



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:12 PM UTC

PDB ID : 4TKR / pdb\_00004tkr  
Title : Native-SAD phasing for ThiT from *Listeria monocytogenes* serovar.  
Authors : Guo, Y.; Liu, Q.; Hendrickson, W.A.; New York Consortium on Membrane Protein Structure (NYCOMPS)  
Deposited on : 2014-05-27  
Resolution : 3.00 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)

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<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>.

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

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

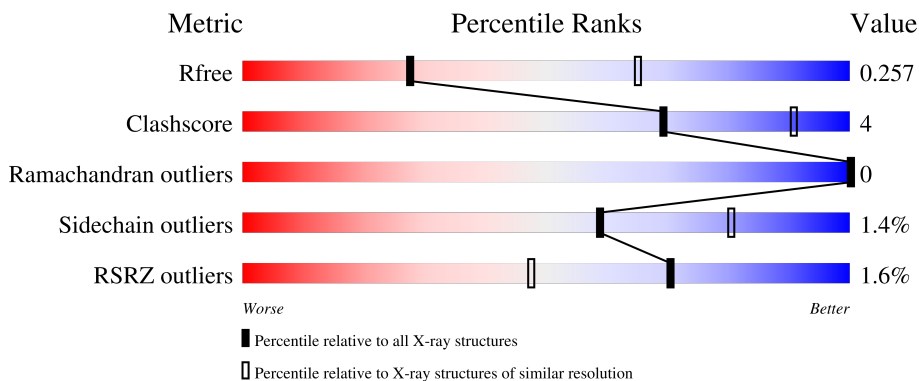
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	214	
1	B	214	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3172 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 Thiamine transporter thia.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	1409	953	223	225	8	0	0	0
1	B	186	1421	958	227	227	9	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

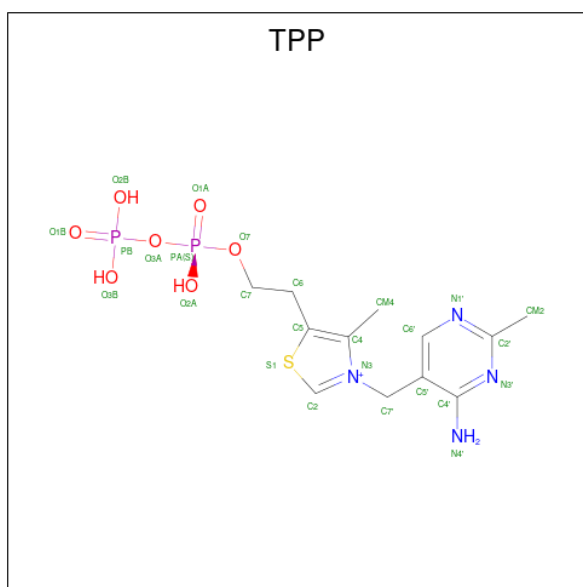
Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP S5L6I0
A	-26	ASP	-	expression tag	UNP S5L6I0
A	-25	TYR	-	expression tag	UNP S5L6I0
A	-24	LYS	-	expression tag	UNP S5L6I0
A	-23	ASP	-	expression tag	UNP S5L6I0
A	-22	ASP	-	expression tag	UNP S5L6I0
A	-21	ASP	-	expression tag	UNP S5L6I0
A	-20	ASP	-	expression tag	UNP S5L6I0
A	-19	LYS	-	expression tag	UNP S5L6I0
A	-18	HIS	-	expression tag	UNP S5L6I0
A	-17	HIS	-	expression tag	UNP S5L6I0
A	-16	HIS	-	expression tag	UNP S5L6I0
A	-15	HIS	-	expression tag	UNP S5L6I0
A	-14	HIS	-	expression tag	UNP S5L6I0
A	-13	HIS	-	expression tag	UNP S5L6I0
A	-12	HIS	-	expression tag	UNP S5L6I0
A	-11	HIS	-	expression tag	UNP S5L6I0
A	-10	HIS	-	expression tag	UNP S5L6I0
A	-9	HIS	-	expression tag	UNP S5L6I0
A	-8	GLU	-	expression tag	UNP S5L6I0
A	-7	ASN	-	expression tag	UNP S5L6I0
A	-6	LEU	-	expression tag	UNP S5L6I0
A	-5	TYR	-	expression tag	UNP S5L6I0
A	-4	PHE	-	expression tag	UNP S5L6I0
A	-3	GLN	-	expression tag	UNP S5L6I0

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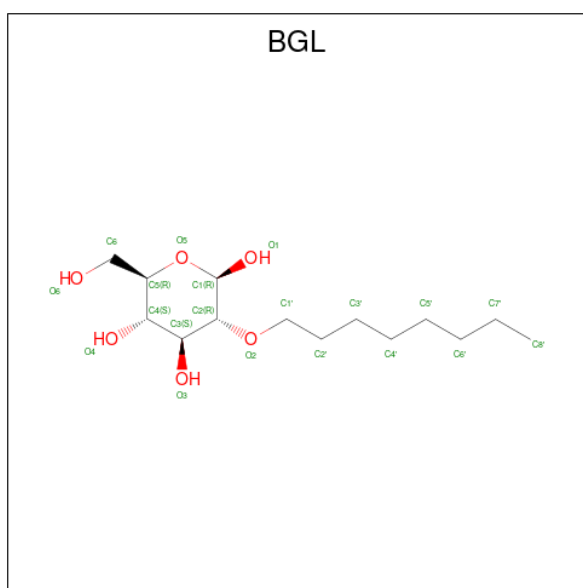
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP S5L6I0
A	-1	TYR	-	expression tag	UNP S5L6I0
A	0	VAL	-	expression tag	UNP S5L6I0
B	-27	MET	-	initiating methionine	UNP S5L6I0
B	-26	ASP	-	expression tag	UNP S5L6I0
B	-25	TYR	-	expression tag	UNP S5L6I0
B	-24	LYS	-	expression tag	UNP S5L6I0
B	-23	ASP	-	expression tag	UNP S5L6I0
B	-22	ASP	-	expression tag	UNP S5L6I0
B	-21	ASP	-	expression tag	UNP S5L6I0
B	-20	ASP	-	expression tag	UNP S5L6I0
B	-19	LYS	-	expression tag	UNP S5L6I0
B	-18	HIS	-	expression tag	UNP S5L6I0
B	-17	HIS	-	expression tag	UNP S5L6I0
B	-16	HIS	-	expression tag	UNP S5L6I0
B	-15	HIS	-	expression tag	UNP S5L6I0
B	-14	HIS	-	expression tag	UNP S5L6I0
B	-13	HIS	-	expression tag	UNP S5L6I0
B	-12	HIS	-	expression tag	UNP S5L6I0
B	-11	HIS	-	expression tag	UNP S5L6I0
B	-10	HIS	-	expression tag	UNP S5L6I0
B	-9	HIS	-	expression tag	UNP S5L6I0
B	-8	GLU	-	expression tag	UNP S5L6I0
B	-7	ASN	-	expression tag	UNP S5L6I0
B	-6	LEU	-	expression tag	UNP S5L6I0
B	-5	TYR	-	expression tag	UNP S5L6I0
B	-4	PHE	-	expression tag	UNP S5L6I0
B	-3	GLN	-	expression tag	UNP S5L6I0
B	-2	SER	-	expression tag	UNP S5L6I0
B	-1	TYR	-	expression tag	UNP S5L6I0
B	0	VAL	-	expression tag	UNP S5L6I0

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	Total	C	0	0
			18	12		
3	A	1	Total	C	0	0
			18	12		

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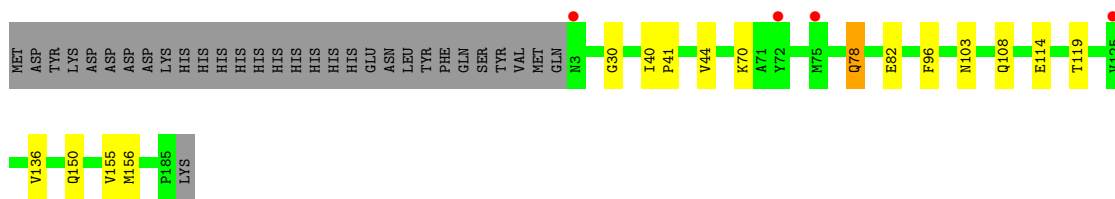
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			18	12	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			18	12	6		
3	B	1	Total	C	O	0	0
			18	12	6		
3	B	1	Total	C	O	0	0
			20	14	6		

### 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.

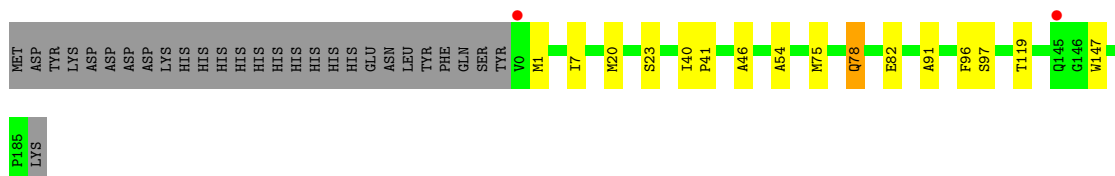
- Molecule 1: Thiamine transporter thia

Chain A: 



- Molecule 1: Thiamine transporter thia

Chain B: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.65Å 95.65Å 125.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.31 – 3.00 39.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.31-3.00) 99.7 (39.31-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.198 , 0.234 0.217 , 0.257	Depositor DCC
$R_{free}$ test set	676 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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

### 5.1 Standard geometry

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

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	0/1450	0.70	0/1971
1	B	0.29	0/1461	0.71	0/1984
All	All	0.29	0/2911	0.70	0/3955

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

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	1409	0	1452	10	0
1	B	1421	0	1463	9	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
3	A	114	0	141	5	0
3	B	176	0	229	2	0
All	All	3172	0	3317	23	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 4.

