



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:32 pm BST

PDB ID : 5F89  
Title : Structure of the Unliganded Fab from HIV-1 Neutralising Antibody CAP248-2B that Binds to the gp120 C-terminus - gp41 Interface  
Authors : Wibmer, C.K.; Gorman, J.; Kwong, P.D.  
Deposited on : 2015-12-09  
Resolution : 2.78 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

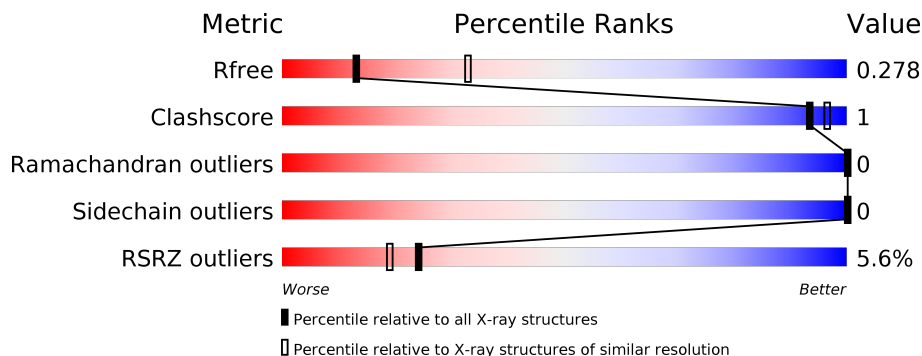
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	229	 7% 94% 6%
1	H	229	 4% 96% .
2	B	225	 4% 96% . .
2	L	225	 7% 96% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13329 atoms, of which 6570 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 CAP248-2B Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	H	228	3388	1082	1674	286	341	5	0	1	0
1	A	228	3426	1094	1691	290	346	5	0	5	0

- Molecule 2 is a protein called CAP248-2B Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	L	221	3225	1022	1592	273	334	4	0	0	0
2	B	222	3267	1039	1613	274	337	4	0	0	0

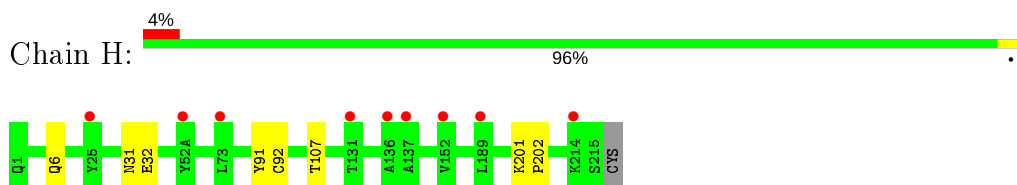
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	6	Total 6 O 6	0	0
3	L	4	Total 4 O 4	0	0
3	A	8	Total 8 O 8	0	0
3	B	5	Total 5 O 5	0	0

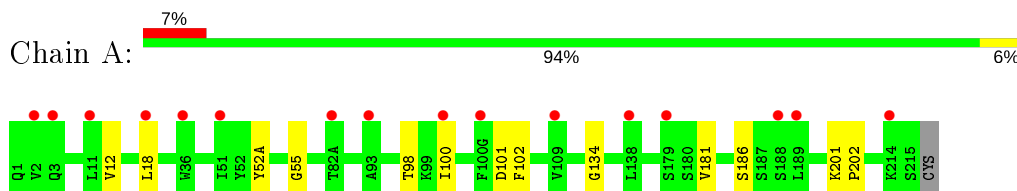
### 3 Residue-property plots [i](#)

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.

