



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2023 – 12:09 AM EDT

PDB ID : 3W0W  
Title : The complex between T36-5 TCR and HLA-A24 bound to HIV-1 Nef134-10(2F) peptide in space group P212121  
Authors : Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.  
Deposited on : 2012-11-05  
Resolution : 2.60 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 : 4.02b-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) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

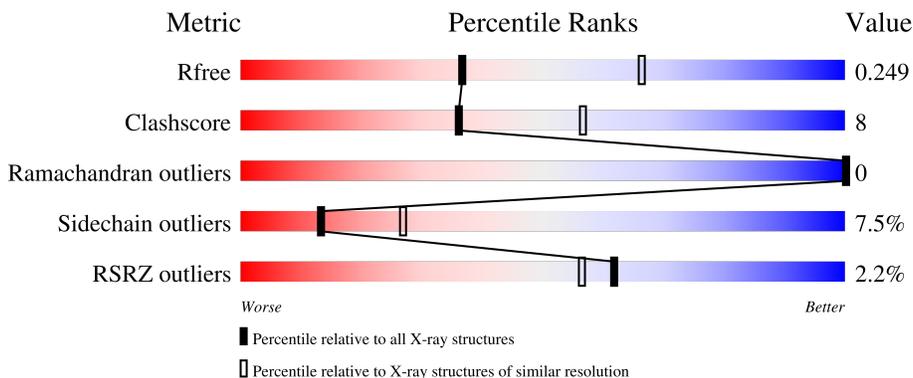
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	291	 3% 75% 19%
2	B	100	 87% 12%
3	C	10	 70% 30%
4	D	205	 4% 75% 21%
5	E	242	 83% 14%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7019 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
			Total	C	N	O	S			
1	A	279	2247	1397	408	432	10	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P05534
A	275	GLY	-	expression tag	UNP P05534
A	276	SER	-	expression tag	UNP P05534
A	277	LEU	-	expression tag	UNP P05534
A	278	GLY	-	expression tag	UNP P05534
A	279	GLY	-	expression tag	UNP P05534
A	280	ILE	-	expression tag	UNP P05534
A	281	PHE	-	expression tag	UNP P05534
A	282	GLU	-	expression tag	UNP P05534
A	283	ALA	-	expression tag	UNP P05534
A	284	MET	-	expression tag	UNP P05534
A	285	LYS	-	expression tag	UNP P05534
A	286	MET	-	expression tag	UNP P05534
A	287	GLU	-	expression tag	UNP P05534
A	288	LEU	-	expression tag	UNP P05534
A	289	ARG	-	expression tag	UNP P05534
A	290	ASP	-	expression tag	UNP P05534

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called 10-mer peptide from Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	10	91	64	14	12	1	0	0	0

- Molecule 4 is a protein called T36-5 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	204	1591	989	263	332	7	0	0	0

- Molecule 5 is a protein called T36-5 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	241	1933	1217	336	372	8	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total 111	O 111	0	0
6	B	53	Total 53	O 53	0	0
6	C	3	Total 3	O 3	0	0
6	D	56	Total 56	O 56	0	0
6	E	97	Total 97	O 97	0	0

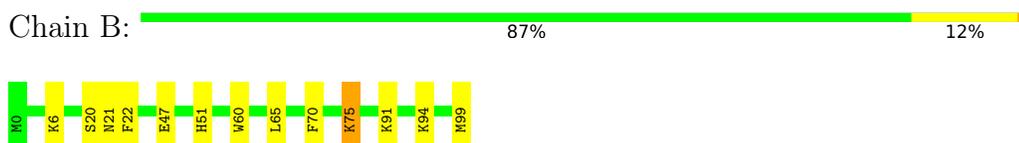
### 3 Residue-property plots [i](#)

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.

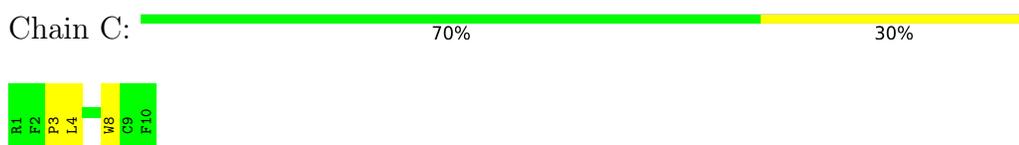
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



