



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:33 AM UTC

PDB ID : 7BKX / pdb_00007bkx
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 Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

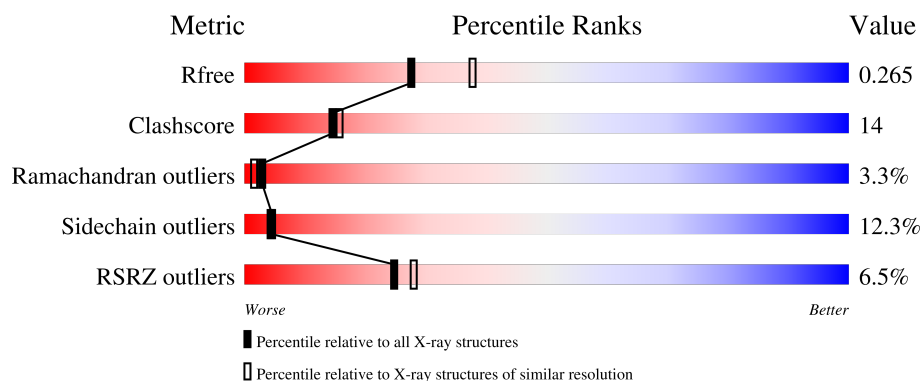
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 ≥ 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	6% 58% 23% 7% 12%
2	AbA	2	100%

2 Entry composition

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
1	AAA	155	Total	C	N	O	S	0	1	0
			1242	798	200	239	5			

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.



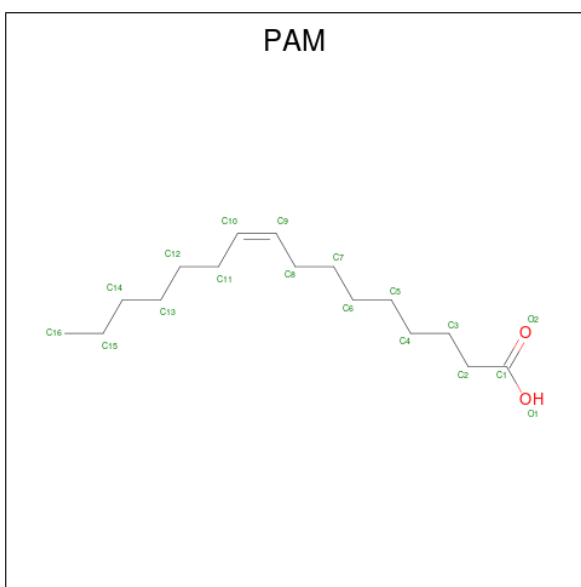
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AbA	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 4 is PALMITOLEIC ACID (CCD ID: 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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

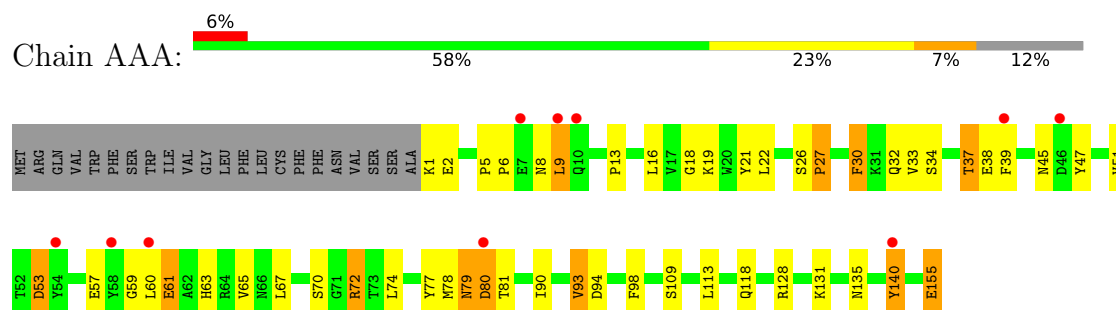
- Molecule 7 is water.

