



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:46 PM UTC

PDB ID : 4LDD / pdb\_00004ldd  
Title : Crystal Structure of Ebola virus VP40 Hexamer  
Authors : Bornholdt, Z.A.; Ableson, D.M.; Sapphire, E.O.  
Deposited on : 2013-06-24  
Resolution : 3.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

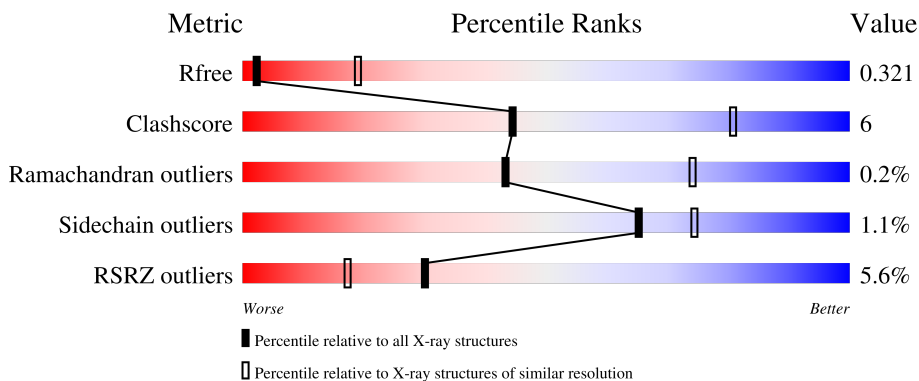
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	297	 2% 41% 5% 54%
1	B	297	 3% 60% 15% 24%
1	C	297	 4% 41% 5% 53%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3883 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 Matrix protein VP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	226	Total 1755	C 1148	N 288	O 313	S 6	0	0	0
1	C	139	Total 1072	C 697	N 178	O 194	S 3	0	0	0
1	A	137	Total 1056	C 687	N 175	O 191	S 3	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP Q05128
B	31	ALA	-	expression tag	UNP Q05128
B	32	HIS	-	expression tag	UNP Q05128
B	33	HIS	-	expression tag	UNP Q05128
B	34	HIS	-	expression tag	UNP Q05128
B	35	HIS	-	expression tag	UNP Q05128
B	36	HIS	-	expression tag	UNP Q05128
B	37	HIS	-	expression tag	UNP Q05128
B	38	VAL	-	expression tag	UNP Q05128
B	39	ASP	-	expression tag	UNP Q05128
B	40	ASP	-	expression tag	UNP Q05128
B	41	ASP	-	expression tag	UNP Q05128
B	42	ASP	-	expression tag	UNP Q05128
B	43	LYS	-	expression tag	UNP Q05128
C	30	MET	-	expression tag	UNP Q05128
C	31	ALA	-	expression tag	UNP Q05128
C	32	HIS	-	expression tag	UNP Q05128
C	33	HIS	-	expression tag	UNP Q05128
C	34	HIS	-	expression tag	UNP Q05128
C	35	HIS	-	expression tag	UNP Q05128
C	36	HIS	-	expression tag	UNP Q05128
C	37	HIS	-	expression tag	UNP Q05128
C	38	VAL	-	expression tag	UNP Q05128

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	39	ASP	-	expression tag	UNP Q05128
C	40	ASP	-	expression tag	UNP Q05128
C	41	ASP	-	expression tag	UNP Q05128
C	42	ASP	-	expression tag	UNP Q05128
C	43	LYS	-	expression tag	UNP Q05128
A	30	MET	-	expression tag	UNP Q05128
A	31	ALA	-	expression tag	UNP Q05128
A	32	HIS	-	expression tag	UNP Q05128
A	33	HIS	-	expression tag	UNP Q05128
A	34	HIS	-	expression tag	UNP Q05128
A	35	HIS	-	expression tag	UNP Q05128
A	36	HIS	-	expression tag	UNP Q05128
A	37	HIS	-	expression tag	UNP Q05128
A	38	VAL	-	expression tag	UNP Q05128
A	39	ASP	-	expression tag	UNP Q05128
A	40	ASP	-	expression tag	UNP Q05128
A	41	ASP	-	expression tag	UNP Q05128
A	42	ASP	-	expression tag	UNP Q05128
A	43	LYS	-	expression tag	UNP Q05128



