



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:05 AM GMT

PDB ID : 3KS8  
Title : Crystal structure of Reston ebolavirus VP35 RNA binding domain in complex with 18bp dsRNA  
Authors : Kimberlin, C.R.; Bornholdt, Z.A.; Li, S.; Woods, V.L.; Macrae, I.J.; Saphire, E.O.  
Deposited on : 2009-11-20  
Resolution : 2.40 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](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

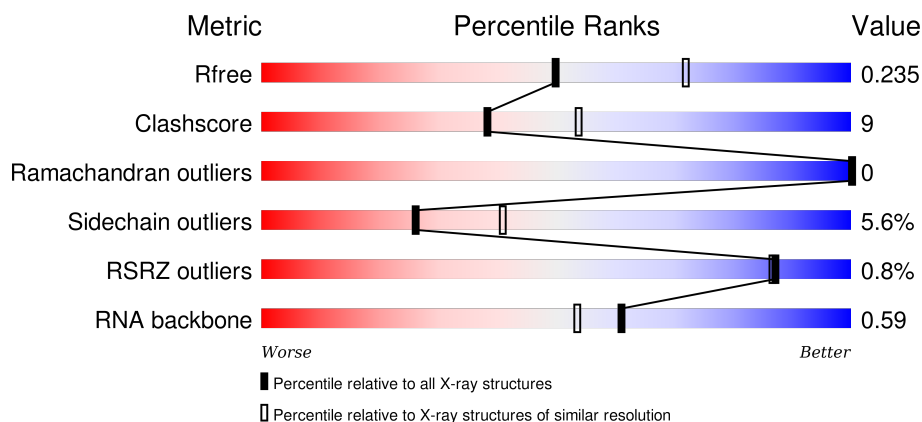
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)
RNA backbone	2183	1073 (2.90-1.90)

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	E	18	<div> <div></div> <div>50%22%22%6%</div> </div>
2	F	18	<div> <div></div> <div>61%33%6%</div> </div>
3	A	184	<div> <div>%</div> <div>56%9%•34%</div> </div>
3	B	184	<div> <div></div> <div>52%14%•33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	184	<div><div></div><div>55%</div><div>10%</div><div>34%</div></div>
3	D	184	<div><div>2%</div><div></div><div>53%</div><div>13%</div><div>33%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4757 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 RNA chain called 5'-R(\*AP\*GP\*AP\*AP\*GP\*GP\*AP\*GP\*GP\*GP\*AP\*GP\*GP\*GP\*AP\*GP\*GP\*GP\*AP\*GP\*GP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			404	180	90	117	17			

- Molecule 2 is a RNA chain called 5'-R(\*UP\*CP\*CP\*UP\*CP\*CP\*CP\*UP\*CP\*CP\*CP\*UP\*CP\*CP\*UP\*UP\*CP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	18	Total	C	N	O	P	0	0	0
			357	162	47	131	17			

- Molecule 3 is a protein called Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	122	Total	C	N	O	S	29	0	0
			952	609	169	168	6			
3	B	124	Total	C	N	O	S	30	0	0
			971	623	171	171	6			
3	C	122	Total	C	N	O	S	28	0	0
			952	609	169	168	6			
3	D	124	Total	C	N	O	S	29	0	0
			971	623	171	171	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	EXPRESSION TAG	UNP Q8JPY0
A	147	ALA	-	EXPRESSION TAG	UNP Q8JPY0
A	148	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	149	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	150	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	151	HIS	-	EXPRESSION TAG	UNP Q8JPY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	152	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	153	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	154	VAL	-	EXPRESSION TAG	UNP Q8JPY0
A	155	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	156	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	157	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	158	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	159	LYS	-	EXPRESSION TAG	UNP Q8JPY0
B	146	MET	-	EXPRESSION TAG	UNP Q8JPY0
B	147	ALA	-	EXPRESSION TAG	UNP Q8JPY0
B	148	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	149	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	150	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	151	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	152	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	153	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	154	VAL	-	EXPRESSION TAG	UNP Q8JPY0
B	155	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	156	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	157	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	158	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	159	LYS	-	EXPRESSION TAG	UNP Q8JPY0
C	146	MET	-	EXPRESSION TAG	UNP Q8JPY0
C	147	ALA	-	EXPRESSION TAG	UNP Q8JPY0
C	148	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	149	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	150	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	151	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	152	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	153	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	154	VAL	-	EXPRESSION TAG	UNP Q8JPY0
C	155	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	156	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	157	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	158	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	159	LYS	-	EXPRESSION TAG	UNP Q8JPY0
D	146	MET	-	EXPRESSION TAG	UNP Q8JPY0
D	147	ALA	-	EXPRESSION TAG	UNP Q8JPY0
D	148	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	149	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	150	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	151	HIS	-	EXPRESSION TAG	UNP Q8JPY0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	152	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	153	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	154	VAL	-	EXPRESSION TAG	UNP Q8JPY0
D	155	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	156	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	157	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	158	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	159	LYS	-	EXPRESSION TAG	UNP Q8JPY0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	30	Total O 30 30	0	0
4	C	33	Total O 33 33	0	0
4	D	35	Total O 35 35	0	0
4	E	13	Total O 13 13	0	0
4	F	7	Total O 7 7	0	0



