



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2022 – 06:04 PM EDT

PDB ID : 7MU5  
Title : Human DCTPP1 bound to Triptolide  
Authors : Hauk, G.; Berger, J.M.  
Deposited on : 2021-05-14  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

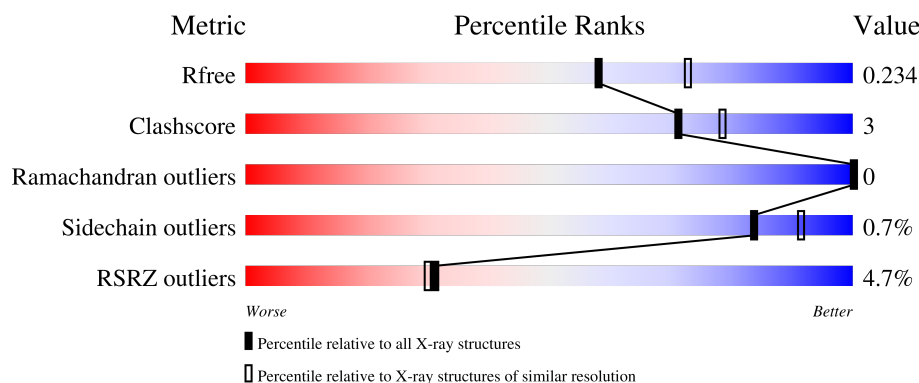
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	110	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>
1	B	110	<div> <div>5%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	C	110	<div> <div>3%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	D	110	<div> <div>5%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
1	E	110	<div> <div>%</div> <div>85%</div> <div>11%</div> <div>5%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	110	<div> <div></div> <div>2%</div> <div>89%</div> <div>7%</div> <div></div> </div>
1	G	110	<div> <div></div> <div>9%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>
1	H	110	<div> <div></div> <div>8%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13830 atoms, of which 6618 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.

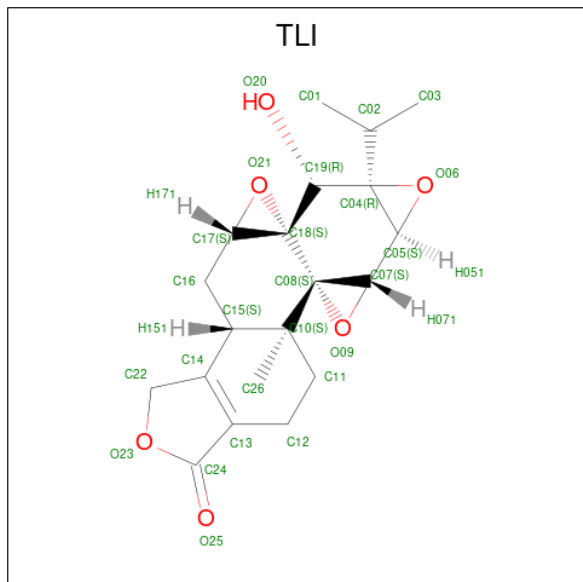
- Molecule 1 is a protein called dCTP pyrophosphatase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	110	Total	C	H	N	O	S	0	0	0
			1702	562	822	156	160	2			
1	B	105	Total	C	H	N	O	S	0	0	0
			1653	545	803	154	149	2			
1	C	104	Total	C	H	N	O	S	0	0	0
			1659	539	819	147	152	2			
1	D	105	Total	C	H	N	O	S	0	0	0
			1648	543	801	150	152	2			
1	E	105	Total	C	H	N	O	S	0	0	0
			1653	542	807	151	151	2			
1	F	106	Total	C	H	N	O	S	0	0	0
			1646	540	806	151	147	2			
1	G	104	Total	C	H	N	O	S	0	0	0
			1630	535	796	147	150	2			
1	H	104	Total	C	H	N	O	S	0	0	0
			1588	527	772	140	147	2			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		

- Molecule 3 is triptolide (three-letter code: TLI) (formula:  $C_{20}H_{24}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			50	20	24	6		
3	A	1	Total	C	H	O	0	0
			50	20	24	6		
3	B	1	Total	C	H	O	0	0
			50	20	24	6		
3	B	1	Total	C	H	O	0	0
			50	20	24	6		
3	C	1	Total	C	H	O	0	0
			50	20	24	6		
3	D	1	Total	C	H	O	0	0
			50	20	24	6		
3	F	1	Total	C	H	O	0	0
			50	20	24	6		
3	G	1	Total	C	H	O	0	0
			50	20	24	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	40	Total	O	0	0
			40	40		

*Continued on next page...*

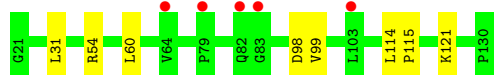
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	39	Total 39	O 39	0	0
4	D	34	Total 34	O 34	0	0
4	E	25	Total 25	O 25	0	0
4	F	17	Total 17	O 17	0	0
4	G	18	Total 18	O 18	0	0
4	H	14	Total 14	O 14	0	0

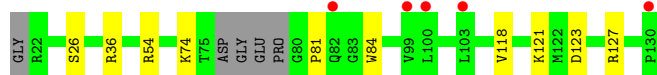
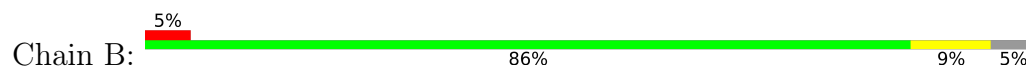
### 3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

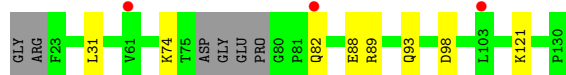
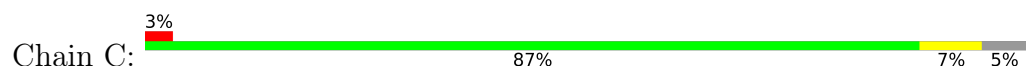
- Molecule 1: dCTP pyrophosphatase 1



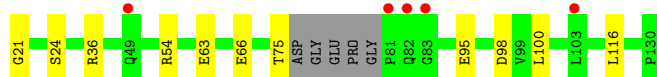
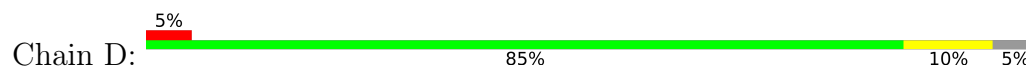
- Molecule 1: dCTP pyrophosphatase 1



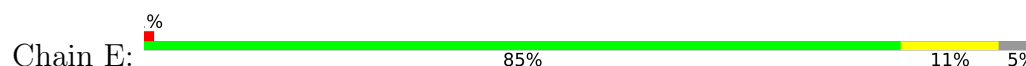
- Molecule 1: dCTP pyrophosphatase 1



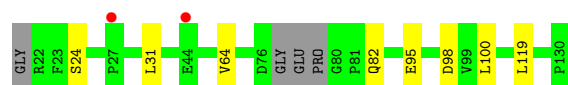
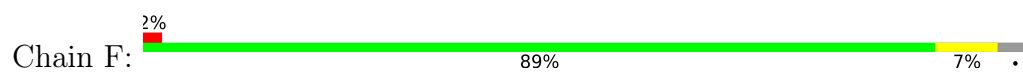
- Molecule 1: dCTP pyrophosphatase 1



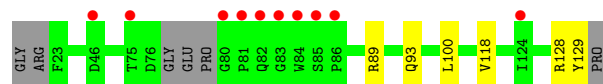
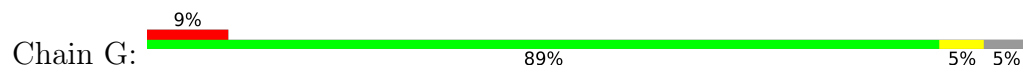
- Molecule 1: dCTP pyrophosphatase 1



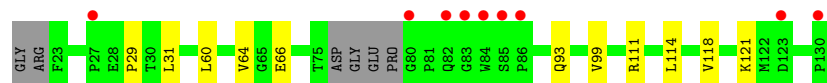
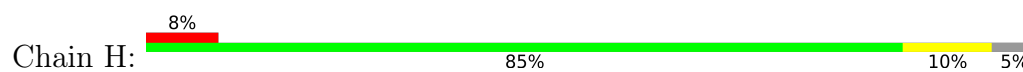
- Molecule 1: dCTP pyrophosphatase 1



- Molecule 1: dCTP pyrophosphatase 1



- Molecule 1: dCTP pyrophosphatase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.16Å 60.92Å 73.46Å 91.46° 101.31° 104.13°	Depositor
Resolution (Å)	29.45 – 2.20 29.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.45-2.20) 98.2 (29.45-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.184 , 0.235 0.183 , 0.234	Depositor DCC
$R_{free}$ test set	1726 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TLI

