



# wwPDB X-ray Structure Validation Summary Report

Dec 15, 2021 – 12:18 pm GMT

PDB ID : 7BKX  
Title : Diploptera punctata inspired lipocalin-like Milk protein expressed in Saccharomyces cerevisiae  
Authors : Banerjee, S.; Kanagavijayan, D.; Subramanian, R.; Santhakumari, P.R.; Chavas, L.M.G.; Ramaswamy, S.  
Deposited on : 2021-01-17  
Resolution : 2.35 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](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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.24  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.24

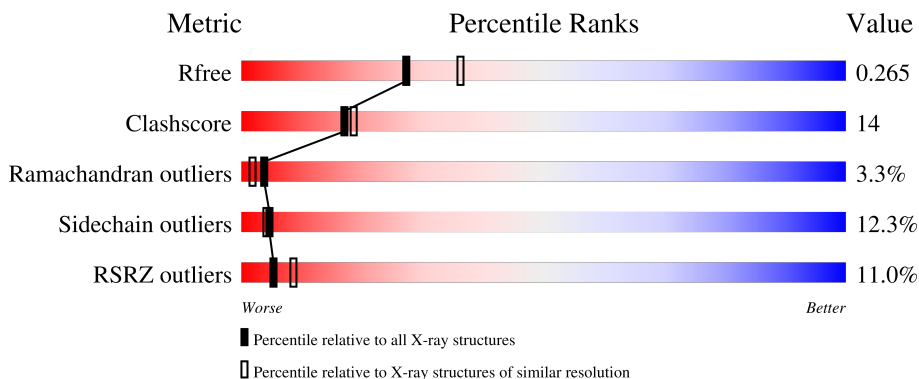
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	AAA	177	
2	AbA	2	

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	NAG	AbA	2	-	-	-	X
3	NAG	AAA	202	-	-	-	X
5	GOL	AAA	205	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 1365 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.

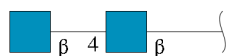
- Molecule 1 is a protein called Milk protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	155	1242	798	200	239	5	0	1	0

There are 22 discrepancies between the modelled and reference sequences:

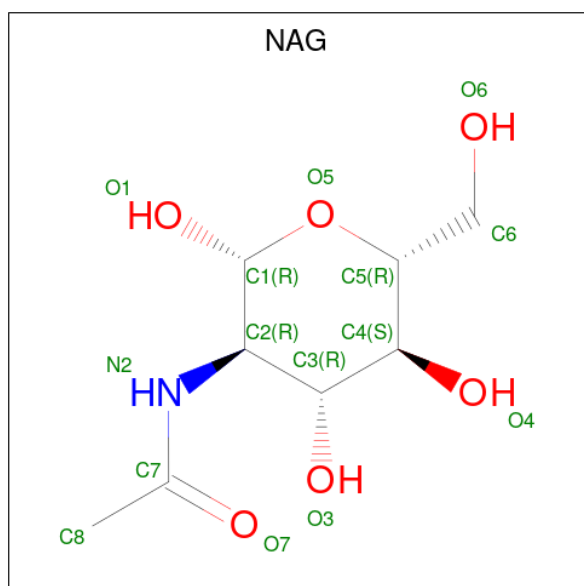
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-21	MET	-	initiating methionine	UNP Q6SVB5
AAA	-20	ARG	-	expression tag	UNP Q6SVB5
AAA	-19	GLN	-	expression tag	UNP Q6SVB5
AAA	-18	VAL	-	expression tag	UNP Q6SVB5
AAA	-17	TRP	-	expression tag	UNP Q6SVB5
AAA	-16	PHE	-	expression tag	UNP Q6SVB5
AAA	-15	SER	-	expression tag	UNP Q6SVB5
AAA	-14	TRP	-	expression tag	UNP Q6SVB5
AAA	-13	ILE	-	expression tag	UNP Q6SVB5
AAA	-12	VAL	-	expression tag	UNP Q6SVB5
AAA	-11	GLY	-	expression tag	UNP Q6SVB5
AAA	-10	LEU	-	expression tag	UNP Q6SVB5
AAA	-9	PHE	-	expression tag	UNP Q6SVB5
AAA	-8	LEU	-	expression tag	UNP Q6SVB5
AAA	-7	CYS	-	expression tag	UNP Q6SVB5
AAA	-6	PHE	-	expression tag	UNP Q6SVB5
AAA	-5	PHE	-	expression tag	UNP Q6SVB5
AAA	-4	ASN	-	expression tag	UNP Q6SVB5
AAA	-3	VAL	-	expression tag	UNP Q6SVB5
AAA	-2	SER	-	expression tag	UNP Q6SVB5
AAA	-1	SER	-	expression tag	UNP Q6SVB5
AAA	0	ALA	-	expression tag	UNP Q6SVB5