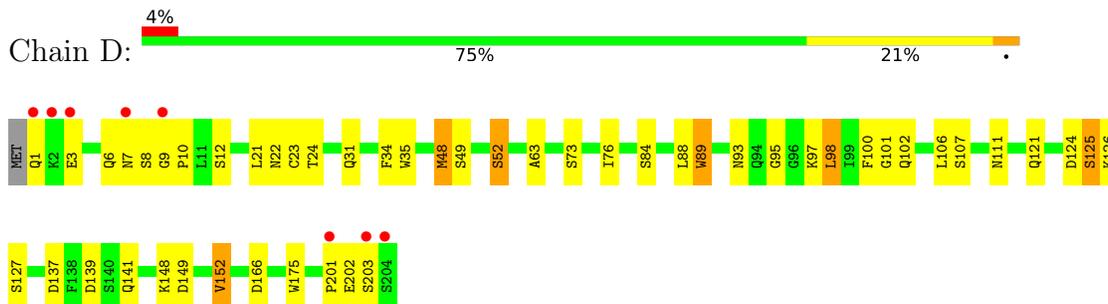
- Molecule 2: Beta-2-microglobulin



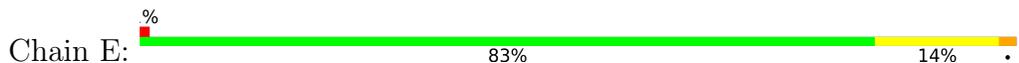
- Molecule 3: 10-mer peptide from Protein Nef

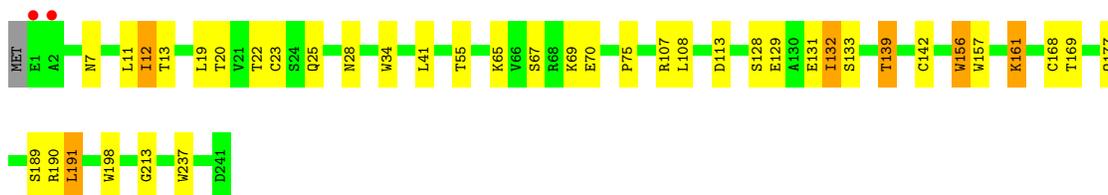


- Molecule 4: T36-5 TCR alpha chain



- Molecule 5: T36-5 TCR beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.92Å 86.44Å 251.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 47.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.60) 99.5 (47.21-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.61Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.186 , 0.250 0.186 , 0.249	Depositor DCC
$R_{free}$ test set	1752 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	0.66	1/2307 (0.0%)	0.72	1/3126 (0.0%)
2	B	0.63	0/860	0.67	0/1162
3	C	1.00	1/96 (1.0%)	0.87	0/128
4	D	0.56	3/1626 (0.2%)	0.67	0/2201
5	E	0.68	4/1986 (0.2%)	0.72	1/2705 (0.0%)
All	All	0.65	9/6875 (0.1%)	0.70	2/9322 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	156	TRP	CD2-CE2	6.14	1.48	1.41
5	E	157	TRP	CD2-CE2	5.78	1.48	1.41
3	C	8	TRP	CD2-CE2	5.67	1.48	1.41
5	E	198	TRP	CD2-CE2	5.49	1.48	1.41
1	A	60	TRP	CD2-CE2	5.40	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	113	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	145	ARG	NE-CZ-NH1	5.84	123.22	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 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	2247	0	2107	58	0
2	B	837	0	803	5	0
3	C	91	0	85	2	0
4	D	1591	0	1495	29	0
5	E	1933	0	1845	15	0
6	A	111	0	0	4	0
6	B	53	0	0	1	0
6	C	3	0	0	0	0
6	D	56	0	0	3	0
6	E	97	0	0	2	0
All	All	7019	0	6335	104	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 8.

The worst 5 of 104 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)
4:D:7:ASN:ND2	4:D:23:CYS:SG	2.37	0.96
1:A:75:ARG:HH11	1:A:75:ARG:HG3	1.36	0.90
4:D:48:MET:HG2	4:D:63:ALA:HB2	1.63	0.79
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.52	0.75
1:A:194:ILE:HG13	1:A:195:SER:N	2.03	0.74

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	Percentiles
1	A	277/291 (95%)	266 (96%)	11 (4%)	0	100 100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
5	E	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
All	All	824/848 (97%)	792 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	232/243 (96%)	218 (94%)	14 (6%)	19	39
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	28
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	11
4	D	182/183 (100%)	166 (91%)	16 (9%)	10	19
5	E	214/215 (100%)	197 (92%)	17 (8%)	12	24
All	All	732/745 (98%)	677 (92%)	55 (8%)	13	27

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	76	ILE
4	D	152	VAL
5	E	191	LEU
5	E	132	ILE
4	D	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	143	ASN
4	D	146	GLN

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Mol	Chain	Res	Type
4	D	189	ASN
1	A	197	HIS
4	D	7	ASN

### 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<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	279/291 (95%)	-0.45	8 (2%) 51 45	16, 28, 91, 123	0
2	B	100/100 (100%)	-0.60	0 100 100	20, 31, 58, 72	0
3	C	10/10 (100%)	-0.75	0 100 100	17, 20, 24, 27	0
4	D	204/205 (99%)	-0.29	8 (3%) 39 32	20, 42, 81, 117	0
5	E	241/242 (99%)	-0.62	2 (0%) 86 84	16, 29, 55, 110	0
All	All	834/848 (98%)	-0.48	18 (2%) 62 56	16, 32, 82, 123	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	203	SER	5.9
1	A	276	SER	5.6
1	A	277	LEU	5.2
4	D	204	SER	4.0
5	E	1	GLU	3.7

### 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.