

# wwPDB X-ray Structure Validation Summary Report (i)

### Apr 30, 2024 – 02:12 PM JST

PDB ID : 8JA6

Title : Structure of the alginate epimerase/lyase complexed with tri-mannuronic acid

 $\begin{array}{cccc} \text{Authors} & : & \text{Fujiwara, T.} \\ \text{Deposited on} & : & 2023\text{-}05\text{-}05 \end{array}$ 

Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) 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 : 2.36.2

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

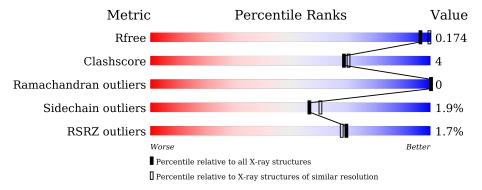
Validation Pipeline (wwPDB-VP) : 2.36.2

## 1 Overall quality at a glance (i)

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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	493	88%	9%	
2	В	3	100%		

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	BEM	В	1	-	-	-	X
4	ACT	A	507	-	-	X	-



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3887 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.

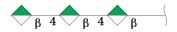
• Molecule 1 is a protein called mannuronan 5-epimerase.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Δ	480	Total	С	N	О	S	0	6	0
1	17	400	3636	2217	632	781	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	LEU	-	expression tag	UNP A0A0C4WKK2
A	487	GLU	-	expression tag	UNP A0A0C4WKK2
A	488	HIS	-	expression tag	UNP A0A0C4WKK2
A	489	HIS	-	expression tag	UNP A0A0C4WKK2
A	490	HIS	-	expression tag	UNP A0A0C4WKK2
A	491	HIS	ı	expression tag	UNP A0A0C4WKK2
A	492	HIS	-	expression tag	UNP A0A0C4WKK2
A	493	HIS	-	expression tag	UNP A0A0C4WKK2

• Molecule 2 is an oligosaccharide called beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.



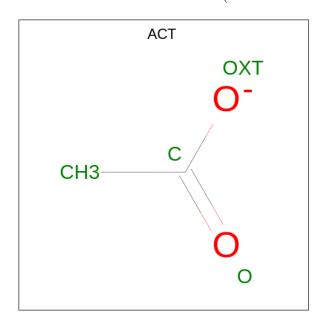
Mol	Chain	Residues	At	oms		ZeroOcc	AltConf	Trace
2	В	3	Total 37	C 18	O 19	0	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Ca 6 6	0	0



 $\bullet$  Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total 4	C 2	O 2	0	0

• Molecule 5 is water.

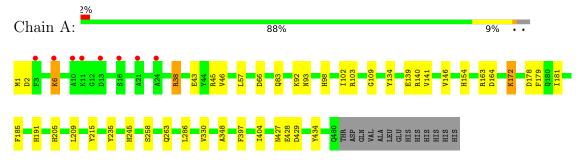
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	204	Total O 204 204	0	0



# 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: mannuronan 5-epimerase



• Molecule 2: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain B: 100%

BEM1 BEM2 BEM3



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	121.71Å 121.71Å 120.69Å	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	48.30 - 2.00	Depositor
Resolution (A)	48.30 - 2.00	EDS
% Data completeness	100.0 (48.30-2.00)	Depositor
(in resolution range)	100.0 (48.30-2.00)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.76 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D.D.	0.154 , 0.178	Depositor
$R, R_{free}$	0.152 , $0.174$	DCC
$R_{free}$ test set	2170 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 42.1	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MLY, BEM, ACT, CA

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	Bo	nd angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.39	0/3636	0.66	1/4923 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	172	MLY	O-C-N	-7.22	111.15	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	MLY	Mainchain

### 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	3636	0	3380	24	0
2	В	37	0	21	0	0
3	A	6	0	0	0	0
4	A	4	0	3	2	0
5	A	204	0	0	2	0
All	All	3887	0	3404	26	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.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:A:43:GLU:OE1	1:A:45:ARG:NH1	2.33	0.61
1:A:428:GLU:OE2	1:A:428:GLU:N	2.28	0.59
1:A:46:VAL:HG11	1:A:57:LEU:HD21	1.90	0.54
1:A:185:PHE:HB2	1:A:209:LEU:HD23	1.90	0.52
1:A:2:ASP:OD1	1:A:38:ARG:NH1	2.46	0.49

