

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 06:30 AM EDT

PDB ID : 7JZJ

Title : Crystal structure demonstrating CTD-CTD interactions of Zaire Ebola virus

VP40 dimer

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Deposited on : 2020-09-02

Resolution : 2.46 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

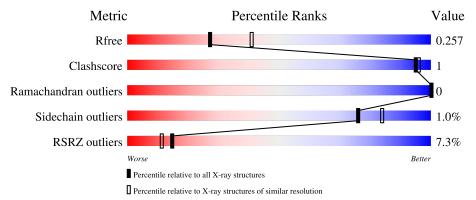
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.46 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	80%	16%
1	В	297	87%	• 10%
1	С	297	78%	19%
1	D	297	8%	17%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14511 atoms, of which 7064 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	A	249	Total	С	Н	N	О	S	0	0	0
1	A	249	3611	1180	1777	308	339	7	0	0	
1	В	267	Total	С	Н	N	О	S	0	0	0
1	Б	207	3943	1275	1961	329	370	8	0	U	U
1	С	240	Total	С	Н	N	О	S	0	0	0
1		240	3300	1098	1587	292	316	7	0	U	0
1	D	246	Total	С	Н	N	О	S	0	0	0
1	D	240	3540	1162	1739	301	330	8	U	U	U

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	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
В	30	MET	-	initiating methionine	UNP Q05128
В	31	ALA	-	expression tag	UNP Q05128
В	32	HIS	-	expression tag	UNP Q05128
В	33	HIS	-	expression tag	UNP Q05128
В	34	HIS	-	expression tag	UNP Q05128
В	35	HIS	-	expression tag	UNP Q05128
В	36	HIS	-	expression tag	UNP Q05128
В	37	HIS	-	expression tag	UNP Q05128

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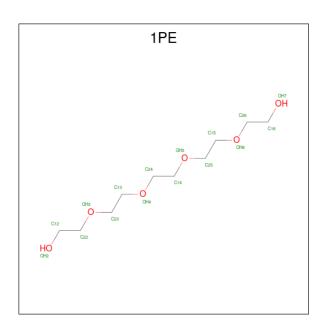


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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
В	38	VAL	-	expression tag	UNP Q05128
В	39	ASP	-	expression tag	UNP Q05128
В	40	ASP	-	expression tag	UNP Q05128
В	41	ASP	-	expression tag	UNP Q05128
В	42	ASP	-	expression tag	UNP Q05128
С	30	MET	-	initiating methionine	UNP Q05128
С	31	ALA	-	expression tag	UNP Q05128
С	32	HIS	-	expression tag	UNP Q05128
С	33	HIS	-	expression tag	UNP Q05128
С	34	HIS	-	expression tag	UNP Q05128
С	35	HIS	-	expression tag	UNP Q05128
С	36	HIS	-	expression tag	UNP Q05128
С	37	HIS	-	expression tag	UNP Q05128
С	38	VAL	-	expression tag	UNP Q05128
С	39	ASP	-	expression tag	UNP Q05128
С	40	ASP	-	expression tag	UNP Q05128
С	41	ASP	-	expression tag	UNP Q05128
С	42	ASP	-	expression tag	UNP Q05128
D	30	MET	-	initiating methionine	UNP Q05128
D	31	ALA	-	expression tag	UNP Q05128
D	32	HIS	-	expression tag	UNP Q05128
D	33	HIS	-	expression tag	UNP Q05128
D	34	HIS	-	expression tag	UNP Q05128
D	35	HIS	-	expression tag	UNP Q05128
D	36	HIS	-	expression tag	UNP Q05128
D	37	HIS	-	expression tag	UNP Q05128
D	38	VAL	-	expression tag	UNP Q05128
D	39	ASP	-	expression tag	UNP Q05128
D	40	ASP	-	expression tag	UNP Q05128
D	41	ASP	-	expression tag	UNP Q05128
D	42	ASP	-	expression tag	UNP Q05128

 \bullet Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\mathrm{C_{10}H_{22}O_6}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Δ	1	Total C O	0	0
	71	1	16 10 6	0	0
2	B	1	Total C O	0	0
2	Ъ	1	16 10 6		0
9	D	1	Total C O	0	0
	ע	1	16 10 6		U

• Molecule 3 is water.

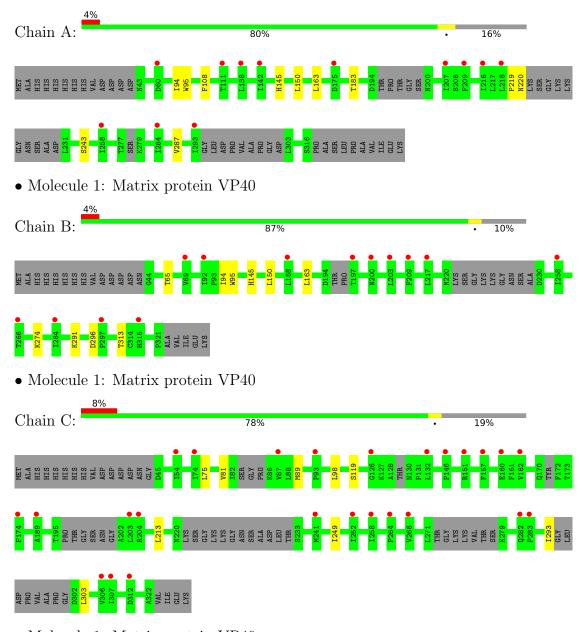
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	В	21	Total O 21 21	0	0
3	С	17	Total O 17 17	0	0
3	D	16	Total O 16 16	0	0



