

Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 04:54 pm BST

PDB ID : 2GWM

Title : Crystal structure of the Salmonella SpvB ATR Domain

Authors : Stebbins, C.E.; Margarit, S.M.

Deposited on : 2006-05-04

Resolution : 1.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

 $\begin{array}{ccc} \text{Xtriage (Phenix)} & : & 1.13 \\ \text{EDS} & : & 2.11 \end{array}$

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

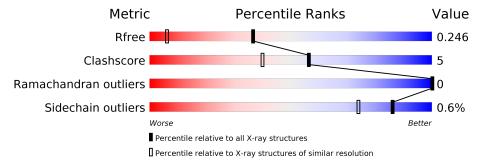
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
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)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	200	90%	10%	•



2 Entry composition (i)

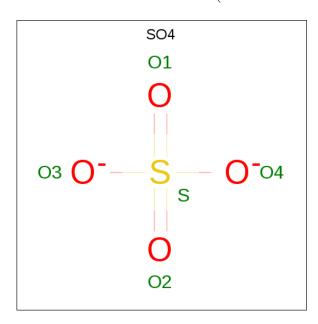
There are 3 unique types of molecules in this entry. The entry contains 1925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 65 kDa virulence protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	200	Total	С	N	О	S	0	0	0
1	Λ	200	1592	1001	271	315	5	0	0	

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

• Molecule 3 is water.

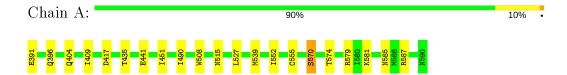
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	323	Total O 323 323	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: 65 kDa virulence protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	55.59Å 55.59Å 143.58Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 - 1.50	Depositor
resolution (A)	39.98 - 1.48	EDS
% Data completeness	97.7 (40.00-1.50)	Depositor
(in resolution range)	95.7 (39.98-1.48)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.62 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.156 , 0.203	Depositor
R, R_{free}	0.203 , 0.246	DCC
R_{free} test set	2119 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 44.4	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1925	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: SO4

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	Boı	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z > 5	RMSZ # Z > 5		
1	Α	0.89	1/1618 (0.1%)	0.90	4/2183 (0.2%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathbf{Ideal}(exttt{\AA})$
1	A	570	SER	CB-OG	5.40	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	A	539	MET	CG-SD-CE	-8.70	86.28	100.20
1	A	587	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	579	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	579	ARG	NE-CZ-NH2	-5.39	117.61	120.30

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	1592	0	1591	16	1
2	A	10	0	0	0	0
3	A	323	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1925	0	1591	16	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 (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f A})$	$oxed{ ext{overlap }(ext{A}) }$
1:A:515:ASN:HD22	1:A:585:ASN:HD22	1.34	0.75
1:A:515:ASN:HD22	1:A:585:ASN:ND2	1.88	0.70
1:A:490:ILE:CD1	1:A:552:ILE:HD12	2.22	0.69
1:A:404:GLN:OE1	3:A:251:HOH:O	2.11	0.69
1:A:490:ILE:HD13	1:A:552:ILE:HD12	1.76	0.67
1:A:574:THR:OG1	3:A:315:HOH:O	2.13	0.65
1:A:409:ILE:HD12	1:A:451:ILE:HG12	1.83	0.60
1:A:490:ILE:HD11	1:A:552:ILE:HD12	1.93	0.51
1:A:417:ASP:HB3	3:A:261:HOH:O	2.09	0.51
1:A:490:ILE:HD11	3:A:45:HOH:O	2.11	0.50
1:A:581:LYS:HE3	3:A:108:HOH:O	2.14	0.47
1:A:391:GLU:OE2	1:A:396:GLN:HG2	2.15	0.47
1:A:508:TRP:HA	1:A:570:SER:HB3	1.99	0.45
1:A:441:GLU:HG3	3:A:298:HOH:O	2.18	0.43
1:A:435:THR:N	3:A:262:HOH:O	2.53	0.42
1:A:396:GLN:HG2	3:A:169:HOH:O	2.19	0.41

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	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:A:555:CYS:SG	1:A:555:CYS:SG[4_555]	2.12	0.08	

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	wed Outliers		Percentiles	
1	A	198/200 (99%)	193 (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	177/177 (100%)	176 (99%)	1 (1%)	86 74		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
1	A	527	LEU	

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

Mol	Chain	Res	Type
1	A	396	GLN
1	A	410	ASN
1	A	422	GLN
1	A	578	ASN
1	A	585	ASN
1	A	590	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are 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 Chair	Chain	Res	Link	Bond lengths		Bond angles				
	Chain			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	SO4	A	591	_	4,4,4	0.26	0	6,6,6	0.40	0
2	SO4	A	592	-	4,4,4	0.41	0	6,6,6	0.27	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