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	478/493 (97%)	463 (97%)	15 (3%)	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	368/374 (98%)	361 (98%)	7 (2%)	57 61	

5 of 7 residues with a non-rotameric sidechain are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type
1	A	66	ASP
1	A	83	GLN
1	A	179	PHE
1	A	163	ARG
1	A	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	Mol Tree		Dog	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
1	MLY	A	76	1	9,10,11	0.56	0	6,11,13	0.85	0
1	MLY	A	436	1	9,10,11	0.67	0	6,11,13	0.86	0
1	MLY	A	255	1	9,10,11	0.70	0	6,11,13	0.78	0
1	MLY	A	60	1	9,10,11	0.62	0	6,11,13	0.63	0



Mol	Т	Chain	Chain	Chain	Chain	Chain	Pag	Link	В	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2					
1	MLY	A	96	1	9,10,11	0.58	0	6,11,13	0.91	0					
1	MLY	A	172	1	9,10,11	0.87	0	6,11,13	0.57	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
1	MLY	A	76	1	-	0/8/9/11	-
1	MLY	A	436	1	-	0/8/9/11	-
1	MLY	A	255	1	-	0/8/9/11	-
1	MLY	A	60	1	-	1/8/9/11	-
1	MLY	A	96	1	-	1/8/9/11	_
1	MLY	A	172	1	-	2/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	96	MLY	O-C-CA-CB
1	A	172	MLY	O-C-CA-CB
1	A	172	MLY	CG-CD-CE-NZ
1	A	60	MLY	CD-CE-NZ-CH1

There are no ring outliers.

No monomer is involved in short contacts.

### 5.5 Carbohydrates (i)

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			В	ond ang	les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BEM	В	1	2	13,13,13	1.23	0	18,19,19	1.51	4 (22%)
2	BEM	В	2	2	12,12,13	1.70	3 (25%)	14,17,19	1.33	2 (14%)
2	BEM	В	3	2	12,12,13	1.42	1 (8%)	14,17,19	1.43	3 (21%)

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	BEM	В	1	2	-	0/4/24/24	0/1/1/1
2	BEM	В	2	2	-	0/4/21/24	0/1/1/1
2	BEM	В	3	2	-	0/4/21/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	2	BEM	C2-C3	3.80	1.58	1.52
2	В	3	BEM	C2-C3	2.98	1.56	1.52
2	В	2	BEM	C5-C6	2.49	1.58	1.53
2	В	2	BEM	O5-C1	-2.20	1.40	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	3	BEM	C3-C4-C5	-3.79	102.75	109.25
2	В	1	BEM	C3-C4-C5	-2.99	104.13	109.25
2	В	1	BEM	O2-C2-C1	2.74	115.50	109.16
2	В	1	BEM	C1-C2-C3	-2.52	105.09	110.31
2	В	2	BEM	C3-C4-C5	-2.49	104.99	109.25

There are no chirality outliers.

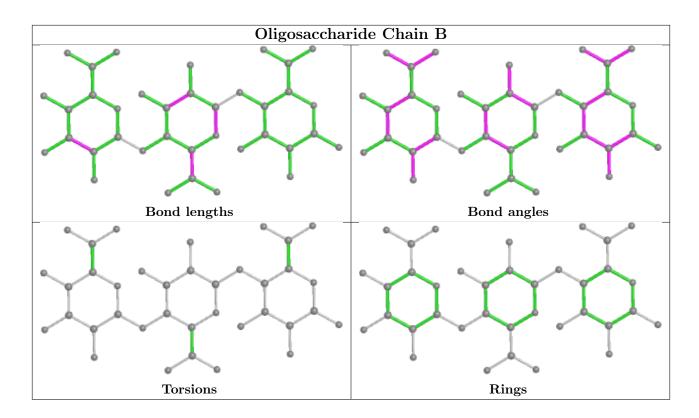
There are no torsion outliers.

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, 6 are monoatomic - leaving 1 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).