MET	ALA	HIS	HIS	HIS	HIS	HIS	VAL	ASP	ASP	ASP	ASP	LYS	PRO	GLY	PRO	ALA	LEU	TYR	GLU	GLU	ASN	ALA	LEU	LYS	GLY	LYS	ILE	ASP	PRO	ASN	SER	TYR	VAL	PRO	ASP	ALA	VAL	GLN	GLU	ALA	TYR	LYS	ASN	LEU	ASP	SER	THR	SER	THR	THR	THR	GLU	GLU	ASN	PHE	GLY	LYS
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● Molecule 3: Polymerase cofactor VP35



MET	ALA	HIS	HIS	HIS	HIS	HIS	VAL	ASP	ASP	ASP	ASP	LYS	PRO	GLY	PRO	ALA	LEU	TYR	GLU	GLU	ASN	ALA	LEU	LYS	GLY	LYS	ILE	ASP	PRO	ASN	SER	TYR	VAL	PRO	ASP	ALA	VAL	GLN	GLU	ALA	TYR	LYS	ASN	LEU	ASP	SER	THR	SER	THR	THR	THR	GLU	GLU	ASN	PHE	GLY	LYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.69Å 85.69Å 108.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.12 – 2.40 37.10 – 2.29	Depositor EDS
% Data completeness (in resolution range)	84.9 (35.12-2.40) 75.0 (37.10-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.27 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_222)	Depositor
R, $R_{free}$	0.198 , 0.239 0.193 , 0.235	Depositor DCC
$R_{free}$ test set	1498 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.0	EDS
Estimated twinning fraction	0.020 for -h,-k,l 0.467 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30271 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	E	0.89	0/457	1.66	6/716 (0.8%)
2	F	0.77	0/392	1.60	1/604 (0.2%)
3	A	0.38	0/974	0.52	0/1317
3	B	0.36	0/995	0.53	0/1346
3	C	0.38	0/974	0.54	0/1317
3	D	0.36	0/995	0.53	0/1346
All	All	0.49	0/4787	0.87	7/6646 (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(°)	Ideal(°)
2	F	14	C	C4'-C3'-C2'	-6.59	96.01	102.60
1	E	16	G	N3-C4-N9	-5.54	122.67	126.00
1	E	9	G	C4'-C3'-C2'	-5.32	97.28	102.60
1	E	13	G	N3-C4-N9	-5.32	122.81	126.00
1	E	12	G	C4'-C3'-C2'	-5.13	97.47	102.60

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	E	404	0	200	6	0
2	F	357	0	193	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	952	0	984	13	1
3	B	971	0	1001	23	0
3	C	952	0	984	11	1
3	D	971	0	1001	22	0
4	A	32	0	0	0	0
4	B	30	0	0	1	0
4	C	33	0	0	0	0
4	D	35	0	0	0	0
4	E	13	0	0	3	0
4	F	7	0	0	0	0
All	All	4757	0	4363	77	1

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.

The worst 5 of 77 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)
3:B:268:GLN:HA	3:B:268:GLN:HE21	1.46	0.79
3:D:268:GLN:HA	3:D:268:GLN:HE21	1.50	0.75
1:E:12:G:N7	4:E:44:HOH:O	2.22	0.73
3:A:287:ARG:CG	3:A:287:ARG:HH11	2.01	0.73
3:C:311:ARG:O	3:C:328:LYS:HE3	1.94	0.68

All (1) 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)
3:A:278:ASP:OD2	3:C:278:ASP:OD2[3_454]	1.84	0.36

## 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	
3	A	120/184 (65%)	117 (98%)	3 (2%)	0	100	100
3	B	122/184 (66%)	117 (96%)	5 (4%)	0	100	100
3	C	120/184 (65%)	117 (98%)	3 (2%)	0	100	100
3	D	122/184 (66%)	116 (95%)	6 (5%)	0	100	100
All	All	484/736 (66%)	467 (96%)	17 (4%)	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	
3	A	106/160 (66%)	101 (95%)	5 (5%)	32	50
3	B	108/160 (68%)	100 (93%)	8 (7%)	17	26
3	C	106/160 (66%)	102 (96%)	4 (4%)	40	60
3	D	108/160 (68%)	101 (94%)	7 (6%)	21	33
All	All	428/640 (67%)	404 (94%)	24 (6%)	26	41

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	283	ILE
3	C	255	SER
3	D	301	ARG
3	B	301	ARG
3	B	311	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	285	HIS
3	D	285	HIS
3	D	263	GLN

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Mol	Chain	Res	Type
3	B	268	GLN
3	C	253	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	17/18 (94%)	4 (23%)	1 (5%)
2	F	17/18 (94%)	3 (17%)	0
All	All	34/36 (94%)	7 (20%)	1 (2%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	9	G
1	E	13	G
1	E	14	G
1	E	15	A
2	F	9	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	9	G

## 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	E	18/18 (100%)	-0.83	0 100 100	30, 50, 77, 80	0
2	F	18/18 (100%)	-0.72	0 100 100	27, 51, 86, 88	0
3	A	122/184 (66%)	-0.55	1 (0%) 87 87	21, 35, 67, 92	7 (5%)
3	B	124/184 (67%)	-0.42	0 100 100	21, 38, 61, 97	7 (5%)
3	C	122/184 (66%)	-0.55	0 100 100	21, 35, 67, 82	7 (5%)
3	D	124/184 (67%)	-0.30	3 (2%) 62 61	21, 38, 62, 106	7 (5%)
All	All	528/772 (68%)	-0.48	4 (0%) 87 87	21, 38, 68, 106	28 (5%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	322	GLY	2.2
3	D	207	TYR	2.2
3	D	206	PRO	2.1
3	D	212	ASP	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.