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	0.68	0/902	0.84	1/1226 (0.1%)
1	B	0.59	0/870	0.79	1/1180 (0.1%)
1	C	0.60	0/860	0.72	0/1168
1	D	0.62	0/867	0.74	0/1176
1	E	0.63	0/866	0.71	0/1175
1	F	0.58	0/860	0.68	0/1169
1	G	0.60	0/853	0.73	0/1158
1	H	0.55	0/836	0.66	0/1139
All	All	0.61	0/6914	0.74	2/9391 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	54	ARG	NE-CZ-NH1	5.58	123.09	120.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	880	822	857	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	850	803	840	9	0
1	C	840	819	822	6	0
1	D	847	801	830	12	0
1	E	846	807	830	9	0
1	F	840	806	819	10	0
1	G	834	796	813	6	0
1	H	816	772	786	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	52	48	0	0	0
3	B	52	48	0	0	0
3	C	26	24	0	0	0
3	D	26	24	0	0	0
3	F	26	24	0	0	0
3	G	26	24	0	0	0
4	A	58	0	0	0	0
4	B	40	0	0	1	0
4	C	39	0	0	0	0
4	D	34	0	0	1	0
4	E	25	0	0	0	0
4	F	17	0	0	0	0
4	G	18	0	0	0	0
4	H	14	0	0	1	0
All	All	7212	6618	6597	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ARG:HD3	4:B:307:HOH:O	1.87	0.74
1:D:36:ARG:HD3	4:D:320:HOH:O	1.87	0.73
1:E:84:TRP:HB3	1:E:88:GLU:HG3	1.72	0.71
1:G:89:ARG:O	1:G:93:GLN:HG3	1.93	0.68
1:F:98:ASP:OD1	1:H:121:LYS:HE2	1.94	0.66
1:H:60:LEU:HD11	1:H:99:VAL:HG13	1.81	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG21	1:D:100:LEU:HD23	1.82	0.62
1:E:118:VAL:HG21	1:G:100:LEU:HD23	1.83	0.61
1:F:100:LEU:HD22	1:H:114:LEU:HD21	1.82	0.61
1:C:74:LYS:NZ	1:C:88:GLU:OE2	2.33	0.60
1:D:66:GLU:HB2	1:D:95:GLU:OE1	2.03	0.58
1:B:26:SER:CB	1:D:116:LEU:HD23	2.34	0.58
1:H:93:GLN:NE2	4:H:201:HOH:O	2.32	0.55
1:D:21:GLY:N	1:E:66:GLU:OE2	2.41	0.54
1:H:60:LEU:CD1	1:H:99:VAL:HG13	2.37	0.54
1:A:121:LYS:HE2	1:C:98:ASP:OD1	2.08	0.53
1:E:100:LEU:HD23	1:G:118:VAL:HG21	1.91	0.52
1:F:82:GLN:NE2	1:H:111:ARG:HG3	2.23	0.52
1:E:84:TRP:HB3	1:E:88:GLU:CG	2.40	0.51
1:G:128:ARG:O	1:G:128:ARG:HG3	2.09	0.51
1:B:81:PRO:HA	1:B:84:TRP:CD1	2.47	0.50
1:F:31:LEU:HD21	1:H:31:LEU:HD21	1.93	0.50
1:B:123:ASP:O	1:B:127:ARG:HG3	2.13	0.48
1:D:66:GLU:CB	1:D:95:GLU:OE1	2.62	0.48
1:G:128:ARG:HG2	1:G:129:TYR:CE2	2.50	0.47
1:D:63:GLU:HG2	1:D:98:ASP:HB3	1.98	0.45
1:F:100:LEU:HD23	1:H:118:VAL:HG21	1.99	0.45
1:E:95:GLU:HA	1:E:95:GLU:OE1	2.17	0.44
1:F:64:VAL:HG21	1:H:64:VAL:HG21	1.99	0.44
1:A:31:LEU:HD21	1:C:31:LEU:HD21	1.99	0.44
1:F:82:GLN:HE21	1:H:111:ARG:HG3	1.81	0.44
1:A:98:ASP:OD2	1:C:121:LYS:HE3	2.18	0.43
1:B:74:LYS:O	1:D:54:ARG:HD3	2.19	0.43
1:B:121:LYS:HE3	1:D:98:ASP:CG	2.39	0.43
1:E:46:ASP:OD2	1:E:49:GLN:NE2	2.51	0.43
1:F:95:GLU:HA	1:F:95:GLU:OE1	2.19	0.43
1:B:26:SER:HB2	1:D:116:LEU:HD23	2.00	0.43
1:A:60:LEU:HD11	1:A:99:VAL:HG13	2.02	0.42
1:A:114:LEU:HB3	1:A:115:PRO:HD3	2.00	0.42
1:D:24:SER:OG	1:G:128:ARG:NH2	2.53	0.42
1:A:98:ASP:CG	1:C:121:LYS:HE3	2.40	0.41
1:C:89:ARG:O	1:C:93:GLN:HG3	2.19	0.41
1:E:81:PRO:HA	1:E:84:TRP:CD1	2.56	0.41
1:B:26:SER:OG	1:D:116:LEU:HD23	2.21	0.41
1:F:82:GLN:CG	1:H:111:ARG:HG3	2.50	0.41
1:E:89:ARG:O	1:E:93:GLN:HG3	2.21	0.40
1:F:119:LEU:HD22	1:H:29:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
1	B	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	C	100/110 (91%)	98 (98%)	2 (2%)	0	100	100
1	D	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	E	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	F	102/110 (93%)	100 (98%)	2 (2%)	0	100	100
1	G	100/110 (91%)	100 (100%)	0	0	100	100
1	H	100/110 (91%)	97 (97%)	3 (3%)	0	100	100
All	All	813/880 (92%)	798 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/93 (97%)	90 (100%)	0	100	100
1	B	87/93 (94%)	87 (100%)	0	100	100
1	C	87/93 (94%)	86 (99%)	1 (1%)	73	85
1	D	87/93 (94%)	86 (99%)	1 (1%)	73	85

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	87/93 (94%)	86 (99%)	1 (1%)	73	85
1	F	84/93 (90%)	83 (99%)	1 (1%)	71	83
1	G	85/93 (91%)	85 (100%)	0	100	100
1	H	82/93 (88%)	81 (99%)	1 (1%)	71	83
All	All	689/744 (93%)	684 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	82	GLN
1	D	75	THR
1	E	128	ARG
1	F	24	SER
1	H	66	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	49	GLN
1	E	52	GLN
1	E	93	GLN
1	F	82	GLN
1	G	93	GLN
1	H	93	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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
3	TLI	A	202	-	29,32,32	2.92	12 (41%)	41,59,59	5.86	26 (63%)
3	TLI	G	202	-	29,32,32	3.11	12 (41%)	41,59,59	5.99	28 (68%)
3	TLI	F	202	-	29,32,32	2.96	12 (41%)	41,59,59	5.93	26 (63%)
3	TLI	B	202	-	29,32,32	2.91	12 (41%)	41,59,59	5.87	26 (63%)
3	TLI	C	202	-	29,32,32	3.00	13 (44%)	41,59,59	5.88	30 (73%)
3	TLI	A	203	-	29,32,32	3.15	11 (37%)	41,59,59	6.01	30 (73%)
3	TLI	B	203	-	29,32,32	2.96	12 (41%)	41,59,59	5.88	25 (60%)
3	TLI	D	201	-	29,32,32	2.89	13 (44%)	41,59,59	5.78	28 (68%)

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
3	TLI	A	202	-	-	1/6/97/97	-
3	TLI	G	202	-	-	0/6/97/97	-
3	TLI	F	202	-	-	3/6/97/97	-
3	TLI	B	202	-	-	0/6/97/97	-
3	TLI	C	202	-	-	0/6/97/97	-
3	TLI	A	203	-	-	0/6/97/97	-
3	TLI	B	203	-	-	1/6/97/97	-
3	TLI	D	201	-	-	0/6/97/97	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	202	TLI	C08-C07	9.76	1.55	1.47
3	A	203	TLI	C08-C07	9.70	1.54	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	TLI	C08-C07	9.53	1.54	1.47
3	B	202	TLI	C08-C07	9.49	1.54	1.47
3	F	202	TLI	C08-C07	9.28	1.54	1.47
3	A	202	TLI	C08-C07	9.23	1.54	1.47
3	B	203	TLI	C08-C07	8.86	1.54	1.47
3	D	201	TLI	C08-C07	8.70	1.54	1.47
3	A	203	TLI	C26-C10	7.78	1.69	1.54
3	G	202	TLI	C26-C10	7.59	1.69	1.54
3	B	203	TLI	C26-C10	6.67	1.67	1.54
3	A	202	TLI	C26-C10	6.49	1.67	1.54
3	C	202	TLI	C26-C10	6.40	1.67	1.54
3	B	202	TLI	C26-C10	6.39	1.67	1.54
3	D	201	TLI	C26-C10	6.39	1.67	1.54
3	A	203	TLI	O21-C18	-6.35	1.37	1.45
3	F	202	TLI	C26-C10	5.97	1.66	1.54
3	B	203	TLI	O21-C18	-5.92	1.38	1.45
3	C	202	TLI	O21-C18	-5.59	1.38	1.45
3	G	202	TLI	O21-C18	-5.52	1.38	1.45
3	D	201	TLI	O21-C18	-5.21	1.39	1.45
3	A	202	TLI	O21-C18	-5.15	1.39	1.45
3	F	202	TLI	O21-C18	-5.13	1.39	1.45
3	B	202	TLI	O21-C18	-5.12	1.39	1.45
3	B	203	TLI	O06-C05	-4.37	1.39	1.45
3	C	202	TLI	O06-C05	-4.32	1.39	1.45
3	F	202	TLI	O06-C05	-4.10	1.39	1.45
3	A	203	TLI	O06-C05	-4.04	1.39	1.45
3	B	202	TLI	O06-C05	-3.93	1.39	1.45
3	A	202	TLI	O06-C05	-3.92	1.39	1.45
3	F	202	TLI	C14-C13	3.85	1.38	1.33
3	D	201	TLI	C14-C13	3.69	1.38	1.33
3	B	203	TLI	C14-C13	3.67	1.38	1.33
3	D	201	TLI	O06-C05	-3.67	1.40	1.45
3	G	202	TLI	C22-C14	3.60	1.54	1.50
3	G	202	TLI	O06-C05	-3.60	1.40	1.45
3	A	203	TLI	C22-C14	3.55	1.54	1.50
3	C	202	TLI	C14-C13	3.53	1.37	1.33
3	A	202	TLI	C14-C13	3.51	1.37	1.33
3	B	202	TLI	C18-C17	3.48	1.52	1.47
3	G	202	TLI	C14-C13	3.43	1.37	1.33
3	B	202	TLI	C14-C13	3.41	1.37	1.33
3	A	203	TLI	C14-C13	3.36	1.37	1.33
3	F	202	TLI	C18-C17	3.34	1.52	1.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	TLI	C18-C17	3.27	1.52	1.47
3	D	201	TLI	C18-C17	3.22	1.52	1.47
3	C	202	TLI	C18-C17	3.21	1.52	1.47
3	A	203	TLI	O09-C07	-3.19	1.40	1.45
3	A	202	TLI	O21-C17	-3.12	1.39	1.45
3	C	202	TLI	O21-C17	-3.11	1.39	1.45
3	F	202	TLI	O21-C17	-3.10	1.39	1.45
3	D	201	TLI	O21-C17	-3.04	1.39	1.45
3	F	202	TLI	C04-C05	3.02	1.52	1.47
3	B	203	TLI	C22-C14	2.98	1.53	1.50
3	G	202	TLI	C18-C17	2.96	1.51	1.47
3	D	201	TLI	O09-C07	-2.95	1.41	1.45
3	F	202	TLI	O09-C07	-2.93	1.41	1.45
3	B	203	TLI	O21-C17	-2.89	1.39	1.45
3	F	202	TLI	C22-C14	2.88	1.53	1.50
3	G	202	TLI	O09-C07	-2.87	1.41	1.45
3	G	202	TLI	C08-C10	2.87	1.58	1.53
3	C	202	TLI	O09-C07	-2.82	1.41	1.45
3	B	203	TLI	C18-C17	2.80	1.51	1.47
3	G	202	TLI	C04-C05	2.79	1.52	1.47
3	A	202	TLI	C22-C14	2.77	1.53	1.50
3	A	203	TLI	O21-C17	-2.71	1.40	1.45
3	A	202	TLI	O09-C07	-2.70	1.41	1.45
3	B	203	TLI	C04-C05	2.68	1.52	1.47
3	B	202	TLI	O09-C07	-2.67	1.41	1.45
3	G	202	TLI	O21-C17	-2.65	1.40	1.45
3	A	202	TLI	C04-C05	2.63	1.52	1.47
3	A	203	TLI	C18-C17	2.63	1.51	1.47
3	D	201	TLI	C04-C05	2.59	1.52	1.47
3	B	203	TLI	O09-C07	-2.59	1.41	1.45
3	C	202	TLI	C04-C05	2.58	1.52	1.47
3	B	202	TLI	O21-C17	-2.57	1.40	1.45
3	D	201	TLI	C22-C14	2.53	1.53	1.50
3	C	202	TLI	C22-C14	2.49	1.53	1.50
3	B	203	TLI	O09-C08	-2.47	1.42	1.45
3	B	202	TLI	O20-C19	-2.47	1.36	1.42
3	A	202	TLI	O09-C08	-2.46	1.42	1.45
3	B	203	TLI	O20-C19	-2.46	1.36	1.42
3	B	202	TLI	C22-C14	2.43	1.53	1.50
3	B	202	TLI	C04-C05	2.41	1.51	1.47
3	A	203	TLI	C04-C05	2.41	1.51	1.47
3	D	201	TLI	O09-C08	-2.33	1.42	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	TLI	C08-C10	2.32	1.57	1.53
3	D	201	TLI	O20-C19	-2.26	1.36	1.42
3	C	202	TLI	O20-C19	-2.24	1.36	1.42
3	A	202	TLI	O20-C19	-2.21	1.36	1.42
3	B	202	TLI	O09-C08	-2.13	1.42	1.45
3	F	202	TLI	O20-C19	-2.12	1.37	1.42
3	C	202	TLI	O09-C08	-2.10	1.42	1.45
3	C	202	TLI	O23-C22	-2.09	1.40	1.44
3	F	202	TLI	C08-C10	2.08	1.57	1.53
3	G	202	TLI	O20-C19	-2.08	1.37	1.42
3	A	203	TLI	O20-C19	-2.01	1.37	1.42

