



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4LDD / pdb_00004ldd
Title : Crystal Structure of Ebola virus VP40 Hexamer
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Deposited on : 2013-06-24
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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
Xtriage (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

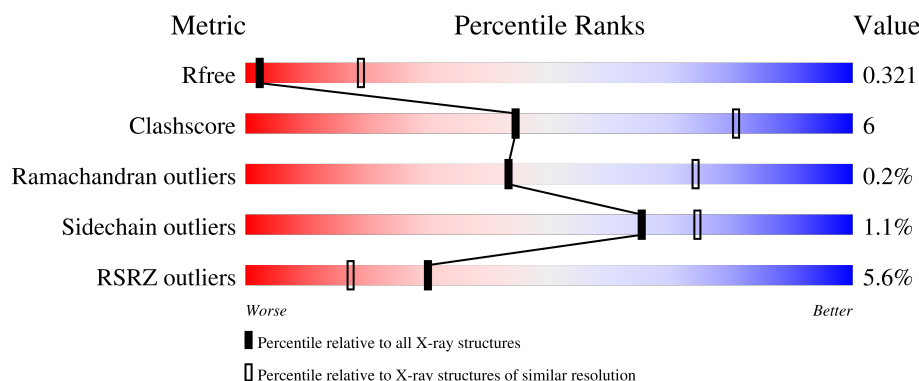
1 Overall quality at a glance

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 ≥ 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	
1	B	297	
1	C	297	

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
1	B	226	Total	C	N	O	S	0	0	0
			1755	1148	288	313	6			
1	C	139	Total	C	N	O	S	0	0	0
			1072	697	178	194	3			
1	A	137	Total	C	N	O	S	0	0	0
			1056	687	175	191	3			

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

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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	A193
ASP	ALA	THR
PHE	THR	THR
LYS	TRP	ASP
ILE	THR	THR
VAL	ASP	THR
ASP	PRO	PRO
PRO	LYS	THR
ILE	ASN	THR
ASP	ILE	GLY
THR	MET	SER
CYS	GLY	ASN
ASP	ILE	GLY
THR	GLU	ALA
CYS	VAL	LEU
HIS	PRO	ARG
SER	GLU	PRO
PRO	THR	GLY
ALA	VAL	ILE
SER	HIS	SER
LEU	LYS	PHE
PRO	LEU	HIS
ALA	THR	PRO
ILE	GLY	LYS
GLU	LYS	LEU
LYS	VAL	ARG
	THR	PRO
	SER	ILE
	LYS	LEU
	ASN	ASN
	GLY	LYS
	PRO	SER
	ILE	GLY
	ILE	LYS
	PRO	GLY
	VAL	ASN
	LEU	SER
	LEU	ALA
	PRO	ASP
	LYS	LEU
	TYR	THR
	ILE	SER
	GLY	PRO
	LEU	GLU
	ASP	LYS
	VAL	ILE
	ALA	GLN
	PRO	ILE
	GLY	MET
	ASP	THR
	LEU	SER
	THR	LEU
	MET	GLN

VAL	ASP
ILE	PHE
THR	LYS
GLN	ILE
ASP	VAL
CYS	PRO
ASP	ILE
THR	ASP
CYS	PRO
HIS	THR
SER	LYS
PRO	ASN
ALA	ILE
SER	MET
LEU	GLY
PRO	ILE
ALA	GLU
VAL	VAL
ILE	PRO
GLU	GLU
LYS	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.48Å)	Xtriage
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 ²)	126.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.087 for -h,l,k 0.040 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3883	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.28	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.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
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

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

The worst 5 of 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	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

The worst 5 of 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

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.