



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 PM GMT

PDB ID : 3VXS
Title : The complex between H27-14 TCR and HLA-A24 bound to HIV-1 Nef134-10(6L) peptide
Authors : Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.
Deposited on : 2012-09-20
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

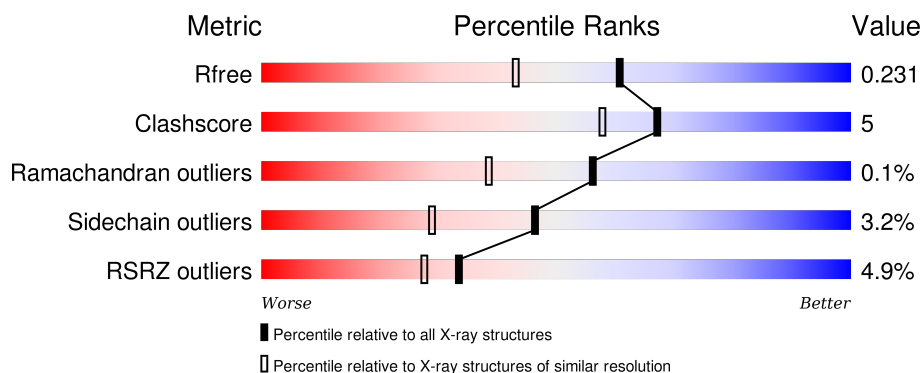
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	275	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	B	100	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	D	207	<div> <div>8%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
4	E	244	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
5	C	10	<div> <div>30%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>

2 Entry composition

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	A	274	Total	C	N	O	S	0	0	0
			2222	1382	403	427	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P05534

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

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

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 H27-14 TCR alpha chain.

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

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

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


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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	10	Total	C	N	O	S	0	0	0
			89	61	14	13	1			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total	O	0	0
			243	243		
6	B	133	Total	O	0	0
			133	133		
6	D	161	Total	O	0	0
			161	161		
6	E	182	Total	O	0	0
			182	182		
6	C	7	Total	O	0	0
			7	7		

- Molecule 5: 10-mer peptide from Protein Nef

Chain C:  30% 80% 10% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.40Å 99.05Å 162.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 31.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-1.80) 98.5 (31.91-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.201 , 0.230 0.202 , 0.231	Depositor DCC
R_{free} test set	5072 reflections (5.34%)	DCC
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 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 100049 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.58	4/2282 (0.2%)	0.68	2/3092 (0.1%)
2	B	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	E	0.56	2/2006 (0.1%)	0.61	0/2724
5	C	0.72	0/93	0.57	0/125
All	All	0.55	8/6844 (0.1%)	0.67	8/9278 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	TRP	CD2-CE2	5.35	1.47	1.41
1	A	217	TRP	CD2-CE2	5.34	1.47	1.41
3	D	177	TRP	CD2-CE2	5.34	1.47	1.41
4	E	222	TRP	CD2-CE2	5.13	1.47	1.41
4	E	200	TRP	CD2-CE2	5.05	1.47	1.41
1	A	51	TRP	CD2-CE2	5.03	1.47	1.41
1	A	147	TRP	CD2-CE2	5.03	1.47	1.41
3	D	35	TRP	CD2-CE2	5.01	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	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	A	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
2	B	45	ARG	NE-CZ-NH2	-7.65	116.47	120.30
3	D	111	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	B	45	ARG	NE-CZ-NH1	5.43	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2222	0	2082	29	0
2	B	836	0	803	11	0
3	D	1575	0	1522	13	0
4	E	1954	0	1850	12	0
5	C	89	0	87	1	0
6	A	243	0	0	9	0
6	B	133	0	0	1	0
6	C	7	0	0	0	0
6	D	161	0	0	1	0
6	E	182	0	0	2	0
All	All	7402	0	6344	63	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 5.

