

Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2023 – 02:03 PM EST

PDB ID : 3DMB

Title: Crystal structure of a putative general stress family protein (xcc2264) from

xanthomonas campestris pv. campestris at 2.30 A resolution

Authors: Joint Center for Structural Genomics (JCSG)

Deposited on : 2008-06-30

Resolution : 2.30 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

 $Mol Probity \quad : \quad 4.02b\text{--}467$

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

Xtriage (Phenix) : 1.13 EDS : 2.31.2

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

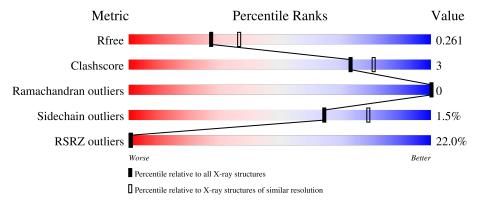
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	
			27%	
1	A	147	91%	7% ••
	_		12%	
1	В	147	91%	7% •
			23%	
1	С	147	87%	9%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3303 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 Putative General Stress Protein 26 with a PNP-Oxidase like Fold.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	1 A 146	Total	С	N	О	Se	0	3	0		
1	A	A 146	1117	712	192	207	6	0	J	U	
1	D	145	Total	С	N	О	Se	0	0	0	
1	Б	140	1100	700	188	208	4	0	U		
1	C	124	Total	С	N	О	Se	0	1	0	
1		134	1022	657	174	187	4	U	1	U	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8P8H7
В	0	GLY	-	expression tag	UNP Q8P8H7
С	0	GLY	-	expression tag	UNP Q8P8H7

• Molecule 2 is water.

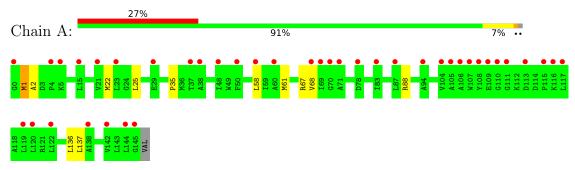
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	В	18	Total O 18 18	0	0
2	С	20	Total O 20 20	0	0



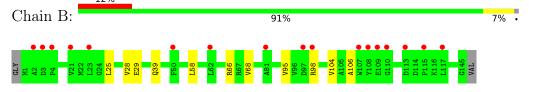
3 Residue-property plots (i)

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.

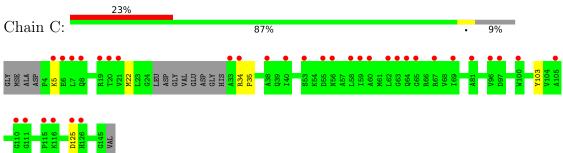
• Molecule 1: Putative General Stress Protein 26 with a PNP-Oxidase like Fold



• Molecule 1: Putative General Stress Protein 26 with a PNP-Oxidase like Fold



 \bullet Molecule 1: Putative General Stress Protein 26 with a PNP-Oxidase like Fold





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	105.32Å 105.32Å 68.34Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.66 - 2.30	Depositor
resolution (A)	28.66 - 2.30	EDS
% Data completeness	99.7 (28.66-2.30)	Depositor
(in resolution range)	99.7 (28.66-2.30)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.49 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.210 , 0.264	Depositor
it, it _{free}	0.214 , 0.261	DCC
R_{free} test set	1006 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34,65.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3303	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.42% 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)

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).

Mal	Mol Chain	Bond	lengths	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.70	0/1147	0.86	$2/1547 \ (0.1\%)$	
1	В	0.63	0/1122	0.81	0/1516	
1	С	0.62	0/1045	0.81	0/1408	
All	All	0.65	0/3314	0.83	2/4471 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	88	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	67	ARG	NE-CZ-NH1	5.23	122.92	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	1117	0	1100	10	0
1	В	1100	0	1072	12	0
1	С	1022	0	1013	3	0
2	A	26	0	0	0	0
2	В	18	0	0	0	0
2	С	20	0	0	0	0
All	All	3303	0	3185	21	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 (21) 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:25:LEU:HD22	1:A:61[A]:MSE:HE3	1.45	0.97
1:B:25:LEU:HD23	1:B:68:VAL:HG12	1.61	0.81
1:B:28:VAL:HG12	1:B:29:GLU:HG2	1.68	0.75
1:B:25:LEU:HD12	1:B:58:LEU:HD22	1.75	0.67
1:B:25:LEU:CD2	1:B:68:VAL:HG12	2.28	0.64
1:A:137:LEU:HD22	1:B:106:ALA:HB2	1.83	0.59
1:B:39:GLN:HE22	1:B:104:VAL:HG22	1.69	0.58
1:A:25:LEU:HD22	1:A:61[A]:MSE:CE	2.29	0.54
1:B:25:LEU:CD1	1:B:58:LEU:HD22	2.38	0.53
1:A:1:MSE:HE2	1:C:103:TYR:CD2	2.44	0.52
1:B:25:LEU:HD11	1:B:58:LEU:HD13	1.91	0.52
1:B:25:LEU:HD23	1:B:68:VAL:CG1	2.36	0.50
1:A:25:LEU:HD12	1:A:68:VAL:HG12	1.94	0.49
1:B:95:VAL:HG22	1:B:98:ARG:HH21	1.78	0.48
1:A:58:LEU:HA	1:A:61[A]:MSE:HE2	1.94	0.48
1:B:25:LEU:CD2	1:B:68:VAL:CG1	2.91	0.47
1:A:136:LEU:HD21	1:C:35:PRO:HG2	1.96	0.46
1:A:2:ALA:HB2	1:C:103:TYR:CE2	2.50	0.46
1:B:25:LEU:HD22	1:B:66:ARG:HD2	1.97	0.45
1:A:22[B]:MSE:HE3	1:A:35:PRO:HB3	1.98	0.44
1:A:25:LEU:HD13	1:A:58:LEU:HD22	2.01	0.42

There are no symmetry-related clashes.

