



# wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 21, 2017 – 05:04 PM EDT

PDB ID : 3JCB  
EMDB ID: : EMD-6542  
Title : Structure of Simian Immunodeficiency Virus Envelope Spikes bound with CD4 and Monoclonal Antibody 36D5  
Authors : Hu, G.; Liu, J.; Roux, K.; Taylor, K.A.  
Deposited on : unknown  
Resolution : unknown (reported)  
Based on PDB ID : 4NCO

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

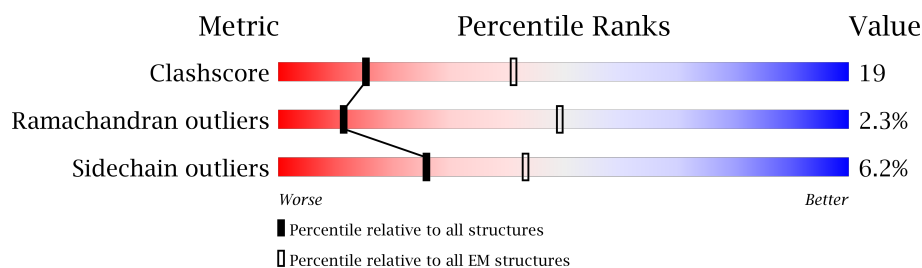
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.

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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	448	54% 35% 6% 6%
1	E	448	55% 33% 6% 6%
1	I	448	55% 33% 5% 6%
2	B	207	84% 13% ..
3	C	232	80% 16% ..
4	D	175	78% 21% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13909 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3096	1937	544	590	25		
1	E	420	Total	C	N	O	S	0	0
			3096	1937	544	590	25		
1	I	420	Total	C	N	O	S	0	0
			3096	1937	544	590	25		

- Molecule 2 is a protein called Antibody 36D5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	202	Total	C	N	O	S	0	0
			1530	964	255	307	4		

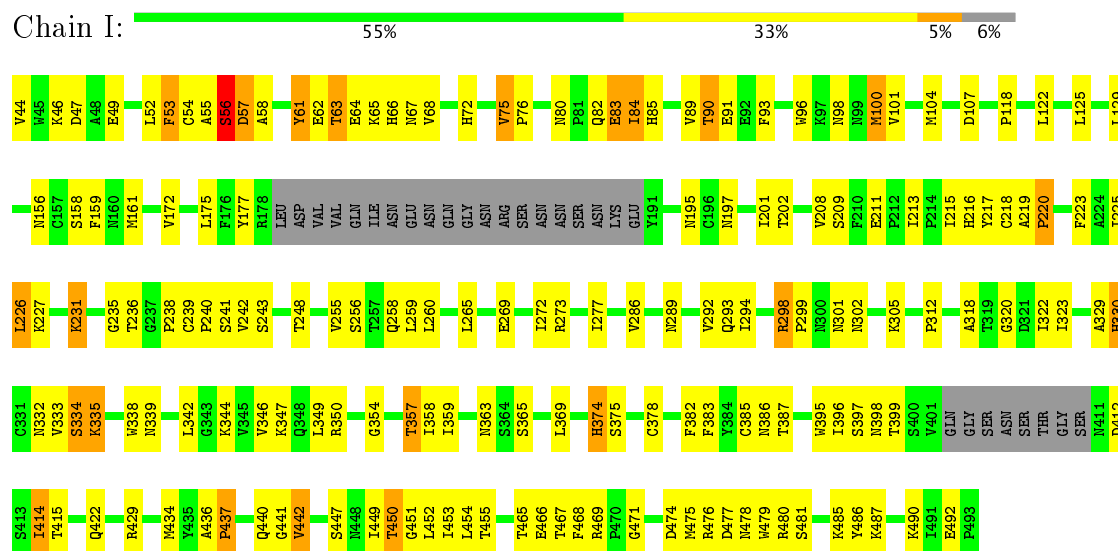
- Molecule 3 is a protein called Antibody 36D5 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	226	Total	C	N	O	S	0	0
			1728	1100	293	330	5		

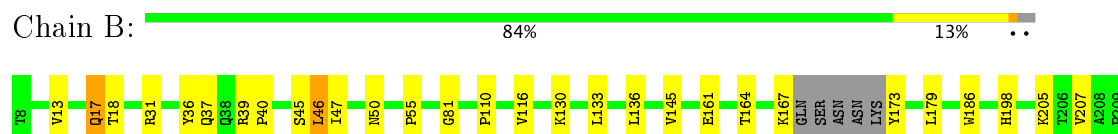
- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1363	851	239	269	4		

