



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 05:14 PM BST

PDB ID : 6XLP  
Title : Structure of the essential inner membrane lipopolysaccharide-PbgA complex  
Authors : Payandeh, J.; Clairefeuille, T.  
Deposited on : 2020-06-29  
Resolution : 2.00 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)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.14.6  
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) : 2.14.6

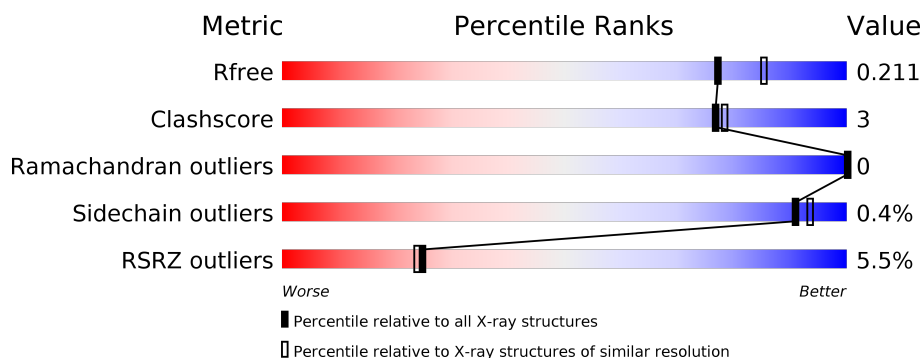
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	596	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VJ4	B	1	-	-	-	X
2	KDO	B	3	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5165 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 LPS binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4677	3015	814	833	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP C3T3G2
A	-1	GLY	-	expression tag	UNP C3T3G2
A	0	SER	-	expression tag	UNP C3T3G2
A	587	GLY	-	expression tag	UNP C3T3G2
A	588	GLU	-	expression tag	UNP C3T3G2
A	589	ASN	-	expression tag	UNP C3T3G2
A	590	LEU	-	expression tag	UNP C3T3G2
A	591	TYR	-	expression tag	UNP C3T3G2
A	592	PHE	-	expression tag	UNP C3T3G2
A	593	GLN	-	expression tag	UNP C3T3G2

- Molecule 2 is an oligosaccharide called 2-deoxy-3-O-[(1R,3R)-1,3-dihydroxytetradecyl]-2-[[3R)-3-hydroxytetradecanoyl]amino}-1-O-phosphono-alpha-D-glucopyranose-(6-1)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)]1,5-anhydro-2-deoxy-2-[[1S,3R)-1-hydroxy-3-(pentanoyloxy)undecyl]amino}-4-O-phosphono-D-glucitol.

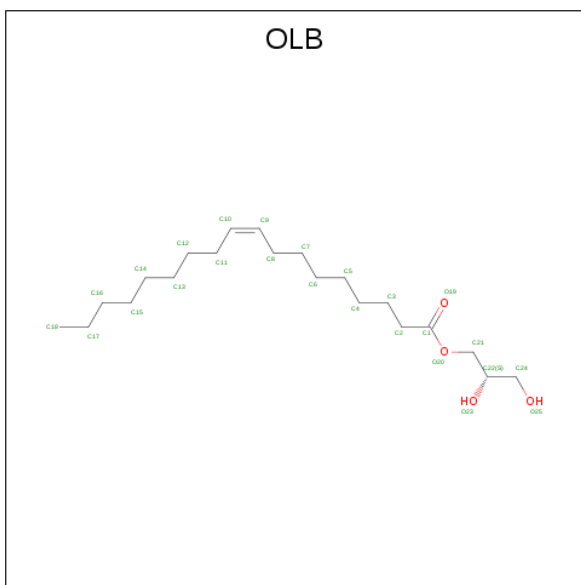
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	P	0	0	0
			97	64	2	29	2			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



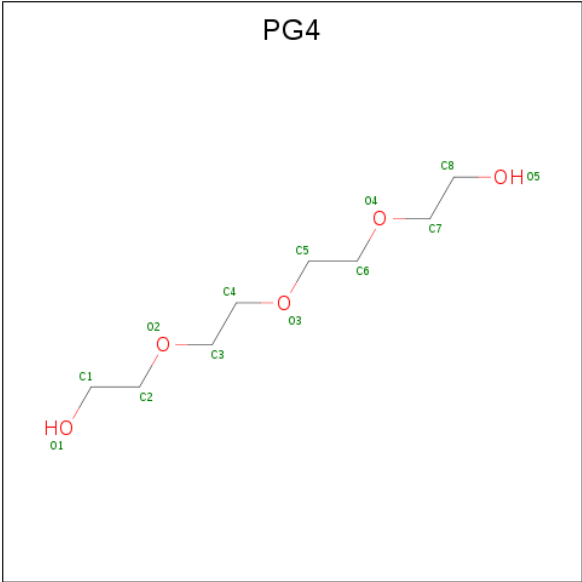
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



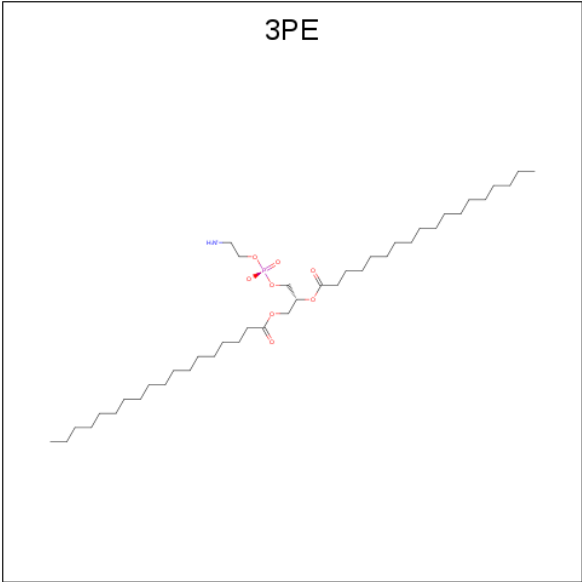
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 19	C 15	O 4	0	0
4	A	1	Total 18	C 14	O 4	0	0
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 14	C 10	O 4	0	0
4	A	1	Total 19	C 15	O 4	0	0
4	A	1	Total 5	C 3	O 2	0	0
4	A	1	Total 19	C 15	O 4	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $\text{C}_8\text{H}_{18}\text{O}_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	18	1	7	1		

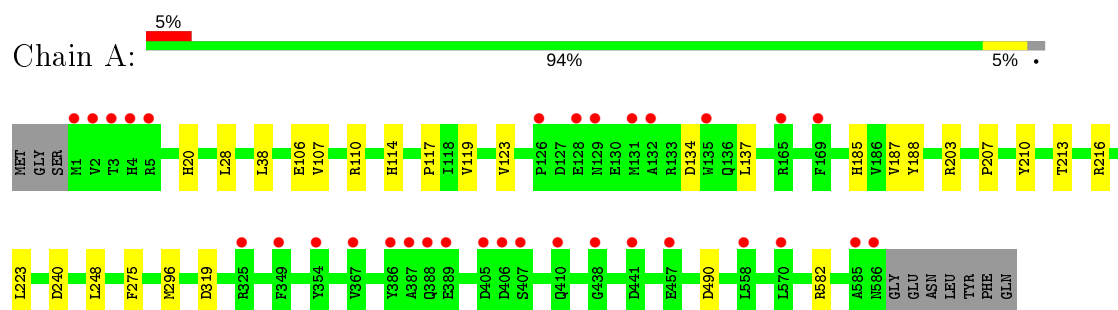
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	146	Total	O	0	0
			146	146		

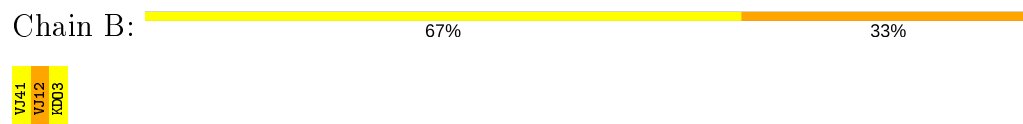
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: LPS binding protein



- Molecule 2: 2-deoxy-3-O-[(1R,3R)-1,3-dihydroxytetradecyl]-2-[[[(3R)-3-hydroxytetradecanoyl]amino}-1-O-phosphono-alpha-D-glucopyranose-(6-1)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)]1,5-anhydro-2-deoxy-2-[[[(1S,3R)-1-hydroxy-3-(pentanoyloxy)undecyl]amino}-4-O-phosphono-D-glucitol



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.27Å 56.33Å 97.36Å 90.00° 106.45° 90.00°	Depositor
Resolution (Å)	24.24 – 2.00 24.24 – 1.85	Depositor EDS
% Data completeness (in resolution range)	88.0 (24.24-2.00) 77.8 (24.24-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.85Å)	Xtriage
Refinement program	PHENIX DEV_2747	Depositor
R, $R_{free}$	0.193 , 0.211 0.193 , 0.211	Depositor DCC
$R_{free}$ test set	2000 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: OLB, KDO, VJ1, VJ4, PG4, SO4, 3PE

