



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:28 PM BST

PDB ID : 2X91  
Title : Crystal structure of AnCE-lisinopril complex  
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Deposited on : 2010-03-14  
Resolution : 1.98 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

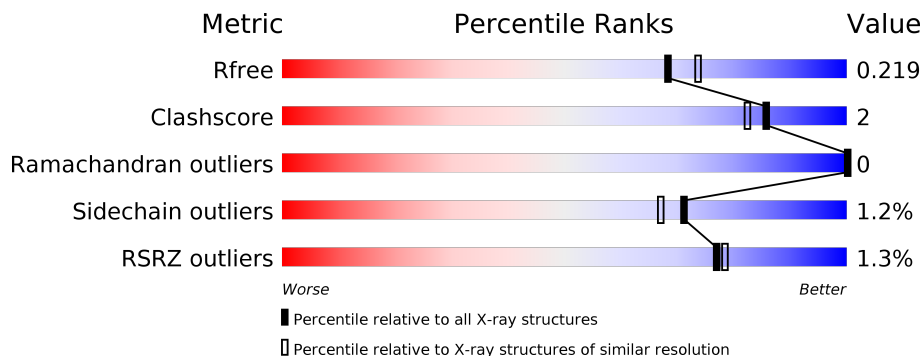
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	598	<p>94% 6%</p>
2	B	6	<p>17% 83%</p>

## 2 Entry composition [i](#)

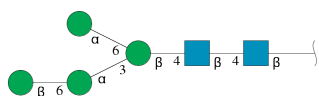
There are 7 unique types of molecules in this entry. The entry contains 5469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANGIOTENSIN CONVERTING ENZYME.

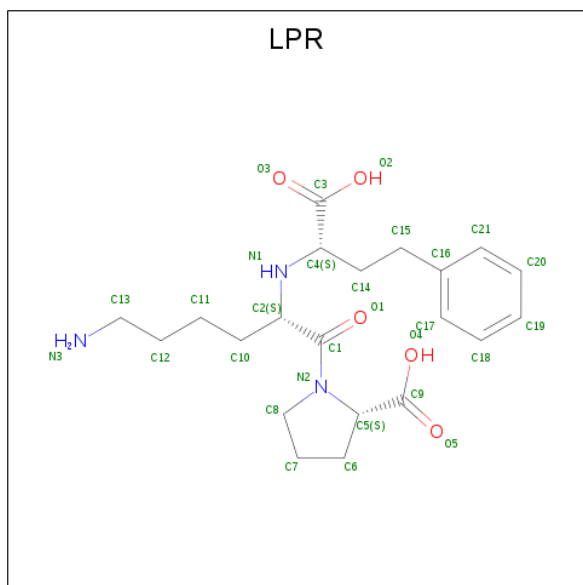
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4863	3110	803	930	20	0	2	0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



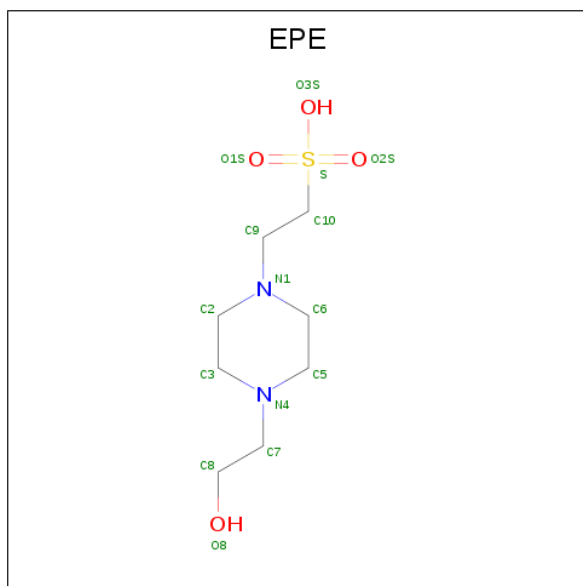
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	72	40	2	30	0	0	0

