



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:12 AM GMT

PDB ID : 3TB8  
Title : Crystal structure of full-length myristoylated HIV-1 Nef  
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Deposited on : 2011-08-05  
Resolution : 3.71 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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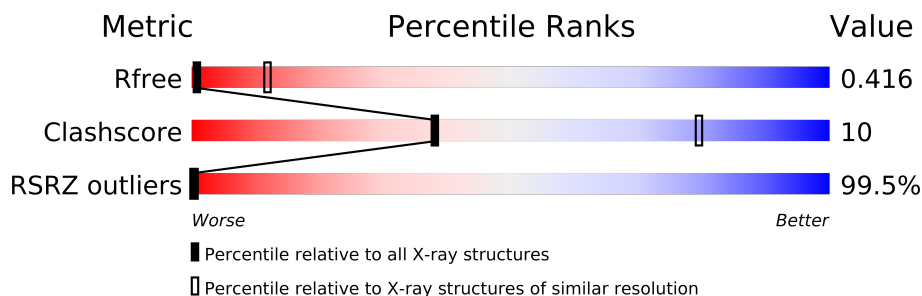
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.71 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))
$R_{free}$	66092	1103 (4.04-3.40)
Clashscore	79885	1026 (3.98-3.46)
RSRZ outliers	66119	1104 (4.04-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	206	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 203 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein Nef.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	203	Total	C	0	0	203
			203	203			

There is a discrepancy between the modelled and reference sequences:

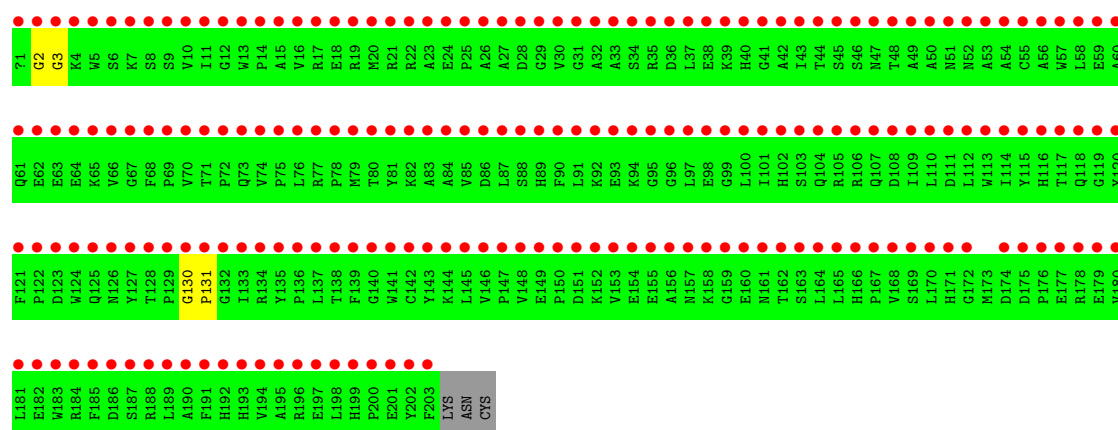
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MYR	-	myristoylated	UNP P03404

### 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 errors 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: Protein Nef

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.33Å 89.33Å 27.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.25 – 3.71 28.25 – 3.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.25-3.71) 99.7 (28.25-3.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.51 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.6.2_432 - Refine	Depositor
R, $R_{free}$	0.231 , 0.337 0.445 , 0.416	Depositor DCC
$R_{free}$ test set	86 reflections (3.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	233.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	1.60 , 81.0	EDS
Estimated twinning fraction	0.487 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 2622 reflections (0.076%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 5$

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	203	0	0	2	0
All	All	203	0	0	2	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:GLY:CA	1:A:3:GLY:CA	2.81	0.59
1:A:130:GLY:CA	1:A:131:PRO:CA	2.98	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains ⓘ

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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.

## 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	A	203/206 (98%)	29.69	202 (99%) 0 0	140, 140, 140, 140	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	CYS	128.5
1	A	58	LEU	118.6
1	A	40	HIS	72.4
1	A	65	LYS	71.8
1	A	24	GLU	71.6
1	A	11	ILE	66.2
1	A	120	TYR	60.7
1	A	112	LEU	59.6
1	A	171	HIS	57.7
1	A	42	ALA	57.0
1	A	12	GLY	55.4
1	A	160	GLU	54.9
1	A	81	TYR	54.2
1	A	15	ALA	54.0
1	A	5	TRP	52.2
1	A	196	ARG	49.9
1	A	22	ARG	48.3
1	A	26	ALA	48.1
1	A	28	ASP	47.6
1	A	151	ASP	47.6
1	A	17	ARG	47.0
1	A	91	LEU	46.3
1	A	117	THR	46.1
1	A	100	LEU	45.7
1	A	25	PRO	45.2
1	A	142	CYS	45.0
1	A	154	GLU	44.0

