



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

Aug 17, 2017 – 08:54 AM EDT

PDB ID : 5FJB  
EMDB ID: : EMD-3076  
Title : Cyclophilin A Stabilize HIV-1 Capsid through a Novel Non- canonical Binding Site  
Authors : Liu, C.; Perilla, J.R.; Ning, J.; Lu, M.; Hou, G.; Ramalhu, R.; Bedwell, G.J.; Ahn, J.; Shi, J.; Gronenborn, A.M.; Prevelige Jr, P.E.; Rousso, I.; Aiken, C.; Polenova, T.; Schulten, K.; Zhang, P.  
Deposited on : unknown  
Resolution : 9.00 Å(reported)  
Based on PDB ID : 3J4F

This is a Full wwPDB/EMDataBank EM Map/Model Validation 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.

---

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

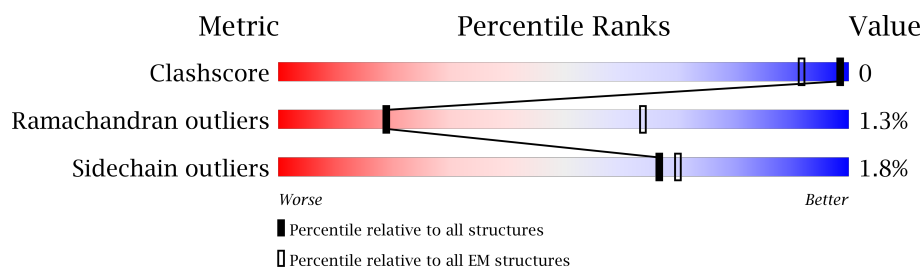
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.00 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)	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	218	
1	B	218	
2	C	164	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4664 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 GAG POLYPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1703	1074	296	320	13		
1	B	218	Total	C	N	O	S	0	0
			1703	1074	296	320	13		

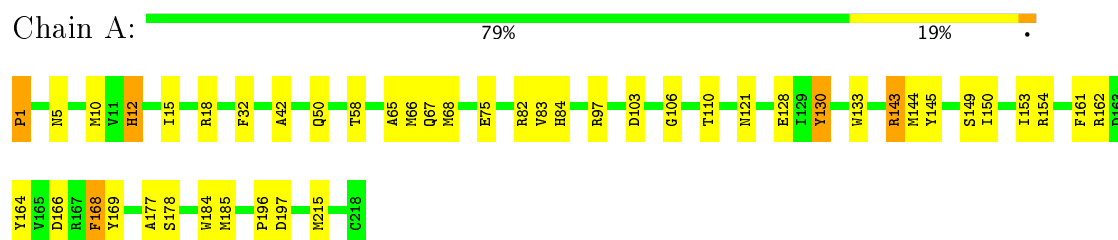
- Molecule 2 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	164	Total	C	N	O	S	0	0
			1258	797	217	236	8		

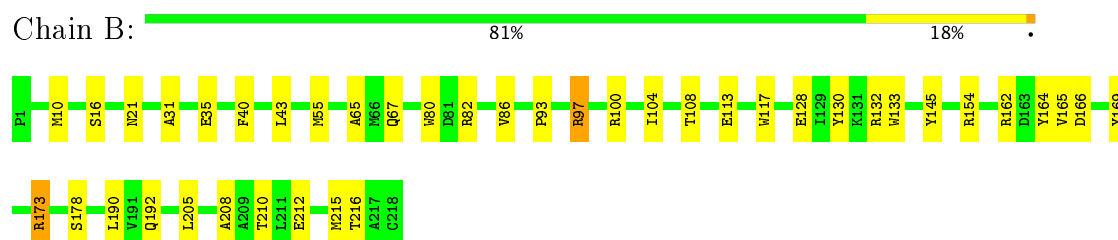
### 3 Residue-property plots [i](#)

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. 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.

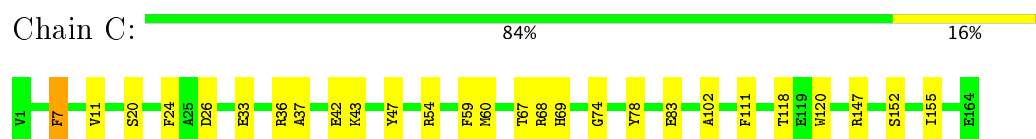
#### • Molecule 1: GAG POLYPROTEIN



#### • Molecule 1: GAG POLYPROTEIN



#### • Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	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	1.66	10/1741 (0.6%)	1.99	32/2368 (1.4%)
1	B	1.59	9/1741 (0.5%)	1.95	35/2368 (1.5%)
2	C	1.67	8/1286 (0.6%)	1.86	22/1723 (1.3%)
All	All	1.64	27/4768 (0.6%)	1.94	89/6459 (1.4%)

