



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 10:02 AM EST

PDB ID : 5VKD  
Title : Crystal structure of C-terminal domain of Ebola (Bundibugyo) nucleoprotein in complex with Fab fragment  
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Deposited on : 2017-04-21  
Resolution : 1.75 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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

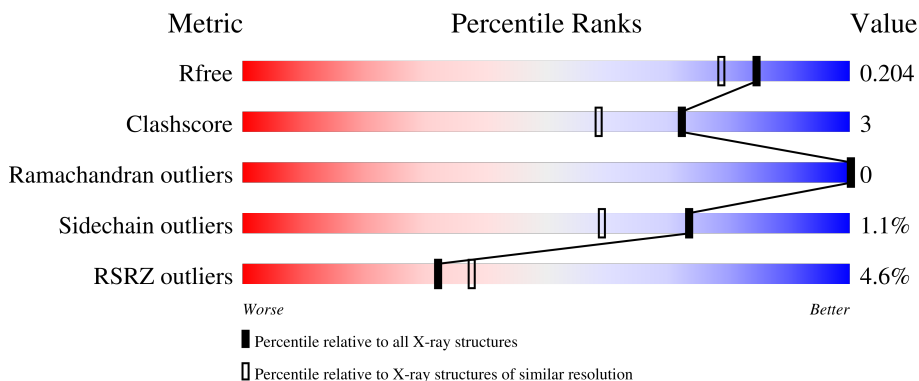
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

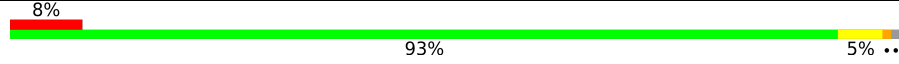
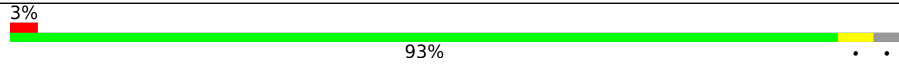
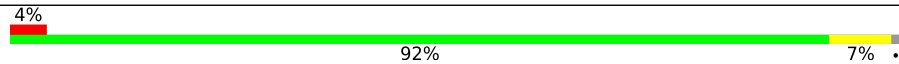
The reported resolution of this entry is 1.75 Å.

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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	103	
2	H	236	
3	L	215	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8848 atoms, of which 4056 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 Nucleoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	102	1646	548	785	141	164	8	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	637	GLY	-	expression tag	UNP R4QJ68
A	638	ALA	-	expression tag	UNP R4QJ68
A	639	MET	-	expression tag	UNP R4QJ68
A	640	ALA	-	expression tag	UNP R4QJ68

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	229	3400	1097	1670	285	342	6	0	2	0

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	213	3235	1019	1601	274	333	8	0	3	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	H	252	Total	O	0	0
			252	252		
4	L	218	Total	O	0	0
			218	218		

### 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.

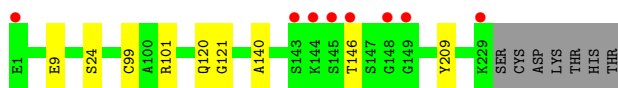
- Molecule 1: Nucleoprotein

Chain A: 

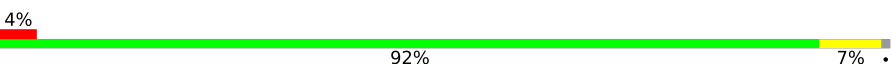


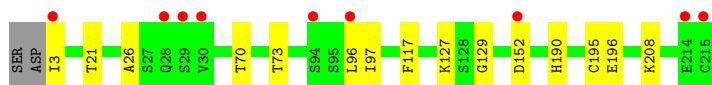
- Molecule 2: Fab Heavy Chain

Chain H: 



- Molecule 3: Fab light chain

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.41Å 87.48Å 130.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.47 – 1.75 42.88 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.47-1.75) 99.8 (42.88-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.176 , 0.202 0.177 , 0.204	Depositor DCC
$R_{free}$ test set	1065 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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	0.26	0/890	0.44	0/1203
2	H	0.28	0/1783	0.49	0/2433
3	L	0.28	0/1678	0.49	0/2277
All	All	0.28	0/4351	0.48	0/5913

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)	H(added)	Clashes	Symm-Clashes
1	A	861	785	799	8	0
2	H	1730	1670	1670	11	0
3	L	1634	1601	1607	13	0
4	A	97	0	0	4	2
4	H	252	0	0	3	0
4	L	218	0	0	4	2
All	All	4792	4056	4076	28	2

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 3.

