	O5-C5-C6-O6
2	k	1	5LS	O5-C5-C6-O6
2	j	1	5LS	O5-C5-C6-O6
2	f	2	GLC	C4-C5-C6-O6
3	i	4	5TJ	C4-C5-C6-O6
2	V	3	PDX	O5-C5-C6-O6
2	W	1	5LS	O5-C5-C6-O6
2	M	1	5LS	O5-C5-C6-O6
2	h	2	GLC	C4-C5-C6-O6
2	X	3	PDX	O5-C5-C6-O6
3	c	2	5TJ	O5-C5-C6-O6
2	N	2	GLC	O5-C5-C6-O6
2	P	2	GLC	C4-C5-C6-O6
3	c	3	5TM	C4-C5-C6-O6
2	j	1	5LS	C4-C5-C6-O6
2	N	1	5LS	O5-C5-C6-O6
2	N	1	5LS	C4-C5-C6-O6
3	c	5	Z4K	O5-C5-C6-O6
2	P	1	5LS	C4-C5-C6-O6
2	Q	1	5LS	C4-C5-C6-O6
2	P	2	GLC	O5-C5-C6-O6
3	c	6	5TK	C4-C5-C6-O6
2	Z	2	GLC	C4-C5-C6-O6
3	O	4	5TJ	C4-C5-C6-O6
2	Y	3	PDX	O5-C5-C6-O6
2	W	3	PDX	C4-C5-C6-O6
2	P	3	PDX	O5-C5-C6-O6
2	N	3	PDX	O5-C5-C6-O6
2	h	2	GLC	O5-C5-C6-O6
2	R	3	PDX	C4-C5-C6-O6
2	Q	1	5LS	O5-C5-C6-O6
2	m	1	5LS	O5-C5-C6-O6
3	O	2	5TJ	O5-C5-C6-O6
2	V	3	PDX	C4-C5-C6-O6
2	e	1	5LS	O5-C5-C6-O6
2	a	2	GLC	C4-C5-C6-O6
2	n	2	GLC	C4-C5-C6-O6
2	l	1	5LS	C4-O4-S2-O07
2	W	1	5LS	C4-C5-C6-O6
3	i	2	5TJ	O5-C5-C6-O6
2	X	3	PDX	C4-C5-C6-O6
2	j	3	PDX	O5-C5-C6-O6

Continued on next page...

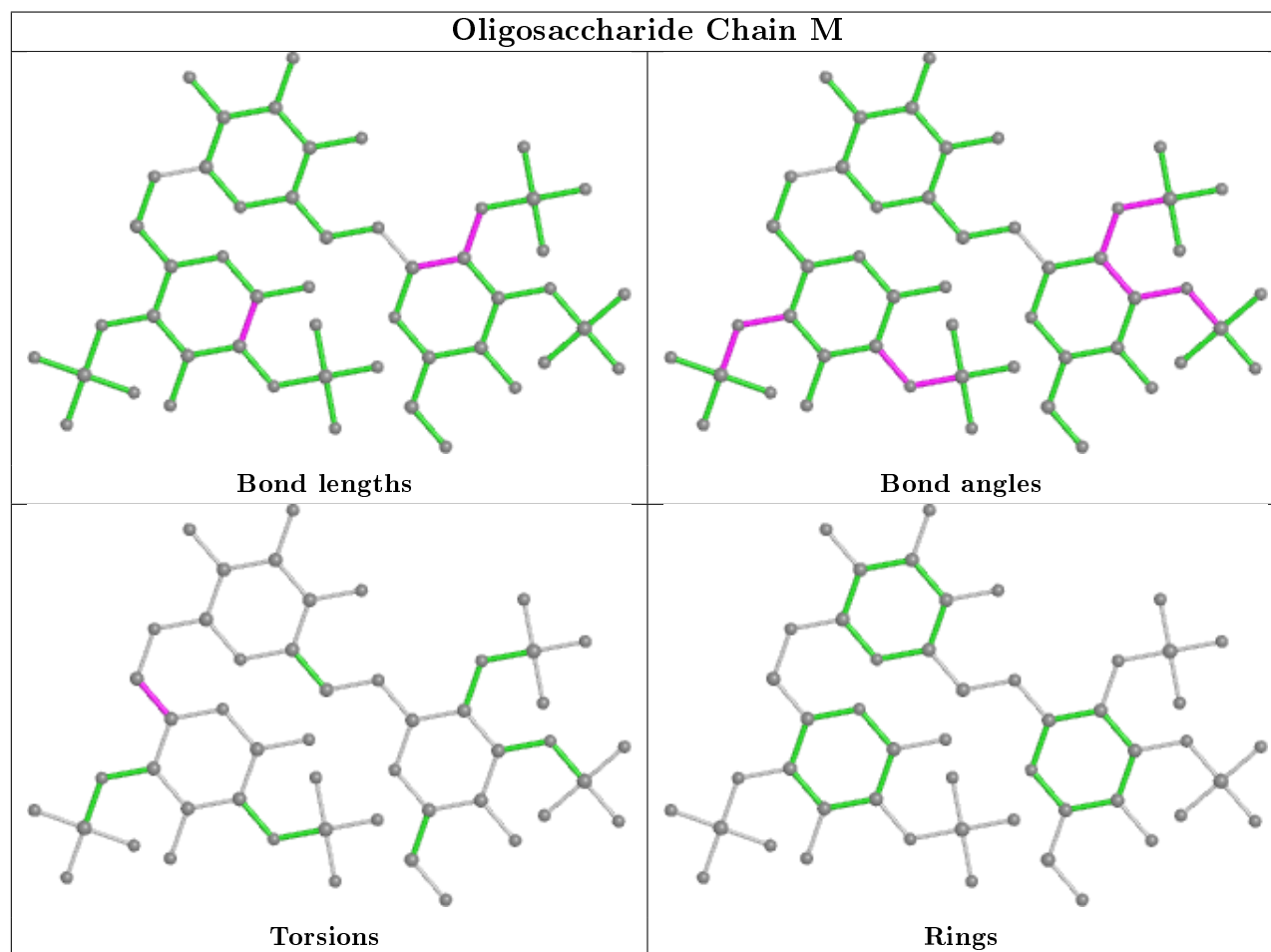
Continued from previous page...

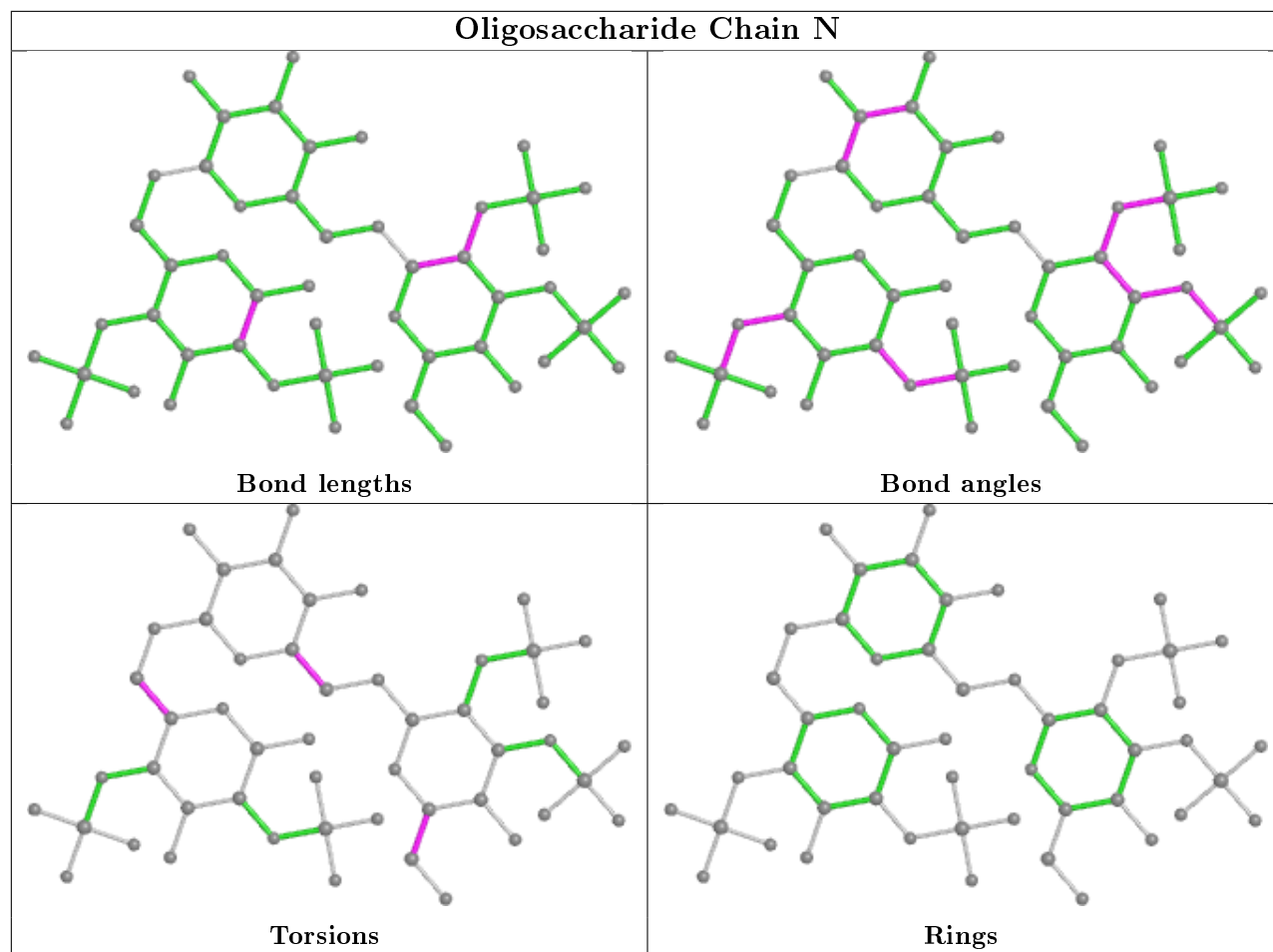
Mol	Chain	Res	Type	Atoms
2	a	2	GLC	O5-C5-C6-O6
3	T	2	5TJ	O5-C5-C6-O6
3	O	7	5TH	C4-C5-C6-O6
3	c	2	5TJ	C4-C5-C6-O6
2	e	2	GLC	O5-C5-C6-O6
2	W	2	GLC	C4-C5-C6-O6
2	Z	2	GLC	O5-C5-C6-O6
2	R	3	PDX	O5-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	n	2	GLC	O5-C5-C6-O6
3	O	5	Z4K	O5-C5-C6-O6
2	V	1	5LS	C4-C5-C6-O6
3	T	6	5TK	O5-C5-C6-O6

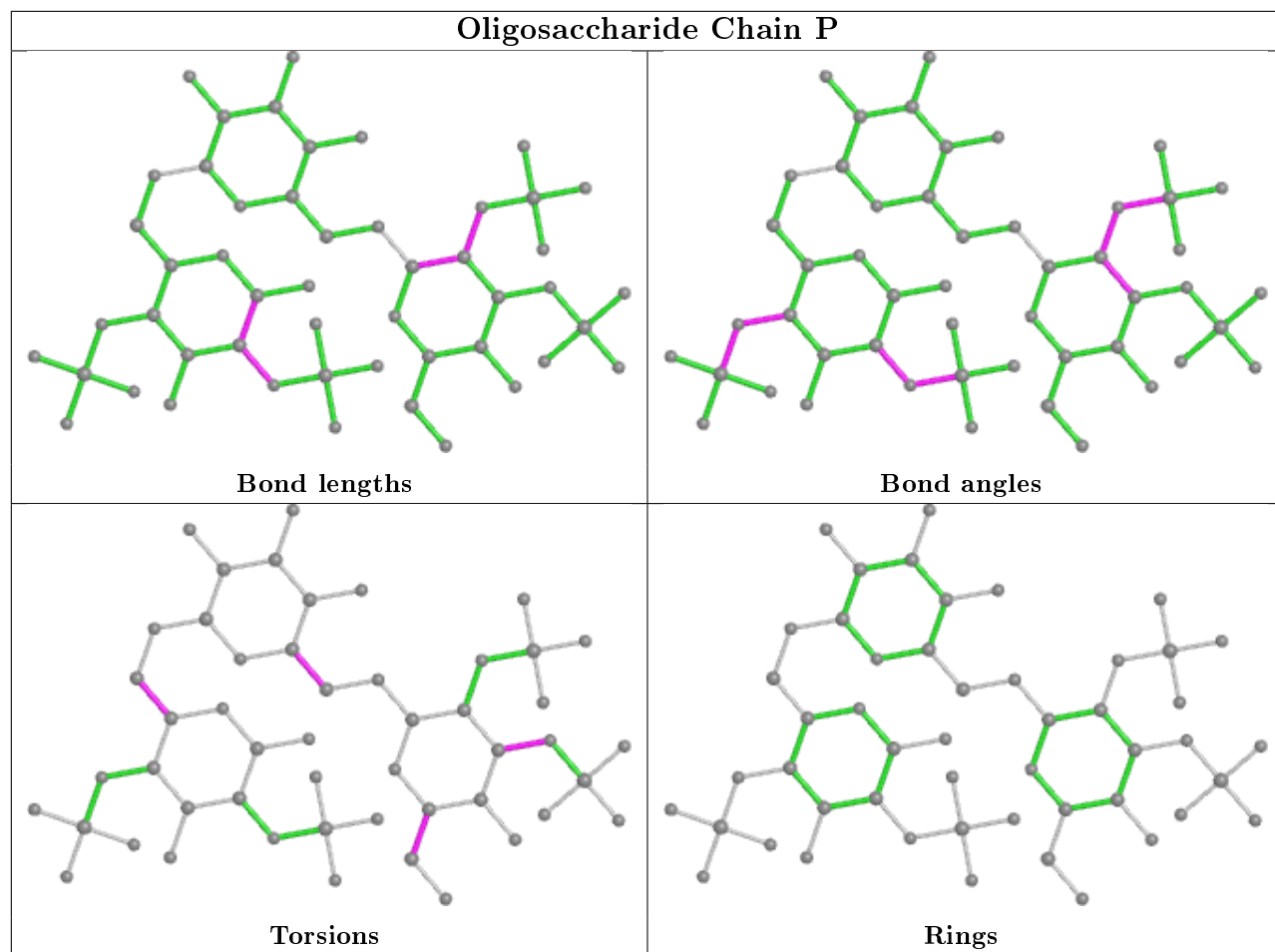
There are no ring outliers.

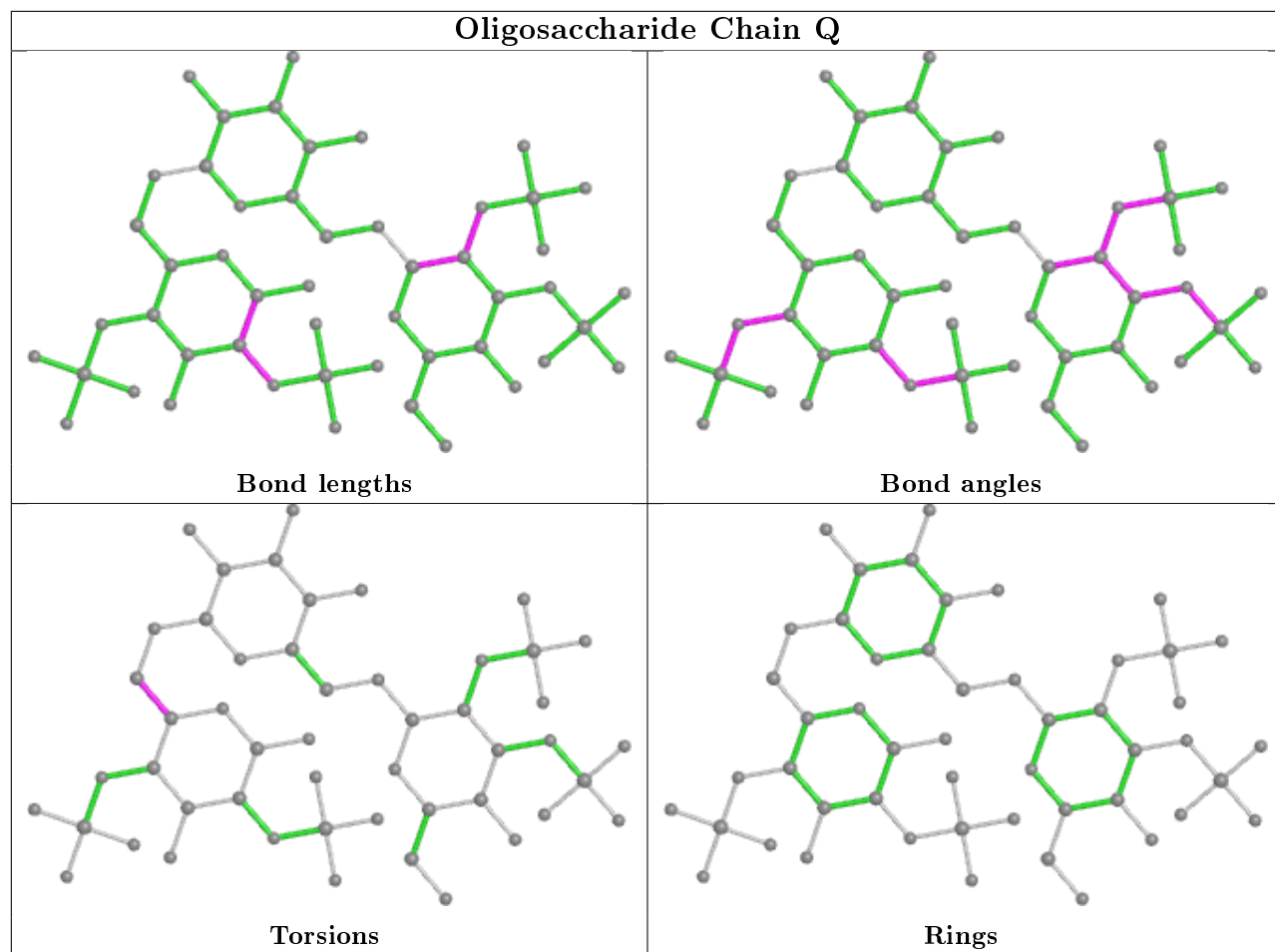
No monomer is involved in short contacts.

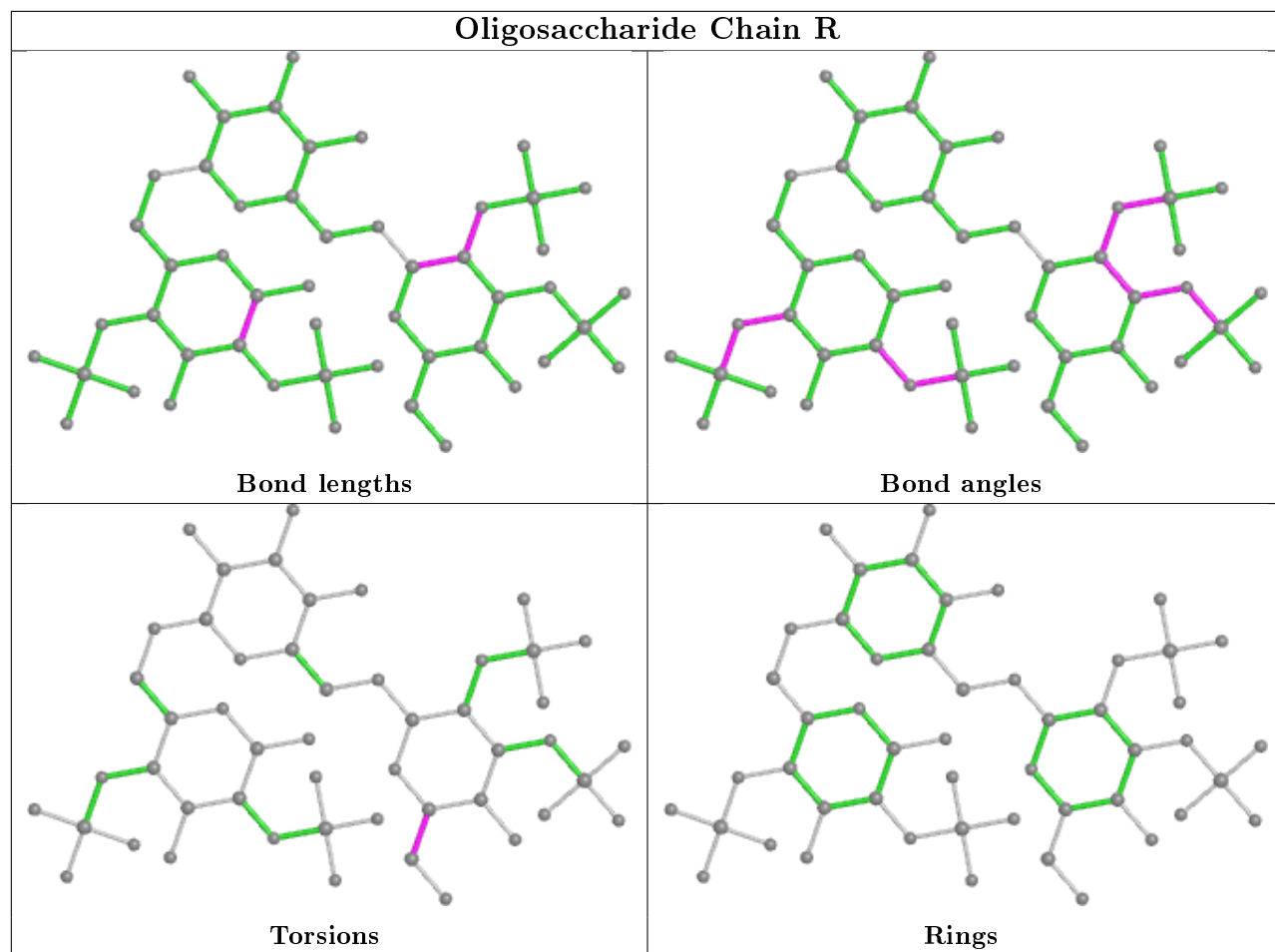
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