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	TLI	C11-C10-C08	14.63	128.50	111.41
3	A	203	TLI	C18-C08-C10	14.54	125.72	117.30
3	F	202	TLI	C11-C10-C08	14.22	128.03	111.41
3	A	202	TLI	C18-C08-C10	14.15	125.50	117.30
3	G	202	TLI	C11-C10-C08	13.97	127.74	111.41
3	C	202	TLI	C11-C10-C08	13.95	127.72	111.41
3	B	203	TLI	C11-C10-C08	13.93	127.69	111.41
3	A	202	TLI	C11-C10-C08	13.64	127.35	111.41
3	B	202	TLI	C11-C10-C08	13.53	127.22	111.41
3	G	202	TLI	C18-C08-C10	13.41	125.07	117.30
3	C	202	TLI	C18-C08-C10	13.27	124.98	117.30
3	F	202	TLI	C18-C08-C10	13.04	124.85	117.30
3	B	203	TLI	C18-C08-C10	12.83	124.73	117.30
3	D	201	TLI	C18-C08-C10	12.70	124.66	117.30
3	A	203	TLI	C26-C10-C11	-12.27	86.91	107.84
3	C	202	TLI	C08-O09-C07	12.25	66.03	60.88
3	A	202	TLI	C08-O09-C07	12.22	66.02	60.88
3	G	202	TLI	C26-C10-C11	-12.20	87.02	107.84
3	G	202	TLI	C08-O09-C07	12.20	66.01	60.88
3	A	203	TLI	C11-C10-C08	12.18	125.65	111.41
3	A	203	TLI	C08-O09-C07	12.18	66.00	60.88
3	B	202	TLI	C18-C08-C10	12.14	124.33	117.30
3	B	202	TLI	C08-O09-C07	12.13	65.98	60.88
3	G	202	TLI	C15-C14-C13	-11.98	118.21	124.51
3	F	202	TLI	C08-O09-C07	11.92	65.89	60.88
3	D	201	TLI	C08-O09-C07	11.84	65.86	60.88
3	B	203	TLI	C08-O09-C07	11.81	65.85	60.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	TLI	C26-C10-C11	-11.61	88.02	107.84
3	F	202	TLI	C26-C10-C11	-11.51	88.20	107.84
3	A	202	TLI	C26-C10-C11	-11.50	88.22	107.84
3	B	202	TLI	C15-C14-C13	-11.33	118.55	124.51
3	B	203	TLI	C08-C07-C05	-11.25	114.03	120.52
3	B	202	TLI	C26-C10-C11	-11.19	88.76	107.84
3	C	202	TLI	C26-C10-C11	-11.15	88.81	107.84
3	A	203	TLI	C15-C14-C13	-10.93	118.76	124.51
3	B	203	TLI	C26-C10-C11	-10.90	89.24	107.84
3	F	202	TLI	C08-C07-C05	-10.55	114.43	120.52
3	F	202	TLI	C26-C10-C08	-10.53	88.43	110.38
3	B	203	TLI	C26-C10-C08	-10.22	89.07	110.38
3	D	201	TLI	C26-C10-C08	-10.21	89.10	110.38
3	G	202	TLI	C26-C10-C08	-10.10	89.32	110.38
3	A	202	TLI	C26-C10-C08	-10.07	89.39	110.38
3	A	203	TLI	C11-C10-C15	9.94	120.09	107.74
3	C	202	TLI	C26-C10-C08	-9.92	89.69	110.38
3	B	202	TLI	C26-C10-C08	-9.91	89.73	110.38
3	C	202	TLI	C08-C07-C05	-9.81	114.86	120.52
3	A	203	TLI	C26-C10-C08	-9.56	90.45	110.38
3	A	202	TLI	C15-C14-C13	-9.07	119.74	124.51
3	A	202	TLI	C11-C10-C15	8.96	118.87	107.74
3	B	203	TLI	C11-C10-C15	8.95	118.86	107.74
3	B	202	TLI	C11-C10-C15	8.72	118.57	107.74
3	F	202	TLI	C08-C10-C15	8.62	114.23	105.72
3	B	202	TLI	C08-C07-C05	-8.50	115.61	120.52
3	D	201	TLI	C11-C10-C15	8.48	118.28	107.74
3	C	202	TLI	C11-C10-C15	8.46	118.24	107.74
3	G	202	TLI	C11-C10-C15	8.44	118.23	107.74
3	A	203	TLI	C08-C10-C15	8.26	113.87	105.72
3	B	202	TLI	C08-C10-C15	8.20	113.81	105.72
3	G	202	TLI	C08-C10-C15	8.19	113.81	105.72
3	A	203	TLI	C10-C08-C07	-8.12	111.49	121.51
3	C	202	TLI	C10-C08-C07	-8.00	111.64	121.51
3	C	202	TLI	C08-C10-C15	7.98	113.60	105.72
3	A	203	TLI	C08-C07-C05	-7.92	115.95	120.52
3	F	202	TLI	C11-C10-C15	7.89	117.54	107.74
3	B	203	TLI	C10-C08-C07	-7.82	111.87	121.51
3	A	202	TLI	C08-C10-C15	7.80	113.42	105.72
3	D	201	TLI	C15-C14-C13	-7.76	120.43	124.51
3	A	202	TLI	C10-C08-C07	-7.69	112.02	121.51
3	B	203	TLI	C15-C14-C13	-7.66	120.48	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	TLI	C10-C08-C07	-7.65	112.07	121.51
3	A	202	TLI	C08-C07-C05	-7.52	116.18	120.52
3	D	201	TLI	C08-C07-C05	-7.46	116.21	120.52
3	D	201	TLI	C08-C10-C15	7.39	113.02	105.72
3	B	203	TLI	C08-C10-C15	7.37	112.99	105.72
3	F	202	TLI	C10-C08-C07	-7.17	112.67	121.51
3	G	202	TLI	C10-C08-C07	-6.89	113.01	121.51
3	D	201	TLI	C10-C08-C07	-6.87	113.04	121.51
3	G	202	TLI	C08-C07-C05	-6.81	116.59	120.52
3	C	202	TLI	C15-C14-C13	-6.75	120.96	124.51
3	D	201	TLI	C10-C15-C14	6.73	117.44	109.64
3	F	202	TLI	C10-C15-C14	6.72	117.43	109.64
3	C	202	TLI	C18-O21-C17	6.64	66.33	60.77
3	F	202	TLI	C18-O21-C17	6.56	66.27	60.77
3	A	202	TLI	C18-O21-C17	6.52	66.24	60.77
3	D	201	TLI	C18-O21-C17	6.45	66.18	60.77
3	F	202	TLI	C15-C14-C13	-6.44	121.13	124.51
3	B	202	TLI	C18-O21-C17	6.36	66.10	60.77
3	B	203	TLI	O09-C07-C05	6.29	129.99	116.43
3	B	203	TLI	C18-O21-C17	6.28	66.03	60.77
3	A	203	TLI	C18-O21-C17	6.18	65.95	60.77
3	G	202	TLI	C18-O21-C17	6.11	65.89	60.77
3	A	202	TLI	C10-C15-C14	6.08	116.69	109.64
3	B	203	TLI	C10-C15-C14	6.08	116.69	109.64
3	B	203	TLI	C04-C05-C07	6.05	125.82	120.96
3	C	202	TLI	C10-C15-C14	6.04	116.65	109.64
3	A	203	TLI	O09-C08-C07	-6.00	56.13	59.36
3	G	202	TLI	C10-C15-C14	6.00	116.60	109.64
3	B	202	TLI	C10-C15-C14	6.00	116.60	109.64
3	F	202	TLI	C04-C05-C07	5.90	125.70	120.96
3	D	201	TLI	C26-C10-C15	-5.76	98.30	110.51
3	C	202	TLI	O09-C07-C05	5.76	128.84	116.43
3	B	202	TLI	C26-C10-C15	-5.66	98.50	110.51
3	G	202	TLI	O06-C05-C07	5.63	128.58	116.43
3	F	202	TLI	O09-C07-C05	5.63	128.58	116.43
3	G	202	TLI	O09-C08-C07	-5.58	56.36	59.36
3	F	202	TLI	C26-C10-C15	-5.56	98.71	110.51
3	D	201	TLI	O06-C05-C07	5.51	128.32	116.43
3	C	202	TLI	C26-C10-C15	-5.48	98.88	110.51
3	B	202	TLI	O09-C07-C05	5.47	128.22	116.43
3	F	202	TLI	O09-C08-C07	-5.44	56.44	59.36
3	A	202	TLI	O06-C05-C07	5.40	128.07	116.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	TLI	O09-C07-C05	5.39	128.05	116.43
3	A	203	TLI	O06-C05-C07	5.37	128.02	116.43
3	B	203	TLI	C26-C10-C15	-5.35	99.17	110.51
3	A	202	TLI	C26-C10-C15	-5.34	99.19	110.51
3	C	202	TLI	O09-C08-C07	-5.29	56.52	59.36
3	A	203	TLI	C10-C15-C14	5.28	115.76	109.64
3	G	202	TLI	C26-C10-C15	-5.26	99.35	110.51
3	D	201	TLI	O09-C07-C05	5.23	127.72	116.43
3	C	202	TLI	C04-C05-C07	5.20	125.14	120.96
3	B	202	TLI	O06-C05-C07	5.19	127.62	116.43
3	A	203	TLI	C26-C10-C15	-5.13	99.61	110.51
3	B	202	TLI	O09-C08-C07	-5.10	56.62	59.36
3	D	201	TLI	O09-C08-C07	-5.03	56.66	59.36
3	A	202	TLI	O09-C07-C05	5.03	127.27	116.43
3	A	202	TLI	O09-C08-C07	-4.88	56.74	59.36
3	A	202	TLI	O09-C07-C08	-4.78	57.24	59.76
3	B	203	TLI	O09-C07-C08	-4.70	57.28	59.76
3	C	202	TLI	O06-C05-C07	4.65	126.46	116.43
3	B	203	TLI	O09-C08-C07	-4.63	56.87	59.36
3	B	203	TLI	O06-C05-C07	4.59	126.34	116.43
3	G	202	TLI	O09-C07-C05	4.54	126.22	116.43
3	B	202	TLI	O09-C07-C08	-4.48	57.40	59.76
3	B	202	TLI	C04-C05-C07	4.45	124.53	120.96
3	G	202	TLI	C22-C14-C13	-4.43	106.10	109.51
3	C	202	TLI	O09-C07-C08	-4.38	57.45	59.76
3	F	202	TLI	C22-C14-C13	-4.38	106.14	109.51
3	D	201	TLI	O09-C07-C08	-4.32	57.48	59.76
3	F	202	TLI	O06-C05-C07	4.06	125.19	116.43
3	G	202	TLI	O09-C07-C08	-4.04	57.63	59.76
3	F	202	TLI	O09-C07-C08	-3.97	57.67	59.76
3	D	201	TLI	C04-C05-C07	3.92	124.11	120.96
3	A	203	TLI	O21-C17-C18	-3.89	56.34	59.54
3	B	203	TLI	C14-C13-C24	-3.87	105.82	108.42
3	A	202	TLI	C04-C05-C07	3.83	124.04	120.96
3	A	203	TLI	C22-C14-C13	-3.70	106.67	109.51
3	A	203	TLI	C16-C15-C10	3.66	118.37	112.89
3	B	203	TLI	O21-C17-C18	-3.60	56.57	59.54
3	A	203	TLI	O09-C07-C08	-3.60	57.86	59.76
3	G	202	TLI	O21-C17-C18	-3.51	56.65	59.54
3	B	202	TLI	O21-C17-C18	-3.51	56.65	59.54
3	C	202	TLI	O21-C17-C18	-3.47	56.68	59.54
3	A	203	TLI	C04-C05-C07	3.44	123.72	120.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	TLI	C22-C14-C13	-3.34	106.94	109.51
3	G	202	TLI	C04-C05-C07	3.29	123.60	120.96
3	D	201	TLI	O21-C17-C18	-3.25	56.86	59.54
3	C	202	TLI	O23-C24-O25	-3.25	116.96	121.07
3	A	203	TLI	C11-C12-C13	3.24	116.80	110.57
3	F	202	TLI	O21-C17-C18	-3.23	56.88	59.54
3	D	201	TLI	C22-C14-C13	-3.20	107.05	109.51
3	A	202	TLI	O21-C17-C18	-3.20	56.90	59.54
3	G	202	TLI	C11-C12-C13	3.06	116.45	110.57
3	A	202	TLI	C14-C13-C24	-3.01	106.40	108.42
3	D	201	TLI	O23-C24-O25	-2.97	117.31	121.07
3	C	202	TLI	C22-C14-C13	-2.94	107.25	109.51
3	G	202	TLI	C16-C15-C10	2.93	117.28	112.89
3	F	202	TLI	C14-C13-C24	-2.85	106.50	108.42
3	D	201	TLI	C12-C13-C14	-2.85	122.73	124.99
3	C	202	TLI	C14-C13-C24	-2.82	106.52	108.42
3	A	203	TLI	C14-C13-C24	-2.78	106.55	108.42
3	G	202	TLI	C12-C13-C14	-2.67	122.88	124.99
3	F	202	TLI	O23-C24-O25	-2.67	117.70	121.07
3	G	202	TLI	C01-C02-C04	-2.57	104.81	113.61
3	G	202	TLI	C14-C13-C24	-2.55	106.70	108.42
3	G	202	TLI	C12-C11-C10	2.54	117.39	112.56
3	F	202	TLI	O21-C18-C17	-2.53	56.85	59.69
3	A	202	TLI	O21-C18-C17	-2.52	56.86	59.69
3	B	202	TLI	C12-C13-C14	-2.48	123.02	124.99
3	B	202	TLI	C01-C02-C04	-2.48	105.11	113.61
3	A	203	TLI	C01-C02-C04	-2.45	105.22	113.61
3	A	202	TLI	C01-C02-C04	-2.44	105.23	113.61
3	F	202	TLI	C12-C11-C10	2.44	117.20	112.56
3	A	202	TLI	C22-C14-C13	-2.44	107.64	109.51
3	D	201	TLI	C01-C02-C04	-2.44	105.26	113.61
3	D	201	TLI	O21-C18-C17	-2.43	56.96	59.69
3	B	202	TLI	C16-C15-C10	2.43	116.53	112.89
3	D	201	TLI	C14-C13-C24	-2.42	106.79	108.42
3	C	202	TLI	O21-C18-C17	-2.41	56.98	59.69
3	A	202	TLI	C16-C15-C10	2.41	116.50	112.89
3	C	202	TLI	C12-C13-C14	-2.40	123.09	124.99
3	F	202	TLI	O25-C24-C13	2.39	133.82	129.78
3	C	202	TLI	C16-C15-C10	2.37	116.44	112.89
3	D	201	TLI	C16-C15-C10	2.34	116.39	112.89
3	F	202	TLI	C11-C12-C13	2.32	115.03	110.57
3	A	203	TLI	C16-C15-C14	-2.32	110.55	113.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	203	TLI	C16-C15-C10	2.31	116.35	112.89
3	C	202	TLI	C01-C02-C04	-2.29	105.75	113.61
3	B	202	TLI	C14-C13-C24	-2.25	106.90	108.42
3	C	202	TLI	C12-C11-C10	2.25	116.84	112.56
3	G	202	TLI	O25-C24-C13	2.21	133.51	129.78
3	B	203	TLI	C01-C02-C04	-2.19	106.10	113.61
3	C	202	TLI	O25-C24-C13	2.18	133.46	129.78
3	B	202	TLI	O21-C18-C17	-2.17	57.25	59.69
3	D	201	TLI	C12-C11-C10	2.15	116.66	112.56
3	B	203	TLI	C12-C11-C10	2.12	116.59	112.56
3	A	203	TLI	C03-C02-C01	2.11	116.35	109.99
3	A	203	TLI	O23-C24-C13	2.10	110.53	108.89
3	D	201	TLI	O25-C24-C13	2.10	133.33	129.78
3	A	202	TLI	O23-C24-O25	-2.10	118.42	121.07
3	B	202	TLI	C12-C11-C10	2.10	116.55	112.56
3	C	202	TLI	C12-C13-C24	2.09	130.39	125.94
3	A	203	TLI	C16-C17-C18	2.09	124.16	121.73
3	A	203	TLI	C22-O23-C24	-2.08	107.41	109.31
3	G	202	TLI	C16-C17-C18	2.07	124.14	121.73
3	A	202	TLI	C11-C12-C13	2.05	114.52	110.57
3	C	202	TLI	O23-C22-C14	2.05	105.74	104.38
3	B	203	TLI	C22-C14-C13	-2.04	107.94	109.51
3	B	203	TLI	O21-C18-C17	-2.04	57.40	59.69
3	A	203	TLI	C12-C11-C10	2.03	116.42	112.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	202	TLI	C01-C02-C04-C05
3	A	202	TLI	C01-C02-C04-C19
3	B	203	TLI	C03-C02-C04-C05
3	F	202	TLI	C03-C02-C04-C05
3	F	202	TLI	C01-C02-C04-O06