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	0.27	0/4802	0.44	0/6548

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	4677	0	4576	27	0
2	B	97	0	12	2	0
3	A	40	0	0	0	0
4	A	142	0	192	13	0
5	A	36	0	49	7	0
6	A	27	0	34	3	0
7	A	146	0	0	1	0
All	All	5165	0	4863	30	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 (30) 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:A:110:ARG:HD2	4:A:611:OLB:H22	1.65	0.78
1:A:210:TYR:H	5:A:618:PG4:H61	1.54	0.71
1:A:185:HIS:CE1	5:A:618:PG4:H62	2.26	0.71
1:A:28:LEU:HB2	4:A:612:OLB:H30	1.74	0.69
1:A:20:HIS:HB3	4:A:609:OLB:H2	1.76	0.67
1:A:187:VAL:HG21	4:A:610:OLB:H19	1.76	0.67
1:A:210:TYR:H	5:A:618:PG4:C6	2.10	0.63
1:A:38:LEU:HD12	4:A:616:OLB:H4	1.83	0.60
1:A:137:LEU:HD22	4:A:611:OLB:H16	1.84	0.60
1:A:185:HIS:HE1	5:A:618:PG4:H62	1.67	0.56
1:A:210:TYR:N	5:A:618:PG4:H61	2.23	0.54
1:A:137:LEU:HD13	4:A:611:OLB:H5	1.92	0.51
1:A:210:TYR:C	5:A:618:PG4:H61	2.31	0.51
1:A:240:ASP:OD2	7:A:701:HOH:O	2.19	0.51
1:A:207:PRO:HB2	6:A:620:3PE:H221	1.92	0.51
1:A:117:PRO:HD3	6:A:620:3PE:H121	1.93	0.49
1:A:106:GLU:HB3	4:A:611:OLB:H2	1.97	0.46
1:A:296:MET:O	1:A:490:ASP:HA	2.16	0.46
1:A:213:THR:O	2:B:2:VJ1:N2	2.49	0.46
1:A:107:VAL:HG11	1:A:119:VAL:HG11	2.00	0.44
5:A:617:PG4:H61	5:A:617:PG4:H81	1.78	0.43
1:A:248:LEU:HD11	1:A:582:ARG:HG2	2.01	0.42
1:A:188:TYR:OH	1:A:203:ARG:HB2	2.20	0.42
4:A:610:OLB:H20	4:A:610:OLB:H5	1.94	0.41
1:A:223:LEU:O	4:A:615:OLB:H21	2.21	0.41
4:A:610:OLB:H2	4:A:610:OLB:H21	1.90	0.41
1:A:114:HIS:HB3	6:A:620:3PE:H32	2.03	0.41
1:A:216:ARG:NH1	2:B:3:KDO:O7	2.53	0.40
1:A:134:ASP:OD2	4:A:611:OLB:H4	2.21	0.40
1:A:123:VAL:HG13	4:A:611:OLB:H4A	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	585/596 (98%)	580 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/522 (94%)	490 (100%)	2 (0%)	91	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	PHE
1	A	319	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	VJ4	B	1	2	33,34,35	1.20	1 (3%)	37,44,46	3.72	5 (13%)
2	VJ1	B	2	2	47,48,48	1.06	2 (4%)	53,60,60	3.09	7 (13%)
2	KDO	B	3	2	12,15,16	0.31	0	16,21,24	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VJ4	B	1	2	-	6/30/48/51	0/1/1/1
2	VJ1	B	2	2	-	8/44/65/65	0/1/1/1
2	KDO	B	3	2	-	1/6/26/30	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	VJ4	O2-C13	-6.02	1.25	1.40
2	B	2	VJ1	O21-C15	-4.87	1.25	1.39
2	B	2	VJ1	C22-N2	4.47	1.43	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	VJ4	C15-O11-C12	20.71	168.78	117.79
2	B	2	VJ1	C23-C22-N2	16.73	138.25	116.33
2	B	2	VJ1	O2-C22-N2	-12.40	102.03	122.95
2	B	1	VJ4	O2-C13-C14	5.23	119.55	109.11
2	B	2	VJ1	O21-C15-C21	4.46	119.11	109.18
2	B	1	VJ4	O11-C12-O10	4.34	134.20	123.70
2	B	2	VJ1	O1-P4B-O8B	3.20	121.76	109.39
2	B	1	VJ4	O11-C12-C21	-3.11	104.80	111.50
2	B	1	VJ4	O7-P1-O4	2.69	118.06	105.99
2	B	2	VJ1	O2-C22-C23	-2.27	118.18	121.50
2	B	2	VJ1	O5-C1-O1	-2.18	108.51	111.36
2	B	2	VJ1	C2-N2-C22	2.16	126.08	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

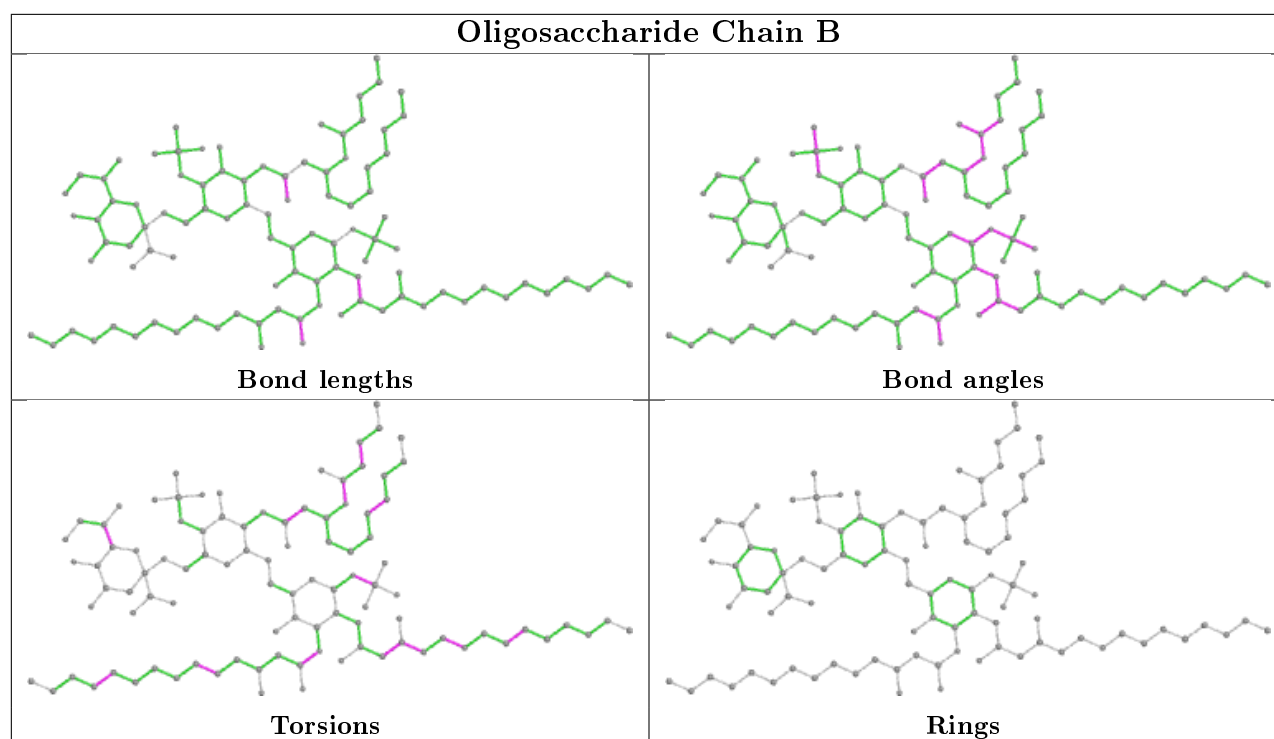
Mol	Chain	Res	Type	Atoms
2	B	2	VJ1	O21-C15-O3-C3
2	B	1	VJ4	O10-C12-O11-C15
2	B	1	VJ4	C21-C12-O11-C15
2	B	1	VJ4	O2-C13-C14-C15
2	B	1	VJ4	C12-C21-C31-C41
2	B	1	VJ4	N2-C13-C14-C15
2	B	2	VJ1	C7-C8-C9-C10
2	B	2	VJ1	C22-C23-C24-O7
2	B	1	VJ4	C18-C7-C8-C9
2	B	2	VJ1	C23-C24-C25-C26
2	B	2	VJ1	C25-C26-C27-C7
2	B	2	VJ1	C91-C16-C17-C18
2	B	2	VJ1	C1-O1-P4B-O9B
2	B	3	KDO	C5-C6-C7-O7
2	B	2	VJ1	C41-C51-C61-C71

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	VJ1	1	0
2	B	3	KDO	1	0

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



## 5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	OLB	A	611	-	17,17,24	0.83	0	18,18,25	0.67	0
5	PG4	A	617	-	12,12,12	0.52	0	11,11,11	0.33	0
3	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.07	0
4	OLB	A	615	-	3,4,24	0.67	0	1,4,25	1.20	0
3	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	608	-	4,4,4	0.14	0	6,6,6	0.10	0
5	PG4	A	619	-	9,9,12	0.51	0	8,8,11	0.23	0
4	OLB	A	612	-	22,22,24	0.36	0	23,23,25	0.30	0
3	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.06	0
4	OLB	A	613	-	13,13,24	0.89	0	14,14,25	0.76	0
4	OLB	A	616	-	18,18,24	0.80	0	18,19,25	0.69	0
3	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.05	0
4	OLB	A	614	-	18,18,24	0.84	0	18,19,25	0.67	0
4	OLB	A	610	-	18,18,24	0.87	1 (5%)	18,19,25	0.82	0
3	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.05	0
6	3PE	A	620	-	26,26,50	0.98	2 (7%)	28,30,55	1.05	1 (3%)
3	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.06	0
5	PG4	A	618	-	12,12,12	0.52	0	11,11,11	0.24	0
4	OLB	A	609	-	24,24,24	0.83	0	25,25,25	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLB	A	611	-	-	12/17/17/24	-
5	PG4	A	617	-	-	5/10/10/10	-
4	OLB	A	615	-	-	2/2/2/24	-
5	PG4	A	619	-	-	2/7/7/10	-
4	OLB	A	612	-	-	11/22/22/24	-
4	OLB	A	613	-	-	6/13/13/24	-
4	OLB	A	616	-	-	4/18/18/24	-
4	OLB	A	610	-	-	8/18/18/24	-
6	3PE	A	620	-	-	13/29/29/54	-
4	OLB	A	614	-	-	10/18/18/24	-
5	PG4	A	618	-	-	1/10/10/10	-
4	OLB	A	609	-	-	8/24/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	620	3PE	O21-C21	2.38	1.41	1.34
6	A	620	3PE	O21-C2	-2.27	1.40	1.46
4	A	610	OLB	O23-C22	-2.07	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	620	3PE	O21-C21-C22	4.00	120.13	111.50

