



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:02 AM UTC

PDB ID : 3VB9 / pdb\_00003vb9  
Title : Crystal structure of VPA0735 from *Vibrio parahaemolyticus* in monoclinic form, NorthEast Structural Genomics target VpR109  
Authors : Seetharaman, J.; Neely, H.; Cunningham, K.; Ciccocanti, C.; Bjelic, S.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2011-12-31  
Resolution : 2.10 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

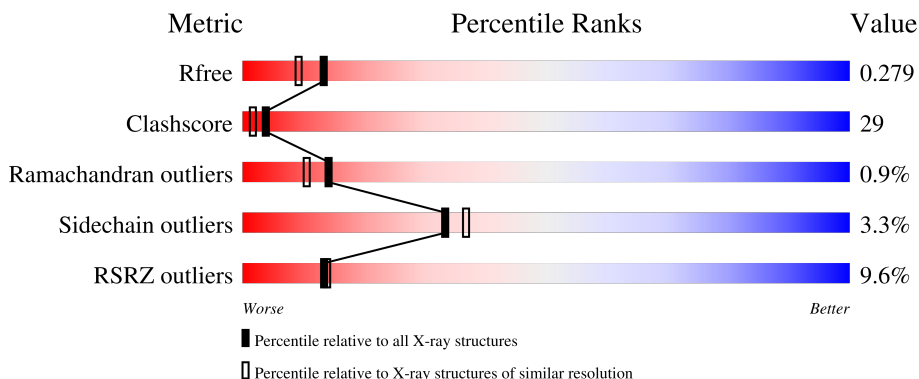
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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	483	
1	B	483	
1	C	483	
1	D	483	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15733 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 Uncharacterized protein VPA0735.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	Se	0	0	0
			3717	2382	623	698	14			
1	B	462	Total	C	N	O	Se	0	0	0
			3736	2393	627	702	14			
1	C	460	Total	C	N	O	Se	0	0	0
			3717	2382	623	698	14			
1	D	460	Total	C	N	O	Se	0	0	0
			3717	2382	623	698	14			

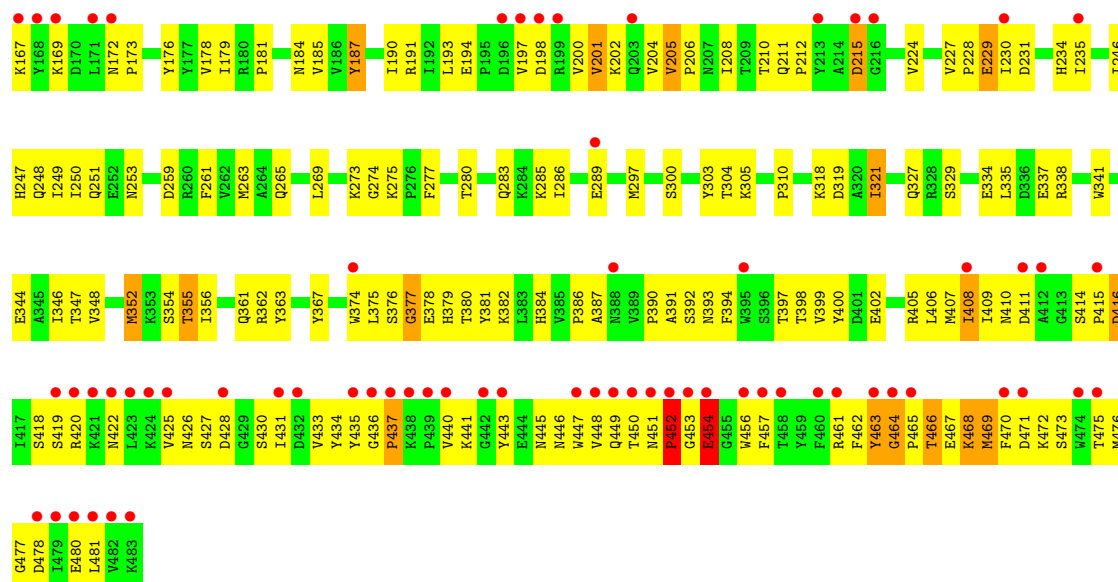
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	1	Total	Mg	0	0
			1	1		
2	D	2	Total	Mg	0	0
			2	2		

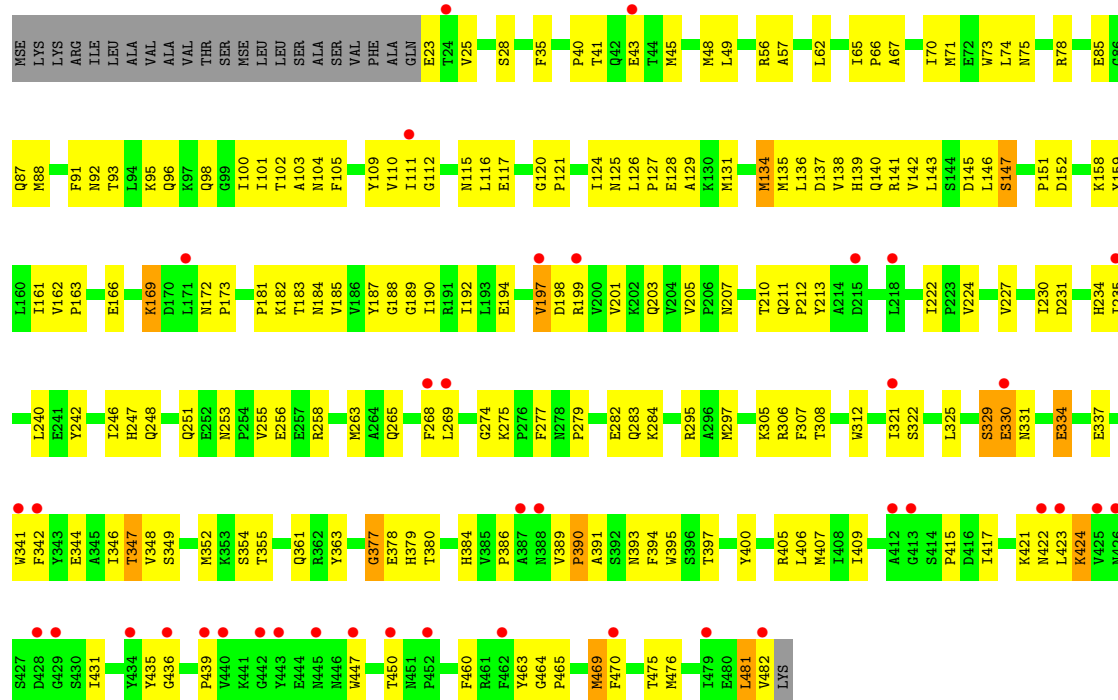
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		
3	B	217	Total	O	0	0
			217	217		
3	C	190	Total	O	0	0
			190	190		
3	D	235	Total	O	0	0
			235	235		