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, α , β , γ	51.61Å 135.66Å 39.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.60 – 2.35 20.60 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.60-2.35) 99.8 (20.60-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.35Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.222 , 0.278 0.223 , 0.265	Depositor DCC
R_{free} test set	573 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1365	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, ZN, PAM, GOL

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	1.13	1/1280 (0.1%)	1.49	9/1749 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	13	PRO	C-O	-5.92	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	27	PRO	N-CA-CB	-8.69	94.12	103.25
1	AAA	27	PRO	CB-CA-C	6.32	121.98	111.56
1	AAA	27	PRO	N-CD-CG	-5.77	94.55	103.20
1	AAA	2	GLU	CB-CG-CD	5.59	122.11	112.60
1	AAA	131	LYS	N-CA-C	-5.47	105.23	111.14
1	AAA	27	PRO	CA-N-CD	-5.46	104.35	112.00
1	AAA	8	ASN	CA-C-N	5.17	131.42	121.54
1	AAA	8	ASN	C-N-CA	5.17	131.42	121.54
1	AAA	30	PHE	CA-CB-CG	-5.12	108.69	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

All (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
4:AAA:203:PAM:O2	4:AAA:203:PAM:H42	1.92	0.69
1:AAA:94:ASP:OD2	1:AAA:128:ARG:NH1	2.31	0.64
1:AAA:65:VAL:HG12	1:AAA:78:MET:CG	2.28	0.63
1:AAA:94:ASP:OD1	1:AAA:128:ARG:NH1	2.31	0.63
1:AAA:19:LYS:NZ	1:AAA:21:TYR:OH	2.29	0.61
1:AAA:47:TYR:HB2	1:AAA:67:LEU:HB2	1.81	0.61
1:AAA:93:VAL:HG22	1:AAA:98:PHE:CE2	2.37	0.59
1:AAA:63:HIS:ND1	1:AAA:80[A]:ASP:OD2	2.36	0.58
1:AAA:94:ASP:CG	1:AAA:128:ARG:NH1	2.61	0.58
1:AAA:9:LEU:HB3	1:AAA:72:ARG:HG2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:118:GLN:HB3	5:AAA:205:GOL:H12	1.88	0.56
1:AAA:38:GLU:HG2	1:AAA:51:VAL:HG22	1.87	0.55
1:AAA:45:ASN:HA	7:AAA:316:HOH:O	2.07	0.55
1:AAA:53:ASP:OD1	1:AAA:61:GLU:OE2	2.26	0.54
1:AAA:9:LEU:CB	1:AAA:72:ARG:HG2	2.40	0.52
1:AAA:9:LEU:HD12	1:AAA:72:ARG:HB3	1.94	0.50
1:AAA:9:LEU:HB3	1:AAA:72:ARG:CG	2.41	0.50
1:AAA:74:LEU:HD12	1:AAA:74:LEU:C	2.37	0.49
1:AAA:30:PHE:HA	1:AAA:33:VAL:O	2.12	0.48
1:AAA:1:LYS:HA	1:AAA:109:SER:O	2.14	0.47
1:AAA:65:VAL:HA	1:AAA:77:TYR:O	2.15	0.47
1:AAA:37:THR:O	1:AAA:51:VAL:HA	2.15	0.47
4:AAA:203:PAM:O2	4:AAA:203:PAM:C4	2.63	0.44
1:AAA:72:ARG:O	1:AAA:90:ILE:HG22	2.20	0.41
1:AAA:18:GLY:O	1:AAA:39:PHE:HA	2.20	0.41
1:AAA:16:LEU:HD22	4:AAA:203:PAM:H162	2.03	0.41
1:AAA:113:LEU:HD13	4:AAA:203:PAM:H9	2.03	0.41
1:AAA:93:VAL:HG22	1:AAA:98:PHE:CZ	2.55	0.41
4:AAA:203:PAM:H61	4:AAA:203:PAM:H31	1.91	0.41
1:AAA:79:ASN:ND2	3:AAA:202:NAG:O7	2.54	0.40
1:AAA:6:PRO:O	1:AAA:9:LEU:CD2	2.69	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	AAA	154/177 (87%)	136 (88%)	13 (8%)	5 (3%)	3 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 ⓘ