- Molecule 3 is [N2-[(S)-1-CARBOXY-3-PHENYLPROPYL]-L-LYSYL-L-PROLINE (three-letter code: LPR) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	21	3	5	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
4	A	1	15	8	2	4	1	0	0

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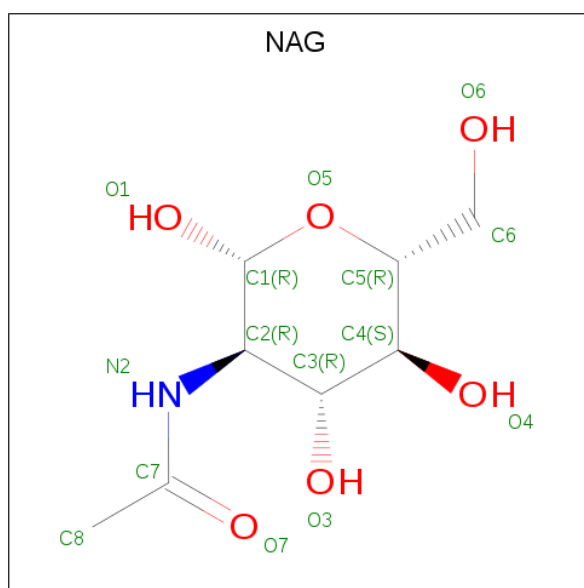
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0

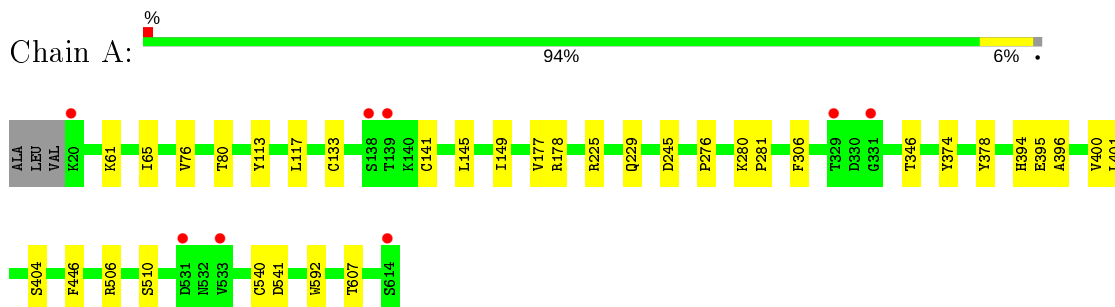
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	431	431	431	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: ANGIOTENSIN CONVERTING ENZYME



- Molecule 2: beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.81Å 172.81Å 102.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.78 – 1.98 31.78 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.6 (31.78-1.98) 79.1 (31.78-1.98)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.192 , 0.209 0.197 , 0.219	Depositor DCC
$R_{free}$ test set	3113 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.127	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.013 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$ 0.008 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.013 for $-h,2/3^*h+1/3^*k+4/3^*l,1/3^*h+2/3^*k-1/3^*l$ 0.024 for $-1/3^*h-2/3^*k+4/3^*l,-2/3^*h-1/3^*k-4/3^*l,1/3^*h-1/3^*k-1/3^*l$ 0.021 for $1/3^*h+2/3^*k-4/3^*l,-k,-2/3^*h-1/3^*k-1/3^*l$ 0.045 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: ZN, BMA, NAG, LPR, EPE, MAN

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	0.39	2/4995 (0.0%)	0.48	0/6768

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	THR	CB-OG1	5.54	1.54	1.43
1	A	607	THR	CB-OG1	5.29	1.53	1.43

There are no bond angle outliers.

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	4863	0	4652	17	0
2	B	72	0	61	0	0
3	A	29	0	29	2	0
4	A	45	0	51	7	0
5	A	1	0	0	0	0
6	A	28	0	26	0	0
7	A	431	0	0	3	0
All	All	5469	0	4819	22	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 2.