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	7
1	B	0	2
2	C	0	2
All	All	0	11

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLY	CA-C	-7.34	1.40	1.51
1	B	16	SER	CA-CB	6.92	1.63	1.52
2	C	83	GLU	CD-OE1	6.88	1.33	1.25
1	B	65	ALA	N-CA	-6.44	1.33	1.46
1	A	145	TYR	CE1-CZ	6.38	1.46	1.38
1	B	205	LEU	C-N	6.19	1.44	1.33
1	B	31	ALA	N-CA	6.05	1.58	1.46
1	A	50	GLN	CA-CB	6.04	1.67	1.53
2	C	36	ARG	CD-NE	5.60	1.55	1.46
2	C	47	TYR	CG-CD2	5.50	1.46	1.39
1	B	133	TRP	CA-CB	5.43	1.66	1.53
2	C	43	LYS	CA-CB	5.40	1.65	1.53
1	A	133	TRP	CE3-CZ3	5.38	1.47	1.38
2	C	147	ARG	CZ-NH1	-5.37	1.26	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	74	GLY	N-CA	5.37	1.54	1.46
1	B	113	GLU	CB-CG	5.31	1.62	1.52
1	A	12	HIS	CG-CD2	-5.28	1.26	1.35
1	A	178	SER	CA-CB	5.26	1.60	1.52
2	C	47	TYR	CZ-OH	5.19	1.46	1.37
1	A	133	TRP	NE1-CE2	-5.18	1.30	1.37
1	B	128	GLU	CD-OE1	5.18	1.31	1.25
2	C	20	SER	CA-CB	5.17	1.60	1.52
1	A	168	PHE	CG-CD1	5.17	1.46	1.38
1	B	178	SER	C-N	5.14	1.45	1.34
1	A	75	GLU	CB-CG	5.11	1.61	1.52
1	A	168	PHE	CE1-CZ	5.08	1.47	1.37
1	B	190	LEU	CA-CB	5.08	1.65	1.53