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

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	5	PRO
1	AAA	22	LEU
1	AAA	32	GLN
1	AAA	34	SER
1	AAA	37	THR
1	AAA	53	ASP
1	AAA	61	GLU
1	AAA	70	SER
1	AAA	72	ARG
1	AAA	79	ASN
1	AAA	80[A]	ASP
1	AAA	80[B]	ASP
1	AAA	81	THR
1	AAA	93	VAL
1	AAA	135	ASN
1	AAA	140	TYR
1	AAA	155	GLU

Sometimes 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 ⓘ

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	2,1	14,14,15	0.68	0	17,19,21	1.28	2 (11%)
2	NAG	AbA	2	2	14,14,15	0.59	0	17,19,21	1.16	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	2,1	-	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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AbA	2	NAG	C4-C3-C2	-2.59	107.22	111.02
2	AbA	1	NAG	O5-C5-C6	2.28	112.10	107.66
2	AbA	2	NAG	O3-C3-C2	2.28	114.14	109.40
2	AbA	1	NAG	O3-C3-C2	2.01	113.58	109.40

There are no chirality outliers.

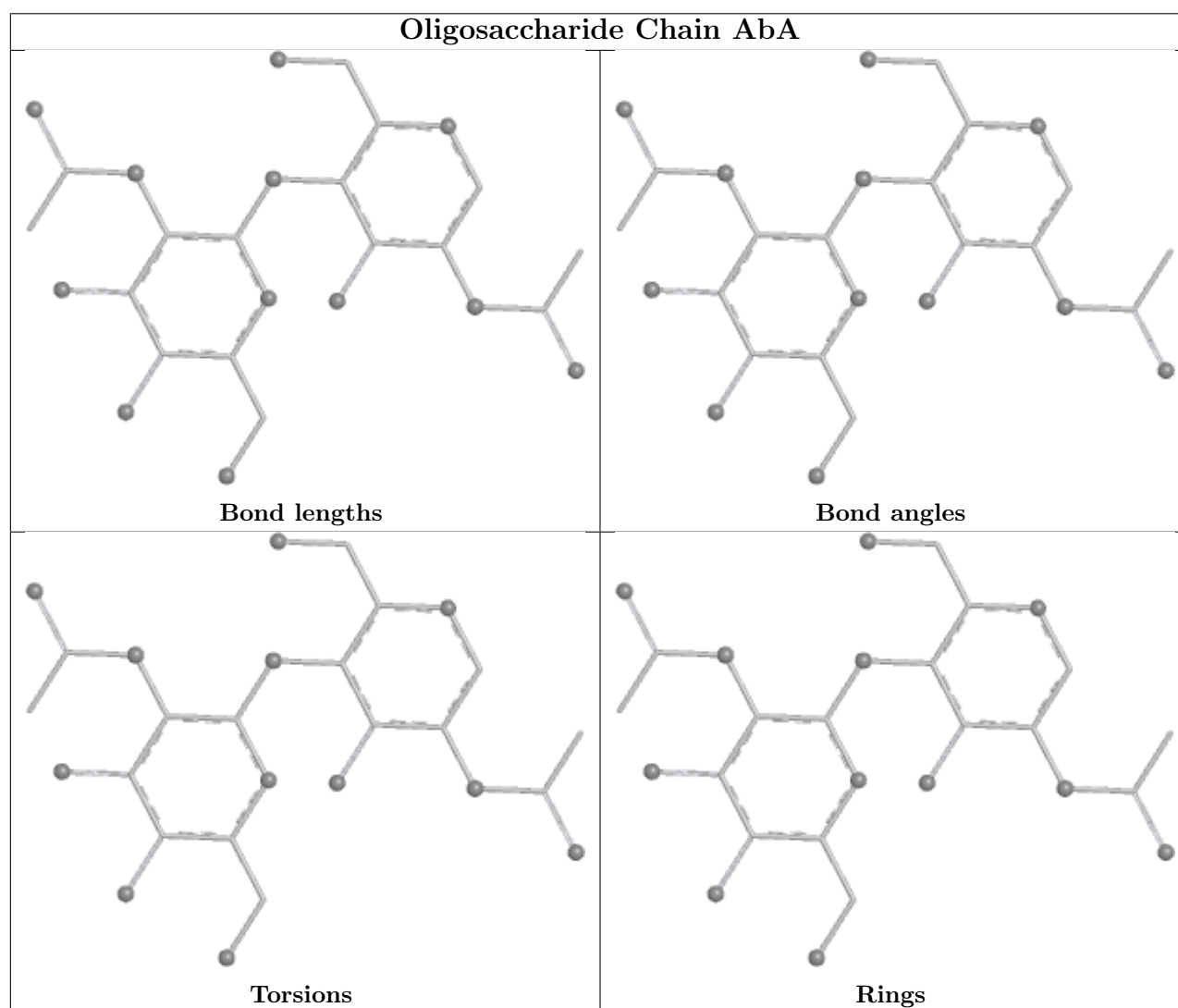
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AbA	1	NAG	O5-C5-C6-O6
2	AbA	1	NAG	C4-C5-C6-O6
2	AbA	2	NAG	O5-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

