

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 3, 2023 – 12:55 AM EDT

:	3VXS
:	The complex between H27-14 TCR and HLA-A24 bound to HIV-1 Nef134-
	10(6L) peptide
:	Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.
	2012-09-20
:	1.80  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

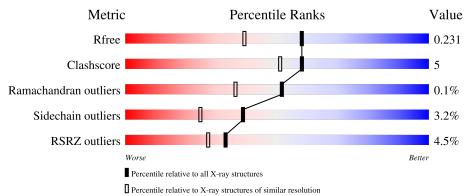
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950(1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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		075	3%	
	A	275	<u>85%</u>	13% •
2	В	100	85%	14% •
			7%	
3	D	207	88%	11% •
		2.4.4	4%	
4	E	244	87%	12% •
F	C	10		
5	C	10	80%	10% 10%



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7402 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 HLA class I histocompatibility antigen, A-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	274	Total 2222	C 1382	N 403	O 427	S 10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	MET	-	expression tag	UNP P05534

• Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 836	C 533	N 141	0 158	S 4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	expression tag	UNP P61769

• Molecule 3 is a protein called H27-14 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	204	Total 1575	C 978	N 266	0 323	S 8	0	0	0

• Molecule 4 is a protein called H27-14 TCR beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	Е	242	Total 1954	C 1226	N 347	0 375	S 6	0	0	0

• Molecule 5 is a protein called 10-mer peptide from Protein Nef.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
۲.	C	10	Total	С	Ν	0	S	0	0	0
0	U	10	89	61	14	13	1	0	0	0

• Molecule 6 is water.

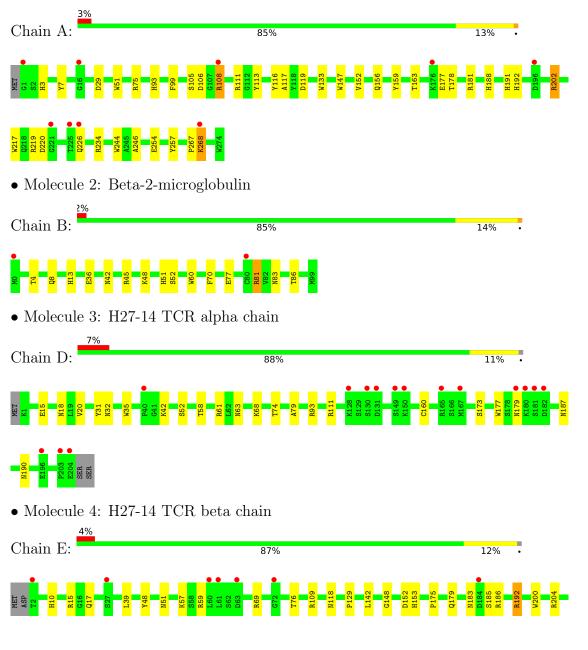
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	243	Total         O           243         243	0	0
6	В	133	Total O 133 133	0	0
6	D	161	Total O 161 161	0	0
6	Е	182	Total         O           182         182	0	0
6	С	7	Total O 7 7	0	0