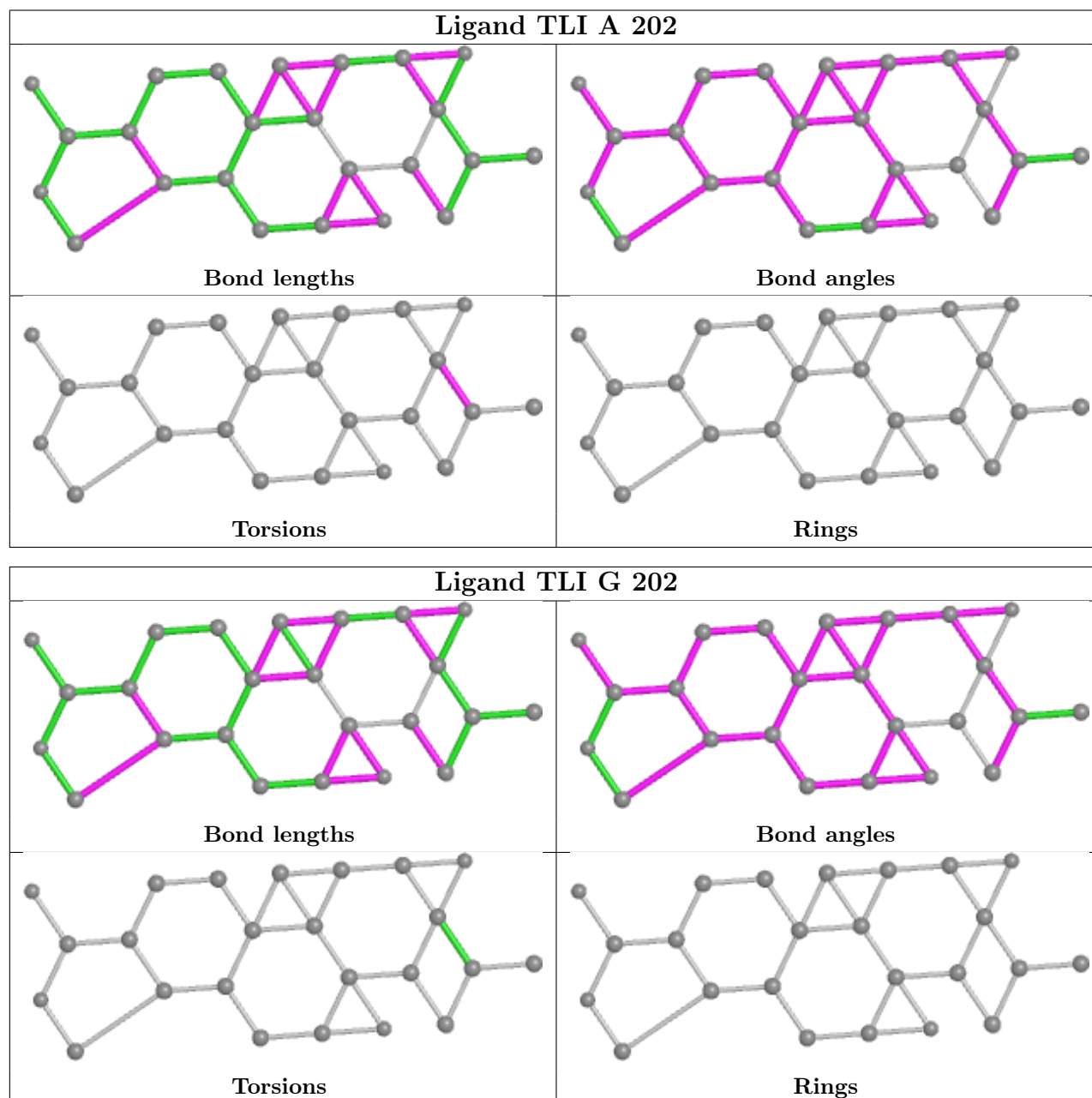
There are no ring outliers.

