



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:10 am GMT

PDB ID : 1R6F  
Title : The structure of Yersinia pestis V-antigen, an essential virulence factor and mediator of immunity against plague  
Authors : Derewenda, U.; Mateja, A.; Devedjiev, Y.; Routzahn, K.M.; Evdokimov, A.G.; Derewenda, Z.S.; Waugh, D.S.  
Deposited on : 2003-10-15  
Resolution : 2.17 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](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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

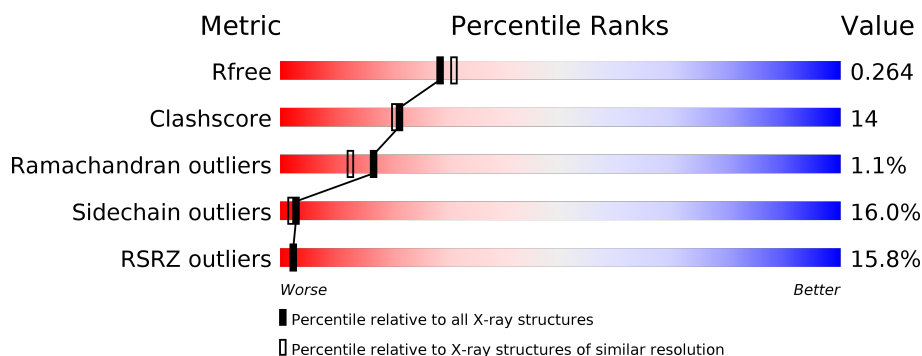
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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	310	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2139 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 Virulence-associated V antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	1
			2139	1343	365	425	6			

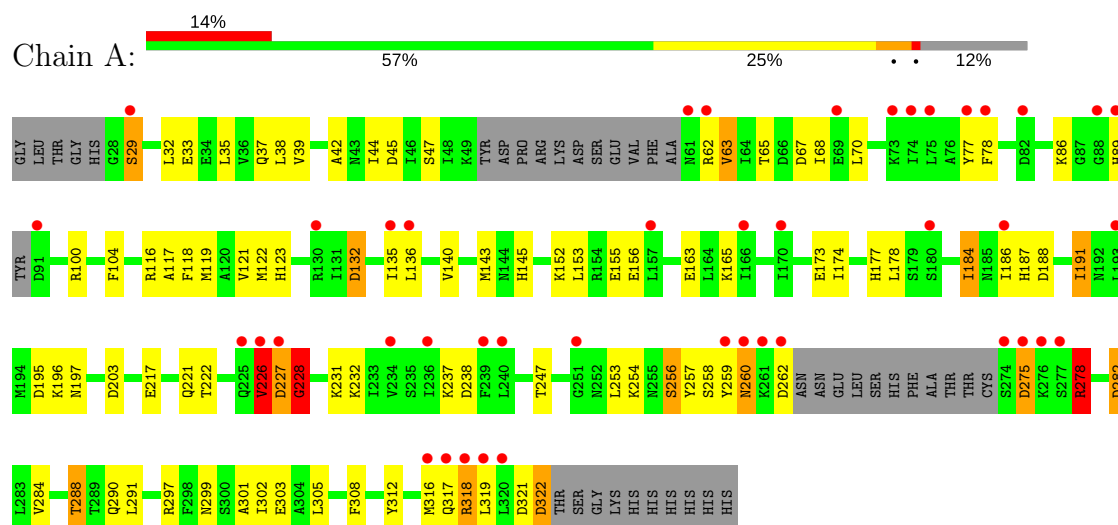
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	CLONING ARTIFACT	UNP P21206
A	40	ALA	LYS	ENGINEERED	UNP P21206
A	41	ALA	ASP	ENGINEERED	UNP P21206
A	42	ALA	LYS	ENGINEERED	UNP P21206
A	327	HIS	-	EXPRESSION TAG	UNP P21206
A	328	HIS	-	EXPRESSION TAG	UNP P21206
A	329	HIS	-	EXPRESSION TAG	UNP P21206
A	330	HIS	-	EXPRESSION TAG	UNP P21206
A	331	HIS	-	EXPRESSION TAG	UNP P21206
A	332	HIS	-	EXPRESSION TAG	UNP P21206