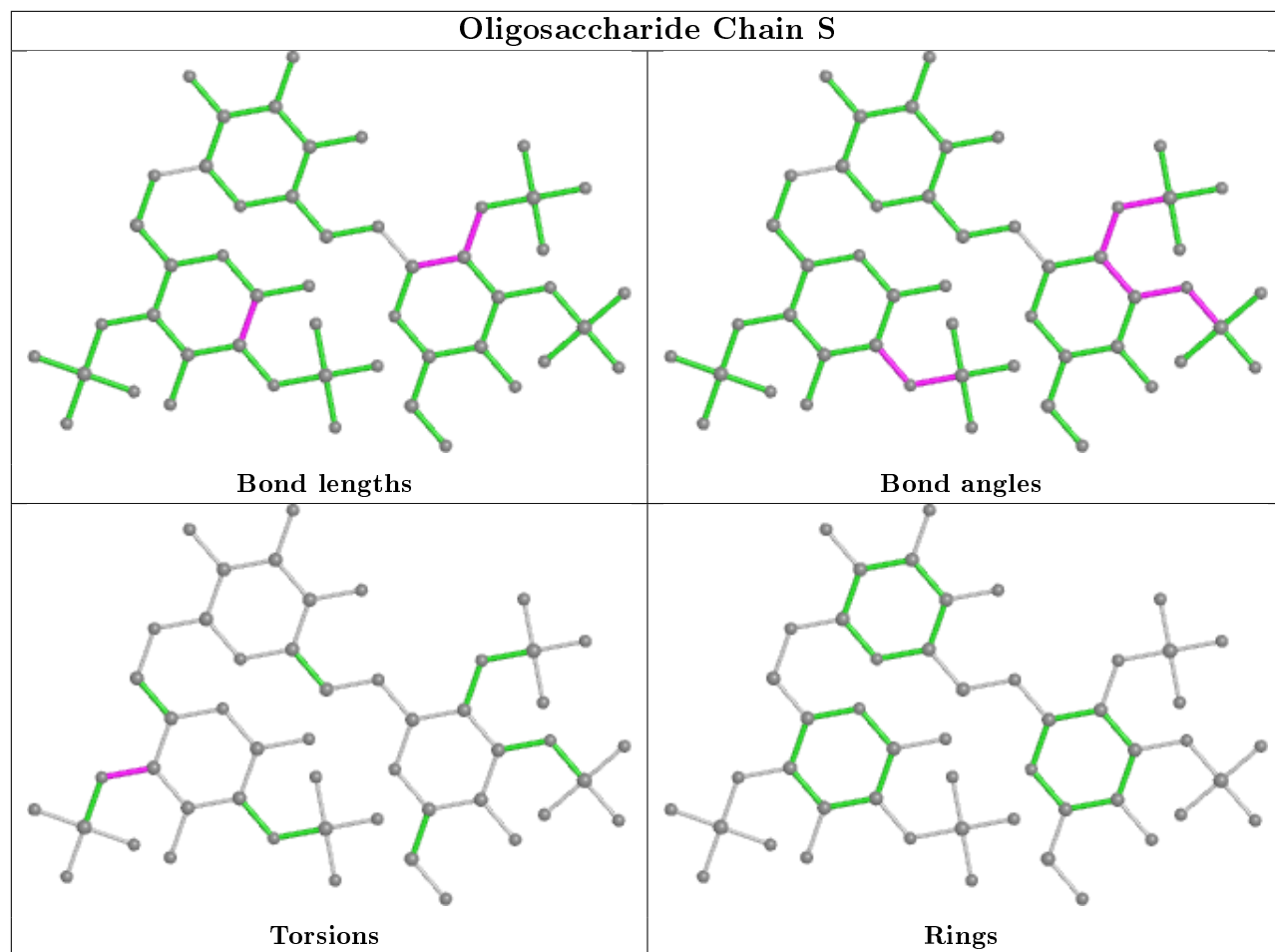


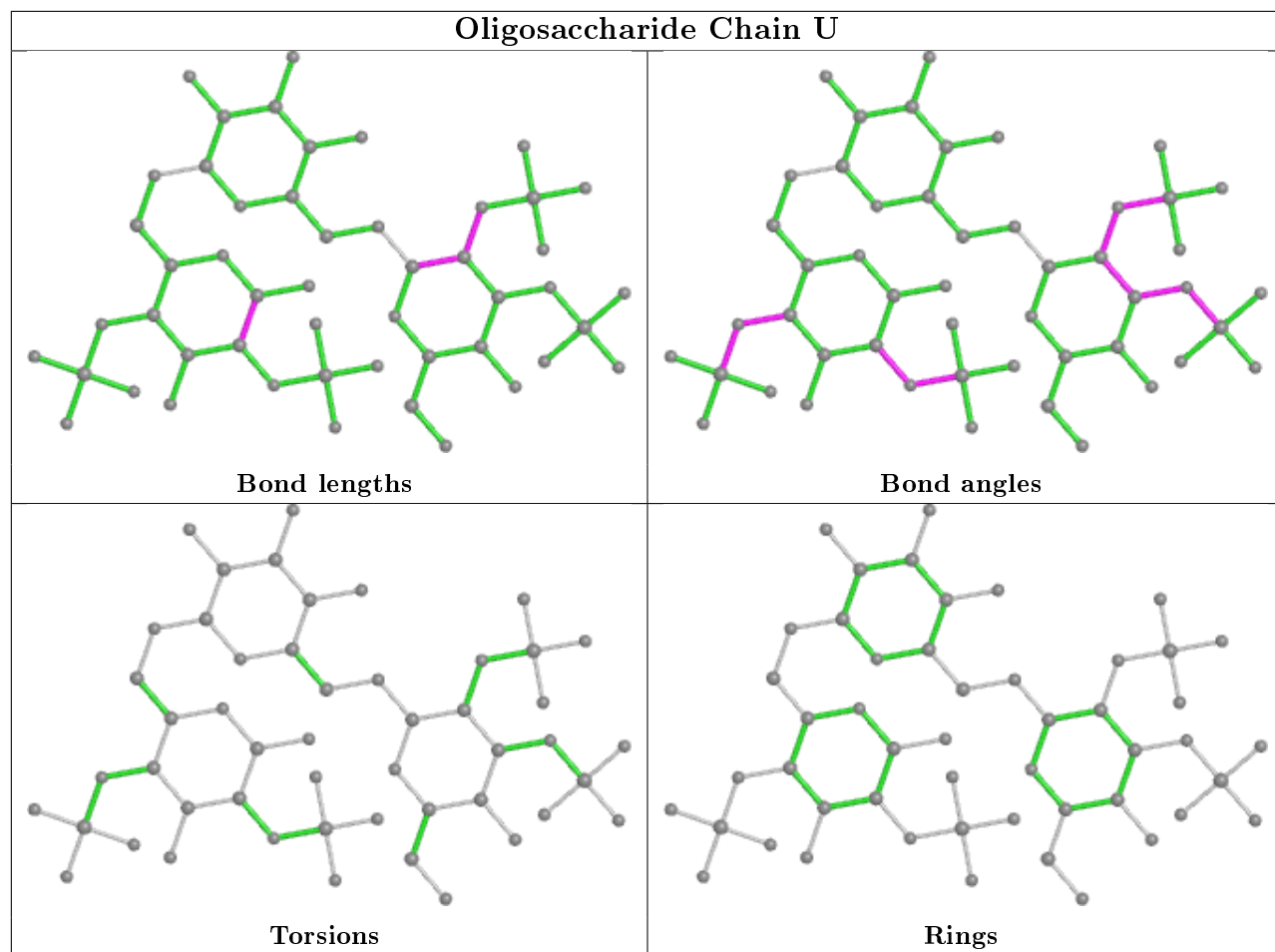


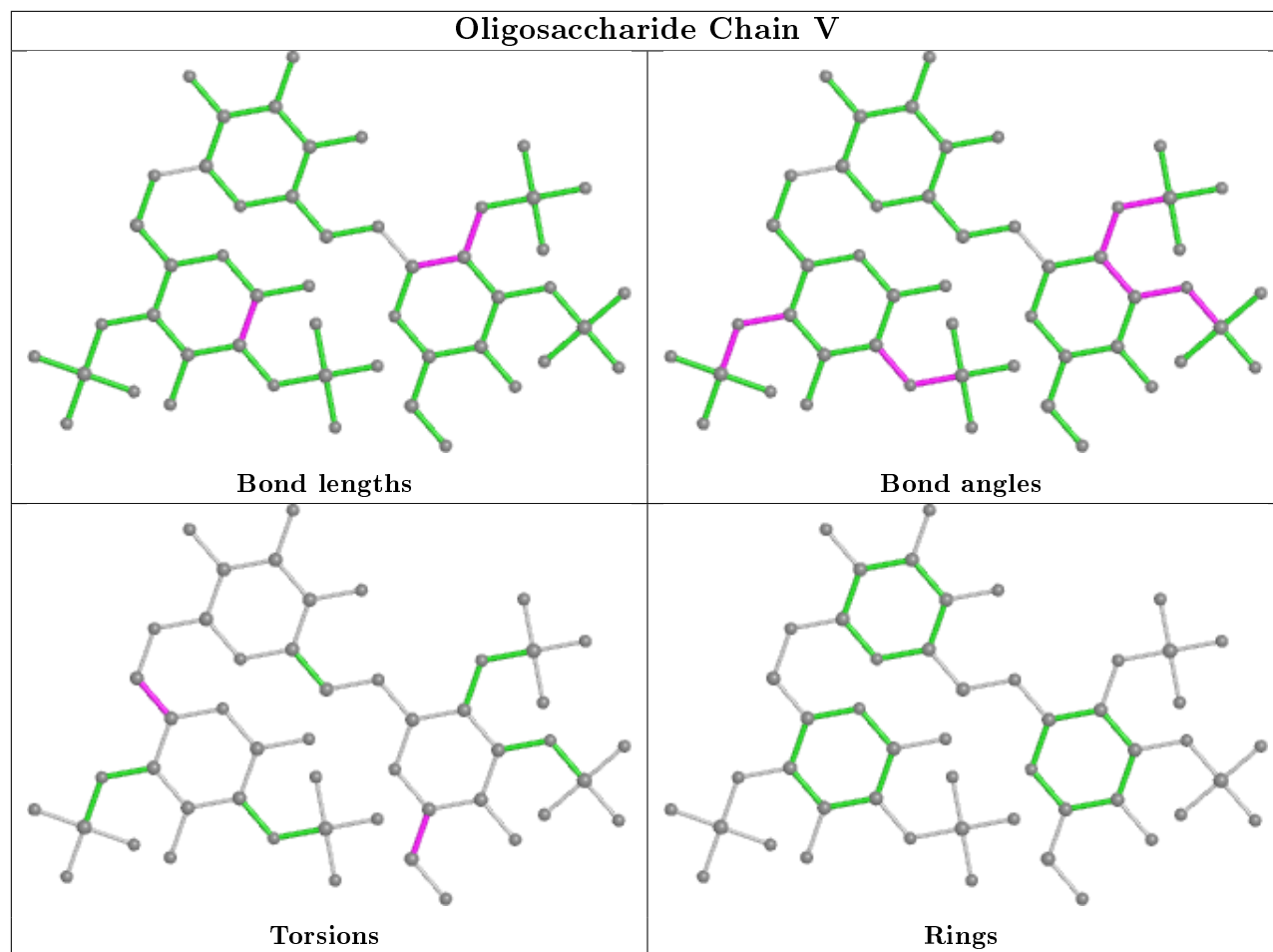


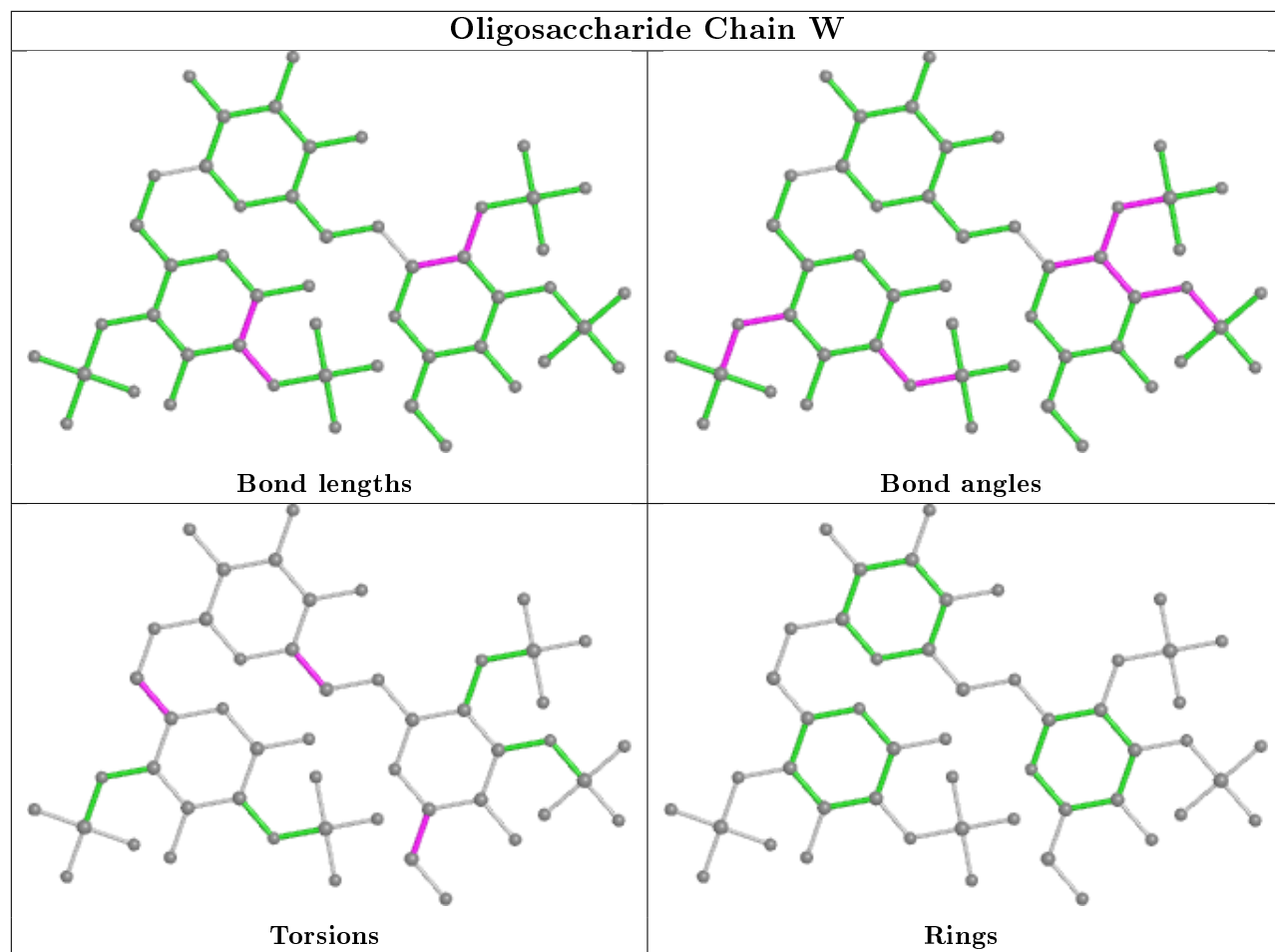


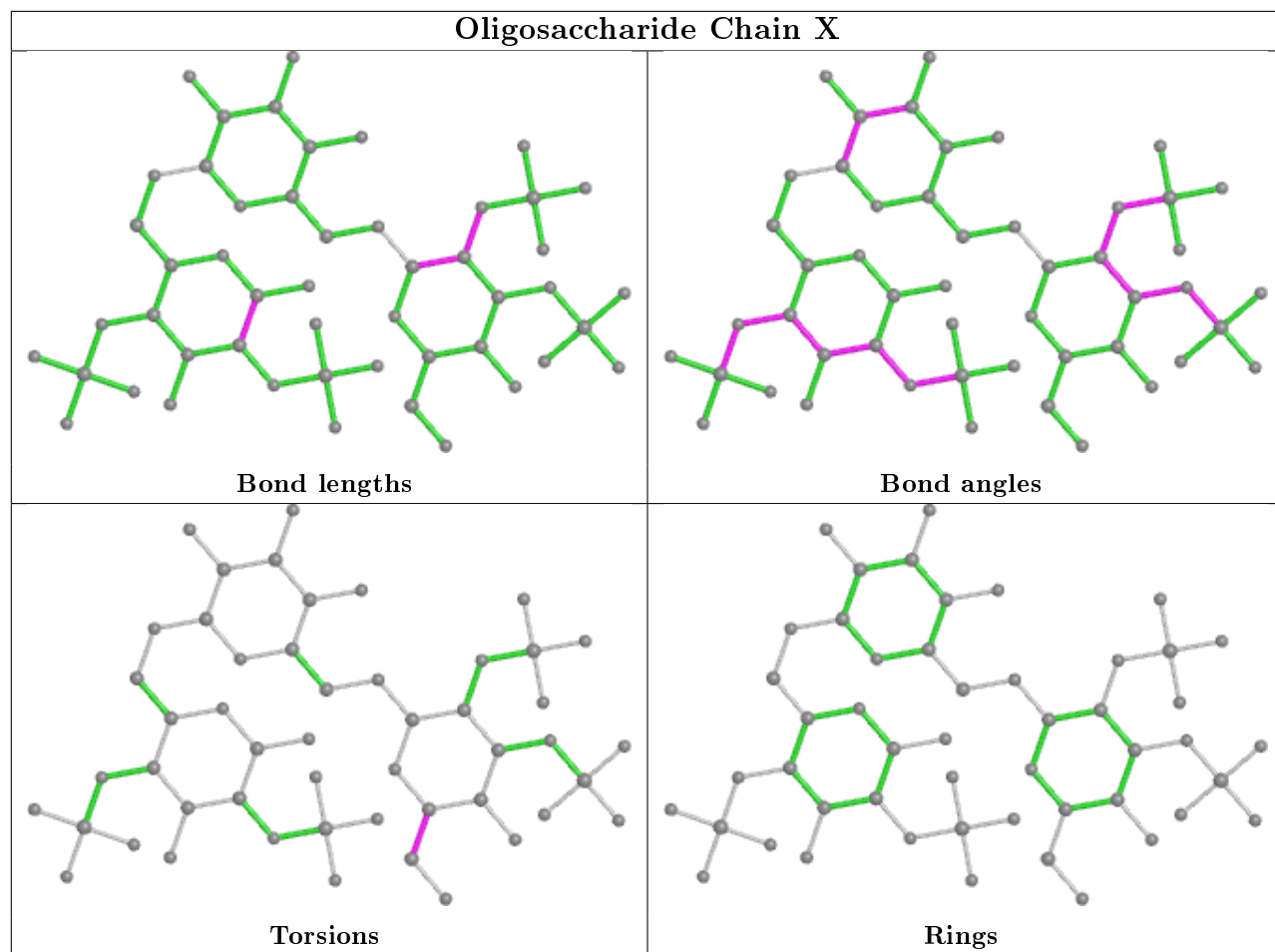


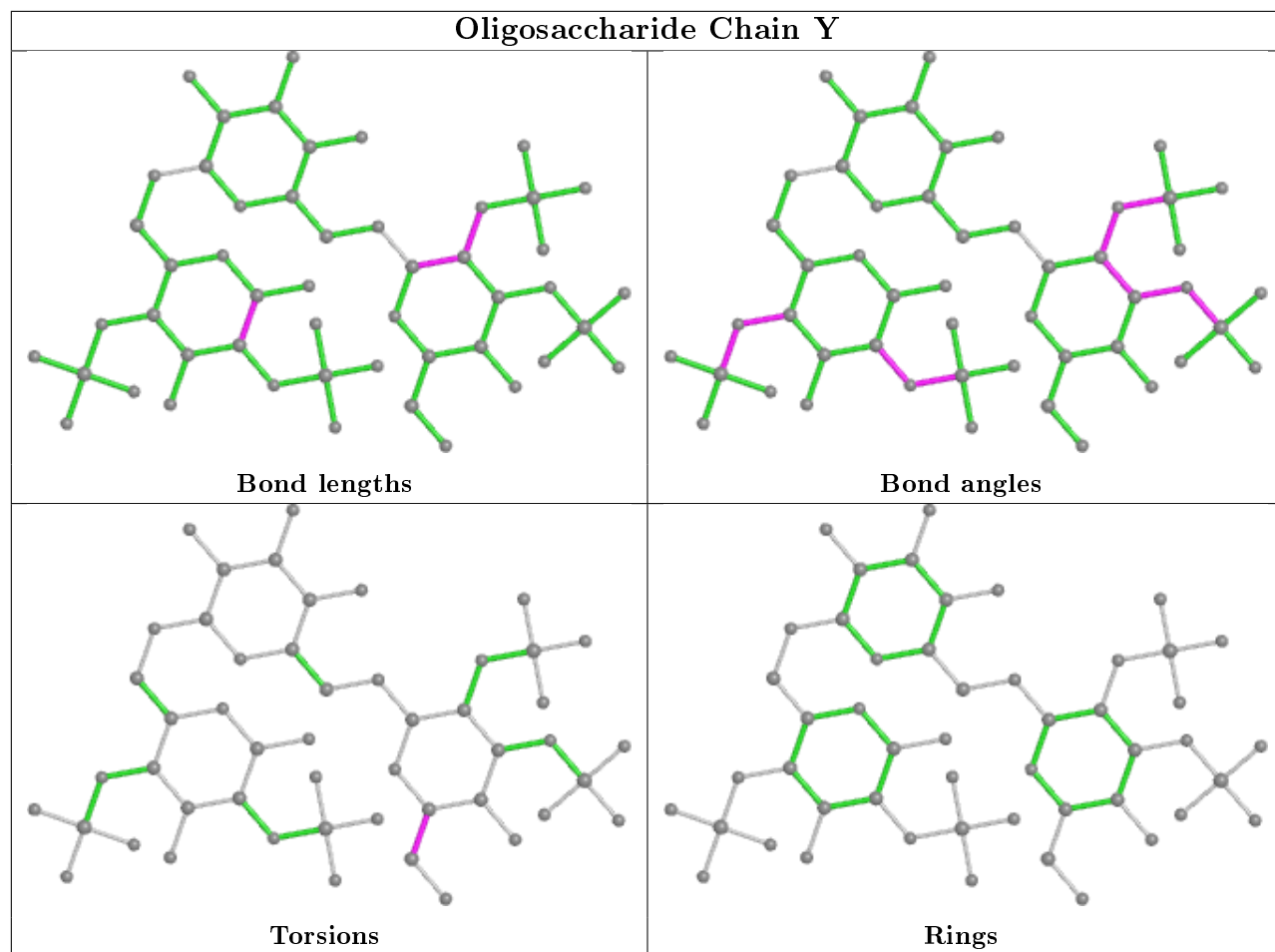


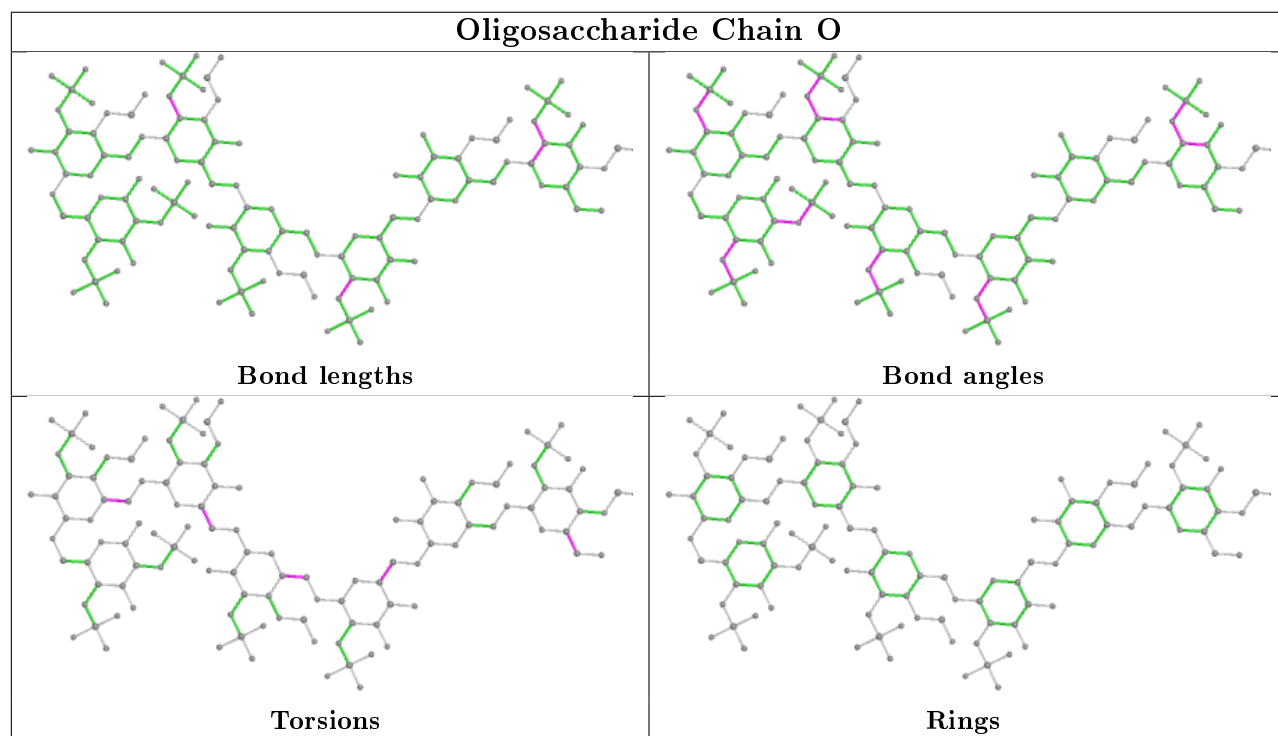
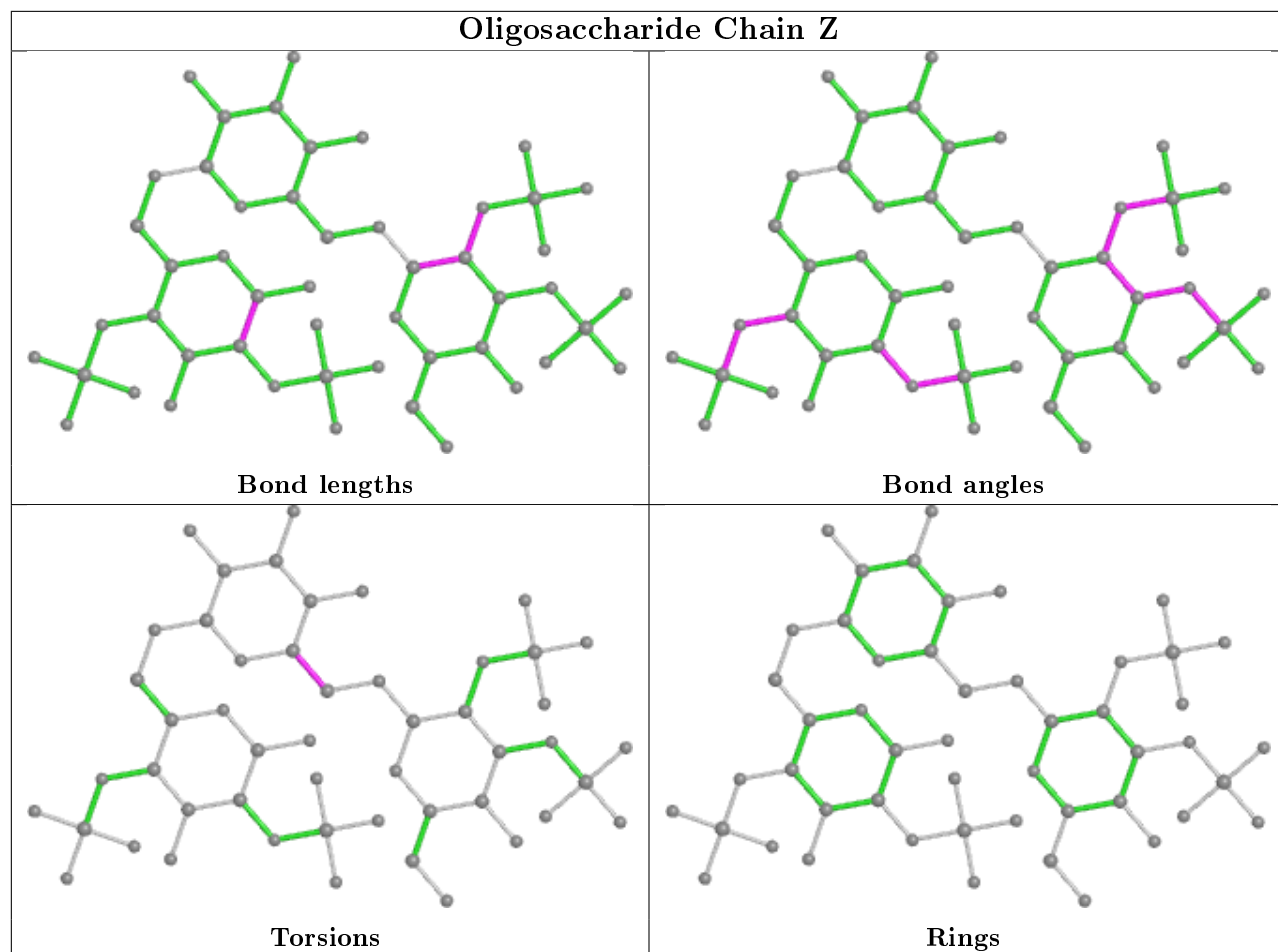


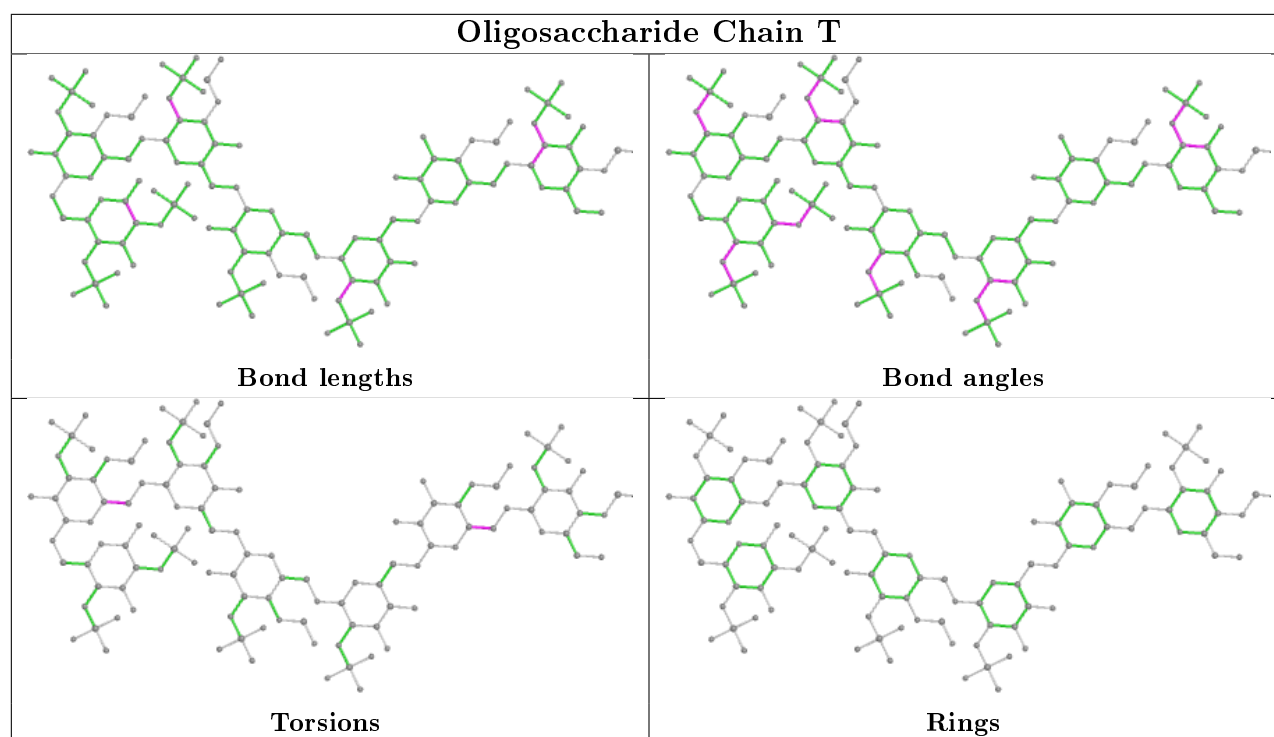












5.6 Ligand geometry [i](#)

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

All (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
4	I	701	5TL	S-N1	-5.99	1.48	1.60
4	J	701	5TL	S-N1	-5.95	1.48	1.60
4	C	701	5TL	S-N1	-5.92	1.48	1.60
4	A	701	5TL	S-N1	-5.75	1.49	1.60
4	D	701	5TL	S-N1	-5.72	1.49	1.60
4	K	701	5TL	S-N1	-5.68	1.49	1.60
4	E	701	5TL	S-N1	-5.67	1.49	1.60
4	G	701	5TL	CAQ-CAR	-4.92	1.33	1.42
4	I	701	5TL	CAQ-CAR	-4.86	1.33	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	5TL	CAQ-CAR	-4.80	1.34	1.42
4	C	701	5TL	CAQ-CAR	-4.79	1.34	1.42
4	J	701	5TL	CAQ-CAR	-4.74	1.34	1.42
4	H	701	5TL	CAQ-CAR	-4.74	1.34	1.42
4	D	701	5TL	CAT-CAU	4.73	1.46	1.38
4	F	701	5TL	CAQ-CAR	-4.72	1.34	1.42
4	D	701	5TL	CAN-CAU	4.71	1.46	1.38
4	L	701	5TL	CAT-CAU	4.70	1.46	1.38
4	J	701	5TL	CAT-CAU	4.67	1.46	1.38
4	E	701	5TL	CAV-NAW	4.64	1.41	1.33
4	I	701	5TL	CAT-CAU	4.64	1.46	1.38
4	C	701	5TL	CAT-CAU	4.63	1.46	1.38
4	B	701	5TL	CAQ-CAR	-4.62	1.34	1.42
4	B	701	5TL	CAT-CAU	4.62	1.46	1.38
4	D	701	5TL	CAQ-CAR	-4.59	1.34	1.42
4	K	701	5TL	CAQ-CAR	-4.56	1.34	1.42
4	A	701	5TL	CAT-CAU	4.56	1.46	1.38
4	E	701	5TL	CAT-CAU	4.55	1.46	1.38
4	E	701	5TL	CAQ-CAR	-4.55	1.34	1.42
4	K	701	5TL	CAT-CAU	4.54	1.46	1.38
4	K	701	5TL	CAV-NAW	4.54	1.41	1.33
4	J	701	5TL	CAN-CAU	4.52	1.45	1.38
4	B	701	5TL	CAN-CAU	4.51	1.45	1.38
4	L	701	5TL	CAN-CAU	4.51	1.45	1.38
4	L	701	5TL	CAQ-CAR	-4.50	1.34	1.42
4	H	701	5TL	CAT-CAU	4.49	1.45	1.38
4	F	701	5TL	CAT-CAU	4.46	1.45	1.38
4	H	701	5TL	CAN-CAU	4.43	1.45	1.38
4	C	701	5TL	CAV-NAW	4.37	1.41	1.33
4	I	701	5TL	CAV-NAW	4.37	1.41	1.33
4	A	701	5TL	CAV-NAW	4.36	1.41	1.33
4	B	701	5TL	CAV-NAW	4.36	1.41	1.33
4	K	701	5TL	CAN-CAU	4.33	1.45	1.38
4	I	701	5TL	CAN-CAU	4.29	1.45	1.38
4	L	701	5TL	CAU-S	4.26	1.83	1.77
4	D	701	5TL	CAV-NAW	4.25	1.41	1.33
4	G	701	5TL	CAV-NAW	4.25	1.41	1.33
4	A	701	5TL	CAN-CAU	4.23	1.45	1.38
4	F	701	5TL	CAN-CAU	4.23	1.45	1.38
4	H	701	5TL	CAV-NAW	4.21	1.41	1.33
4	L	701	5TL	CAV-NAW	4.20	1.41	1.33
4	F	701	5TL	CAV-NAW	4.19	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	701	5TL	CAV-NAW	4.19	1.41	1.33
4	E	701	5TL	CAN-CAU	4.19	1.45	1.38
