



# wwPDB X-ray Structure Validation Summary Report

Aug 19, 2014 – 04:39 PM EDT

PDB ID : 4L3E  
Title : The complex between high affinity TCR DMF5(alpha-D26Y,beta-L98W)and human Class I MHC HLA-A2 with the bound MART-1(26-35)(A27L) peptide  
Authors : Hellman, L.M.  
Deposited on : 2013-06-05  
Resolution : 2.56 Å(reported)

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

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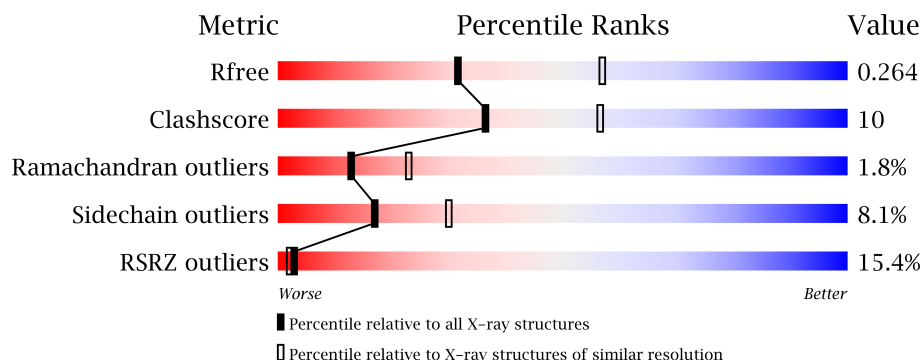
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
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)	:	stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.56 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	2347 (2.60-2.52)
Clashscore	79885	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)
RSRZ outliers	66119	2347 (2.60-2.52)

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	275	
2	B	100	
3	C	10	
4	D	199	
5	E	242	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6615 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- 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
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called Melanoma antigen recognized by T-cells 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	45	10	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LEU	ALA	ENGINEERED MUTATION	UNP Q16655

- Molecule 4 is a protein called DMF5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1549	970	255	316	8			

- Molecule 5 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total 1902	C 1196	N 334	O 364	S 8	0	0	0

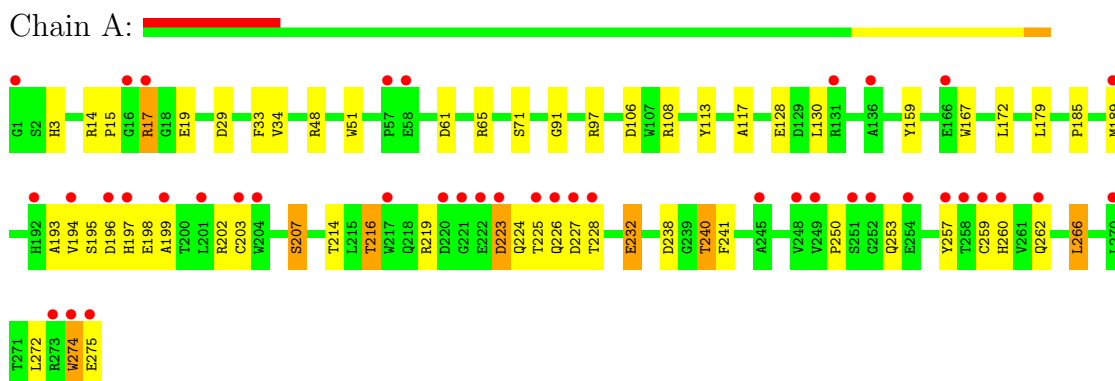
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	O 4	0	0
6	B	2	Total 2	O 2	0	0
6	C	1	Total 1	O 1	0	0
6	D	3	Total 3	O 3	0	0
6	E	2	Total 2	O 2	0	0

