



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:10 pm BST

PDB ID : 3INO  
Title : 1.95A Resolution Structure of Protective Antigen Domain 4  
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Deposited on : 2009-08-12  
Resolution : 1.95 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.

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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	:	2.11
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)	:	2.11

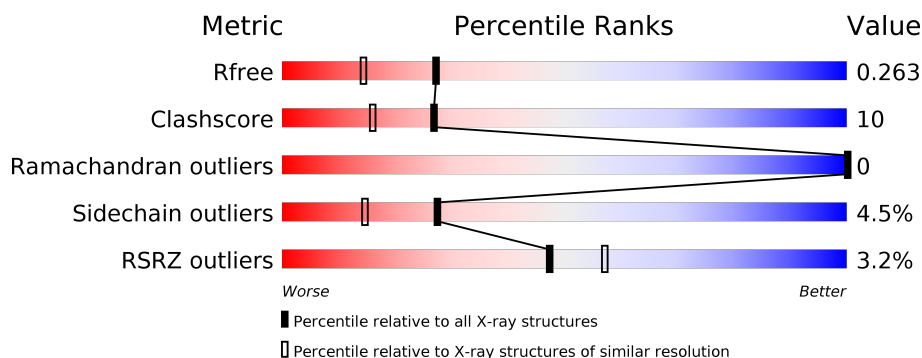
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	143	 83% 15% •
1	B	143	 6% 76% 16% • 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2358 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 Protective antigen PA-63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	7	0
			1166	740	195	229	2			
1	B	134	Total	C	N	O	S	0	2	0
			1081	685	183	211	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	593	GLY	-	EXPRESSION TAG	UNP P13423
A	594	SER	-	EXPRESSION TAG	UNP P13423
B	593	GLY	-	EXPRESSION TAG	UNP P13423
B	594	SER	-	EXPRESSION TAG	UNP P13423


- Molecule 2 is water.

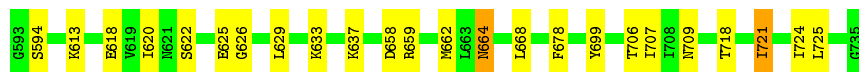
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	39	Total	O	0	0
			39	39		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

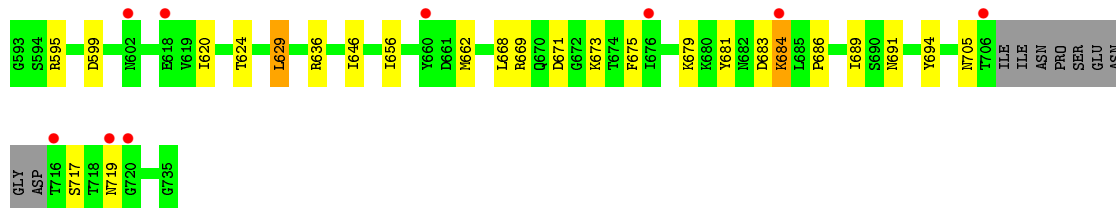
- Molecule 1: Protective antigen PA-63

Chain A:  83% 15% .



- Molecule 1: Protective antigen PA-63

Chain B:  6% 76% 16% . 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.73Å 35.85Å 129.09Å 90.00° 99.29° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 18.95 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.00-1.95) 97.8 (18.95-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 1.94Å)	Xtriage
Refinement program	REFMAC refmac _5.5.0066	Depositor
R, $R_{free}$	0.199 , 0.258 0.206 , 0.263	Depositor DCC
$R_{free}$ test set	1050 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.040 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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	1.02	0/1203	1.02	0/1619
1	B	0.93	0/1101	0.96	2/1479 (0.1%)
All	All	0.98	0/2304	0.99	2/3098 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	629	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	599	ASP	CB-CG-OD2	-5.20	113.62	118.30

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	1166	0	1191	30	0
1	B	1081	0	1095	23	1
2	A	72	0	0	1	0
2	B	39	0	0	1	1
All	All	2358	0	2286	46	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 10.