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	611	OLB	C2-C1-O20-C21
4	A	611	OLB	O19-C1-O20-C21
4	A	611	OLB	C21-C22-C24-O25
4	A	615	OLB	O20-C21-C22-O23
4	A	609	OLB	C21-C22-C24-O25
6	A	620	3PE	C1-O11-P-O14
6	A	620	3PE	C11-O13-P-O12
6	A	620	3PE	C11-O13-P-O14
6	A	620	3PE	C1-C2-C3-O31
6	A	620	3PE	O21-C2-C3-O31
4	A	610	OLB	C2-C1-O20-C21
4	A	610	OLB	O20-C21-C22-C24
4	A	614	OLB	C9-C10-C11-C12
4	A	610	OLB	O19-C1-O20-C21
4	A	611	OLB	C4-C5-C6-C7
4	A	614	OLB	O20-C21-C22-O23
4	A	610	OLB	C5-C6-C7-C8
4	A	614	OLB	O20-C21-C22-C24
5	A	617	PG4	O3-C5-C6-O4
4	A	611	OLB	O20-C21-C22-O23
4	A	610	OLB	O20-C21-C22-O23
5	A	617	PG4	O2-C3-C4-O3
4	A	612	OLB	C1-C2-C3-C4
4	A	609	OLB	O20-C21-C22-O23
6	A	620	3PE	C11-O13-P-O11
4	A	609	OLB	C11-C12-C13-C14
4	A	611	OLB	O20-C21-C22-C24
4	A	609	OLB	O20-C21-C22-C24
4	A	612	OLB	C4-C5-C6-C7
4	A	612	OLB	C2-C3-C4-C5
4	A	610	OLB	C3-C4-C5-C6
4	A	613	OLB	C3-C4-C5-C6
4	A	611	OLB	C1-C2-C3-C4
4	A	609	OLB	C10-C11-C12-C13
6	A	620	3PE	C25-C26-C27-C28
4	A	611	OLB	O23-C22-C24-O25
4	A	609	OLB	O23-C22-C24-O25
4	A	612	OLB	C5-C6-C7-C8
6	A	620	3PE	C24-C25-C26-C27
4	A	613	OLB	C2-C1-O20-C21

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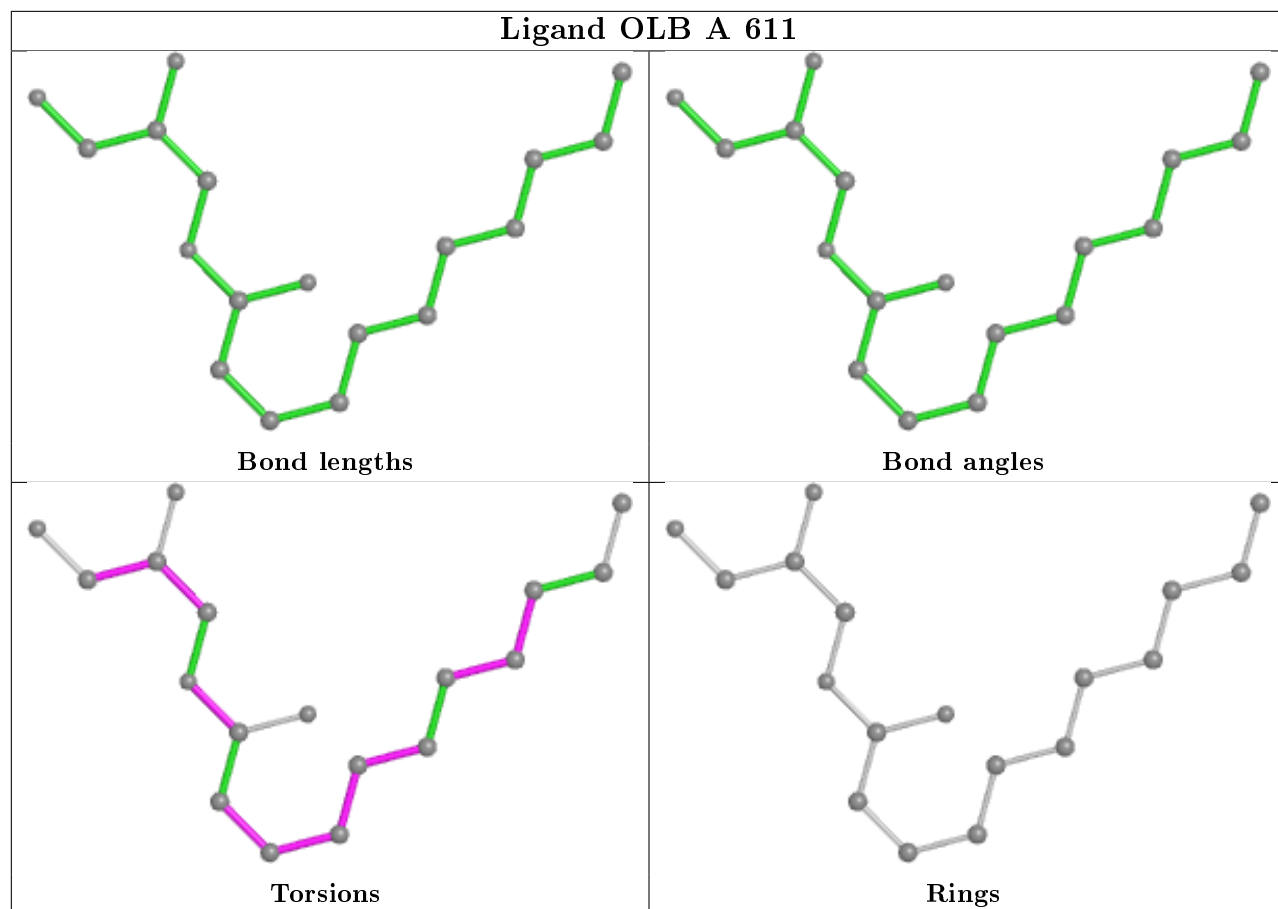
Mol	Chain	Res	Type	Atoms
4	A	616	OLB	C9-C10-C11-C12
4	A	612	OLB	C6-C7-C8-C9
4	A	612	OLB	C10-C11-C12-C13
4	A	613	OLB	O20-C21-C22-C24
4	A	613	OLB	O19-C1-O20-C21
4	A	610	OLB	C4-C5-C6-C7
5	A	617	PG4	C4-C3-O2-C2
4	A	611	OLB	C3-C4-C5-C6
4	A	616	OLB	C2-C3-C4-C5
4	A	614	OLB	C4-C5-C6-C7
4	A	612	OLB	C13-C14-C15-C16
6	A	620	3PE	O11-C1-C2-C3
6	A	620	3PE	C1-O11-P-O13
4	A	616	OLB	C4-C5-C6-C7
4	A	613	OLB	O20-C21-C22-O23
4	A	609	OLB	C3-C4-C5-C6
6	A	620	3PE	O11-C1-C2-O21
5	A	619	PG4	C6-C5-O3-C4
4	A	612	OLB	O23-C22-C24-O25
4	A	611	OLB	C6-C7-C8-C9
5	A	619	PG4	C5-C6-O4-C7
5	A	617	PG4	C8-C7-O4-C6
4	A	611	OLB	C2-C3-C4-C5
4	A	613	OLB	C2-C3-C4-C5
4	A	616	OLB	C5-C6-C7-C8
4	A	612	OLB	C11-C10-C9-C8
4	A	610	OLB	C2-C3-C4-C5
4	A	611	OLB	C7-C8-C9-C10
4	A	614	OLB	C7-C8-C9-C10
5	A	618	PG4	C6-C5-O3-C4
4	A	609	OLB	C7-C8-C9-C10
6	A	620	3PE	O22-C21-O21-C2
4	A	612	OLB	C9-C10-C11-C12
4	A	614	OLB	C2-C3-C4-C5
4	A	615	OLB	O20-C21-C22-C24
4	A	614	OLB	O20-C1-C2-C3
4	A	614	OLB	C3-C4-C5-C6
4	A	612	OLB	C21-C22-C24-O25
4	A	614	OLB	C5-C6-C7-C8
5	A	617	PG4	C5-C6-O4-C7
4	A	614	OLB	O19-C1-C2-C3
6	A	620	3PE	C22-C21-O21-C2

