



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:16 AM UTC

PDB ID : 7O78 / pdb\_00007o78  
Title : Structure of the PL6 family chondroitinase B from Pseudopedobacter saltans, Pedsa3807  
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Deposited on : 2021-04-13  
Resolution : 1.58 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
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

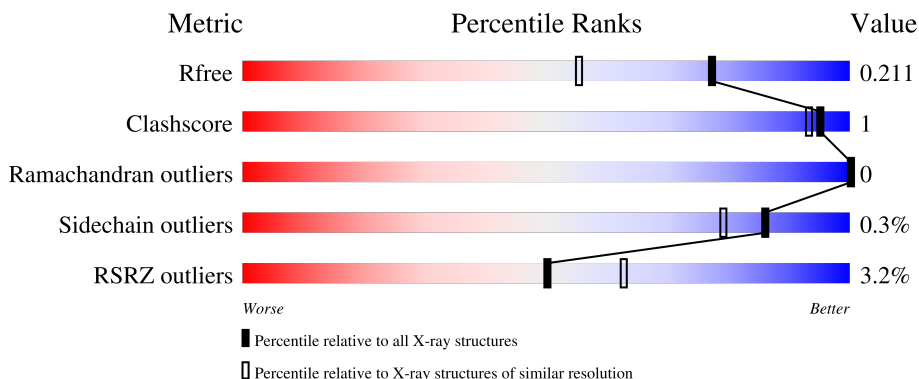
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	A	492	 5% 97%
1	B	492	 % 95%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8525 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 Polysaccharide lyase from Pseudopedobacter saltans, Pedsa3807.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	Total 3798	C 2409	N 661	O 719	S 9	0	0	0
1	B	492	Total 3819	C 2421	N 663	O 726	S 9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP F0S763
B	15	GLY	-	expression tag	UNP F0S763

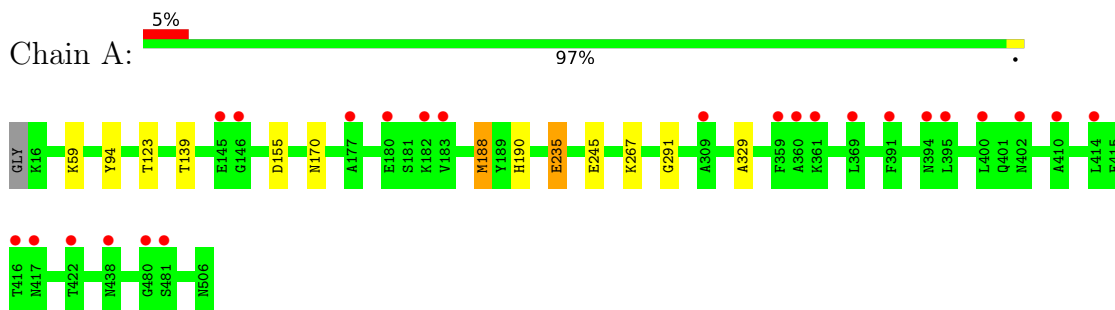
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	422	Total 422	O 422	0	0
2	B	486	Total 486	O 486	0	0

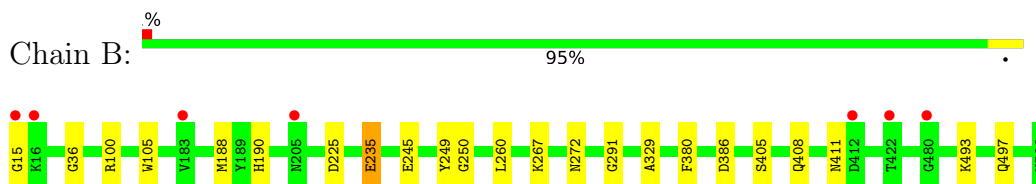
### 3 Residue-property plots [i](#)

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: Polysaccharide lyase from *Pseudopedobacter saltans*, Pedsa3807



