



wwPDB X-ray Structure Validation Summary Report

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PDB ID : 3LM6
Title : Crystal Structure of Stage V sporulation protein AD (spoVAD) from *Bacillus subtilis*, Northeast Structural Genomics Consortium Target SR525
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Deposited on : 2010-01-29
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

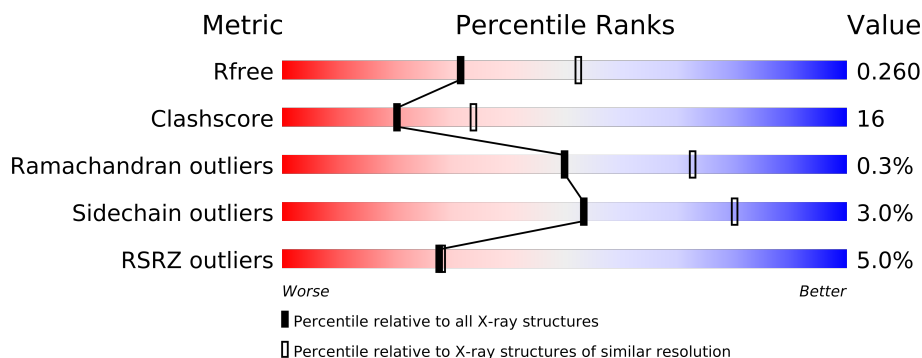
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	346	
1	B	346	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5021 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Stage V sporulation protein AD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	Se	0	0	0
			2505	1572	425	493	6	9			
1	B	322	Total	C	N	O	S	Se	0	0	0
			2401	1505	407	474	6	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	LEU	-	expression tag	UNP P40869
A	340	GLU	-	expression tag	UNP P40869
A	341	HIS	-	expression tag	UNP P40869
A	342	HIS	-	expression tag	UNP P40869
A	343	HIS	-	expression tag	UNP P40869
A	344	HIS	-	expression tag	UNP P40869
A	345	HIS	-	expression tag	UNP P40869
A	346	HIS	-	expression tag	UNP P40869
B	339	LEU	-	expression tag	UNP P40869
B	340	GLU	-	expression tag	UNP P40869
B	341	HIS	-	expression tag	UNP P40869
B	342	HIS	-	expression tag	UNP P40869
B	343	HIS	-	expression tag	UNP P40869
B	344	HIS	-	expression tag	UNP P40869
B	345	HIS	-	expression tag	UNP P40869
B	346	HIS	-	expression tag	UNP P40869

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	43	Total	O	0	0
			43	43		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.97Å 87.66Å 130.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 29.23 – 2.49	Depositor EDS
% Data completeness (in resolution range)	82.1 (19.92-2.50) 95.9 (29.23-2.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.188 , 0.241 0.210 , 0.260	Depositor DCC
R_{free} test set	1879 reflections (9.57%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 21.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37869 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5021	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 9.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.39	0/2543	0.60	0/3438
1	B	0.38	0/2434	0.60	0/3289
All	All	0.39	0/4977	0.60	0/6727

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2480	94	0
1	B	2401	0	2385	75	0
2	A	72	0	0	9	0
2	B	43	0	0	2	0
All	All	5021	0	4865	154	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:HIS:O	1:A:293:GLN:HG2	1.81	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:ALA:HB2	1:B:324:THR:HG23	1.64	0.78
1:A:115:GLU:O	1:A:119:VAL:HG12	1.84	0.78
1:A:208:ALA:HB2	1:A:324:THR:HG23	1.64	0.78
1:A:216:HIS:HE1	1:A:227:TYR:OH	1.66	0.78

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	332/346 (96%)	314 (95%)	17 (5%)	1 (0%)	50	73
1	B	318/346 (92%)	301 (95%)	16 (5%)	1 (0%)	50	73
All	All	650/692 (94%)	615 (95%)	33 (5%)	2 (0%)	50	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	ASP
1	B	269	ASP

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	270/270 (100%)	261 (97%)	9 (3%)	50	76
1	B	260/270 (96%)	253 (97%)	7 (3%)	57	83
All	All	530/540 (98%)	514 (97%)	16 (3%)	53	80

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	LEU
1	A	269	ASP
1	B	131	ARG
1	A	152	GLU
1	B	136	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	271	GLN
1	B	181	GLN
1	A	181	GLN
1	A	216	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	334/346 (96%)	0.17	9 (2%) 52 54	7, 24, 48, 65	0
1	B	322/346 (93%)	0.42	24 (7%) 14 14	4, 26, 52, 69	0
All	All	656/692 (94%)	0.30	33 (5%) 28 28	4, 25, 51, 69	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	5.9
1	B	311	LEU	4.6
1	B	199	PHE	4.2
1	A	310	LEU	4.2
1	B	145	ARG	4.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.