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



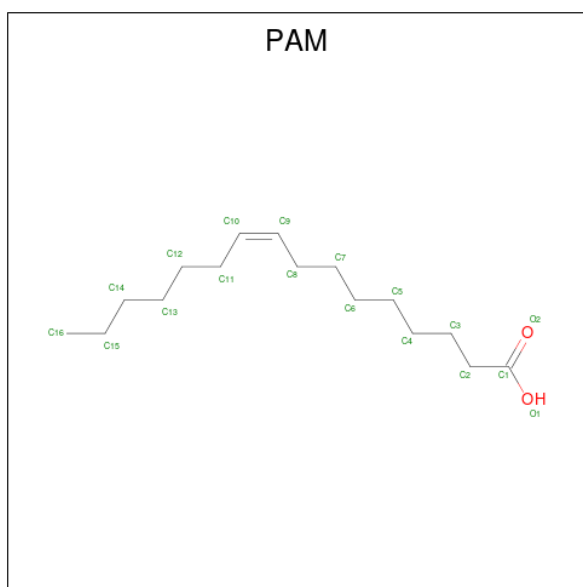
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	AbA	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	AAA	1	14	8	1	5	0	0
3	AAA	1	14	8	1	5	0	0
3	AAA	1	14	8	1	5	0	0

- Molecule 4 is PALMITOLEIC ACID (three-letter code: PAM) (formula:  $C_{16}H_{30}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			18	16	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	3	Total 3	Zn 3	0	0

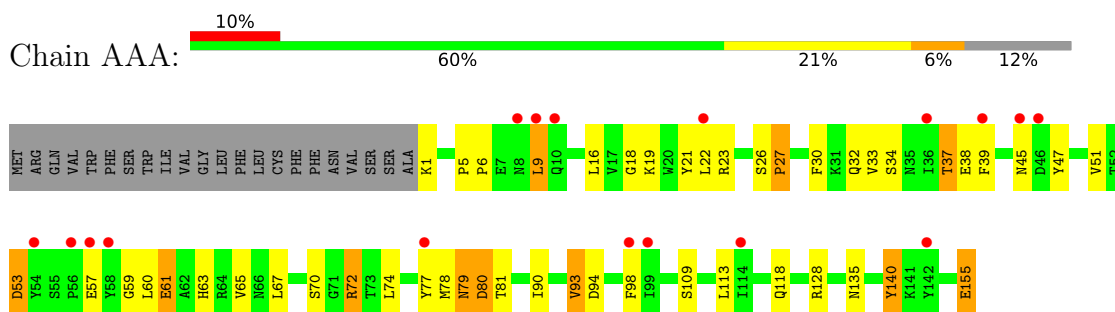
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	26	Total 26	O 26	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: Milk protein



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.61Å 135.66Å 39.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.60 – 2.35 20.61 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.60-2.35) 100.0 (20.61-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.35Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, $R_{free}$	0.222 , 0.278 0.221 , 0.265	Depositor DCC
$R_{free}$ test set	573 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: ZN, PAM, GOL, NAG

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	AAA	0.80	0/1280	1.05	4/1749 (0.2%)

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	AAA	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	23	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	AAA	27	PRO	N-CA-CB	-7.65	94.12	103.30
1	AAA	27	PRO	N-CD-CG	-5.77	94.55	103.20
1	AAA	27	PRO	CA-N-CD	-5.10	104.35	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	26	SER	Peptide,Mainchain
1	AAA	59	GLY	Peptide

## 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	AAA	1242	0	1134	33	0
2	AbA	28	0	25	0	0
3	AAA	42	0	39	3	0
4	AAA	18	0	29	5	0
5	AAA	6	0	8	1	0
6	AAA	3	0	0	1	0
7	AAA	26	0	0	2	0
All	All	1365	0	1235	36	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 14.

