



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:41 AM GMT

PDB ID : 2I8B  
Title : Crystal structure of the C-terminal domain of Ebola virus VP30  
Authors : Muziol, T.M.; Hartlieb, B.; Becker, S.; Weissenhorn, W.  
Deposited on : 2006-09-01  
Resolution : 2.00 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

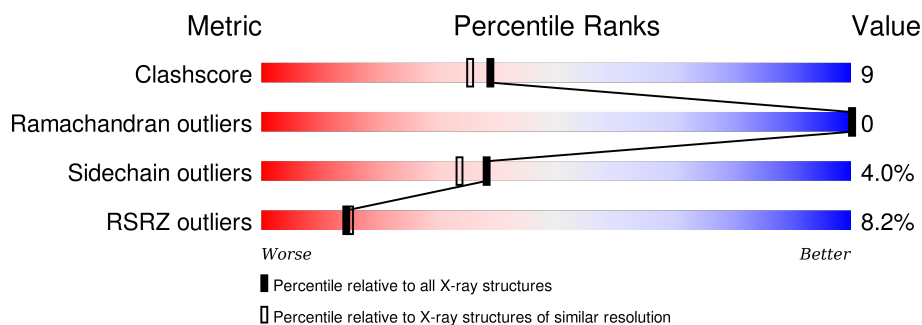
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	152	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	152	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2253 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 Minor nucleoprotein VP30.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	Se	0	4	0
			1020	649	178	187	3	3			
1	B	132	Total	C	N	O	S	Se	0	2	0
			1059	676	185	192	3	3			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	HIS	-	CLONING ARTIFACT	UNP Q05323
A	122	HIS	-	CLONING ARTIFACT	UNP Q05323
A	123	HIS	-	CLONING ARTIFACT	UNP Q05323
A	124	HIS	-	CLONING ARTIFACT	UNP Q05323
A	125	HIS	-	CLONING ARTIFACT	UNP Q05323
A	126	HIS	-	CLONING ARTIFACT	UNP Q05323
A	127	ASP	-	CLONING ARTIFACT	UNP Q05323
A	128	TYR	-	CLONING ARTIFACT	UNP Q05323
A	129	ASP	-	CLONING ARTIFACT	UNP Q05323
A	130	ILE	-	CLONING ARTIFACT	UNP Q05323
A	131	PRO	-	CLONING ARTIFACT	UNP Q05323
A	132	THR	-	CLONING ARTIFACT	UNP Q05323
A	133	THR	-	CLONING ARTIFACT	UNP Q05323
A	134	GLU	-	CLONING ARTIFACT	UNP Q05323
A	135	ASN	-	CLONING ARTIFACT	UNP Q05323
A	136	LEU	-	CLONING ARTIFACT	UNP Q05323
A	137	TYR	-	CLONING ARTIFACT	UNP Q05323
A	138	PHE	-	CLONING ARTIFACT	UNP Q05323
A	139	GLN	-	CLONING ARTIFACT	UNP Q05323
A	140	GLY	-	CLONING ARTIFACT	UNP Q05323
A	141	ALA	-	CLONING ARTIFACT	UNP Q05323
A	177	MSE	MET	MODIFIED RESIDUE	UNP Q05323
A	237	MSE	MET	MODIFIED RESIDUE	UNP Q05323
B	121	HIS	-	CLONING ARTIFACT	UNP Q05323
B	122	HIS	-	CLONING ARTIFACT	UNP Q05323

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Chain	Residue	Modelled	Actual	Comment	Reference
B	123	HIS	-	CLONING ARTIFACT	UNP Q05323
B	124	HIS	-	CLONING ARTIFACT	UNP Q05323
B	125	HIS	-	CLONING ARTIFACT	UNP Q05323
B	126	HIS	-	CLONING ARTIFACT	UNP Q05323
B	127	ASP	-	CLONING ARTIFACT	UNP Q05323
B	128	TYR	-	CLONING ARTIFACT	UNP Q05323
B	129	ASP	-	CLONING ARTIFACT	UNP Q05323
B	130	ILE	-	CLONING ARTIFACT	UNP Q05323
B	131	PRO	-	CLONING ARTIFACT	UNP Q05323
B	132	THR	-	CLONING ARTIFACT	UNP Q05323
B	133	THR	-	CLONING ARTIFACT	UNP Q05323
B	134	GLU	-	CLONING ARTIFACT	UNP Q05323
B	135	ASN	-	CLONING ARTIFACT	UNP Q05323
B	136	LEU	-	CLONING ARTIFACT	UNP Q05323
B	137	TYR	-	CLONING ARTIFACT	UNP Q05323
B	138	PHE	-	CLONING ARTIFACT	UNP Q05323
B	139	GLN	-	CLONING ARTIFACT	UNP Q05323
B	140	GLY	-	CLONING ARTIFACT	UNP Q05323
B	141	ALA	-	CLONING ARTIFACT	UNP Q05323
B	177	MSE	MET	MODIFIED RESIDUE	UNP Q05323
B	237	MSE	MET	MODIFIED RESIDUE	UNP Q05323