4	G	701	5TL	CAT-CAU	4.17	1.45	1.38
4	C	701	5TL	CAN-CAU	4.16	1.45	1.38
4	D	701	5TL	CAU-S	4.16	1.83	1.77
4	G	701	5TL	CAN-CAU	4.12	1.45	1.38
4	B	701	5TL	CAU-S	4.10	1.83	1.77
4	E	701	5TL	CAU-S	4.01	1.83	1.77
4	J	701	5TL	CAU-S	3.99	1.83	1.77
4	I	701	5TL	CAU-S	3.98	1.83	1.77
4	C	701	5TL	CAU-S	3.91	1.83	1.77
4	H	701	5TL	CAU-S	3.84	1.83	1.77
4	A	701	5TL	CAU-S	3.83	1.83	1.77
4	F	701	5TL	CAU-S	3.81	1.83	1.77
4	D	701	5TL	CAR-NAY	3.76	1.49	1.37
4	F	701	5TL	CAR-NAY	3.71	1.49	1.37
4	L	701	5TL	CAR-NAY	3.71	1.49	1.37
4	J	701	5TL	CAR-NAY	3.69	1.49	1.37
4	H	701	5TL	CAR-NAY	3.67	1.49	1.37
4	K	701	5TL	CAR-NAY	3.66	1.48	1.37
4	A	701	5TL	CAR-NAY	3.64	1.48	1.37
4	G	701	5TL	CAR-NAY	3.64	1.48	1.37
4	K	701	5TL	CAU-S	3.63	1.82	1.77
4	E	701	5TL	CAR-NAY	3.62	1.48	1.37
4	B	701	5TL	CAR-NAY	3.58	1.48	1.37
4	I	701	5TL	CAR-NAY	3.57	1.48	1.37
4	C	701	5TL	CAR-NAY	3.55	1.48	1.37
4	A	701	5TL	CAG-CAH	-3.50	1.40	1.49
4	G	701	5TL	CAU-S	3.44	1.82	1.77
4	E	701	5TL	CAG-CAH	-3.42	1.40	1.49
4	L	701	5TL	CAG-CAH	-3.39	1.40	1.49
4	B	701	5TL	CAG-CAH	-3.37	1.40	1.49
4	H	701	5TL	CAG-CAH	-3.35	1.40	1.49
4	I	701	5TL	CAG-CAH	-3.34	1.40	1.49
4	K	701	5TL	CAG-CAH	-3.28	1.40	1.49
4	C	701	5TL	CAG-CAH	-3.24	1.41	1.49
4	D	701	5TL	CAG-CAH	-3.21	1.41	1.49
4	J	701	5TL	CAG-CAH	-3.21	1.41	1.49
4	G	701	5TL	CAG-CAH	-3.21	1.41	1.49
4	F	701	5TL	CAG-CAH	-3.11	1.41	1.49
4	L	701	5TL	CAS-CAL	-3.10	1.32	1.39
4	H	701	5TL	CAS-CAL	-3.07	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	5TL	CAS-CAL	-2.97	1.33	1.39
4	G	701	5TL	CAS-CAL	-2.95	1.33	1.39
4	C	701	5TL	CAS-CAL	-2.94	1.33	1.39
4	B	701	5TL	CAS-CAL	-2.88	1.33	1.39
4	D	701	5TL	CAS-CAL	-2.85	1.33	1.39
4	E	701	5TL	CAS-CAL	-2.82	1.33	1.39
4	J	701	5TL	CAS-CAL	-2.81	1.33	1.39
4	I	701	5TL	CAS-CAL	-2.80	1.33	1.39
4	G	701	5TL	CAQ-CAV	-2.76	1.46	1.50
4	F	701	5TL	CAS-CAL	-2.75	1.33	1.39
4	K	701	5TL	CAS-CAL	-2.67	1.33	1.39
4	J	701	5TL	CAQ-CAV	-2.53	1.46	1.50
4	D	701	5TL	CAQ-CAV	-2.41	1.46	1.50
4	H	701	5TL	CAQ-CAV	-2.35	1.46	1.50
4	L	701	5TL	CAQ-CAV	-2.29	1.47	1.50
4	A	701	5TL	CAI-CAJ	-2.28	1.36	1.39
4	B	701	5TL	CAQ-CAV	-2.18	1.47	1.50
4	I	701	5TL	CAI-CAJ	-2.15	1.36	1.39
4	C	701	5TL	CAQ-CAV	-2.15	1.47	1.50
4	E	701	5TL	CAI-CAJ	-2.15	1.36	1.39
4	C	701	5TL	CAI-CAJ	-2.15	1.36	1.39
4	F	701	5TL	CAI-CAJ	-2.13	1.36	1.39
4	H	701	5TL	CAS-CAT	2.10	1.42	1.38
4	A	701	5TL	CAQ-CAV	-2.08	1.47	1.50
4	B	701	5TL	CAS-CAT	2.06	1.42	1.38
4	K	701	5TL	CAI-CAJ	-2.05	1.36	1.39
4	G	701	5TL	CAI-CAJ	-2.05	1.36	1.39
4	A	701	5TL	CAI-CAH	-2.00	1.36	1.39
4	B	701	5TL	CAI-CAJ	-2.00	1.36	1.39