The worst 5 of 36 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:AAA:155:GLU:O	7:AAA:301:HOH:O	1.95	0.84
1:AAA:79:ASN:O	3:AAA:202:NAG:O7	2.08	0.72
1:AAA:77:TYR:HB2	3:AAA:204:NAG:H82	1.73	0.71
1:AAA:61:GLU:OE2	6:AAA:206:ZN:ZN	1.39	0.71
1:AAA:65:VAL:HG12	1:AAA:78:MET:HG2	1.71	0.71

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	AAA	154/177 (87%)	136 (88%)	13 (8%)	5 (3%)	4 2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	27	PRO
1	AAA	60	LEU
1	AAA	9	LEU
1	AAA	57	GLU
1	AAA	140	TYR

### 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	AAA	131/160 (82%)	114 (87%)	17 (13%)	4 4

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	135	ASN
1	AAA	155	GLU
1	AAA	70	SER
1	AAA	72	ARG
1	AAA	79	ASN

Sometimes 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](#)

2 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	AbA	1	1,2	14,14,15	0.65	0	17,19,21	1.38	1 (5%)
2	NAG	AbA	2	2	14,14,15	0.59	0	17,19,21	1.15	2 (11%)

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	AbA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	AbA	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AbA	1	NAG	O5-C5-C6	3.13	112.10	107.20
2	AbA	2	NAG	C4-C3-C2	-2.59	107.22	111.02
2	AbA	2	NAG	O3-C3-C2	2.26	114.14	109.47

There are no chirality outliers.

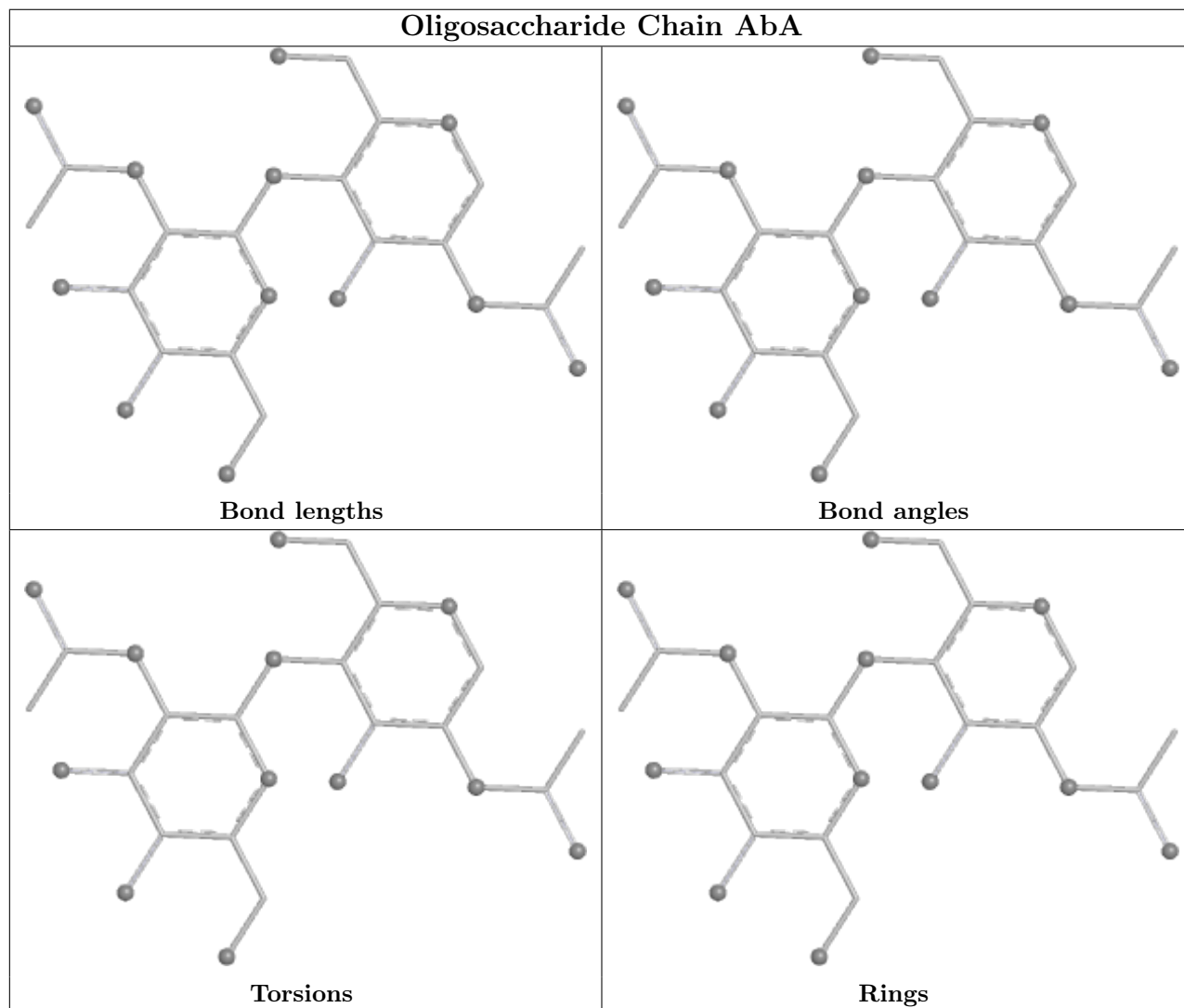
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AbA	1	NAG	O5-C5-C6-O6
2	AbA	2	NAG	O5-C5-C6-O6
2	AbA	1	NAG	C4-C5-C6-O6
2	AbA	2	NAG	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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	AAA	202	1	14,14,15	0.65	0	17,19,21	2.26	4 (23%)
5	GOL	AAA	205	-	5,5,5	0.17	0	5,5,5	0.34	0
3	NAG	AAA	204	1	14,14,15	0.62	0	17,19,21	2.39	8 (47%)
3	NAG	AAA	201	1	14,14,15	1.11	1 (7%)	17,19,21	2.08	6 (35%)
4	PAM	AAA	203	-	14,17,17	0.50	0	13,17,17	0.28	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
3	NAG	AAA	202	1	-	3/6/23/26	0/1/1/1
5	GOL	AAA	205	-	-	2/4/4/4	-
3	NAG	AAA	204	1	-	0/6/23/26	0/1/1/1
3	NAG	AAA	201	1	-	0/6/23/26	0/1/1/1
4	PAM	AAA	203	-	-	9/13/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	201	NAG	O5-C5	2.90	1.49	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	202	NAG	C1-C2-N2	5.89	120.56	110.49
3	AAA	202	NAG	C2-N2-C7	5.09	130.15	122.90
3	AAA	204	NAG	C1-O5-C5	-4.92	105.52	112.19
3	AAA	201	NAG	C1-O5-C5	4.11	117.76	112.19
3	AAA	204	NAG	O3-C3-C2	-3.74	101.72	109.47