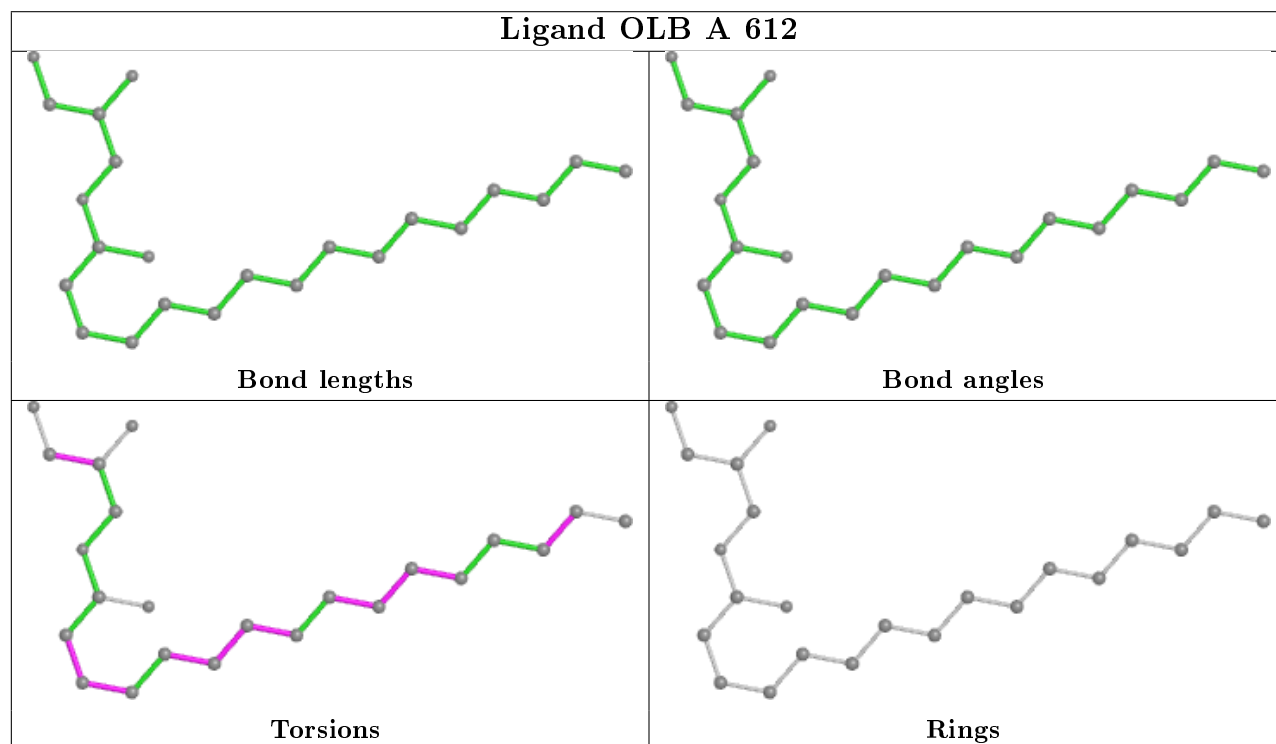
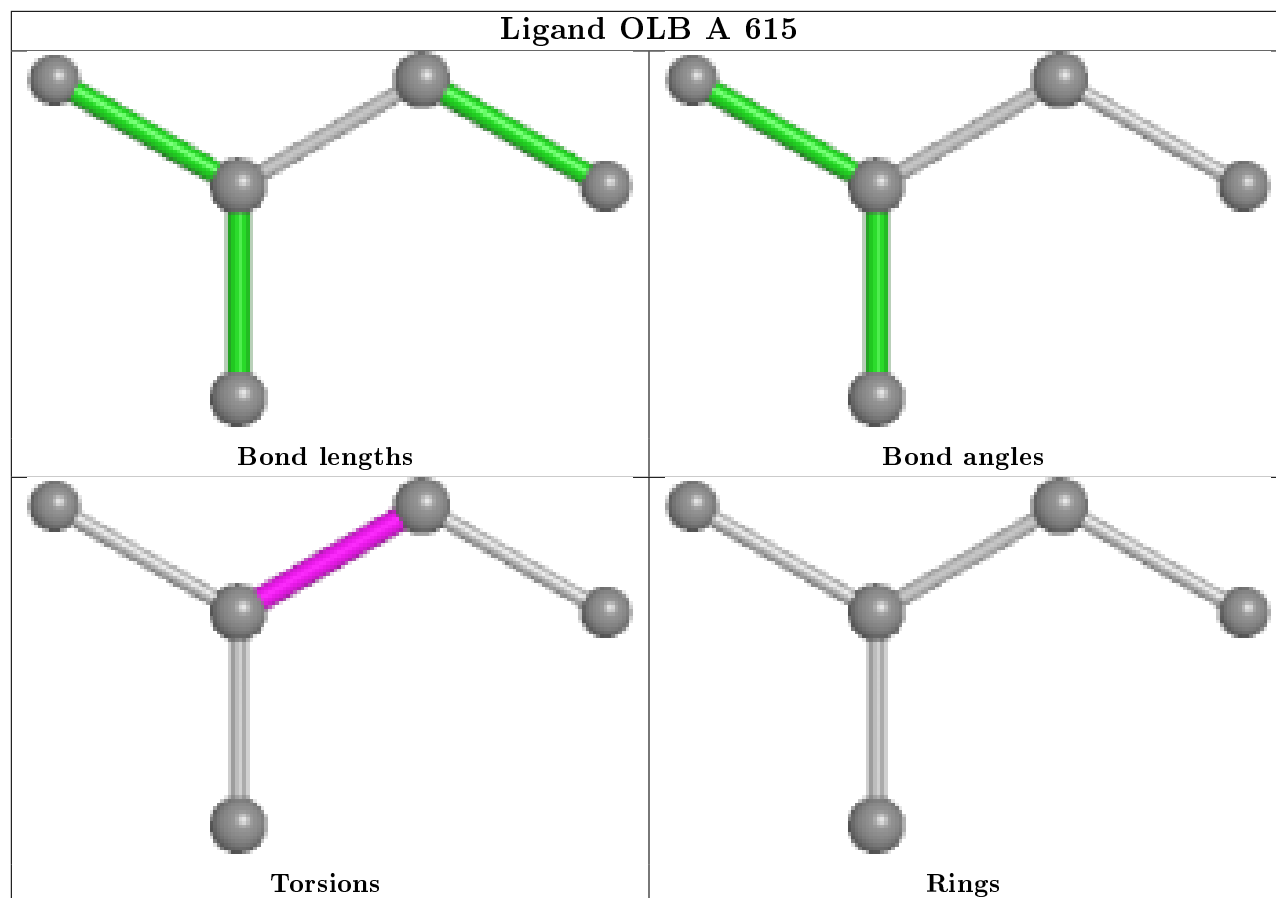
There are no ring outliers.