P187	ALA	THR	TRP	THR	ASP	ASP	THR	THR	PRO	THR	GLY	SER	ASN	ALA	LEU	ARG	PRO	GLY	ILE	SER	PHE	HIS	PRO	LYS	LEU	ARG	PRO	ILE	LEU	PRO	ASN	LYS	SER	GLY	LYS	GLY	GLY	ASN	SER	ALA	ASP	THR	THR	PRO	GLY	LYS	LEU	GLN	LEU	GLN
------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	PHE	LYS	ILE	VAL	PRO	ILE	ASP	PRO	PRO	THR	LYS	ASN	ILE	MET	GLY	ILE	GLU	VAL	PRO	GLU	THR	LYS	LEU	THR	GLY	LYS	VAL	THR	SER	LYS	ASN	GLY	GLN	PRO	ILE	ILE	PRO	VAL	LEU	LEU	PRO	LYS	TYR	THR	SER	ILE	GLY	LEU	ASP	PRO	ILE	VAL	GLN	ALA	PRO	ILE	GLY	ASP	LEU	THR	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	ILE	THR	GLN	ASP	CYS	ASP	THR	CYS	HIS	SER	PRO	ALA	SER	LEU	PRO	ALA	VAL	ILE	GLU	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.48Å 134.48Å 136.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.88 – 3.50 44.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.88-3.50) 98.6 (44.88-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1150)	Depositor
R, $R_{free}$	0.306 , 0.323 0.310 , 0.321	Depositor DCC
$R_{free}$ test set	823 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.8	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.087 for -h,l,k 0.040 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.28	0/1084	0.79	2/1484 (0.1%)
1	B	0.30	0/1799	0.87	5/2461 (0.2%)
1	C	0.29	0/1101	0.75	0/1508
All	All	0.29	0/3984	0.82	7/5453 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LEU	CA-C-N	-7.16	112.56	120.14
1	A	168	LEU	C-N-CA	-7.16	112.56	120.14
1	B	252	ILE	N-CA-C	-5.34	107.40	111.62
1	B	210	HIS	CA-C-N	5.30	126.46	119.84
1	B	210	HIS	C-N-CA	5.30	126.46	119.84
1	B	285	ILE	CA-C-N	5.04	125.05	120.21
1	B	285	ILE	C-N-CA	5.04	125.05	120.21

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	1056	0	1069	8	0
1	B	1755	0	1826	30	0
1	C	1072	0	1088	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3883	0	3983	47	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 6.