3 Residue-property plots (i)

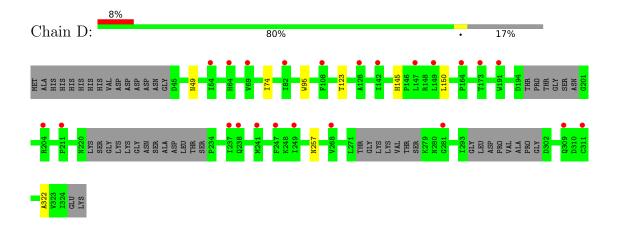
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Matrix protein VP40







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants	159.94Å 159.94Å 89.76Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.17 - 2.46	Depositor
Resolution (A)	79.97 - 2.46	EDS
% Data completeness	91.7 (46.17-2.46)	Depositor
(in resolution range)	91.9 (79.97-2.46)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.59 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
D D	0.249 , 0.258	Depositor
R, R_{free}	0.248 , 0.257	DCC
R_{free} test set	2191 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 77.2	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14511	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE

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	
IVIOI	Chain	RMSZ $ \# Z > 5$		RMSZ	# Z > 5
1	A	0.63	0/1880	0.88	0/2582
1	В	0.62	0/2034	0.89	0/2796
1	С	0.66	0/1755	0.89	0/2414
1	D	0.61	0/1847	0.85	0/2541
All	All	0.63	0/7516	0.88	0/10333

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 (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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1834	1777	1777	5	0
1	В	1982	1961	1961	5	5
1	С	1713	1587	1589	4	0
1	D	1801	1739	1746	4	5
2	A	16	0	22	1	0
2	В	16	0	22	2	0
2	D	16	0	22	2	0
3	A	15	0	0	0	0
3	В	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	17	0	0	0	0
3	D	16	0	0	0	0
All	All	7447	7064	7139	18	5

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 1.

The worst 5 of 18 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:95:TRP:CZ3	2:B:401:1PE:H261	2.39	0.58
1:C:249:ILE:HD11	1:C:303:LEU:HD21	1.85	0.57
1:B:291:LYS:HG3	2:B:401:1PE:H142	1.89	0.55
1:D:257:ASN:HB2	2:D:401:1PE:H131	1.90	0.54
1:A:94:ILE:HD12	1:A:163:LEU:CD2	2.39	0.53

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:274:LYS:NZ	1:D:322:ALA:O[5_554]	1.38	0.82
1:B:274:LYS:CE	1:D:322:ALA:O[5_554]	1.72	0.48
1:B:274:LYS:HZ1	1:D:322:ALA:O[5_554]	1.23	0.37
1:B:274:LYS:HE3	1:D:322:ALA:O[5_554]	1.47	0.13
1:B:274:LYS:HZ2	1:D:322:ALA:O[5_554]	1.48	0.12

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	Perce	\mathbf{ntiles}
1	A	239/297 (80%)	237 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	В	261/297 (88%)	258 (99%)	3 (1%)	0	100	100
1	С	224/297 (75%)	219 (98%)	5 (2%)	0	100	100
1	D	$236/297 \ (80\%)$	235 (100%)	1 (0%)	0	100	100
All	All	960/1188 (81%)	949 (99%)	11 (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	Perce	ntiles
1	A	195/259~(75%)	193 (99%)	2 (1%)	76	84
1	В	218/259 (84%)	215 (99%)	3 (1%)	67	77
1	\mathbf{C}	171/259~(66%)	170 (99%)	1 (1%)	86	91
1	D	191/259 (74%)	189 (99%)	2 (1%)	76	84
All	All	775/1036 (75%)	767 (99%)	8 (1%)	76	84

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	123	THR
1	D	49	ASN
1	В	313	THR
1	В	296	ASP
1	С	119	SER

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

Mol	Chain	Res	Type
1	С	124	HIS



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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Во	nd leng	$ ag{ths}$	В	ond ang	les
WIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1PE	D	401	-	15,15,15	0.40	0	14,14,14	0.35	0
2	1PE	A	401	-	15,15,15	0.55	0	14,14,14	0.25	0
2	1PE	В	401	-	15,15,15	0.37	0	14,14,14	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
2	1PE	D	401	-	-	5/13/13/13	-
2	1PE	A	401	-	-	5/13/13/13	-
2	1PE	В	401	-	-	8/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	401	1PE	C13-C23-OH3-C22
2	D	401	1PE	C14-C24-OH4-C13
2	A	401	1PE	OH5-C14-C24-OH4
2	A	401	1PE	ОН7-С16-С26-ОН6
2	В	401	1PE	OH5-C14-C24-OH4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	1PE	2	0
2	A	401	1PE	1	0
2	В	401	1PE	2	0

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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	249/297 (83%)	0.68	12 (4%) 30 28	59, 90, 130, 156	0
1	В	267/297 (89%)	0.67	13 (4%) 29 27	51, 77, 130, 154	0
1	С	240/297 (80%)	0.72	25 (10%) 6 4	60, 92, 150, 172	0
1	D	246/297 (82%)	0.75	23 (9%) 8 5	61, 90, 147, 179	0
All	All	1002/1188 (84%)	0.70	73 (7%) 15 11	51, 88, 140, 179	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	TRP	4.2
1	В	200	ASN	4.0
1	С	151	ARG	3.9
1	D	238	GLN	3.6
1	С	132	LEU	3.5

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q<0.9
2	1PE	A	401	16/16	0.77	0.20	102,103,105,105	0
2	1PE	D	401	16/16	0.84	0.23	114,117,119,119	0
2	1PE	В	401	16/16	0.96	0.15	67,71,73,74	16

6.5 Other polymers (i)

There are no such residues in this entry.