All (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
4	L	701	5TL	CAT-CAS-CAL	-13.09	102.29	121.13
4	A	701	5TL	CAT-CAS-CAL	-13.05	102.34	121.13
4	C	701	5TL	CAT-CAS-CAL	-13.01	102.40	121.13
4	K	701	5TL	CAT-CAS-CAL	-12.99	102.43	121.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	701	5TL	CAS-CAL-CAM	12.98	143.47	117.59
4	H	701	5TL	CAS-CAL-CAM	12.97	143.45	117.59
4	G	701	5TL	CAT-CAS-CAL	-12.95	102.50	121.13
4	E	701	5TL	CAT-CAS-CAL	-12.93	102.52	121.13
4	E	701	5TL	CAS-CAL-CAM	12.93	143.37	117.59
4	H	701	5TL	CAT-CAS-CAL	-12.92	102.53	121.13
4	I	701	5TL	CAT-CAS-CAL	-12.90	102.56	121.13
4	A	701	5TL	CAS-CAL-CAM	12.86	143.23	117.59
4	F	701	5TL	CAS-CAL-CAM	12.85	143.21	117.59
4	C	701	5TL	CAS-CAL-CAM	12.83	143.16	117.59
4	I	701	5TL	CAS-CAL-CAM	12.81	143.13	117.59
4	G	701	5TL	CAS-CAL-CAM	12.81	143.12	117.59
4	B	701	5TL	CAS-CAL-CAM	12.76	143.03	117.59
4	B	701	5TL	CAT-CAS-CAL	-12.72	102.82	121.13
4	F	701	5TL	CAT-CAS-CAL	-12.18	103.60	121.13
4	K	701	5TL	CAM-CAN-CAU	-11.06	108.00	119.45
4	C	701	5TL	CAM-CAN-CAU	-10.98	108.08	119.45
4	G	701	5TL	CAM-CAN-CAU	-10.89	108.17	119.45
4	E	701	5TL	CAM-CAN-CAU	-10.85	108.21	119.45
4	A	701	5TL	CAM-CAN-CAU	-10.82	108.25	119.45
4	I	701	5TL	CAM-CAN-CAU	-10.72	108.35	119.45
4	J	701	5TL	CAM-CAN-CAU	-10.70	108.37	119.45
4	D	701	5TL	CAM-CAN-CAU	-10.68	108.39	119.45
4	H	701	5TL	CAM-CAN-CAU	-10.60	108.47	119.45
4	B	701	5TL	CAM-CAN-CAU	-10.58	108.49	119.45
4	L	701	5TL	CAM-CAN-CAU	-10.58	108.50	119.45
4	F	701	5TL	CAN-CAU-S	-9.64	105.75	119.73
4	F	701	5TL	CAM-CAN-CAU	-9.64	109.47	119.45
4	J	701	5TL	CAS-CAL-CAJ	-8.81	106.63	120.91
4	B	701	5TL	CAS-CAL-CAJ	-8.78	106.68	120.91
4	L	701	5TL	CAS-CAL-CAJ	-8.76	106.73	120.91
4	H	701	5TL	CAS-CAL-CAJ	-8.70	106.81	120.91
4	E	701	5TL	CAN-CAU-S	-8.67	107.16	119.73
4	K	701	5TL	CAS-CAL-CAJ	-8.67	106.87	120.91
4	D	701	5TL	CAS-CAL-CAJ	-8.66	106.88	120.91
4	E	701	5TL	CAS-CAL-CAJ	-8.64	106.91	120.91
4	C	701	5TL	CAN-CAU-S	-8.61	107.25	119.73
4	G	701	5TL	CAS-CAL-CAJ	-8.60	106.97	120.91
4	A	701	5TL	CAS-CAL-CAJ	-8.54	107.07	120.91
4	K	701	5TL	CAN-CAU-S	-8.51	107.39	119.73
4	A	701	5TL	CAN-CAU-S	-8.46	107.47	119.73
4	I	701	5TL	CAN-CAU-S	-8.45	107.48	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	5TL	CAS-CAL-CAJ	-8.44	107.24	120.91
4	G	701	5TL	CAN-CAU-S	-8.41	107.53	119.73
4	I	701	5TL	CAS-CAL-CAJ	-8.39	107.33	120.91
4	D	701	5TL	CAN-CAU-S	-8.34	107.64	119.73
4	L	701	5TL	CAN-CAU-S	-8.32	107.67	119.73
4	F	701	5TL	CAM-CAL-CAJ	-8.32	107.43	120.91
4	B	701	5TL	CAN-CAU-S	-8.28	107.73	119.73
4	J	701	5TL	CAN-CAU-S	-8.18	107.87	119.73
4	H	701	5TL	CAN-CAU-S	-8.16	107.91	119.73
4	F	701	5TL	CAS-CAL-CAJ	-7.94	108.05	120.91
4	D	701	5TL	CAM-CAL-CAJ	-7.79	108.29	120.91
4	J	701	5TL	CAM-CAL-CAJ	-7.64	108.53	120.91
4	L	701	5TL	CAM-CAL-CAJ	-7.63	108.55	120.91
4	E	701	5TL	CAM-CAL-CAJ	-7.55	108.68	120.91
4	I	701	5TL	CAM-CAL-CAJ	-7.51	108.74	120.91
4	K	701	5TL	CAM-CAL-CAJ	-7.49	108.78	120.91
4	H	701	5TL	CAM-CAL-CAJ	-7.48	108.80	120.91
4	K	701	5TL	O2-S-O4	-7.46	106.49	118.76
4	B	701	5TL	CAM-CAL-CAJ	-7.46	108.83	120.91
4	C	701	5TL	CAM-CAL-CAJ	-7.38	108.95	120.91
4	G	701	5TL	CAM-CAL-CAJ	-7.32	109.06	120.91
4	A	701	5TL	CAM-CAL-CAJ	-7.30	109.08	120.91
4	J	701	5TL	O2-S-O4	-7.28	106.78	118.76
4	G	701	5TL	O2-S-O4	-6.95	107.34	118.76
4	F	701	5TL	O2-S-O4	-6.90	107.41	118.76
4	D	701	5TL	O2-S-O4	-6.71	107.73	118.76
4	C	701	5TL	O2-S-O4	-6.64	107.84	118.76
4	A	701	5TL	O2-S-O4	-6.58	107.94	118.76
4	I	701	5TL	O2-S-O4	-6.57	107.95	118.76
4	L	701	5TL	O2-S-O4	-6.36	108.30	118.76
4	B	701	5TL	O2-S-O4	-6.27	108.46	118.76
4	K	701	5TL	CAT-CAU-CAN	6.22	129.13	120.44
4	H	701	5TL	O2-S-O4	-6.17	108.61	118.76
4	E	701	5TL	O2-S-O4	-5.96	108.97	118.76
4	E	701	5TL	CAT-CAU-CAN	5.86	128.63	120.44
4	G	701	5TL	CAT-CAU-CAN	5.82	128.56	120.44
4	C	701	5TL	CAT-CAU-CAN	5.77	128.50	120.44
4	J	701	5TL	CAT-CAU-CAN	5.73	128.44	120.44
4	A	701	5TL	CAT-CAU-CAN	5.70	128.40	120.44
4	I	701	5TL	CAT-CAU-CAN	5.67	128.35	120.44
4	D	701	5TL	CAT-CAU-CAN	5.59	128.25	120.44
4	F	701	5TL	CAT-CAU-CAN	5.57	128.22	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	701	5TL	CAT-CAU-CAN	5.53	128.17	120.44
4	B	701	5TL	CAT-CAU-CAN	5.49	128.11	120.44
4	L	701	5TL	CAT-CAU-CAN	5.30	127.84	120.44
4	D	701	5TL	O4-S-CAU	5.27	113.23	107.35
4	C	701	5TL	O4-S-CAU	5.03	112.97	107.35
4	I	701	5TL	O4-S-CAU	4.78	112.69	107.35
4	E	701	5TL	OAO-CAV-NAW	-4.73	115.86	122.58
4	A	701	5TL	O4-S-CAU	4.73	112.62	107.35
4	H	701	5TL	O4-S-CAU	4.69	112.58	107.35
4	L	701	5TL	O4-S-CAU	4.68	112.58	107.35
4	K	701	5TL	O4-S-CAU	4.64	112.53	107.35
4	F	701	5TL	CAN-CAM-CAL	-4.64	114.45	121.13
4	G	701	5TL	CAI-CAJ-CAL	4.64	127.23	118.58
4	B	701	5TL	O4-S-CAU	4.63	112.52	107.35
4	K	701	5TL	OAO-CAV-NAW	-4.57	116.09	122.58
4	J	701	5TL	O4-S-CAU	4.49	112.36	107.35
4	G	701	5TL	O4-S-CAU	4.46	112.33	107.35
4	H	701	5TL	CAI-CAJ-CAL	4.40	126.78	118.58
4	C	701	5TL	CAI-CAJ-CAL	4.34	126.67	118.58
4	D	701	5TL	CAI-CAJ-CAL	4.32	126.63	118.58
4	E	701	5TL	CAI-CAJ-CAL	4.32	126.63	118.58
4	I	701	5TL	CAI-CAJ-CAL	4.30	126.59	118.58
4	F	701	5TL	CAT-CAU-S	4.30	125.96	119.73
4	K	701	5TL	CAI-CAJ-CAL	4.27	126.55	118.58
4	L	701	5TL	CAI-CAJ-CAL	4.27	126.54	118.58
4	D	701	5TL	CAN-CAM-CAL	-4.27	114.99	121.13
4	I	701	5TL	OAO-CAV-NAW	-4.27	116.52	122.58
4	B	701	5TL	CAI-CAJ-CAL	4.26	126.53	118.58
4	J	701	5TL	CAI-CAJ-CAL	4.23	126.47	118.58
4	J	701	5TL	CAN-CAM-CAL	-4.23	115.05	121.13
4	A	701	5TL	CAI-CAJ-CAL	4.21	126.42	118.58
4	C	701	5TL	OAO-CAV-NAW	-4.20	116.61	122.58
4	F	701	5TL	CAI-CAJ-CAL	4.17	126.34	118.58
4	F	701	5TL	OAO-CAV-NAW	-4.08	116.78	122.58
4	L	701	5TL	CAN-CAM-CAL	-4.07	115.28	121.13
4	H	701	5TL	CAN-CAM-CAL	-4.03	115.33	121.13
4	K	701	5TL	CAN-CAM-CAL	-4.01	115.36	121.13
4	E	701	5TL	CAN-CAM-CAL	-4.00	115.38	121.13
4	E	701	5TL	O4-S-CAU	3.94	111.74	107.35
4	I	701	5TL	CAN-CAM-CAL	-3.93	115.48	121.13
4	B	701	5TL	CAN-CAM-CAL	-3.88	115.54	121.13
4	G	701	5TL	CAN-CAM-CAL	-3.88	115.55	121.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	5TL	OAQ-CAV-NAW	-3.85	117.11	122.58
4	E	701	5TL	CAQ-CAV-NAW	3.85	124.21	118.29
4	A	701	5TL	CAN-CAM-CAL	-3.81	115.64	121.13
4	L	701	5TL	OAQ-CAV-NAW	-3.81	117.16	122.58
4	F	701	5TL	CAU-S-N1	3.81	113.77	108.38
4	C	701	5TL	CAN-CAM-CAL	-3.79	115.67	121.13
4	H	701	5TL	OAQ-CAV-NAW	-3.78	117.21	122.58
4	G	701	5TL	OAQ-CAV-NAW	-3.70	117.32	122.58
4	B	701	5TL	OAQ-CAV-NAW	-3.66	117.38	122.58
4	J	701	5TL	OAQ-CAV-NAW	-3.60	117.46	122.58
4	D	701	5TL	OAQ-CAV-NAW	-3.59	117.48	122.58
4	I	701	5TL	CAQ-CAV-NAW	3.53	123.72	118.29
4	J	701	5TL	CAU-S-N1	3.50	113.33	108.38
4	F	701	5TL	O4-S-CAU	3.43	111.18	107.35
4	C	701	5TL	CAQ-CAV-NAW	3.41	123.53	118.29
4	J	701	5TL	CAQ-CAV-NAW	3.37	123.48	118.29
4	L	701	5TL	CAQ-CAV-NAW	3.37	123.47	118.29
4	K	701	5TL	CAQ-CAV-NAW	3.36	123.46	118.29
4	G	701	5TL	CAQ-CAV-NAW	3.29	123.35	118.29
4	D	701	5TL	CAQ-CAV-NAW	3.29	123.35	118.29
4	L	701	5TL	CAT-CAU-S	3.24	124.43	119.73
4	A	701	5TL	O2-S-CAU	-3.23	103.75	107.35
4	H	701	5TL	CAQ-CAV-NAW	3.23	123.25	118.29
4	F	701	5TL	CAQ-CAV-NAW	3.16	123.15	118.29
4	B	701	5TL	CAQ-CAV-NAW	3.15	123.14	118.29
4	C	701	5TL	CAT-CAU-S	3.07	124.19	119.73
4	E	701	5TL	CAT-CAU-S	3.05	124.16	119.73
4	L	701	5TL	CAU-S-N1	3.03	112.67	108.38
4	I	701	5TL	CAT-CAU-S	3.02	124.11	119.73
4	B	701	5TL	CAT-CAU-S	3.01	124.11	119.73
4	D	701	5TL	CAU-S-N1	3.01	112.64	108.38
4	A	701	5TL	CAT-CAU-S	2.98	124.05	119.73
4	H	701	5TL	CAU-S-N1	2.97	112.59	108.38
4	D	701	5TL	CAT-CAU-S	2.97	124.04	119.73
4	B	701	5TL	CAU-S-N1	2.94	112.54	108.38
4	A	701	5TL	CAU-S-N1	2.89	112.47	108.38
4	A	701	5TL	CAQ-CAV-NAW	2.86	122.69	118.29
4	H	701	5TL	CAT-CAU-S	2.85	123.86	119.73
4	G	701	5TL	CAT-CAU-S	2.83	123.84	119.73
4	G	701	5TL	CAP-CAQ-CAV	-2.79	114.67	121.53
4	F	701	5TL	CAL-CAJ-CAR	-2.72	115.86	121.63
4	G	701	5TL	CAU-S-N1	2.69	112.19	108.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	701	5TL	O4-S-N1	2.69	111.35	107.36
4	J	701	5TL	CAT-CAU-S	2.69	123.63	119.73
4	D	701	5TL	O2-S-CAU	-2.69	104.35	107.35
4	C	701	5TL	CAU-S-N1	2.67	112.16	108.38
4	I	701	5TL	CAU-S-N1	2.66	112.15	108.38
4	C	701	5TL	O2-S-CAU	-2.64	104.40	107.35
4	G	701	5TL	CAI-CAJ-CAR	-2.64	115.45	119.13
4	E	701	5TL	CAU-S-N1	2.62	112.09	108.38
4	J	701	5TL	O2-S-CAU	-2.62	104.43	107.35
4	F	701	5TL	O2-S-CAU	-2.60	104.45	107.35
4	I	701	5TL	O2-S-CAU	-2.57	104.48	107.35
4	K	701	5TL	CAU-S-N1	2.56	112.01	108.38
4	B	701	5TL	O2-S-CAU	-2.55	104.50	107.35
4	K	701	5TL	CAT-CAU-S	2.55	123.43	119.73
4	F	701	5TL	O4-S-N1	2.52	111.10	107.36
4	C	701	5TL	CAP-CAQ-CAV	-2.51	115.34	121.53
4	J	701	5TL	O4-S-N1	2.47	111.03	107.36
4	D	701	5TL	CAP-CAQ-CAV	-2.46	115.47	121.53
4	L	701	5TL	CAP-CAQ-CAV	-2.45	115.50	121.53
4	D	701	5TL	CAL-CAJ-CAR	-2.44	116.46	121.63
4	J	701	5TL	CAP-CAQ-CAV	-2.42	115.58	121.53
4	B	701	5TL	CAP-CAQ-CAV	-2.41	115.60	121.53
4	H	701	5TL	CAP-CAQ-CAV	-2.40	115.61	121.53
4	G	701	5TL	CAJ-CAR-NAY	-2.37	116.05	120.28
4	I	701	5TL	CAL-CAJ-CAR	-2.36	116.63	121.63
4	G	701	5TL	CAQ-CAP-CAH	-2.36	116.52	120.97
4	A	701	5TL	O4-S-N1	2.36	110.86	107.36
4	E	701	5TL	CAP-CAQ-CAV	-2.31	115.83	121.53
4	J	701	5TL	CAL-CAJ-CAR	-2.31	116.74	121.63
4	A	701	5TL	CAP-CAQ-CAV	-2.29	115.89	121.53
4	K	701	5TL	CAQ-CAR-CAJ	2.29	124.88	119.45
4	C	701	5TL	CAJ-CAR-NAY	-2.28	116.21	120.28
4	A	701	5TL	CAJ-CAR-NAY	-2.27	116.22	120.28
4	G	701	5TL	CAQ-CAR-CAJ	2.27	124.83	119.45
4	I	701	5TL	CAP-CAQ-CAV	-2.26	115.96	121.53
4	H	701	5TL	CAL-CAJ-CAR	-2.26	116.84	121.63
4	K	701	5TL	CAP-CAQ-CAV	-2.26	115.97	121.53
4	H	701	5TL	O2-S-CAU	-2.26	104.83	107.35
4	B	701	5TL	CAL-CAJ-CAR	-2.23	116.90	121.63
4	C	701	5TL	CAL-CAJ-CAR	-2.21	116.94	121.63
4	L	701	5TL	CAL-CAJ-CAR	-2.21	116.94	121.63
4	E	701	5TL	CAL-CAJ-CAR	-2.21	116.95	121.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	701	5TL	CAJ-CAR-NAY	-2.19	116.37	120.28
4	L	701	5TL	CAJ-CAR-NAY	-2.19	116.37	120.28
4	K	701	5TL	CAL-CAJ-CAR	-2.18	117.01	121.63
4	L	701	5TL	O2-S-CAU	-2.17	104.92	107.35
4	A	701	5TL	CAQ-CAP-CAH	-2.17	116.87	120.97
4	E	701	5TL	CAJ-CAR-NAY	-2.17	116.40	120.28
4	I	701	5TL	O4-S-N1	2.15	110.55	107.36
4	A	701	5TL	CAQ-CAR-CAJ	2.15	124.54	119.45
4	A	701	5TL	CAI-CAJ-CAR	-2.14	116.14	119.13
4	C	701	5TL	CAI-CAJ-CAR	-2.14	116.15	119.13
4	E	701	5TL	CAQ-CAR-CAJ	2.14	124.52	119.45
4	G	701	5TL	CAL-CAJ-CAR	-2.14	117.10	121.63
4	H	701	5TL	CAQ-CAR-CAJ	2.13	124.50	119.45
4	H	701	5TL	CAJ-CAR-NAY	-2.13	116.48	120.28
4	G	701	5TL	O2-S-CAU	-2.12	104.99	107.35
4	A	701	5TL	CAL-CAJ-CAR	-2.11	117.15	121.63
4	H	701	5TL	CAI-CAJ-CAR	-2.11	116.19	119.13
4	B	701	5TL	CAQ-CAP-CAH	-2.10	117.01	120.97
4	C	701	5TL	CAQ-CAR-CAJ	2.06	124.35	119.45
4	G	701	5TL	O4-S-N1	2.06	110.42	107.36
4	K	701	5TL	CAI-CAJ-CAR	-2.06	116.27	119.13
4	B	701	5TL	CAJ-CAR-NAY	-2.05	116.62	120.28
4	I	701	5TL	CAJ-CAR-NAY	-2.04	116.63	120.28
4	G	701	5TL	CAF-CAG-CAH	-2.03	117.83	121.36
4	C	701	5TL	O4-S-N1	2.03	110.38	107.36
4	L	701	5TL	CAQ-CAP-CAH	-2.03	117.14	120.97
4	B	701	5TL	CAF-CAG-CAD	2.02	121.62	117.59
4	E	701	5TL	CAI-CAJ-CAR	-2.02	116.32	119.13
4	I	701	5TL	CAQ-CAR-CAJ	2.02	124.23	119.45

There are no chirality outliers.

All (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
4	F	701	5TL	CAR-CAJ-CAL-CAS
4	E	701	5TL	CAR-CAJ-CAL-CAM
4	E	701	5TL	CAR-CAJ-CAL-CAS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	701	5TL	CAR-CAJ-CAL-CAM
4	G	701	5TL	CAR-CAJ-CAL-CAS
4	H	701	5TL	CAR-CAJ-CAL-CAM
4	H	701	5TL	CAR-CAJ-CAL-CAS
4	J	701	5TL	CAR-CAJ-CAL-CAM
4	J	701	5TL	CAR-CAJ-CAL-CAS
4	I	701	5TL	CAR-CAJ-CAL-CAM
4	I	701	5TL	CAR-CAJ-CAL-CAS
4	L	701	5TL	CAR-CAJ-CAL-CAM
4	L	701	5TL	CAR-CAJ-CAL-CAS
4	K	701	5TL	CAR-CAJ-CAL-CAM
4	K	701	5TL	CAR-CAJ-CAL-CAS
4	B	701	5TL	CAR-CAJ-CAL-CAM
4	A	701	5TL	CAR-CAJ-CAL-CAM
4	A	701	5TL	CAR-CAJ-CAL-CAS
4	B	701	5TL	CAR-CAJ-CAL-CAS
4	E	701	5TL	CAI-CAJ-CAL-CAM
4	H	701	5TL	CAI-CAJ-CAL-CAM
4	J	701	5TL	CAI-CAJ-CAL-CAM
4	L	701	5TL	CAI-CAJ-CAL-CAM
4	D	701	5TL	CAI-CAJ-CAL-CAM
4	F	701	5TL	CAI-CAJ-CAL-CAM
4	G	701	5TL	CAI-CAJ-CAL-CAM
4	I	701	5TL	CAI-CAJ-CAL-CAM
4	K	701	5TL	CAI-CAJ-CAL-CAM
4	C	701	5TL	CAI-CAJ-CAL-CAM
4	B	701	5TL	CAI-CAJ-CAL-CAM
4	A	701	5TL	CAI-CAJ-CAL-CAM
4	B	701	5TL	CAI-CAJ-CAL-CAS
4	D	701	5TL	CAI-CAJ-CAL-CAS
4	C	701	5TL	CAI-CAJ-CAL-CAS
4	F	701	5TL	CAI-CAJ-CAL-CAS
4	E	701	5TL	CAI-CAJ-CAL-CAS
4	G	701	5TL	CAI-CAJ-CAL-CAS
4	H	701	5TL	CAI-CAJ-CAL-CAS
4	J	701	5TL	CAI-CAJ-CAL-CAS
4	I	701	5TL	CAI-CAJ-CAL-CAS
4	L	701	5TL	CAI-CAJ-CAL-CAS
4	K	701	5TL	CAI-CAJ-CAL-CAS
4	A	701	5TL	CAI-CAJ-CAL-CAS
4	C	701	5TL	CAT-CAU-S-O2
4	C	701	5TL	CAT-CAU-S-N1

Continued on next page...

Continued from previous page...

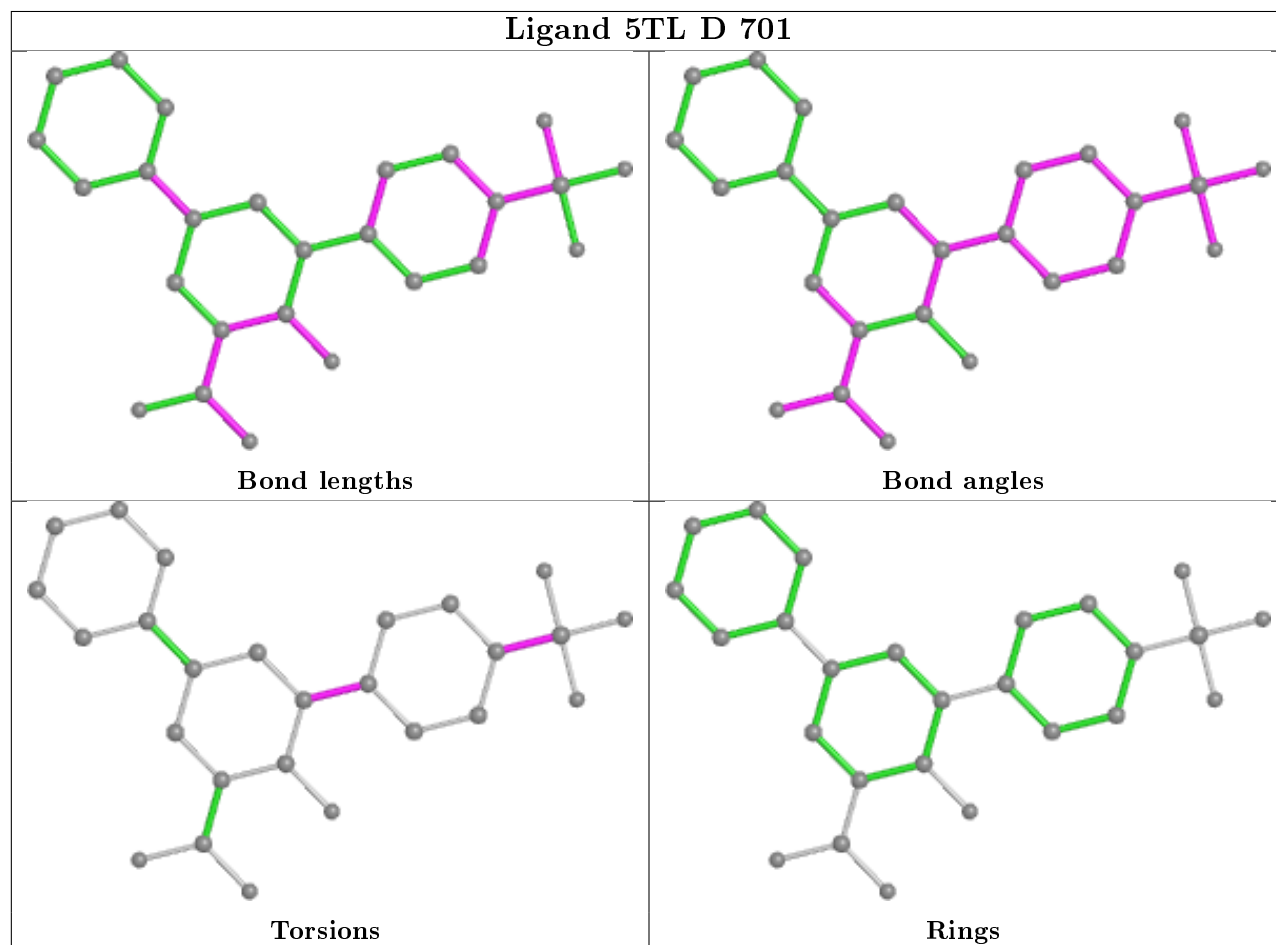
Mol	Chain	Res	Type	Atoms
4	J	701	5TL	CAN-CAU-S-O2
4	D	701	5TL	CAN-CAU-S-N1
4	I	701	5TL	CAT-CAU-S-O2
4	C	701	5TL	CAN-CAU-S-O2
4	E	701	5TL	CAN-CAU-S-N1
4	J	701	5TL	CAN-CAU-S-N1
4	J	701	5TL	CAT-CAU-S-N1
4	K	701	5TL	CAT-CAU-S-O2
4	D	701	5TL	CAT-CAU-S-N1
4	E	701	5TL	CAT-CAU-S-N1
4	J	701	5TL	CAT-CAU-S-O2
4	A	701	5TL	CAT-CAU-S-O2
4	F	701	5TL	CAT-CAU-S-O2
4	I	701	5TL	CAT-CAU-S-N1
4	I	701	5TL	CAN-CAU-S-O2
4	K	701	5TL	CAN-CAU-S-O2
4	K	701	5TL	CAT-CAU-S-N1
4	C	701	5TL	CAN-CAU-S-N1
4	F	701	5TL	CAN-CAU-S-O2
4	F	701	5TL	CAT-CAU-S-N1
4	E	701	5TL	CAT-CAU-S-O4
4	A	701	5TL	CAT-CAU-S-N1
4	A	701	5TL	CAN-CAU-S-O2
4	E	701	5TL	CAN-CAU-S-O4
4	I	701	5TL	CAN-CAU-S-N1
4	K	701	5TL	CAN-CAU-S-N1
4	B	701	5TL	CAT-CAU-S-O2
4	H	701	5TL	CAN-CAU-S-O2
4	H	701	5TL	CAT-CAU-S-O2
4	B	701	5TL	CAN-CAU-S-O2
4	F	701	5TL	CAN-CAU-S-N1
4	L	701	5TL	CAN-CAU-S-O4
4	A	701	5TL	CAN-CAU-S-N1
4	G	701	5TL	CAN-CAU-S-O4

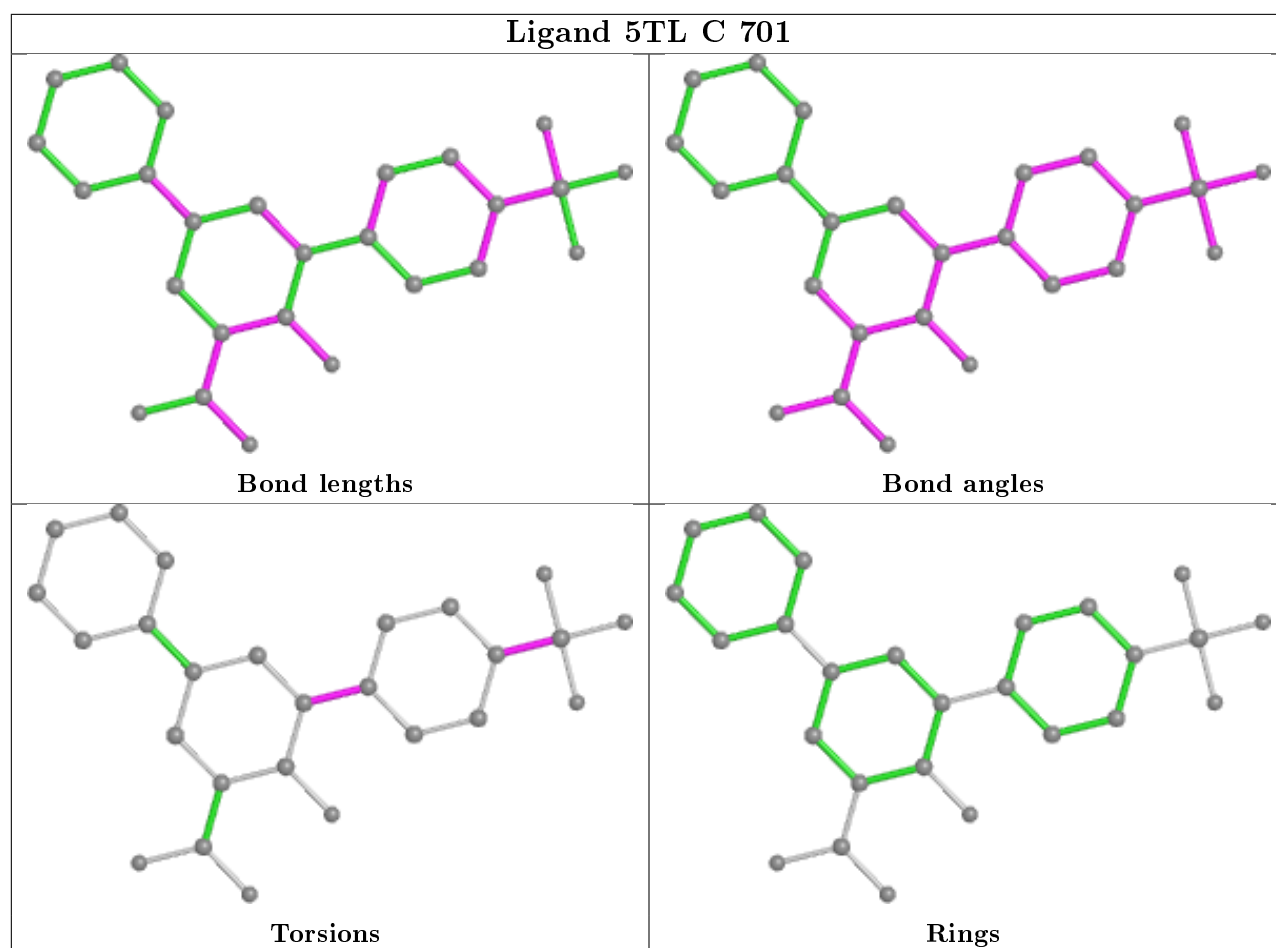
There are no ring outliers.