### 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 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: Virulence-associated V antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.88Å 45.09Å 46.91Å 76.20° 78.42° 77.17°	Depositor
Resolution (Å)	18.50 – 2.17 17.64 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.2 (18.50-2.17) 89.3 (17.64-2.16)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.42 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.217 , 0.284 0.265 , 0.264	Depositor DCC
$R_{free}$ test set	1370 reflections (9.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 28.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.40	0/2163	1.02	11/2909 (0.4%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASP	CB-CG-OD2	6.75	124.37	118.30
1	A	228	GLY	N-CA-C	6.64	129.70	113.10
1	A	45	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	275	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	67	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	132	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	278	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	262	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	227	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	203	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	195	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2139	0	2141	58	0
All	All	2139	0	2141	58	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 14.

All (58) 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:118:PHE:HD2	1:A:119:MET:HE2	1.42	0.85
1:A:284:VAL:O	1:A:288:THR:HG23	1.76	0.84
1:A:153:LEU:HG	1:A:302:ILE:CD1	2.09	0.82
1:A:118:PHE:HD2	1:A:119:MET:CE	1.94	0.81
1:A:278:ARG:HG2	1:A:278:ARG:HH11	1.48	0.78
1:A:173:GLU:HG2	1:A:191:ILE:HG12	1.69	0.73
1:A:153:LEU:HG	1:A:302:ILE:HD13	1.72	0.72
1:A:35:LEU:O	1:A:38:LEU:HB2	1.94	0.67
1:A:118:PHE:CD2	1:A:119:MET:CE	2.78	0.66
1:A:174:ILE:HA	1:A:184:ILE:HD13	1.78	0.66
1:A:254:LYS:HE2	1:A:257:TYR:CE2	2.31	0.65
1:A:322:ASP:N	1:A:322:ASP:OD1	2.27	0.65
1:A:153:LEU:CG	1:A:302:ILE:HD13	2.31	0.60
1:A:78:PHE:CZ	1:A:123:HIS:HB2	2.36	0.60
1:A:186:ILE:HG13	1:A:237:LYS:HB2	1.85	0.59
1:A:318:ARG:HH11	1:A:318:ARG:CG	2.16	0.59
1:A:318:ARG:NH1	1:A:318:ARG:HG3	2.17	0.58
1:A:319:LEU:HG	1:A:319:LEU:O	2.04	0.58
1:A:78:PHE:HZ	1:A:123:HIS:HB2	1.70	0.57
1:A:47:SER:HB3	1:A:63:VAL:HA	1.87	0.56
1:A:135:ILE:HG21	1:A:301:ALA:CB	2.36	0.55
1:A:187:HIS:CG	1:A:188:ASP:H	2.25	0.54
1:A:318:ARG:HH11	1:A:318:ARG:HG3	1.73	0.54
1:A:222:THR:HG23	1:A:238:ASP:OD1	2.08	0.53
1:A:153:LEU:CD2	1:A:302:ILE:HD13	2.38	0.53
1:A:118:PHE:CD2	1:A:119:MET:HE1	2.42	0.53
1:A:221:GLN:NE2	1:A:232:LYS:HB3	2.24	0.52
1:A:121:VAL:HG22	1:A:140:VAL:HG21	1.92	0.52
1:A:121:VAL:CG2	1:A:140:VAL:HG21	2.39	0.51
1:A:163:GLU:OE2	1:A:247:THR:OG1	2.23	0.51
1:A:163:GLU:HB3	1:A:291:LEU:HD21	1.93	0.51
1:A:254:LYS:HG3	1:A:257:TYR:CZ	2.46	0.50
1:A:143:MET:HE1	1:A:308:PHE:HE2	1.76	0.50
1:A:47:SER:HB2	1:A:62:ARG:O	2.13	0.49
1:A:104:PHE:CZ	1:A:136:LEU:HB3	2.48	0.48
1:A:118:PHE:CZ	1:A:122:MET:HE2	2.47	0.48
1:A:318:ARG:NH1	1:A:318:ARG:CG	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:CG	1:A:188:ASP:N	2.81	0.47
1:A:152:LYS:NZ	1:A:155:GLU:OE2	2.39	0.47
1:A:226:VAL:HB	1:A:227:ASP:H	1.57	0.46
1:A:118:PHE:CD2	1:A:119:MET:HE2	2.34	0.46
1:A:135:ILE:HG21	1:A:301:ALA:HB2	1.99	0.44
1:A:116:ARG:HG3	1:A:312:TYR:CE1	2.52	0.44
1:A:117:ALA:HB2	1:A:143:MET:HB3	2.00	0.43
1:A:221:GLN:HE22	1:A:232:LYS:HB3	1.81	0.43
1:A:132:ASP:HB2	1:A:297:ARG:NH1	2.34	0.43
1:A:29:SER:O	1:A:33:GLU:HG2	2.18	0.43
1:A:254:LYS:HE2	1:A:257:TYR:CD2	2.53	0.43
1:A:118:PHE:CZ	1:A:122:MET:CE	3.02	0.42
1:A:174:ILE:O	1:A:178:LEU:HG	2.20	0.42
1:A:77:TYR:HE2	1:A:319:LEU:HD13	1.85	0.41
1:A:227:ASP:OD1	1:A:228:GLY:N	2.51	0.41
1:A:254:LYS:HG3	1:A:257:TYR:CE1	2.55	0.41
1:A:254:LYS:HD2	1:A:256:SER:O	2.21	0.41
1:A:39:VAL:O	1:A:42:ALA:O	2.39	0.41
1:A:177:HIS:CD2	1:A:184:ILE:HD12	2.56	0.41
1:A:278:ARG:HG2	1:A:282:ASP:OD2	2.22	0.40
1:A:116:ARG:HG3	1:A:312:TYR:CD1	2.57	0.40

