



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2022 – 03:31 pm GMT

PDB ID : 7QFI  
Title : Crystal structure of S-layer protein SlpX from *Lactobacillus acidophilus*, domain I (aa 31-182)  
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Deposited on : 2021-12-06  
Resolution : 1.50 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.

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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
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) : 2.31.3

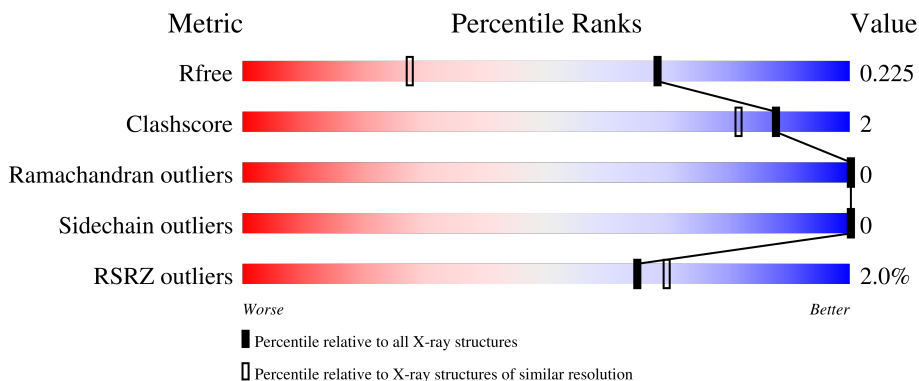
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	162	 76% 22%
1	B	162	 74% 6% 20%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4228 atoms, of which 1983 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 SlpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	127	2009	624	997	173	214	1	34	6	0
1	B	129	1986	620	986	170	209	1	31	3	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	initiating methionine	UNP Q5FLN0
A	30	GLY	-	expression tag	UNP Q5FLN0
A	183	LEU	-	expression tag	UNP Q5FLN0
A	184	GLU	-	expression tag	UNP Q5FLN0
A	185	HIS	-	expression tag	UNP Q5FLN0
A	186	HIS	-	expression tag	UNP Q5FLN0
A	187	HIS	-	expression tag	UNP Q5FLN0
A	188	HIS	-	expression tag	UNP Q5FLN0
A	189	HIS	-	expression tag	UNP Q5FLN0
A	190	HIS	-	expression tag	UNP Q5FLN0
B	29	MET	-	initiating methionine	UNP Q5FLN0
B	30	GLY	-	expression tag	UNP Q5FLN0
B	183	LEU	-	expression tag	UNP Q5FLN0
B	184	GLU	-	expression tag	UNP Q5FLN0
B	185	HIS	-	expression tag	UNP Q5FLN0
B	186	HIS	-	expression tag	UNP Q5FLN0
B	187	HIS	-	expression tag	UNP Q5FLN0
B	188	HIS	-	expression tag	UNP Q5FLN0
B	189	HIS	-	expression tag	UNP Q5FLN0
B	190	HIS	-	expression tag	UNP Q5FLN0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	114	Total 114	O 114	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.35Å 38.35Å 82.75Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	41.28 – 1.50 41.28 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.28-1.50) 98.9 (41.28-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.187 , 0.222 0.188 , 0.225	Depositor DCC
$R_{free}$ test set	1877 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.106	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>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section:  
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		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.78	0/1026	0.87	1/1395 (0.1%)
1	B	0.73	0/1015	0.86	0/1382
All	All	0.76	0/2041	0.87	1/2777 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	GLY	CA-C-O	-5.27	111.12	120.60

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	1012	997	990	2	0
1	B	1000	986	977	6	0
2	B	1	0	0	0	0
3	A	118	0	0	1	0
3	B	114	0	0	1	1
All	All	2245	1983	1967	8	1

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 2.

The worst 5 of 8 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:A:81:ARG:NE	3:A:201:HOH:O	2.17	0.71
1:B:103[A]:VAL:HG23	1:B:116:VAL:HG21	1.82	0.62
1:B:152:LYS:HE2	3:B:307:HOH:O	2.09	0.53
1:B:103[A]:VAL:HG23	1:B:116:VAL:CG2	2.40	0.51
1:B:55:GLN:O	1:B:109:ASN:HB2	2.10	0.50

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:387:HOH:O	3:B:395:HOH:O[2_455]	2.13	0.07