No monomer is involved in short contacts.

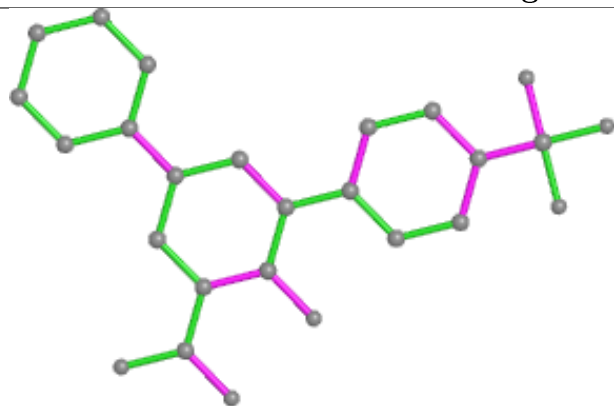
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

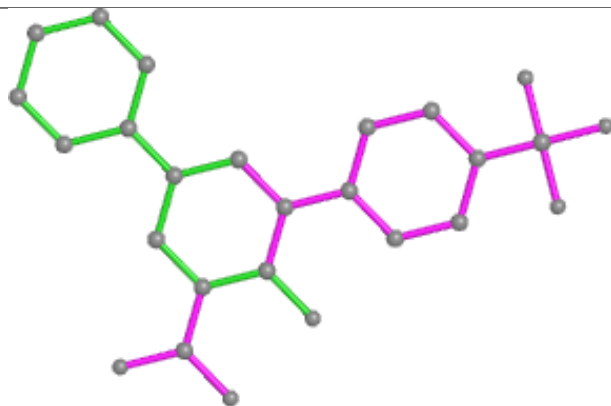




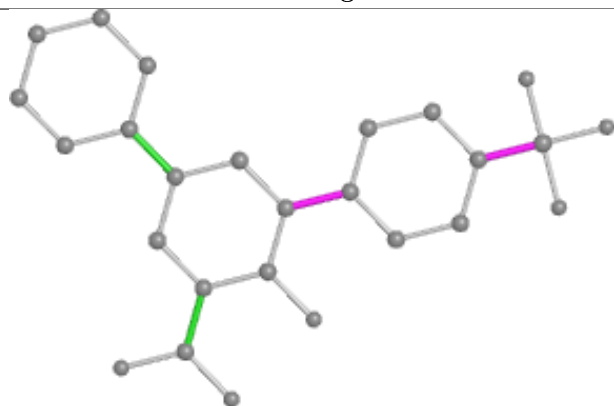
Ligand 5TL F 701



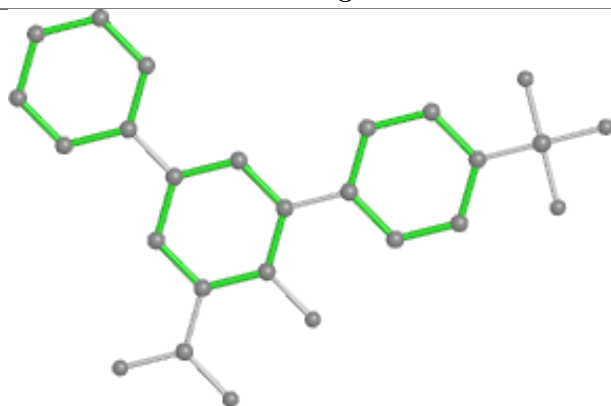
Bond lengths



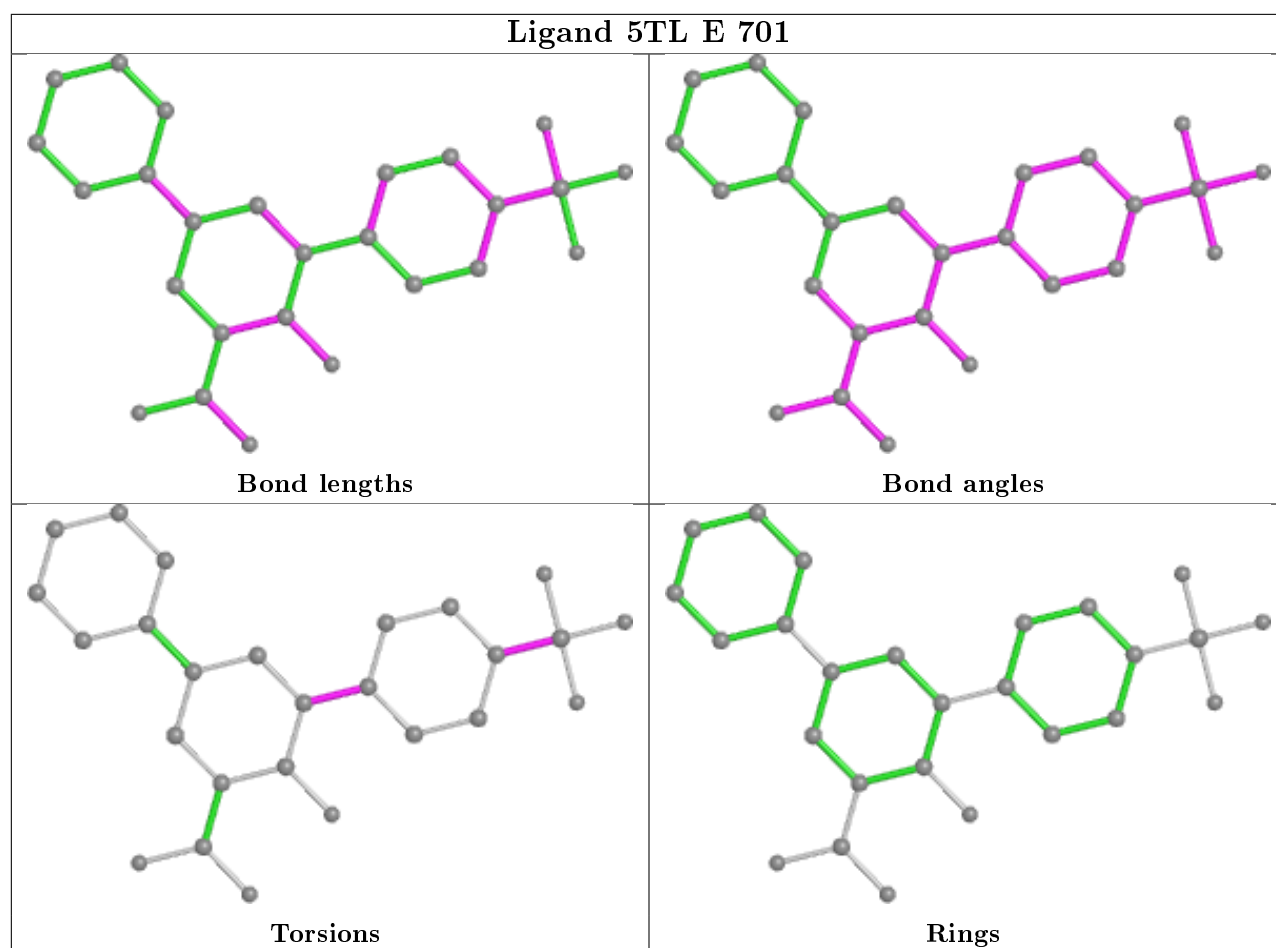
Bond angles

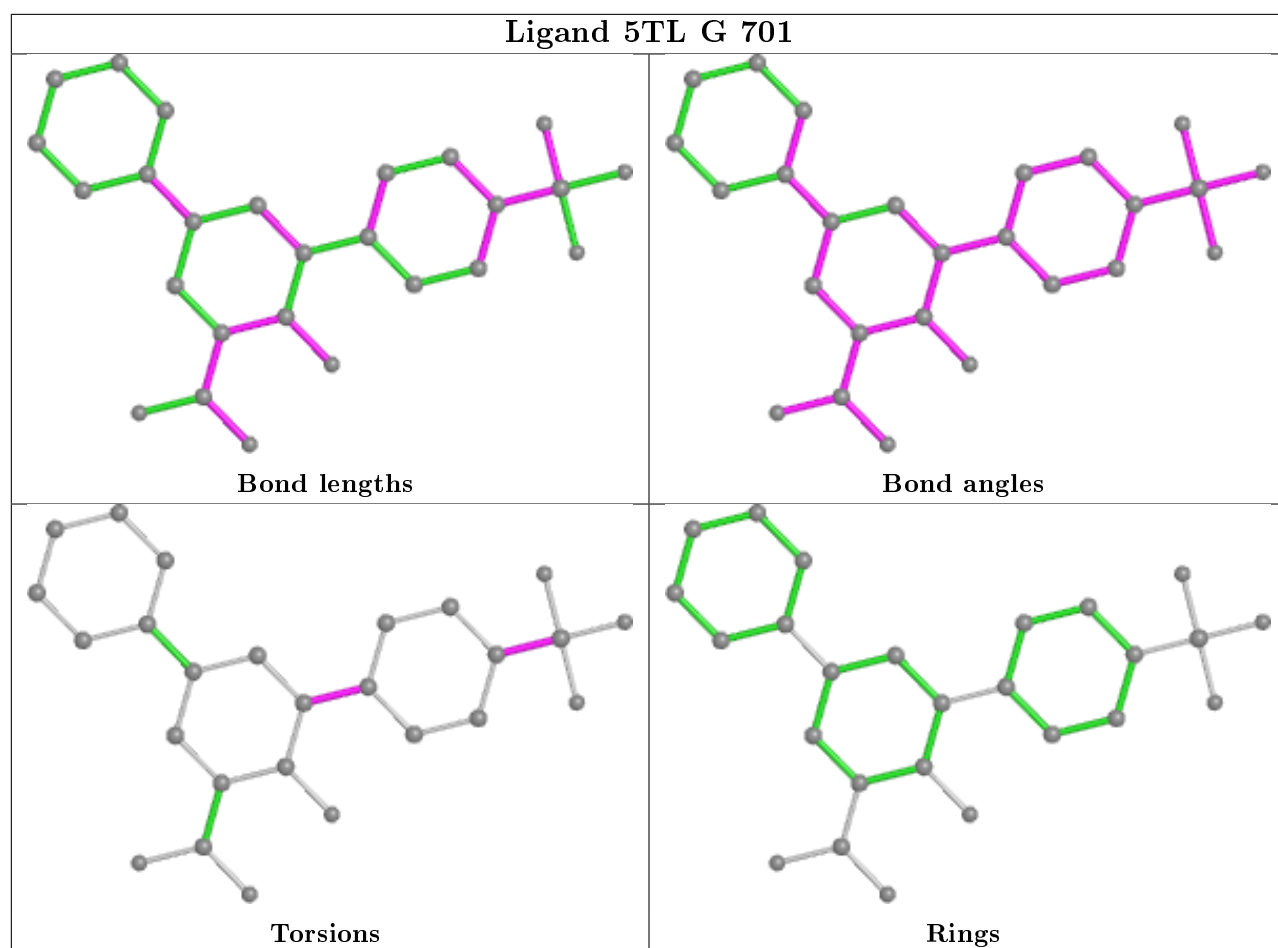


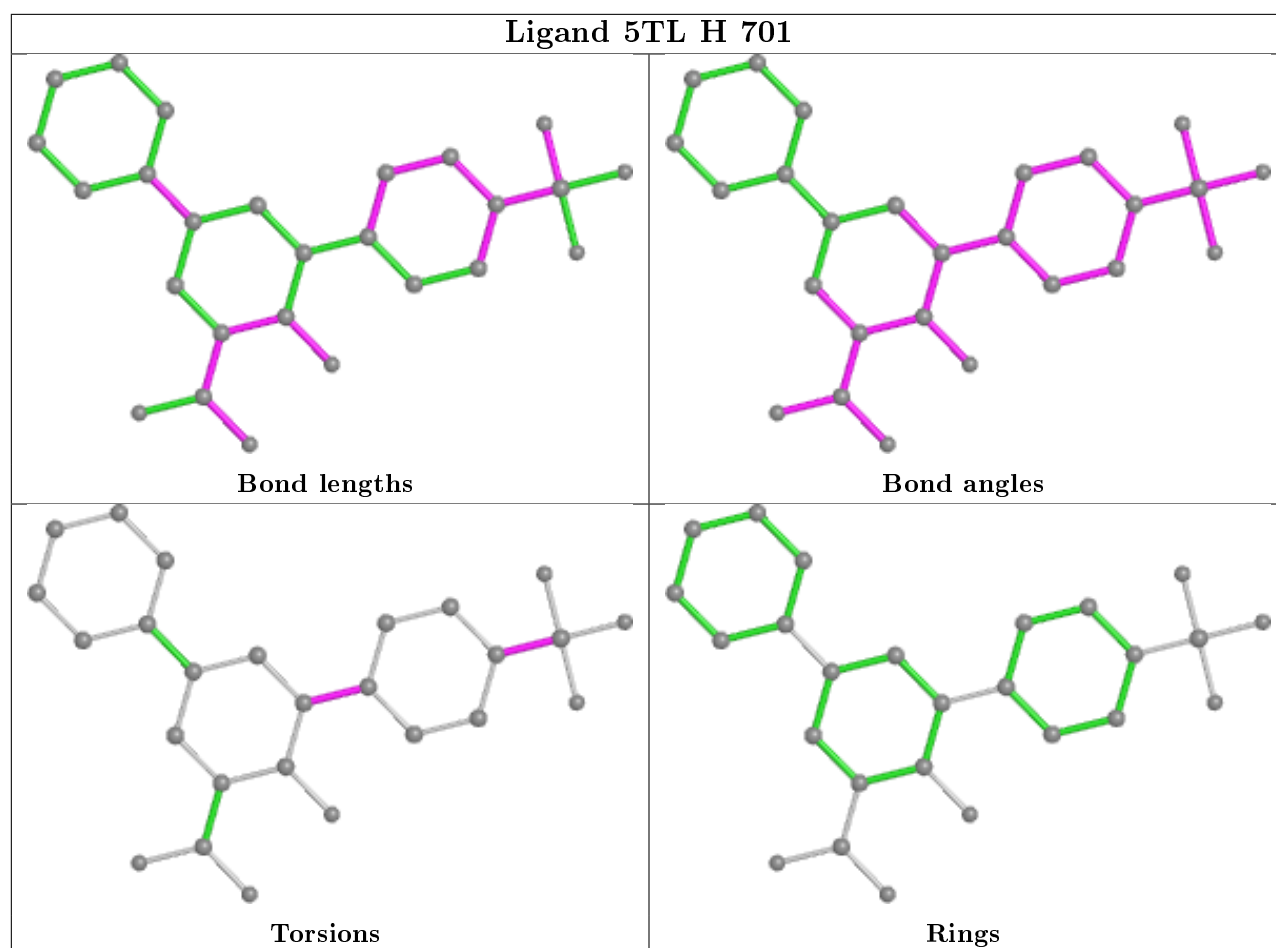
Torsions

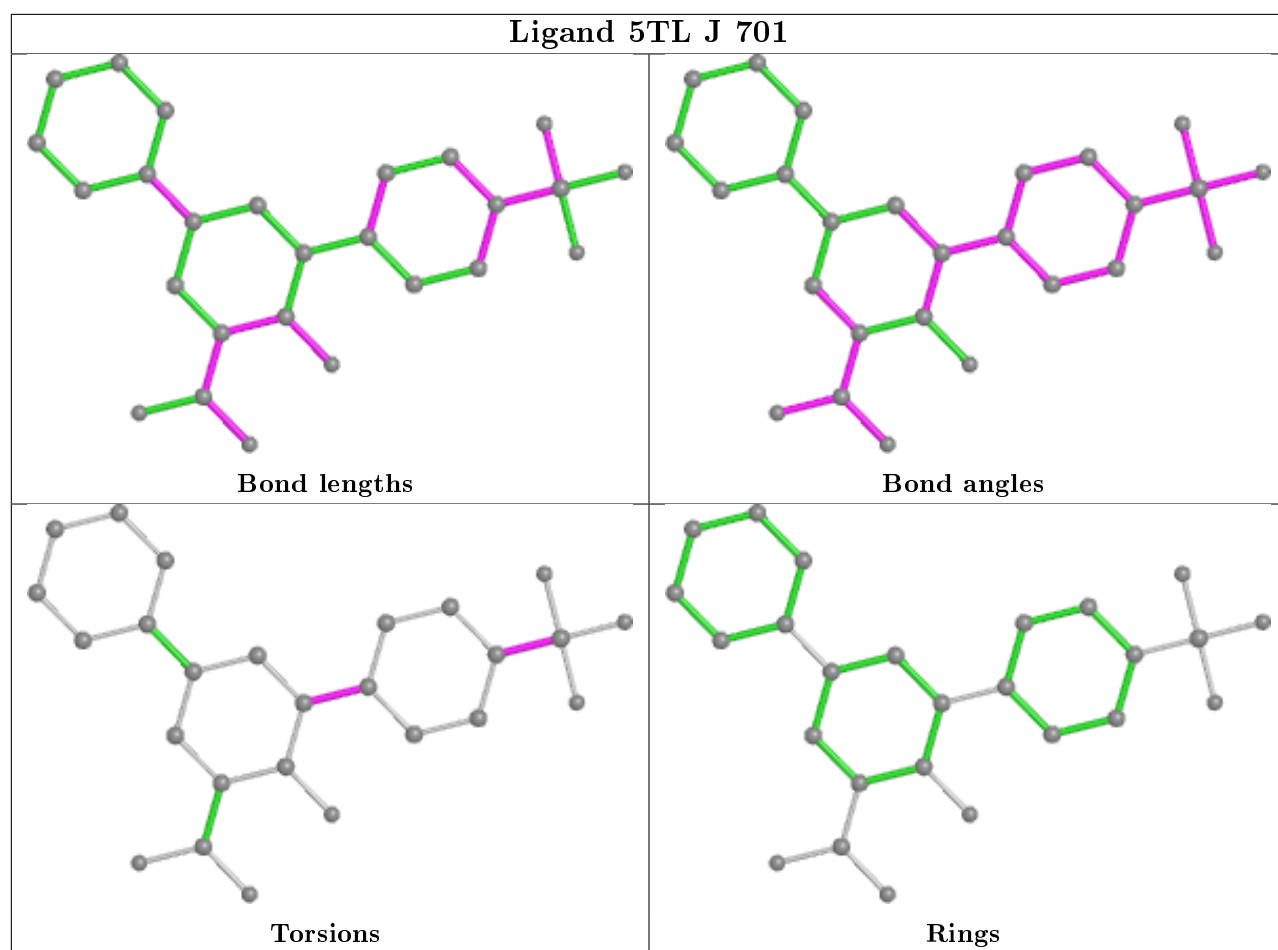


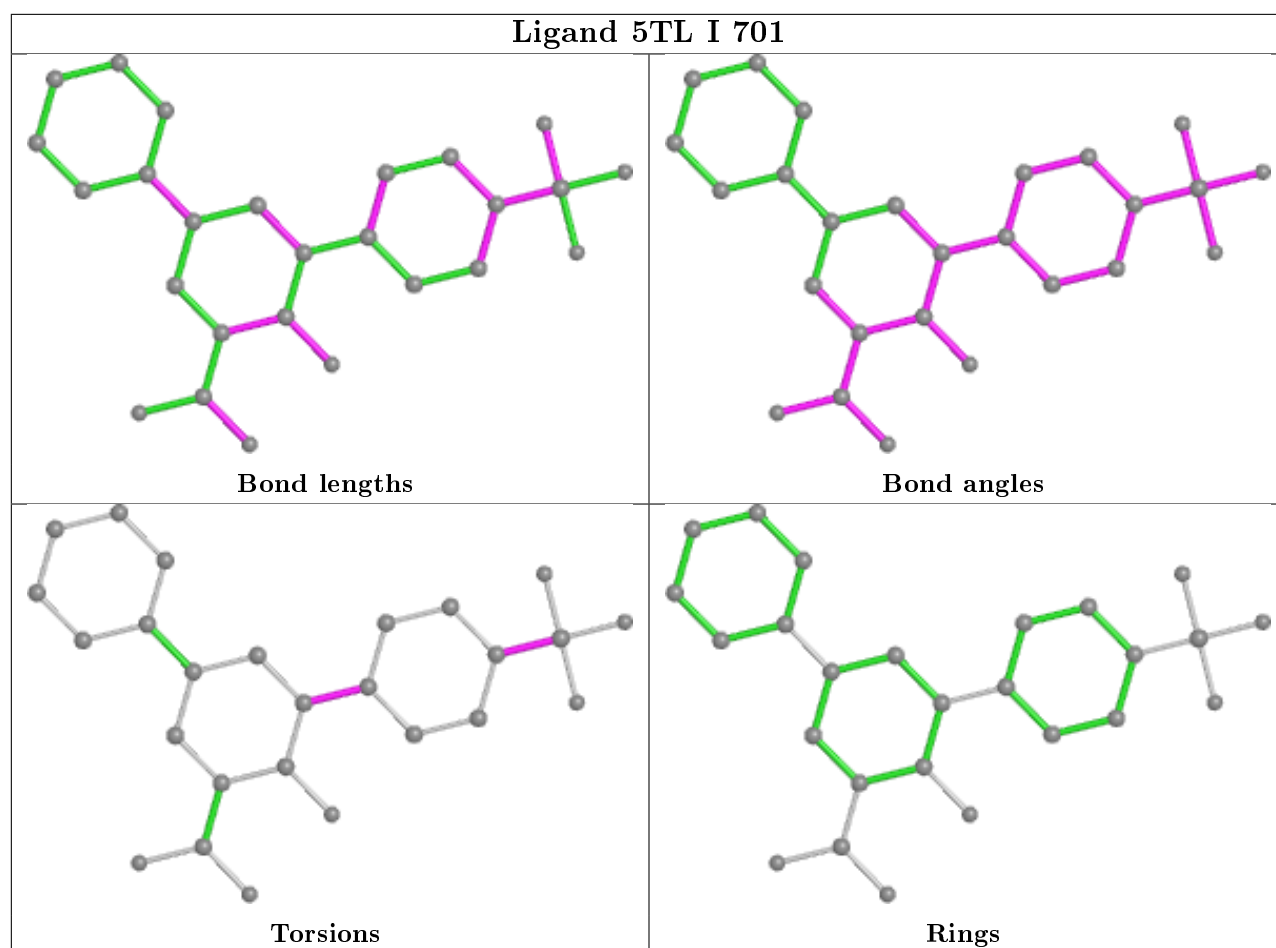
Rings

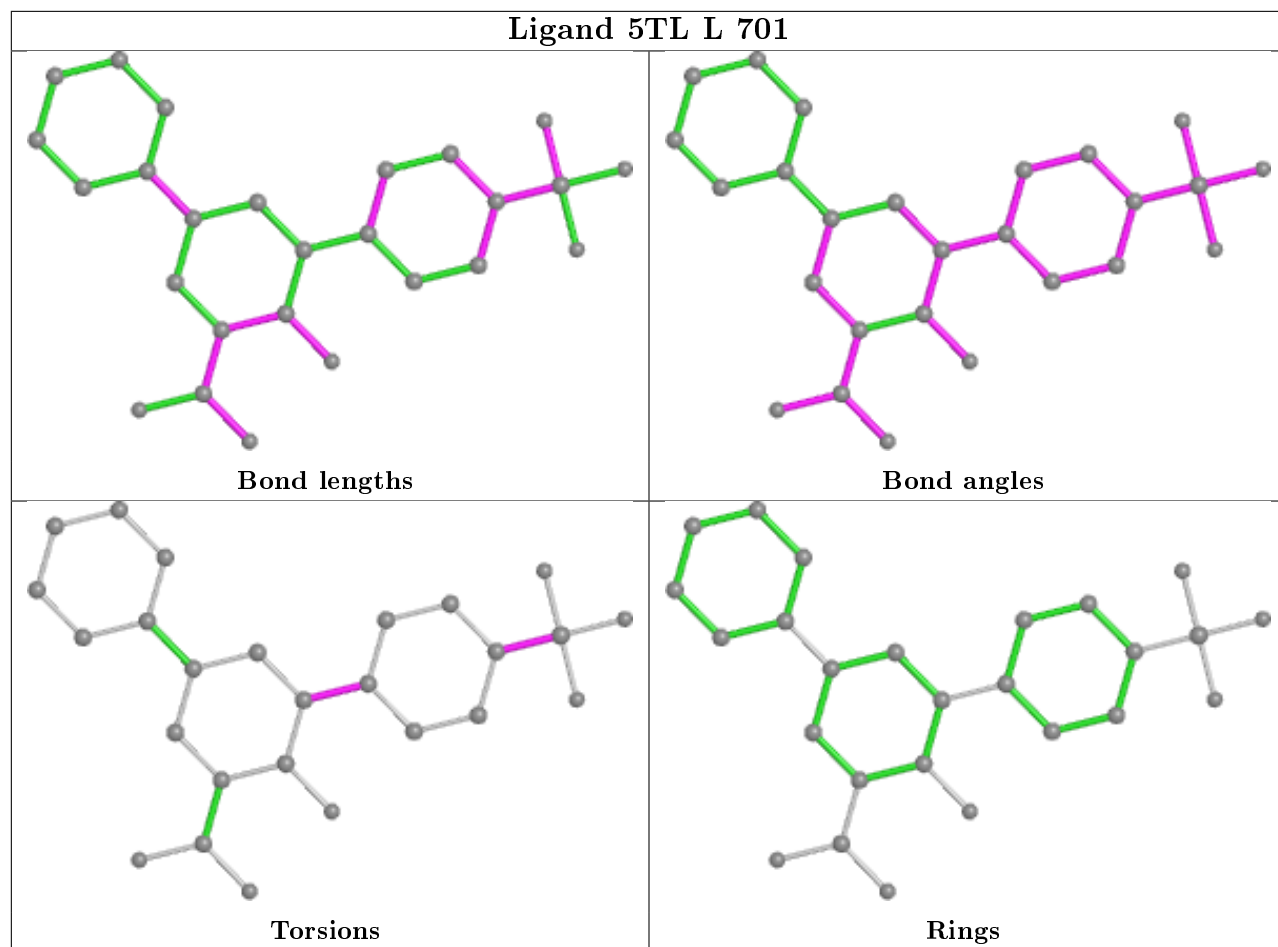




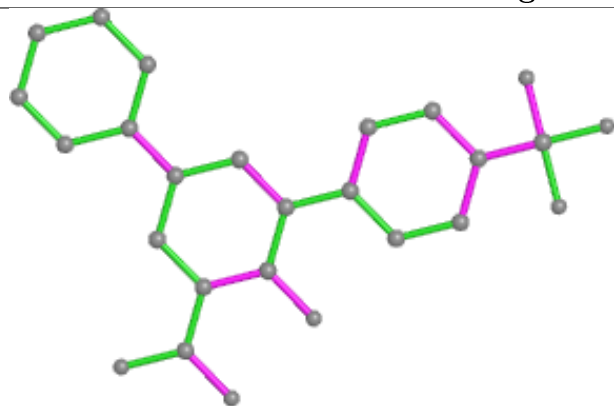




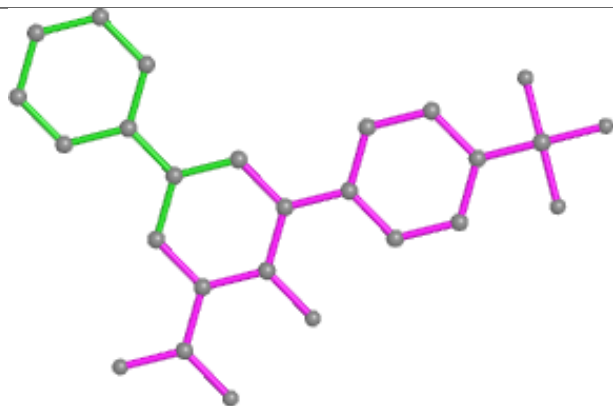




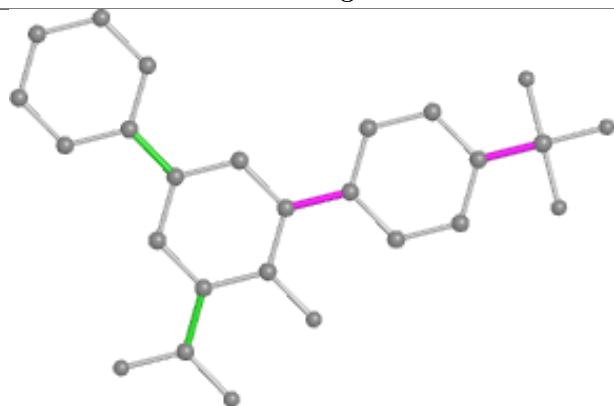
Ligand 5TL K 701



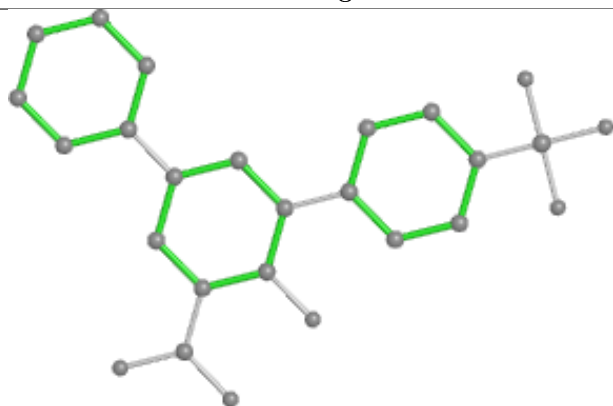