Mo	l Type	Chain	Pog	Link	Bond lengths			Bond angles		
IVIO	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	ACT	A	507	-	3,3,3	0.71	0	3,3,3	1.60	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
4	A	507	ACT	OXT-C-O	2.18	130.08	122.05

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	ACT	2	0

# 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	474/493 (96%)	-0.20	8 (1%) 70 68	28, 45, 80, 111	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	4.2
1	A	16	SER	3.2
1	A	6	LYS	3.2
1	A	13	ASP	3.0
1	A	24	ALA	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	MLY	A	172	11/12	0.91	0.18	41,44,60,65	0
1	MLY	A	76	11/12	0.94	0.17	65,70,76,84	0
1	MLY	A	96	11/12	0.96	0.11	47,52,61,62	0
1	MLY	A	60	11/12	0.97	0.14	54,58,75,76	0
1	MLY	A	255	11/12	0.97	0.16	27,30,39,39	0
1	MLY	A	436	11/12	0.97	0.09	36,38,56,58	0

### 6.3 Carbohydrates (i)

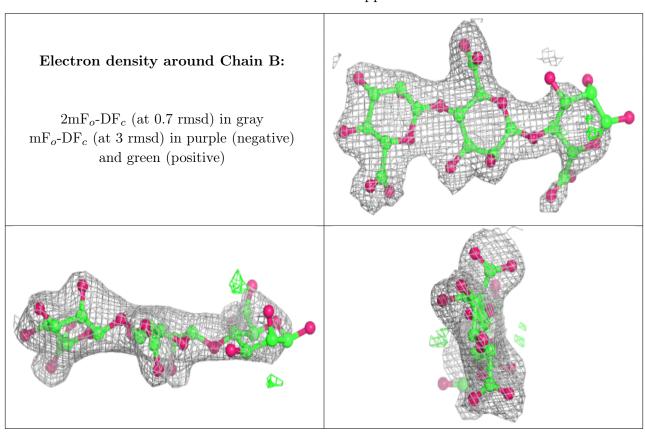
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column



Tabelled we visit have the number of adding with decubation less than the	labelled ' $Q < 0.9$	o' lists the number	of atoms with occu	pancy less than 0.9.
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BEM	В	1	13/13	0.74	0.42	67,76,81,81	13
2	BEM	В	2	12/13	0.88	0.12	55,62,65,68	12
2	BEM	В	3	12/13	0.91	0.08	54,59,66,67	12

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,  $95^{th}$  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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
4	ACT	A	507	4/4	0.92	0.17	29,37,40,46	4
3	CA	A	506	1/1	0.97	0.05	70,70,70,70	1
3	CA	A	501	1/1	0.97	0.09	46,46,46,46	1
3	CA	A	505	1/1	0.98	0.04	47,47,47,47	0