All (22) 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:1615:LPR:H18	4:A:1616:EPE:H31	1.75	0.68
1:A:61:LYS:O	1:A:65:ILE:HG12	1.98	0.64
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.38	0.59
1:A:404:SER:HB2	1:A:541:ASP:HA	1.85	0.58
1:A:506:ARG:HH12	4:A:1616:EPE:H32	1.72	0.55
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.43	0.54
1:A:306:PHE:CD2	1:A:401:LEU:HD13	2.46	0.51
1:A:395:GLU:HB2	1:A:510:SER:HB2	1.94	0.50
1:A:133:CYS:HA	1:A:141:CYS:HA	1.94	0.49
1:A:178:ARG:NH1	7:A:2102:HOH:O	2.47	0.47
4:A:1617:EPE:H32	7:A:2416:HOH:O	2.16	0.45
1:A:177:VAL:HG13	1:A:177:VAL:O	2.17	0.45
1:A:225:ARG:O	1:A:229:GLN:HG2	2.16	0.45
1:A:506:ARG:HH22	4:A:1616:EPE:H52	1.82	0.44
1:A:145:LEU:HA	1:A:149:ILE:HB	2.00	0.43
4:A:1616:EPE:H72	7:A:2339:HOH:O	2.19	0.43
1:A:280:LYS:HB3	1:A:281:PRO:HD2	2.00	0.42
1:A:396:ALA:O	1:A:400:VAL:HG23	2.19	0.42
1:A:177:VAL:CG1	1:A:177:VAL:O	2.68	0.41
3:A:1615:LPR:C18	4:A:1616:EPE:H31	2.46	0.41
1:A:76:VAL:O	1:A:80:THR:HG23	2.21	0.40
4:A:1617:EPE:H101	4:A:1617:EPE:H61	1.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/598 (100%)	587 (99%)	8 (1%)	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	519/520 (100%)	513 (99%)	6 (1%)	71	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	ASP
1	A	374	TYR
1	A	378	TYR
1	A	394	HIS
1	A	446	PHE
1	A	540	CYS

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

### 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](#)

6 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	NAG	B	1	1,2	14,14,15	0.49	0	17,19,21	0.73	1 (5%)
2	NAG	B	2	2	14,14,15	0.47	0	17,19,21	1.38	2 (11%)
2	BMA	B	3	2	11,11,12	0.64	0	15,15,17	0.84	0
2	MAN	B	4	2	11,11,12	0.55	0	15,15,17	1.17	1 (6%)
2	BMA	B	5	2	11,11,12	0.58	0	15,15,17	1.06	2 (13%)
2	MAN	B	6	2	11,11,12	0.62	0	15,15,17	1.03	2 (13%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	C1-O5-C5	3.46	116.87	112.19
2	B	2	NAG	C2-N2-C7	3.06	127.26	122.90
2	B	5	BMA	C1-O5-C5	3.06	116.33	112.19
2	B	2	NAG	C1-O5-C5	2.92	116.15	112.19
2	B	6	MAN	C1-C2-C3	2.24	112.42	109.67
2	B	5	BMA	C1-C2-C3	2.23	112.41	109.67
2	B	6	MAN	C1-O5-C5	2.11	115.05	112.19
2	B	1	NAG	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