Bond lengths



Bond angles

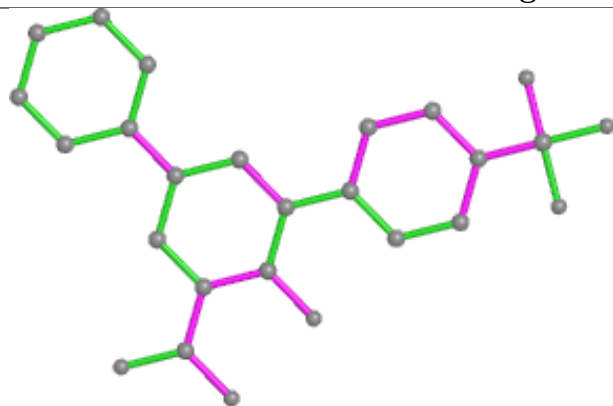


Torsions

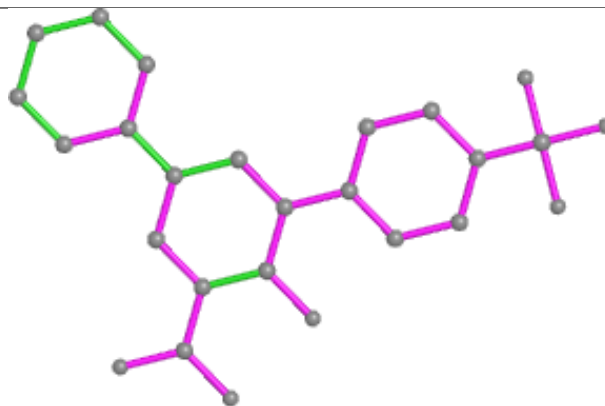


Rings

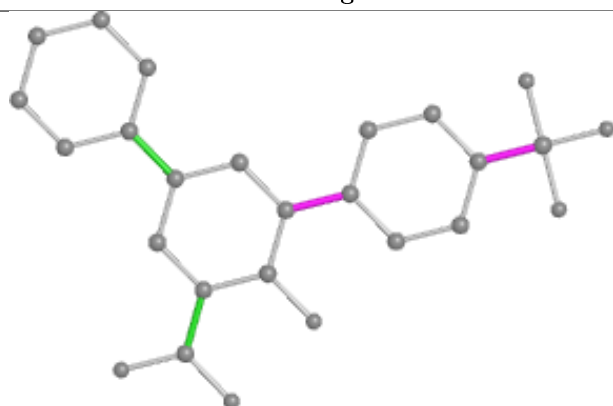
Ligand 5TL B 701



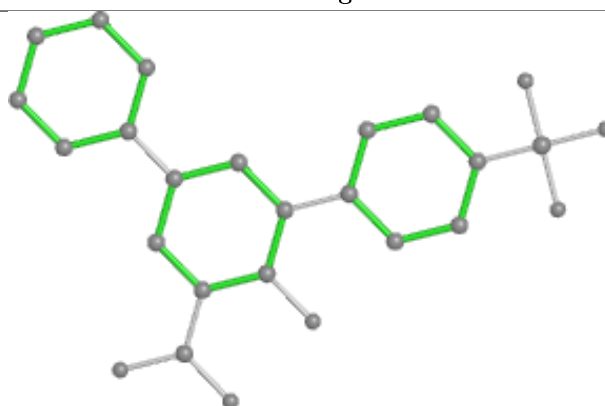
Bond lengths



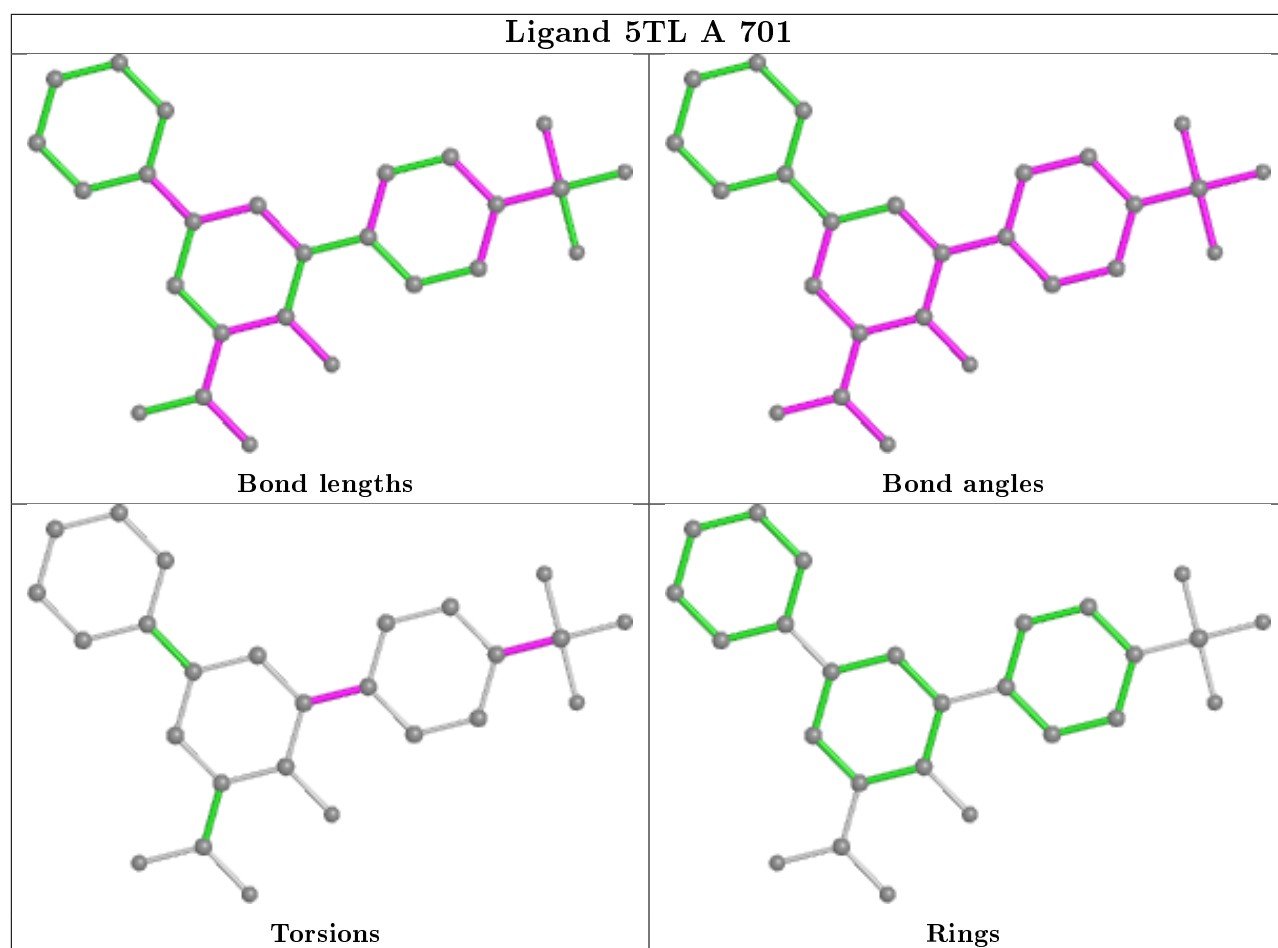
Bond angles



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.

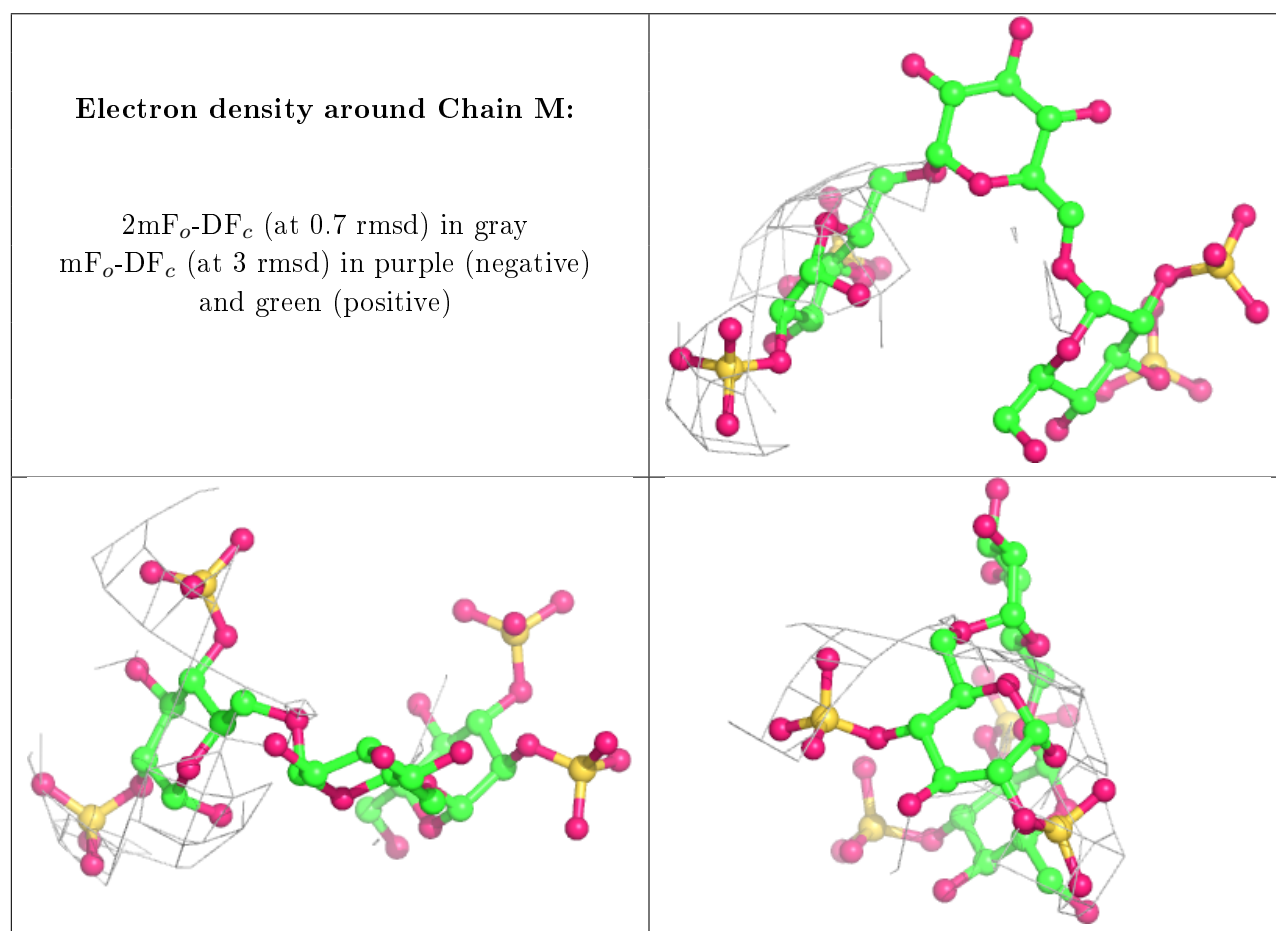
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

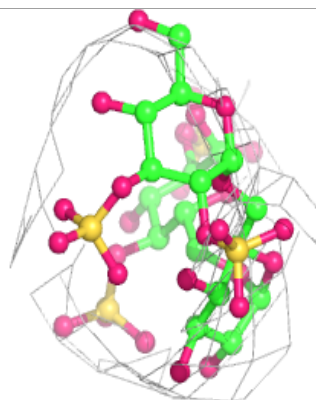
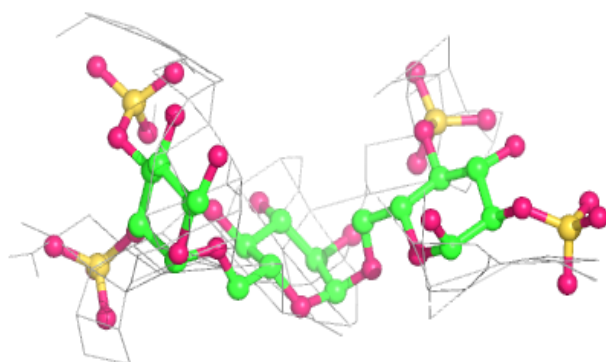
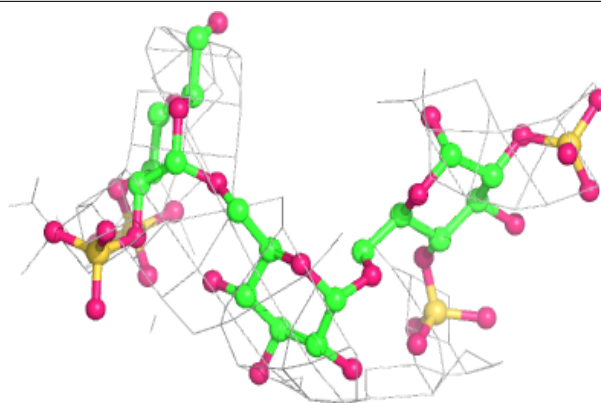
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

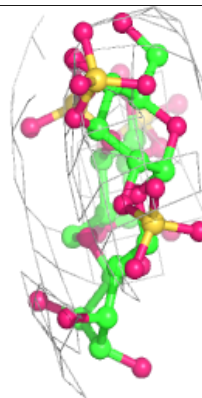
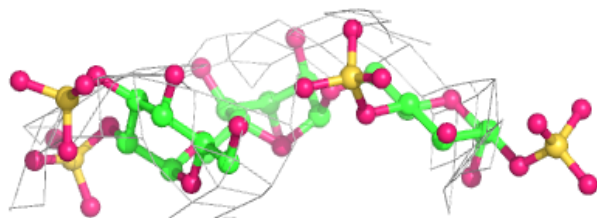
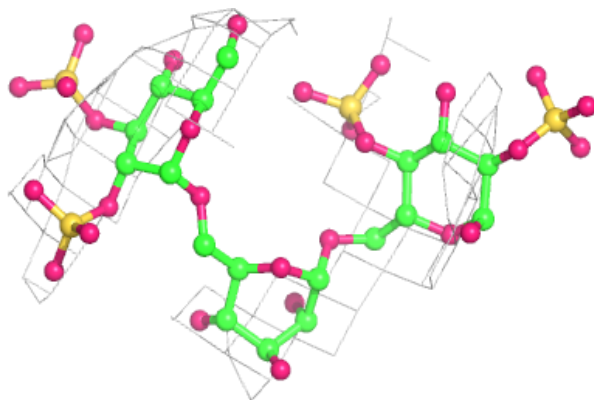