All (23) 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)
3:A:305:BGL:H1	3:A:306:BGL:H1'1	1.61	0.82
3:A:305:BGL:H5	3:A:306:BGL:H2	1.71	0.71
1:A:30:GLY:HA3	3:A:303:BGL:H1	1.78	0.66
1:A:114:GLU:HG2	3:A:305:BGL:H2	1.78	0.65
1:A:78:GLN:NE2	1:A:82:GLU:OE1	2.32	0.62
1:A:96:PHE:HB2	1:A:119:THR:HB	1.83	0.60
1:B:96:PHE:HB2	1:B:119:THR:HB	1.85	0.58
1:A:82:GLU:OE2	2:A:301:TPP:N4'	2.36	0.55
1:A:136:VAL:HG22	1:A:150:GLN:HA	1.91	0.52
1:B:46:ALA:O	1:B:97:SER:OG	2.25	0.50
1:B:82:GLU:OE2	2:B:301:TPP:N4'	2.41	0.50
3:A:305:BGL:H3'2	3:A:306:BGL:H5'1	1.94	0.49
1:B:1:MET:HA	1:B:7:ILE:HD11	1.95	0.48
1:A:78:GLN:HE21	1:A:78:GLN:HB2	1.59	0.44
3:B:306:BGL:H4	3:B:310:BGL:H3	2.00	0.43
1:B:75:MET:O	1:B:78:GLN:HG3	2.19	0.43
1:B:147:TRP:HE1	3:B:302:BGL:H1	1.83	0.42
1:B:40:ILE:HB	1:B:41:PRO:HD3	2.01	0.42
1:B:54:ALA:HB3	1:B:91:ALA:HA	2.02	0.41
1:A:155:VAL:HG12	1:A:156:MET:HE2	2.02	0.41
1:A:40:ILE:HB	1:A:41:PRO:HD3	2.02	0.41
1:B:20:MET:HE3	1:B:23:SER:HB2	2.01	0.41
1:A:103:ASN:HB3	1:A:108:GLN:HB2	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	181/214 (85%)	178 (98%)	3 (2%)	0	100	100
1	B	184/214 (86%)	181 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	365/428 (85%)	359 (98%)	6 (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	141/174 (81%)	138 (98%)	3 (2%)	47	75
1	B	141/174 (81%)	140 (99%)	1 (1%)	76	86
All	All	282/348 (81%)	278 (99%)	4 (1%)	59	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	70	LYS
1	A	78	GLN
1	B	78	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	B	103	ASN
1	B	107	ASN
1	B	157	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 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$
3	BGL	A	306	-	20,20,20	1.17	2 (10%)	24,25,25	1.23	3 (12%)
3	BGL	A	304	-	20,20,20	1.19	3 (15%)	24,25,25	1.12	2 (8%)
3	BGL	A	305	-	20,20,20	1.24	2 (10%)	24,25,25	1.14	3 (12%)
3	BGL	B	303	-	20,20,20	1.22	2 (10%)	24,25,25	1.25	3 (12%)
3	BGL	B	307	-	20,20,20	1.14	3 (15%)	24,25,25	1.36	2 (8%)
3	BGL	B	302	-	20,20,20	1.19	4 (20%)	24,25,25	1.26	4 (16%)
3	BGL	B	309	-	18,18,20	1.24	3 (16%)	22,23,25	1.31	3 (13%)
3	BGL	A	307	-	18,18,20	1.25	3 (16%)	22,23,25	1.17	2 (9%)
2	TPP	A	301	-	26,27,27	1.83	7 (26%)	38,40,40	1.56	10 (26%)
3	BGL	B	304	-	20,20,20	1.18	2 (10%)	24,25,25	1.31	3 (12%)
3	BGL	B	305	-	20,20,20	1.20	3 (15%)	24,25,25	1.22	4 (16%)
3	BGL	A	303	-	18,18,20	1.23	4 (22%)	22,23,25	1.27	2 (9%)
3	BGL	B	308	-	18,18,20	1.29	2 (11%)	22,23,25	1.29	3 (13%)
3	BGL	A	302	-	18,18,20	1.25	3 (16%)	22,23,25	1.24	3 (13%)
3	BGL	B	310	-	20,20,20	1.20	3 (15%)	24,25,25	1.23	3 (12%)
2	TPP	B	301	-	26,27,27	1.83	8 (30%)	38,40,40	1.56	11 (28%)
3	BGL	B	306	-	20,20,20	1.18	3 (15%)	24,25,25	1.21	2 (8%)

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	BGL	A	306	-	-	5/11/31/31	0/1/1/1
3	BGL	A	304	-	-	1/11/31/31	0/1/1/1
3	BGL	A	305	-	-	3/11/31/31	0/1/1/1
3	BGL	B	303	-	-	4/11/31/31	0/1/1/1
3	BGL	B	307	-	-	7/11/31/31	0/1/1/1
3	BGL	B	302	-	-	4/11/31/31	0/1/1/1
3	BGL	B	309	-	-	1/9/29/31	0/1/1/1
3	BGL	A	307	-	-	4/9/29/31	0/1/1/1
2	TPP	A	301	-	-	4/17/17/17	0/2/2/2
3	BGL	B	304	-	-	3/11/31/31	0/1/1/1
3	BGL	B	305	-	-	2/11/31/31	0/1/1/1
3	BGL	A	303	-	-	2/9/29/31	0/1/1/1
3	BGL	B	308	-	-	4/9/29/31	0/1/1/1
3	BGL	A	302	-	-	2/9/29/31	0/1/1/1
3	BGL	B	310	-	-	3/11/31/31	0/1/1/1
2	TPP	B	301	-	-	4/17/17/17	0/2/2/2
3	BGL	B	306	-	-	1/11/31/31	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	TPP	C5-S1	-5.11	1.59	1.72
2	B	301	TPP	C5-S1	-5.03	1.59	1.72
3	A	305	BGL	C1-C2	-3.32	1.50	1.52
3	B	308	BGL	C1-C2	-3.26	1.50	1.52
3	B	303	BGL	C1-C2	-3.15	1.50	1.52
3	B	310	BGL	C1-C2	-3.00	1.50	1.52
3	B	305	BGL	C1-C2	-2.92	1.50	1.52
3	B	304	BGL	C1-C2	-2.90	1.50	1.52
2	B	301	TPP	C2-S1	-2.90	1.60	1.69
3	A	306	BGL	C1-C2	-2.88	1.50	1.52
3	A	302	BGL	C1-C2	-2.86	1.50	1.52
3	A	307	BGL	C1-C2	-2.85	1.50	1.52
2	A	301	TPP	C2-S1	-2.84	1.60	1.69
3	A	304	BGL	C1-C2	-2.79	1.50	1.52
3	B	307	BGL	C1-C2	-2.77	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	309	BGL	C1-C2	-2.77	1.50	1.52
2	A	301	TPP	C2'-N1'	2.66	1.38	1.34
3	B	306	BGL	C1-C2	-2.65	1.50	1.52
2	B	301	TPP	C2'-N1'	2.65	1.38	1.34
2	A	301	TPP	C2'-N3'	2.64	1.38	1.34
2	B	301	TPP	C2'-N3'	2.63	1.38	1.34
2	A	301	TPP	C4'-N3'	2.62	1.38	1.35
2	B	301	TPP	C4'-N3'	2.62	1.38	1.35
3	B	302	BGL	C1-C2	-2.53	1.50	1.52
3	A	303	BGL	C1-C2	-2.50	1.50	1.52
3	B	302	BGL	C3-C2	-2.45	1.45	1.52
3	B	308	BGL	C3-C2	-2.40	1.45	1.52
3	B	310	BGL	C3-C2	-2.38	1.45	1.52
3	A	302	BGL	C3-C2	-2.37	1.45	1.52
3	B	305	BGL	C3-C2	-2.35	1.45	1.52
3	B	304	BGL	C3-C2	-2.35	1.45	1.52
3	B	303	BGL	C3-C2	-2.35	1.45	1.52
3	A	307	BGL	C3-C2	-2.34	1.45	1.52
2	A	301	TPP	C2-N3	2.33	1.38	1.32
3	A	305	BGL	C3-C2	-2.33	1.46	1.52
3	A	304	BGL	C3-C2	-2.31	1.46	1.52
3	A	303	BGL	C3-C2	-2.31	1.46	1.52
2	B	301	TPP	C2-N3	2.31	1.37	1.32
3	B	306	BGL	C3-C2	-2.30	1.46	1.52
3	B	309	BGL	C3-C2	-2.28	1.46	1.52
3	A	306	BGL	C3-C2	-2.25	1.46	1.52
3	A	303	BGL	O5-C1	2.15	1.48	1.42
2	A	301	TPP	C4-N3	-2.14	1.35	1.39
3	B	302	BGL	O5-C1	2.14	1.48	1.42
3	B	306	BGL	O5-C1	2.12	1.48	1.42
2	B	301	TPP	C4-N3	-2.11	1.35	1.39
2	B	301	TPP	C5'-C4'	-2.08	1.39	1.42
3	B	305	BGL	O5-C1	2.08	1.48	1.42
3	B	307	BGL	C3-C2	-2.08	1.46	1.52
3	B	309	BGL	O5-C1	2.07	1.47	1.42
3	A	302	BGL	O5-C1	2.05	1.47	1.42
3	A	304	BGL	O5-C1	2.04	1.47	1.42
3	B	310	BGL	O5-C1	2.03	1.47	1.42
3	B	307	BGL	O5-C1	2.02	1.47	1.42
3	A	303	BGL	C4-C3	-2.02	1.47	1.52
3	B	302	BGL	C4-C3	-2.01	1.47	1.52
3	A	307	BGL	O5-C1	2.00	1.47	1.42

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	307	BGL	C1'-O2-C2	3.58	121.97	114.02
2	B	301	TPP	N1'-C2'-N3'	-3.26	120.10	125.53
2	A	301	TPP	N1'-C2'-N3'	-3.26	120.11	125.53
2	A	301	TPP	C6'-C5'-C4'	3.24	119.53	115.55
2	B	301	TPP	C6'-C5'-C4'	3.21	119.49	115.55
3	B	309	BGL	C1'-O2-C2	3.16	121.04	114.02
3	B	306	BGL	C1'-O2-C2	3.04	120.77	114.02
3	B	304	BGL	C1'-O2-C2	3.04	120.76	114.02
3	A	303	BGL	C1'-O2-C2	3.02	120.72	114.02
3	A	306	BGL	C1'-O2-C2	2.89	120.44	114.02
3	B	302	BGL	C1'-O2-C2	2.86	120.37	114.02
2	A	301	TPP	C6-C5-S1	-2.84	114.24	120.90
3	B	310	BGL	C1'-O2-C2	2.72	120.06	114.02
3	B	308	BGL	C1'-O2-C2	2.72	120.05	114.02
3	B	304	BGL	O5-C5-C4	2.70	114.56	109.70
3	A	307	BGL	C1'-O2-C2	2.70	120.01	114.02
2	B	301	TPP	C6-C5-S1	-2.68	114.63	120.90
3	B	305	BGL	O2-C1'-C2'	2.67	118.41	109.37
3	A	302	BGL	C1'-O2-C2	2.66	119.94	114.02
3	A	304	BGL	O2-C1'-C2'	2.64	118.32	109.37
3	A	305	BGL	C1'-O2-C2	2.64	119.88	114.02
3	B	303	BGL	C1'-O2-C2	2.62	119.84	114.02
3	B	308	BGL	O5-C5-C4	2.60	114.39	109.70
3	A	306	BGL	O2-C1'-C2'	2.57	118.09	109.37
3	A	304	BGL	C1'-O2-C2	2.52	119.62	114.02
3	B	308	BGL	O2-C1'-C2'	2.50	117.86	109.37
3	B	303	BGL	O5-C5-C4	2.50	114.20	109.70
3	B	305	BGL	O5-C5-C4	2.48	114.17	109.70
3	B	310	BGL	O2-C1'-C2'	2.46	117.72	109.37
3	B	303	BGL	O2-C1'-C2'	2.45	117.68	109.37
3	A	302	BGL	O2-C1'-C2'	2.43	117.60	109.37
2	B	301	TPP	CM2-C2'-N1'	2.42	119.78	117.20
2	A	301	TPP	C6'-N1'-C2'	2.41	120.03	116.07
3	B	310	BGL	O5-C5-C4	2.40	114.03	109.70
3	A	305	BGL	O2-C1'-C2'	2.40	117.51	109.37
3	A	307	BGL	O2-C1'-C2'	2.38	117.44	109.37
2	B	301	TPP	C6'-N1'-C2'	2.36	119.95	116.07
3	B	302	BGL	C1-O5-C5	2.36	118.21	113.65
3	B	306	BGL	O2-C1'-C2'	2.35	117.34	109.37
3	A	303	BGL	O2-C1'-C2'	2.35	117.33	109.37
2	A	301	TPP	CM2-C2'-N1'	2.33	119.68	117.20
3	B	304	BGL	O2-C1'-C2'	2.33	117.27	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	BGL	O5-C5-C4	2.32	113.89	109.70
3	B	309	BGL	O2-C1'-C2'	2.31	117.21	109.37
3	B	305	BGL	C1'-O2-C2	2.31	119.15	114.02
3	A	302	BGL	O5-C5-C4	2.30	113.84	109.70
3	B	302	BGL	O2-C1'-C2'	2.27	117.06	109.37
3	B	307	BGL	O5-C5-C4	2.26	113.77	109.70
2	A	301	TPP	C4-C5-S1	2.26	114.08	110.56
2	A	301	TPP	C2-N3-C4	-2.20	111.08	114.06
2	A	301	TPP	C5'-C6'-N1'	-2.20	120.25	123.83
3	B	309	BGL	O5-C5-C4	2.19	113.64	109.70
2	B	301	TPP	C2-S1-C5	2.18	92.66	91.22
2	B	301	TPP	C5'-C6'-N1'	-2.17	120.30	123.83
2	B	301	TPP	C2-N3-C4	-2.16	111.14	114.06
3	A	305	BGL	O5-C5-C4	2.12	113.51	109.70
2	B	301	TPP	CM4-C4-N3	2.09	125.40	120.57
2	A	301	TPP	CM4-C4-N3	2.09	125.39	120.57
2	B	301	TPP	C4-C5-S1	2.08	113.81	110.56
2	B	301	TPP	N4'-C4'-N3'	2.07	119.82	117.03
2	A	301	TPP	CM2-C2'-N3'	2.06	120.21	117.13
3	B	305	BGL	C1-O5-C5	2.03	117.58	113.65
3	B	302	BGL	O5-C5-C4	2.01	113.31	109.70

