



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4UIC / pdb_00004uic
Title : Crystal structure of the S-layer protein rSbsC(31-844)
Authors : Pavkov-Keller, T.; Dordic, A.; Egelseer, E.M.; Sleytr, U.B.; Keller, W.
Deposited on : 2015-03-27
Resolution : 2.90 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
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

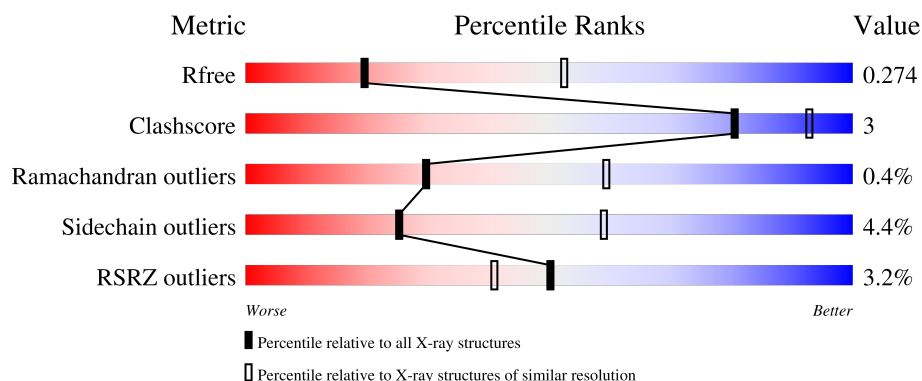
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	814	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5385 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 SURFACE LAYER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5351	3382	875	1091	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.40Å 98.52Å 108.58Å 90.00° 93.50° 90.00°	Depositor
Resolution (Å)	49.26 – 2.90 49.26 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.7 (49.26-2.90) 89.7 (49.26-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.62 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.230 , 0.274 0.230 , 0.274	Depositor DCC
R_{free} test set	1218 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5385	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [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	0.56	0/5416	0.91	0/7353

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	A	5351	0	5459	28	0
2	A	34	0	0	0	0
All	All	5385	0	5459	28	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 3.

All (28) 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:576:LYS:HG2	1:A:616:THR:HG22	1.82	0.62
1:A:578:THR:HG22	1:A:614:GLU:HG2	1.81	0.61
1:A:137:MET:SD	1:A:160:ILE:HG22	2.48	0.54
1:A:560:VAL:HG11	1:A:640:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:SER:HB2	1:A:518:VAL:HG23	1.91	0.51
1:A:463:THR:HB	1:A:471:PHE:HB2	1.94	0.47
1:A:524:VAL:HG12	1:A:526:PRO:HD3	1.97	0.47
1:A:597:LYS:HB3	1:A:600:THR:HG22	1.96	0.47
1:A:164:LEU:HD22	1:A:192:GLN:HG2	1.97	0.46
1:A:278:THR:HG22	1:A:317:THR:HG22	1.96	0.46
1:A:90:GLY:HA2	1:A:94:LYS:HD3	1.97	0.46
1:A:630:THR:HG22	1:A:639:LYS:HG2	1.97	0.45
1:A:701:SER:HB3	1:A:739:LEU:HD23	1.99	0.45
1:A:375:SER:HA	1:A:414:ASN:OD1	2.17	0.44
1:A:537:LYS:HB3	1:A:542:THR:HG22	2.00	0.44
1:A:137:MET:HE1	1:A:163:GLU:HG3	1.99	0.43
1:A:629:ILE:HG22	1:A:640:VAL:HB	1.99	0.43
1:A:451:GLU:HG2	1:A:488:LYS:HB2	2.00	0.43
1:A:137:MET:HB3	1:A:160:ILE:CG2	2.50	0.42
1:A:342:THR:C	1:A:344:GLY:H	2.26	0.42
1:A:181:GLU:HG3	1:A:184:ARG:HH21	1.85	0.42
1:A:565:VAL:HB	1:A:642:VAL:HG22	2.02	0.42
1:A:518:VAL:HG21	1:A:534:VAL:HG23	2.03	0.41
1:A:173:ARG:NH1	1:A:772:ILE:HB	2.36	0.41
1:A:100:ASP:O	1:A:104:ILE:HD12	2.21	0.40
1:A:50:TYR:HB3	1:A:54:HIS:ND1	2.36	0.40
1:A:207:LYS:HB3	1:A:230:VAL:HG23	2.04	0.40
1:A:230:VAL:O	1:A:234:VAL:HG23	2.22	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	700/814 (86%)	676 (97%)	21 (3%)	3 (0%)	30 59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	ALA
1	A	634	GLY
1	A	720	GLY

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	A	587/673 (87%)	561 (96%)	26 (4%)	25 59

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	VAL
1	A	150	LEU
1	A	160	ILE
1	A	171	LEU
1	A	202	ILE
1	A	213	ASP
1	A	227	LEU
1	A	229	GLN
1	A	278	THR
1	A	365	THR
1	A	373	GLU
1	A	416	THR
1	A	430	THR
1	A	467	ASN
1	A	477	GLN
1	A	478	ILE
1	A	485	LEU
1	A	527	ILE
1	A	594	THR
1	A	629	ILE
1	A	652	ASN
1	A	696	ASP

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Mol	Chain	Res	Type
1	A	697	VAL
1	A	723	VAL
1	A	740	THR
1	A	745	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	192	GLN
1	A	512	ASN
1	A	571	GLN
1	A	585	ASN
1	A	719	ASN

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 ⓘ

There are no ligands in this entry.

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

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, 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	710/814 (87%)	0.30	23 (3%)	50 41	35, 72, 117, 147	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	755	VAL	6.2
1	A	774	LEU	4.8
1	A	708	GLY	4.3
1	A	760	LEU	3.8
1	A	478	ILE	3.0
1	A	646	ALA	3.0
1	A	681	TYR	3.0
1	A	678	LEU	2.8
1	A	343	ALA	2.7
1	A	622	VAL	2.6
1	A	724	TYR	2.5
1	A	729	ASN	2.5
1	A	563	THR	2.5
1	A	676	VAL	2.4
1	A	623	ALA	2.4
1	A	527	ILE	2.4
1	A	718	ALA	2.3
1	A	600	THR	2.3
1	A	577	VAL	2.3
1	A	621	GLY	2.1
1	A	677	GLN	2.1
1	A	657	VAL	2.1
1	A	727	THR	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.