



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:04 PM UTC

PDB ID : 8BT9 / pdb_00008bt9
Title : Crystal structure of SlpA domain II (aa 201-310), domain that is involved in the self-assembly and dimerization of the S-layer from *Lactobacillus acidophilus*
Authors : Sagmeister, T.; Grininger, C.; Pavkov-Keller, T.
Deposited on : 2022-11-28
Resolution : 2.10 Å(reported)

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

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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
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

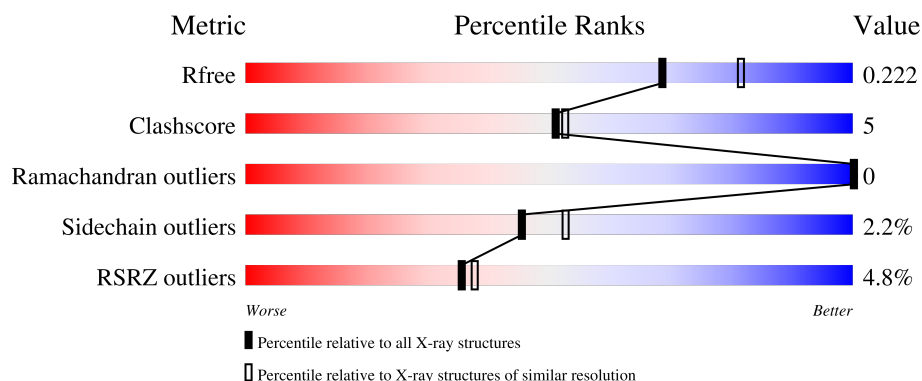
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	A	120	2% 85% 6% 8%
1	B	120	3% 87% 8%
1	C	120	8% 73% 17% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4995 atoms, of which 2304 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 S-layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	H	N	O	0	4	0
			1592	517	759	147	169			
1	C	109	Total	C	H	N	O	0	0	0
			1556	505	748	141	162			
1	B	115	Total	C	H	N	O	0	4	0
			1681	550	793	162	176			

There are 30 discrepancies between the modelled and reference sequences:

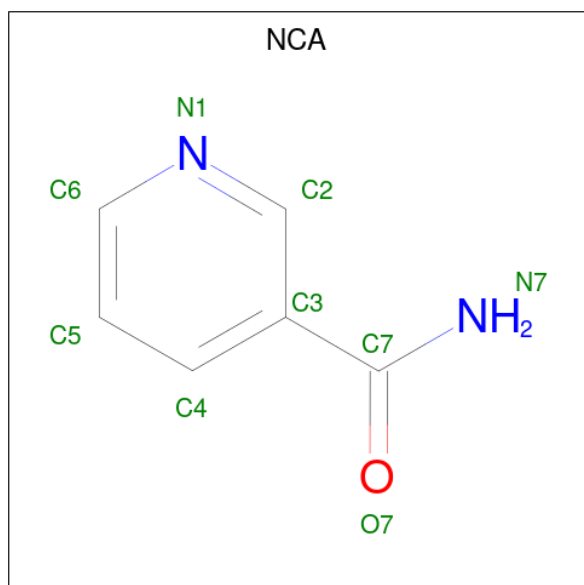
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	MET	-	initiating methionine	UNP P35829
A	200	GLY	-	expression tag	UNP P35829
A	311	LEU	VAL	conflict	UNP P35829
A	312	GLU	ALA	conflict	UNP P35829
A	313	HIS	GLU	conflict	UNP P35829
A	314	HIS	-	expression tag	UNP P35829
A	315	HIS	-	expression tag	UNP P35829
A	316	HIS	-	expression tag	UNP P35829
A	317	HIS	-	expression tag	UNP P35829
A	318	HIS	-	expression tag	UNP P35829
C	199	MET	-	initiating methionine	UNP P35829
C	200	GLY	-	expression tag	UNP P35829
C	311	LEU	VAL	conflict	UNP P35829
C	312	GLU	ALA	conflict	UNP P35829
C	313	HIS	GLU	conflict	UNP P35829
C	314	HIS	-	expression tag	UNP P35829
C	315	HIS	-	expression tag	UNP P35829
C	316	HIS	-	expression tag	UNP P35829
C	317	HIS	-	expression tag	UNP P35829
C	318	HIS	-	expression tag	UNP P35829
B	199	MET	-	initiating methionine	UNP P35829
B	200	GLY	-	expression tag	UNP P35829
B	311	LEU	VAL	conflict	UNP P35829