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

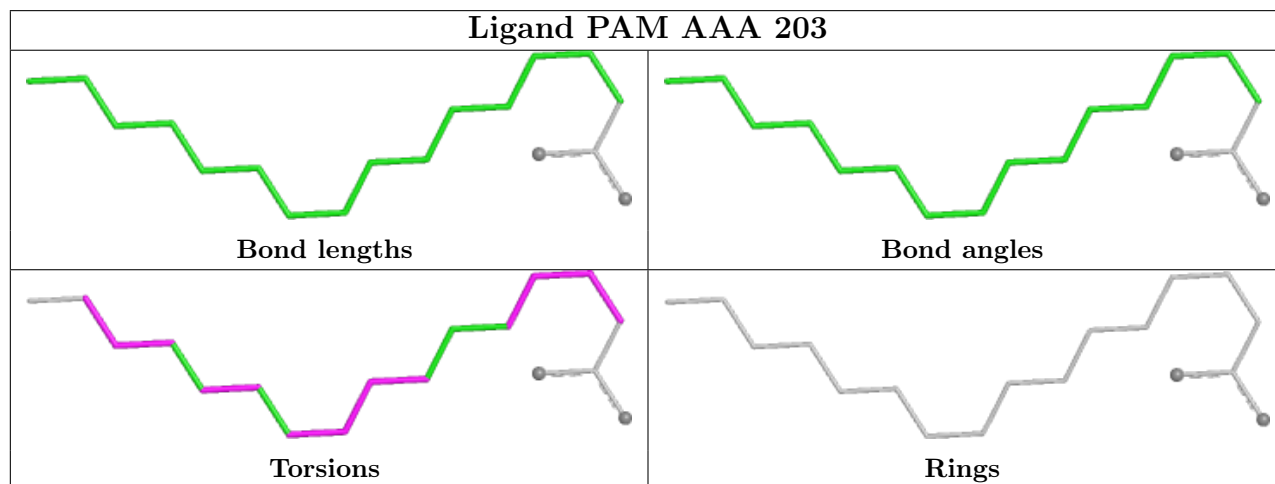
Mol	Chain	Res	Type	Atoms
4	AAA	203	PAM	C1-C2-C3-C4
5	AAA	205	GOL	O1-C1-C2-C3
3	AAA	202	NAG	C1-C2-N2-C7
3	AAA	202	NAG	O5-C5-C6-O6
3	AAA	202	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	202	NAG	2	0
5	AAA	205	GOL	1	0
3	AAA	204	NAG	1	0
4	AAA	203	PAM	5	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	AAA	155/177 (87%)	0.53	17 (10%) <b>5</b> <b>8</b>	30, 60, 92, 111	1 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	114	ILE	4.1
1	AAA	22	LEU	3.8
1	AAA	54	TYR	3.8
1	AAA	142	TYR	3.5
1	AAA	9	LEU	2.9