No monomer is involved in short contacts.

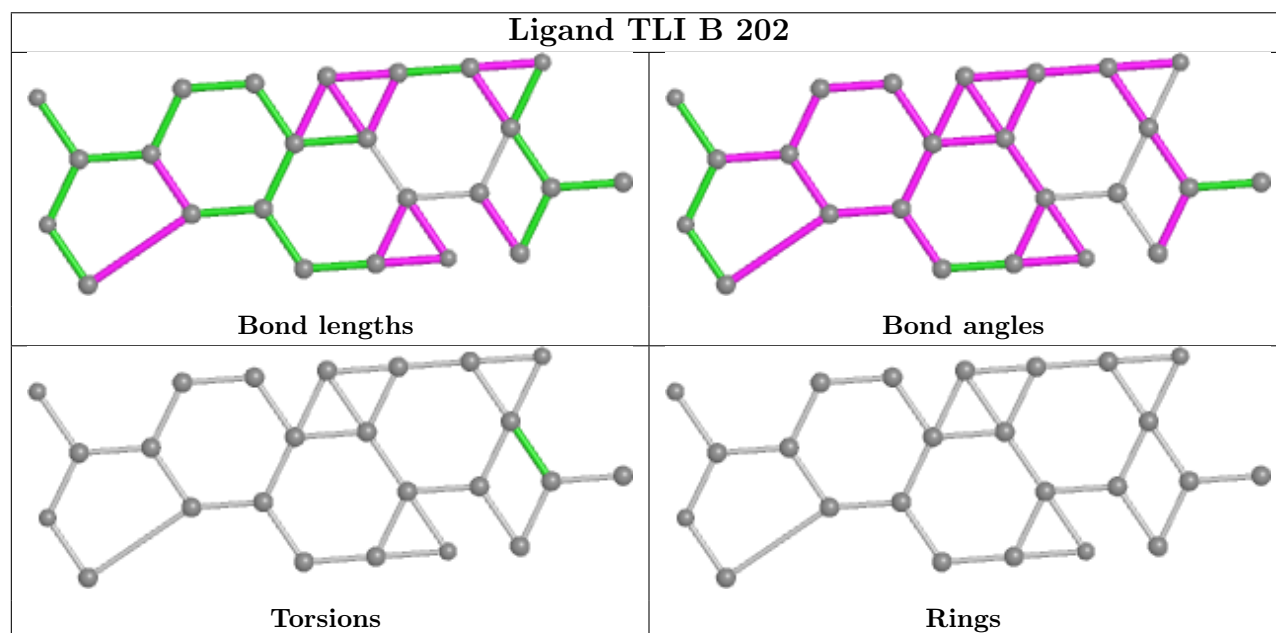
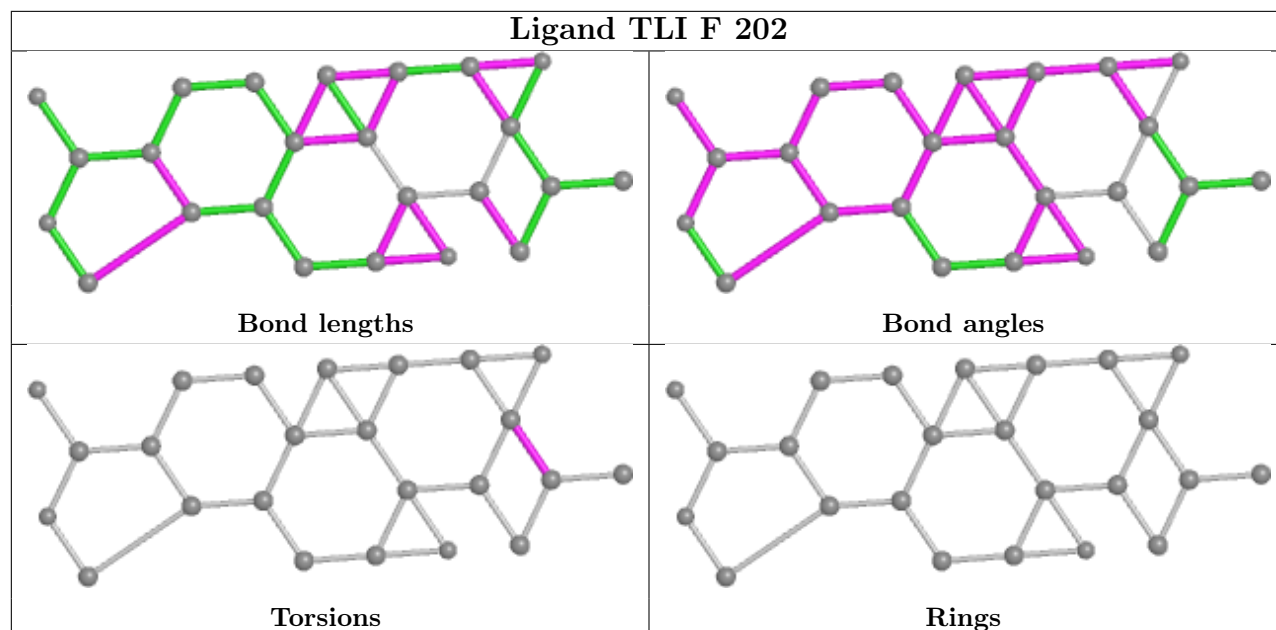
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