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Chain	Residue	Modelled	Actual	Comment	Reference
B	312	GLU	ALA	conflict	UNP P35829
B	313	HIS	GLU	conflict	UNP P35829
B	314	HIS	-	expression tag	UNP P35829
B	315	HIS	-	expression tag	UNP P35829
B	316	HIS	-	expression tag	UNP P35829
B	317	HIS	-	expression tag	UNP P35829
B	318	HIS	-	expression tag	UNP P35829

- Molecule 2 is NICOTINAMIDE (CCD ID: NCA) (formula: $C_6H_6N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			13	6	4	2	1		

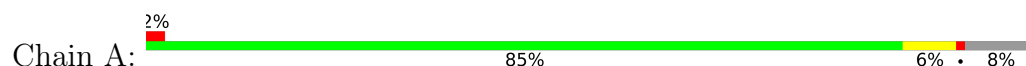
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	C	30	Total	O	0	0
			30	30		
3	B	45	Total	O	0	0
			45	45		

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.

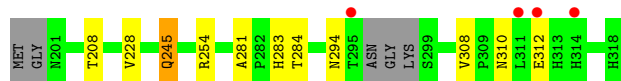
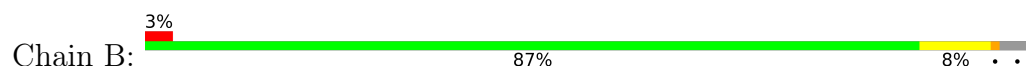
- Molecule 1: S-layer protein



- Molecule 1: S-layer protein



- Molecule 1: S-layer protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.69Å 137.69Å 51.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.12 – 2.10 47.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.12-2.10) 100.0 (47.12-2.10)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.189 , 0.222 0.190 , 0.222	Depositor DCC
R_{free} test set	1696 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: NCA

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	0.67	0/858	0.99	2/1171 (0.2%)
1	B	0.63	0/922	1.04	0/1257
1	C	0.62	0/818	1.07	3/1116 (0.3%)
All	All	0.64	0/2598	1.03	5/3544 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	THR	CA-CB-OG1	-6.60	99.70	109.60
1	C	206	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	214	THR	CA-CB-OG1	-5.74	100.99	109.60
1	A	225	GLN	CB-CG-CD	-5.25	103.67	112.60
1	C	258	THR	CB-CA-C	5.07	119.21	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	833	759	806	7	0
1	B	888	793	847	9	0
1	C	808	748	806	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	4	6	1	0
3	A	78	0	0	0	1
3	B	45	0	0	1	0
3	C	30	0	0	3	0
All	All	2691	2304	2465	26	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 5.