- Molecule 1: Polysaccharide lyase from *Pseudopedobacter saltans*, Pedsa3807



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.33Å 87.45Å 148.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.35 – 1.58 58.35 – 1.58	Depositor EDS
% Data completeness (in resolution range)	96.0 (58.35-1.58) 96.0 (58.35-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 1.58Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.178 , 0.210 0.179 , 0.211	Depositor DCC
$R_{free}$ test set	6756 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtrriage
Anisotropy	0.481	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8504e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.78	3/3881 (0.1%)	0.85	0/5269
1	B	0.79	1/3902 (0.0%)	0.87	2/5295 (0.0%)
All	All	0.78	4/7783 (0.1%)	0.86	2/10564 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	C-O	-5.79	1.19	1.24
1	B	235	GLU	C-O	-5.42	1.18	1.24
1	A	188	MET	SD-CE	-5.11	1.66	1.79
1	A	94	TYR	C-O	-5.00	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ASN	CA-C-N	6.27	129.53	120.38
1	B	411	ASN	C-N-CA	6.27	129.53	120.38

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3594	6	0
1	B	3819	0	3621	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	422	0	0	1	0
2	B	486	0	0	0	0
All	All	8525	0	7215	17	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 1.

All (17) 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:B:493:LYS:O	1:B:497:GLN:HG3	1.96	0.65
1:A:59:LYS:HB2	2:A:939:HOH:O	2.09	0.52
1:A:139:THR:HG22	1:A:170:ASN:HB2	1.96	0.47
1:B:15:GLY:HA2	1:B:36:GLY:O	2.14	0.47
1:A:245:GLU:HA	1:A:267:LYS:O	2.16	0.46
1:A:291:GLY:O	1:A:329:ALA:HA	2.15	0.46
1:B:100:ARG:HD2	1:B:105:TRP:CE2	2.52	0.45
1:A:188:MET:HB3	1:A:190:HIS:CD2	2.54	0.43
1:B:386:ASP:OD1	1:B:408:GLN:OE1	2.37	0.42
1:A:123:THR:HA	1:A:155:ASP:O	2.19	0.42
1:B:245:GLU:HA	1:B:267:LYS:O	2.19	0.42
1:B:291:GLY:O	1:B:329:ALA:HA	2.19	0.41
1:B:260:LEU:HD23	1:B:260:LEU:C	2.45	0.41
1:B:380:PHE:O	1:B:405:SER:HA	2.21	0.40
1:B:250:GLY:HA2	1:B:272:ASN:O	2.20	0.40
1:B:225:ASP:HA	1:B:249:TYR:O	2.22	0.40
1:B:188:MET:HB3	1:B:190:HIS:CD2	2.56	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	A	489/492 (99%)	475 (97%)	14 (3%)	0	100	100
1	B	490/492 (100%)	480 (98%)	10 (2%)	0	100	100
All	All	979/984 (100%)	955 (98%)	24 (2%)	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	390/422 (92%)	389 (100%)	1 (0%)	86	79
1	B	394/422 (93%)	393 (100%)	1 (0%)	86	79
All	All	784/844 (93%)	782 (100%)	2 (0%)	86	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	B	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	GLN
1	A	435	GLN
1	A	490	GLN
1	B	99	ASN
1	B	128	ASN
1	B	261	ASN
1	B	402	ASN
1	B	408	GLN
1	B	490	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](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	491/492 (99%)	0.38	24 (4%) 35 46	14, 23, 39, 48	0
1	B	492/492 (100%)	0.01	7 (1%) 73 81	14, 21, 34, 48	1 (0%)
All	All	983/984 (99%)	0.20	31 (3%) 50 63	14, 22, 36, 48	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ALA	3.6
1	A	183	VAL	3.2
1	A	395	LEU	3.2
1	A	369	LEU	3.1
1	A	422	THR	3.0
1	A	400	LEU	3.0
1	A	360	ALA	2.9
1	B	15	GLY	2.9
1	B	480	GLY	2.9
1	A	414	LEU	2.7
1	A	417	ASN	2.6
1	B	183	VAL	2.6
1	A	391	PHE	2.6
1	B	412	ASP	2.5
1	A	182	LYS	2.4
1	A	145	GLU	2.4
1	A	146	GLY	2.4
1	A	480	GLY	2.3
1	A	309	ALA	2.3
1	A	481	SER	2.3
1	A	402	ASN	2.3
1	A	394	ASN	2.2
1	A	416	THR	2.2
1	A	438	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	205	ASN	2.2
1	A	361	LYS	2.1
1	A	180	GLU	2.1
1	A	359	PHE	2.1
1	B	16	LYS	2.0
1	B	422	THR	2.0
1	A	410	ALA	2.0

## 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](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.