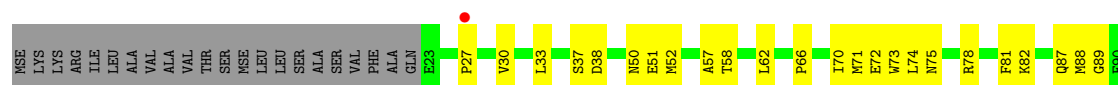




• Molecule 1: Uncharacterized protein VPA0735



• Molecule 1: Uncharacterized protein VPA0735





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.27Å 106.93Å 157.18Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	39.99 – 2.10 39.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.99-2.10) 92.1 (39.99-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.274 0.224 , 0.279	Depositor DCC
$R_{free}$ test set	19578 reflections (8.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3721e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG

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	0.41	0/3803	0.98	19/5137 (0.4%)
1	B	0.41	0/3822	0.96	18/5160 (0.3%)
1	C	0.40	0/3803	0.91	7/5137 (0.1%)
1	D	0.41	0/3803	0.94	11/5137 (0.2%)
All	All	0.41	0/15231	0.95	55/20571 (0.3%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLY	N-CA-C	13.96	132.62	115.31
1	A	352	MSE	N-CA-C	-12.76	96.21	113.30
1	A	352	MSE	N-CA-CB	-10.89	94.17	110.61
1	A	204	VAL	N-CA-C	10.12	119.95	110.74
1	B	414	SER	CA-C-N	7.74	127.38	119.56

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	3717	0	3643	250	0
1	B	3736	0	3664	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3717	0	3643	209	0
1	D	3717	0	3643	153	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	197	0	0	12	0
3	B	217	0	0	18	0
3	C	190	0	0	11	0
3	D	235	0	0	9	0
All	All	15733	0	14593	844	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 29.

The worst 5 of 844 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:300:SER:HA	1:B:45:MSE:HE2	1.18	1.14
1:C:105:PHE:HB2	1:C:407:MSE:HE1	1.32	1.11
1:C:135:MSE:HE3	1:C:146:LEU:HD11	1.32	1.10
1:A:303:TYR:HB2	1:B:45:MSE:HE1	1.30	1.09
1:C:45:MSE:HE1	1:D:303:TYR:HB2	1.24	1.09

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	458/483 (95%)	436 (95%)	20 (4%)	2 (0%)	30 28
1	B	460/483 (95%)	428 (93%)	26 (6%)	6 (1%)	9 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	11	8
1	D	458/483 (95%)	432 (94%)	23 (5%)	3 (1%)	18	15
All	All	1834/1932 (95%)	1731 (94%)	87 (5%)	16 (1%)	14	10

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	419	SER
1	B	452	PRO
1	C	334	GLU
1	A	334	GLU
1	B	437	PRO

### 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	405/408 (99%)	387 (96%)	18 (4%)	25	26
1	B	407/408 (100%)	391 (96%)	16 (4%)	28	31
1	C	405/408 (99%)	396 (98%)	9 (2%)	45	53
1	D	405/408 (99%)	395 (98%)	10 (2%)	42	48
All	All	1622/1632 (99%)	1569 (97%)	53 (3%)	33	37

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	352	MSE
1	C	134	MSE
1	D	230	ILE
1	B	408	ILE
1	B	468	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	140	GLN
1	D	247	HIS
1	B	234	HIS
1	B	203	GLN
1	D	251	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	446/483 (92%)	0.51	35 (7%) 19 20	10, 24, 45, 55	0
1	B	448/483 (92%)	0.97	73 (16%) 4 4	8, 24, 51, 68	0
1	C	446/483 (92%)	0.58	39 (8%) 16 16	8, 24, 45, 64	0
1	D	446/483 (92%)	0.41	25 (5%) 30 32	10, 21, 40, 59	0
All	All	1786/1932 (92%)	0.62	172 (9%) 13 14	8, 23, 45, 68	0

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	TRP	14.4
1	B	463	TYR	7.7
1	B	437	PRO	7.2
1	B	474	TRP	7.1
1	B	215	ASP	7.0

### 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](#)

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	502	1/1	0.95	0.25	20,20,20,20	0
2	MG	B	502	1/1	0.97	0.26	21,21,21,21	0
2	MG	A	502	1/1	0.98	0.25	16,16,16,16	0
2	MG	B	501	1/1	0.98	0.12	18,18,18,18	0
2	MG	C	501	1/1	0.99	0.02	13,13,13,13	0
2	MG	D	501	1/1	0.99	0.05	14,14,14,14	0
2	MG	A	501	1/1	0.99	0.05	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.