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TPP	C7-O7-PA-O2A
2	B	301	TPP	C7-O7-PA-O1A
2	B	301	TPP	C7-O7-PA-O3A
3	B	308	BGL	C2'-C1'-O2-C2
3	A	306	BGL	O5-C5-C6-O6
3	B	310	BGL	O5-C5-C6-O6
3	A	307	BGL	O5-C5-C6-O6
3	B	307	BGL	O5-C5-C6-O6
3	B	302	BGL	C4-C5-C6-O6
3	B	307	BGL	C4-C5-C6-O6
3	B	308	BGL	O5-C5-C6-O6
3	A	307	BGL	C4-C5-C6-O6
3	A	306	BGL	C4-C5-C6-O6
3	B	305	BGL	C2'-C3'-C4'-C5'
3	B	310	BGL	C4-C5-C6-O6
3	B	302	BGL	O5-C5-C6-O6

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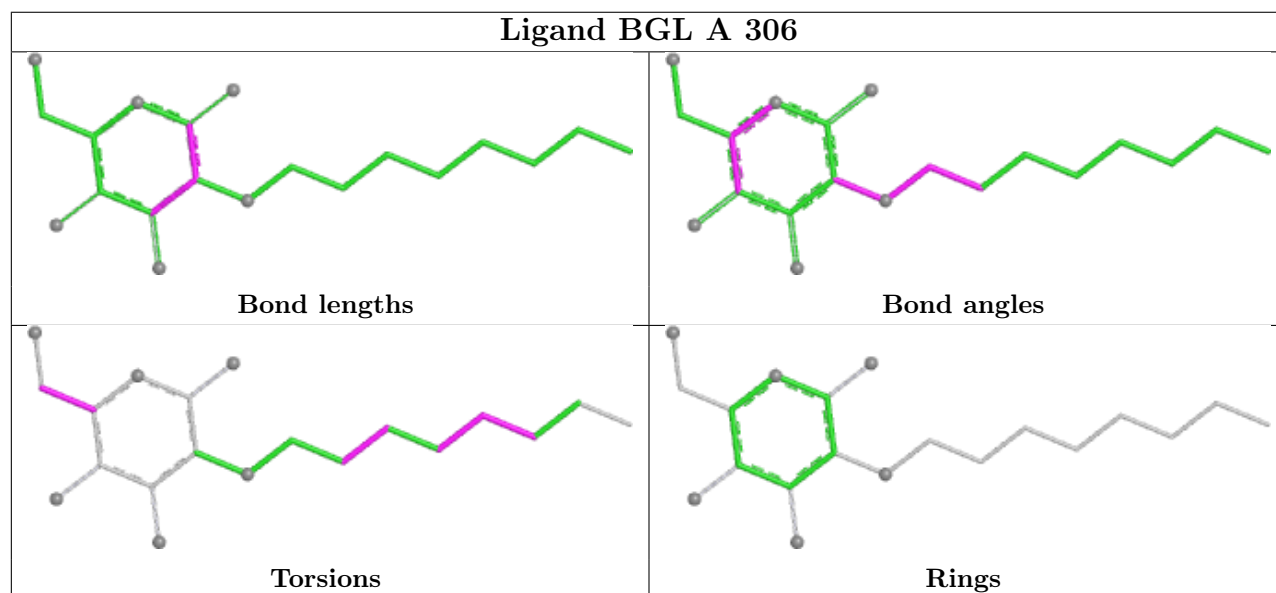
Mol	Chain	Res	Type	Atoms
3	B	309	BGL	O5-C5-C6-O6
3	B	302	BGL	C2'-C1'-O2-C2
3	B	307	BGL	C2'-C1'-O2-C2
3	B	307	BGL	O2-C1'-C2'-C3'
3	A	302	BGL	C1'-C2'-C3'-C4'
3	A	305	BGL	C1'-C2'-C3'-C4'
3	B	307	BGL	C1'-C2'-C3'-C4'
3	A	306	BGL	C4'-C5'-C6'-C7'
3	B	305	BGL	C4'-C5'-C6'-C7'
3	B	302	BGL	O2-C1'-C2'-C3'
3	B	303	BGL	O5-C5-C6-O6
3	B	304	BGL	O5-C5-C6-O6
3	B	303	BGL	C1'-C2'-C3'-C4'
3	B	304	BGL	C2'-C3'-C4'-C5'
3	A	305	BGL	O2-C1'-C2'-C3'
3	A	303	BGL	O5-C5-C6-O6
3	A	307	BGL	C3'-C4'-C5'-C6'
3	B	307	BGL	C4'-C5'-C6'-C7'
2	B	301	TPP	PB-O3A-PA-O1A
3	B	308	BGL	C4-C5-C6-O6
3	B	303	BGL	C4-C5-C6-O6
3	A	306	BGL	C3'-C4'-C5'-C6'
3	B	308	BGL	O2-C1'-C2'-C3'
3	A	305	BGL	C4'-C5'-C6'-C7'
3	A	307	BGL	C1'-C2'-C3'-C4'
3	A	304	BGL	O2-C1'-C2'-C3'
3	A	303	BGL	C1'-C2'-C3'-C4'
2	A	301	TPP	C7-O7-PA-O1A
2	A	301	TPP	C7-O7-PA-O3A
3	B	307	BGL	C2'-C3'-C4'-C5'
3	B	306	BGL	O2-C1'-C2'-C3'
3	A	306	BGL	C1'-C2'-C3'-C4'
3	B	303	BGL	C2'-C1'-O2-C2
3	B	304	BGL	C1'-C2'-C3'-C4'
2	B	301	TPP	PB-O3A-PA-O2A
3	B	310	BGL	C3'-C4'-C5'-C6'
3	A	302	BGL	O2-C1'-C2'-C3'
2	A	301	TPP	PB-O3A-PA-O2A

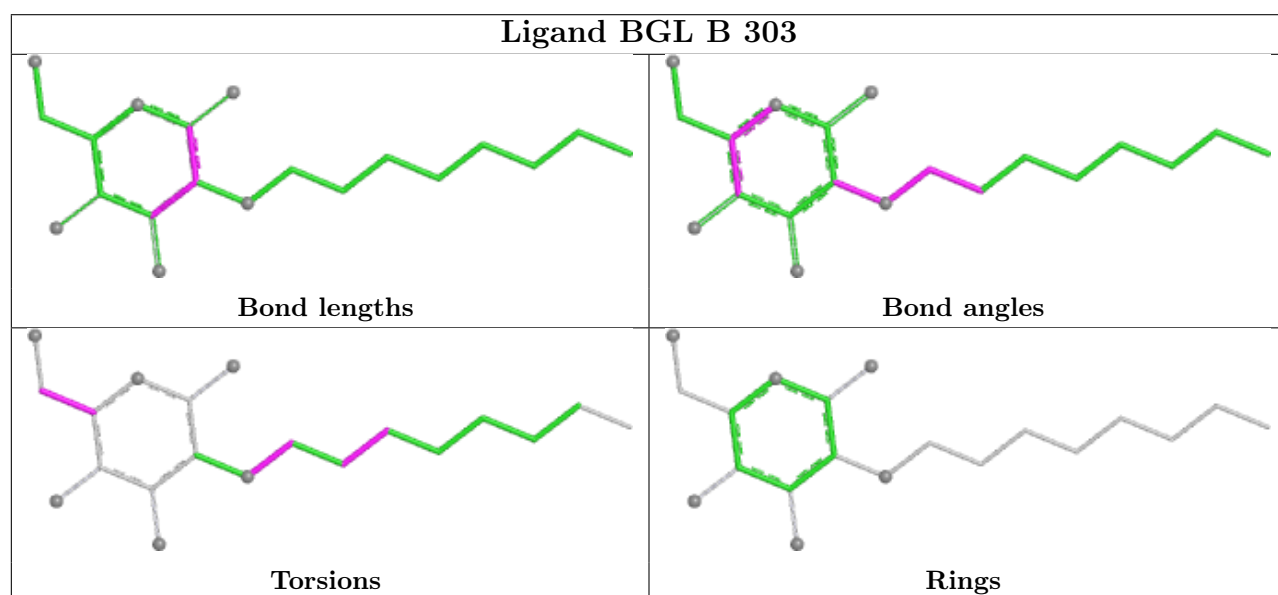
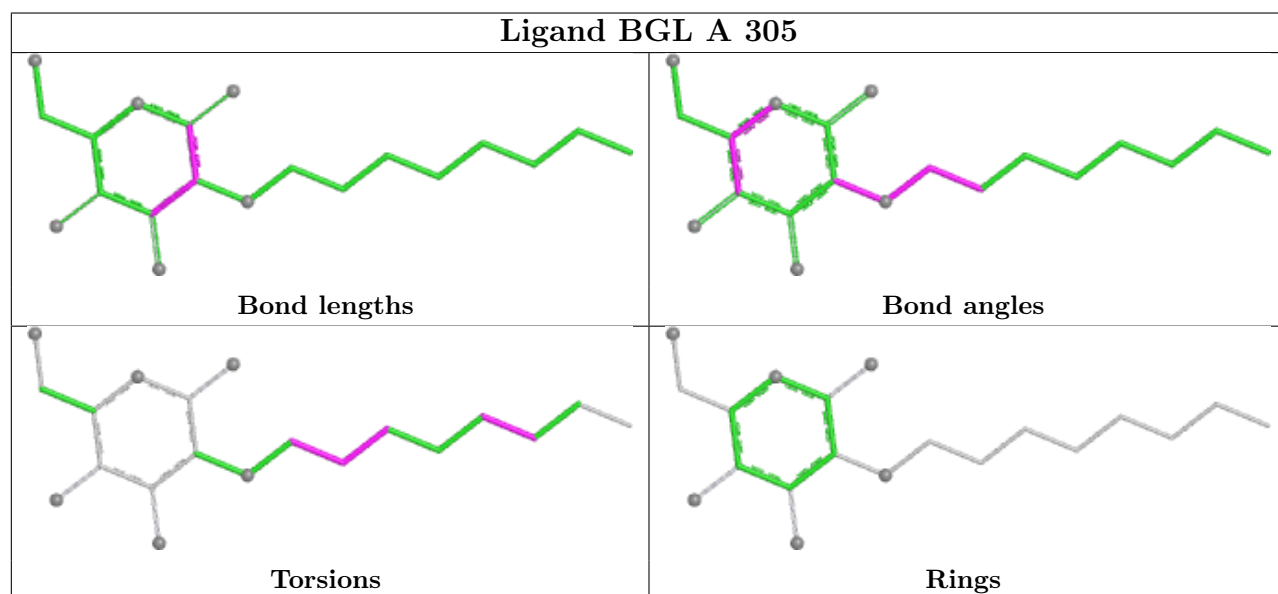
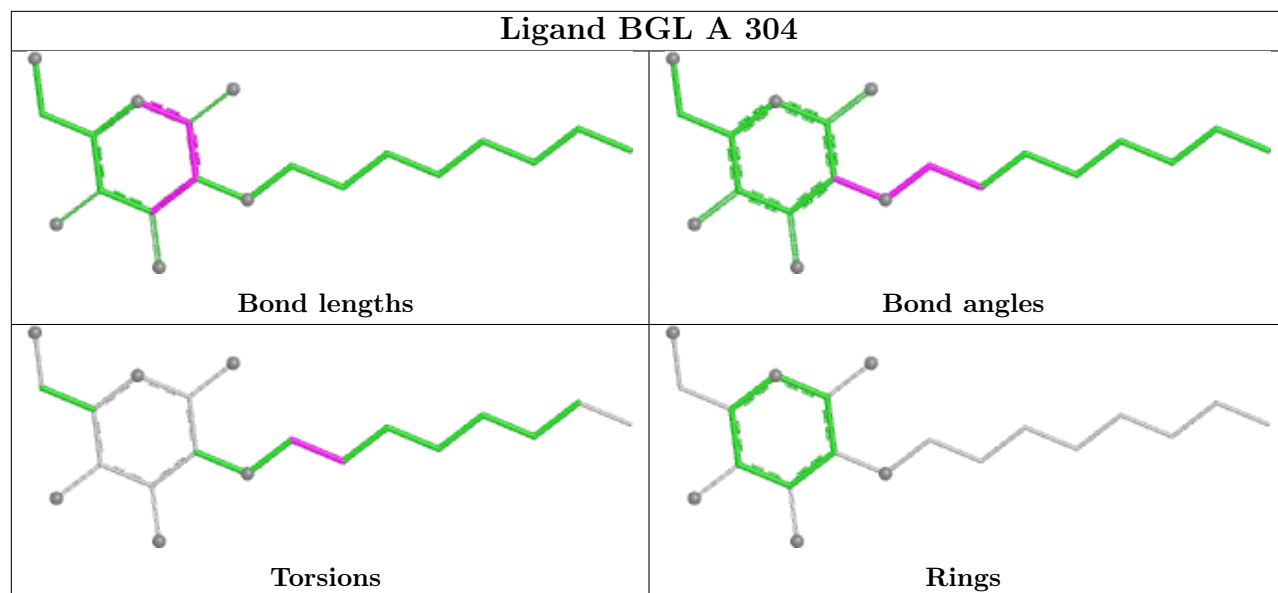
There are no ring outliers.