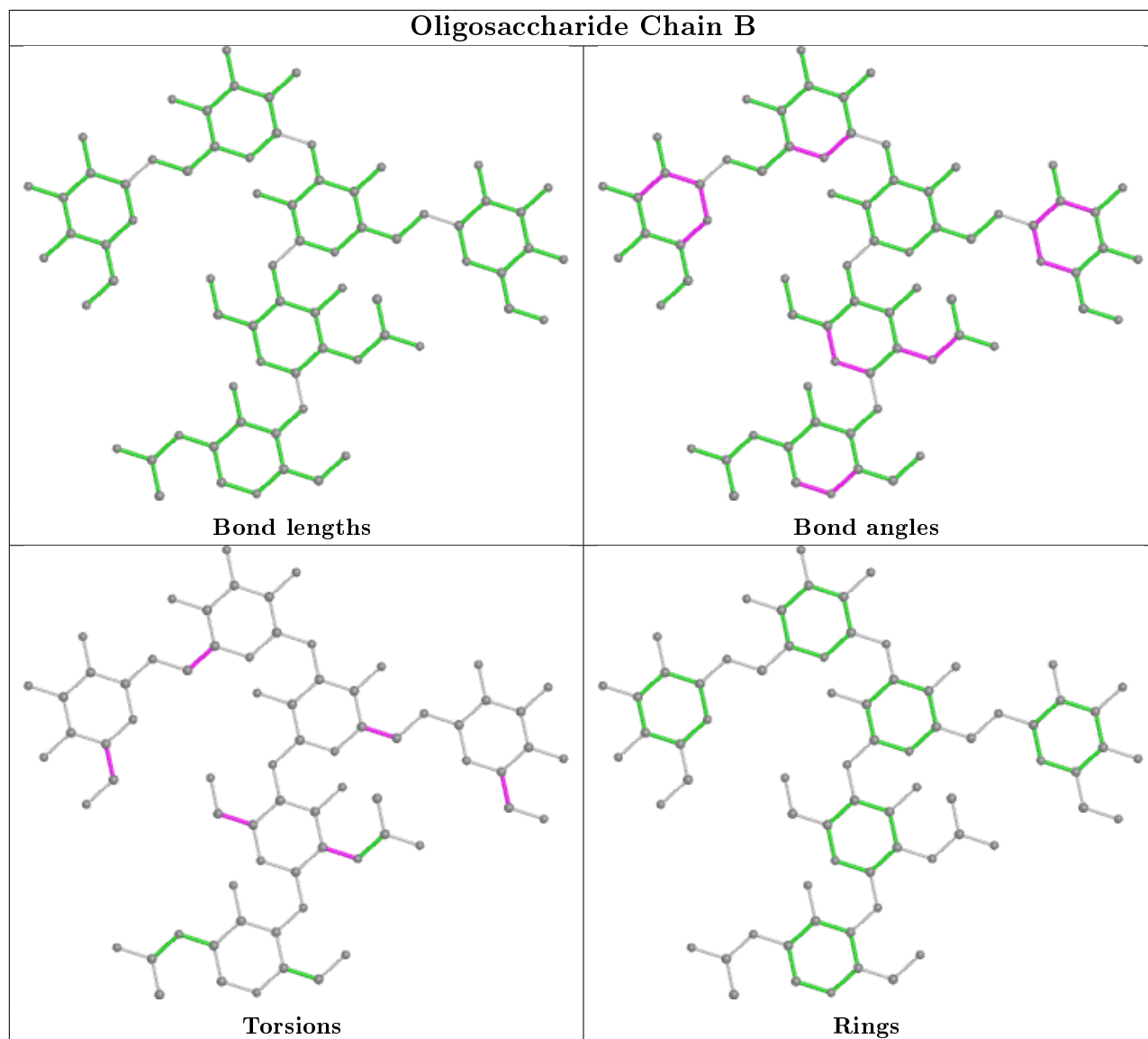
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	5	BMA	O5-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
2	B	5	BMA	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	B	2	NAG	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z  > 2$
6	NAG	A	1626	1	14,14,15	0.60	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EPE	A	1617	-	15,15,15	0.79	1 (6%)	18,20,20	1.96	4 (22%)
4	EPE	A	1618	-	15,15,15	0.87	1 (6%)	18,20,20	1.87	4 (22%)
4	EPE	A	1616	-	15,15,15	0.82	1 (6%)	18,20,20	1.86	6 (33%)
3	LPR	A	1615	5	24,30,30	2.00	10 (41%)	29,39,39	1.04	1 (3%)
6	NAG	A	1625	1	14,14,15	0.57	0	17,19,21	0.70	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
6	NAG	A	1626	1	-	2/6/23/26	0/1/1/1
4	EPE	A	1617	-	-	6/9/19/19	0/1/1/1
4	EPE	A	1618	-	-	2/9/19/19	0/1/1/1
4	EPE	A	1616	-	-	5/9/19/19	0/1/1/1
3	LPR	A	1615	5	-	3/22/40/40	0/2/2/2
6	NAG	A	1625	1	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1615	LPR	C4-N1	4.32	1.53	1.47
3	A	1615	LPR	C7-C6	-3.51	1.37	1.51
3	A	1615	LPR	O1-C1	3.08	1.27	1.22