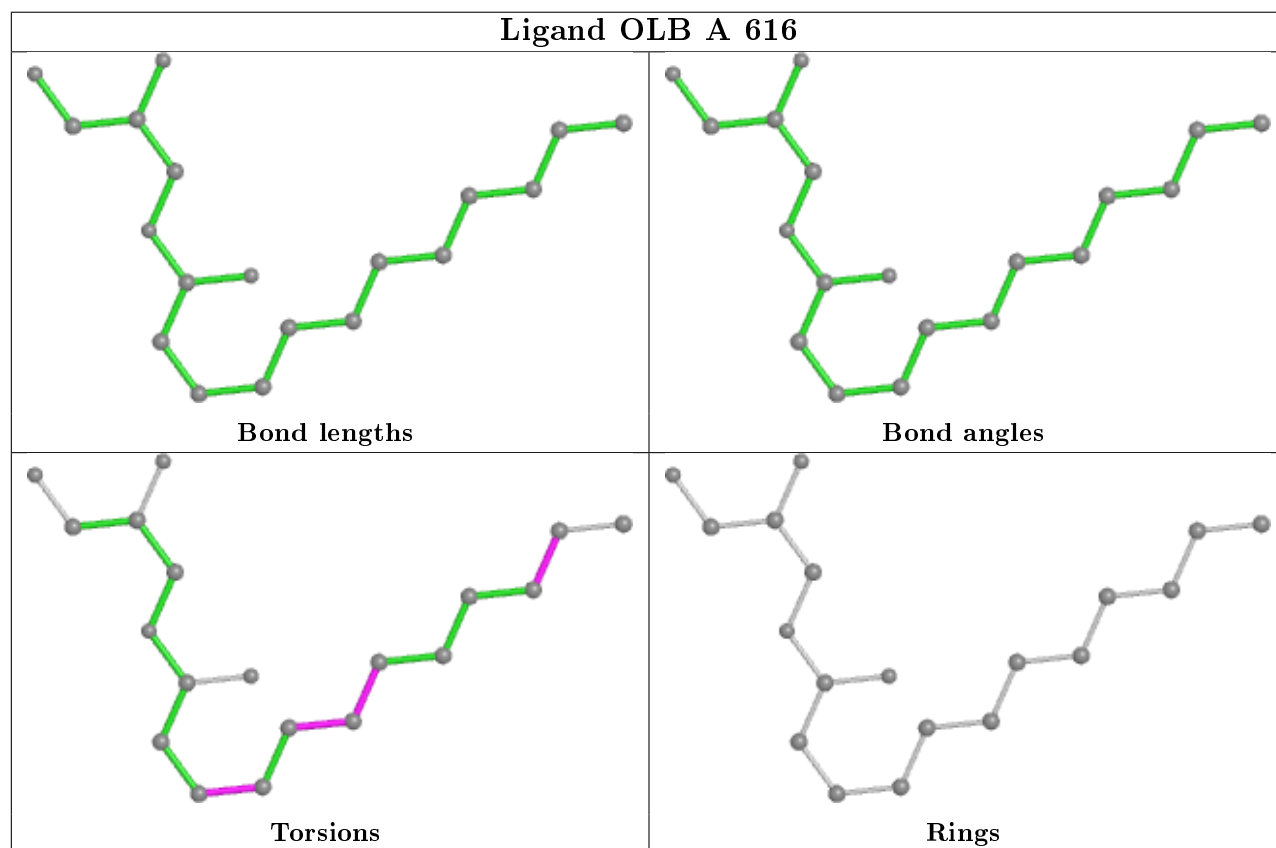
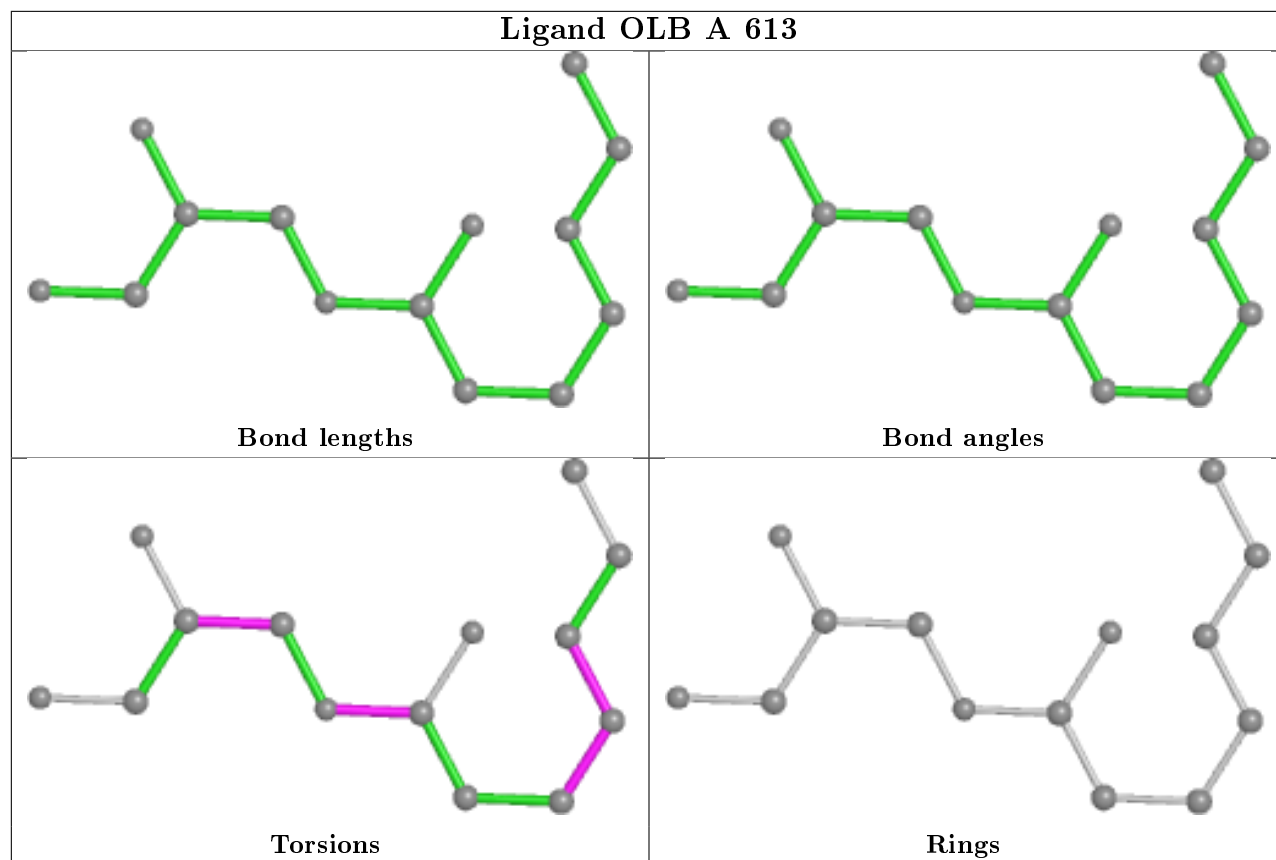
9 monomers are involved in 23 short contacts:

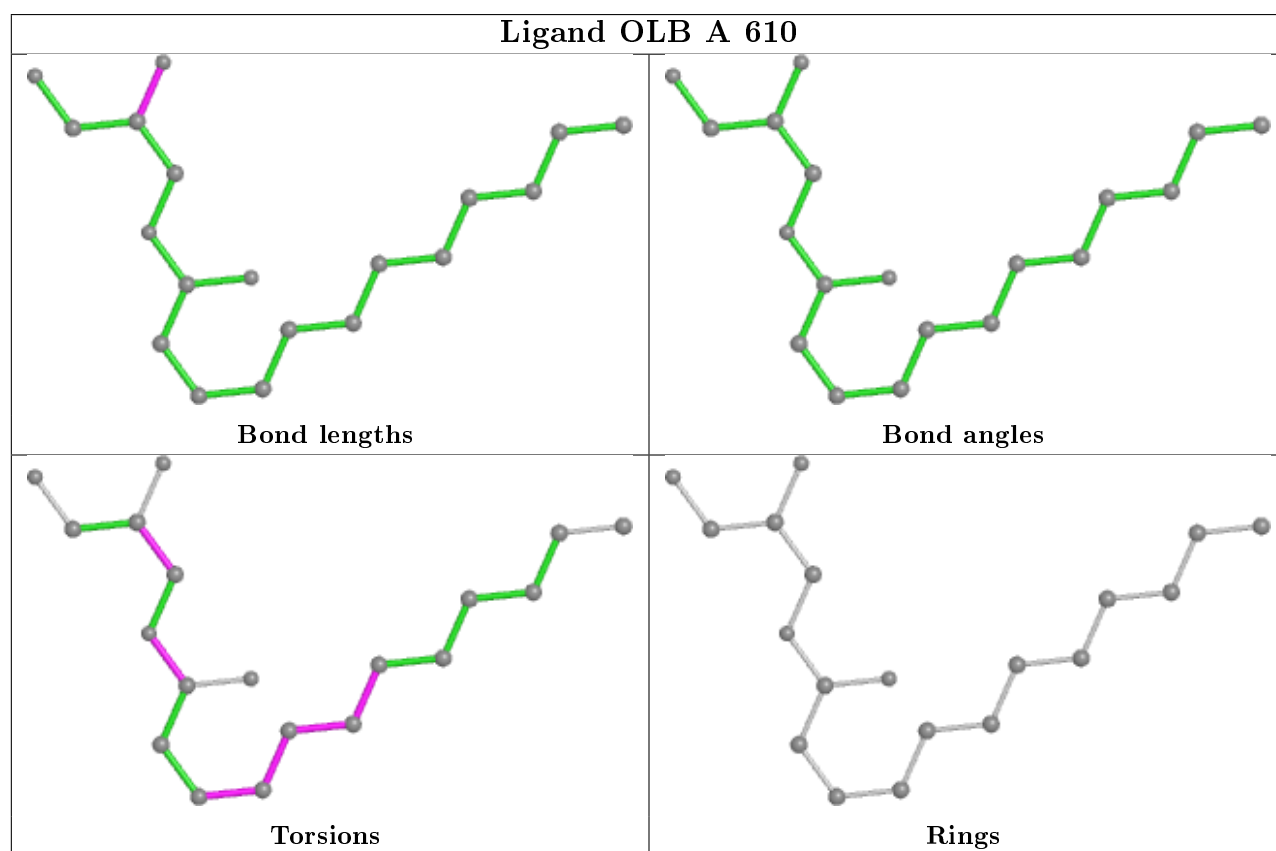
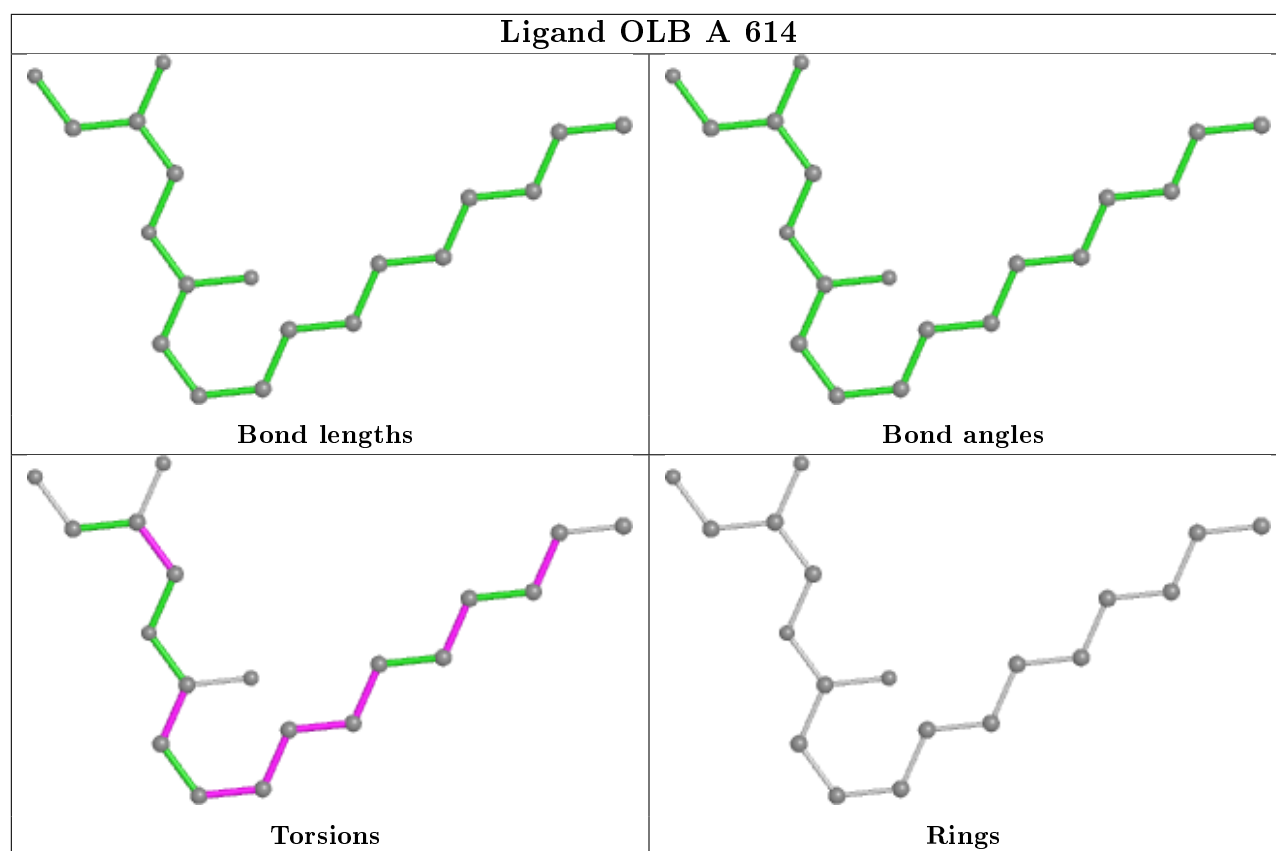
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	OLB	6	0
5	A	617	PG4	1	0
4	A	615	OLB	1	0
4	A	612	OLB	1	0
4	A	616	OLB	1	0
4	A	610	OLB	3	0
6	A	620	3PE	3	0
5	A	618	PG4	6	0
4	A	609	OLB	1	0

