



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1NO7  
Title : Structure of the Large Protease Resistant Upper Domain of VP5, the Major Capsid Protein of Herpes Simplex Virus-1  
Authors : Bowman, B.R.; Baker, M.L.; Rixon, F.J.; Chiu, W.; Quijcho, F.A.  
Deposited on : 2003-01-15  
Resolution : 2.90 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

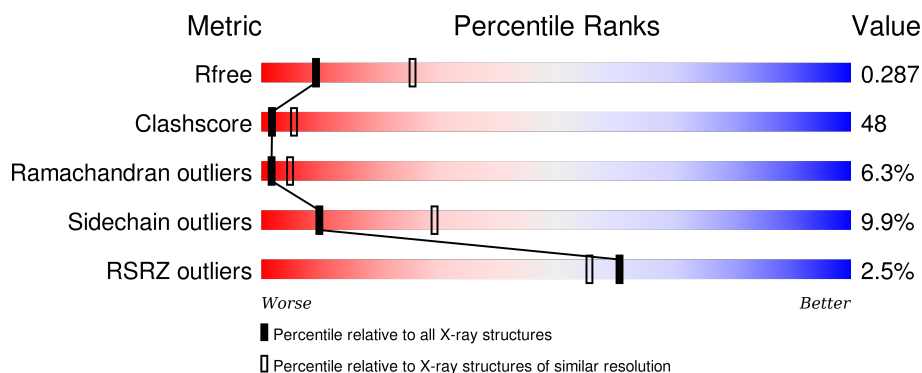
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	A	604	
1	B	604	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8179 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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4121	2609	747	740	25			
1	B	534	Total	C	N	O	S	0	0	0
			4058	2573	734	726	25			





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.07Å 99.07Å 454.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.90 48.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (47.09-2.90) 91.4 (48.40-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.289 0.253 , 0.287	Depositor DCC
$R_{free}$ test set	4746 reflections (10.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 64.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	2 of 51090 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

### 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	0.65	4/4235 (0.1%)	1.00	16/5798 (0.3%)
1	B	0.59	2/4169 (0.0%)	0.98	12/5704 (0.2%)
All	All	0.62	6/8404 (0.1%)	0.99	28/11502 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	1	1
All	All	2	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	GLY	C-N	-16.74	0.95	1.34
1	A	800	HIS	CB-CG	-15.89	1.21	1.50
1	B	800	HIS	CB-CG	-15.58	1.22	1.50
1	B	801	ARG	CB-CG	-11.61	1.21	1.52
1	A	555	ASP	C-N	-9.62	1.11	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	677	TYR	CB-CG-CD2	-29.83	103.10	121.00
1	B	677	TYR	CB-CG-CD1	29.36	138.61	121.00
1	A	677	TYR	CB-CG-CD2	-29.19	103.49	121.00
1	A	677	TYR	CB-CG-CD1	28.97	138.38	121.00
1	A	800	HIS	CA-CB-CG	14.48	138.21	113.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	554	ALA	CA
1	B	554	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	552	GLY	Mainchain
1	A	801	ARG	Mainchain
1	B	801	ARG	Mainchain

## 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	4121	0	3986	400	0
1	B	4058	0	3932	381	0
All	All	8179	0	7918	774	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 48.

The worst 5 of 774 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:618:PHE:HA	1:A:940:MET:HE3	1.13	1.10
1:B:926:MET:HE2	1:B:926:MET:HA	1.24	1.08
1:A:610:THR:HG22	1:A:689:VAL:HA	1.37	1.07
1:B:618:PHE:HA	1:B:940:MET:HE3	1.09	1.05
1:A:949:ILE:HD12	1:A:949:ILE:H	1.20	1.03

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	536/604 (89%)	379 (71%)	122 (23%)	35 (6%)	1	4
1	B	524/604 (87%)	367 (70%)	125 (24%)	32 (6%)	2	5
All	All	1060/1208 (88%)	746 (70%)	247 (23%)	67 (6%)	2	5

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	HIS
1	A	660	ARG
1	A	837	ALA
1	B	660	ARG
1	B	837	ALA

### 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	416/467 (89%)	372 (89%)	44 (11%)	8	25
1	B	409/467 (88%)	371 (91%)	38 (9%)	11	32
All	All	825/934 (88%)	743 (90%)	82 (10%)	10	29

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	937	ILE

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Mol	Chain	Res	Type
1	B	500	ASP
1	B	926	MET
1	A	949	ILE
1	A	1003	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	986	GLN
1	B	485	ASN
1	B	997	ASN
1	A	1018	ASN
1	B	503	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 carbohydrates 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, 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	542/604 (89%)	-0.23	17 (3%)	52 45	8, 54, 122, 193	0
1	B	534/604 (88%)	-0.21	10 (1%)	70 66	13, 58, 124, 166	0
All	All	1076/1208 (89%)	-0.22	27 (2%)	61 55	8, 55, 124, 193	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	714	LEU	7.6
1	A	715	GLY	5.8
1	B	565	PRO	5.5
1	B	714	LEU	5.0
1	A	716	GLY	4.5

### 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 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.