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	204	1	14,14,15	0.60	0	17,19,21	2.42	8 (47%)
5	GOL	AAA	205	-	5,5,5	0.18	0	5,5,5	0.34	0
4	PAM	AAA	203	-	17,17,17	0.55	0	17,17,17	0.80	0
3	NAG	AAA	201	1	14,14,15	1.12	1 (7%)	17,19,21	2.11	6 (35%)
3	NAG	AAA	202	1	14,14,15	0.68	0	17,19,21	2.39	4 (23%)

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	204	1	-	0/6/23/26	0/1/1/1
5	GOL	AAA	205	-	-	2/4/4/4	-
4	PAM	AAA	203	-	-	9/15/15/15	-
3	NAG	AAA	201	1	-	0/6/23/26	0/1/1/1
3	NAG	AAA	202	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	201	NAG	O5-C5	3.03	1.49	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	202	NAG	C1-C2-N2	6.42	120.56	110.43
3	AAA	202	NAG	C2-N2-C7	5.41	130.15	122.90
3	AAA	204	NAG	C1-O5-C5	-4.97	105.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	201	NAG	C1-O5-C5	4.16	117.76	112.19
3	AAA	204	NAG	O3-C3-C2	-3.70	101.72	109.40
3	AAA	201	NAG	C1-C2-N2	3.68	116.22	110.43
3	AAA	204	NAG	C8-C7-N2	-3.59	110.17	116.12
3	AAA	204	NAG	O5-C1-C2	3.30	116.40	111.29
3	AAA	201	NAG	O6-C6-C5	-3.12	100.72	111.33
3	AAA	204	NAG	C1-C2-N2	-2.86	105.92	110.43
3	AAA	202	NAG	O3-C3-C2	2.68	114.97	109.40
3	AAA	201	NAG	C8-C7-N2	-2.65	111.72	116.12
3	AAA	201	NAG	O5-C5-C4	2.61	117.17	110.83
3	AAA	202	NAG	C1-O5-C5	2.48	115.51	112.19
3	AAA	204	NAG	O3-C3-C4	2.47	116.19	110.38
3	AAA	201	NAG	C6-C5-C4	-2.36	107.22	113.02
3	AAA	204	NAG	C4-C3-C2	2.28	114.36	111.02
3	AAA	204	NAG	C3-C4-C5	2.09	114.02	110.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	202	NAG	C1-C2-N2-C7
5	AAA	205	GOL	O1-C1-C2-C3
3	AAA	202	NAG	O5-C5-C6-O6
4	AAA	203	PAM	C1-C2-C3-C4
3	AAA	202	NAG	C4-C5-C6-O6
4	AAA	203	PAM	C3-C4-C5-C6
4	AAA	203	PAM	C10-C11-C12-C13
4	AAA	203	PAM	C2-C3-C4-C5
4	AAA	203	PAM	C6-C7-C8-C9
5	AAA	205	GOL	O1-C1-C2-O2
4	AAA	203	PAM	C11-C10-C9-C8
4	AAA	203	PAM	C13-C14-C15-C16
4	AAA	203	PAM	C12-C13-C14-C15
4	AAA	203	PAM	C7-C8-C9-C10

