



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 22, 2017 – 03:46 AM EDT

PDB ID : 3JCC
EMDB ID: : EMD-6543
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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

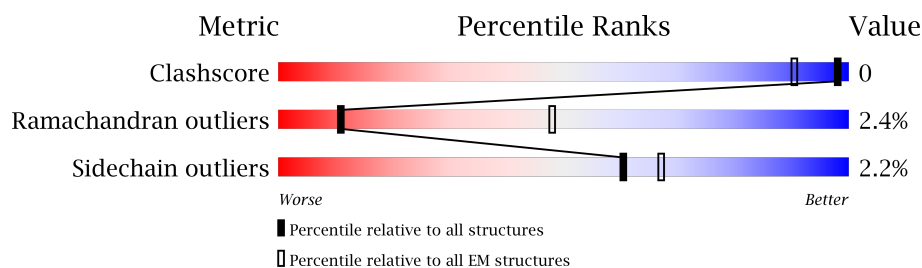
1 Overall quality at a glance

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 ≥ 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	
1	E	448	
1	I	448	
2	B	207	
3	C	232	
4	D	175	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14521 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
			3299	2065	581	626	27		
1	E	420	Total	C	N	O	S	0	0
			3299	2065	581	626	27		
1	I	420	Total	C	N	O	S	0	0
			3299	2065	581	626	27		

- 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
			1531	964	255	308	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
			1729	1100	293	331	5		

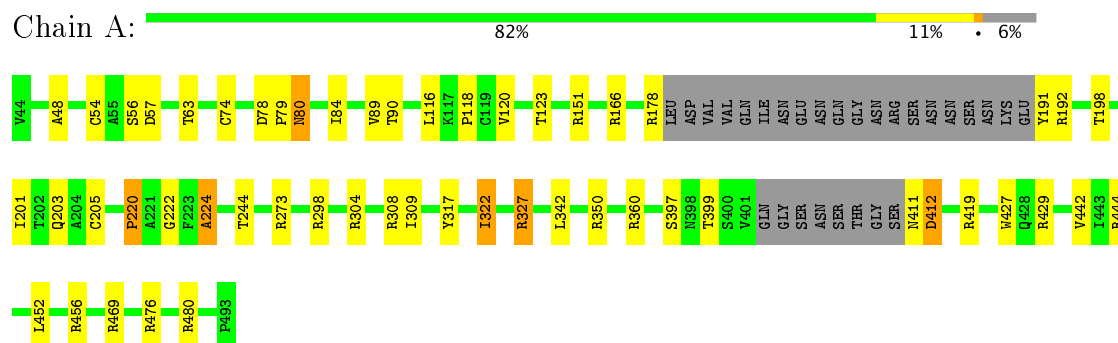
- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1364	851	239	270	4		

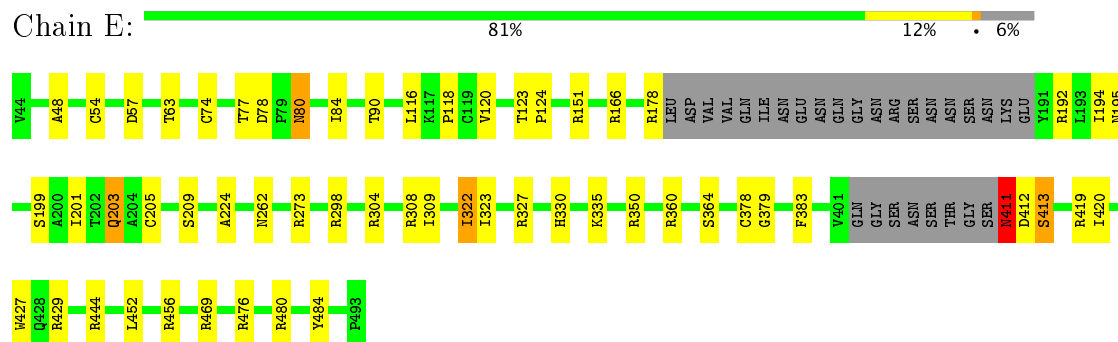
3 Residue-property plots

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. 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. 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.