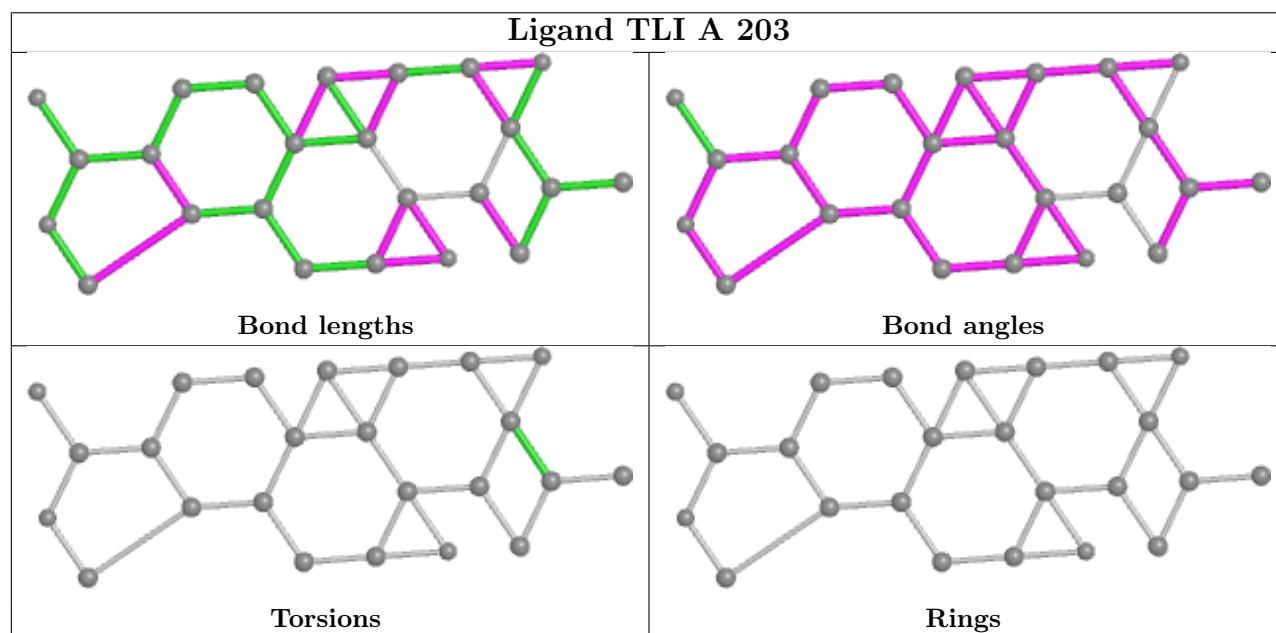
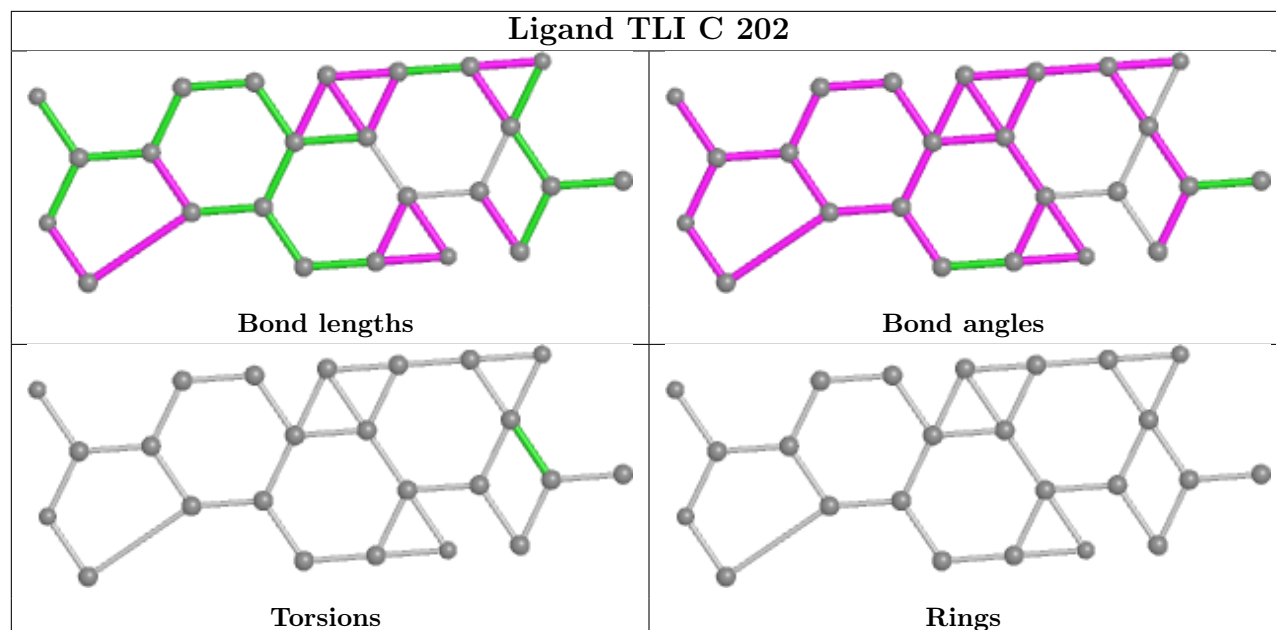


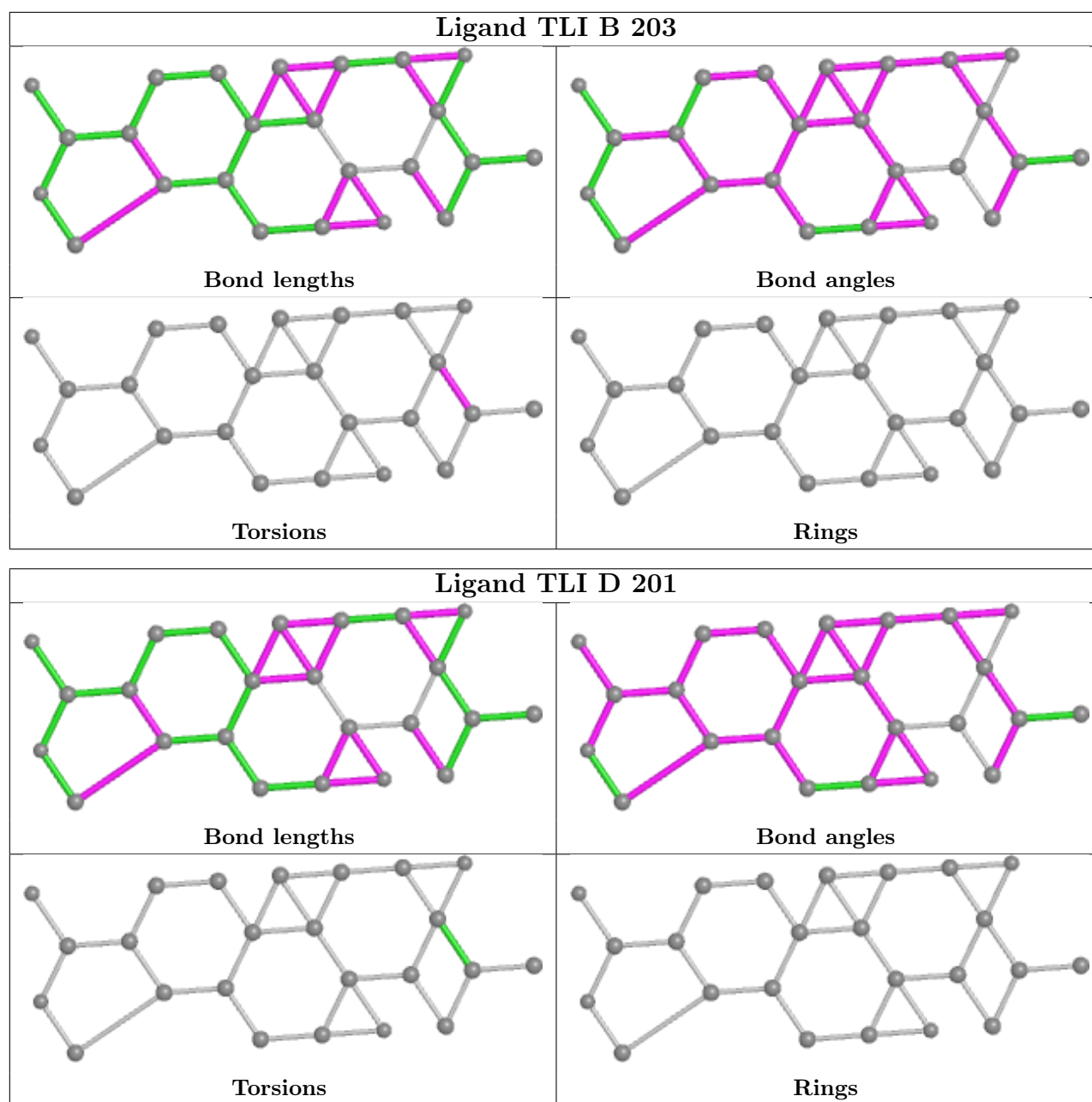
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	110/110 (100%)	0.10	5 (4%) 33 32	26, 36, 55, 65	0
1	B	105/110 (95%)	0.13	5 (4%) 30 29	27, 35, 51, 56	0
1	C	104/110 (94%)	0.05	3 (2%) 51 49	27, 36, 47, 55	0
1	D	105/110 (95%)	0.28	5 (4%) 30 29	28, 38, 53, 67	0
1	E	105/110 (95%)	0.08	1 (0%) 82 81	30, 41, 55, 71	0
1	F	106/110 (96%)	0.03	2 (1%) 66 65	29, 45, 57, 61	0
1	G	104/110 (94%)	0.45	10 (9%) 8 6	28, 43, 62, 69	0
1	H	104/110 (94%)	0.49	9 (8%) 10 8	29, 46, 66, 78	0
All	All	843/880 (95%)	0.20	40 (4%) 31 30	26, 39, 57, 78	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	GLY	5.0
1	H	83	GLY	4.8
1	H	82	GLN	4.3
1	D	82	GLN	4.2
1	A	82	GLN	4.2
1	H	80	GLY	3.9
1	G	83	GLY	3.8
1	H	84	TRP	3.8
1	C	82	GLN	3.8
1	G	86	PRO	3.6
1	D	103	LEU	3.0
1	B	82	GLN	2.9
1	H	85	SER	2.9
1	B	103	LEU	2.8
1	G	80	GLY	2.7
1	H	27	PRO	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	46	ASP	2.6
1	G	82	GLN	2.6
1	G	81	PRO	2.6
1	G	84	TRP	2.5
1	E	61	VAL	2.5
1	B	99	VAL	2.4
1	G	75	THR	2.4
1	A	79	PRO	2.3
1	A	64	VAL	2.3
1	H	130	PRO	2.3
1	C	103	LEU	2.3
1	C	61	VAL	2.3
1	D	81	PRO	2.2
1	H	123	ASP	2.2
1	H	86	PRO	2.2
1	A	83	GLY	2.2
1	F	27	PRO	2.2
1	G	85	SER	2.1
1	A	103	LEU	2.1
1	G	124	ILE	2.1
1	B	130	PRO	2.1
1	D	49	GLN	2.0
1	F	44	GLU	2.0
1	B	100	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