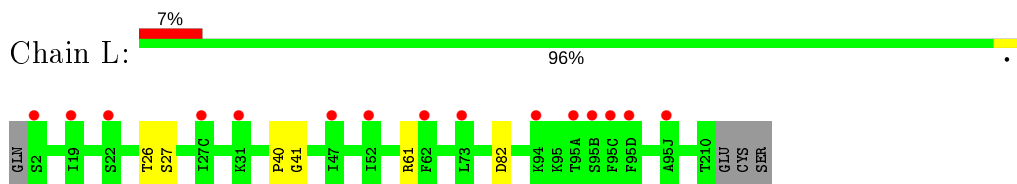
- Molecule 1: CAP248-2B Heavy Chain



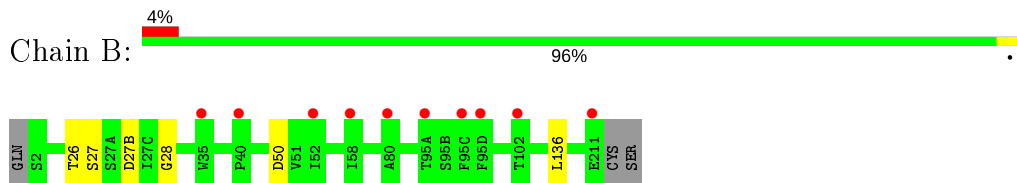
- Molecule 1: CAP248-2B Heavy Chain



- Molecule 2: CAP248-2B Light Chain



- Molecule 2: CAP248-2B Light Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.00Å 68.28Å 85.73Å 95.59° 99.82° 102.54°	Depositor
Resolution (Å)	41.82 – 2.78 41.82 – 2.78	Depositor EDS
% Data completeness (in resolution range)	88.1 (41.82-2.78) 80.2 (41.82-2.78)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.08 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.228 , 0.279 0.230 , 0.278	Depositor DCC
$R_{free}$ test set	1027 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtrriage
Anisotropy	0.557	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 17.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	0.27	0/1780	0.45	0/2434
1	H	0.28	0/1758	0.46	0/2404
2	B	0.26	0/1695	0.42	0/2311
2	L	0.25	0/1672	0.42	0/2281
All	All	0.26	0/6905	0.44	0/9430

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

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	1735	1691	1680	8	0
1	H	1714	1674	1662	5	0
2	B	1654	1613	1612	4	0
2	L	1633	1592	1592	3	0
3	A	8	0	0	0	0
3	B	5	0	0	0	0
3	H	6	0	0	0	0
3	L	4	0	0	0	0
All	All	6759	6570	6546	18	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 1.

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:B:27(B):ASP:O	2:B:28:GLY:N	2.32	0.61
1:H:31:ASN:OD1	1:H:32:GLU:N	2.36	0.59
1:H:6:GLN:HE22	1:H:91:TYR:HA	1.72	0.55
1:H:6:GLN:OE1	1:H:107:THR:HG23	2.07	0.54
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.40	0.51
1:A:134:GLY:O	1:A:186:SER:N	2.41	0.50
1:H:6:GLN:NE2	1:H:92:CYS:H	2.12	0.47
2:B:26:THR:OG1	2:B:27:SER:N	2.47	0.47
1:A:52(A):TYR:O	1:A:55:GLY:N	2.48	0.46
1:A:101:ASP:OD1	1:A:102:PHE:N	2.49	0.46
1:A:12:VAL:HG21	1:A:18:LEU:HD13	1.98	0.46
1:A:181:VAL:HG21	2:B:136:LEU:CD1	2.47	0.44
1:A:98:THR:OG1	2:B:50:ASP:OD2	2.37	0.42
1:A:201:LYS:N	1:A:202:PRO:CD	2.83	0.42
2:L:26:THR:OG1	2:L:27:SER:N	2.49	0.41
1:H:201:LYS:N	1:H:202:PRO:CD	2.84	0.41
2:L:40:PRO:HA	2:L:41:GLY:HA2	1.82	0.40
1:A:100:ILE:N	1:A:100:ILE:HD12	2.37	0.40