Electron density around Chain N:

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

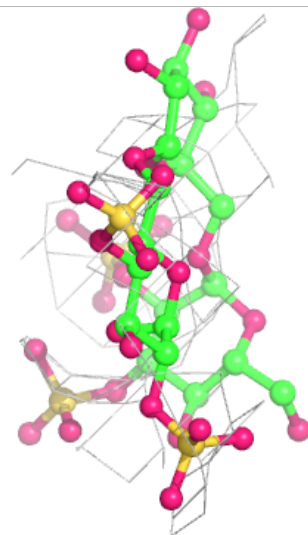
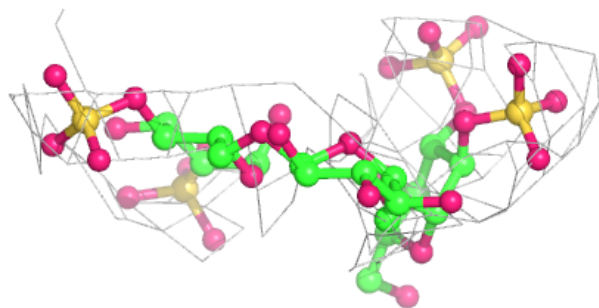
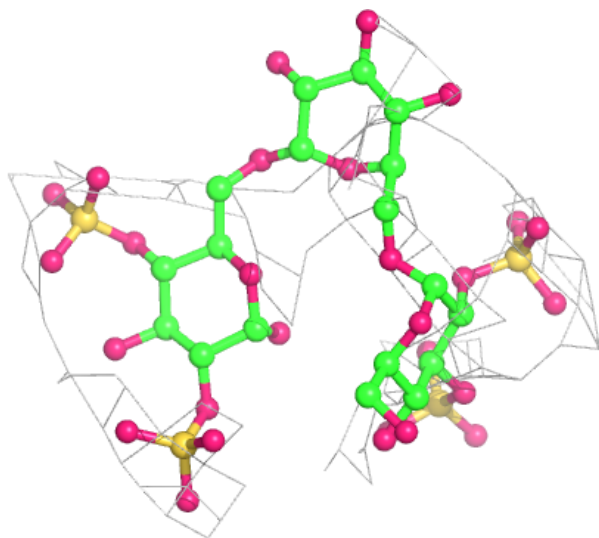
**Electron density around Chain P:**

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



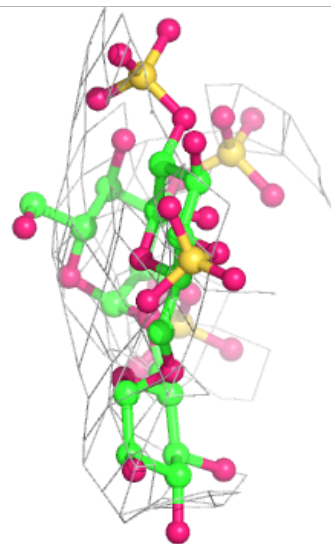
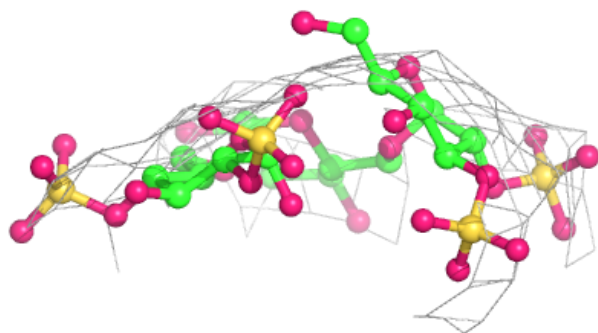
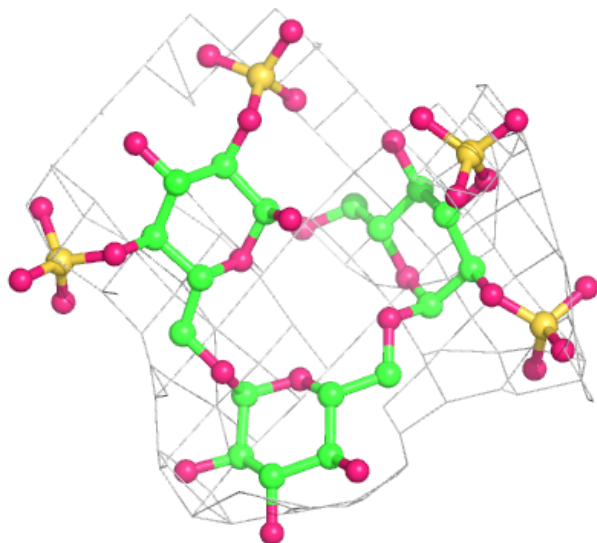
Electron density around Chain Q:

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



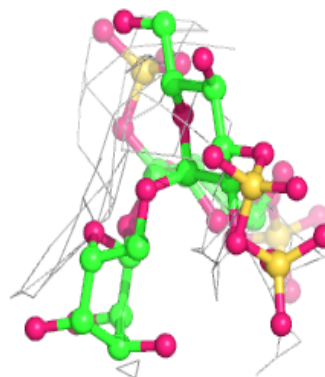
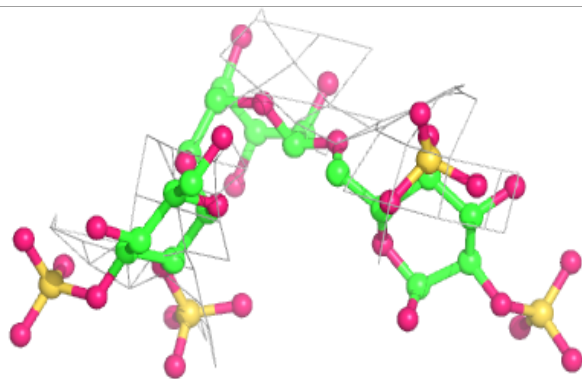
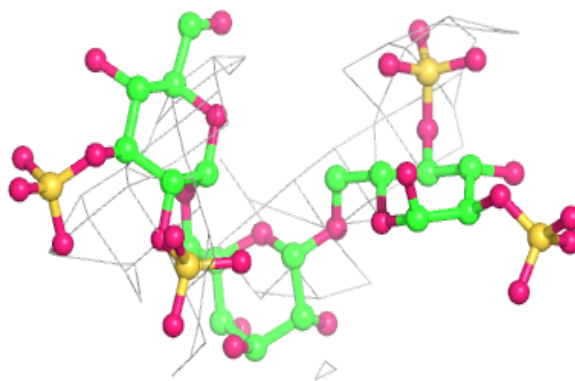
Electron density around Chain R:

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



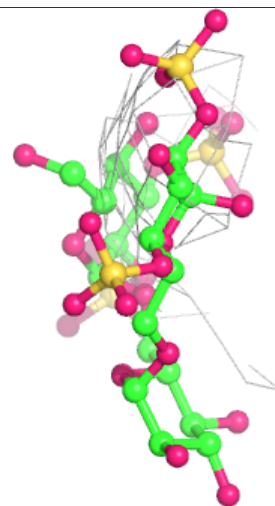
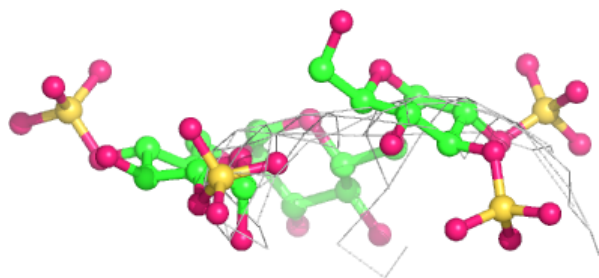
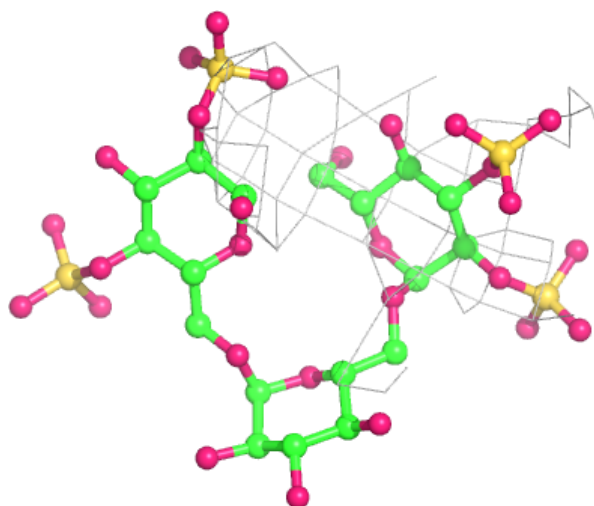
Electron density around Chain S:

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



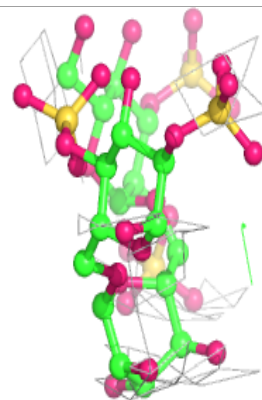
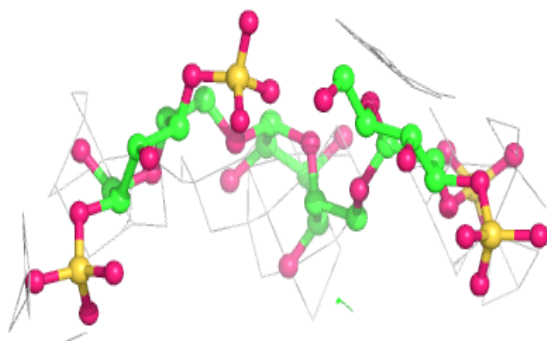
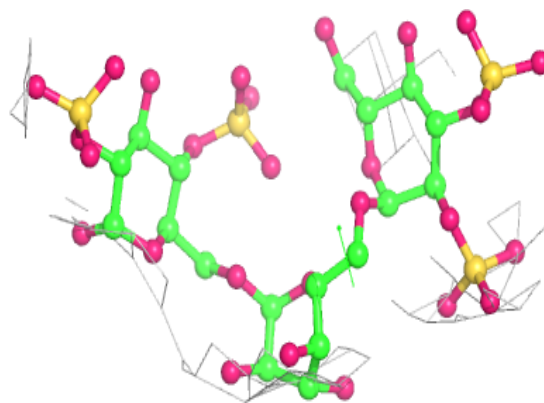
Electron density around Chain U:

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



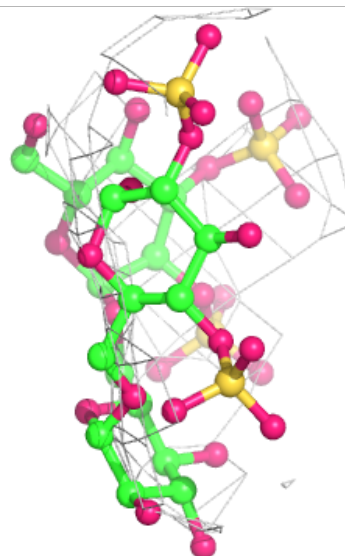
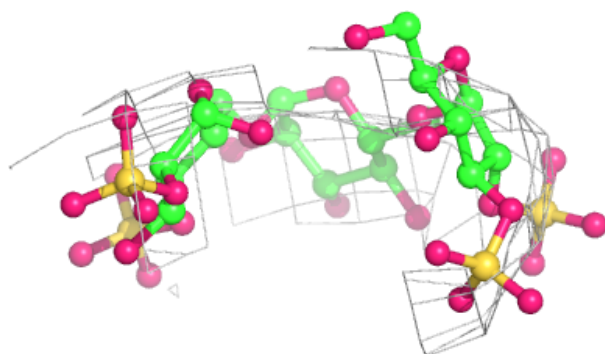
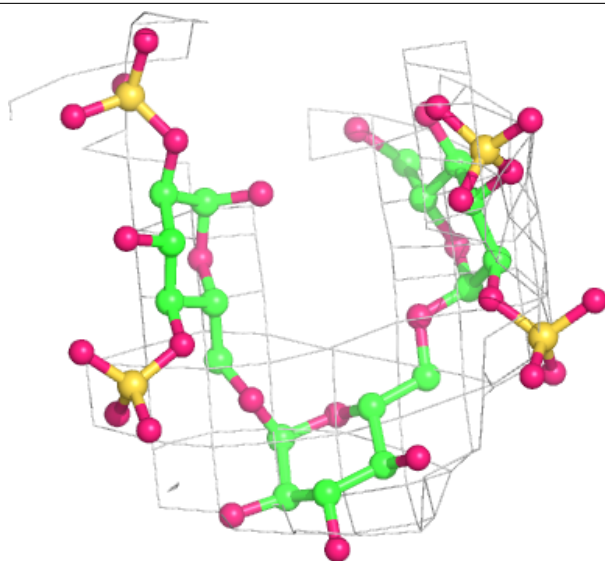
Electron density around Chain V:

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



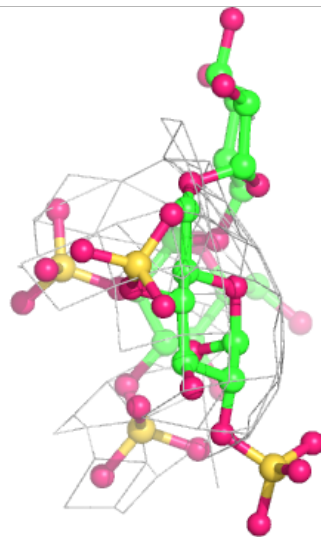
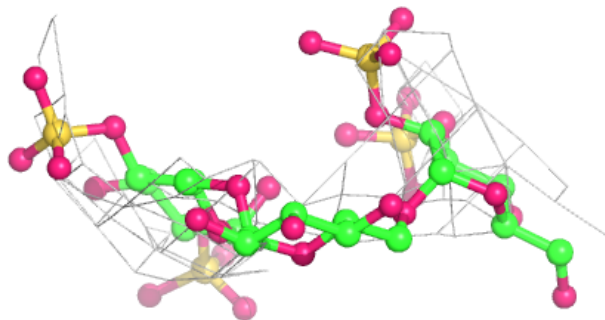
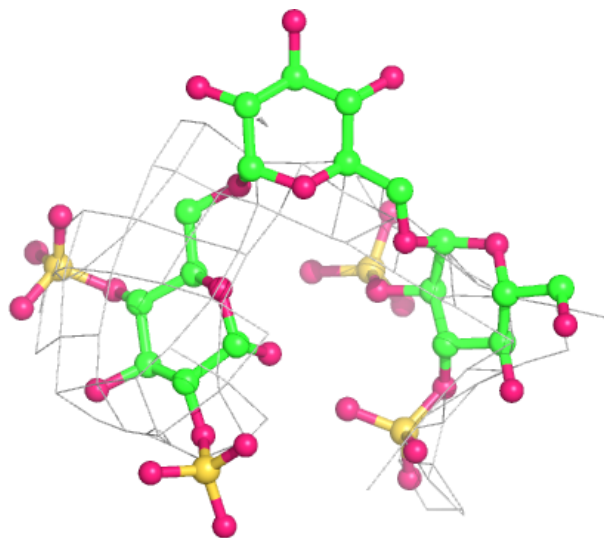
Electron density around Chain W:

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



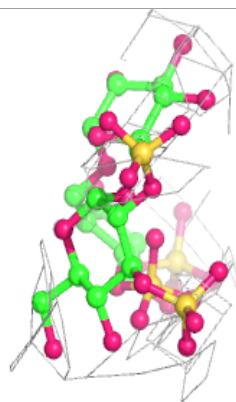
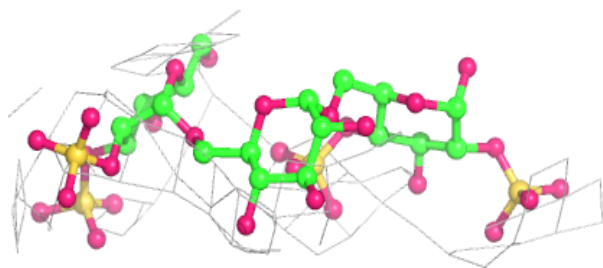
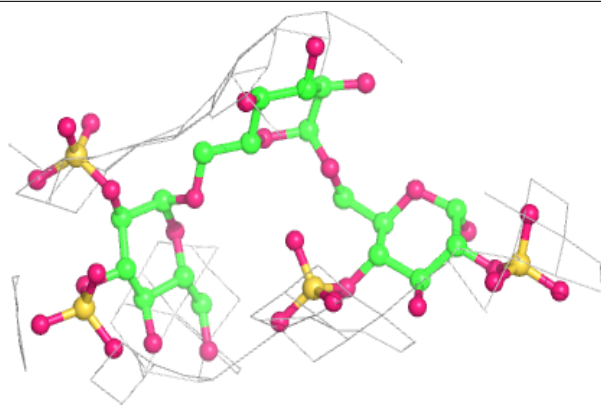
Electron density around Chain X:

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

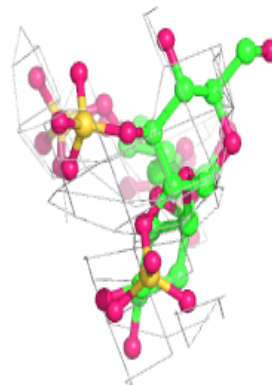
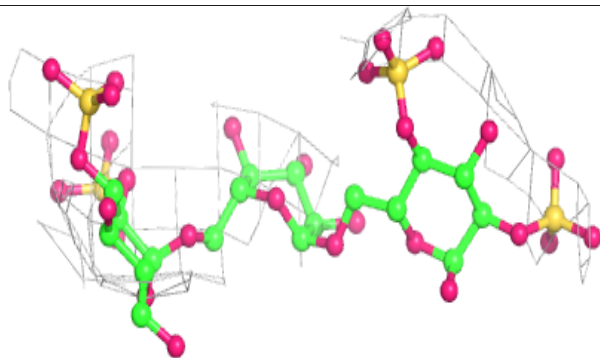
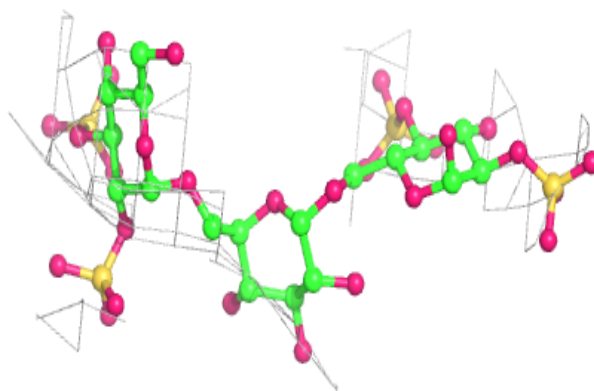


Electron density around Chain Y:

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

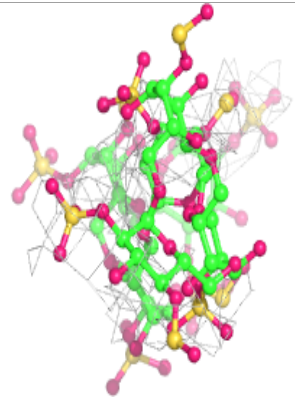
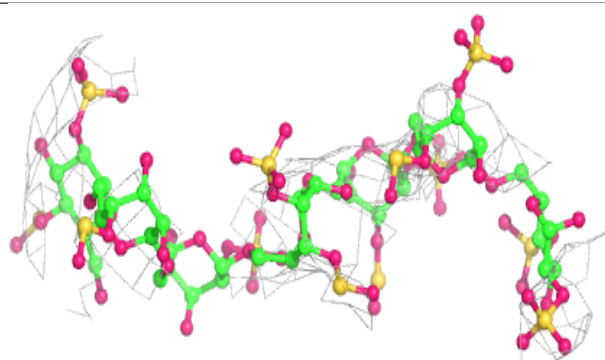
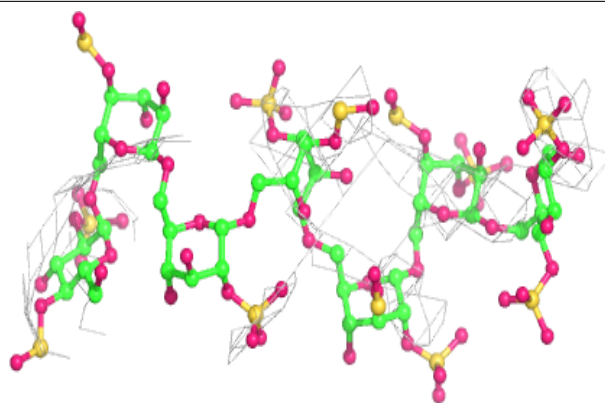
**Electron density around Chain Z:**

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

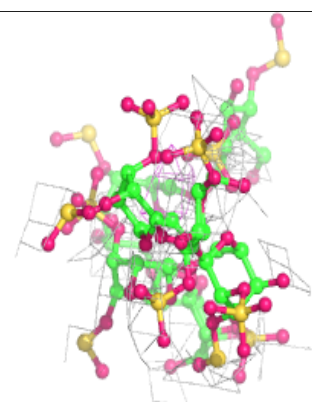
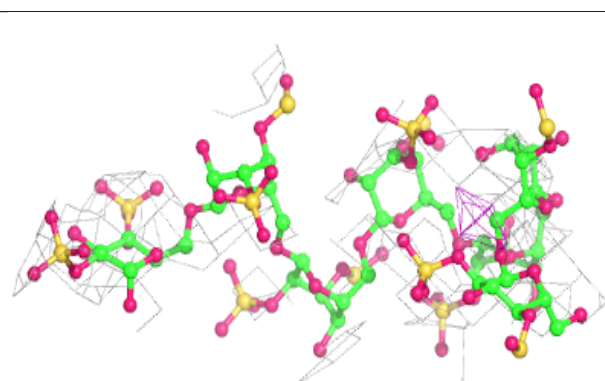
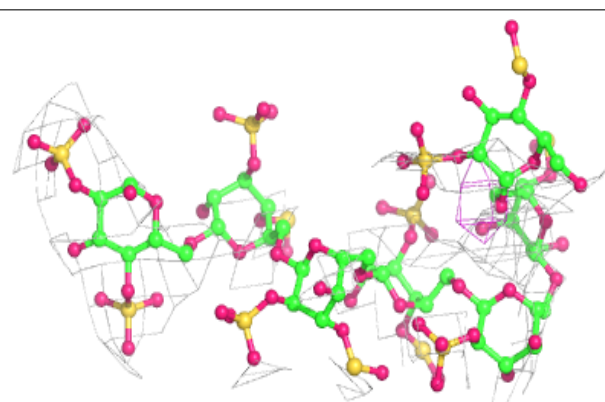


Electron density around Chain O:

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

**Electron density around Chain T:**

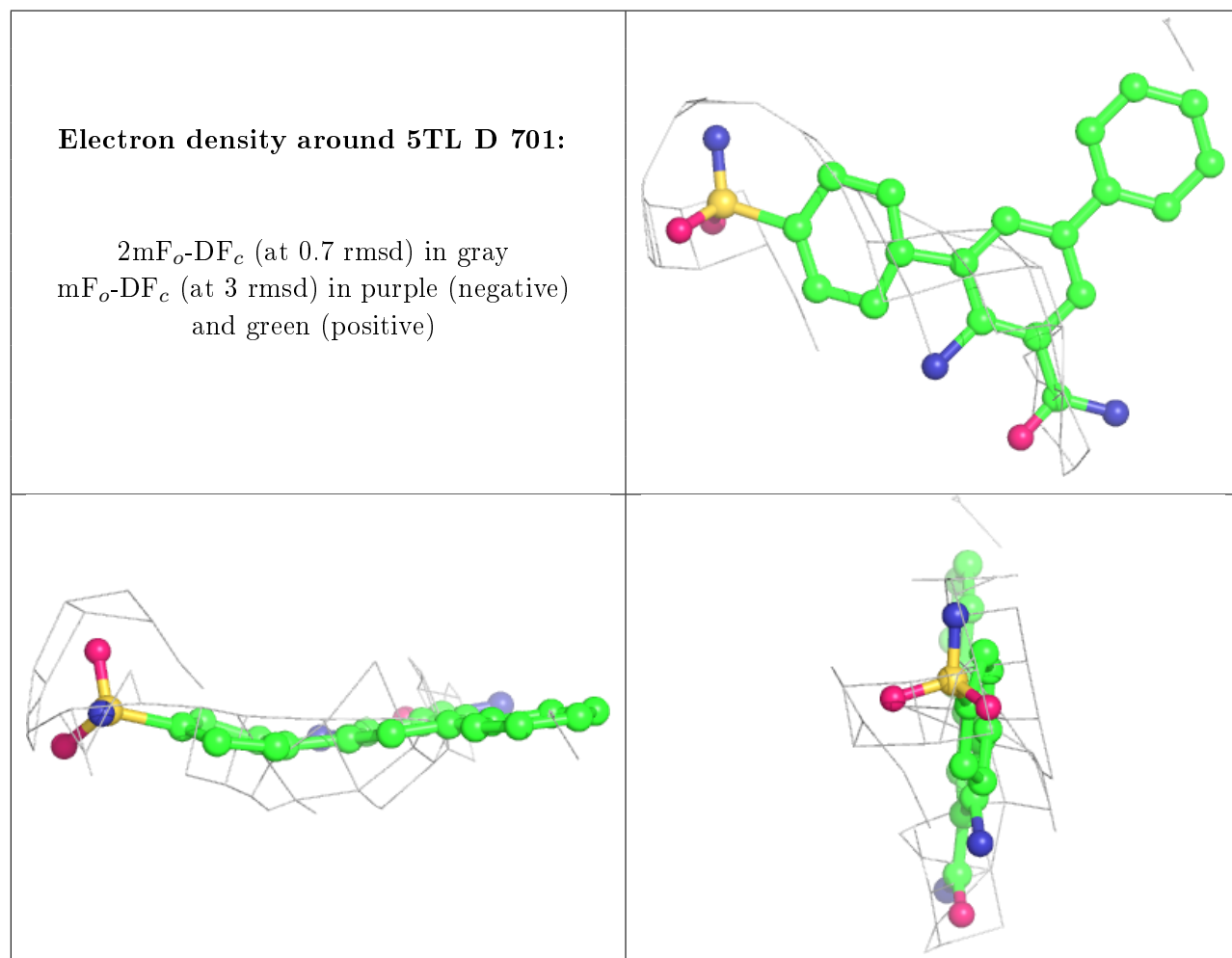
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands ⓘ

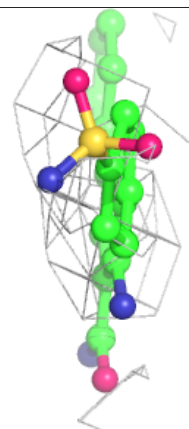
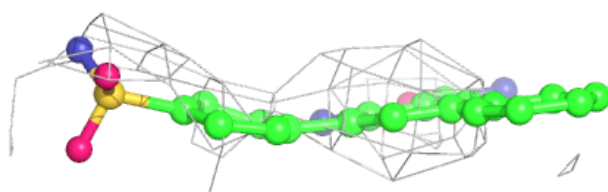
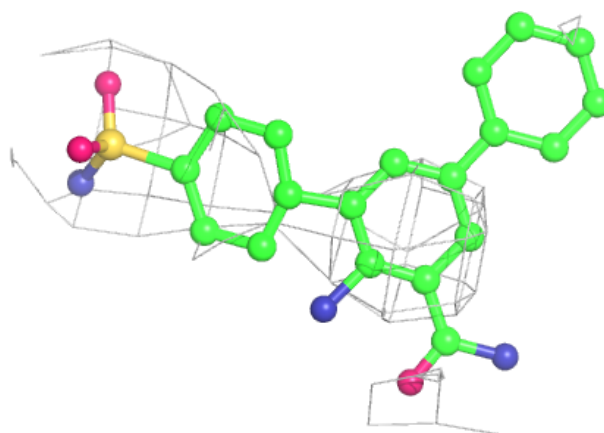
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

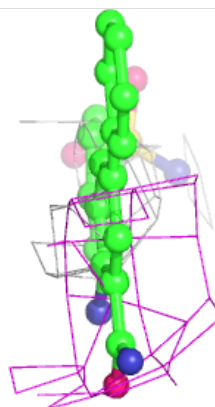
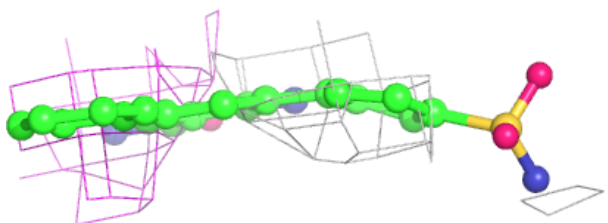
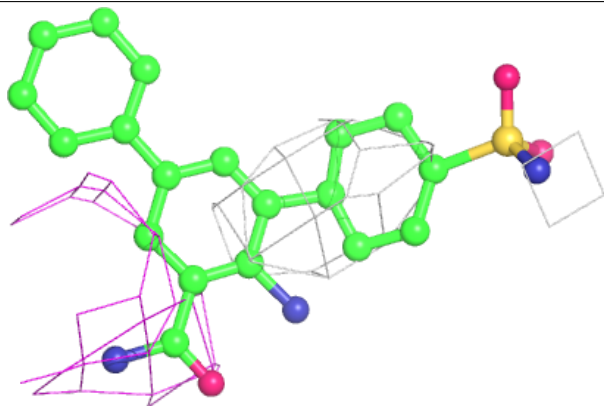


Electron density around 5TL C 701:

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

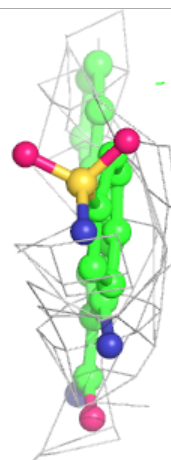
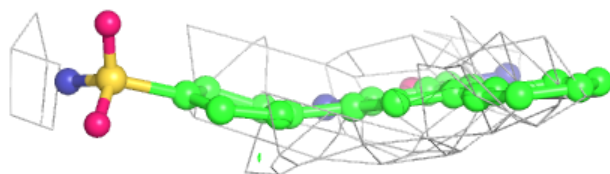
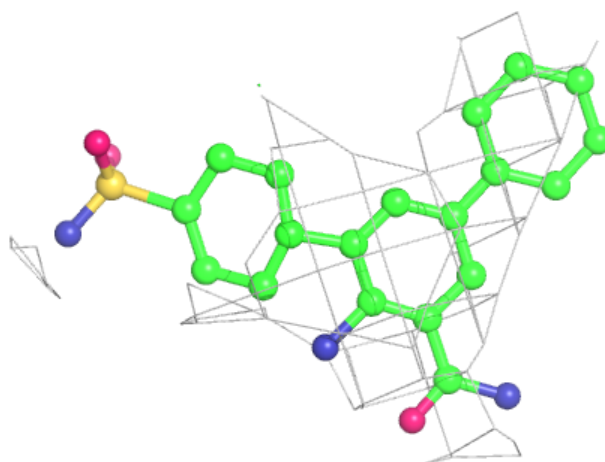
**Electron density around 5TL F 701:**

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



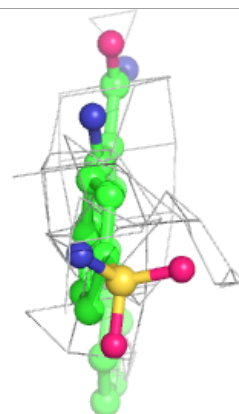
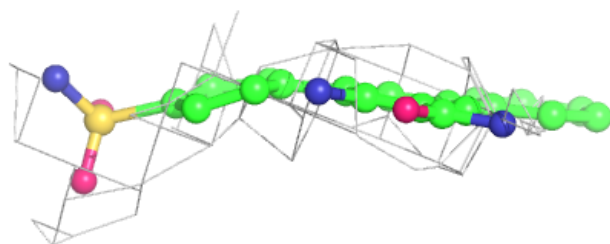
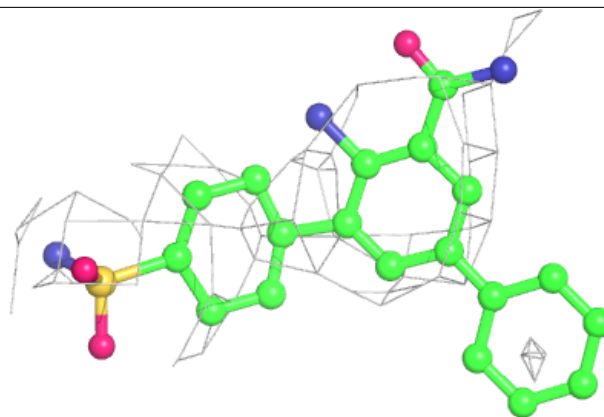
Electron density around 5TL E 701:

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

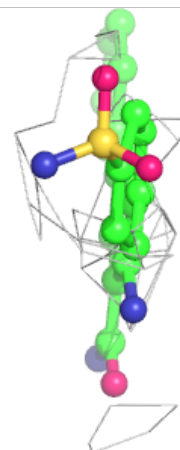
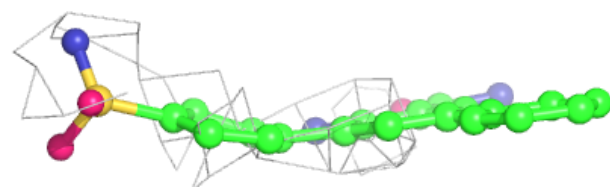
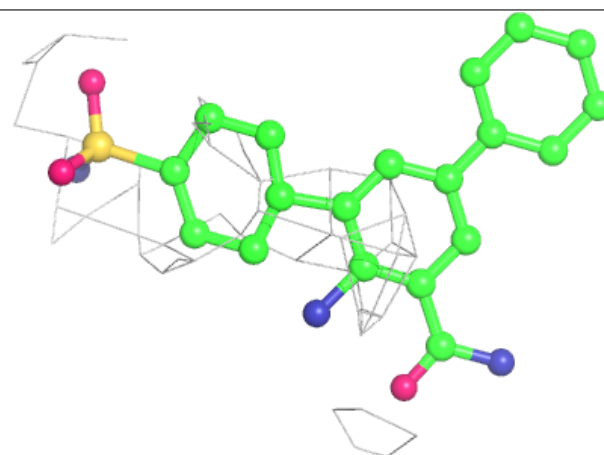


Electron density around 5TL G 701:

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

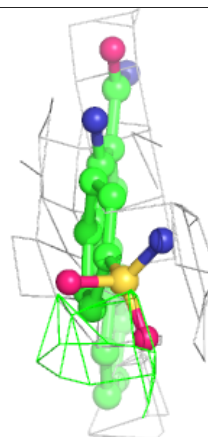
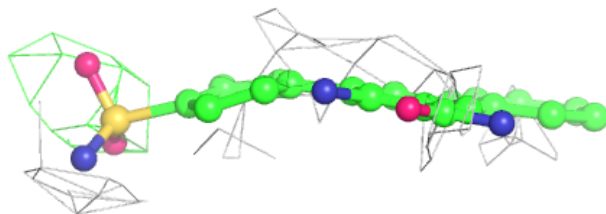
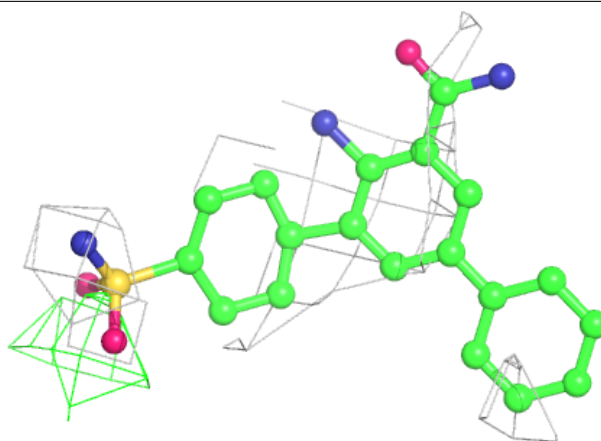
**Electron density around 5TL H 701:**

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



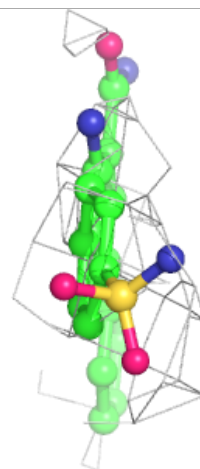
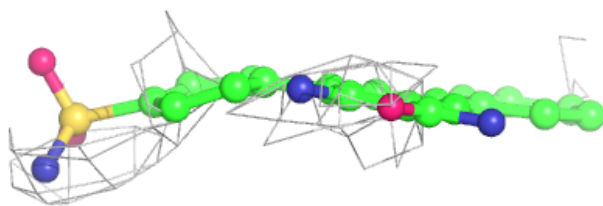
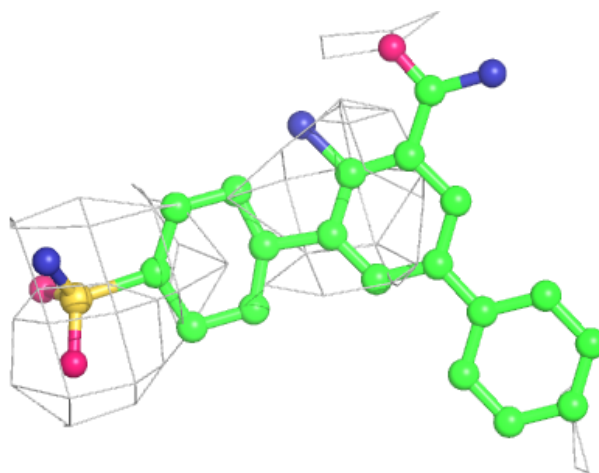
Electron density around 5TL J 701:

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



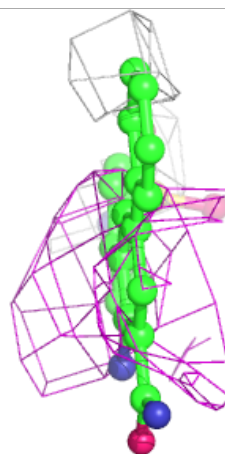
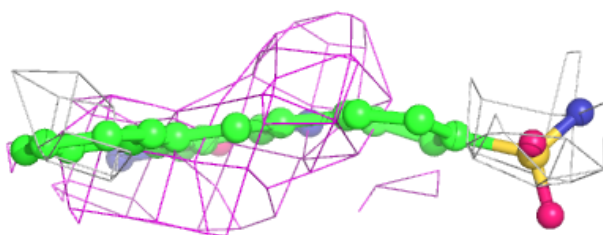
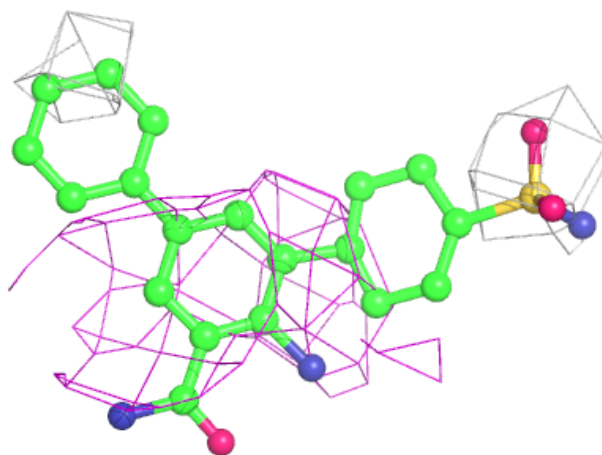
Electron density around 5TL I 701:

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



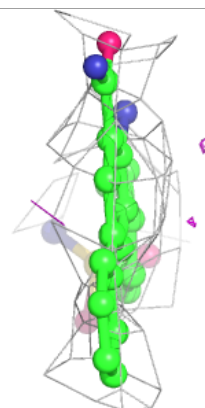
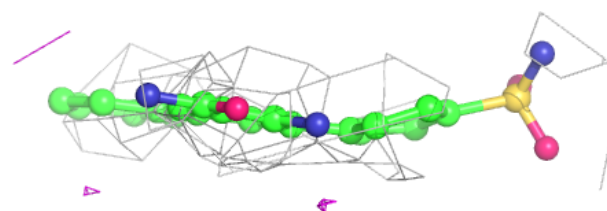
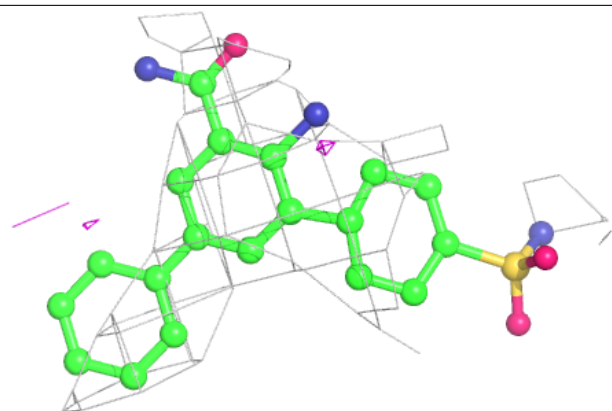
Electron density around 5TL L 701:

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

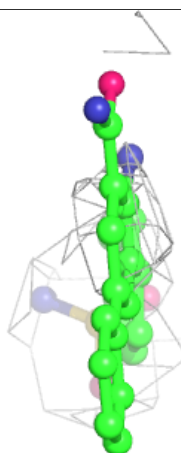
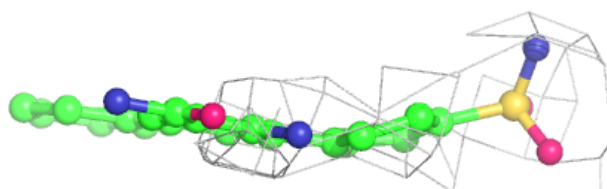
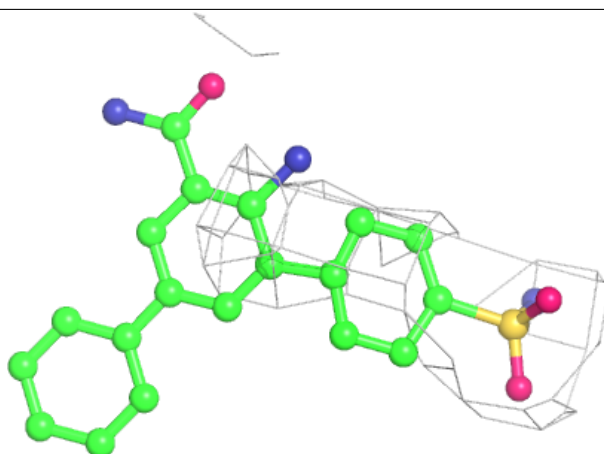


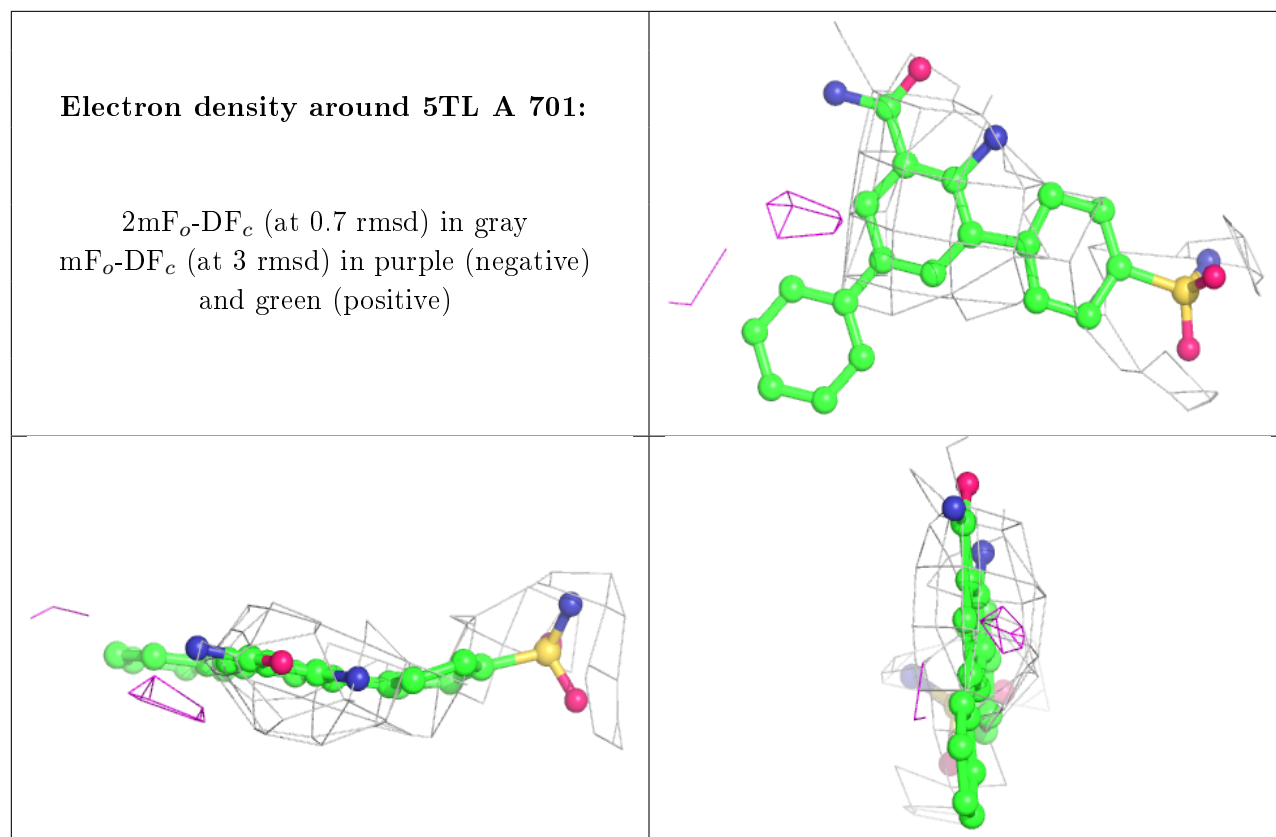
Electron density around 5TL K 701:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

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