

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

#### Mar 5, 2024 – 03:14 AM EST

PDB ID	:	8V05
Title	:	Crystal structure of mouse PLD3
Authors	:	Yuan, M.; Zhu, X.; Wilson, I.A.
Deposited on	:	2023-11-17
Resolution	:	2.08  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:

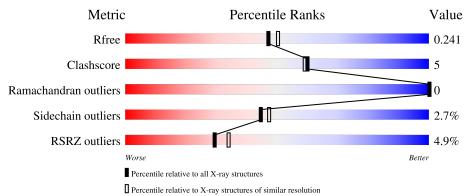
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.08 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	6189(2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	А	467	4%	81%	10% • 9%
2	В	3		100%	
3	С	2		100%	
4	D	7	29%	71%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	В	1	-	-	-	Х
2	NAG	В	2	-	-	-	Х
2	BMA	В	3	-	-	-	Х
4	MAN	D	5	-	-	-	Х

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7169 atoms, of which 3423 are hydrogens and 0 are deuteriums.

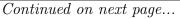
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called 5'-3' exonuclease PLD3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total 6630	C 2126	Н 3266	N 594	O 627	S 17	0	5	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	22	HIS	-	expression tag	UNP O35405
А	23	HIS	_	expression tag	UNP O35405
А	24	HIS	-	expression tag	UNP O35405
А	25	HIS	-	expression tag	UNP O35405
А	26	HIS	-	expression tag	UNP O35405
А	27	HIS	-	expression tag	UNP O35405
А	28	GLY	-	expression tag	UNP O35405
А	29	PRO	-	expression tag	UNP O35405
А	30	LEU	-	expression tag	UNP O35405
А	31	VAL	-	expression tag	UNP O35405
А	32	ASP	-	expression tag	UNP O35405
А	33	VAL	-	expression tag	UNP O35405
А	34	ALA	-	expression tag	UNP O35405
А	35	SER	-	expression tag	UNP O35405
А	36	ASN	-	expression tag	UNP O35405
А	37	GLU	-	expression tag	UNP O35405
А	38	GLN	-	expression tag	UNP O35405
А	39	LYS	-	expression tag	UNP O35405
А	40	LEU	-	expression tag	UNP O35405
А	41	ILE	-	expression tag	UNP O35405
А	42	SER	-	expression tag	UNP O35405
А	43	GLU	-	expression tag	UNP O35405
А	44	GLU	-	expression tag	UNP O35405
А	45	ASP	-	expression tag	UNP O35405
А	46	LEU	-	expression tag	UNP O35405
А	47	ALA	-	expression tag	UNP O35405
А	48	SER	-	expression tag	UNP O35405

There are 41 discrepancies between the modelled and reference sequences:

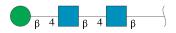




Chain	Residue	Modelled	Actual	Comment	Reference
А	49	MET	-	expression tag	UNP O35405
А	50	THR	-	expression tag	UNP O35405
А	51	GLY	-	expression tag	UNP O35405
А	52	GLY	-	expression tag	UNP O35405
А	53	GLN	-	expression tag	UNP O35405
А	54	GLN	-	expression tag	UNP O35405
A	55	MET	-	expression tag	UNP O35405
A	56	GLY	-	expression tag	UNP O35405
А	57	ARG	-	expression tag	UNP O35405
А	58	ASP	-	expression tag	UNP O35405
А	59	ILE	-	expression tag	UNP O35405
А	60	GLU	-	expression tag	UNP O35405
А	61	GLY	-	expression tag	UNP O35405
А	62	ARG	-	expression tag	UNP O35405

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	3	Total 73	C	Н 34	N 2	O 15	0	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	2	Total	С	Η	Ν	0	0	0	0
	Ű	-	53	16	25	2	10		5	, , , , , , , , , , , , , , , , , , ,

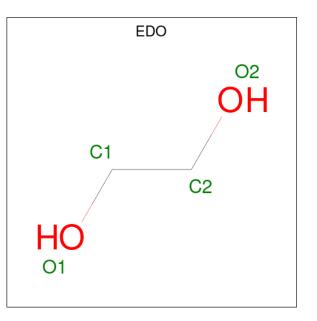
• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total 153	C 46	Н 70	N 2	O 35	0	0	0

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

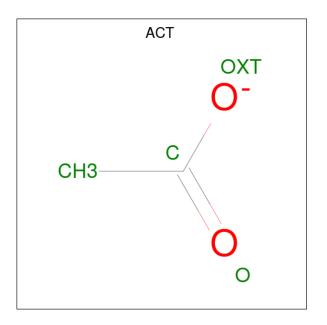


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccccc} \mathrm{Total} & \mathrm{C} & \mathrm{H} & \mathrm{O} \\ 10 & 2 & 6 & 2 \end{array}$	0	0
5	А	1	Total         C         H         O           10         2         6         2	0	0
5	А	1	Total         C         H         O           10         2         6         2	0	0

• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).

