



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 05:29 pm GMT

PDB ID : 5U3J  
Title : Crystal Structure of DH511.1 Fab in Complex with HIV-1 gp41 MPER Peptide  
Authors : Ofek, G.; Wu, L.; Loughheed, C.S.; Williams, L.D.; Nicely, N.I.; Haynes, B.F.  
Deposited on : 2016-12-02  
Resolution : 2.74 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 : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

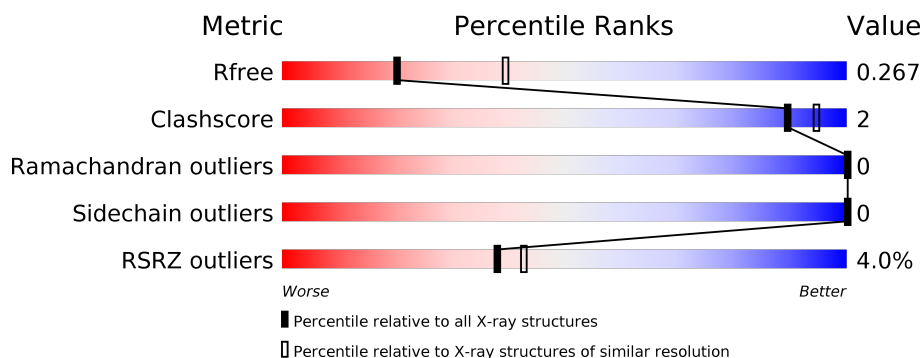
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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))
$R_{free}$	111664	1033 (2.76-2.72)
Clashscore	122126	1084 (2.76-2.72)
Ramachandran outliers	120053	1064 (2.76-2.72)
Sidechain outliers	120020	1065 (2.76-2.72)
RSRZ outliers	108989	1008 (2.76-2.72)

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	H	235	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
2	L	215	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
3	A	34	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7218 atoms, of which 3530 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 DH511.1 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	235	Total	C	H	N	O	S	0	0	0
			3492	1120	1724	300	341	7			

- Molecule 2 is a protein called DH511.1 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	215	Total	C	H	N	O	S	0	0	0
			3238	1031	1591	277	334	5			

- Molecule 3 is a protein called gp41 MPER peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	29	Total	C	H	N	O	0	0	0
			465	170	215	40	40			

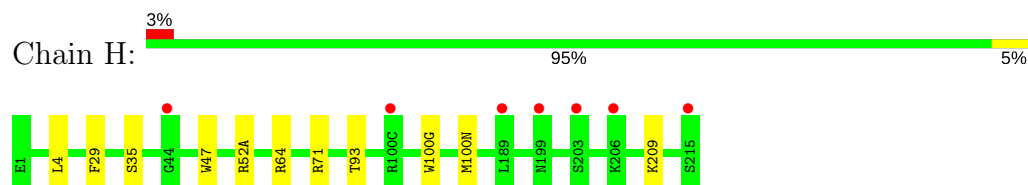
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	16	Total O 16 16	0	0
4	L	6	Total O 6 6	0	0
4	A	1	Total O 1 1	0	0

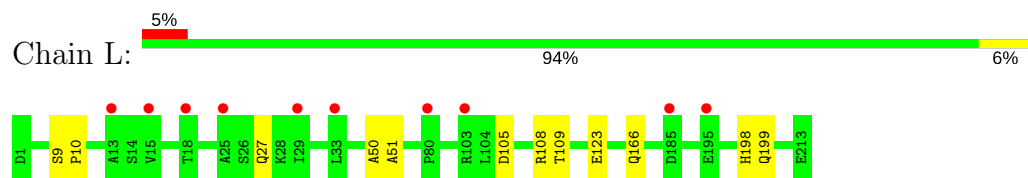
### 3 Residue-property plots [i](#)

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.