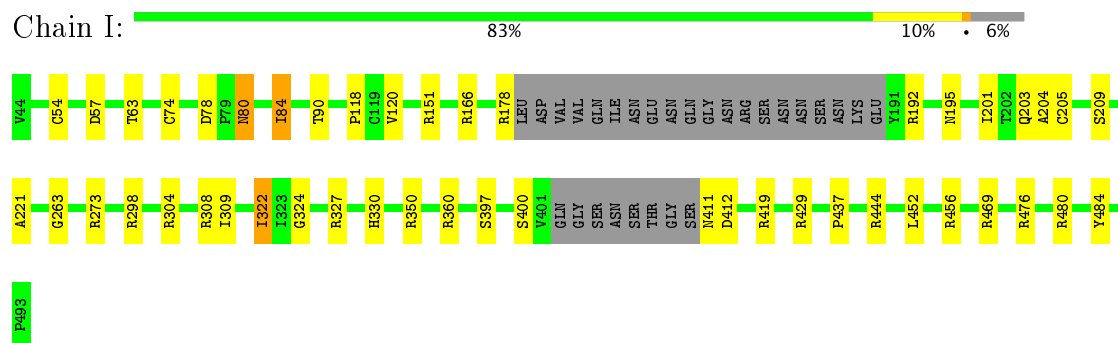
- Molecule 1: Envelope glycoprotein gp120



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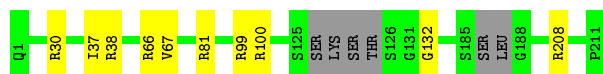
- Molecule 2: Antibody 36D5 light chain

Chain B:  92% 5% •



- Molecule 3: Antibody 36D5 heavy chain

Chain C:  93% • •



- Molecule 4: T-cell surface glycoprotein CD4

Chain D:  97% •



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	1796	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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.62	0/3369	1.11	24/4574 (0.5%)
1	E	0.63	0/3369	1.08	26/4574 (0.6%)
1	I	0.63	0/3369	1.09	20/4574 (0.4%)
2	B	0.62	0/1573	0.98	9/2154 (0.4%)
3	C	0.62	0/1777	0.98	8/2427 (0.3%)
4	D	0.53	0/1383	0.95	6/1863 (0.3%)
All	All	0.62	0/14840	1.05	93/20166 (0.5%)

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	1	5
1	E	1	5
1	I	1	2
2	B	0	2
3	C	0	1
All	All	3	15

There are no bond length outliers.

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	298	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	298	ARG	NE-CZ-NH1	9.81	125.21	120.30
4	D	54	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	E	444	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	I	166	ARG	NE-CZ-NH2	9.12	124.86	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	411	ASN	CA
1	E	411	ASN	CA
1	I	411	ASN	CA

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ALA	Peptide
1	A	317	TYR	Sidechain
1	A	327	ARG	Sidechain
1	A	56	SER	Peptide
1	A	80	ASN	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	3299	0	3241	4	0
1	E	3299	0	3241	6	0
1	I	3299	0	3241	2	0
2	B	1531	0	1473	0	0
3	C	1729	0	1701	0	0
4	D	1364	0	1389	0	0
All	All	14521	0	14286	12	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 0.

The worst 5 of 12 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:120:VAL:HG12	1:A:201:ILE:HG22	1.67	0.77
1:E:120:VAL:HG13	1:E:203:GLN:HA	1.84	0.60
1:I:120:VAL:HG12	1:I:201:ILE:HG22	1.85	0.58
1:E:120:VAL:HG12	1:E:201:ILE:HG22	1.91	0.50
1:I:120:VAL:HG13	1:I:203:GLN:HA	1.94	0.48

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 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	418/448 (93%)	359 (86%)	43 (10%)	16 (4%)	4	4
1	E	418/448 (93%)	363 (87%)	42 (10%)	13 (3%)	5	5
1	I	418/448 (93%)	352 (84%)	51 (12%)	15 (4%)	4	4
2	B	200/207 (97%)	194 (97%)	6 (3%)	0	100	100
3	C	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
4	D	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
All	All	1851/1958 (94%)	1656 (90%)	151 (8%)	44 (2%)	11	7

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	220	PRO
1	A	322	ILE
1	A	412	ASP
1	E	57	ASP

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 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	375/400 (94%)	364 (97%)	11 (3%)	48	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	375/400 (94%)	362 (96%)	13 (4%)	41	41
1	I	375/400 (94%)	365 (97%)	10 (3%)	50	50
2	B	171/176 (97%)	170 (99%)	1 (1%)	89	89
3	C	196/202 (97%)	194 (99%)	2 (1%)	80	80
4	D	159/159 (100%)	159 (100%)	0	100	100
All	All	1651/1737 (95%)	1614 (98%)	37 (2%)	60	57

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	123	THR
1	E	330	HIS
1	I	411	ASN
1	E	194	ILE
1	E	209	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	133	ASN
1	A	216	HIS
4	D	164	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.