4	A	1618	EPE	C10-S	2.89	1.81	1.77
4	A	1616	EPE	C10-S	2.68	1.81	1.77
4	A	1617	EPE	C10-S	2.65	1.81	1.77
3	A	1615	LPR	C14-C4	2.50	1.56	1.53
3	A	1615	LPR	C5-N2	2.43	1.51	1.47
3	A	1615	LPR	C21-C16	2.38	1.44	1.38
3	A	1615	LPR	C19-C18	2.22	1.43	1.38
3	A	1615	LPR	C2-C1	2.10	1.57	1.53
3	A	1615	LPR	C17-C16	2.08	1.43	1.38
3	A	1615	LPR	C20-C19	2.06	1.43	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1618	EPE	C5-N4-C3	5.01	120.10	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1617	EPE	C5-N4-C3	4.95	119.96	108.83
4	A	1616	EPE	C5-N4-C3	4.57	119.12	108.83
4	A	1617	EPE	C7-N4-C5	3.96	121.37	111.23
4	A	1618	EPE	C7-N4-C5	3.39	119.89	111.23
4	A	1616	EPE	C7-N4-C5	3.33	119.75	111.23
4	A	1617	EPE	O3S-S-C10	3.11	110.81	105.77
4	A	1618	EPE	C7-N4-C3	3.10	119.17	111.23
4	A	1616	EPE	C7-N4-C3	2.76	118.28	111.23
4	A	1618	EPE	O3S-S-C10	2.63	110.02	105.77
4	A	1616	EPE	O1S-S-C10	2.55	109.98	106.92
4	A	1617	EPE	C7-N4-C3	2.51	117.66	111.23
4	A	1616	EPE	O3S-S-C10	2.15	109.24	105.77
4	A	1616	EPE	O2S-S-C10	2.14	109.49	106.92
3	A	1615	LPR	C6-C7-C8	2.04	110.76	104.98