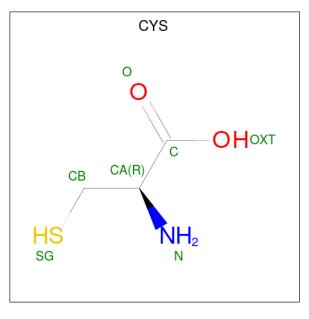






Mo	Chain	Residues	Atoms		ZeroOcc	AltConf		
6	А	1	Total 7	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	H	O 2	0	0

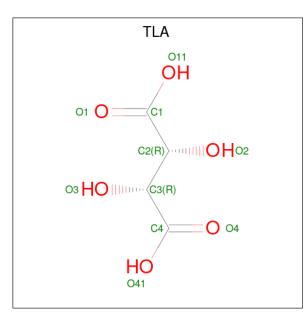
• Molecule 7 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
7	А	1	Total 10	${ m C} { m 3}$	Н 3	N 1	O 2	S 1	0	0

• Molecule 8 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
8	А	1	Total 14	С 4	H 4	O 6	0	0

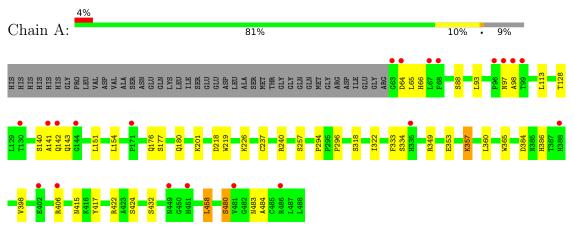
• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	199	Total O 199 199	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: 5'-3' exonuclease PLD3

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

Chain B:

100%

#### NAG1 NAG2 BMA3

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain C:

100%

#### NAG1 NAG2

 $\label{eq:mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-b$ 

Chain D: 29% 71%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN6 MAN6



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	94.16Å 94.16Å 109.37Å	Denesiton
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	47.08 - 2.08	Depositor
Resolution (A)	47.08 - 2.08	EDS
% Data completeness	99.9 (47.08-2.08)	Depositor
(in resolution range)	99.9 (47.08-2.08)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.32 (at 2.08 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
D D	0.206 , $0.243$	Depositor
$R, R_{free}$	0.206 , $0.241$	DCC
$R_{free}$ test set	1679 reflections $(4.92\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.3	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, $47.2$	EDS
L-test for $twinning^2$	$<  L  > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7169	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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: EDO, ACT, TLA, BMA, NAG, 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	А	0.26	0/3470	0.53	0/4731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (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	А	3364	3266	3264	31	0
2	В	39	34	34	0	0
3	С	28	25	25	0	0
4	D	83	70	70	1	0
5	А	12	18	18	2	0
6	А	4	3	3	0	0
7	А	7	3	3	0	0
8	А	10	4	4	0	0
9	А	199	0	0	8	0
All	All	3746	3423	3421	32	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 5.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:OE1	9:A:601:HOH:O	1.98	0.80
1:A:140:SER:O	9:A:601:HOH:O	1.99	0.80
1:A:237:CYS:SG	9:A:616:HOH:O	2.45	0.75
1:A:432:SER:OG	9:A:602:HOH:O	2.08	0.71
1:A:142:GLN:CG	1:A:143:GLN:N	2.68	0.55

The worst 5 of 32 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	5
1	А	429/467~(92%)	413 (96%)	16 (4%)	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.

Mo	l Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	369/398~(93%)	360~(98%)	9~(2%)	49 52

5 of 9 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	458	LEU
1	А	480	SER
1	А	365	TRP
1	А	406	ARG
1	А	415	ASN

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

Mol	Chain	Res	Type
1	А	273	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)

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

### 5.5 Carbohydrates (i)

12 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).