All (28) 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:638:ALA:N	4:A:801:HOH:O	2.05	0.89
3:L:152:ASP:OD2	3:L:190:HIS:ND1	2.07	0.88
1:A:739:ARG:CZ	1:A:739:ARG:HA	2.09	0.82
3:L:196:GLU:OE1	4:L:301:HOH:O	2.01	0.78
1:A:711:ARG:NH2	4:A:802:HOH:O	2.19	0.75
1:A:739:ARG:HA	1:A:739:ARG:NE	2.00	0.75
1:A:711:ARG:CZ	4:A:802:HOH:O	2.39	0.71
2:H:140:ALA:O	4:H:301:HOH:O	2.11	0.69
2:H:120:GLN:OE1	4:H:302:HOH:O	2.12	0.67
1:A:695:GLU:OE2	1:A:711:ARG:NH1	2.29	0.62
2:H:209:TYR:OH	4:H:303:HOH:O	2.16	0.60
2:H:146:THR:HG23	3:L:117:PHE:CD2	2.39	0.57
3:L:26:ALA:O	3:L:70:THR:OG1	2.30	0.50
2:H:146:THR:CG2	3:L:117:PHE:CE2	2.95	0.49
1:A:638:ALA:CA	4:A:801:HOH:O	2.62	0.44
3:L:3:ILE:HG21	3:L:96:LEU:HD22	1.99	0.44
1:A:739:ARG:NE	1:A:739:ARG:CA	2.76	0.43
2:H:146:THR:HG23	3:L:117:PHE:CE2	2.54	0.42
3:L:127:LYS:NZ	4:L:311:HOH:O	2.52	0.42
2:H:9[B]:GLU:OE2	2:H:99:CYS:N	2.53	0.42
2:H:9[B]:GLU:OE1	2:H:121:GLY:HA2	2.20	0.42
3:L:21:THR:HG23	3:L:73[A]:THR:HG23	2.02	0.42
3:L:129:GLY:O	4:L:302:HOH:O	2.21	0.42
3:L:96:LEU:HD23	3:L:97:ILE:N	2.36	0.41
3:L:208:LYS:NZ	4:L:304:HOH:O	2.35	0.41
2:H:9[B]:GLU:HA	2:H:24:SER:O	2.21	0.41
2:H:146:THR:HG23	3:L:117:PHE:HD2	1.81	0.41
2:H:9[A]:GLU:HA	2:H:24:SER:O	2.21	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
4:A:869:HOH:O	4:L:490:HOH:O[3_745]	2.05	0.15
4:A:802:HOH:O	4:L:376:HOH:O[3_745]	2.18	0.02

## 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	101/103 (98%)	101 (100%)	0	0	100	100
2	H	229/236 (97%)	224 (98%)	5 (2%)	0	100	100
3	L	215/215 (100%)	206 (96%)	9 (4%)	0	100	100
All	All	545/554 (98%)	531 (97%)	14 (3%)	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	93/92 (101%)	90 (97%)	3 (3%)	39	15
2	H	192/198 (97%)	191 (100%)	1 (0%)	88	83
3	L	192/190 (101%)	189 (98%)	3 (2%)	62	44
All	All	477/480 (99%)	470 (98%)	7 (2%)	73	47

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	ASP
1	A	727	HIS
1	A	739	ARG
2	H	101	ARG
3	L	195[A]	CYS

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Mol	Chain	Res	Type
3	L	195[B]	CYS
3	L	195[C]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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	102/103 (99%)	0.05	8 (7%) 13 17	22, 32, 69, 90	0
2	H	229/236 (97%)	-0.12	8 (3%) 44 49	20, 28, 61, 111	0
3	L	213/215 (99%)	-0.04	9 (4%) 36 41	20, 32, 61, 96	0
All	All	544/554 (98%)	-0.06	25 (4%) 32 38	20, 30, 66, 111	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	30	VAL	10.7
3	L	215	CYS	7.5
2	H	146	THR	6.8
3	L	3	ILE	6.3
2	H	145	SER	6.1
1	A	739	ARG	5.7
2	H	144	LYS	5.5
3	L	96	LEU	3.5
1	A	639	MET	3.3
1	A	640	ALA	3.3
1	A	642	ALA	3.3
1	A	643	GLN	3.1
3	L	94	SER	3.1
2	H	229	LYS	3.0
1	A	638	ALA	3.0
3	L	28	GLN	2.9
2	H	1	GLU	2.8
3	L	29	SER	2.6
2	H	148	GLY	2.6
2	H	149	GLY	2.5
1	A	645	GLU	2.4
3	L	152	ASP	2.3
3	L	214	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	143	SER	2.2
1	A	644	SER	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.