



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:21 am BST

PDB ID : 6UCE  
Title : N123-VRC34\_pI3 HIV neutralizing antibody in complex with HIV fusion peptide residue 512-519  
Authors : Xu, K.; Kwong, P.D.  
Deposited on : 2019-09-16  
Resolution : 1.38 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

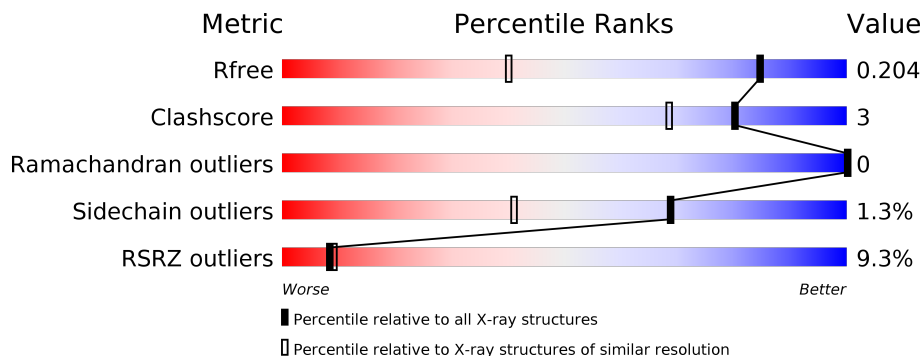
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.38 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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	L	214	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">7% <span style="margin-left: 100px;">93%</span> <span style="margin-left: 100px;">7%</span></p>
2	H	233	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">11% <span style="margin-left: 100px;">92%</span> <span style="margin-left: 100px;">5%</span> •</p>
3	C	8	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: center;">13% <span style="margin-left: 100px;">100%</span></p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4147 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 N123-VRC34\_pI3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	214	1641	1030	275	330	6	0	0	0

- Molecule 2 is a protein called N123-VRC34\_pI3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	228	1720	1087	288	336	9	0	0	0

- Molecule 3 is a protein called HIV fusion peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	51	35	8	8	0	0	0

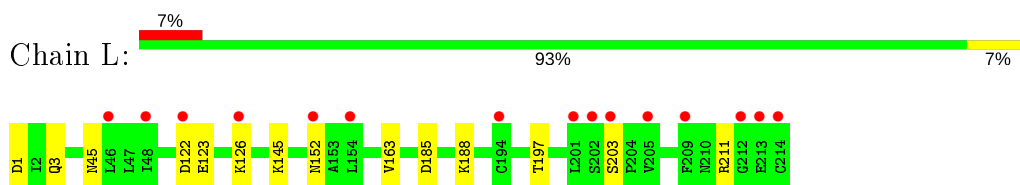
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	367	Total 367	O 367	0	0
4	H	357	Total 357	O 357	0	0
4	C	11	Total 11	O 11	0	0

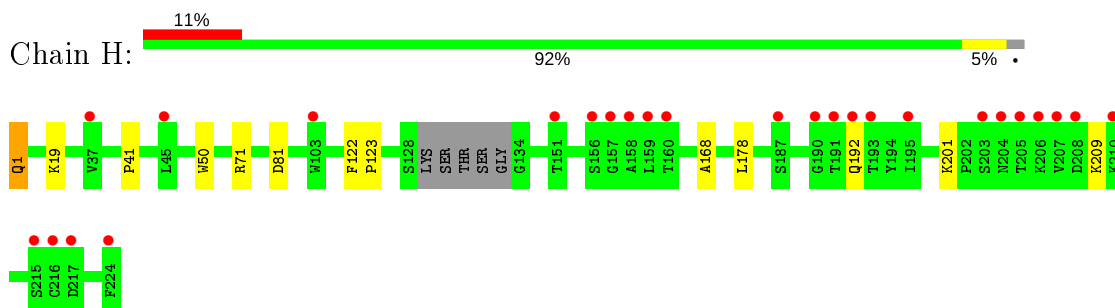
### 3 Residue-property plots [i](#)

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.

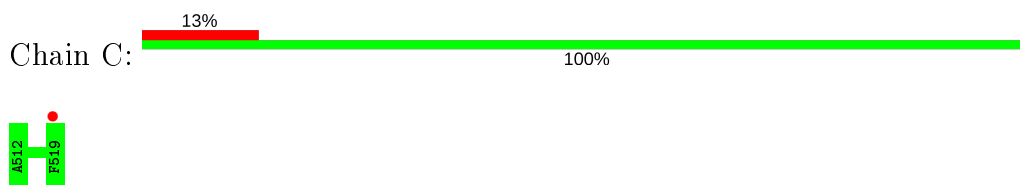
- Molecule 1: N123-VRC34\_pI3 light chain