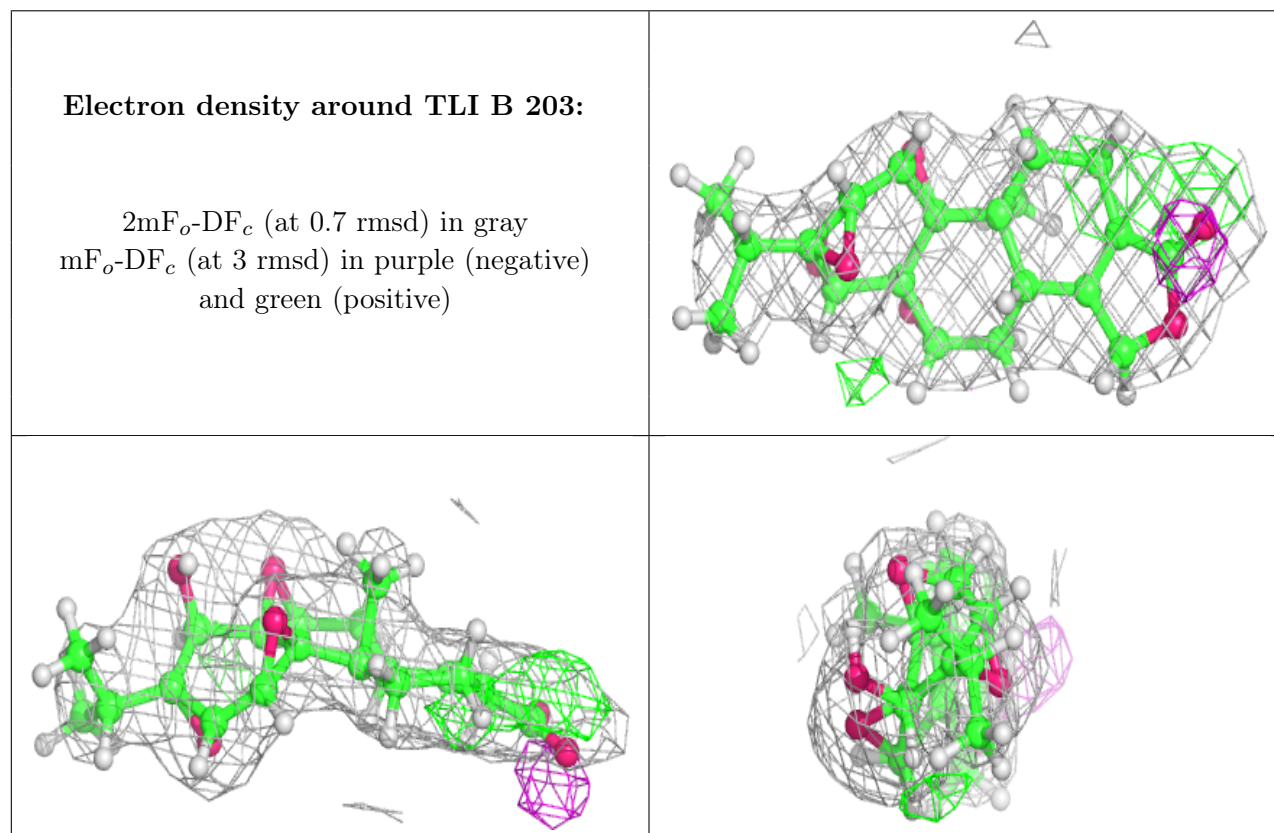
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

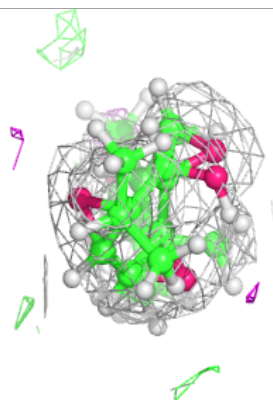
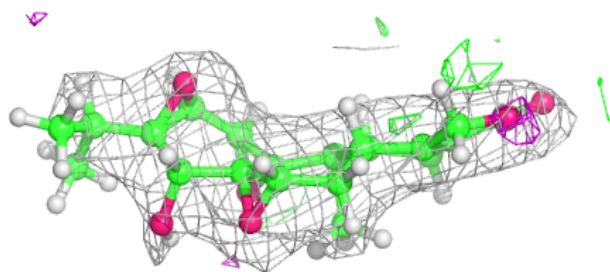
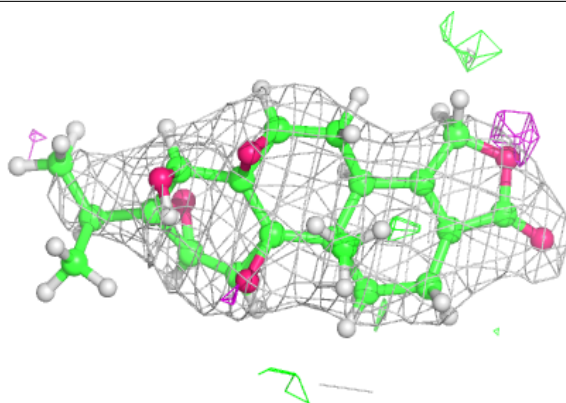
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TLI	B	203	26/26	0.82	0.16	35,45,59,60	0
3	TLI	D	201	26/26	0.83	0.24	47,58,81,87	0
3	TLI	A	203	26/26	0.85	0.22	39,51,72,77	0
3	TLI	B	202	26/26	0.85	0.24	43,53,71,81	0
3	TLI	G	202	26/26	0.85	0.30	46,61,80,82	0
3	TLI	A	202	26/26	0.88	0.20	41,53,76,78	0
2	MG	G	201	1/1	0.89	0.31	62,62,62,62	0
3	TLI	F	202	26/26	0.89	0.17	45,56,72,87	0
3	TLI	C	202	26/26	0.89	0.17	36,44,56,57	0
2	MG	C	201	1/1	0.93	0.26	43,43,43,43	0
2	MG	B	201	1/1	0.94	0.16	34,34,34,34	0
2	MG	F	201	1/1	0.95	0.20	39,39,39,39	0
2	MG	A	201	1/1	0.95	0.21	35,35,35,35	0
2	MG	E	201	1/1	0.96	0.22	32,32,32,32	0

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

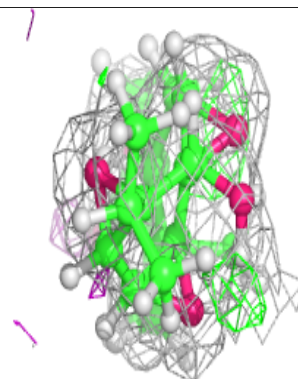
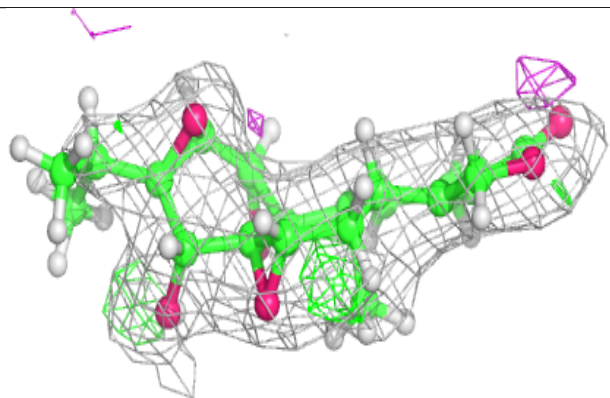
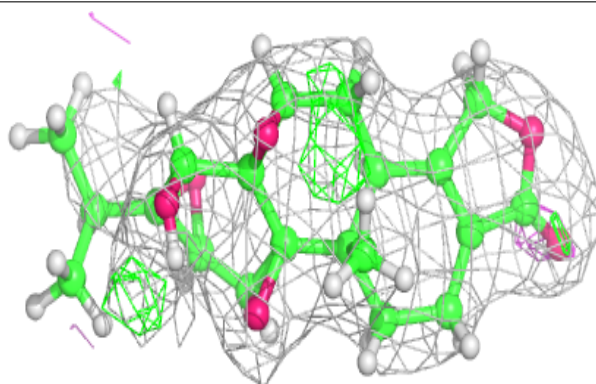


**Electron density around TLI D 201:**

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

**Electron density around TLI A 203:**

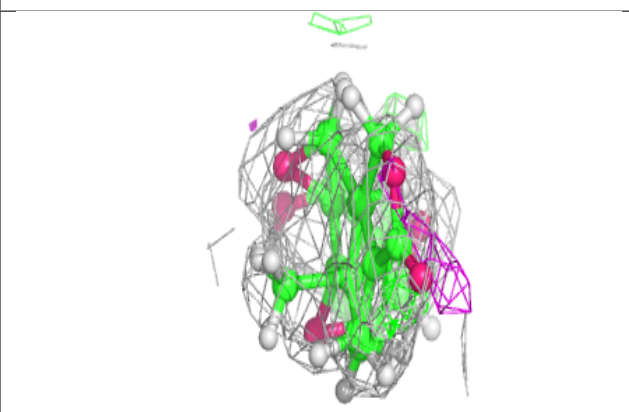
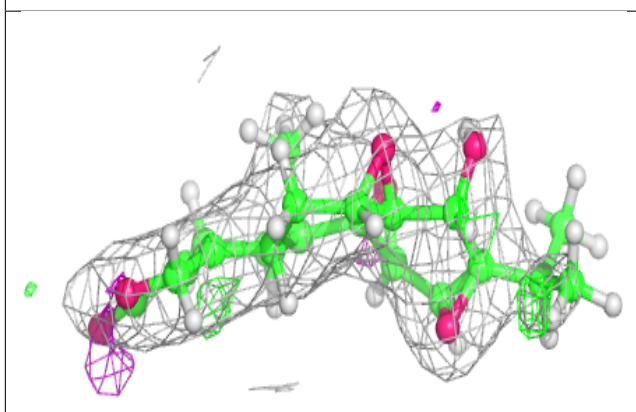
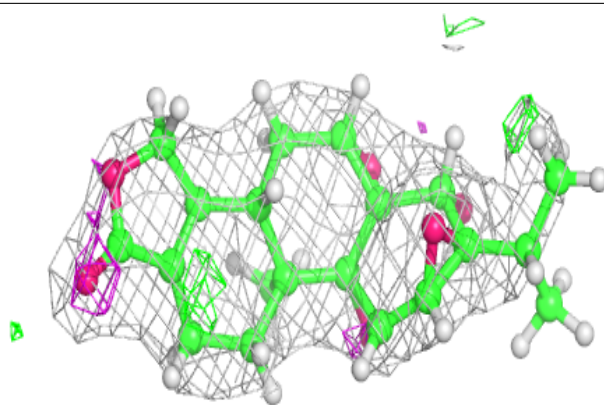
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