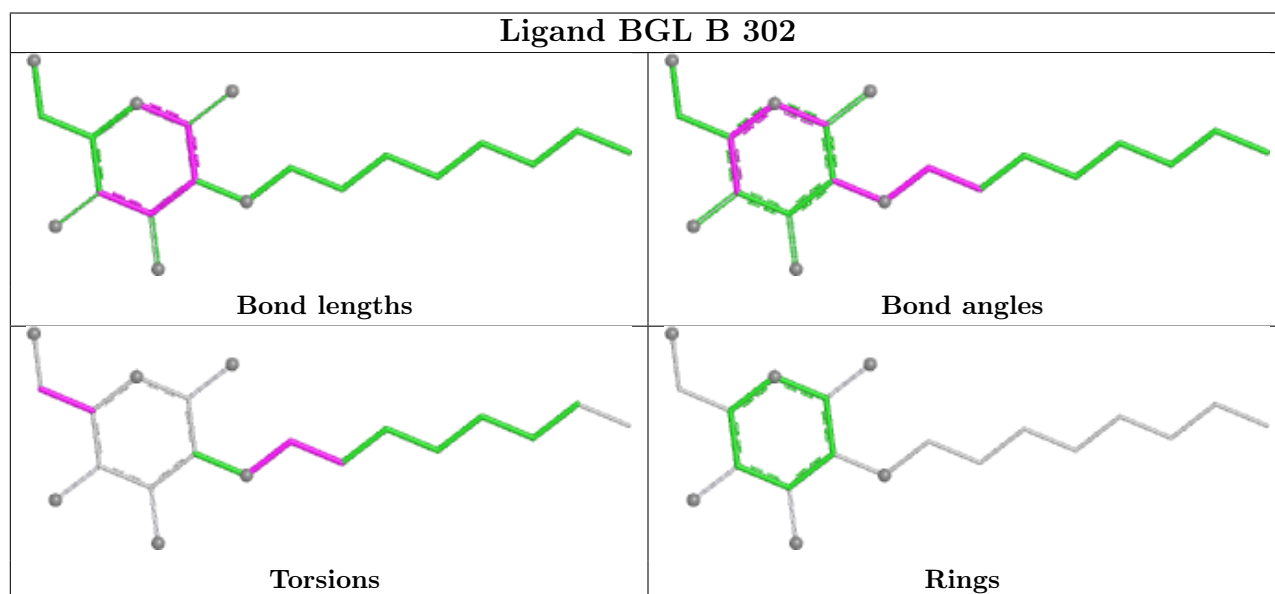
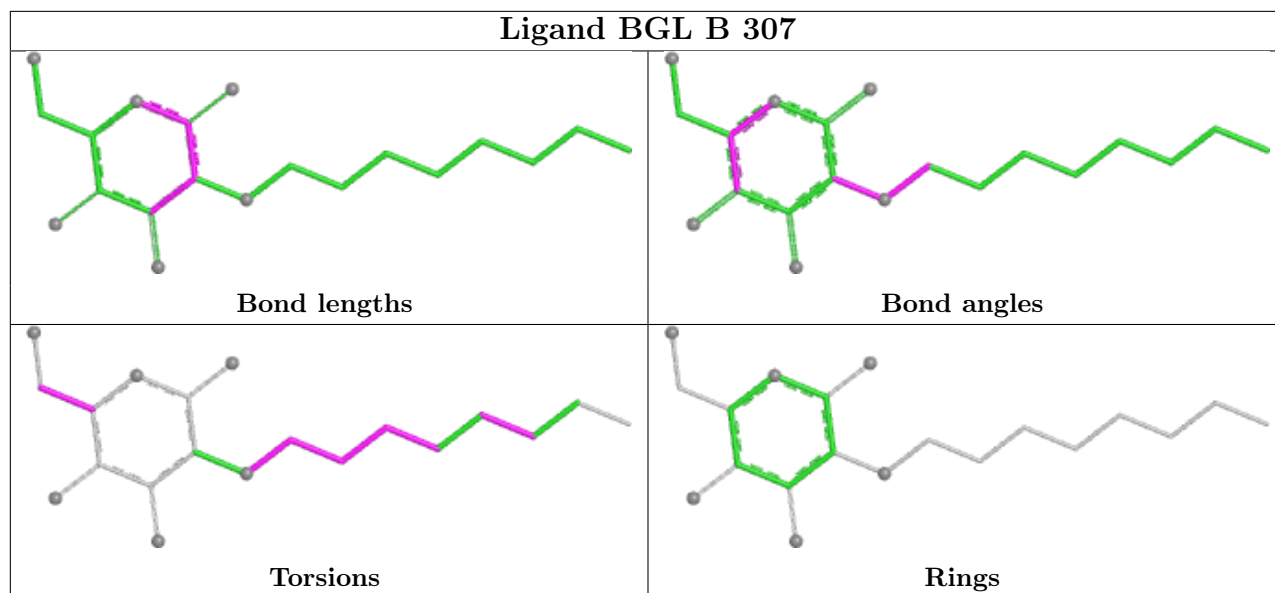
8 monomers are involved in 9 short contacts:

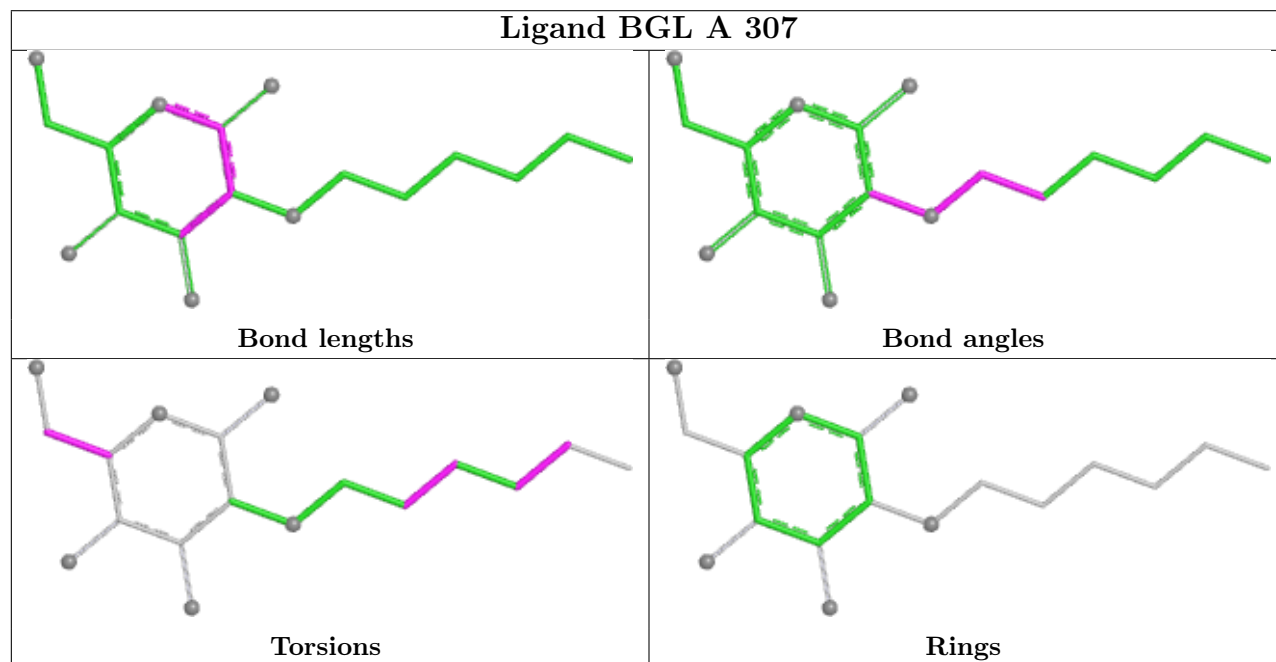
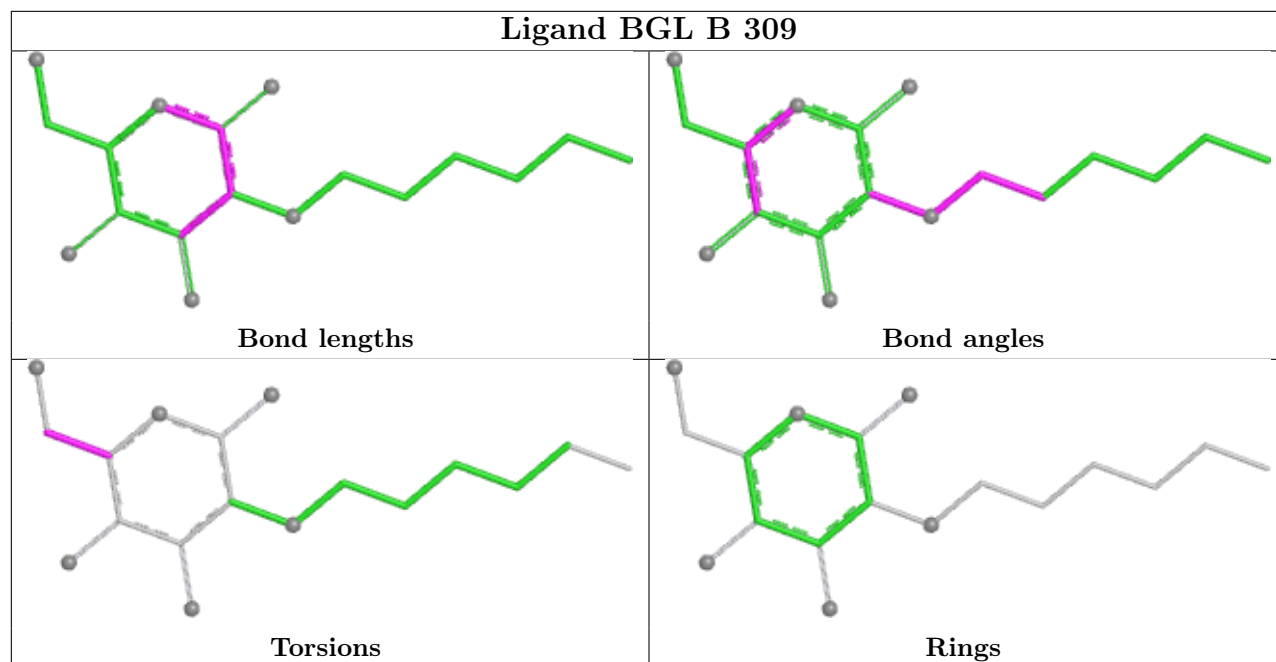
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	BGL	3	0
3	A	305	BGL	4	0
3	B	302	BGL	1	0
2	A	301	TPP	1	0
3	A	303	BGL	1	0
3	B	310	BGL	1	0
2	B	301	TPP	1	0
3	B	306	BGL	1	0