There are no ring outliers.

4 monomers are involved in 9 short contacts:

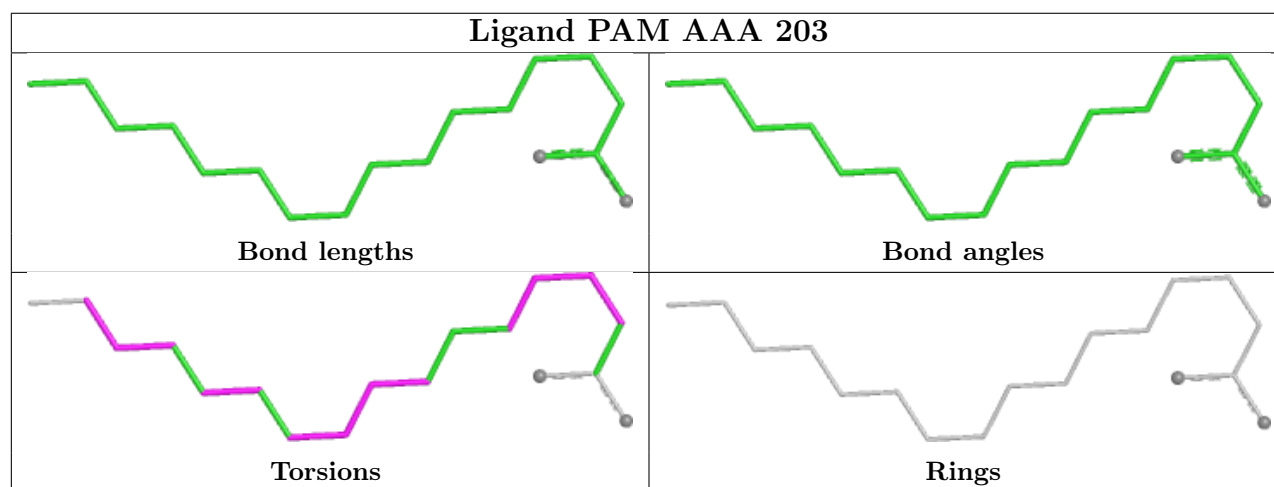
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	204	NAG	1	0
5	AAA	205	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	203	PAM	5	0
3	AAA	202	NAG	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, 95th 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 ²)	Q<0.9
1	AAA	155/177 (87%)	0.44	10 (6%) 25 28	30, 60, 90, 111	2 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	58	TYR	4.3
1	AAA	7	GLU	3.5
1	AAA	46	ASP	3.2
1	AAA	54	TYR	3.0
1	AAA	39	PHE	2.6
1	AAA	9	LEU	2.4
1	AAA	80[A]	ASP	2.4
1	AAA	60	LEU	2.4
1	AAA	140	TYR	2.2
1	AAA	10	GLN	2.2