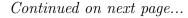
5.3 Torsion angles (i)

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	Perce	ntiles
1	A	147/147 (100%)	141 (96%)	6 (4%)	0	100	100





Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	143/147~(97%)	140 (98%)	3 (2%)	0	100	100
1	\mathbf{C}	$131/147\ (89\%)$	127 (97%)	4 (3%)	0	100	100
All	All	421/441 (96%)	408 (97%)	13 (3%)	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	113/111 (102%)	112 (99%)	1 (1%)	78	89
1	В	111/111 (100%)	111 (100%)	0	100	100
1	С	103/111 (93%)	98 (95%)	5 (5%)	25	35
All	All	327/333 (98%)	321 (98%)	6 (2%)	65	75

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

Mol	Mol Chain		Type	
1	A	1	MSE	
1	С	5	LYS	
1	С	22[A]	MSE	
1	С	22[B]	MSE	
1	С	34	ARG	
1	С	125	ASP	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	39	GLN



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} 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		$OWAB(A^2)$	Q < 0.9	
1	A	142/147~(96%)	1.42	40 (28%)	0	0	57, 66, 80, 87	0
1	В	141/147 (95%)	0.98	17 (12%)	4	6	58, 67, 80, 91	0
1	С	131/147 (89%)	1.37	34 (25%)	0	0	57, 67, 78, 81	0
All	All	414/441 (93%)	1.25	91 (21%)	0	1	57, 67, 79, 91	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	2	ALA	7.5
1	A	110	GLY	5.6
1	В	109	GLU	5.5
1	В	110	GLY	5.4
1	A	144	LEU	5.4
1	С	6	GLU	5.2
1	A	29	GLU	5.0
1	A	0	GLY	4.8
1	С	33	ALA	4.8
1	A	107	TRP	4.7
1	С	126	HIS	4.5
1	A	115	PRO	4.4
1	С	8	GLN	4.3
1	A	108	TYR	4.3
1	С	56	ASN	4.2
1	С	5	LYS	4.2
1	С	58	LEU	4.1
1	В	108	TYR	4.1
1	A	21	VAL	4.1
1	С	59	ILE	4.0
1	С	67	ARG	3.9
1	В	113	ASP	3.9
1	A	142	VAL	3.9

Continued on next page...



Continued from previous page...

Mol	nued fron Chain	Res	Type	RSRZ
1	A	106	ALA	3.9
1	В	3	ASP	3.8
1	A	105	ALA	3.8
1	В	4	PRO	3.6
1	A	23	LEU	3.6
1	В	21	VAL	3.6
1	A	109	GLU	3.6
1	С	21	VAL	3.5
1	A	120	LEU	3.5
1	С	63	GLY	3.5
1	A	4	PRO	3.4
1	С	7	LEU	3.4
1	A	83	ILE	3.3
1	A	145	GLY	3.3
1		125	ASP	3.3
1	C C C C A	53	SER	3.2
1	С	34	ARG	3.2
1	С	115	PRO	3.1
1	С	96	VAL	3.1
1	A	70	GLY	3.1
1	С	38	ALA	3.0
1	С	62	LEU	3.0
1	A	38	ALA	3.0
1	A	87	LEU	2.9
1	В	98	ARG	2.9
1	A	68	VAL	2.9
1	С	81	ALA	2.9
1	A	94	ALA	2.8
1	A	60	ALA	2.8
1	A	71	ALA	2.8
1	A	111	GLY	2.8
1	A	5	LYS	2.8
1	В	115	PRO	2.8
1	В	97	ASP	2.7
1	A	119	LEU	2.7
1	С	116	LYS	2.7
1	A	113	ASP	2.7
1	С	111	GLY	2.7
1	С	69	ILE	2.7
1	С	100	TRP	2.7
1	A	122	LEU	2.5
1	В	23	LEU	2.5

Continued on next page...



Continued from previous page...

Mol	nuea jron Chain	Res	Type	RSRZ
1	С	55	ASP	2.5
1	В	81	ALA	2.5
1	В	117	LEU	2.5
1	A	138	ALA	2.5
1	A	78	ASP	2.5
1	С	110	GLY	2.4
1	С	64	GLN	2.4
1	A	69	ILE	2.4
1	A	116	LYS	2.3
1	С	97	ASP	2.3
1	С	60	ALA	2.3
1	A	48	ILE	2.2
1	A	58	LEU	2.2
1	A	117	LEU	2.2
1	A	50	PHE	2.2
1	С	65	GLY	2.2
1	С	19	ARG	2.2
1	В	107	TRP	2.1
1	С	40	ILE	2.1
1	С	20	THR	2.1
1	A	15	LEU	2.1
1	A	37	THR	2.1
1	С	105	ALA	2.1
1	A	104	VAL	2.1
1	В	50	PHE	2.0
1	В	62	LEU	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 monosaccharides 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.