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	264/310 (85%)	249 (94%)	12 (4%)	3 (1%)	17	12

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	228	GLY
1	A	260	ASN
1	A	226	VAL

### 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	238/277 (86%)	200 (84%)	38 (16%)	<b>3</b> <b>2</b>

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	32	LEU
1	A	37	GLN
1	A	44	ILE
1	A	63	VAL
1	A	65	THR
1	A	68	ILE
1	A	70	LEU
1	A	86	LYS
1	A	89	HIS
1	A	100	ARG
1	A	145	HIS
1	A	156	GLU
1	A	165	LYS
1	A	184	ILE
1	A	191	ILE
1	A	196	LYS
1	A	197	ASN
1	A	217	GLU
1	A	226	VAL
1	A	231	LYS
1	A	253	LEU
1	A	256	SER
1	A	258	SER

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Mol	Chain	Res	Type
1	A	259	TYR
1	A	260	ASN
1	A	275	ASP
1	A	278	ARG
1	A	288	THR
1	A	290	GLN
1	A	299	ASN
1	A	303	GLU
1	A	305	LEU
1	A	316	MET
1	A	317	GLN
1	A	318	ARG
1	A	321	ASP
1	A	322	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	197	ASN
1	A	221	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 carbohydrates 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 ⓘ

### 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, 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	272/310 (87%)	1.09	43 (15%) 2 2	18, 25, 32, 38	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	SER	10.4
1	A	275	ASP	7.8
1	A	262	ASP	7.2
1	A	259	TYR	6.0
1	A	88	GLY	5.8
1	A	261	LYS	5.8
1	A	226	VAL	5.6
1	A	260	ASN	4.8
1	A	277	SER	4.2
1	A	89	HIS	3.9
1	A	320	LEU	3.6
1	A	69	GLU	3.4
1	A	136	LEU	3.4
1	A	78	PHE	3.2
1	A	318	ARG	3.0
1	A	317	GLN	2.9
1	A	74	ILE	2.8
1	A	316	MET	2.8
1	A	91	ASP	2.7
1	A	29	SER	2.7
1	A	225	GLN	2.6
1	A	251	GLY	2.5
1	A	236	ILE	2.5
1	A	276	LYS	2.5
1	A	157	LEU	2.4
1	A	135	ILE	2.4
1	A	186	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	61	ASN	2.3
1	A	75	LEU	2.3
1	A	180	SER	2.3
1	A	82	ASP	2.3
1	A	62	ARG	2.2
1	A	234	VAL	2.2
1	A	166	ILE	2.2
1	A	130	ARG	2.2
1	A	240	LEU	2.2
1	A	319	LEU	2.1
1	A	77	TYR	2.1
1	A	73	LYS	2.1
1	A	227	ASP	2.1
1	A	193	LEU	2.0
1	A	239	PHE	2.0
1	A	170	ILE	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 carbohydrates 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.