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

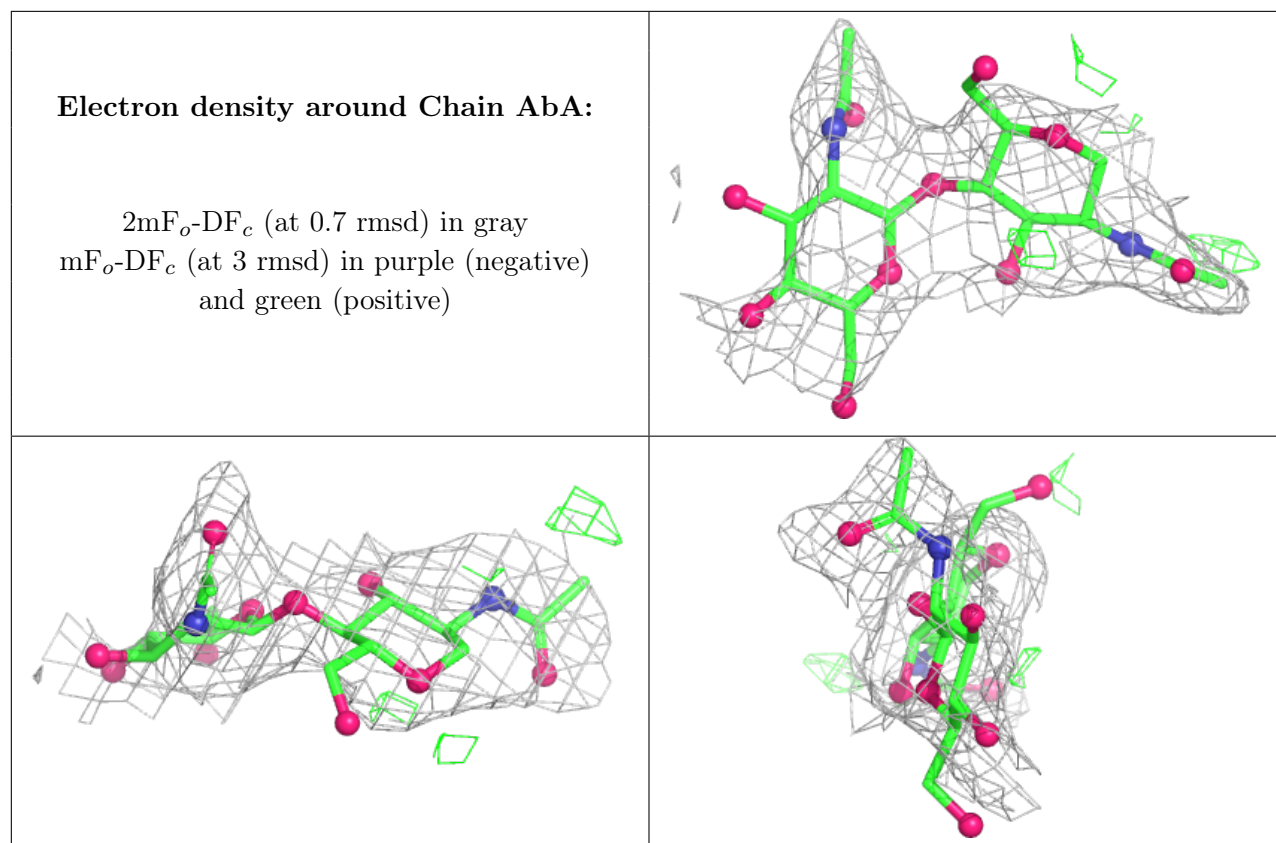
There are no non-standard protein/DNA/RNA residues in this entry.