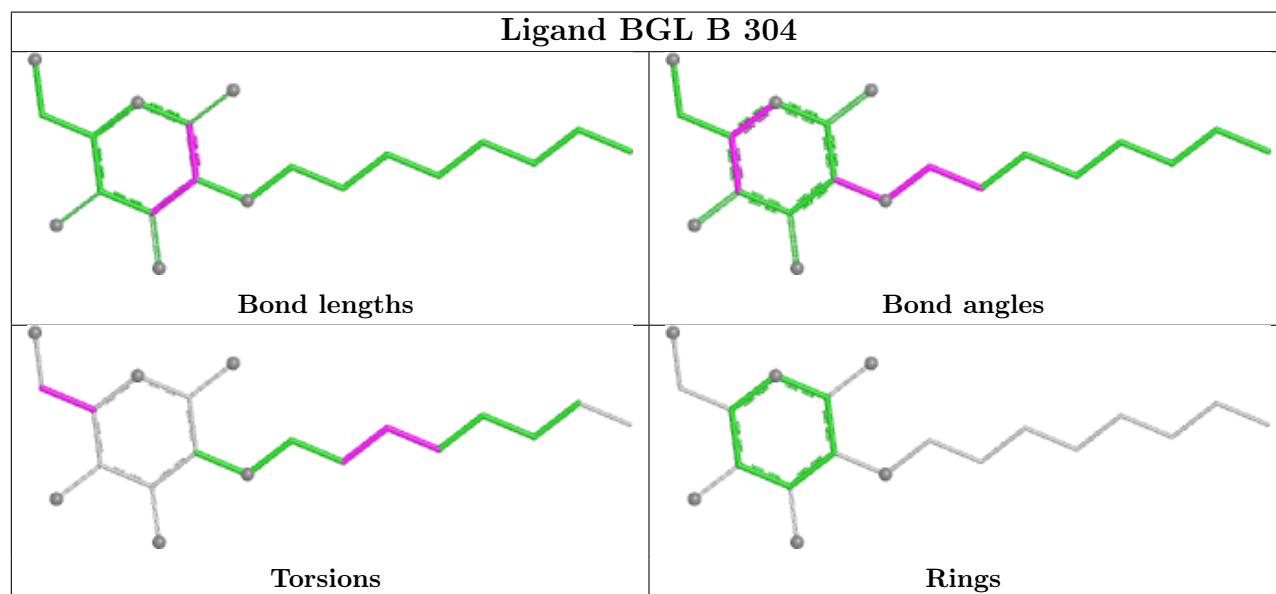
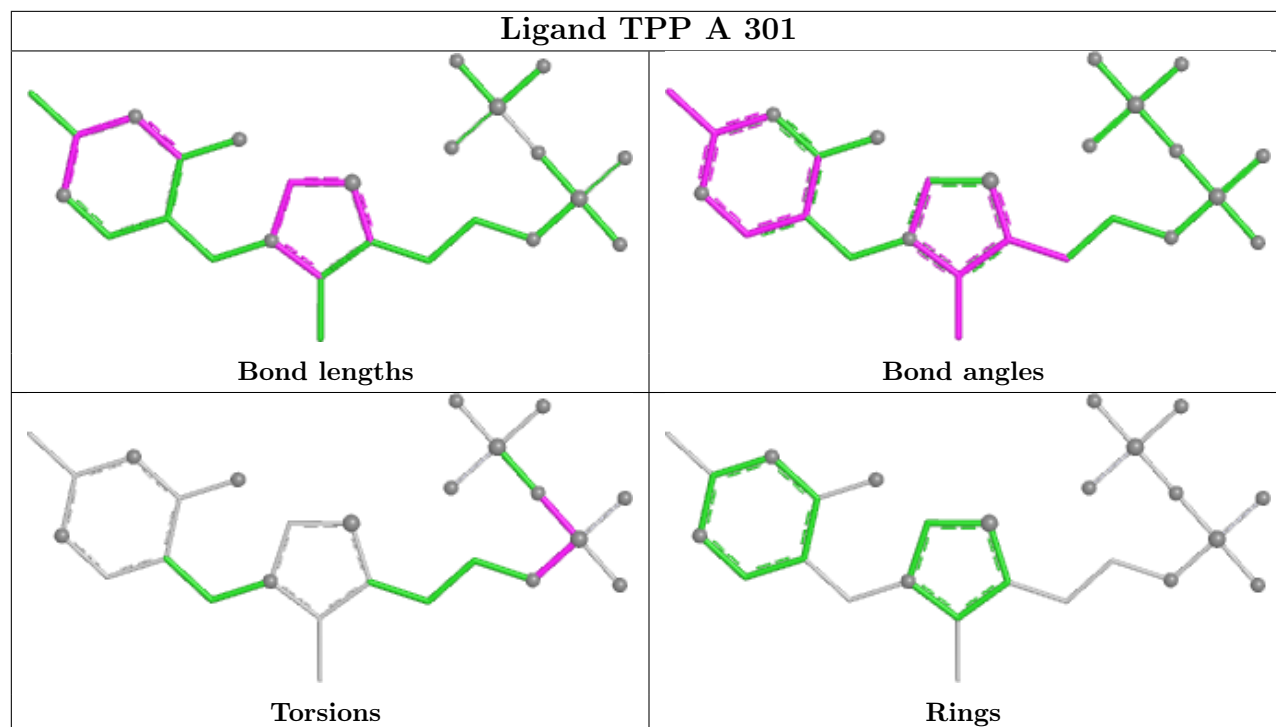
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

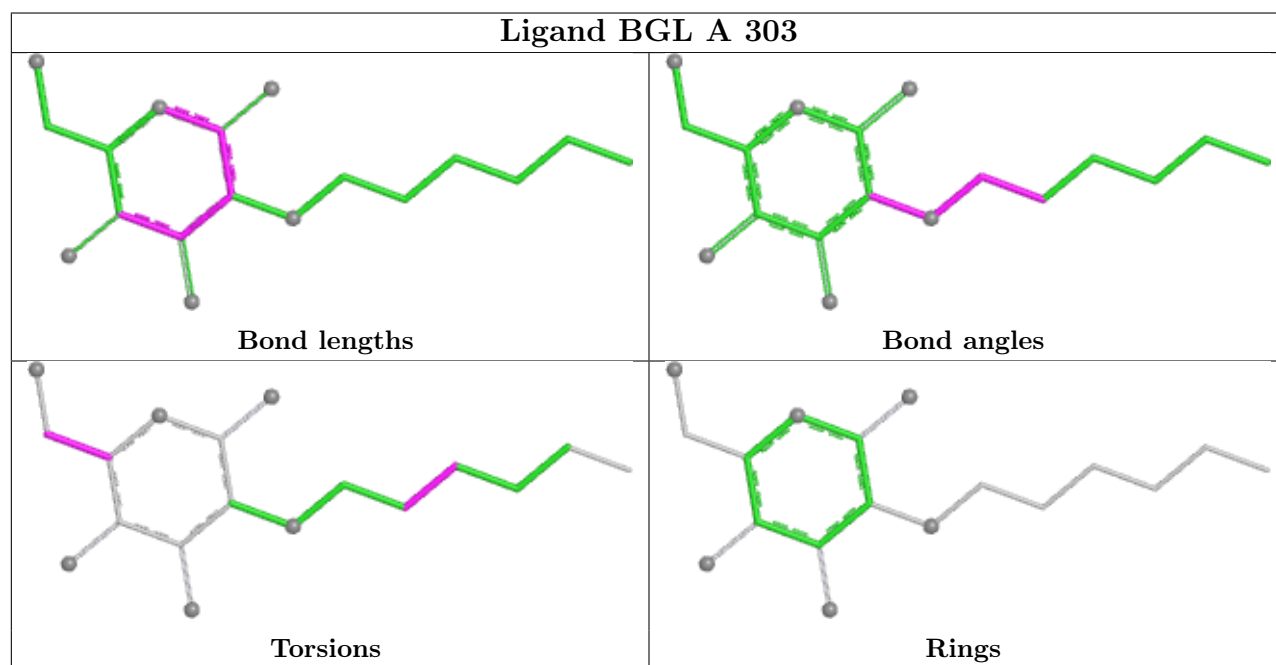
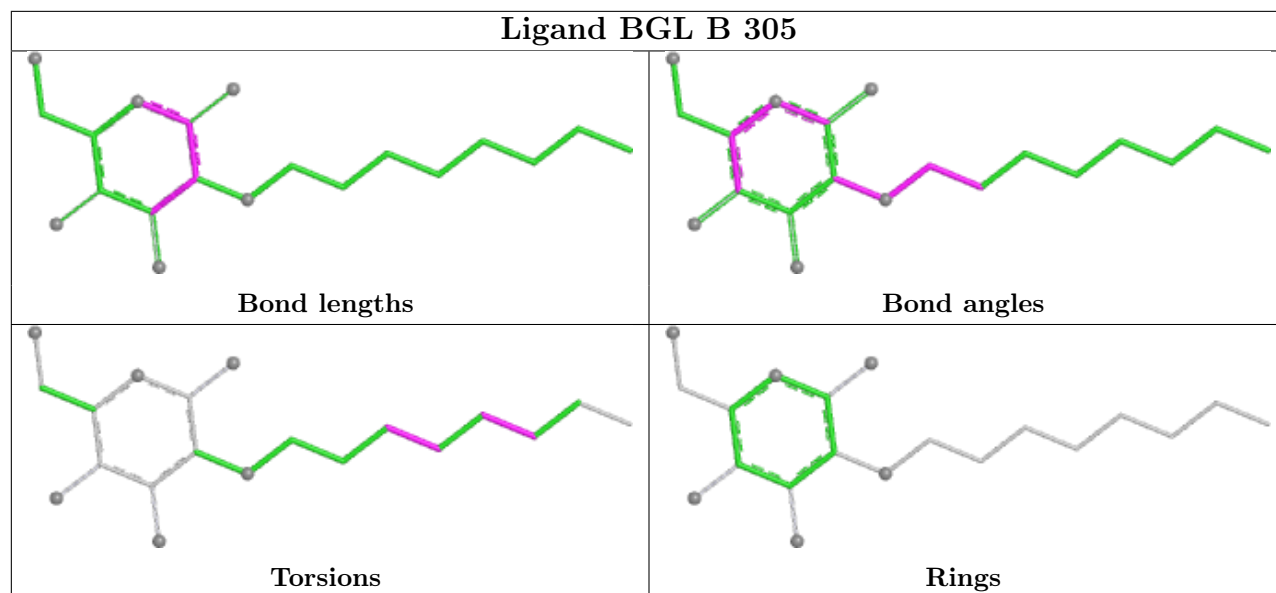


