



# wwPDB X-ray Structure Validation Summary Report

Mar 6, 2026 – 03:41 PM UTC

PDB ID : 4EN2 / pdb\_00004en2  
Title : HIV-1 Nef in complex with MHC-I cytoplasmic domain and Mu1 adaptin subunit of AP1 adaptor (second domain)  
Authors : Jia, X.; Xiong, Y.  
Deposited on : 2012-04-12  
Resolution : 2.58 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

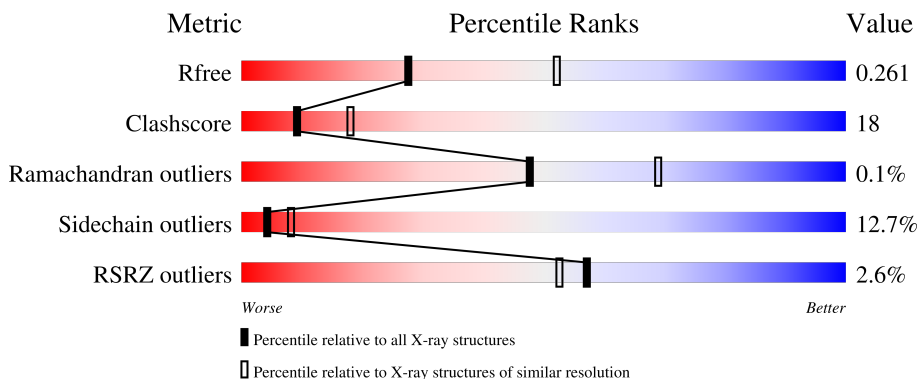
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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.



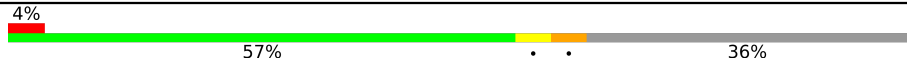
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	A	266	
1	M	266	
2	B	206	
2	C	206	
3	D	28	

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Mol	Chain	Length	Quality of chain
3	E	28	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '4%', a large green segment in the middle labeled '57%', and a grey segment on the right labeled '36%'. There are two small black dots on the bar, one near the end of the green segment and one at the end of the grey segment.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6783 atoms, of which 0 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 AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	256	Total 2085	C 1339	N 365	O 375	S 6	0	0	0
1	A	255	Total 2081	C 1335	N 366	O 374	S 6	0	1	0

- Molecule 2 is a protein called Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	149	Total 1238	C 798	N 218	O 219	S 3	0	0	0
2	C	133	Total 1123	C 733	N 195	O 192	S 3	0	0	0

- Molecule 3 is a protein called MHC-I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	12	Total 81	C 46	N 14	O 21	0	0	0
3	E	18	Total 121	C 68	N 24	O 29	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	18	Total 18 O 18	0	0
4	B	16	Total 16 O 16	0	0
4	C	4	Total 4 O 4	0	0
4	A	13	Total 14 O 14	0	1

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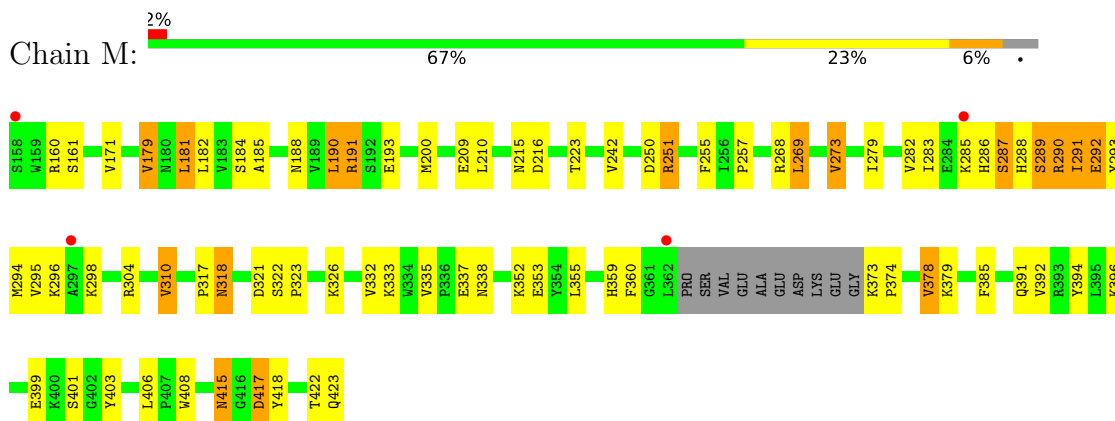
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0