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	231/229 (101%)	217 (94%)	14 (6%)	0	100	100
1	H	227/229 (99%)	215 (95%)	12 (5%)	0	100	100
2	B	220/225 (98%)	204 (93%)	16 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	219/225 (97%)	199 (91%)	20 (9%)	0	100	100
All	All	897/908 (99%)	835 (93%)	62 (7%)	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	197/195 (101%)	197 (100%)	0	100	100
1	H	195/195 (100%)	195 (100%)	0	100	100
2	B	186/189 (98%)	186 (100%)	0	100	100
2	L	183/189 (97%)	183 (100%)	0	100	100
All	All	761/768 (99%)	761 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PCA	A	1	1	7,8,9	2.21	2 (28%)	9,10,12	2.43	5 (55%)
1	PCA	H	1	1	7,8,9	2.14	2 (28%)	9,10,12	2.26	5 (55%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	4.70	1.47	1.34
1	H	1	PCA	CD-N	4.60	1.46	1.34
1	A	1	PCA	CA-N	3.33	1.50	1.46
1	H	1	PCA	CA-N	3.11	1.50	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CA-C	-4.17	106.97	112.70
1	H	1	PCA	CB-CA-C	-3.23	108.26	112.70
1	A	1	PCA	OE-CD-CG	-3.18	121.21	126.76
1	H	1	PCA	CA-N-CD	-3.08	103.02	113.58
1	H	1	PCA	OE-CD-CG	-3.01	121.51	126.76
1	A	1	PCA	CA-N-CD	-3.00	103.30	113.58
1	H	1	PCA	CB-CA-N	2.70	111.05	103.30
1	A	1	PCA	CB-CA-N	2.54	110.58	103.30
1	H	1	PCA	CG-CD-N	2.50	114.87	108.39
1	A	1	PCA	CG-CD-N	2.42	114.66	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	227/229 (99%)	0.64	16 (7%) 16 11	50, 65, 74, 83	0
1	H	227/229 (99%)	0.58	9 (3%) 38 33	47, 54, 64, 73	0
2	B	222/225 (98%)	0.70	10 (4%) 33 27	48, 61, 77, 83	0
2	L	221/225 (98%)	0.63	15 (6%) 17 12	47, 59, 69, 92	0
All	All	897/908 (98%)	0.64	50 (5%) 24 19	47, 58, 74, 92	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	95(D)	PHE	6.5
2	L	95(C)	PHE	6.5
2	L	95(A)	THR	5.7
2	L	95(B)	SER	4.1
1	A	109	VAL	4.0
2	L	31	LYS	3.8
2	B	211	GLU	3.5
1	A	18	LEU	3.2
2	L	19	ILE	3.2
1	H	73	LEU	3.1
2	B	40	PRO	3.0
2	L	95(D)	PHE	3.0
1	A	214	LYS	2.9
1	A	82(A)	THR	2.9
2	B	80	ALA	2.8
2	L	52	ILE	2.8
1	H	137	ALA	2.7
2	L	2	SER	2.7
1	A	51	ILE	2.7
1	A	100	ILE	2.7
1	A	11[A]	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	214	LYS	2.7
1	A	189	LEU	2.7
2	L	73	LEU	2.6
2	L	62	PHE	2.6
2	L	27(C)	ILE	2.5
2	B	35	TRP	2.5
2	B	58	ILE	2.5
2	B	95(A)	THR	2.5
2	L	22	SER	2.4
1	H	136	ALA	2.4
2	L	47	ILE	2.4
1	A	3	GLN	2.3
1	A	138	LEU	2.3
1	A	36	TRP	2.3
1	A	93	ALA	2.3
2	L	95(J)	ALA	2.3
1	H	152	VAL	2.3
2	B	102	THR	2.2
2	B	95(C)	PHE	2.2
1	A	100(G)	PHE	2.2
1	A	2	VAL	2.2
1	A	179	SER	2.2
1	H	52(A)	TYR	2.2
2	B	52	ILE	2.1
2	L	94	LYS	2.0
1	H	131	THR	2.0
1	H	189	LEU	2.0
1	H	25	TYR	2.0
1	A	188	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	A	1	8/9	0.85	0.43	66,68,81,81	0
1	PCA	H	1	8/9	0.91	0.22	58,61,74,74	0

### 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.