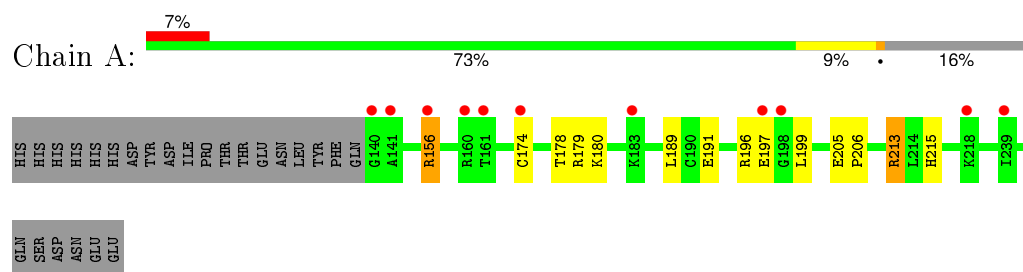
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	88	Total O 88 88	0	0
2	B	86	Total O 86 86	0	0

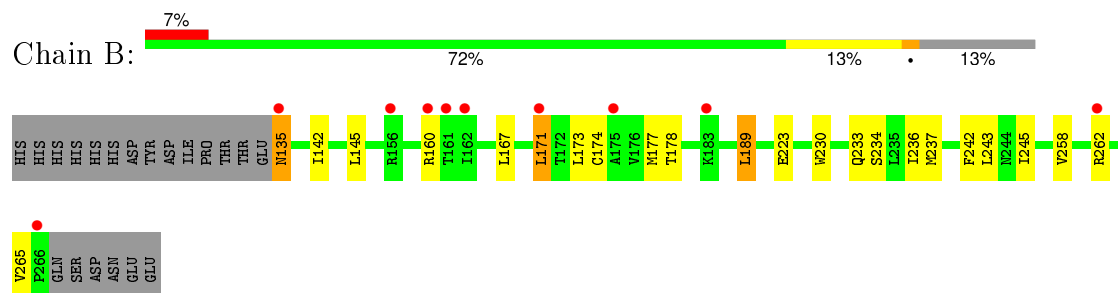
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Minor nucleoprotein VP30



#### • Molecule 1: Minor nucleoprotein VP30



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.37Å 63.59Å 80.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 22.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.00) 99.8 (22.94-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.59 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.195 , 0.241 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 20788 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2253	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 32.76 % 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 8.9205e-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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	0/1046	0.55	0/1411
1	B	0.47	0/1081	0.57	0/1459
All	All	0.46	0/2127	0.56	0/2870

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	1020	0	1059	17	0
1	B	1059	0	1091	23	0
2	A	88	0	0	3	0
2	B	86	0	0	0	0
All	All	2253	0	2150	38	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 9.