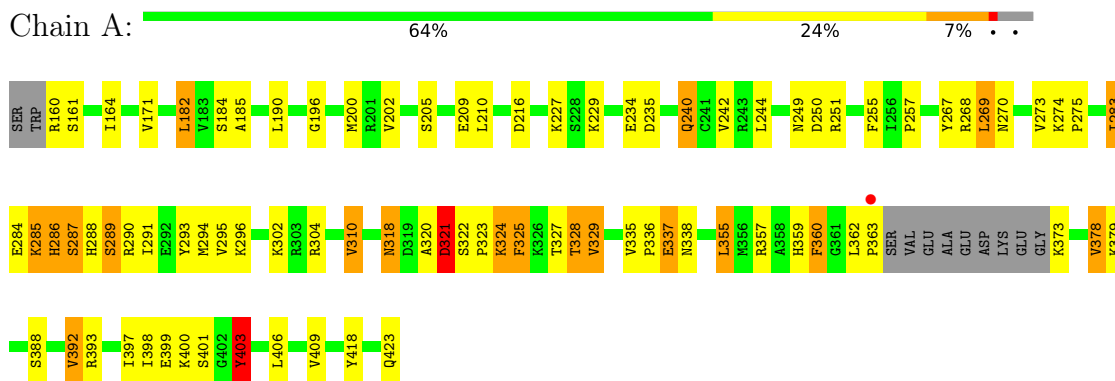
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

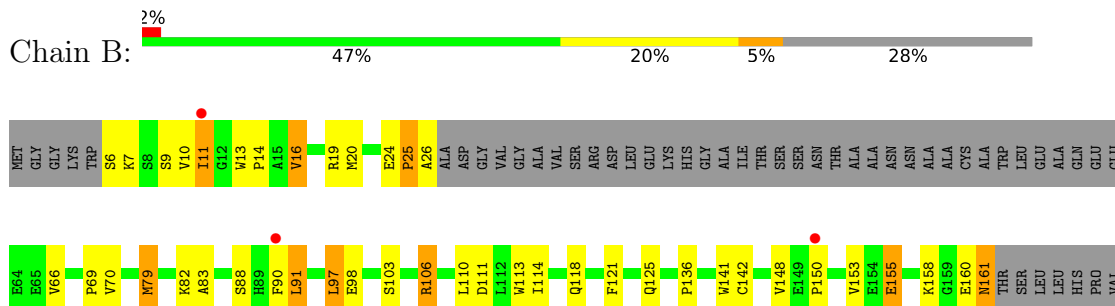
- Molecule 1: AP-1 complex subunit mu-1

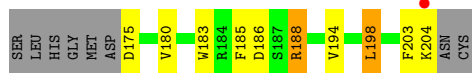


- Molecule 1: AP-1 complex subunit mu-1

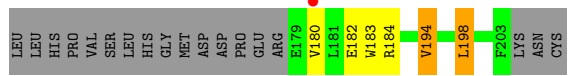
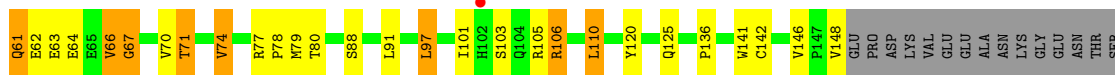
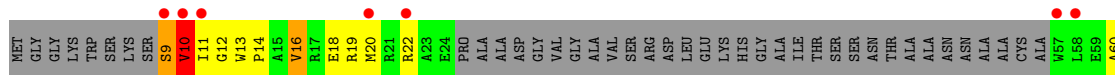