All (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
3:D:187:ASN:HA	3:D:190:ASN:ND2	2.00	0.76
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.24	0.73
3:D:58:THR:HG22	3:D:63:ASN:ND2	2.03	0.73
3:D:173:SER:OG	4:E:192:ARG:HD3	1.89	0.72
1:A:188:HIS:HD2	6:A:302:HOH:O	1.72	0.71
3:D:18:ASN:HD22	3:D:79:ALA:H	1.39	0.70
2:B:81:ARG:NH1	2:B:81:ARG:HG2	2.08	0.68
2:B:4:THR:HG22	2:B:86:THR:HB	1.76	0.67
1:A:220:ASP:HA	6:A:354:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD2	6:A:391:HOH:O	1.94	0.66
3:D:18:ASN:ND2	3:D:79:ALA:H	1.94	0.64
3:D:32:ASN:ND2	3:D:93:ARG:HH11	1.96	0.63
4:E:10:HIS:CD2	4:E:153:HIS:ND1	2.66	0.62
3:D:32:ASN:HD21	3:D:93:ARG:NH1	1.99	0.59
2:B:13:HIS:HE1	6:B:122:HOH:O	1.84	0.58
1:A:111:ARG:HD3	6:A:466:HOH:O	2.03	0.58
1:A:106:ASP:OD2	1:A:108:ARG:CD	2.48	0.57
1:A:234:ARG:HH11	2:B:8:GLN:NE2	2.02	0.57
3:D:52:SER:HB2	3:D:68:LYS:HD2	1.87	0.57
4:E:148:GLY:O	4:E:186:ARG:HD2	2.05	0.56
4:E:204:ARG:HD2	4:E:204:ARG:O	2.06	0.54
1:A:202:ARG:CD	1:A:244:TRP:CE3	2.90	0.54
3:D:20:VAL:HG13	3:D:74:THR:HG23	1.90	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
2:B:81:ARG:CG	2:B:81:ARG:HH11	2.10	0.53
1:A:192:HIS:CD2	6:A:360:HOH:O	2.62	0.53
2:B:36:GLU:HB2	2:B:83:ASN:HB3	1.90	0.52
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.45	0.51
4:E:153:HIS:HB2	6:E:339:HOH:O	2.12	0.50
1:A:191:HIS:HE1	1:A:254:GLU:OE1	1.94	0.50
3:D:31:TYR:HD2	3:D:32:ASN:HD22	1.58	0.49
1:A:219:ARG:HD3	1:A:257:TYR:CZ	2.48	0.49
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.96	0.48
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.49	0.48
1:A:178:THR:HA	1:A:181:ARG:HD3	1.96	0.47
1:A:152:VAL:HG13	1:A:156:GLN:HE21	1.79	0.47
3:D:20:VAL:HG13	3:D:74:THR:CG2	2.44	0.47
2:B:42:ASN:ND2	2:B:77:GLU:H	2.13	0.46
4:E:51:ASN:O	4:E:69:ARG:HD3	2.15	0.46
1:A:219:ARG:HB2	1:A:257:TYR:CE1	2.51	0.46
5:C:2:TYR:CD2	5:C:3:PRO:HD2	2.51	0.45
1:A:192:HIS:HD2	6:A:360:HOH:O	1.96	0.45
2:B:81:ARG:CG	2:B:81:ARG:NH1	2.73	0.45
1:A:111:ARG:HG2	6:A:313:HOH:O	2.15	0.45
4:E:152:ASP:HB2	4:E:175:PRO:HG2	1.99	0.44
4:E:179:GLN:O	4:E:185:SER:HB2	2.18	0.44
1:A:219:ARG:HG2	6:A:491:HOH:O	2.18	0.43
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.54	0.43
1:A:267:PRO:HB2	1:A:268:LYS:HD3	2.00	0.43
3:D:179:ASN:N	6:D:410:HOH:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:HE1	6:A:536:HOH:O	2.02	0.42
1:A:7:TYR:HB2	1:A:99:PHE:CE1	2.54	0.42
4:E:216:LEU:HD22	4:E:229:PRO:HG2	2.02	0.42
4:E:129:PRO:HD3	4:E:142:LEU:HG	2.03	0.41
2:B:51:HIS:HD2	2:B:52:SER:O	2.04	0.41
4:E:15:ARG:NH1	6:E:441:HOH:O	2.54	0.41
1:A:202:ARG:HD3	1:A:246:ALA:HB2	2.02	0.40
1:A:159:TYR:CD1	1:A:163:THR:HB	2.56	0.40