- Molecule 2: N123-VRC34\_pI3 heavy chain



- Molecule 3: HIV fusion peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.81Å 80.73Å 69.82Å 90.00° 102.31° 90.00°	Depositor
Resolution (Å)	31.42 – 1.38 31.42 – 1.38	Depositor EDS
% Data completeness (in resolution range)	94.6 (31.42-1.38) 94.6 (31.42-1.38)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.38Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.180 , 0.204 0.180 , 0.204	Depositor DCC
$R_{free}$ test set	4485 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtrriage
Anisotropy	0.338	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.6	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	0.96	EDS
Total number of atoms	4147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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	L	0.29	0/1678	0.54	0/2279
2	H	0.29	0/1762	0.54	0/2400
3	C	0.31	0/51	0.52	0/68
All	All	0.29	0/3491	0.54	0/4747

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	L	1641	0	1592	10	0
2	H	1720	0	1681	10	0
3	C	51	0	53	0	0
4	C	11	0	0	0	0
4	H	357	0	0	5	5
4	L	367	0	0	5	5
All	All	4147	0	3326	18	6

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 (18) 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)
2:H:19:LYS:NZ	4:H:303:HOH:O	2.11	0.83
1:L:211:ARG:O	4:L:301:HOH:O	1.98	0.80
1:L:1:ASP:OD1	4:L:302:HOH:O	2.00	0.79
2:H:192:GLN:O	4:H:301:HOH:O	2.03	0.76
1:L:152:ASN:O	4:L:303:HOH:O	2.05	0.74
2:H:81:ASP:OD1	4:H:302:HOH:O	2.09	0.69
1:L:163:VAL:HG21	4:L:647:HOH:O	2.00	0.61
1:L:45:ASN:ND2	4:L:308:HOH:O	2.33	0.61
1:L:123:GLU:OE2	2:H:209:LYS:NZ	2.34	0.58
2:H:201:LYS:NZ	4:H:312:HOH:O	2.38	0.56
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.89	0.54
2:H:1:GLN:OE1	2:H:1:GLN:N	2.41	0.50
2:H:41:PRO:HG2	4:H:582:HOH:O	2.13	0.47
1:L:185:ASP:HA	1:L:188:LYS:HD3	1.97	0.46
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.01	0.43
1:L:123:GLU:HG2	2:H:122:PHE:CE1	2.55	0.41
1:L:145:LYS:HB3	1:L:197:THR:HB	2.03	0.41
1:L:122:ASP:O	1:L:126:LYS:HG2	2.21	0.40

All (6) 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:L:508:HOH:O	4:H:362:HOH:O 1_556]	1.85	0.35
4:H:405:HOH:O	4:H:531:HOH:O 1_454]	1.97	0.23
4:L:642:HOH:O	4:L:657:HOH:O 1_556]	2.01	0.19
4:L:640:HOH:O	4:H:604:HOH:O 1_554]	2.02	0.18
4:L:332:HOH:O	4:H:478:HOH:O 1_655]	2.05	0.15
4:L:365:HOH:O	4:H:536:HOH:O 2_645]	2.16	0.04

## 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	L	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	H	224/233 (96%)	222 (99%)	2 (1%)	0	100	100
3	C	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
All	All	442/455 (97%)	432 (98%)	10 (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	L	187/187 (100%)	185 (99%)	2 (1%)	73	48
2	H	192/196 (98%)	189 (98%)	3 (2%)	62	33
3	C	4/4 (100%)	4 (100%)	0	100	100
All	All	383/387 (99%)	378 (99%)	5 (1%)	69	41

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	203	SER
2	H	1	GLN
2	H	50	TRP
2	H	71	ARG

Some 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 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

### 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	L	214/214 (100%)	0.64	15 (7%) 16 17	10, 21, 37, 74	0
2	H	228/233 (97%)	0.79	26 (11%) 5 4	10, 21, 52, 63	0
3	C	8/8 (100%)	0.87	1 (12%) 3 4	14, 16, 24, 43	0
All	All	450/455 (98%)	0.72	42 (9%) 8 9	10, 21, 47, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	214	CYS	11.6
1	L	212	GLY	6.0
2	H	195	ILE	5.6
2	H	215	SER	5.3
2	H	216	CYS	5.3
3	C	519	PHE	5.0
2	H	187	SER	4.9
2	H	193	THR	4.4
2	H	191	THR	4.2
1	L	202	SER	4.1
2	H	205	THR	4.1
1	L	154	LEU	4.1
2	H	151	THR	3.9
2	H	217	ASP	3.7
1	L	213	GLU	3.7
1	L	126	LYS	3.5
2	H	157	GLY	3.5
2	H	156	SER	3.5
2	H	206	LYS	3.3
2	H	208	ASP	3.1
2	H	159	LEU	3.1
2	H	158	ALA	3.1
2	H	160	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	37	VAL	2.9
1	L	122	ASP	2.8
2	H	210	LYS	2.8
1	L	152	ASN	2.8
1	L	203	SER	2.7
2	H	204	ASN	2.6
2	H	192	GLN	2.5
1	L	201	LEU	2.3
1	L	209	PHE	2.3
2	H	103	TRP	2.3
1	L	205	VAL	2.3
2	H	224	PHE	2.3
1	L	48	ILE	2.2
1	L	46	LEU	2.2
2	H	45	LEU	2.1
1	L	194	CYS	2.1
2	H	190	GLY	2.1
2	H	203	SER	2.1
2	H	207	VAL	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 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.