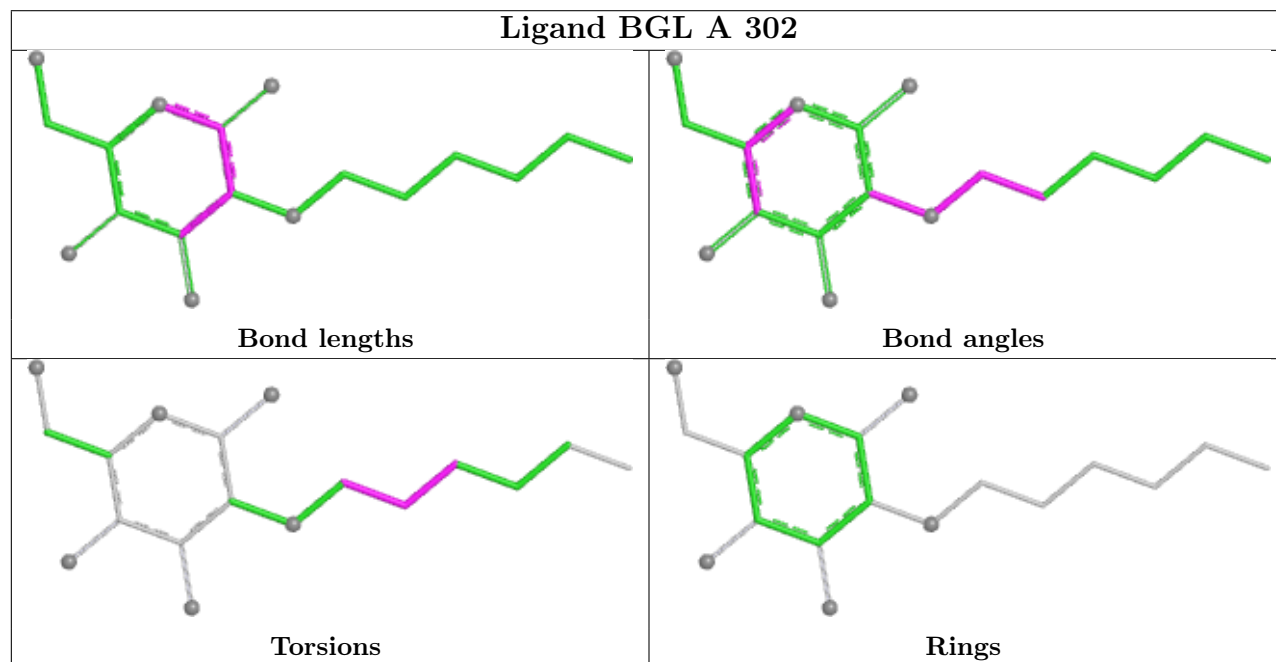
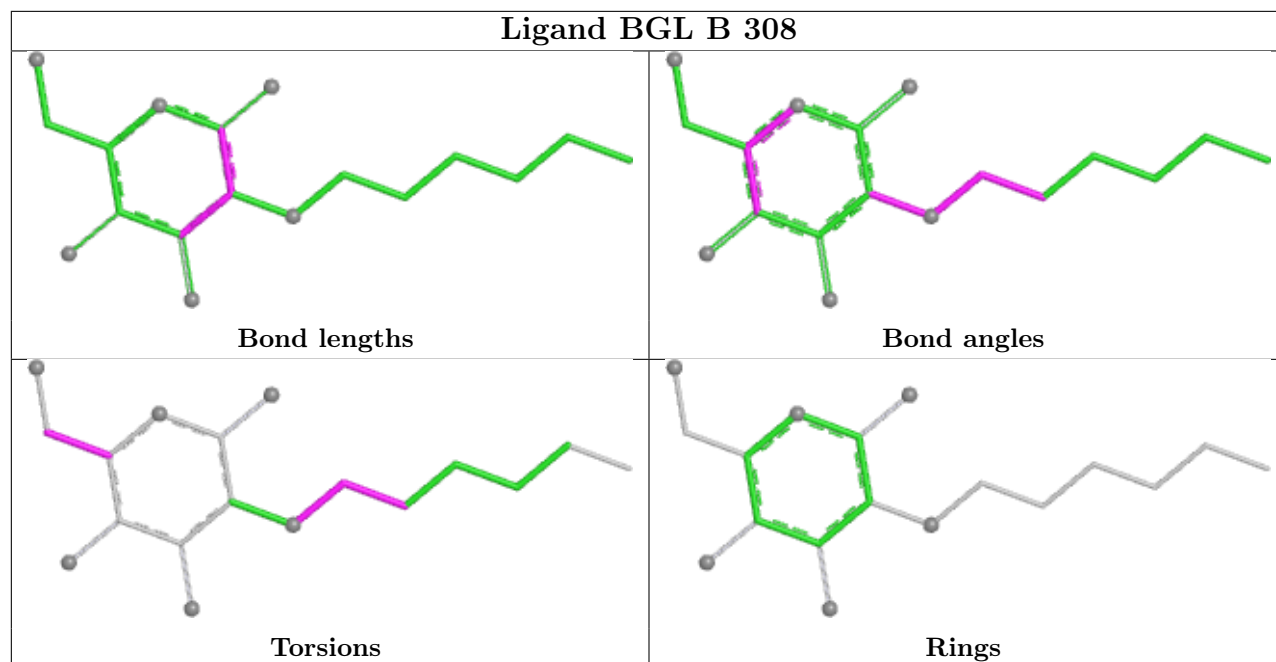


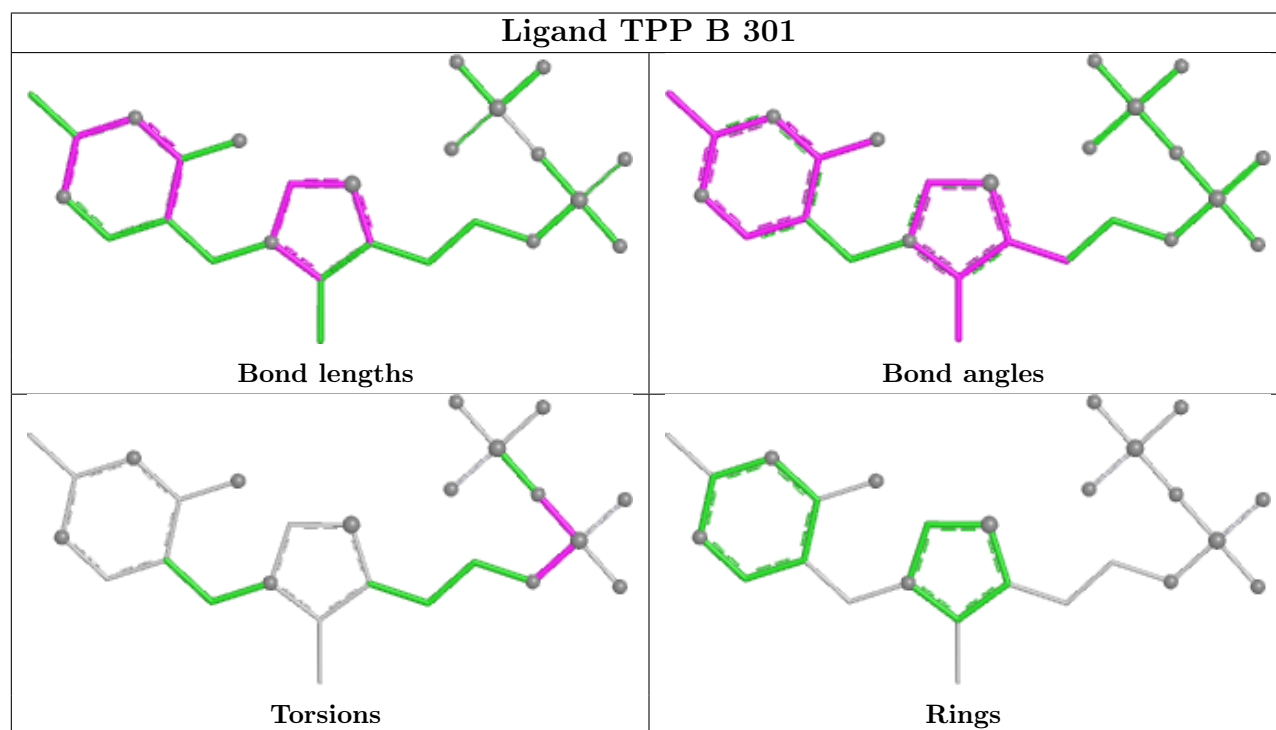
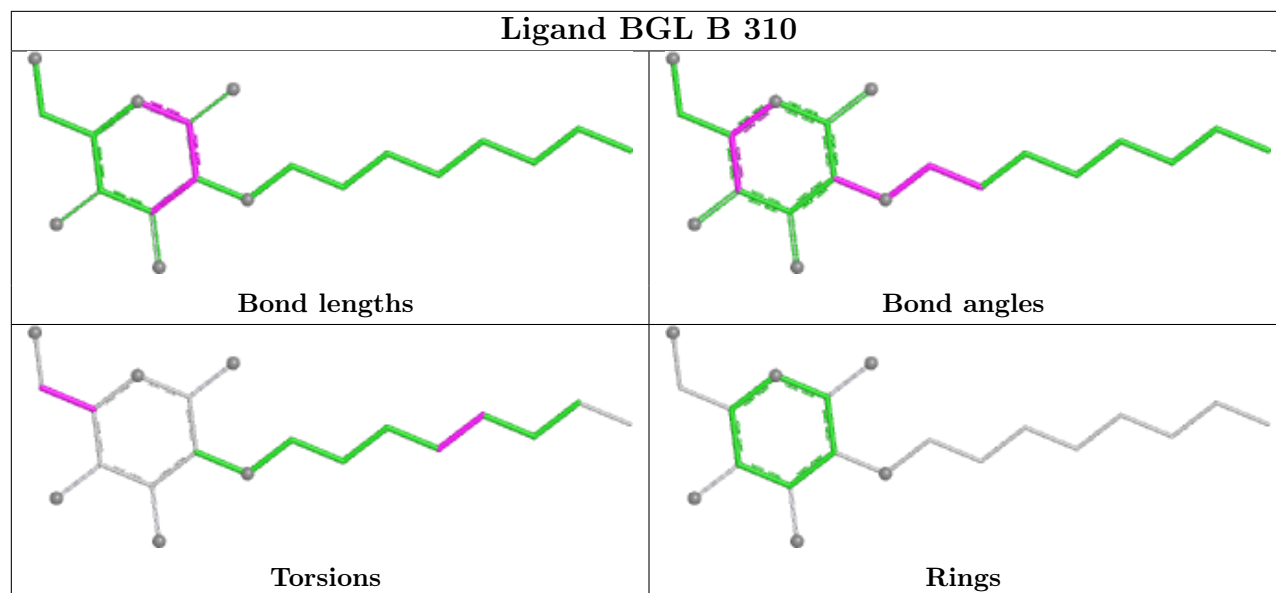


