



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:51 PM GMT

PDB ID : 4AQ1  
Title : Structure of the SbsB S-layer protein of *Geobacillus stearothermophilus* PV72p2 in complex with nanobody KB6  
Authors : Baranova, E.; Remaut, H.  
Deposited on : 2012-04-12  
Resolution : 2.42 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

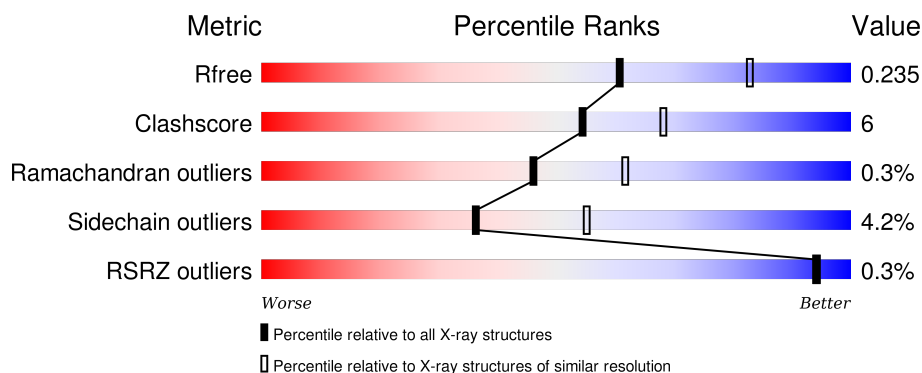
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	892	
2	B	130	
2	D	130	
3	C	892	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12335 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 SBSB PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	82	0	0
			5363	3356	881	1124	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	EXPRESSION TAG	UNP Q45664
A	86	GLY	ASP	CONFLICT	UNP Q45664
A	139	ALA	ARG	CONFLICT	UNP Q45664
A	140	HIS	TYR	CONFLICT	UNP Q45664
A	500	GLU	ASP	CONFLICT	UNP Q45664
A	812	GLU	LYS	CONFLICT	UNP Q45664
A	921	GLY	-	EXPRESSION TAG	UNP Q45664
A	922	SER	-	EXPRESSION TAG	UNP Q45664

- Molecule 2 is a protein called NBKB6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	2	0	0
			924	572	163	184	5			
2	D	124	Total	C	N	O	S	7	0	0
			924	572	163	184	5			

- Molecule 3 is a protein called SBSB PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	627	Total	C	N	O	S	26	0	0
			4641	2899	761	979	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	MET	-	EXPRESSION TAG	UNP Q45664
C	86	GLY	ASP	CONFLICT	UNP Q45664
C	139	ALA	ARG	CONFLICT	UNP Q45664
C	140	HIS	TYR	CONFLICT	UNP Q45664
C	402	THR	SER	CONFLICT	UNP Q45664
C	500	GLU	ASP	CONFLICT	UNP Q45664
C	812	GLU	LYS	CONFLICT	UNP Q45664
C	921	GLY	-	EXPRESSION TAG	UNP Q45664
C	922	SER	-	EXPRESSION TAG	UNP Q45664

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Ca 4 4	0	0
4	C	4	Total Ca 4 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	253	Total O 253 253	0	0
5	B	21	Total O 21 21	0	0
5	C	173	Total O 173 173	0	0
5	D	28	Total O 28 28	0	0



Chain C:  63% 7% 30%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.50Å 88.50Å 95.20Å 112.50° 101.60° 84.70°	Depositor
Resolution (Å)	43.81 – 2.42 43.81 – 2.42	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.81-2.42) 85.5 (43.81-2.42)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.183 , 0.236 0.186 , 0.235	Depositor DCC
$R_{free}$ test set	3729 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74479 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.67	3/5430 (0.1%)	0.77	1/7406 (0.0%)
2	B	0.70	1/943 (0.1%)	0.71	0/1271
2	D	0.70	0/943	0.76	0/1271
3	C	0.63	1/4698 (0.0%)	0.74	1/6409 (0.0%)
All	All	0.66	5/12014 (0.0%)	0.75	2/16357 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	GLU	CA-CB	-10.73	1.30	1.53
1	A	275	LYS	CG-CD	-6.83	1.29	1.52
2	B	36	TRP	CD2-CE2	5.83	1.48	1.41
1	A	278	LYS	CD-CE	5.11	1.64	1.51
3	C	833	TRP	CD2-CE2	5.09	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ASP	CB-CG-OD1	5.21	122.99	118.30
3	C	523	GLY	N-CA-C	-5.11	100.34	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	548	GLY	Peptide