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1617	EPE	C10-C9-N1-C6
4	A	1617	EPE	C8-C7-N4-C5
4	A	1617	EPE	S-C10-C9-N1
4	A	1616	EPE	S-C10-C9-N1
4	A	1616	EPE	C9-C10-S-O1S
4	A	1616	EPE	C9-C10-S-O2S
6	A	1625	NAG	O5-C5-C6-O6
4	A	1618	EPE	N4-C7-C8-O8
6	A	1626	NAG	O5-C5-C6-O6
4	A	1616	EPE	C9-C10-S-O3S
6	A	1625	NAG	C4-C5-C6-O6
4	A	1617	EPE	N4-C7-C8-O8
4	A	1617	EPE	C10-C9-N1-C2
6	A	1626	NAG	C4-C5-C6-O6
4	A	1618	EPE	C8-C7-N4-C3
4	A	1616	EPE	C8-C7-N4-C3
3	A	1615	LPR	C10-C11-C12-C13
4	A	1617	EPE	C8-C7-N4-C3
3	A	1615	LPR	C14-C15-C16-C21
3	A	1615	LPR	C14-C15-C16-C17

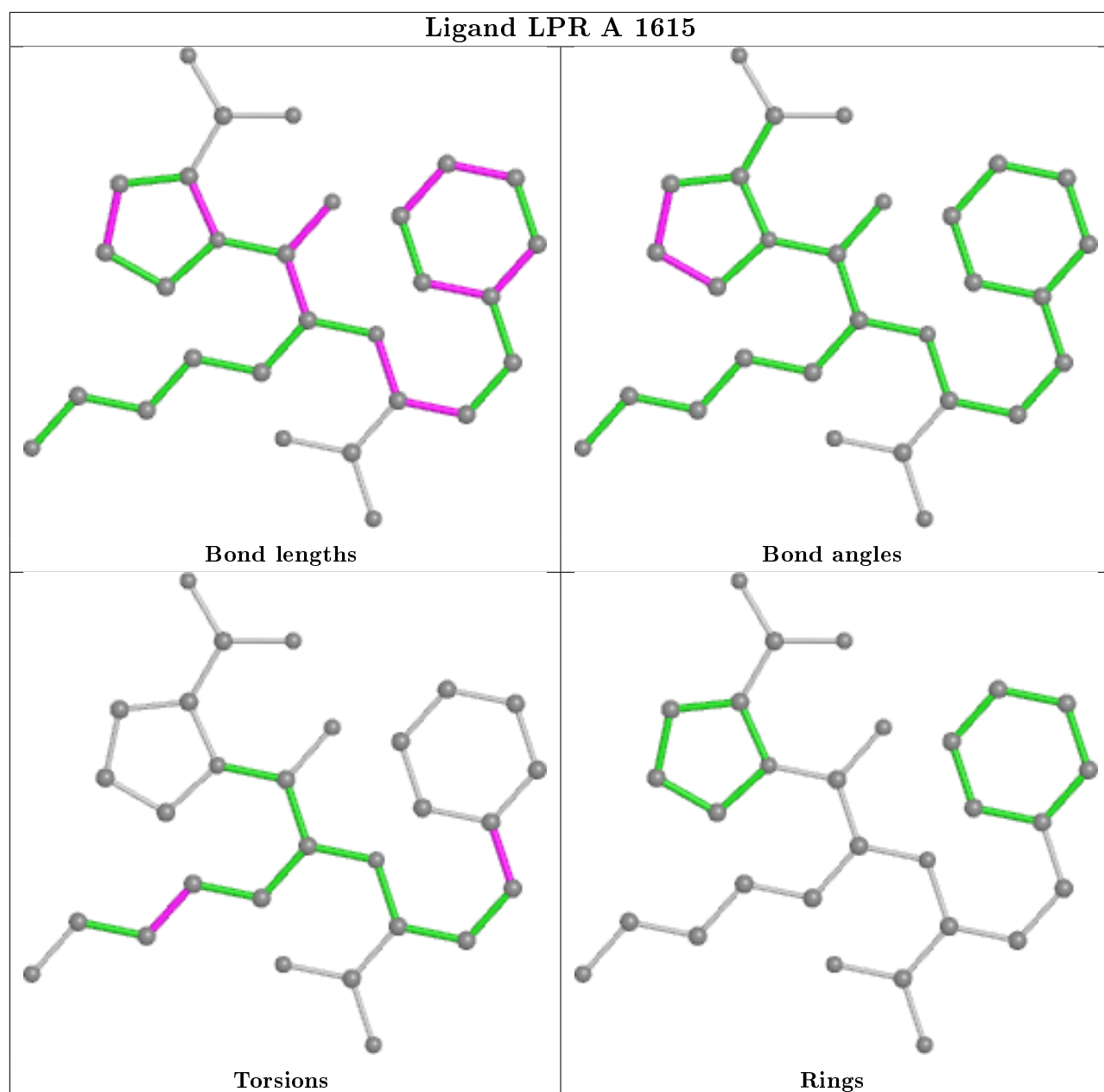
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1617	EPE	2	0
4	A	1616	EPE	5	0
3	A	1615	LPR	2	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	595/598 (99%)	-0.21	8 (1%) 77 78	18, 28, 39, 47	7 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	THR	5.1
1	A	20	LYS	3.4
1	A	533	VAL	3.3
1	A	331	GLY	3.2
1	A	614	SER	3.0
1	A	531	ASP	2.5
1	A	138	SER	2.2
1	A	329	THR	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](#)

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.