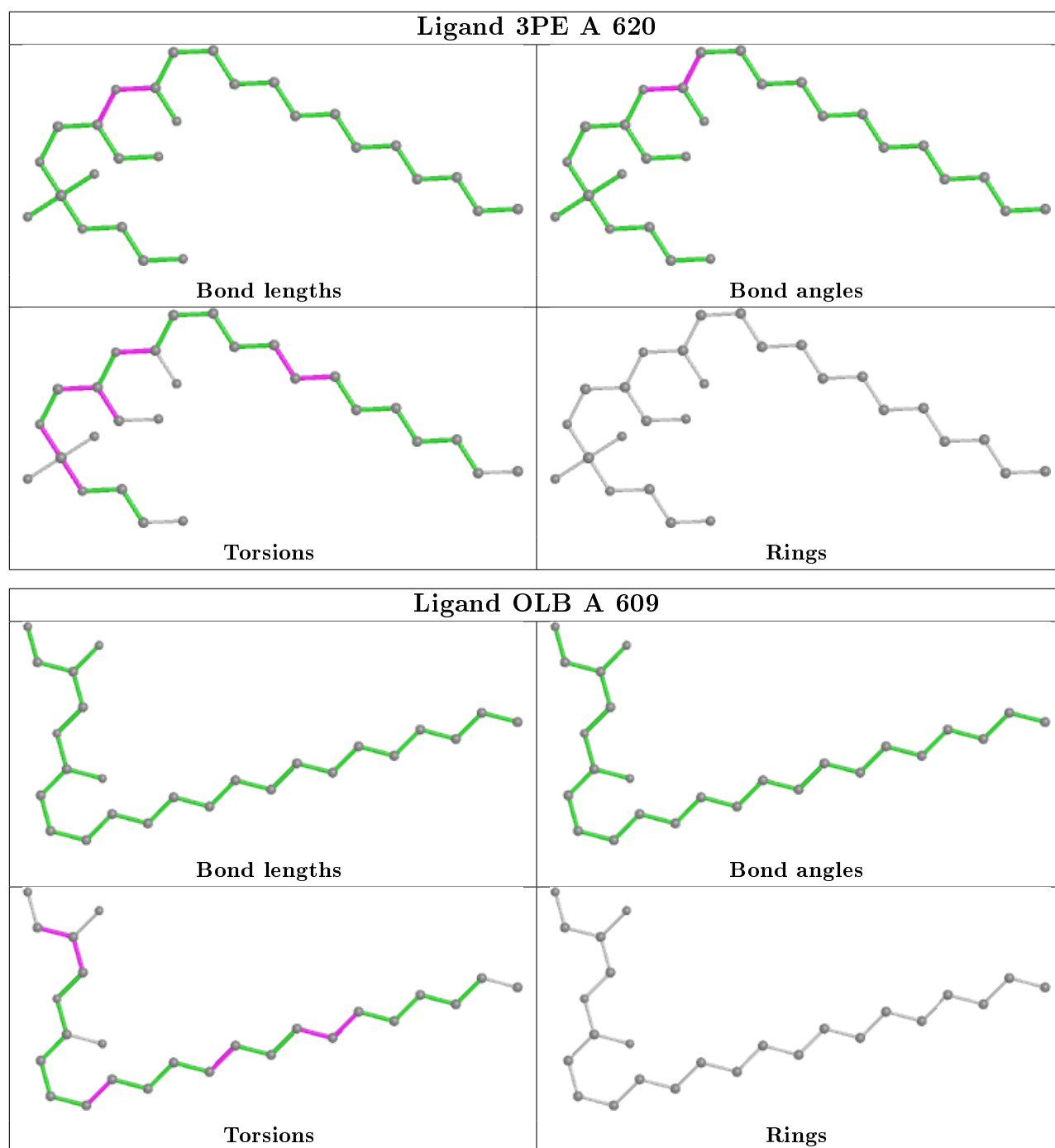
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 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	586/596 (98%)	0.03	32 (5%) 25 24	26, 44, 88, 119	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	GLN	5.8
1	A	131	MET	5.3
1	A	129	ASN	4.9
1	A	4	HIS	4.1
1	A	132	ALA	4.0
1	A	405	ASP	3.8
1	A	386	TYR	3.6
1	A	406	ASP	3.6
1	A	135	TRP	3.4
1	A	128	GLU	3.3
1	A	367	VAL	3.3
1	A	387	ALA	3.3
1	A	457	GLU	3.2
1	A	1	MET	3.2
1	A	349	PHE	3.1
1	A	126	PRO	3.0
1	A	586	ASN	2.9
1	A	570	LEU	2.9
1	A	438	GLY	2.7
1	A	354	TYR	2.5
1	A	407	SER	2.5
1	A	585	ALA	2.4
1	A	410	GLN	2.3
1	A	5	ARG	2.3
1	A	389	GLU	2.3
1	A	2	VAL	2.2
1	A	3	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	558	LEU	2.1
1	A	169	PHE	2.1
1	A	325	ARG	2.1
1	A	165	ARG	2.0
1	A	441	ASP	2.0

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

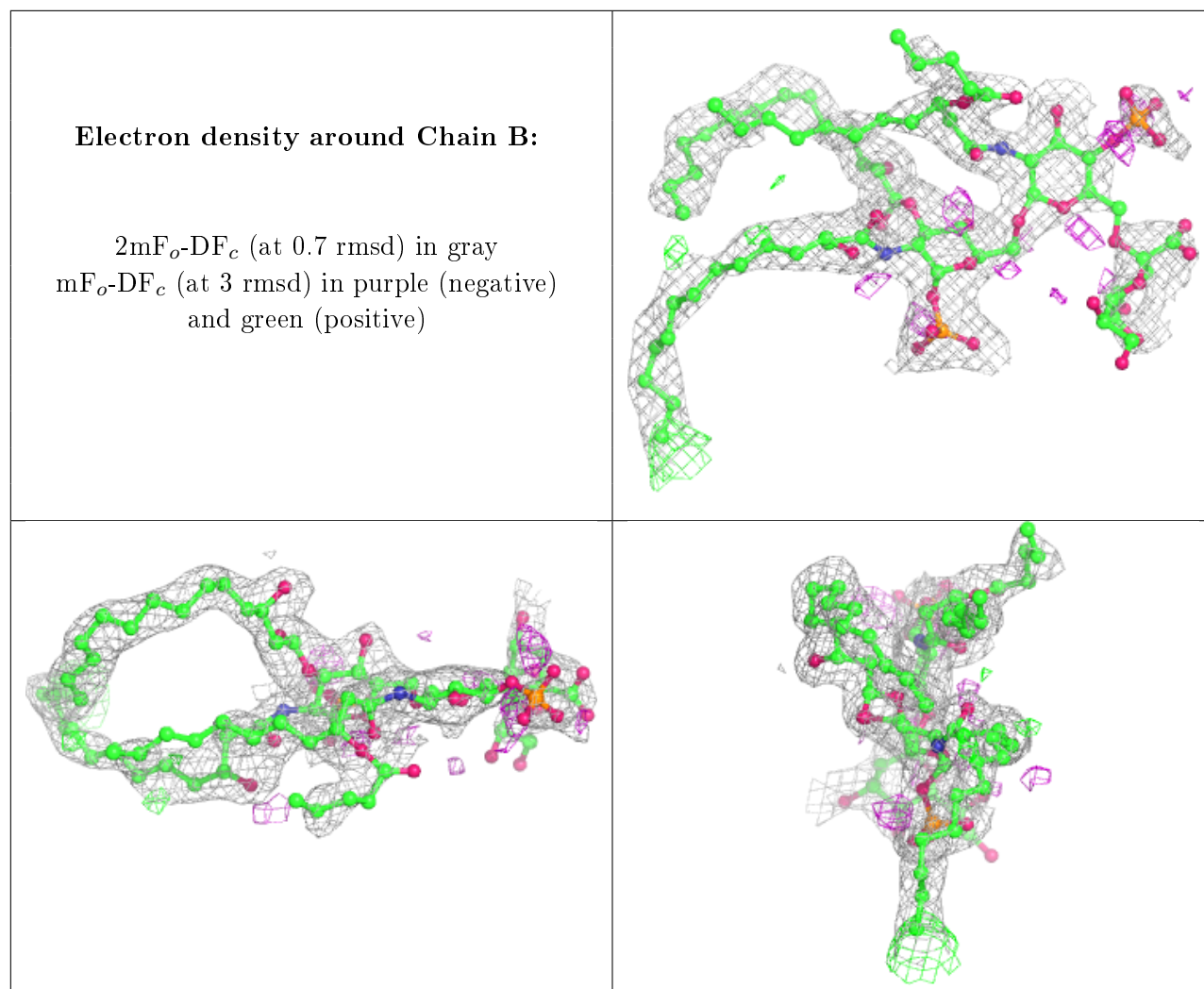
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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(Å <sup>2</sup> )	Q<0.9
2	VJ4	B	1	34/35	0.64	0.45	84,93,135,138	0
2	KDO	B	3	15/16	0.80	0.52	110,111,116,116	0
2	VJ1	B	2	48/48	0.94	0.13	38,61,81,84	0