Mal	Trune	Chain	Dec	Link	Bo	ond leng	ths	В	ond ang	jles
Mol	Type	Chain	$\operatorname{Res}$	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	В	1	2,1	14,14,15	0.21	0	17,19,21	0.39	0
2	NAG	В	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	BMA	В	3	2	11,11,12	0.63	0	$15,\!15,\!17$	0.90	0
3	NAG	С	1	3,1	14,14,15	0.27	0	17,19,21	0.56	0
3	NAG	С	2	3	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	D	1	4,1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.18	0	17,19,21	0.41	0
4	BMA	D	3	4	11,11,12	0.63	0	$15,\!15,\!17$	0.75	0



Mol	Turne	Chain	Res	Link	Bo	ond leng	$\mathbf{ths}$	Bond angles			
	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	MAN	D	4	4	$11,\!11,\!12$	0.62	0	$15,\!15,\!17$	0.96	2 (13%)	
4	MAN	D	5	4	$11,\!11,\!12$	0.66	0	$15,\!15,\!17$	1.12	2 (13%)	
4	MAN	D	6	4	11,11,12	0.65	0	$15,\!15,\!17$	0.97	2 (13%)	
4	MAN	D	7	4	11,11,12	0.77	1 (9%)	$15,\!15,\!17$	1.06	1 (6%)	

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	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	2/6/23/26	0/1/1/1
2	BMA	В	3	2	-	1/2/19/22	0/1/1/1
3	NAG	С	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1
4	MAN	D	6	4	-	1/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	7	MAN	C1-C2	2.13	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\mathbf{Ideal}(^{o})$
4	D	5	MAN	C1-O5-C5	3.02	116.28	112.19
4	D	6	MAN	C1-O5-C5	2.40	115.44	112.19
4	D	7	MAN	O2-C2-C3	-2.29	105.54	110.14
4	D	5	MAN	O2-C2-C3	-2.23	105.67	110.14
4	D	4	MAN	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:



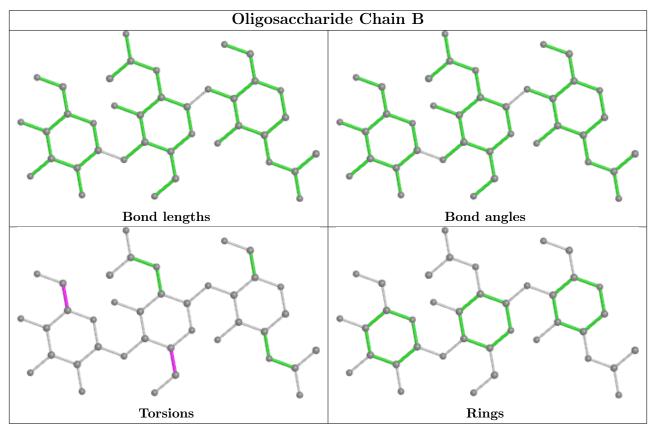
Mol	Chain	Res	Type	Atoms
4	D	5	MAN	O5-C5-C6-O6
2	В	2	NAG	O5-C5-C6-O6
4	D	5	MAN	C4-C5-C6-O6
2	В	3	BMA	O5-C5-C6-O6
2	В	2	NAG	C4-C5-C6-O6

There are no ring outliers.

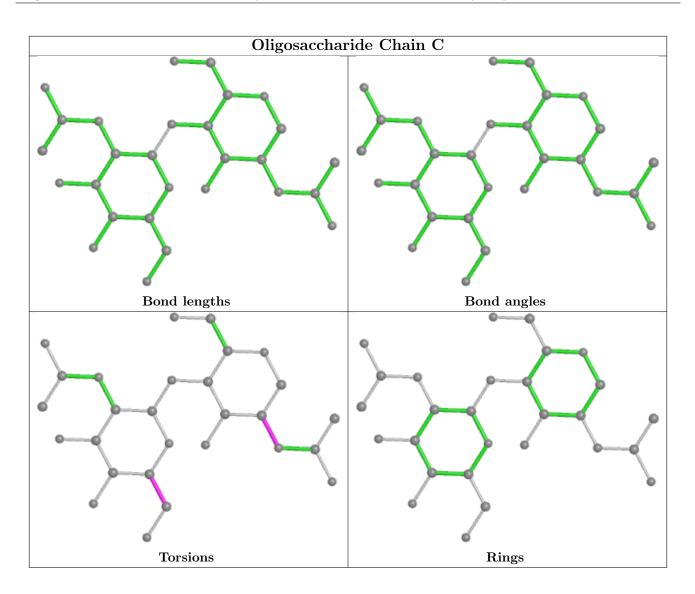
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