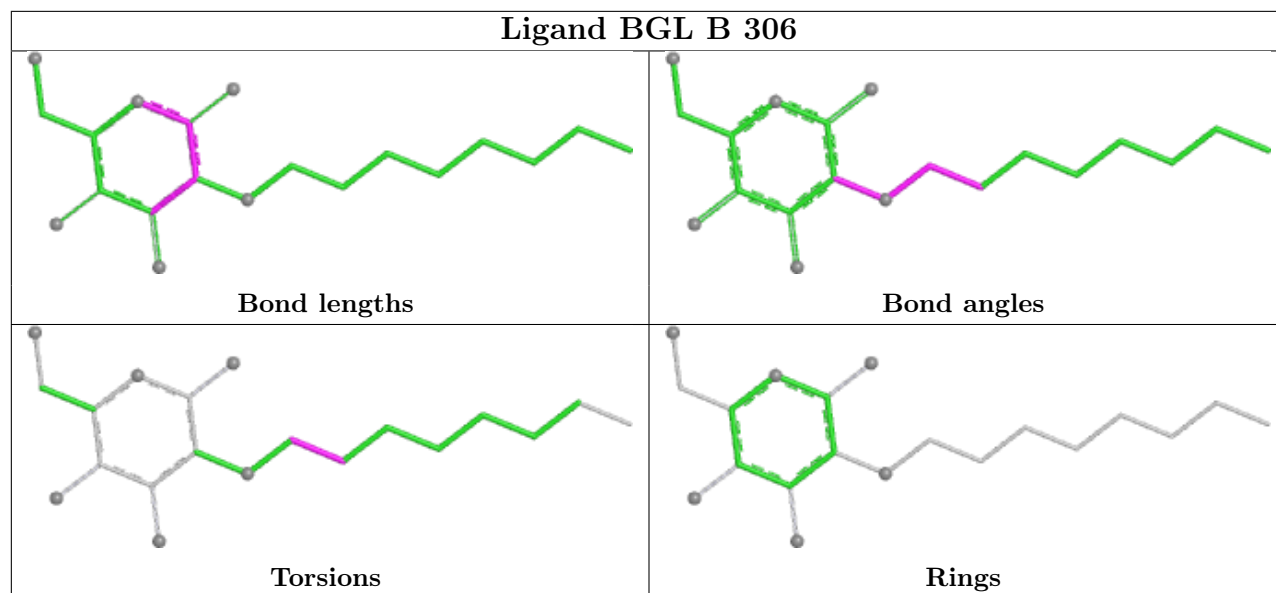












## 5.7 Other polymers [i](#)

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 [i](#)

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

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	183/214 (85%)	-0.16	4 (2%) 62 39	25, 51, 73, 99	1 (0%)
1	B	186/214 (86%)	-0.22	2 (1%) 78 57	36, 51, 74, 104	0
All	All	369/428 (86%)	-0.19	6 (1%) 70 47	25, 51, 75, 104	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	VAL	3.2
1	A	3	ASN	2.6
1	A	75	MET	2.3
1	A	72	TYR	2.2
1	A	125	VAL	2.2
1	B	145	GLN	2.1

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

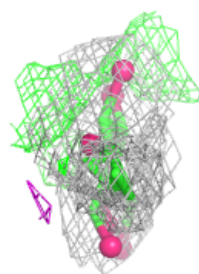
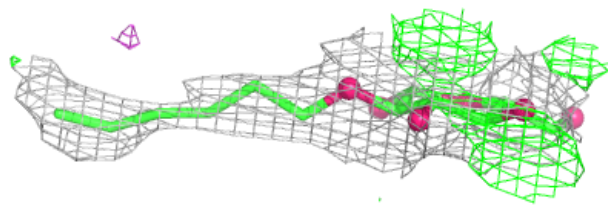
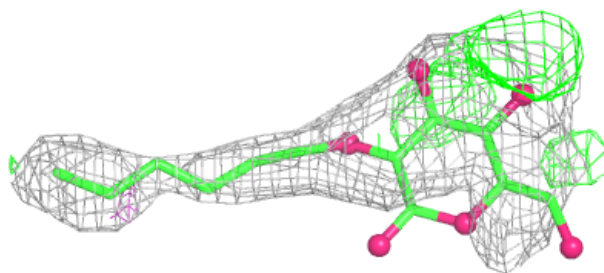
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	BGL	A	302	18/20	0.72	0.27	46,112,130,133	0
3	BGL	B	309	18/20	0.76	0.24	46,93,109,122	0
3	BGL	A	307	18/20	0.79	0.18	54,80,90,94	0
3	BGL	B	308	18/20	0.84	0.15	39,72,80,84	0
3	BGL	B	307	20/20	0.85	0.16	40,81,105,108	0
3	BGL	A	303	18/20	0.86	0.19	46,95,106,111	0
3	BGL	A	306	20/20	0.87	0.16	46,89,106,112	0
3	BGL	B	304	20/20	0.87	0.18	30,107,116,117	0
3	BGL	B	306	20/20	0.87	0.14	31,74,101,106	0
3	BGL	A	304	20/20	0.88	0.15	40,72,88,97	0
3	BGL	B	310	20/20	0.88	0.13	42,86,102,104	0
3	BGL	A	305	20/20	0.89	0.16	47,88,102,109	0
3	BGL	B	303	20/20	0.89	0.14	32,64,102,103	0
3	BGL	B	302	20/20	0.90	0.14	30,79,101,106	0
3	BGL	B	305	20/20	0.92	0.13	29,78,84,85	0
2	TPP	B	301	26/26	0.94	0.09	41,55,74,188	0
2	TPP	A	301	26/26	0.94	0.10	36,45,86,113	0

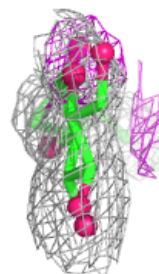
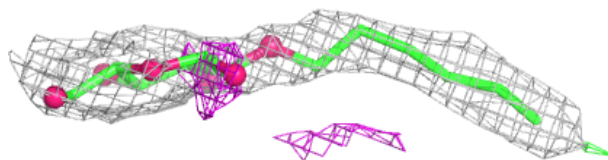
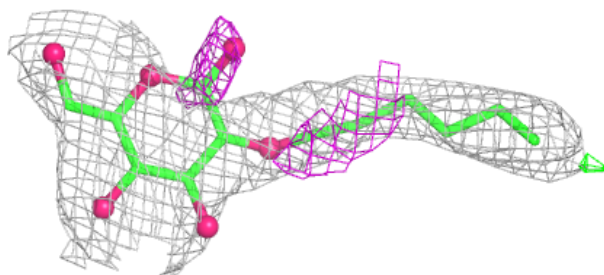
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BGL A 302:**

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

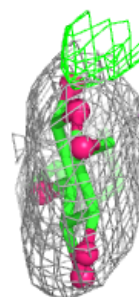
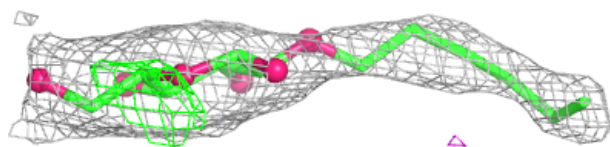
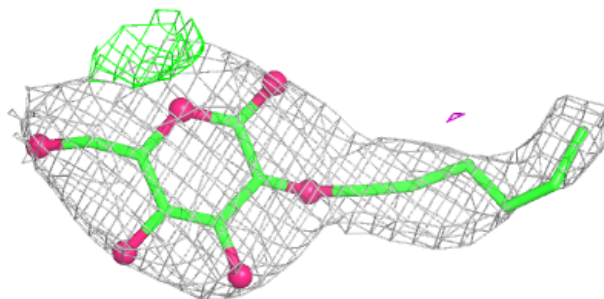
**Electron density around BGL B 309:**

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

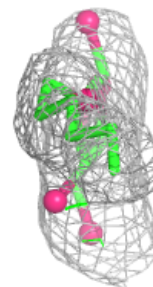
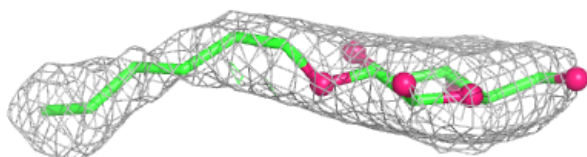
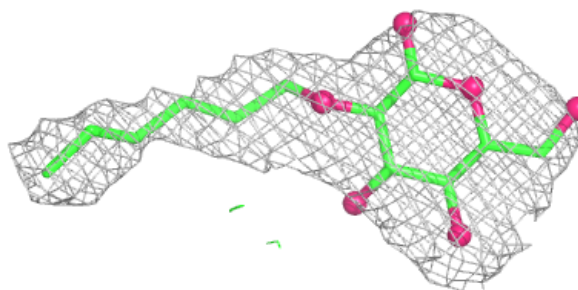


**Electron density around BGL A 307:**

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

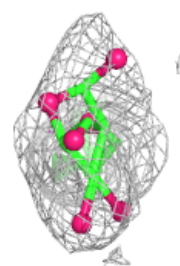
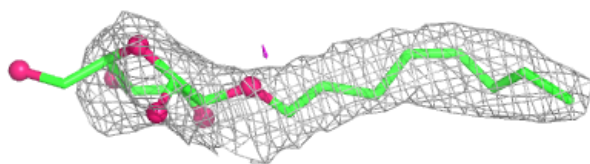
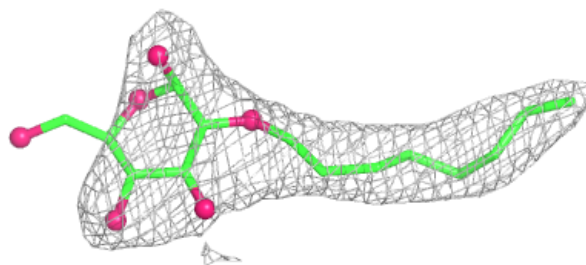
**Electron density around BGL B 308:**

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

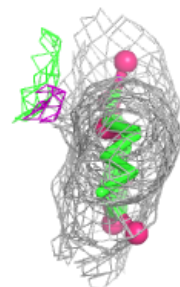
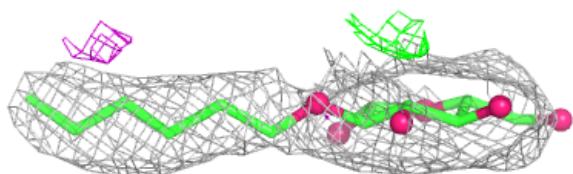
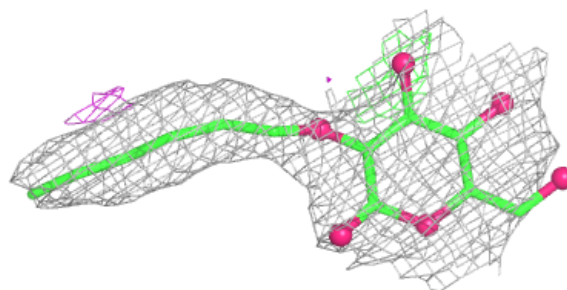


**Electron density around BGL B 307:**

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

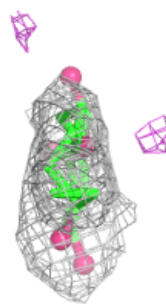
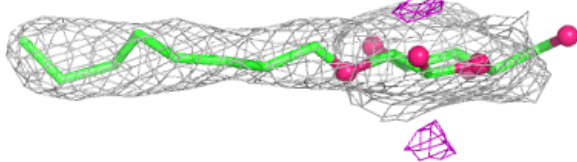
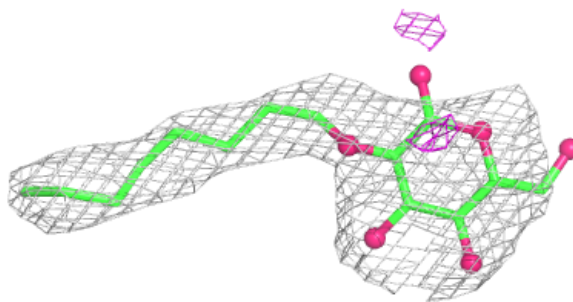
**Electron density around BGL A 303:**