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



## 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(Å <sup>2</sup> )	Q<0.9
4	OLB	A	615	5/25	0.51	0.18	63,66,68,68	0
4	OLB	A	613	14/25	0.52	0.32	59,77,87,89	0
6	3PE	A	620	27/51	0.58	0.23	51,81,110,112	0
4	OLB	A	611	18/25	0.60	0.30	77,81,94,95	0
4	OLB	A	610	19/25	0.64	0.28	70,73,83,84	0
4	OLB	A	614	19/25	0.68	0.21	55,67,79,79	0
4	OLB	A	612	23/25	0.69	0.21	60,75,87,89	0
4	OLB	A	609	25/25	0.72	0.16	45,52,78,81	0
3	SO4	A	607	5/5	0.81	0.24	124,124,124,125	0

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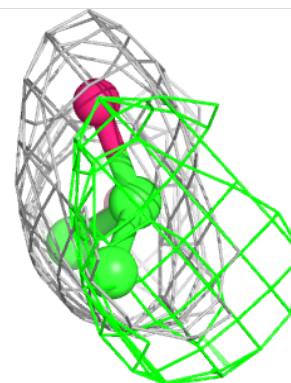
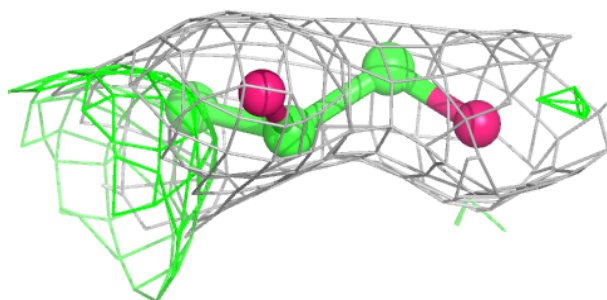
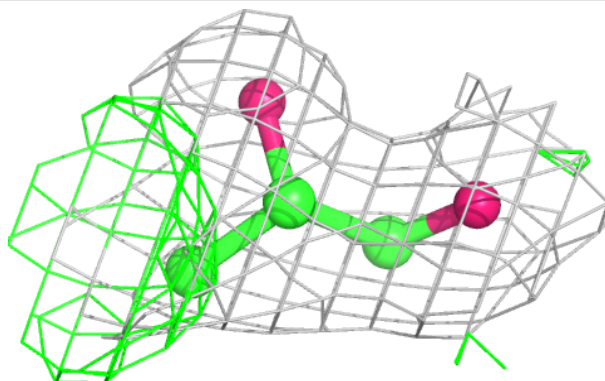
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	604	5/5	0.82	0.37	115,115,117,118	0
5	PG4	A	618	13/13	0.85	0.15	36,52,62,62	0
5	PG4	A	619	10/13	0.88	0.15	57,62,67,67	0
5	PG4	A	617	13/13	0.88	0.14	66,67,73,73	0
3	SO4	A	602	5/5	0.89	0.21	119,119,119,120	0
3	SO4	A	606	5/5	0.91	0.19	62,70,74,75	0
4	OLB	A	616	19/25	0.91	0.18	43,49,56,56	0
3	SO4	A	605	5/5	0.94	0.18	111,111,111,112	0
3	SO4	A	601	5/5	0.95	0.18	94,96,97,98	0
3	SO4	A	603	5/5	0.96	0.28	121,122,122,122	0
3	SO4	A	608	5/5	0.97	0.15	73,73,74,75	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.

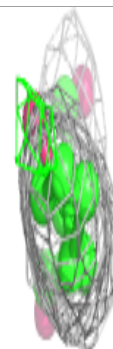
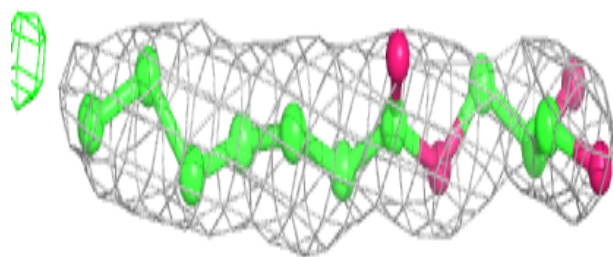
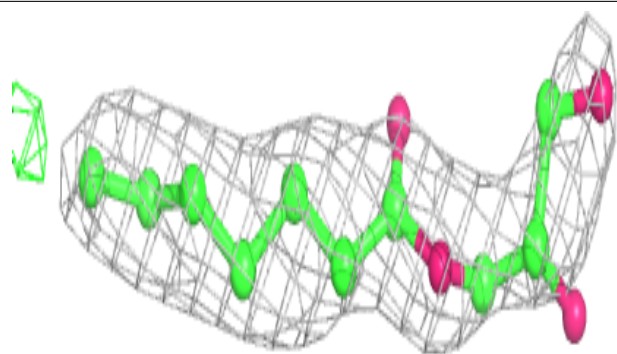
**Electron density around OLB A 615:**

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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

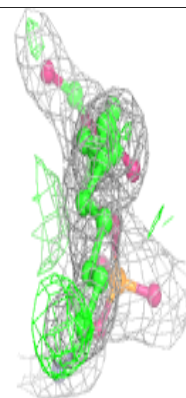
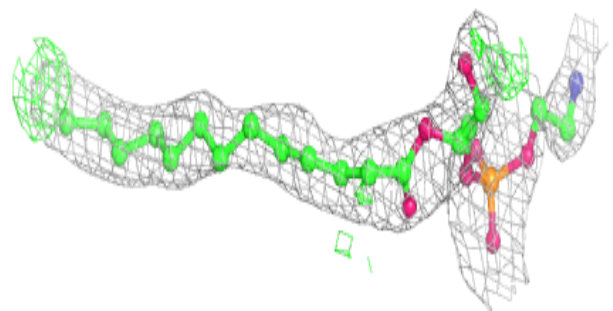
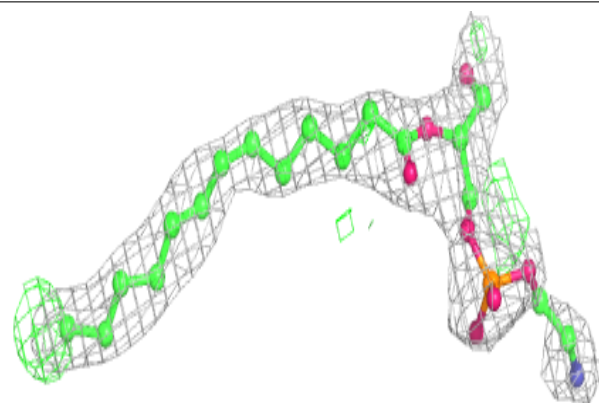


**Electron density around OLB A 613:**

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and green (positive)