All (47) 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:265:GLU:HB3	1:B:269:HIS:HE1	1.31	0.95
1:B:265:GLU:HB3	1:B:269:HIS:CE1	2.06	0.89
1:B:205:PRO:HB3	1:B:305:MET:HE1	1.79	0.65
1:B:265:GLU:O	1:B:269:HIS:ND1	2.30	0.63
1:B:242:THR:O	1:B:245:GLN:NE2	2.29	0.62
1:B:253:ASP:OD1	1:B:255:THR:OG1	2.18	0.56
1:C:124:HIS:HB2	1:C:174:PHE:HE2	1.73	0.54
1:B:124:HIS:HB2	1:B:174:PHE:HE2	1.74	0.53
1:A:124:HIS:HB2	1:A:174:PHE:HE2	1.73	0.53
1:C:48:SER:HB3	1:C:174:PHE:HB2	1.92	0.52
1:A:48:SER:HB3	1:A:174:PHE:HB2	1.92	0.52
1:B:48:SER:HB3	1:B:174:PHE:HB2	1.92	0.51
1:A:145:HIS:CE1	1:A:150:LEU:HD12	2.45	0.51
1:C:145:HIS:CE1	1:C:150:LEU:HD12	2.46	0.50
1:C:78:MET:HE1	1:A:187:PRO:HG2	1.94	0.49
1:B:145:HIS:CE1	1:B:150:LEU:HD12	2.47	0.49
1:B:156:ALA:O	1:B:214:ARG:NH2	2.47	0.48
1:B:210:HIS:CG	1:B:211:PRO:HD2	2.50	0.47
1:A:124:HIS:HB2	1:A:174:PHE:CE2	2.50	0.46
1:C:124:HIS:HB2	1:C:174:PHE:CE2	2.49	0.46
1:B:124:HIS:HB2	1:B:174:PHE:CE2	2.50	0.46
1:A:53:PRO:HG2	1:A:116:MET:HA	1.99	0.45
1:C:82:ILE:HG22	1:C:87:VAL:HG12	1.99	0.45
1:B:262:GLU:OE1	1:B:282:GLN:NE2	2.49	0.45
1:C:162:VAL:HG23	1:C:163:LEU:HG	1.99	0.45
1:B:53:PRO:HG2	1:B:116:MET:HA	1.99	0.44
1:B:162:VAL:HG23	1:B:163:LEU:HG	1.99	0.44
1:C:53:PRO:HG2	1:C:116:MET:HA	1.99	0.44
1:B:82:ILE:HG22	1:B:87:VAL:HG12	1.99	0.44
1:A:162:VAL:HG23	1:A:163:LEU:HG	1.99	0.44
1:B:184:GLN:HG2	1:B:258:ILE:HD12	1.99	0.43
1:B:216:ILE:HD12	1:B:216:ILE:H	1.84	0.43
1:B:282:GLN:HA	1:B:283:PRO:HD2	1.81	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:HD22	1:B:289:LEU:HB3	1.85	0.42
1:B:251:PRO:HA	1:B:259:MET:HA	2.02	0.42
1:B:207:ILE:O	1:B:216:ILE:HB	2.19	0.42
1:B:208:SER:HB2	1:B:215:PRO:HA	2.02	0.41
1:B:265:GLU:C	1:B:269:HIS:HD1	2.29	0.41
1:B:78:MET:HE1	1:B:93:PRO:HB3	2.02	0.41
1:B:287:VAL:HG13	1:B:289:LEU:HB2	2.03	0.41
1:B:89:MET:HB3	1:B:92:ILE:HD11	2.03	0.41
1:B:86:LYS:HE3	1:B:86:LYS:HB2	1.85	0.41
1:A:78:MET:HE1	1:A:93:PRO:HB3	2.03	0.41
1:B:184:GLN:HA	1:B:185:PRO:HD3	1.81	0.41
1:C:186:LEU:HA	1:C:187:PRO:HD2	1.93	0.40
1:B:106:TYR:OH	1:B:143:PRO:O	2.38	0.40
1:C:86:LYS:HE3	1:C:86:LYS:HB2	1.84	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	129/297 (43%)	127 (98%)	2 (2%)	0	100	100
1	B	214/297 (72%)	202 (94%)	11 (5%)	1 (0%)	24	57
1	C	133/297 (45%)	128 (96%)	5 (4%)	0	100	100
All	All	476/891 (53%)	457 (96%)	18 (4%)	1 (0%)	43	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	PRO

### 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	119/259 (46%)	118 (99%)	1 (1%)	73	77
1	B	202/259 (78%)	199 (98%)	3 (2%)	57	71
1	C	121/259 (47%)	120 (99%)	1 (1%)	73	77
All	All	442/777 (57%)	437 (99%)	5 (1%)	65	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	VAL
1	B	218	LEU
1	B	289	LEU
1	C	135	VAL
1	A	135	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	GLN
1	B	257	ASN
1	B	309	GLN
1	C	170	GLN
1	A	170	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](#)

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	137/297 (46%)	0.41	6 (4%) 39 21	19, 56, 106, 123	0
1	B	226/297 (76%)	0.35	10 (4%) 39 21	20, 77, 121, 140	0
1	C	139/297 (46%)	0.71	12 (8%) 16 11	18, 56, 111, 120	0
All	All	502/891 (56%)	0.47	28 (5%) 30 17	18, 62, 116, 140	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	PHE	7.2
1	C	83	SER	5.4
1	A	173	THR	4.1
1	C	144	ASP	3.8
1	A	126	GLY	3.7
1	C	46	THR	3.2
1	B	83	SER	3.1
1	B	269	HIS	3.0
1	C	89	MET	2.8
1	C	169	PRO	2.7
1	B	212	LYS	2.7
1	B	291	LYS	2.7
1	C	87	VAL	2.7
1	B	290	PRO	2.6
1	A	172	PHE	2.5
1	B	265	GLU	2.5
1	C	171	TYR	2.4
1	C	154	ASN	2.4
1	B	244	LEU	2.3
1	B	293	ILE	2.2
1	C	187	PRO	2.2
1	A	69	VAL	2.1
1	C	81	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	2.1
1	C	84	GLY	2.1
1	A	175	ASP	2.1
1	B	283	PRO	2.1
1	C	86	LYS	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 oligosaccharides 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.