## 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	5363	0	5396	87	0
2	B	924	0	872	15	0
2	D	924	0	872	12	0
3	C	4641	0	4657	39	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	253	0	0	9	0
5	B	21	0	0	0	0
5	C	173	0	0	4	0
5	D	28	0	0	1	0
All	All	12335	0	11797	149	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 6.

The worst 5 of 149 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:440:THR:HG21	5:A:2087:HOH:O	1.46	1.15
1:A:275:LYS:HG3	1:A:281:THR:HG22	1.34	1.04
1:A:271:ALA:HB1	1:A:274:ILE:HD11	1.44	0.98
1:A:293:VAL:HG22	1:A:296:ALA:HB2	1.47	0.96
1:A:838:GLN:HE22	1:A:845:PHE:H	1.15	0.89

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	719/892 (81%)	692 (96%)	23 (3%)	4 (1%)	30	41
2	B	122/130 (94%)	114 (93%)	8 (7%)	0	100	100
2	D	122/130 (94%)	119 (98%)	3 (2%)	0	100	100
3	C	625/892 (70%)	608 (97%)	16 (3%)	1 (0%)	52	69
All	All	1588/2044 (78%)	1533 (96%)	50 (3%)	5 (0%)	46	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	277	LEU
1	A	204	PRO
3	C	867	VAL
1	A	279	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	617/753 (82%)	586 (95%)	31 (5%)	30	47
2	B	92/98 (94%)	86 (94%)	6 (6%)	21	32
2	D	92/98 (94%)	91 (99%)	1 (1%)	80	91
3	C	534/753 (71%)	516 (97%)	18 (3%)	44	64
All	All	1335/1702 (78%)	1279 (96%)	56 (4%)	36	55

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	729	ILE
2	B	12	VAL
3	C	816	THR
1	A	744	THR
1	A	864	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
3	C	377	ASN
3	C	838	GLN
2	B	84	ASN
2	B	119	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are 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 [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<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	721/892 (80%)	-0.39	2 (0%) 94 94	16, 34, 70, 109	26 (3%)
2	B	124/130 (95%)	-0.11	1 (0%) 87 87	20, 45, 95, 127	1 (0%)
2	D	124/130 (95%)	-0.20	0 100 100	19, 36, 68, 86	3 (2%)
3	C	627/892 (70%)	-0.37	2 (0%) 94 94	18, 37, 65, 91	8 (1%)
All	All	1596/2044 (78%)	-0.35	5 (0%) 94 94	16, 36, 71, 127	38 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	295	ASP	2.4
2	B	122	VAL	2.4
3	C	371	ASP	2.3
1	A	277	LEU	2.2
1	A	922	SER	2.1

### 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](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	C	1922	1/1	0.99	0.09	-0.73	28,28,28,28	0
4	CA	C	1925	1/1	0.97	0.08	-1.36	33,33,33,33	0
4	CA	A	1923	1/1	0.99	0.06	-2.03	25,25,25,25	0
4	CA	A	1926	1/1	0.99	0.07	-2.33	27,27,27,27	0
4	CA	C	1924	1/1	0.99	0.06	-2.54	24,24,24,24	0
4	CA	C	1923	1/1	0.99	0.04	-2.67	29,29,29,29	0
4	CA	A	1925	1/1	0.99	0.04	-3.17	22,22,22,22	0
4	CA	A	1924	1/1	0.99	0.04	-6.82	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.