All (26) 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)
2:A:401:NCA:HN72	1:C:219:SER:H	1.31	0.79
1:B:284[B]:THR:HG22	1:B:284[B]:THR:O	2.02	0.59
1:B:281:ALA:HB1	1:B:308:VAL:HG21	1.84	0.59
1:C:202:VAL:HG12	1:C:298:LYS:O	2.04	0.58
1:B:245:GLN:NE2	1:B:254:ARG:HH11	2.06	0.54
1:C:258:THR:HG22	3:C:419:HOH:O	2.09	0.51
1:A:208:THR:HG21	1:C:239:SER:CB	2.40	0.51
1:B:283:HIS:CE1	1:B:312:GLU:HG3	2.46	0.50
1:C:201:ASN:HB3	1:C:297:GLY:HA3	1.95	0.48
1:A:208:THR:HG21	1:C:239:SER:HB3	1.96	0.48
1:C:254:ARG:HH11	1:C:294:ASN:ND2	2.13	0.47
1:C:227:GLN:HE22	1:C:280:LYS:HB2	1.82	0.45
1:B:283:HIS:NE2	1:B:312:GLU:HG3	2.32	0.45
1:A:307:THR:HG21	1:C:307:THR:HG21	2.00	0.43
1:C:284:THR:HG22	3:C:425:HOH:O	2.17	0.43
1:B:245:GLN:CD	1:B:254:ARG:HH11	2.26	0.43
1:C:203:ASN:OD1	3:C:401:HOH:O	2.21	0.42
1:B:208:THR:HG23	3:B:434:HOH:O	2.20	0.42
1:B:228:VAL:HG23	1:B:281:ALA:HB2	2.00	0.41
1:B:245:GLN:HE22	1:B:294:ASN:H	1.67	0.41
1:A:208:THR:HG21	1:C:239:SER:HB2	2.03	0.41
1:A:214:THR:HG22	1:A:215:ASN:OD1	2.21	0.41
1:A:239[A]:SER:OG	1:C:208:THR:HG22	2.21	0.41
1:C:254:ARG:NH1	1:C:294:ASN:ND2	2.68	0.41
1:C:276:VAL:O	1:C:276:VAL:HG22	2.20	0.41
1:A:276:VAL:HG23	1:A:278:TYR:HD2	1.85	0.40

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:A:577:HOH:O	3:A:577:HOH:O[6_554]	1.75	0.45

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	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
1	B	115/120 (96%)	111 (96%)	4 (4%)	0	100	100
1	C	105/120 (88%)	103 (98%)	2 (2%)	0	100	100
All	All	330/360 (92%)	323 (98%)	7 (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	93/98 (95%)	92 (99%)	1 (1%)	65	74
1	B	99/98 (101%)	97 (98%)	2 (2%)	48	56
1	C	88/98 (90%)	85 (97%)	3 (3%)	32	35
All	All	280/294 (95%)	274 (98%)	6 (2%)	45	54

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	THR
1	C	214	THR
1	C	267	LYS
1	C	290	LYS
1	B	245	GLN
1	B	310	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	227	GLN
1	A	232	ASN
1	C	201	ASN
1	C	227	GLN
1	C	232	ASN
1	C	245	GLN
1	C	294	ASN
1	B	215	ASN
1	B	224	ASN
1	B	294	ASN
1	B	314	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	NCA	A	401	-	9,9,9	0.62	0	11,11,11	0.86	1 (9%)

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	NCA	A	401	-	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NCA	C5-C4-C3	-2.10	118.30	120.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NCA	1	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, 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	A	110/120 (91%)	-0.05	3 (2%)	56 59	26, 59, 93, 131	3 (2%)
1	B	115/120 (95%)	0.19	4 (3%)	47 49	28, 68, 112, 138	3 (2%)
1	C	109/120 (90%)	0.73	9 (8%)	17 18	56, 88, 132, 158	0
All	All	334/360 (92%)	0.29	16 (4%)	35 38	26, 70, 126, 158	6 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283[A]	HIS	4.8
1	B	295	THR	2.9
1	C	251	LEU	2.8
1	C	249	LYS	2.7
1	A	295	THR	2.7
1	B	311	LEU	2.6
1	B	312	GLU	2.5
1	C	283	HIS	2.5
1	C	311	LEU	2.3
1	C	246	TYR	2.3
1	B	314	HIS	2.2
1	C	247	ALA	2.2
1	A	312	GLU	2.1
1	C	201	ASN	2.1
1	C	276	VAL	2.1
1	C	294	ASN	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](#)

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($\text{\AA}^2$)	Q<0.9
2	NCA	A	401	9/9	0.97	0.06	44,46,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.