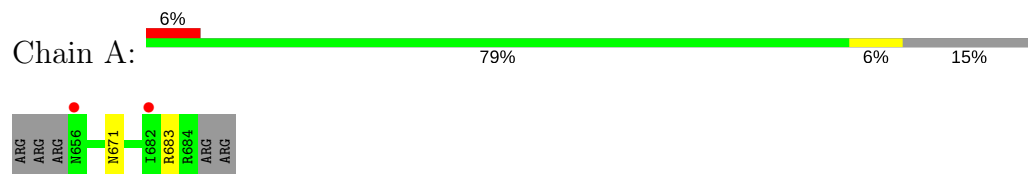
- Molecule 1: DH511.1 Heavy Chain



- Molecule 2: DH511.1 Light Chain



- Molecule 3: gp41 MPER peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.09Å 133.96Å 179.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.30 – 2.74 37.29 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.30-2.74) 92.6 (37.29-2.74)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.71 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.229 , 0.264 0.232 , 0.267	Depositor DCC
$R_{free}$ test set	999 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

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	H	0.26	0/1813	0.45	0/2467
2	L	0.25	0/1683	0.43	0/2288
3	A	0.23	0/261	0.33	0/360
All	All	0.25	0/3757	0.43	0/5115

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	H	1768	1724	1723	8	0
2	L	1647	1591	1590	7	0
3	A	250	215	214	2	0
4	A	1	0	0	0	0
4	H	16	0	0	2	0
4	L	6	0	0	1	0
All	All	3688	3530	3527	14	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 2.

All (14) 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:L:105:ASP:OD1	2:L:166:GLN:NE2	2.13	0.81
2:L:198:HIS:ND1	2:L:199:GLN:O	2.16	0.77
1:H:4:LEU:O	4:H:301:HOH:O	2.03	0.76
1:H:29:PHE:O	1:H:71:ARG:NH2	2.39	0.56
1:H:100(G):TRP:O	3:A:683:ARG:NH1	2.40	0.55
2:L:108:ARG:NH1	2:L:109:THR:O	2.41	0.54
1:H:64:ARG:NH1	4:H:304:HOH:O	2.41	0.51
1:H:35:SER:OG	1:H:47:TRP:NE1	2.44	0.49
1:H:52(A):ARG:NH1	3:A:671:ASN:OD1	2.48	0.47
2:L:9:SER:CB	2:L:10:PRO:HD3	2.49	0.43
1:H:209:LYS:NZ	2:L:123:GLU:OE2	2.41	0.42
2:L:27:GLN:NE2	4:L:303:HOH:O	2.46	0.41
2:L:50:ALA:O	2:L:51:ALA:HB3	2.21	0.40
1:H:93:THR:HG21	1:H:100(N):MET:HB3	2.04	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	H	233/235 (99%)	224 (96%)	9 (4%)	0	100	100
2	L	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
3	A	27/34 (79%)	25 (93%)	2 (7%)	0	100	100
All	All	473/484 (98%)	448 (95%)	25 (5%)	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	H	193/198 (98%)	193 (100%)	0	100	100
2	L	184/187 (98%)	184 (100%)	0	100	100
3	A	22/33 (67%)	22 (100%)	0	100	100
All	All	399/418 (96%)	399 (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](#)

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	H	235/235 (100%)	0.46	7 (2%)	50	58	44, 69, 117, 149	0
2	L	215/215 (100%)	0.76	10 (4%)	31	35	57, 94, 131, 217	0
3	A	29/34 (85%)	0.79	2 (6%)	17	19	57, 78, 155, 166	0
All	All	479/484 (98%)	0.62	19 (3%)	38	43	44, 82, 127, 217	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	656	ASN	4.0
2	L	13	ALA	3.3
2	L	18	THR	3.2
1	H	215	SER	3.0
2	L	80	PRO	2.8
1	H	189	LEU	2.6
2	L	15	VAL	2.5
3	A	682	ILE	2.4
1	H	203	SER	2.4
2	L	103	ARG	2.3
1	H	44	GLY	2.3
2	L	195	GLU	2.2
1	H	199	ASN	2.1
1	H	206	LYS	2.1
2	L	25	ALA	2.1
1	H	100(C)	ARG	2.1
2	L	29	ILE	2.0
2	L	33	LEU	2.0
2	L	185	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.