All (38) 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:213:ARG:HH11	1:A:213:ARG:HG2	1.08	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191[B]:GLU:HG2	2:A:330:HOH:O	1.81	0.80
1:A:213:ARG:HH11	1:A:213:ARG:CG	1.95	0.77
1:A:213:ARG:NH1	1:A:213:ARG:HG2	1.89	0.76
1:B:177:MSE:HE3	1:B:242:PHE:HE2	1.56	0.70
1:A:196:ARG:HB3	1:A:199:LEU:HD22	1.73	0.69
1:B:177:MSE:HE1	1:B:243:LEU:CD2	2.22	0.69
1:B:233:GLN:O	1:B:237[A]:MSE:HG3	1.95	0.66
1:A:258:VAL:HG22	1:B:142:ILE:HD12	1.78	0.65
1:B:177:MSE:HE3	1:B:242:PHE:CE2	2.32	0.65
1:B:189:LEU:HD23	1:B:245:ILE:CG2	2.33	0.59
1:B:177:MSE:HE1	1:B:243:LEU:HD23	1.85	0.57
1:B:174:CYS:HA	1:B:177:MSE:CE	2.34	0.57
1:B:258:VAL:O	1:B:262:ARG:HG2	2.06	0.55
1:B:262:ARG:O	1:B:265:VAL:HG22	2.07	0.54
1:A:174:CYS:O	1:A:178:THR:HG23	2.09	0.52
1:B:189:LEU:HD23	1:B:245:ILE:HG22	1.91	0.52
1:B:171:LEU:O	1:B:171:LEU:HD22	2.10	0.52
1:B:174:CYS:HA	1:B:177:MSE:HE3	1.92	0.50
1:A:179:ARG:HG2	1:A:215:HIS:O	2.12	0.50
1:B:160:ARG:HA	1:B:236:ILE:HD13	1.93	0.50
1:A:258:VAL:HA	1:B:142:ILE:CD1	2.42	0.50
1:B:171:LEU:HD13	1:B:223:GLU:HG3	1.93	0.49
1:B:171:LEU:HD13	1:B:223:GLU:CG	2.43	0.49
1:A:199:LEU:HB3	2:A:291:HOH:O	2.13	0.49
1:A:205:GLU:HB2	1:A:206:PRO:HD3	1.95	0.48
1:B:234:SER:HA	1:B:237[A]:MSE:HE2	1.95	0.48
1:B:177:MSE:HE1	1:B:243:LEU:HD21	1.96	0.47
1:A:213:ARG:NH1	1:A:213:ARG:CG	2.63	0.47
1:B:174:CYS:O	1:B:178:THR:HG23	2.16	0.46
1:A:156:ARG:HD2	1:A:156:ARG:H	1.80	0.46
1:A:197:GLU:HG2	2:A:329:HOH:O	2.16	0.46
1:A:189:LEU:HD22	1:A:245:ILE:HG22	1.97	0.45
1:A:180:LYS:HA	1:A:180:LYS:HD3	1.87	0.43
1:B:189:LEU:HD23	1:B:245:ILE:HG21	2.02	0.42
1:B:171:LEU:HD22	1:B:171:LEU:C	2.40	0.42
1:B:135:ASN:HD22	1:B:135:ASN:HA	1.61	0.42

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	129/152 (85%)	128 (99%)	1 (1%)	0	100	100
1	B	132/152 (87%)	131 (99%)	1 (1%)	0	100	100
All	All	261/304 (86%)	259 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	114/133 (86%)	112 (98%)	2 (2%)	66	69
1	B	117/133 (88%)	110 (94%)	7 (6%)	24	17
All	All	231/266 (87%)	222 (96%)	9 (4%)	38	35

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ARG
1	A	213	ARG
1	B	135	ASN
1	B	145	LEU
1	B	167	LEU
1	B	171	LEU
1	B	173	LEU
1	B	189	LEU

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Mol	Chain	Res	Type
1	B	230	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	B	135	ASN
1	B	233	GLN
1	B	244	ASN

### 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	125/152 (82%)	0.36	11 (8%) 12 13	19, 27, 41, 48	0
1	B	130/152 (85%)	0.26	10 (7%) 16 17	15, 24, 40, 46	0
All	All	255/304 (83%)	0.31	21 (8%) 14 15	15, 26, 41, 48	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	LYS	5.7
1	A	140	GLY	5.0
1	B	161	THR	4.3
1	B	135	ASN	3.9
1	A	160	ARG	3.3
1	B	160	ARG	2.9
1	A	141	ALA	2.8
1	B	183	LYS	2.8
1	A	198	GLY	2.7
1	B	266	PRO	2.6
1	B	156	ARG	2.5
1	B	162	ILE	2.5
1	A	183	LYS	2.4
1	A	197	GLU	2.3
1	A	174	CYS	2.3
1	B	262	ARG	2.3
1	B	171	LEU	2.2
1	A	156	ARG	2.1
1	A	161	THR	2.0
1	A	239	ILE	2.0
1	B	175	ALA	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.