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Mol	Chain	Res	Type	RSRZ
1	A	150	PRO	43.4
1	A	97	LEU	42.8
1	A	159	GLY	42.6
1	A	141	TRP	42.2
1	A	49	ALA	41.9
1	A	75	PRO	41.8
1	A	125	GLN	41.4
1	A	79	MET	40.7
1	A	8	SER	40.2
1	A	94	LYS	40.2
1	A	7	LYS	39.6
1	A	43	ILE	38.7
1	A	19	ARG	38.2
1	A	74	VAL	38.1
1	A	165	LEU	38.0
1	A	201	GLU	37.1
1	A	52	ASN	37.0
1	A	195	ALA	36.6
1	A	16	VAL	36.6
1	A	34	SER	36.5
1	A	191	PHE	36.4
1	A	44	THR	36.4
1	A	170	LEU	36.2
1	A	143	TYR	35.9
1	A	70	VAL	35.9
1	A	149	GLU	35.7
1	A	128	THR	35.5
1	A	32	ALA	35.0
1	A	121	PHE	35.0
1	A	64	GLU	34.9
1	A	140	GLY	34.9
1	A	133	ILE	34.7
1	A	106	ARG	34.6
1	A	126	ASN	34.5
1	A	124	TRP	34.5
1	A	153	VAL	34.4
1	A	38	GLU	34.3
1	A	189	LEU	34.1
1	A	174	ASP	34.0
1	A	27	ALA	33.9
1	A	101	ILE	33.8
1	A	105	ARG	33.4

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Mol	Chain	Res	Type	RSRZ
1	A	162	THR	33.4
1	A	194	VAL	33.1
1	A	87	LEU	33.1
1	A	176	PRO	32.8
1	A	138	THR	32.7
1	A	80	THR	32.5
1	A	23	ALA	32.5
1	A	78	PRO	32.4
1	A	188	ARG	32.2
1	A	56	ALA	32.2
1	A	109	ILE	32.1
1	A	203	PHE	31.9
1	A	39	LYS	31.7
1	A	132	GLY	31.6
1	A	95	GLY	30.3
1	A	178	ARG	30.2
1	A	147	PRO	30.2
1	A	29	GLY	30.1
1	A	30	VAL	29.9
1	A	60	ALA	29.5
1	A	186	ASP	29.3
1	A	33	ALA	29.1
1	A	107	GLN	29.1
1	A	98	GLU	29.1
1	A	10	VAL	29.1
1	A	62	GLU	29.0
1	A	113	TRP	28.8
1	A	161	ASN	28.8
1	A	158	LYS	28.5
1	A	20	MET	28.3
1	A	169	SER	28.1
1	A	155	GLU	28.1
1	A	118	GLN	28.1
1	A	114	ILE	27.2
1	A	36	ASP	26.9
1	A	2	GLY	26.6
1	A	3	GLY	26.5
1	A	71	THR	26.5
1	A	9	SER	26.5
1	A	116	HIS	25.9
1	A	18	GLU	25.8
1	A	35	ARG	25.8

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	25.8
1	A	13	TRP	25.7
1	A	157	ASN	25.6
1	A	111	ASP	25.2
1	A	37	LEU	25.2
1	A	48	THR	25.2
1	A	144	LYS	25.2
1	A	108	ASP	25.2
1	A	77	ARG	25.0
1	A	63	GLU	24.9
1	A	50	ALA	24.9
1	A	127	TYR	24.9
1	A	119	GLY	24.8
1	A	83	ALA	24.7
1	A	145	LEU	24.7
1	A	152	LYS	24.6
1	A	199	HIS	24.5
1	A	156	ALA	24.4
1	A	179	GLU	23.9
1	A	46	SER	23.5
1	A	164	LEU	23.5
1	A	104	GLN	23.0
1	A	192	HIS	22.7
1	A	66	VAL	22.6
1	A	110	LEU	22.6
1	A	183	TRP	22.5
1	A	187	SER	22.4
1	A	184	ARG	22.4
1	A	31	GLY	22.4
1	A	148	VAL	22.3
1	A	85	VAL	22.3
1	A	92	LYS	22.1
1	A	168	VAL	21.8
1	A	129	PRO	21.4
1	A	14	PRO	21.3
1	A	123	ASP	21.0
1	A	73	GLN	20.9
1	A	59	GLU	20.8
1	A	82	LYS	20.8
1	A	21	ARG	20.0
1	A	99	GLY	20.0
1	A	198	LEU	19.6

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLU	19.6
1	A	72	PRO	19.3
1	A	193	HIS	19.0
1	A	84	ALA	19.0
1	A	61	GLN	19.0
1	A	185	PHE	19.0
1	A	122	PRO	18.9
1	A	93	GLU	18.8
1	A	76	LEU	18.7
1	A	41	GLY	18.6
1	A	139	PHE	18.2
1	A	197	GLU	18.1
1	A	89	HIS	17.6
1	A	175	ASP	17.3
1	A	130	GLY	17.3
1	A	190	ALA	16.9
1	A	1	MYR	16.7
1	A	115	TYR	16.4
1	A	163	SER	16.2
1	A	96	GLY	15.5
1	A	103	SER	15.4
1	A	67	GLY	14.8
1	A	90	PHE	14.2
1	A	137	LEU	13.6
1	A	51	ASN	13.5
1	A	131	PRO	12.8
1	A	4	LYS	12.5
1	A	202	TYR	12.1
1	A	57	TRP	12.0
1	A	53	ALA	11.4
1	A	45	SER	11.3
1	A	88	SER	11.3
1	A	6	SER	10.8
1	A	166	HIS	10.6
1	A	167	PRO	10.4
1	A	136	PRO	10.3
1	A	200	PRO	9.9
1	A	182	GLU	9.8
1	A	69	PRO	9.7
1	A	68	PHE	8.9
1	A	102	HIS	8.5
1	A	47	ASN	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	54	ALA	6.8
1	A	146	VAL	6.8
1	A	135	TYR	6.3
1	A	181	LEU	4.9
1	A	172	GLY	3.7
1	A	134	ARG	3.5
1	A	180	VAL	3.4

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.