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

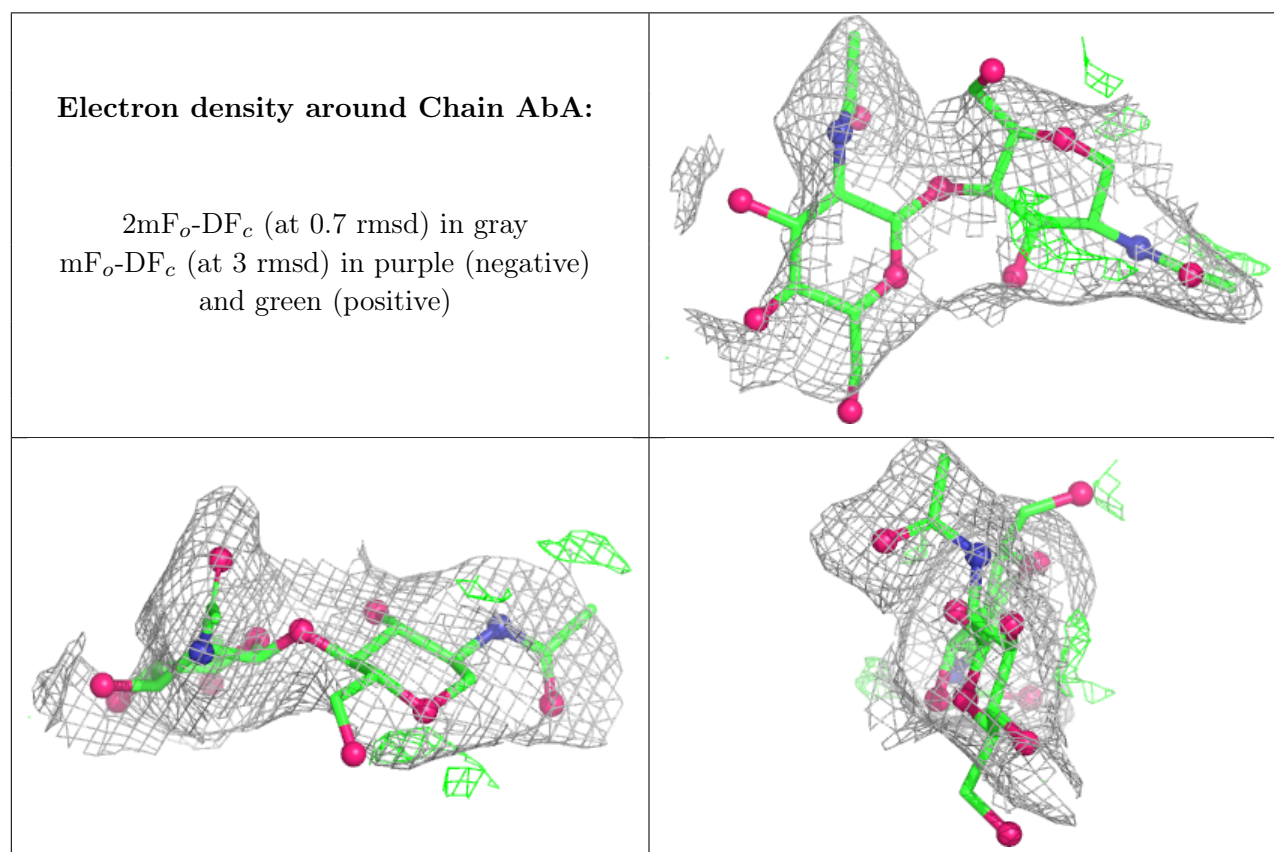
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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 ²)	Q<0.9
2	NAG	AbA	1	14/15	-	-	89,100,117,118	0
2	NAG	AbA	2	14/15	-	-	105,130,142,143	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.