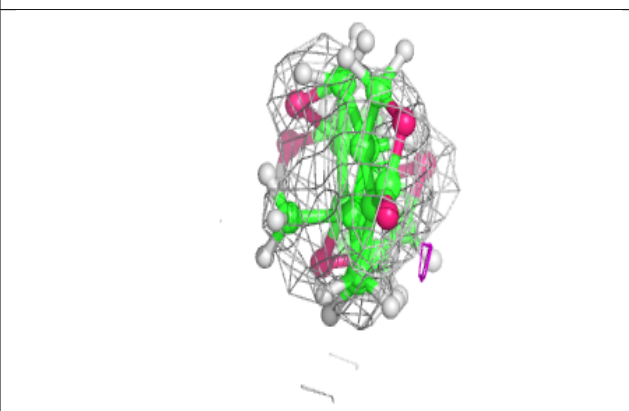
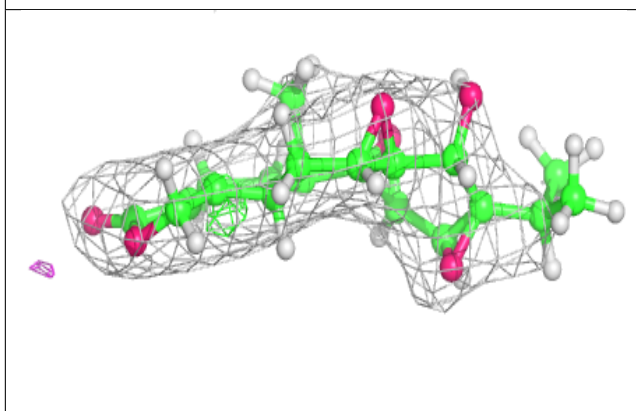
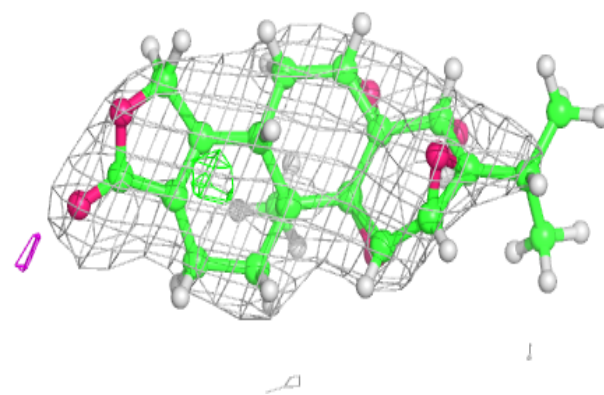


**Electron density around TLI B 202:**

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

**Electron density around TLI G 202:**

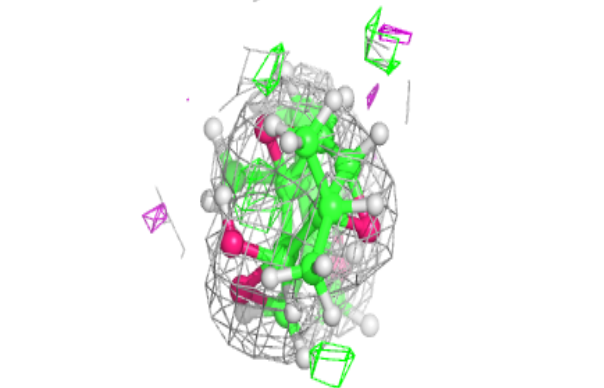
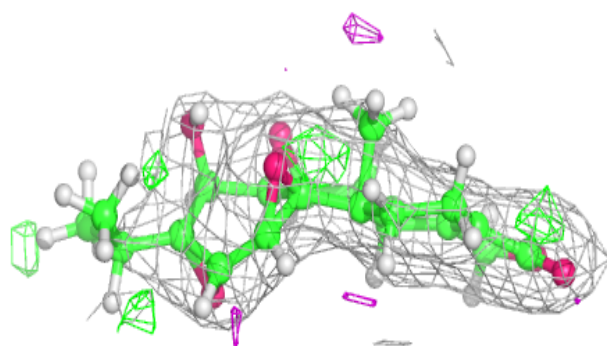
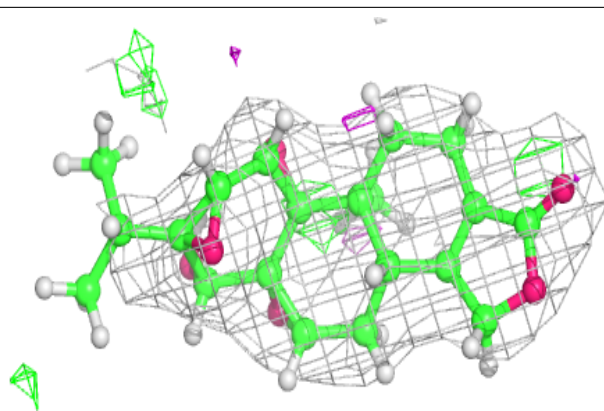
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



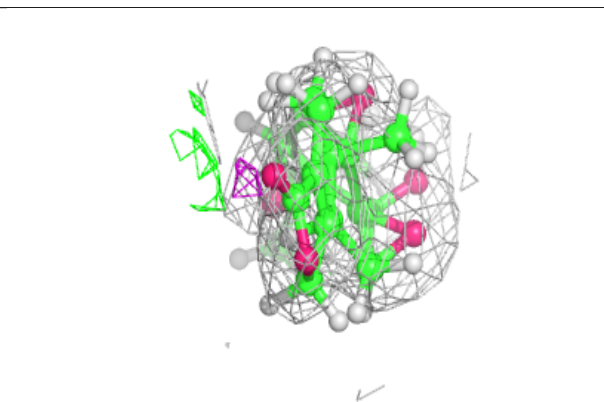
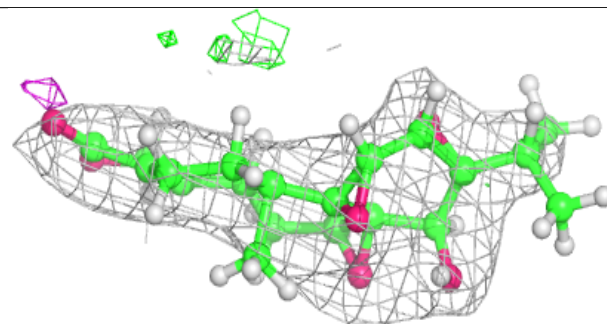
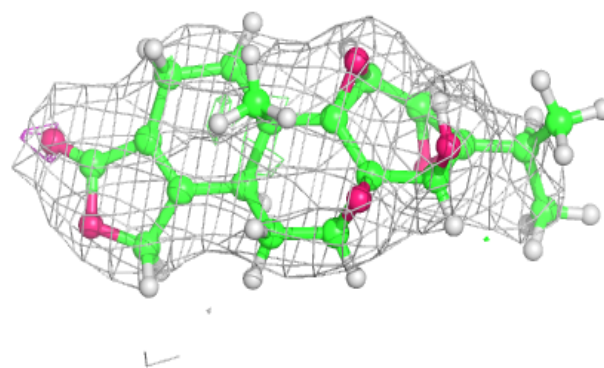


**Electron density around TLI A 202:**

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

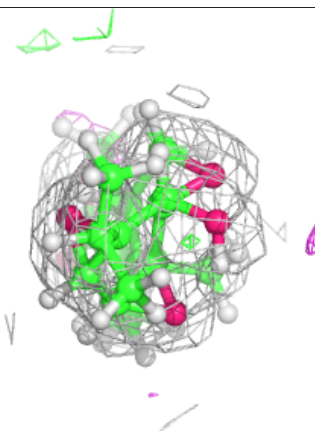
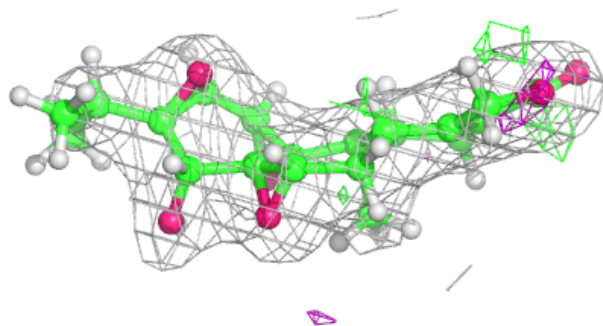
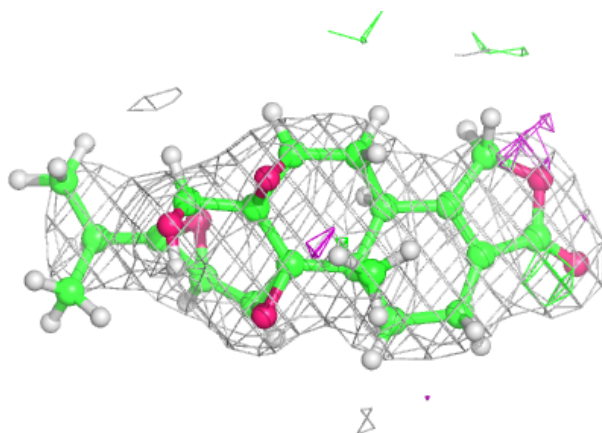
**Electron density around TLI F 202:**

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



**Electron density around TLI C 202:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.