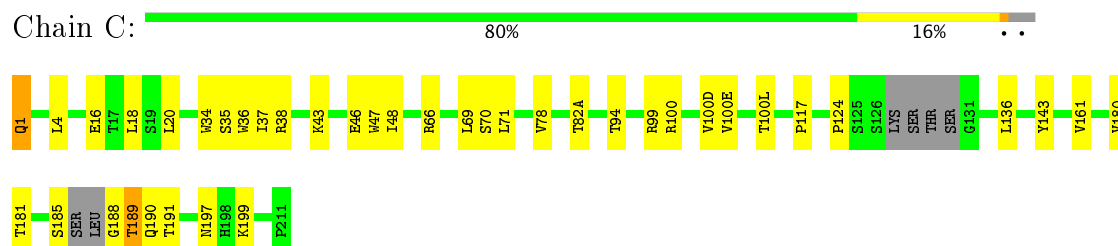




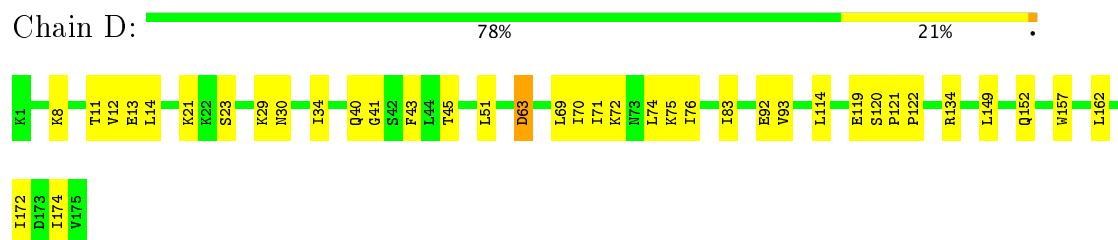
• Molecule 2: Antibody 36D5 light chain



• Molecule 3: Antibody 36D5 heavy chain



• Molecule 4: T-cell surface glycoprotein CD4



## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	1181	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	100	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	31000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor

## 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  >2	RMSZ	# Z  >2
1	A	0.33	0/3161	0.71	4/4306 (0.1%)
1	E	0.34	0/3161	0.71	4/4306 (0.1%)
1	I	0.34	0/3161	0.71	3/4306 (0.1%)
2	B	0.28	0/1571	0.54	1/2151 (0.0%)
3	C	0.31	0/1774	0.57	0/2421
4	D	0.26	0/1382	0.53	0/1863
All	All	0.32	0/14210	0.66	12/19353 (0.1%)

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	0	3
1	E	0	3
1	I	0	3
2	B	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	LYS	N-CA-C	6.19	127.72	111.00
1	I	335	LYS	N-CA-C	6.19	127.71	111.00
1	E	335	LYS	N-CA-C	6.18	127.70	111.00
1	E	450	THR	C-N-CA	-5.98	109.74	122.30
1	A	450	THR	C-N-CA	-5.97	109.76	122.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
1	A	56	SER	Peptide
1	A	80	ASN	Peptide
2	B	110	PRO	Peptide
1	E	56	SER	Peptide

## 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	3096	0	2836	159	0
1	E	3096	0	2836	127	0
1	I	3096	0	2835	150	0
2	B	1530	0	1472	19	0
3	C	1728	0	1699	37	0
4	D	1363	0	1386	61	0
All	All	13909	0	13064	501	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 19.

The worst 5 of 501 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)
4:D:21:LYS:CE	1:I:62:GLU:HG3	1.41	1.49
1:A:472:GLY:O	4:D:40:GLN:HG3	1.16	1.27
4:D:21:LYS:HE3	1:I:62:GLU:CG	1.63	1.26
1:A:325:ASP:O	3:C:100(E):VAL:HG23	1.15	1.25
1:A:474:ASP:OD1	4:D:41:GLY:HA3	1.04	1.22

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	414/448 (92%)	349 (84%)	51 (12%)	14 (3%)	4	4
1	E	414/448 (92%)	348 (84%)	52 (13%)	14 (3%)	4	4
1	I	414/448 (92%)	349 (84%)	51 (12%)	14 (3%)	4	4
2	B	198/207 (96%)	191 (96%)	7 (4%)	0	100	100
3	C	220/232 (95%)	213 (97%)	6 (3%)	1 (0%)	32	32
4	D	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
All	All	1833/1958 (94%)	1608 (88%)	182 (10%)	43 (2%)	11	7

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	83	GLU
1	A	323	ILE
1	A	429	ARG
1	E	57	ASP

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	317/400 (79%)	293 (92%)	24 (8%)	15	15
1	E	317/400 (79%)	293 (92%)	24 (8%)	15	15
1	I	317/400 (79%)	293 (92%)	24 (8%)	15	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	171/176 (97%)	164 (96%)	7 (4%)	35	35
3	C	196/202 (97%)	189 (96%)	7 (4%)	40	40
4	D	159/159 (100%)	154 (97%)	5 (3%)	45	45
All	All	1477/1737 (85%)	1386 (94%)	91 (6%)	26	21

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	152	GLN
1	E	125	LEU
1	I	374	HIS
4	D	162	LEU
1	E	75	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	112	GLN
1	E	130	GLN
1	I	289	ASN
4	D	103	ASN
1	I	330	HIS

### 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 ⓘ

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.