



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:05 PM 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 validation 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>

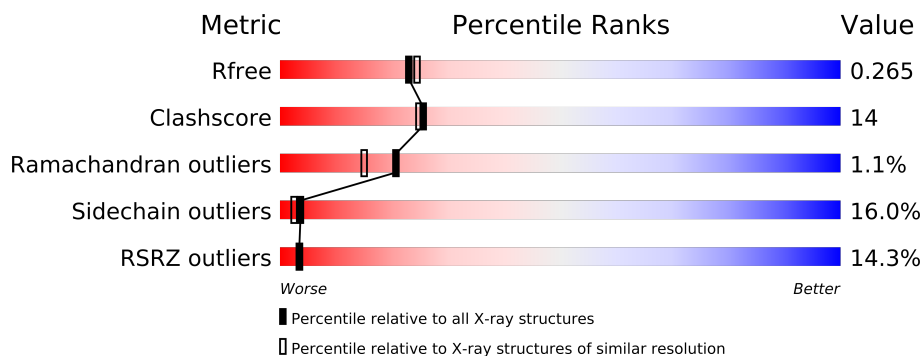
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.17 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}	66092	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (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 ≥ 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	310	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2139 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 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:

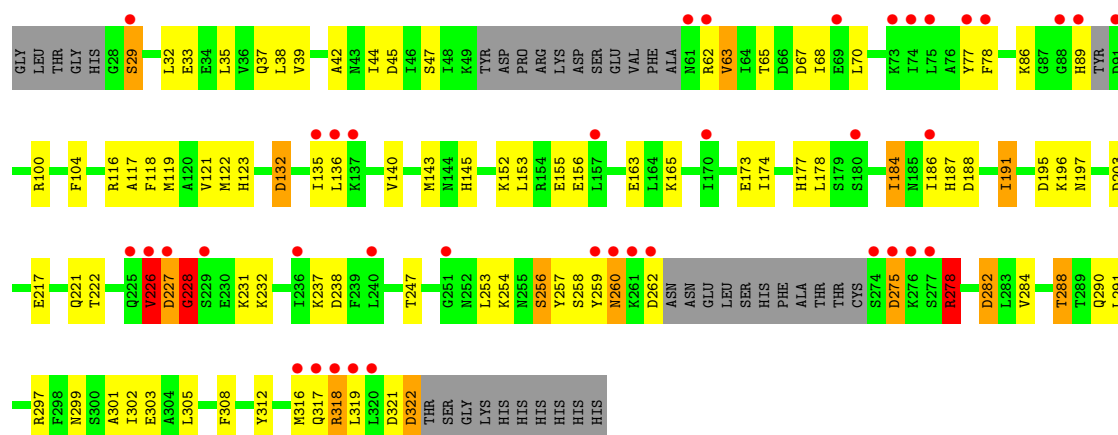
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	CLONING ARTIFACT	UNP P21206
A	40	ALA	LYS	ENGINEERED	UNP P21206
A	41	ALA	ASP	ENGINEERED	UNP P21206
A	42	ALA	LYS	ENGINEERED	UNP P21206
A	327	HIS	-	EXPRESSION TAG	UNP P21206
A	328	HIS	-	EXPRESSION TAG	UNP P21206
A	329	HIS	-	EXPRESSION TAG	UNP P21206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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.2 (17.64-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.284 0.267 , 0.265	Depositor DCC
R_{free} test set	1383 reflections (9.81%)	DCC
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 19.0	EDS
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 14116 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2139	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.40	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 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	2139	0	2141	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2139	0	2141	58	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 14.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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%)	21	15

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%)	3 2

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
1	A	259	TYR

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Mol	Chain	Res	Type
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 ⓘ

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	272/310 (87%)	1.09	39 (14%) 3 3	18, 25, 32, 38	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	SER	9.4
1	A	275	ASP	7.5
1	A	262	ASP	7.1
1	A	88	GLY	5.7
1	A	261	LYS	5.7
1	A	259	TYR	5.6
1	A	226	VAL	5.2
1	A	260	ASN	5.1
1	A	89	HIS	3.9
1	A	277	SER	3.8
1	A	69	GLU	3.5
1	A	136	LEU	3.1
1	A	320	LEU	3.0
1	A	78	PHE	3.0
1	A	318	ARG	2.8
1	A	276	LYS	2.7
1	A	251	GLY	2.7
1	A	180	SER	2.6
1	A	225	GLN	2.6
1	A	186	ILE	2.6
1	A	74	ILE	2.5
1	A	317	GLN	2.5
1	A	135	ILE	2.5
1	A	316	MET	2.4
1	A	75	LEU	2.4
1	A	29	SER	2.4
1	A	227	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	2.3
1	A	91	ASP	2.2
1	A	157	LEU	2.2
1	A	236	ILE	2.2
1	A	62	ARG	2.2
1	A	77	TYR	2.1
1	A	61	ASN	2.1
1	A	137	LYS	2.1
1	A	229	SER	2.1
1	A	240	LEU	2.0
1	A	170	ILE	2.0
1	A	73	LYS	2.0

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.