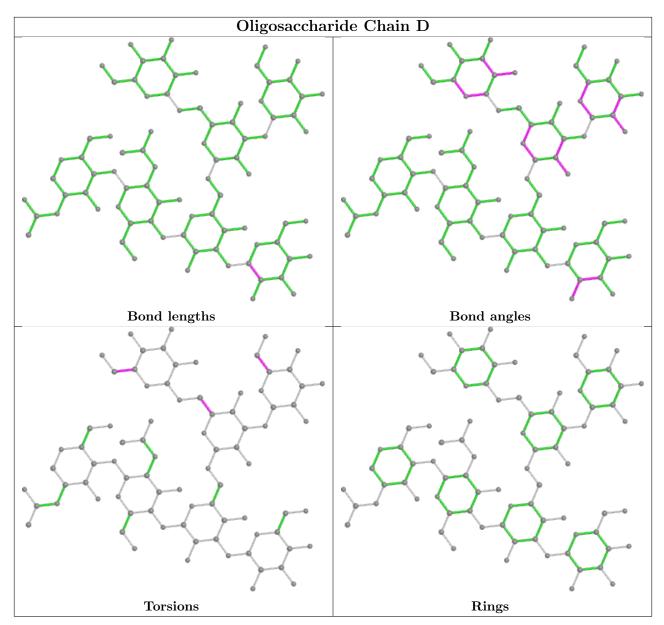
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











### 5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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



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Page 1	8	WW	vPDB .	X-ray S	tructure \	/alidatior	n Summary	Report		8V05
Mol	Type	Chain	Res	Link	B	ond leng		В	ond ang	
wioi	турс	Cham	ites		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
[	[	[	1							-
Mol	Type	Chain	Res	Link		Bond lengths			ond ang	
10101	турс	Cham	Ites		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	ACT	А	503	-	3,3,3	1.32	0	$3,\!3,\!3$	1.38	0
5	EDO	А	505	-	3,3,3	0.47	0	$2,\!2,\!2$	0.24	0
5	EDO	А	502	-	3,3,3	0.47	0	$2,\!2,\!2$	0.24	0
5	EDO	А	501	-	3,3,3	0.46	0	$2,\!2,\!2$	0.29	0
7	CYS	А	504	1	$5,\!6,\!6$	1.02	1(20%)	5,7,7	1.55	2(40%)

0.99

0

12,12,12

1.34

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.

9,9,9

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	А	505	-	-	1/1/1/1	-
5	EDO	А	502	-	-	0/1/1/1	-
5	EDO	А	501	-	-	1/1/1/1	-
7	CYS	А	504	1	-	2/6/6/6	-
8	TLA	А	506	-	-	3/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
7	А	504	CYS	OXT-C	-2.12	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
7	А	504	CYS	OXT-C-O	-2.63	118.12	124.09
8	А	506	TLA	O41-C4-C3	2.50	120.03	113.27
8	А	506	TLA	O11-C1-C2	2.49	120.01	113.27
7	А	504	CYS	OXT-C-CA	2.21	120.92	113.38

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	А	504	CYS	N-CA-CB-SG
7	А	504	CYS	C-CA-CB-SG

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2(16%)



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Mol	Chain	Res	Type	Atoms
5	А	501	EDO	O1-C1-C2-O2
5	А	505	EDO	O1-C1-C2-O2
8	А	506	TLA	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	505	EDO	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	426/467~(91%)	0.26	21 (4%) 29 34	29, 46, 93, 130	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	63	GLY	8.7
1	А	449	ASN	4.6
1	А	451	HIS	3.8
1	А	335	HIS	3.4
1	А	64	ASP	3.1

## 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,  $95^{th}$  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	$B-factors(Å^2)$	Q<0.9
4	MAN	D	5	11/12	0.36	0.56	121,137,160,166	0
2	NAG	В	1	14/15	0.44	0.41	79,112,141,146	0
2	NAG	В	2	14/15	0.61	0.47	116,136,159,164	0
4	MAN	D	7	11/12	0.65	0.36	119,134,162,164	0
4	MAN	D	6	11/12	0.69	0.32	102,122,147,151	0
4	MAN	D	4	11/12	0.71	0.21	109,120,145,145	0
2	BMA	В	3	11/12	0.73	0.48	133,144,171,174	0