### 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	NAG	AbA	2	14/15	<b>0.73</b>	<b>0.42</b>	105,130,142,143	0
2	NAG	AbA	1	14/15	0.84	0.28	89,100,117,118	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.

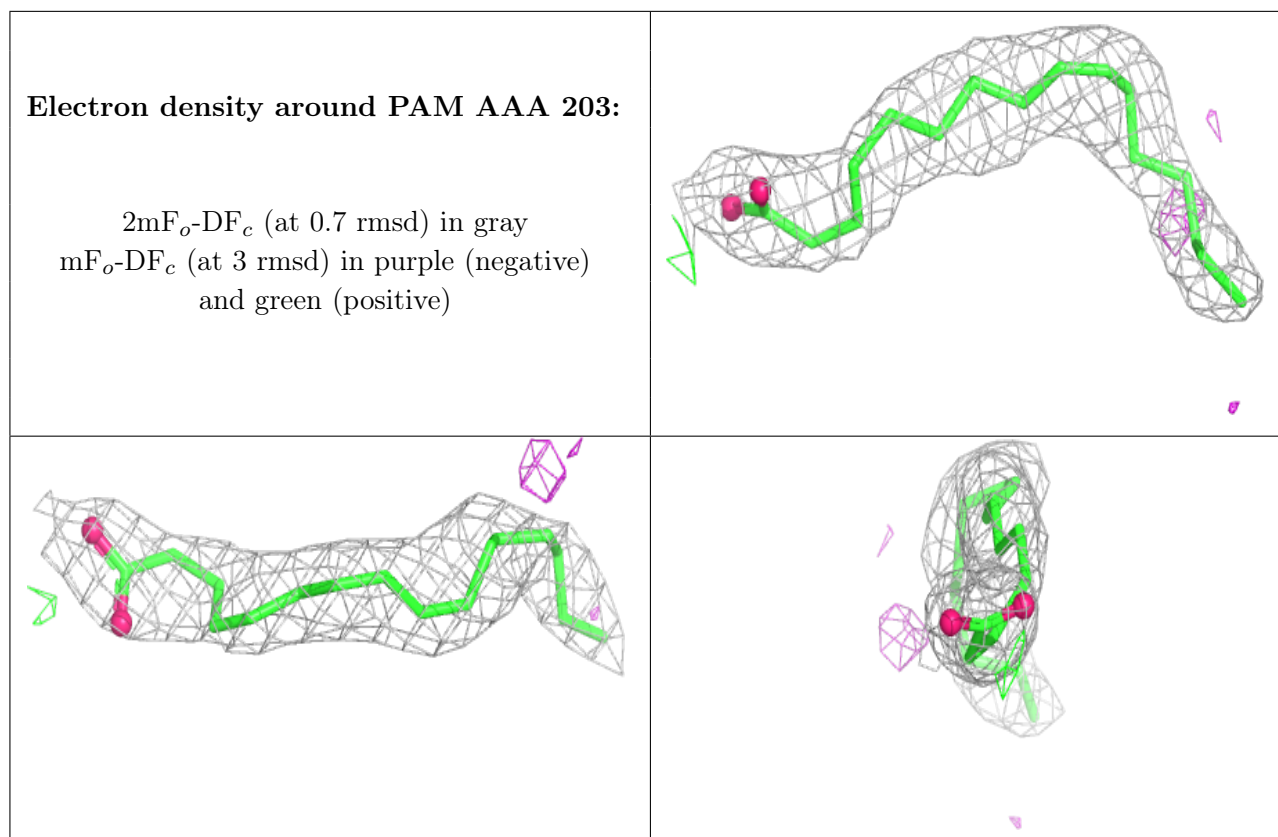


## 6.4 Ligands [i](#)

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
3	NAG	AAA	202	14/15	0.68	0.50	110,121,128,133	0
5	GOL	AAA	205	6/6	0.71	0.52	87,93,101,107	0
3	NAG	AAA	204	14/15	0.83	0.30	88,99,106,109	0
4	PAM	AAA	203	18/18	0.87	0.38	55,58,76,82	0
3	NAG	AAA	201	14/15	0.91	0.20	52,69,79,79	0
6	ZN	AAA	207	1/1	0.97	0.06	58,58,58,58	0
6	ZN	AAA	208	1/1	0.98	0.07	49,49,49,49	1
6	ZN	AAA	206	1/1	0.99	0.03	78,78,78,78	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.