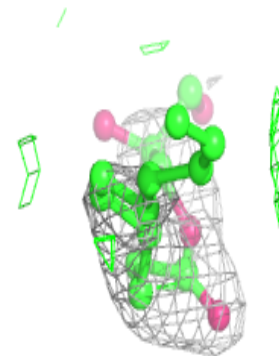
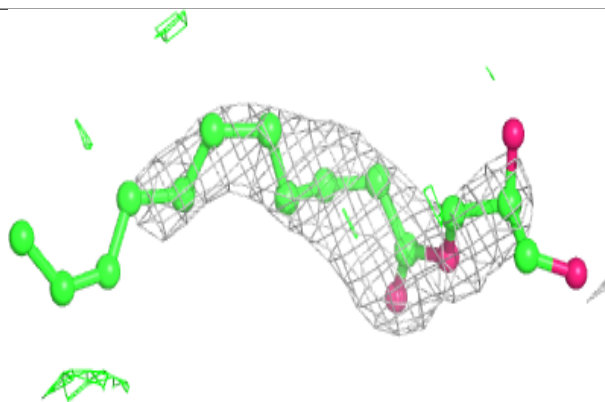
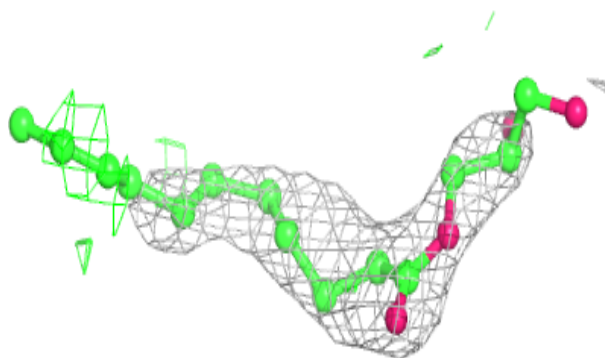
**Electron density around 3PE A 620:**

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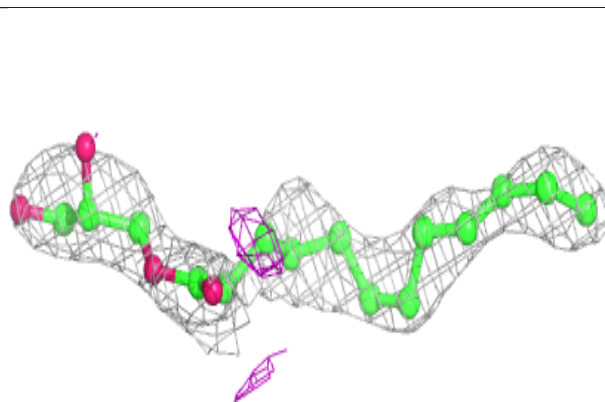
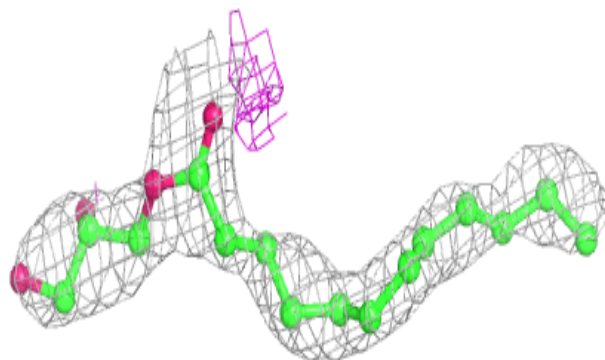


**Electron density around OLB A 611:**

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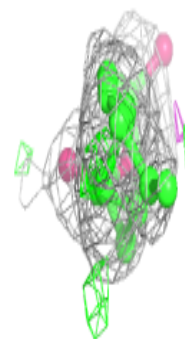
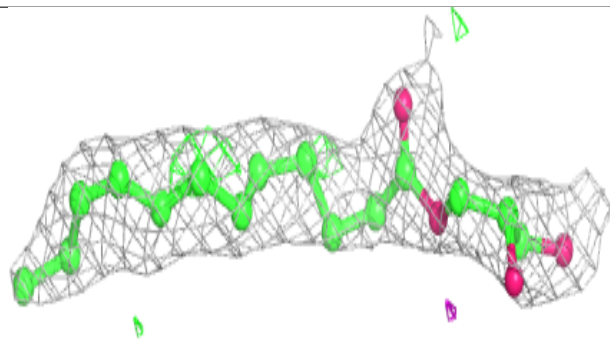
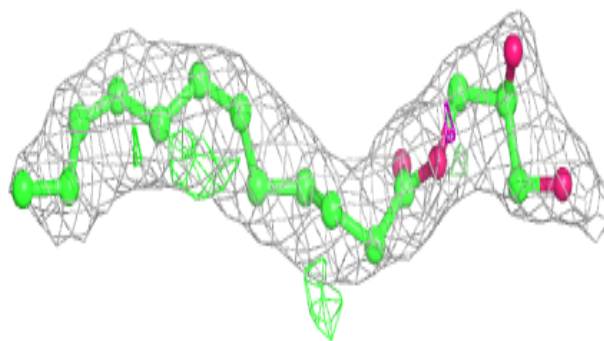
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and green (positive)

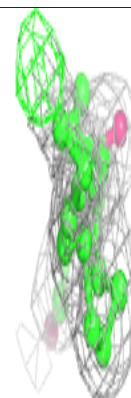
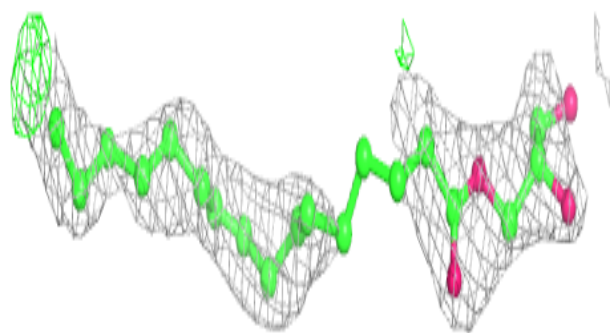
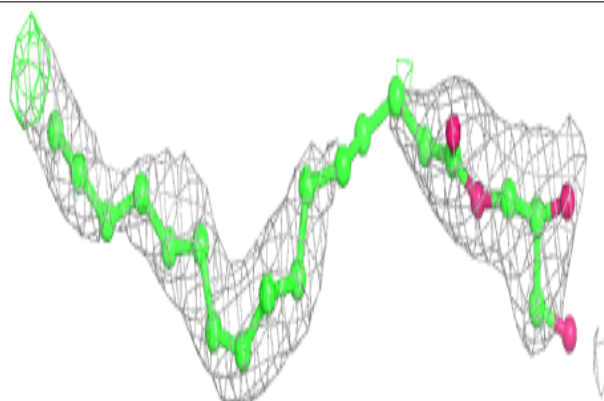


**Electron density around OLB A 614:**

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and green (positive)

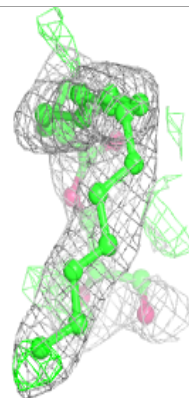
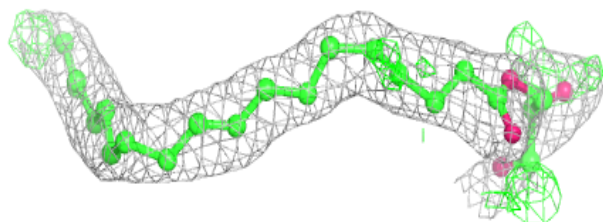
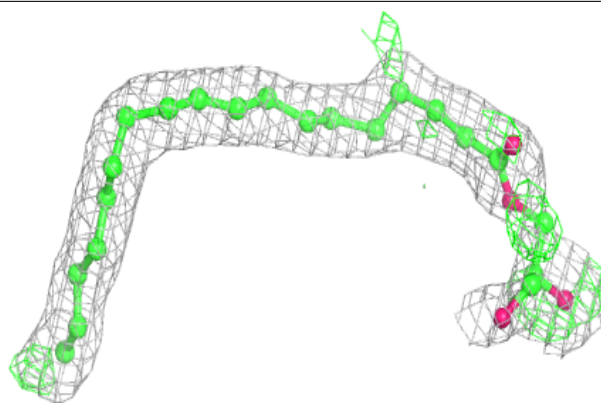
**Electron density around OLB A 612:**

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

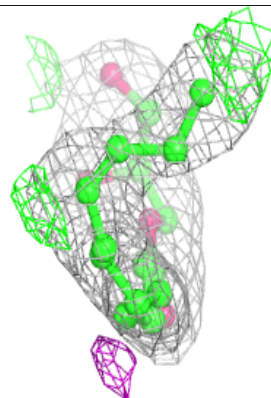
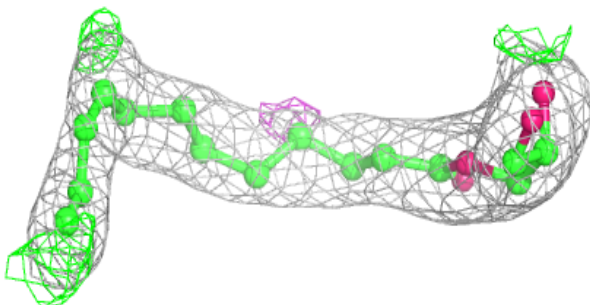
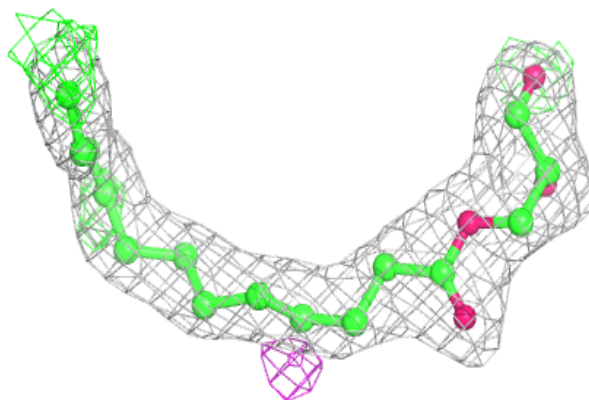


**Electron density around OLB A 609:**

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

**Electron density around OLB A 616:**

$2mF_o-DF_c$  (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.