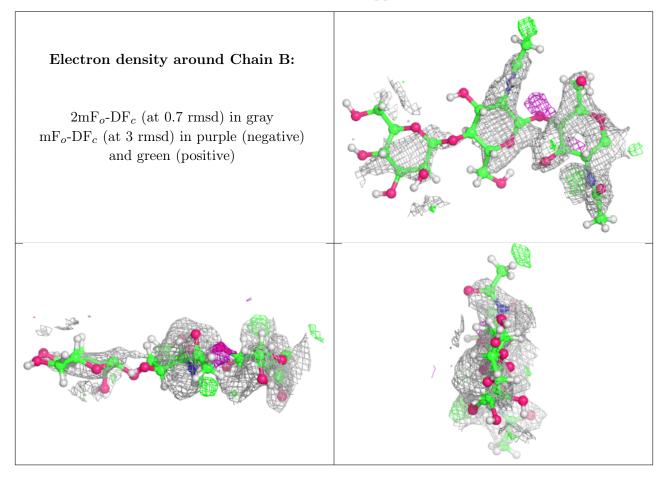
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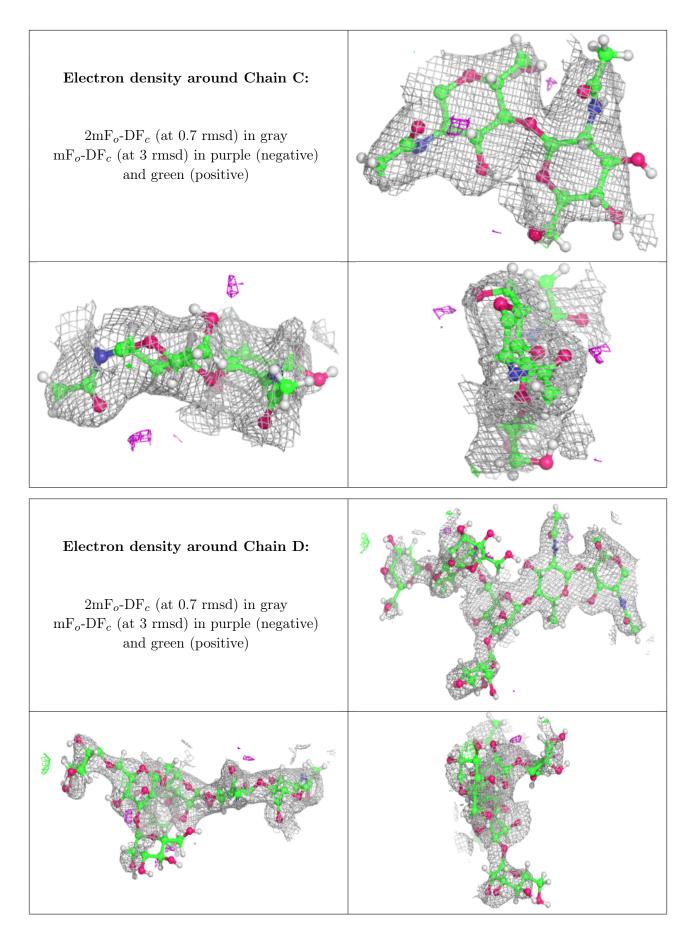
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
4	BMA	D	3	11/12	0.76	0.23	98,109,131,136	0
3	NAG	С	2	14/15	0.80	0.29	83,103,123,133	0
4	NAG	D	2	14/15	0.85	0.23	58,89,107,113	0
3	NAG	С	1	14/15	0.90	0.15	47,62,81,83	0
4	NAG	D	1	14/15	0.95	0.21	49,65,77,80	0

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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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
6	ACT	А	503	4/4	0.70	0.20	$50,\!61,\!65,\!67$	0
7	CYS	А	504	7/7	0.73	0.32	$65,\!85,\!91,\!96$	0
8	TLA	А	506	10/10	0.81	0.22	60,73,91,95	0
5	EDO	А	505	4/4	0.90	0.32	53,64,75,75	0
5	EDO	А	501	4/4	0.92	0.28	49,61,68,78	0
5	EDO	А	502	4/4	0.94	0.11	45,54,55,64	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