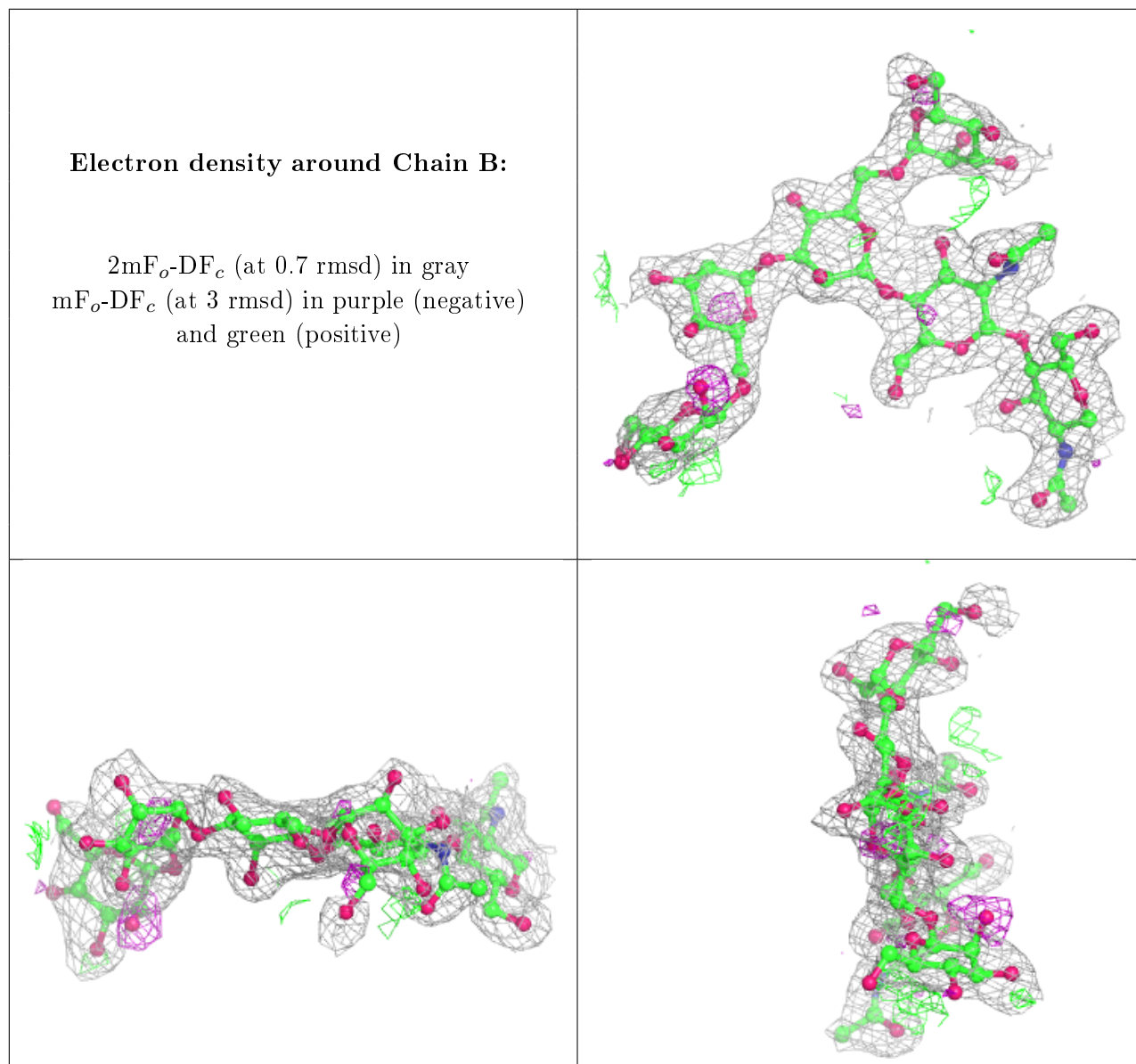
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	B	6	11/12	0.78	0.31	62,64,64,64	0
2	BMA	B	5	11/12	0.81	0.24	67,68,69,69	0
2	MAN	B	4	11/12	0.89	0.18	60,61,63,65	0
2	BMA	B	3	11/12	0.90	0.17	53,56,58,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.95	0.15	39,42,44,48	0
2	NAG	B	1	14/15	0.97	0.07	30,31,33,36	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.