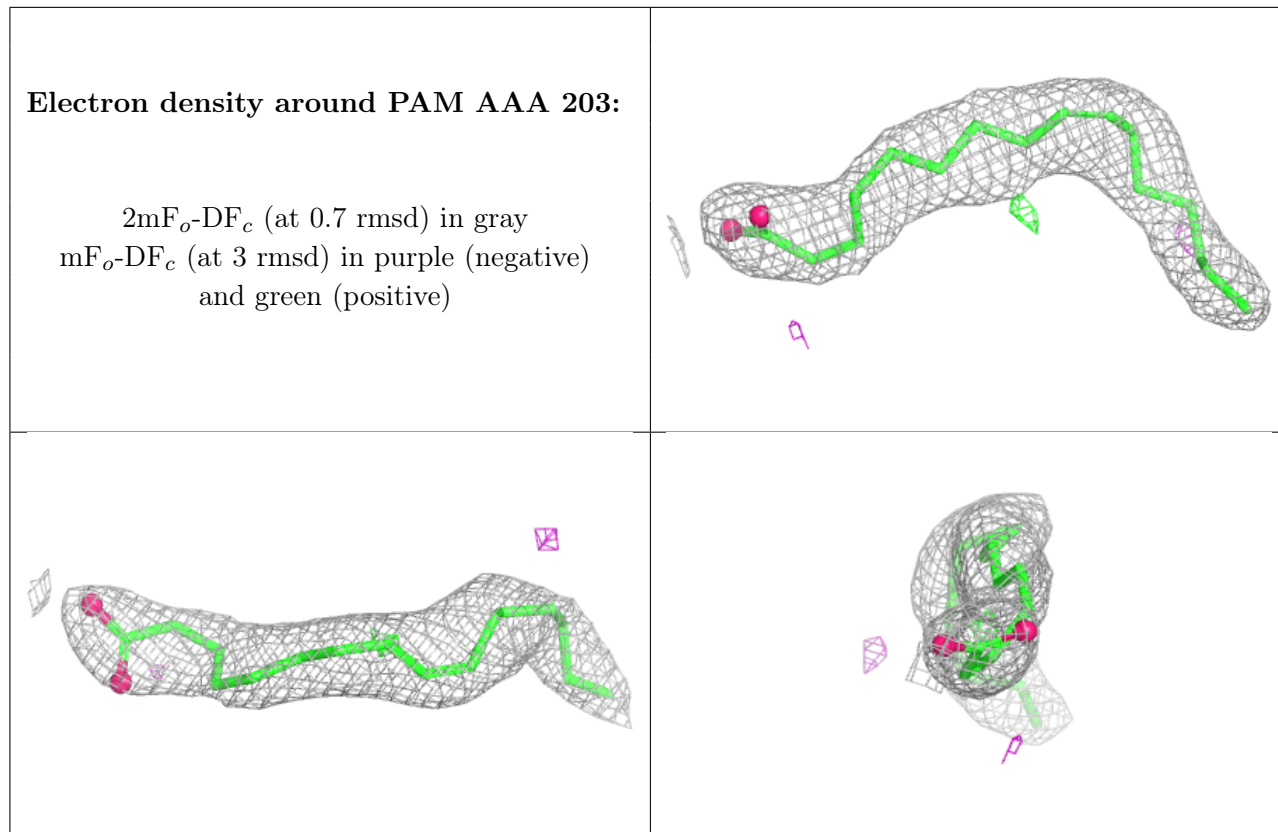
6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
3	NAG	AAA	202	14/15	0.50	0.16	110,121,128,133	0
5	GOL	AAA	205	6/6	0.70	0.19	87,93,101,107	0
3	NAG	AAA	204	14/15	0.80	0.15	88,99,106,109	0
3	NAG	AAA	201	14/15	0.87	0.12	52,69,79,79	0
4	PAM	AAA	203	18/18	0.93	0.15	55,58,76,82	0
6	ZN	AAA	206	1/1	0.99	0.04	78,78,78,78	0
6	ZN	AAA	207	1/1	0.99	0.03	58,58,58,58	0
6	ZN	AAA	208	1/1	0.99	0.02	49,49,49,49	1

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 ⓘ

There are no such residues in this entry.