All (46) 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:709:ASN:ND2	1:B:669:ARG:NH1	2.11	0.98
1:A:633:LYS:O	1:A:637[A]:LYS:HG3	1.64	0.95
1:A:709:ASN:ND2	1:B:669:ARG:HH11	1.70	0.87
1:B:671:ASP:OD2	1:B:673:LYS:NZ	2.07	0.87
1:A:659:ARG:HB2	1:A:662[B]:MET:HE2	1.56	0.86
1:A:658:ASP:O	1:A:718:THR:HG23	1.80	0.81
1:A:709:ASN:HD21	1:B:669:ARG:NH1	1.75	0.79
1:A:709:ASN:HD21	1:B:669:ARG:HH11	1.27	0.78
1:B:662[A]:MET:HE2	1:B:681:TYR:HB3	1.67	0.76
1:A:664:ASN:HD22	1:A:664:ASN:H	1.31	0.76
1:B:662[A]:MET:HE1	2:B:92:HOH:O	1.90	0.70
1:A:718:THR:HA	1:A:721:ILE:HG13	1.75	0.68
1:A:709:ASN:OD1	1:B:675:PHE:CE1	2.47	0.68
1:A:706:THR:HG22	1:A:707:ILE:N	2.09	0.67
1:B:620:ILE:N	1:B:620:ILE:HD13	2.08	0.67
1:B:683:ASP:O	1:B:684:LYS:HG2	1.99	0.63
1:A:718:THR:CA	1:A:721:ILE:HG13	2.28	0.63
1:B:679:LYS:HE3	1:B:686:PRO:HD3	1.85	0.59
1:A:709:ASN:ND2	1:B:669:ARG:HH12	1.99	0.59
1:A:618:GLU:HB2	2:A:59:HOH:O	2.03	0.59
1:A:659:ARG:H	1:A:662[B]:MET:CE	2.17	0.58
1:A:626:GLY:HA2	1:A:678:PHE:CD2	2.40	0.57
1:A:659:ARG:HB2	1:A:662[B]:MET:CE	2.32	0.55
1:B:662[A]:MET:CE	1:B:681:TYR:HB3	2.33	0.55
1:A:659:ARG:HB2	1:A:662[A]:MET:HG3	1.88	0.55
1:B:646:ILE:HD12	1:B:656:ILE:HD11	1.89	0.55
1:A:659:ARG:H	1:A:662[B]:MET:HE2	1.72	0.55
1:A:613:LYS:NZ	1:A:725:LEU:O	2.43	0.51
1:B:662[A]:MET:HE2	1:B:681:TYR:CB	2.40	0.51
1:A:620[A]:ILE:HG12	1:A:629:LEU:HA	1.95	0.49
1:A:709:ASN:OD1	1:B:675:PHE:CD1	2.67	0.48
1:A:659:ARG:CB	1:A:662[B]:MET:HE2	2.35	0.48
1:A:664:ASN:HD22	1:A:664:ASN:N	2.04	0.47
1:A:718:THR:O	1:A:721:ILE:HG13	2.14	0.47
1:A:718:THR:HA	1:A:721:ILE:CG1	2.43	0.47
1:B:624:THR:HG22	1:B:689:ILE:CD1	2.46	0.45
1:A:706:THR:CG2	1:A:707:ILE:N	2.77	0.45
1:A:626:GLY:HA2	1:A:678:PHE:CG	2.52	0.45
1:B:691:ASN:HB3	1:B:694:TYR:CD1	2.53	0.44
1:A:699:TYR:HA	1:A:724:ILE:O	2.18	0.43
1:B:683:ASP:C	1:B:684:LYS:HG2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:THR:HG22	1:B:689:ILE:HD12	2.01	0.43
1:B:705:ASN:HD22	1:B:705:ASN:HA	1.66	0.42
1:B:679:LYS:HE2	1:B:679:LYS:HB3	1.78	0.42
1:B:673:LYS:HZ2	1:B:673:LYS:HG3	1.75	0.41

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)
1:B:595:ARG:CD	2:B:47:HOH:O[1_565]	2.14	0.06

## 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	148/143 (104%)	145 (98%)	3 (2%)	0	100	100
1	B	132/143 (92%)	130 (98%)	2 (2%)	0	100	100
All	All	280/286 (98%)	275 (98%)	5 (2%)	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	134/129 (104%)	129 (96%)	5 (4%)	34	22
1	B	122/129 (95%)	116 (95%)	6 (5%)	25	12
All	All	256/258 (99%)	245 (96%)	11 (4%)	27	16

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	594	SER
1	A	625	GLU
1	A	664	ASN
1	A	668	LEU
1	A	721	ILE
1	B	629	LEU
1	B	636	ARG
1	B	668	LEU
1	B	684	LYS
1	B	717	SER
1	B	719	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	664	ASN
1	A	705	ASN
1	A	709	ASN
1	A	719	ASN
1	B	697	ASN
1	B	705	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	143/143 (100%)	0.01	0 <span>100</span> <span>100</span>	20, 26, 38, 45	0
1	B	134/143 (93%)	0.30	9 (6%) <span>17</span> <span>26</span>	24, 31, 41, 46	0
All	All	277/286 (96%)	0.15	9 (3%) <span>47</span> <span>57</span>	20, 29, 40, 46	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	720	GLY	4.0
1	B	716	THR	2.7
1	B	719	ASN	2.6
1	B	618	GLU	2.5
1	B	602	ASN	2.5
1	B	676	ILE	2.3
1	B	684	LYS	2.3
1	B	660	TYR	2.3
1	B	706	THR	2.3

### 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

There are no such residues in this entry.