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 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	272/275 (99%)	269 (99%)	3 (1%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	0	100	100
3	D	202/207 (98%)	199 (98%)	3 (2%)	0	100	100
4	E	240/244 (98%)	232 (97%)	7 (3%)	1 (0%)	39	23
5	C	8/10 (80%)	8 (100%)	0	0	100	100
All	All	820/836 (98%)	806 (98%)	13 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	218	GLU

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 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	230/231 (100%)	225 (98%)	5 (2%)	60	45
2	B	95/95 (100%)	92 (97%)	3 (3%)	46	29
3	D	182/185 (98%)	179 (98%)	3 (2%)	70	59
4	E	213/215 (99%)	202 (95%)	11 (5%)	29	12
5	C	9/9 (100%)	8 (89%)	1 (11%)	8	1
All	All	729/735 (99%)	706 (97%)	23 (3%)	46	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	SER
1	A	108	ARG
1	A	177	GLU
1	A	226	GLN
1	A	268	LYS
2	B	48	LYS
2	B	70	PHE
2	B	81	ARG
3	D	15	GLU
3	D	42	LYS
3	D	160	CYS
4	E	17	GLN
4	E	39	LEU
4	E	48	TYR
4	E	57	LYS
4	E	59	ARG
4	E	76	THR
4	E	109	ARG
4	E	118	ASN
4	E	183	ASN
4	E	192	ARG
4	E	219	ASN
5	C	2	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	72	GLN
1	A	93	HIS
1	A	188	HIS
1	A	191	HIS
2	B	8	GLN
2	B	13	HIS
2	B	24	ASN
2	B	42	ASN
2	B	51	HIS
3	D	18	ASN
3	D	32	ASN
3	D	63	ASN
3	D	148	GLN
3	D	190	ASN
4	E	10	HIS
4	E	17	GLN
4	E	41	GLN
4	E	51	ASN
4	E	179	GLN
4	E	183	ASN
4	E	206	HIS
4	E	219	ASN

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 [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 ⓘ

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, 95th 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	A	274/275 (99%)	0.12	10 (3%) 46 40	14, 25, 48, 60	0
2	B	100/100 (100%)	-0.08	2 (2%) 68 64	14, 20, 36, 55	0
3	D	204/207 (98%)	0.27	16 (7%) 16 12	14, 25, 57, 78	0
4	E	242/244 (99%)	0.14	10 (4%) 41 35	16, 28, 47, 70	0
5	C	10/10 (100%)	1.38	3 (30%) 1 0	16, 20, 28, 33	0
All	All	830/836 (99%)	0.15	41 (4%) 33 27	14, 25, 49, 78	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	2	THR	6.1
3	D	204	GLU	5.3
3	D	182	ASP	4.7
3	D	130	SER	4.5
4	E	60	LEU	4.5
3	D	131	ASP	4.2
3	D	40	PRO	4.2
3	D	203	PRO	4.1
1	A	226	GLN	3.8
3	D	181	SER	3.7
1	A	221	GLY	3.2
1	A	16	GLY	3.2
4	E	61	LEU	3.0
3	D	150	LYS	2.9
4	E	218	GLU	2.9
3	D	165	ARG	2.9
1	A	268	LYS	2.9
1	A	225	THR	2.8
1	A	108	ARG	2.7
2	B	80	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	E	72	GLY	2.6
4	E	27	SER	2.6
3	D	128	LYS	2.5
1	A	1	GLY	2.5
4	E	219	ASN	2.4
4	E	63	ASP	2.4
3	D	167	MET	2.4
3	D	149	SER	2.4
2	B	0	MET	2.4
3	D	180	LYS	2.3
4	E	243	ASP	2.3
5	C	8	TRP	2.2
3	D	179	ASN	2.1
1	A	196	ASP	2.1
3	D	196	GLU	2.1
4	E	184	ASP	2.1
1	A	176	LYS	2.1
5	C	6	LEU	2.0
3	D	143	GLN	2.0
1	A	197	HIS	2.0
5	C	4	LEU	2.0

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 carbohydrates 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.