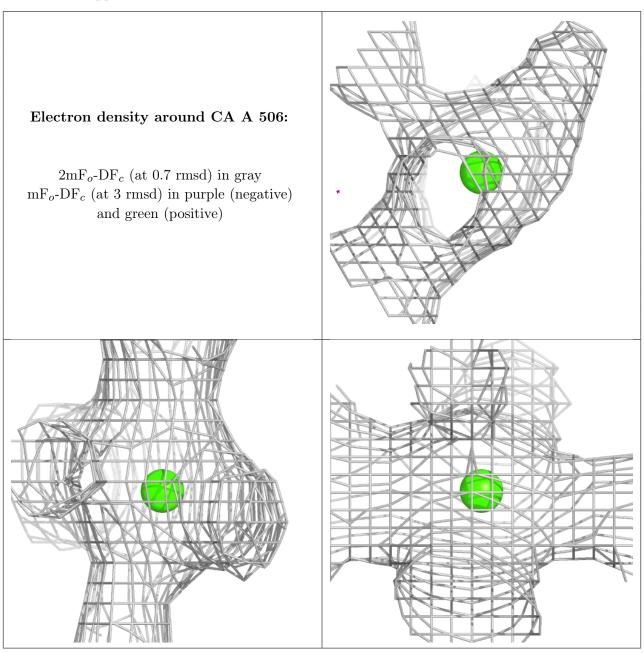
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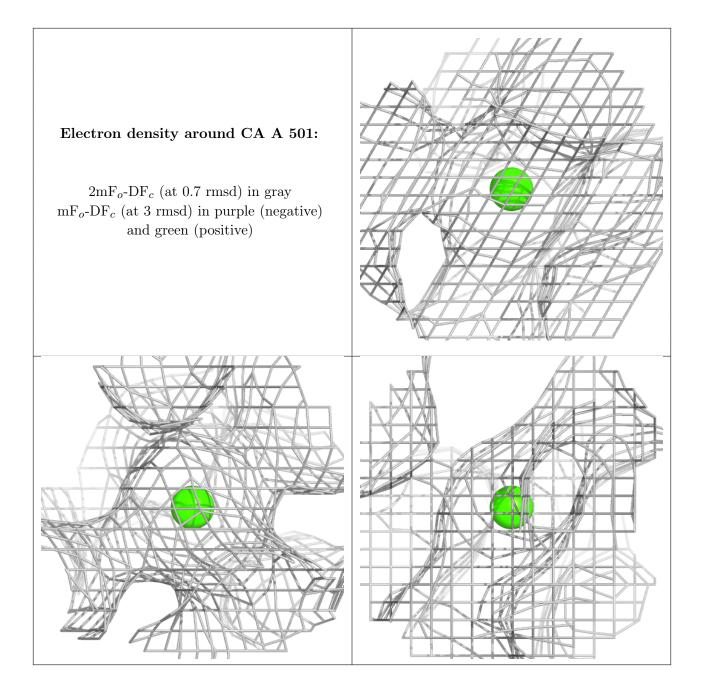
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	CA	A	504	1/1	0.99	0.07	41,41,41,41	0
3	CA	A	503	1/1	0.99	0.10	34,34,34,34	0
3	CA	A	502	1/1	1.00	0.10	31,31,31,31	0

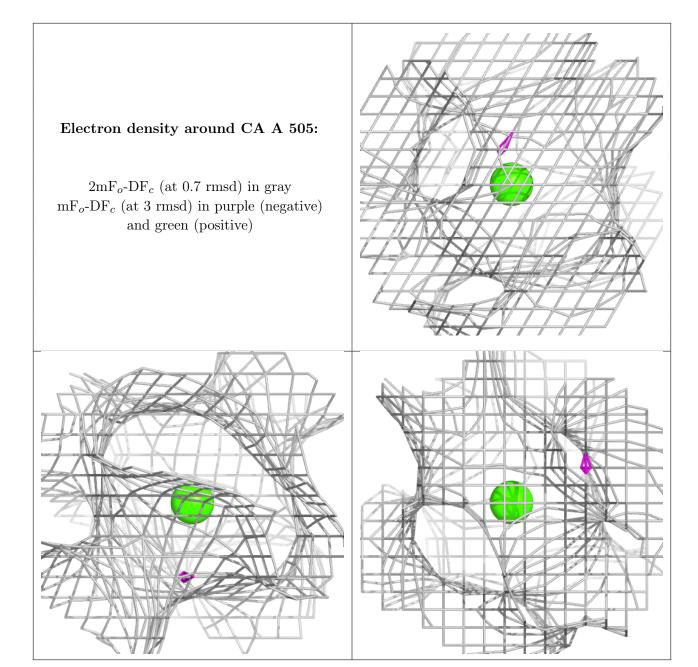
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