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

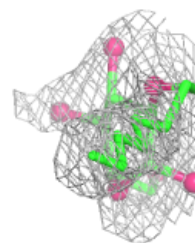
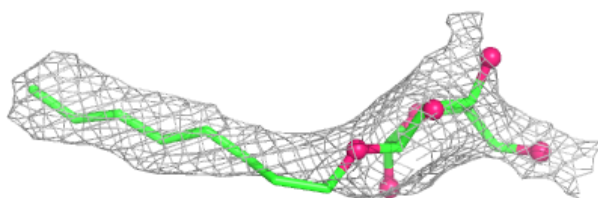
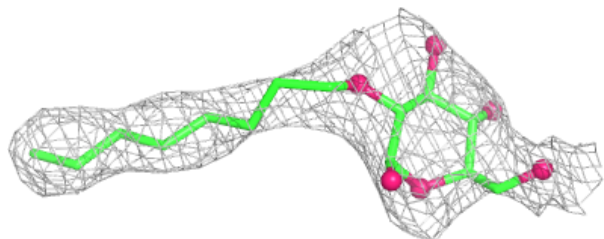


**Electron density around BGL A 306:**

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

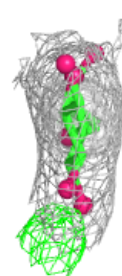
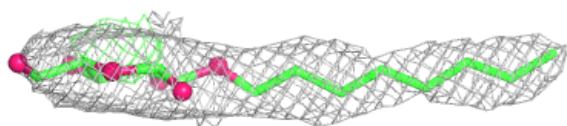
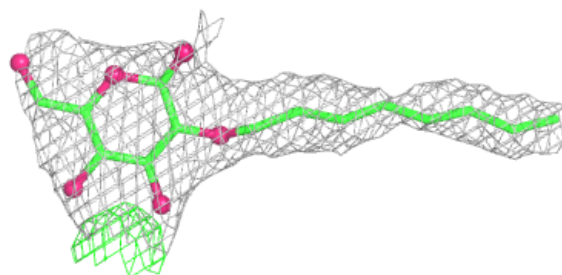
**Electron density around BGL B 304:**

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

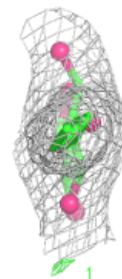
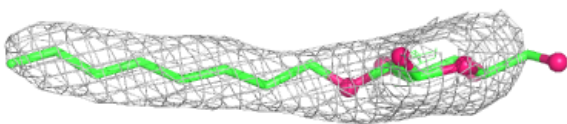


**Electron density around BGL B 306:**

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

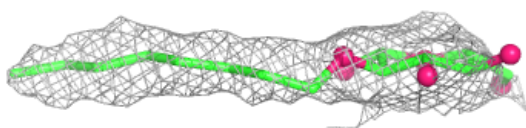
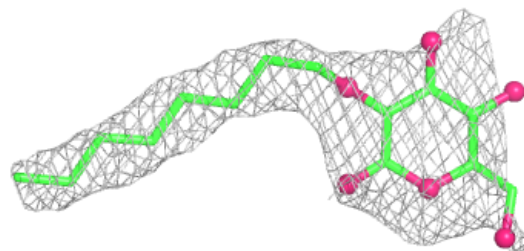
**Electron density around BGL A 304:**

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

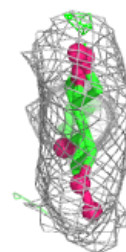
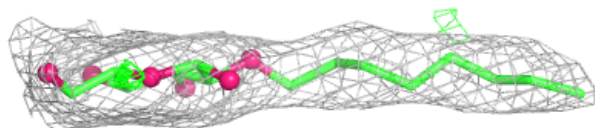
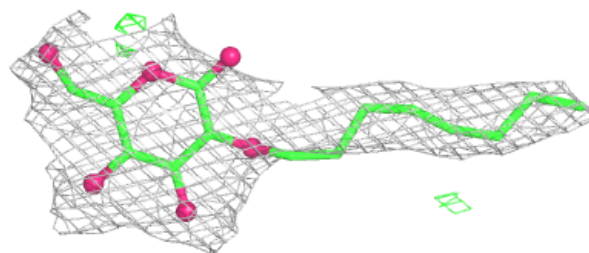


**Electron density around BGL B 310:**

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

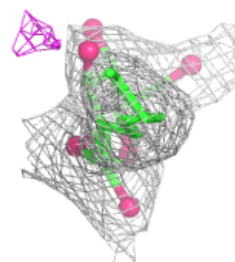
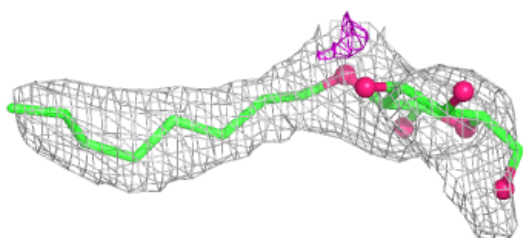
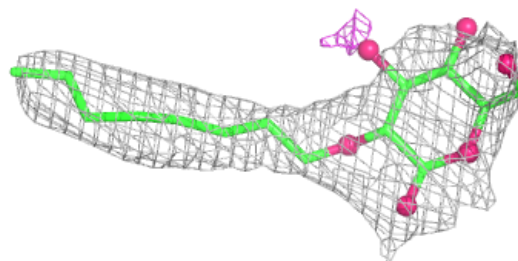
**Electron density around BGL A 305:**

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

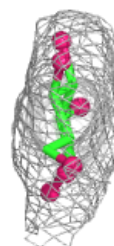
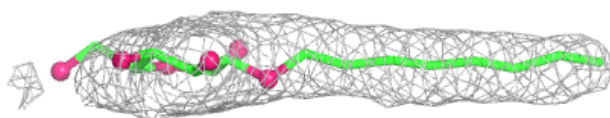
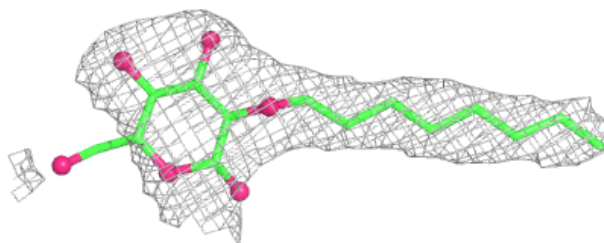


**Electron density around BGL B 303:**

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

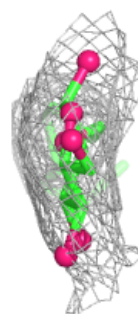
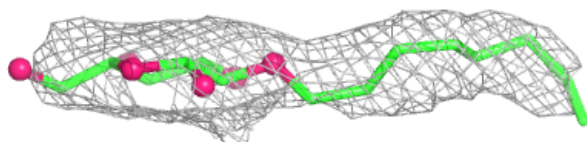
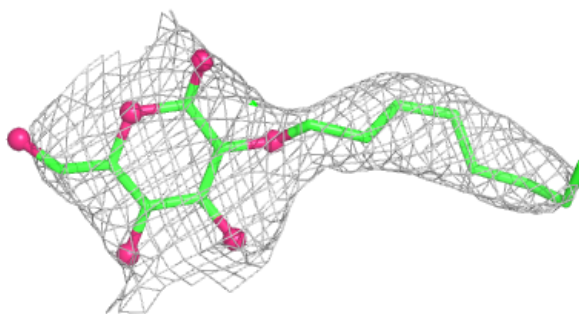
**Electron density around BGL B 302:**

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

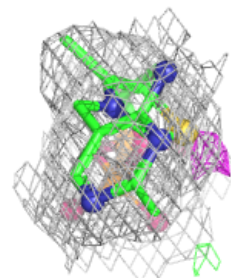
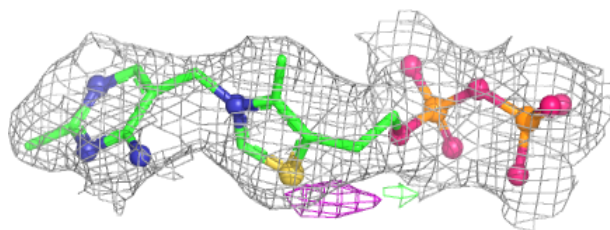
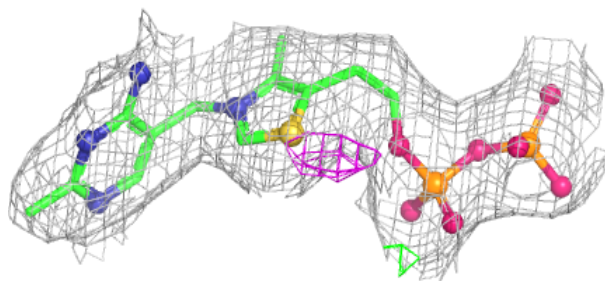


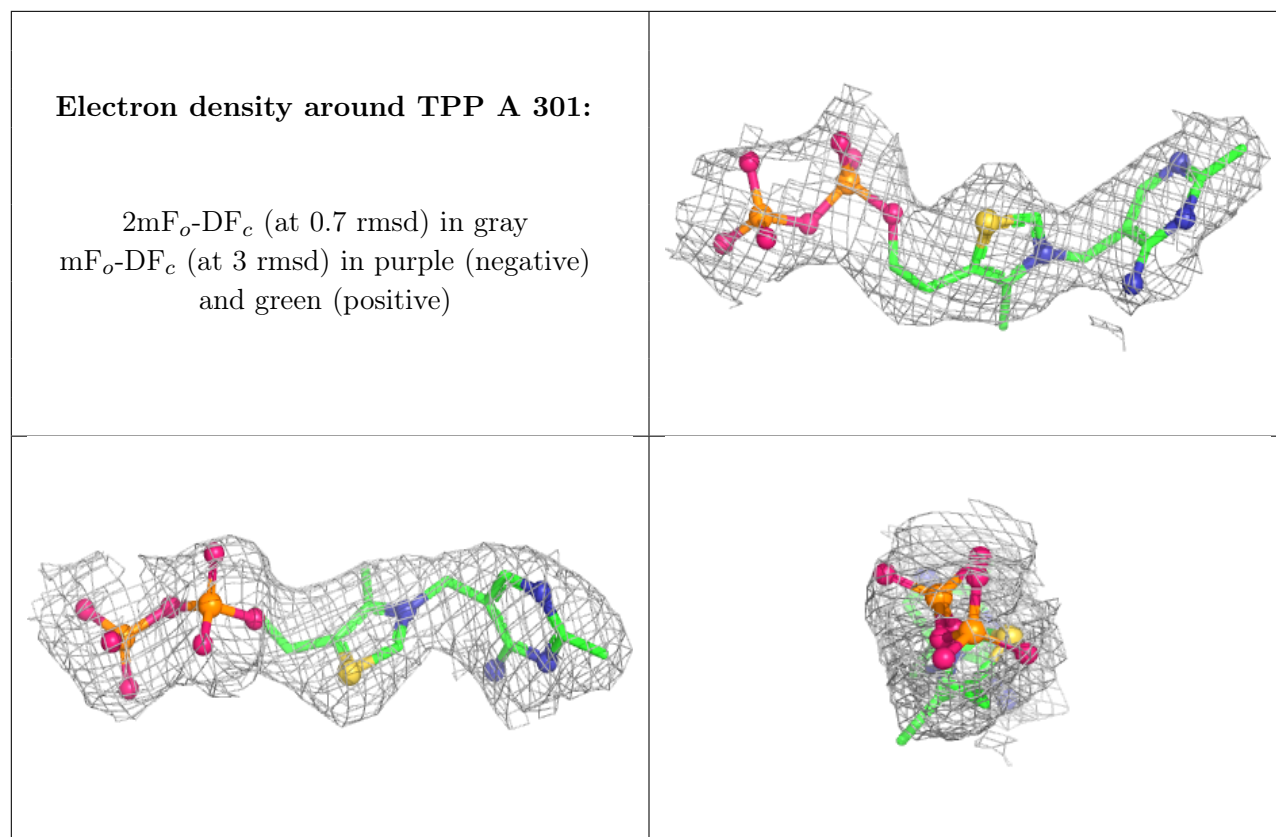
**Electron density around BGL B 305:**

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

**Electron density around TPP B 301:**

$2mF_o-DF_c$  (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.