## 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: HLA class I histocompatibility antigen, A-24 alpha chain







• Molecule 5: 10-mer peptide from Protein Nef

-	10%		
Chain C:	80%	10%	10%
R1 P3 W8 C9 F10			



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.40Å 99.05Å 162.97Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 1.80	Depositor
Resolution (A)	31.91 - 1.80	EDS
% Data completeness	98.5 (50.00-1.80)	Depositor
(in resolution range)	98.5 (31.91-1.80)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.07	Depositor
$< I/\sigma(I) > 1$	$5.71 (at 1.80 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
D D.	0.201 , 0.230	Depositor
$R, R_{free}$	0.202 , $0.231$	DCC
$R_{free}$ test set	4997 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $41.6$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7402	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	
			# Z  > 5	RMSZ	# Z  > 5
1	А	0.58	4/2282~(0.2%)	0.68	2/3092~(0.1%)
2	В	0.57	0/859	0.68	2/1162~(0.2%)
3	D	0.46	2/1604~(0.1%)	0.74	4/2175~(0.2%)
4	Ε	0.56	2/2006~(0.1%)	0.61	0/2724
5	С	0.72	0/93	0.57	0/125
All	All	0.55	8/6844~(0.1%)	0.67	8/9278~(0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	133	TRP	CD2-CE2	5.35	1.47	1.41
1	А	217	TRP	CD2-CE2	5.34	1.47	1.41
3	D	177	TRP	CD2-CE2	5.34	1.47	1.41
4	Е	222	TRP	CD2-CE2	5.13	1.47	1.41
4	Е	200	TRP	CD2-CE2	5.05	1.47	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	202	ARG	NE-CZ-NH2	-12.04	114.28	120.30
3	D	61	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	А	202	ARG	NE-CZ-NH1	10.56	125.58	120.30
3	D	111	ARG	NE-CZ-NH2	-8.99	115.81	120.30
3	D	61	ARG	NE-CZ-NH1	8.40	124.50	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2222	0	2082	29	0
2	В	836	0	803	11	0
3	D	1575	0	1522	13	0
4	Ε	1954	0	1850	12	0
5	С	89	0	87	1	0
6	А	243	0	0	9	0
6	В	133	0	0	1	0
6	С	7	0	0	0	0
6	D	161	0	0	1	0
6	Е	182	0	0	2	0
All	All	7402	0	6344	63	0

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.

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 5.

The worst 5 of 63 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)
2:B:81:ARG:HH11	2:B:81:ARG:HG2	1.30	0.95
1:A:106:ASP:OD2	1:A:108:ARG:HD2	1.65	0.94
3:D:32:ASN:HD21	3:D:93:ARG:HH11	1.26	0.82
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.63	0.79
4:E:10:HIS:HD2	4:E:153:HIS:ND1	1.80	0.79

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 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	Perce	ntiles
1	А	272/275~(99%)	269~(99%)	3(1%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$\mathbf{ntiles}$
2	В	98/100~(98%)	98 (100%)	0	0	100	100
3	D	202/207~(98%)	199~(98%)	3~(2%)	0	100	100
4	Ε	240/244~(98%)	232~(97%)	7 (3%)	1 (0%)	34	21
5	С	8/10 (80%)	8 (100%)	0	0	100	100
All	All	820/836~(98%)	806 (98%)	13 (2%)	1 (0%)	51	36

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All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Ε	218	GLU

#### 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	А	230/231~(100%)	225~(98%)	5(2%)	52 39
2	В	95/95~(100%)	92~(97%)	3(3%)	39 25
3	D	182/185~(98%)	179~(98%)	3 (2%)	62 54
4	Ε	213/215~(99%)	202~(95%)	11 (5%)	23 10
5	С	9/9~(100%)	8 (89%)	1 (11%)	6 1
All	All	729/735~(99%)	706~(97%)	23 (3%)	39 25

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Е	57	LYS
4	Е	109	ARG
4	Е	76	THR
4	Е	118	ASN
2	В	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:



Mol	Chain	Res	Type
3	D	190	ASN
4	Е	41	GLN
4	Е	17	GLN
4	Е	51	ASN
2	В	13	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 monosaccharides 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,  $95^{th}$  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	$OWAB(Å^2)$	Q<0.9
1	А	274/275~(99%)	0.08	9 (3%) 46 40	14, 25, 48, 60	0
2	В	100/100~(100%)	-0.12	2 (2%) 65 61	14, 20, 36, 55	0
3	D	204/207~(98%)	0.23	15 (7%) 14 11	14, 25, 57, 78	0
4	Е	242/244~(99%)	0.10	10 (4%) 37 31	16, 28, 47, 70	0
5	С	10/10 (100%)	1.32	1 (10%) 7 5	16, 20, 28, 33	0
All	All	830/836~(99%)	0.11	37 (4%) 33 27	14, 25, 49, 78	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Ε	2	THR	6.1
3	D	204	GLU	5.2
3	D	182	ASP	4.6
3	D	130	SER	4.4
4	Е	60	LEU	4.4

### 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 monosaccharides in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.



## 6.5 Other polymers (i)

There are no such residues in this entry.