- Molecule 2: Protein Nef

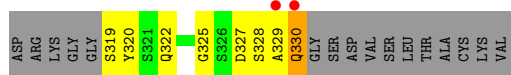




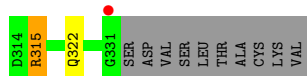
• Molecule 2: Protein Nef



• Molecule 3: MHC-I



• Molecule 3: MHC-I



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.03Å 98.13Å 112.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.58 48.88 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.88-2.58) 98.4 (48.88-2.58)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.58Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.208 , 0.258 0.211 , 0.261	Depositor DCC
$R_{free}$ test set	1561 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [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  >5	RMSZ	# Z  >5
1	A	1.02	0/2132	1.09	3/2875 (0.1%)
1	M	1.00	0/2134	1.09	6/2880 (0.2%)
2	B	1.06	0/1279	0.98	1/1736 (0.1%)
2	C	0.99	0/1163	1.00	4/1582 (0.3%)
3	D	0.94	0/81	0.85	0/108
3	E	1.08	0/121	1.06	1/159 (0.6%)
All	All	1.02	0/6910	1.05	15/9340 (0.2%)

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
2	C	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	251	ARG	CG-CD-NE	-6.68	97.31	112.00
2	C	10	VAL	N-CA-C	6.45	117.13	110.36
2	C	67	GLY	N-CA-C	6.31	122.15	112.81
1	M	415	ASN	N-CA-C	6.22	117.94	111.03
1	M	417	ASP	N-CA-C	5.89	118.33	107.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	64	GLU	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	2081	0	2115	103	0
1	M	2085	0	2111	62	1
2	B	1238	0	1191	41	1
2	C	1123	0	1075	43	0
3	D	81	0	66	10	0
3	E	121	0	105	1	0
4	A	14	0	0	1	0
4	B	16	0	0	0	0
4	C	4	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	M	18	0	0	1	0
All	All	6783	0	6663	243	1

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 18.

The worst 5 of 243 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:M:296:LYS:HG2	1:M:355:LEU:CD2	1.43	1.45
1:M:296:LYS:CG	1:M:355:LEU:HD21	1.63	1.26
1:A:323:PRO:CA	1:A:360:PHE:HB3	1.84	1.08
1:A:320:ALA:HB2	1:A:362:LEU:HD12	1.31	1.04
2:B:79:MET:HE2	2:B:83:ALA:HB3	1.43	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:352:LYS:NZ	2:B:24:GLU:OE2[4_445]	1.90	0.30

## 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	A	252/266 (95%)	240 (95%)	12 (5%)	0	100	100
1	M	252/266 (95%)	238 (94%)	14 (6%)	0	100	100
2	B	143/206 (69%)	138 (96%)	4 (3%)	1 (1%)	18	36
2	C	127/206 (62%)	121 (95%)	6 (5%)	0	100	100
3	D	10/28 (36%)	10 (100%)	0	0	100	100
3	E	16/28 (57%)	16 (100%)	0	0	100	100
All	All	800/1000 (80%)	763 (95%)	36 (4%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	PRO

### 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	A	234/242 (97%)	202 (86%)	32 (14%)	3	6
1	M	234/242 (97%)	208 (89%)	26 (11%)	6	11
2	B	131/173 (76%)	115 (88%)	16 (12%)	5	9
2	C	117/173 (68%)	101 (86%)	16 (14%)	3	6
3	D	8/20 (40%)	6 (75%)	2 (25%)	0	1
3	E	11/20 (55%)	10 (91%)	1 (9%)	9	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	735/870 (84%)	642 (87%)	93 (13%)	<b>4</b> <b>8</b>

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	198	LEU
1	A	287	SER
1	A	164	ILE
1	A	249	ASN
1	A	318	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	GLN
3	E	322	GLN
3	E	330	GLN
3	D	330	GLN
2	B	199	HIS

### 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 oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	255/266 (95%)	0.10	1 (0%) 88 87	33, 70, 119, 153	1 (0%)
1	M	256/266 (96%)	0.18	4 (1%) 70 67	48, 71, 108, 137	0
2	B	149/206 (72%)	0.29	4 (2%) 56 52	48, 67, 115, 157	0
2	C	133/206 (64%)	0.53	9 (6%) 23 19	55, 81, 155, 210	0
3	D	12/28 (42%)	0.60	2 (16%) 4 3	62, 77, 115, 122	0
3	E	18/28 (64%)	0.38	1 (5%) 30 25	60, 70, 116, 118	0
All	All	823/1000 (82%)	0.24	21 (2%) 57 52	33, 72, 120, 210	1 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	PRO	4.7
1	M	297	ALA	4.0
2	C	11	ILE	3.9
2	C	10	VAL	3.5
1	M	362	LEU	3.4

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.