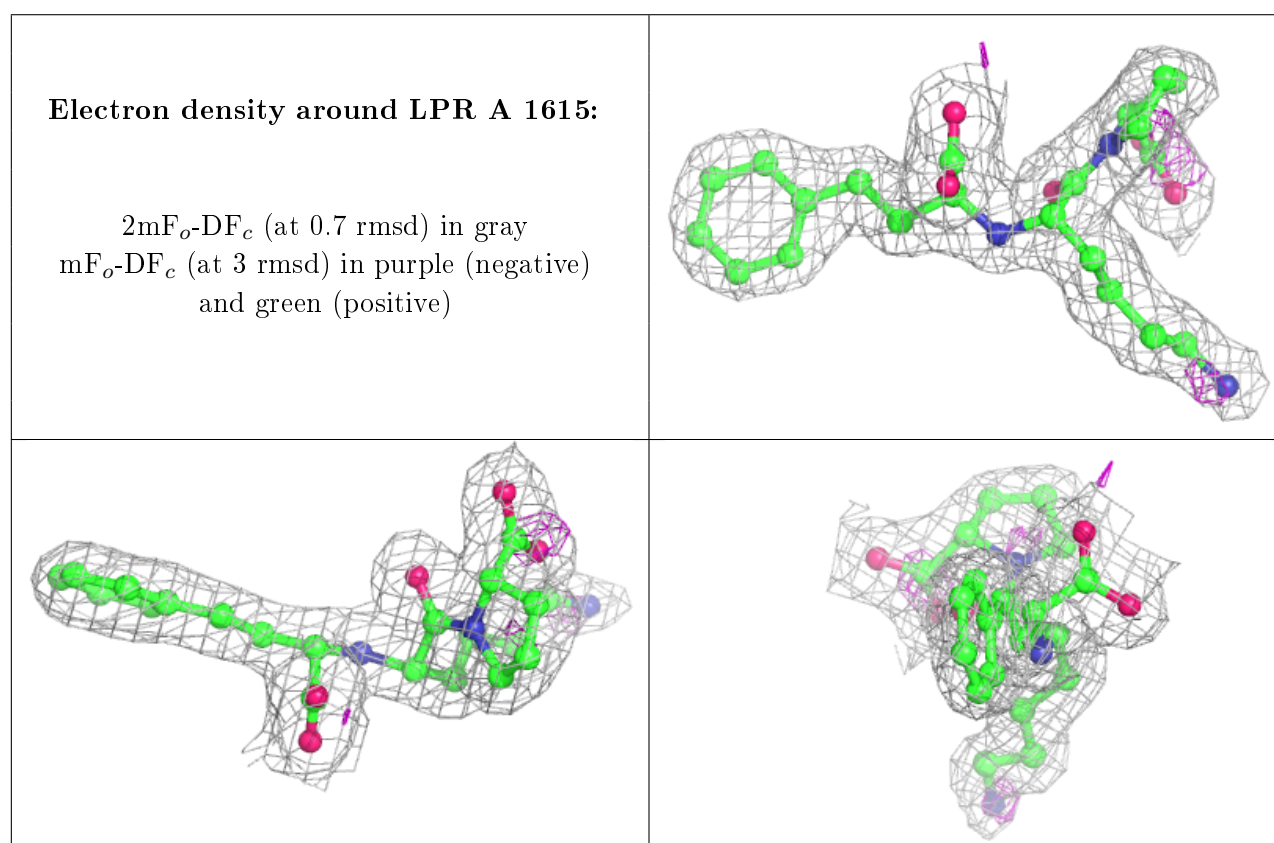


## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	1625	14/15	0.78	0.39	36,37,38,38	14
6	NAG	A	1626	14/15	0.81	0.39	44,45,45,45	14
4	EPE	A	1616	15/15	0.82	0.26	70,72,73,73	0
4	EPE	A	1617	15/15	0.94	0.15	48,49,51,52	0
4	EPE	A	1618	15/15	0.95	0.11	45,48,51,52	0
3	LPR	A	1615	29/29	0.97	0.14	22,24,30,33	0
5	ZN	A	1619	1/1	1.00	0.08	21,21,21,21	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.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.