



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 09:28 AM EDT

PDB ID : 3L29  
Title : Crystal Structure of Zaire Ebola VP35 interferon inhibitory domain  
K319A/R322A mutant  
Authors : Leung, D.W.; Ramanan, P.; Borek, D.M.; Amarasinghe, G.K.  
Deposited on : 2009-12-14  
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 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) : 2.23.2

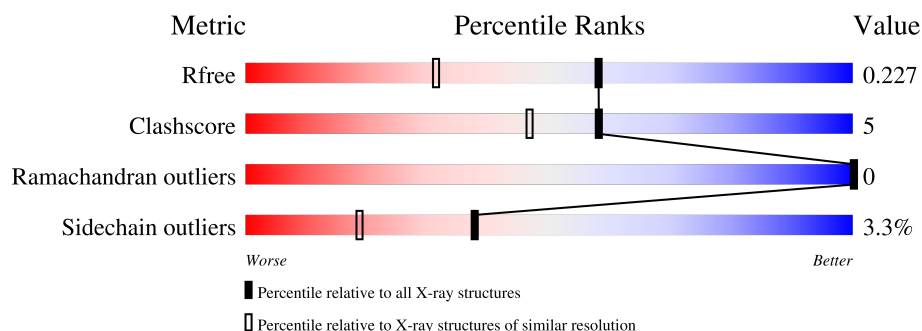
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	129	 91% . . 5%
1	B	129	 85% 12% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2316 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 Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	7	0
			1000	632	178	184	6			
1	B	127	Total	C	N	O	S	0	11	0
			1061	668	192	194	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	GLY	-	expression tag	UNP Q05127
A	213	HIS	-	expression tag	UNP Q05127
A	214	MET	-	expression tag	UNP Q05127
A	319	ALA	LYS	engineered mutation	UNP Q05127
A	322	ALA	ARG	engineered mutation	UNP Q05127
B	212	GLY	-	expression tag	UNP Q05127
B	213	HIS	-	expression tag	UNP Q05127
B	214	MET	-	expression tag	UNP Q05127
B	319	ALA	LYS	engineered mutation	UNP Q05127
B	322	ALA	ARG	engineered mutation	UNP Q05127

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	123	Total 123	O 123	0	0

### 3 Residue-property plots


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. 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. 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: Polymerase cofactor VP35

Chain A:  91% . . 5%



- Molecule 1: Polymerase cofactor VP35

Chain B:  85% 12% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.43Å 66.07Å 72.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.32 – 1.70 36.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.32-1.70) 97.2 (36.32-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.191 , 0.232 0.193 , 0.227	Depositor DCC
$R_{free}$ test set	1372 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.341	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.68 % 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 3.0601e-04. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.72	0/1023	0.72	0/1388
1	B	0.75	0/1085	0.70	0/1470
All	All	0.74	0/2108	0.71	0/2858

There are no bond length outliers.

There are no bond angle outliers.

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	1000	0	1000	5	0
1	B	1061	0	1062	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	130	0	0	2	0
3	B	123	0	0	5	0
All	All	2316	0	2062	20	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 5.

All (20) 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:B:266[B]:SER:OG	1:B:279[B]:GLN:OE1	1.76	1.02
1:B:275[B]:CYS:O	1:B:279[B]:GLN:HG3	1.60	1.01
1:B:311:LEU:C	1:B:312:ARG:HD2	2.04	0.79
1:B:312:ARG:HG2	3:B:156:HOH:O	1.84	0.77
1:A:229:TYR:OH	1:A:244[B]:GLN:HG2	1.95	0.66
1:A:244[B]:GLN:NE2	3:A:118:HOH:O	2.37	0.58
1:B:312:ARG:HD2	1:B:312:ARG:N	2.21	0.52
1:B:312:ARG:NH1	3:B:354:HOH:O	2.45	0.49
1:A:231[B]:HIS:HE1	3:A:186:HOH:O	1.94	0.49
1:B:271:ASP:OD2	1:B:279[B]:GLN:NE2	2.47	0.48
1:B:248:LYS:NZ	3:B:205:HOH:O	2.46	0.48
1:B:298:ARG:HG2	1:B:331:GLN:NE2	2.30	0.46
1:B:288:GLN:HG3	3:B:359:HOH:O	2.15	0.45
1:B:271:ASP:OD2	1:B:279[B]:GLN:OE1	2.35	0.44
1:B:314:VAL:HG21	1:B:335[B]:THR:HG22	1.98	0.44
1:B:327:VAL:HG13	1:B:335[B]:THR:HG22	2.02	0.41
1:B:269[A]:GLU:HG2	3:B:169:HOH:O	2.21	0.41
1:A:229:TYR:OH	1:A:244[B]:GLN:CG	2.68	0.40
1:A:240:HIS:O	1:A:244[B]:GLN:HG3	2.21	0.40
1:B:311:LEU:O	1:B:312:ARG:HD2	2.21	0.40

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	128/129 (99%)	126 (98%)	2 (2%)	0	100	100
1	B	136/129 (105%)	135 (99%)	1 (1%)	0	100	100
All	All	264/258 (102%)	261 (99%)	3 (1%)	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	111/108 (103%)	107 (96%)	4 (4%)	35	16
1	B	118/108 (109%)	114 (97%)	4 (3%)	37	18
All	All	229/216 (106%)	221 (96%)	8 (4%)	38	17

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244[A]	GLN
1	A	244[B]	GLN
1	A	298	ARG
1	A	331	GLN
1	B	216	LYS
1	B	300	ARG
1	B	312	ARG
1	B	329	GLN

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

Mol	Chain	Res	Type
1	B	331	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](#)

Of 2 ligands modelled in this entry, 2 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.