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH1	22.44	131.52	120.30
1	B	97	ARG	NE-CZ-NH2	-20.21	110.19	120.30
1	A	82	ARG	NE-CZ-NH1	18.10	129.35	120.30
1	B	132	ARG	NE-CZ-NH1	15.42	128.01	120.30
1	B	97	ARG	NE-CZ-NH1	15.29	127.95	120.30
2	C	36	ARG	NE-CZ-NH1	14.37	127.49	120.30
1	A	82	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	B	132	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	154	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	A	162	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	B	145	TYR	CB-CG-CD2	-10.00	115.00	121.00
1	B	100	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	B	173	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	B	162	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	B	169	TYR	CD1-CE1-CZ	-9.34	111.40	119.80
1	A	143	ARG	NE-CZ-NH2	-9.01	115.79	120.30
2	C	36	ARG	NH1-CZ-NH2	-8.93	109.58	119.40
1	A	168	PHE	CB-CG-CD1	8.70	126.89	120.80
1	A	185	MET	CG-SD-CE	-8.68	86.31	100.20
1	A	110	THR	CA-CB-CG2	-8.17	100.96	112.40
2	C	68	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	A	197	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	130	TYR	CB-CG-CD2	-7.61	116.43	121.00
2	C	152	SER	CB-CA-C	-7.52	95.81	110.10
1	B	164	TYR	CB-CG-CD2	-7.40	116.56	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	TYR	CB-CG-CD2	7.37	125.42	121.00
1	A	168	PHE	CB-CG-CD2	-7.30	115.69	120.80
1	A	66	MET	CG-SD-CE	-7.29	88.53	100.20
2	C	59	PHE	CB-CG-CD1	-7.29	115.70	120.80
1	B	169	TYR	CZ-CE2-CD2	-7.19	113.33	119.80
1	B	166	ASP	CB-CG-OD1	7.04	124.64	118.30
2	C	37	ALA	O-C-N	-6.99	111.52	122.70
1	A	97	ARG	NE-CZ-NH1	6.99	123.79	120.30
2	C	120	TRP	CB-CG-CD2	6.99	135.68	126.60
1	B	215	MET	CG-SD-CE	-6.86	89.22	100.20
1	A	144	MET	CG-SD-CE	-6.85	89.24	100.20
2	C	102	ALA	N-CA-CB	-6.80	100.59	110.10
2	C	78	TYR	CB-CG-CD1	-6.78	116.94	121.00
1	A	83	VAL	CG1-CB-CG2	-6.74	100.12	110.90
1	A	215	MET	CA-CB-CG	6.64	124.58	113.30
2	C	67	THR	N-CA-CB	6.42	122.49	110.30
1	B	145	TYR	CB-CG-CD1	6.39	124.84	121.00
2	C	42	GLU	OE1-CD-OE2	-6.28	115.76	123.30
1	B	166	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	166	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	55	MET	CG-SD-CE	-6.12	90.41	100.20
1	B	10	MET	N-CA-C	6.08	127.40	111.00
2	C	59	PHE	CG-CD1-CE1	-5.97	114.23	120.80
2	C	33	GLU	OE1-CD-OE2	-5.86	116.27	123.30
2	C	24	PHE	CB-CG-CD1	5.79	124.85	120.80
1	A	128	GLU	OE1-CD-OE2	-5.78	116.37	123.30
1	B	169	TYR	CG-CD2-CE2	5.77	125.92	121.30
1	A	161	PHE	CB-CG-CD1	5.74	124.81	120.80
1	B	212	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	B	21	ASN	O-C-N	-5.65	113.66	122.70
1	B	108	THR	CA-CB-CG2	-5.62	104.54	112.40
1	A	68	MET	CG-SD-CE	-5.60	91.25	100.20
1	A	154	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	A	103	ASP	CB-CG-OD2	5.47	123.22	118.30
2	C	118	THR	OG1-CB-CG2	-5.47	97.42	110.00
2	C	7	PHE	CB-CA-C	-5.46	99.49	110.40
1	A	84	HIS	CA-CB-CG	-5.43	104.37	113.60
1	B	169	TYR	CB-CG-CD1	5.40	124.24	121.00
1	B	104	ILE	O-C-N	-5.38	114.09	122.70
1	B	82	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	40	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	B	93	PRO	N-CA-C	5.32	125.92	112.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	152	SER	N-CA-CB	5.30	118.46	110.50
2	C	26	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	130	TYR	CG-CD1-CE1	-5.29	117.06	121.30
1	B	208	ALA	CB-CA-C	5.28	118.03	110.10
1	B	67	GLN	CG-CD-OE1	5.28	132.16	121.60
1	A	42	ALA	N-CA-CB	-5.26	102.73	110.10
2	C	54	ARG	CD-NE-CZ	5.26	130.96	123.60
2	C	7	PHE	N-CA-CB	5.25	120.05	110.60
1	A	15	ILE	O-C-N	5.25	131.09	122.70
1	A	65	ALA	O-C-N	-5.21	114.36	122.70
1	B	130	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	A	133	TRP	NE1-CE2-CD2	5.19	112.49	107.30
1	B	210	THR	N-CA-CB	5.17	120.13	110.30
1	B	117	TRP	NE1-CE2-CZ2	5.17	136.09	130.40
1	B	205	LEU	CB-CG-CD2	5.17	119.79	111.00
2	C	147	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	43	LEU	CB-CG-CD2	5.15	119.76	111.00
1	A	184	TRP	CB-CG-CD1	-5.04	120.45	127.00
1	B	165	VAL	CA-CB-CG2	-5.03	103.36	110.90
1	A	103	ASP	OD1-CG-OD2	-5.01	113.78	123.30
1	B	80	TRP	CB-CG-CD2	-5.00	120.09	126.60
2	C	78	TYR	CB-CG-CD2	5.00	124.00	121.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PRO	Peptide
1	A	121	ASN	Peptide
1	A	130	TYR	Sidechain
1	A	168	PHE	Sidechain
1	A	169	TYR	Sidechain
1	A	18	ARG	Sidechain
1	A	32	PHE	Sidechain
1	B	173	ARG	Sidechain
1	B	97	ARG	Sidechain
2	C	111	PHE	Sidechain
2	C	7	PHE	Sidechain

## 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	1703	0	1704	1	0
1	B	1703	0	1704	0	0
2	C	1258	0	1228	1	0
All	All	4664	0	4636	2	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.

All (2) 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:150:ILE:HD12	1:A:153:ILE:HG13	1.82	0.61
2:C:11:VAL:HG22	2:C:155:ILE:HD12	2.03	0.41

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	216/218 (99%)	199 (92%)	12 (6%)	5 (2%)	7	43
1	B	216/218 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
2	C	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	28	71
All	All	594/600 (99%)	553 (93%)	33 (6%)	8 (1%)	19	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	149	SER
1	A	177	ALA
2	C	69	HIS
1	A	5	ASN
1	B	35	GLU
1	B	86	VAL
1	A	196	PRO

### 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	186/186 (100%)	181 (97%)	5 (3%)	50	74
1	B	186/186 (100%)	183 (98%)	3 (2%)	68	85
2	C	132/132 (100%)	131 (99%)	1 (1%)	85	92
All	All	504/504 (100%)	495 (98%)	9 (2%)	67	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	12	HIS
1	A	58	THR
1	A	67	GLN
1	A	143	ARG
1	B	154	ARG
1	B	192	GLN
1	B	216	THR
2	C	60	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	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 ⓘ

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.