## 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	131/162 (81%)	129 (98%)	2 (2%)	0	100	100
1	B	130/162 (80%)	127 (98%)	3 (2%)	0	100	100
All	All	261/324 (81%)	256 (98%)	5 (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	119/139 (86%)	119 (100%)	0	100	100
1	B	116/139 (84%)	116 (100%)	0	100	100
All	All	235/278 (84%)	235 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	63	ASN
1	A	169	ASN
1	B	121	ASN
1	B	168	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	A	127/162 (78%)	-0.05	2 (1%) 72 77	10, 14, 31, 52	0
1	B	129/162 (79%)	0.09	3 (2%) 60 65	10, 21, 42, 55	0
All	All	256/324 (79%)	0.02	5 (1%) 65 70	10, 18, 38, 55	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ASN	3.6
1	B	72	GLN	2.4
1	B	182	GLY	2.2
1	A	117	THR	2.0
1	B	73	SER	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](#)

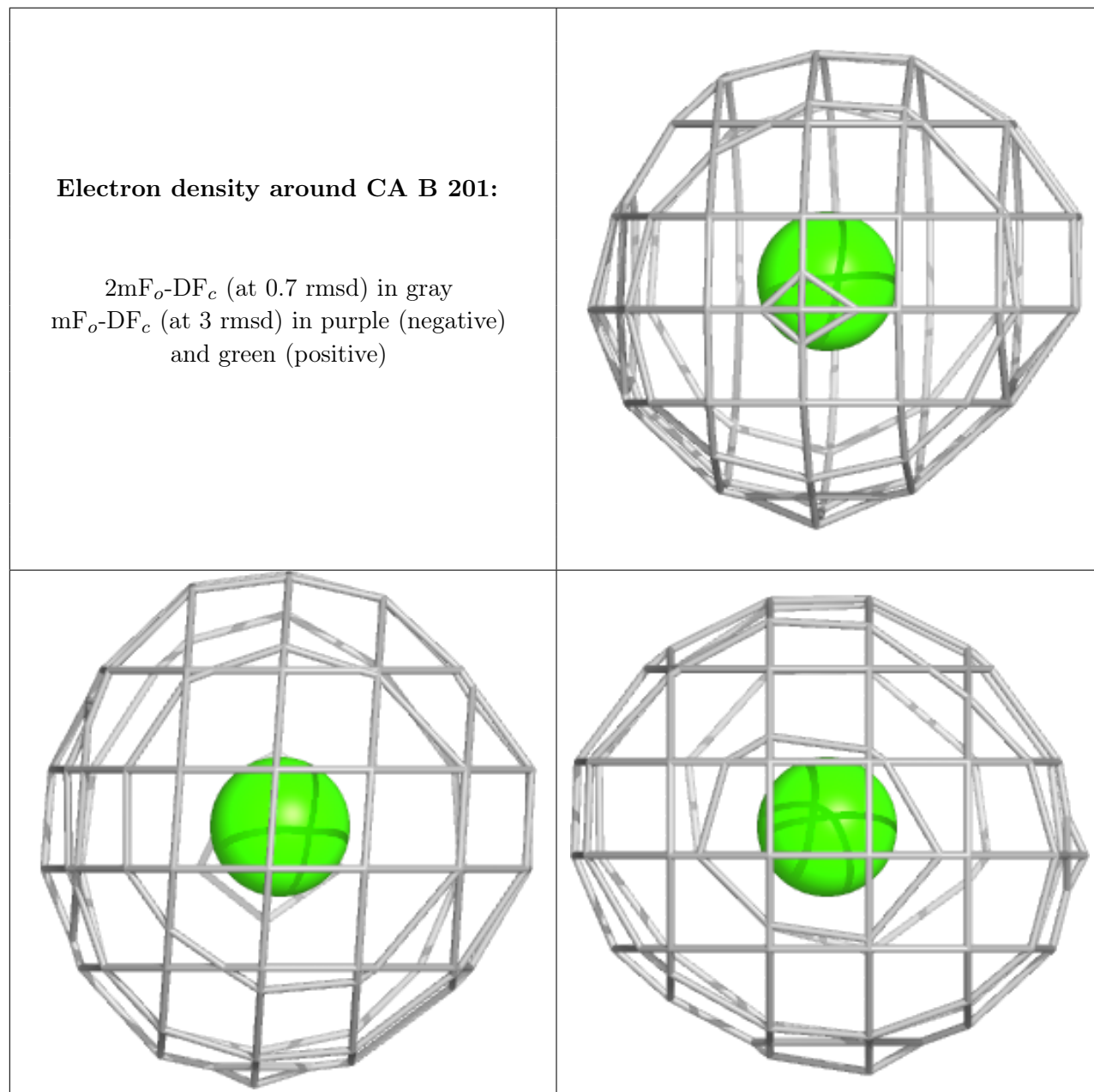
There are no monosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
2	CA	B	201	1/1	0.99	0.04	22,22,22,22	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.