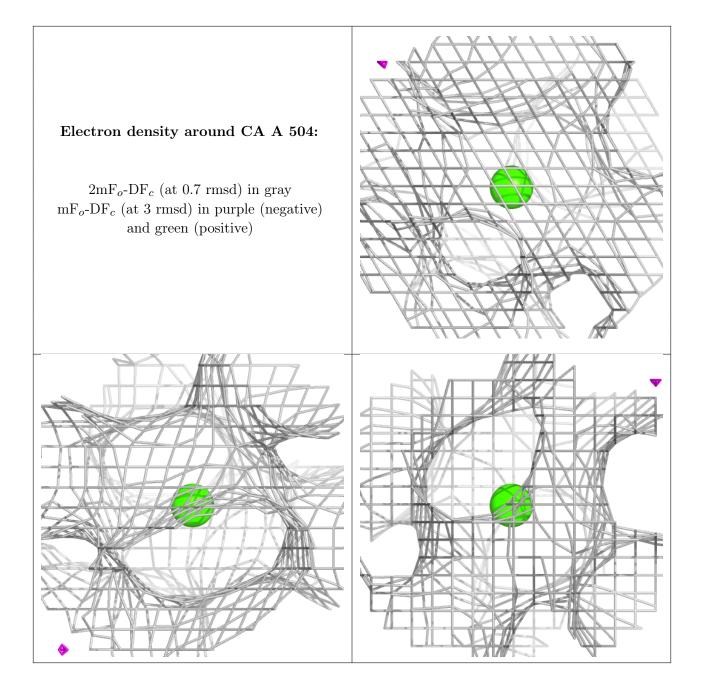




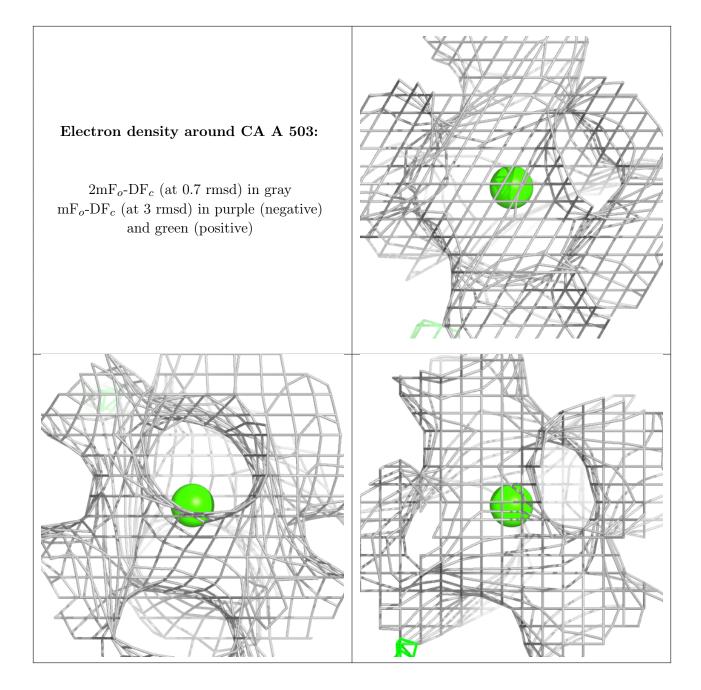




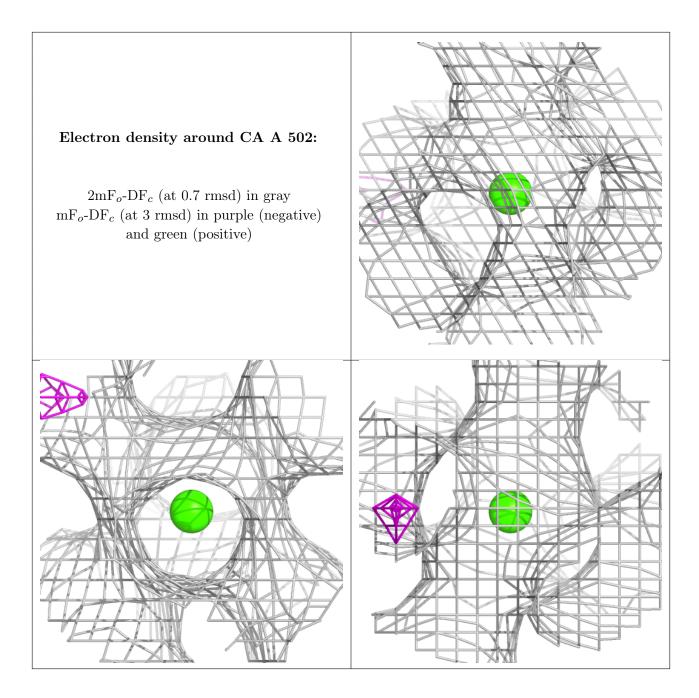












# 6.5 Other polymers (i)

There are no such residues in this entry.