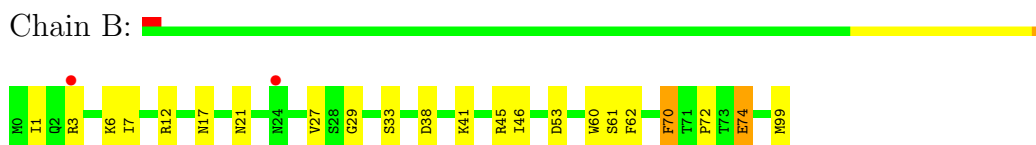
### 3 Residue-property plots

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: HLA class I histocompatibility antigen, A-2 alpha chain



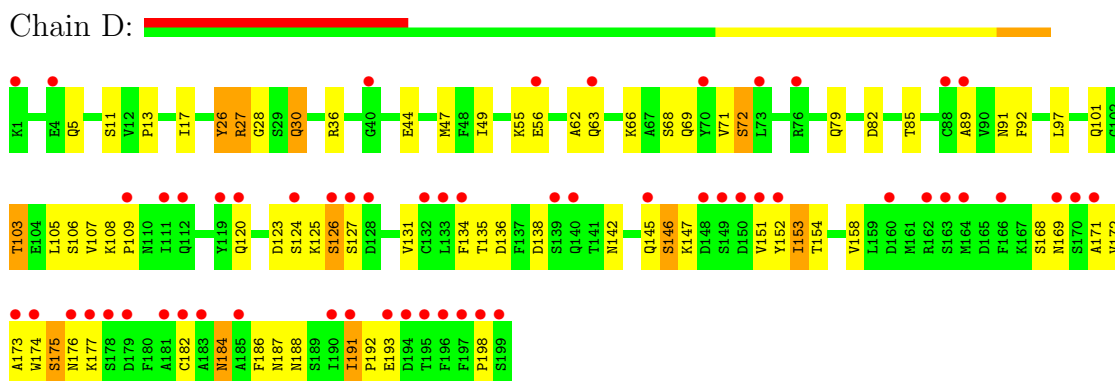
- Molecule 2: Beta-2-microglobulin



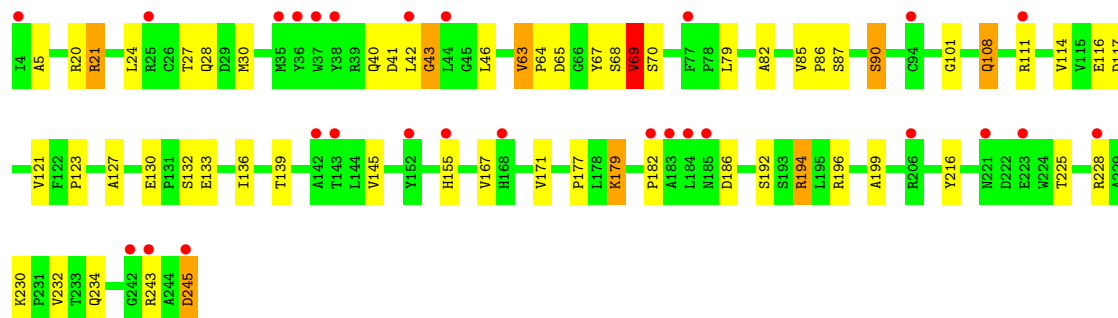
- Molecule 3: Melanoma antigen recognized by T-cells 1



- Molecule 4: DMF5 alpha chain



## ● Molecule 5: DMF5 beta chain

Chain E: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.04Å 49.32Å 92.89Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	20.05 – 2.56 20.05 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.05-2.56) 94.8 (20.05-2.56)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.229 , 0.266 0.226 , 0.264	Depositor DCC
$R_{free}$ test set	1625 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 31904 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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

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	0.43	0/2311	0.60	0/3137
2	B	0.44	0/860	0.58	0/1162
3	C	0.79	0/68	0.78	0/90
4	D	0.49	0/1583	0.59	0/2142
5	E	0.45	1/1953 (0.1%)	0.60	1/2663 (0.0%)
All	All	0.46	1/6775 (0.0%)	0.59	1/9194 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	64	PRO	N-CD	5.33	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	63	VAL	C-N-CD	5.52	139.99	128.40

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	2246	0	2096	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	837	0	803	15	0
3	C	69	0	79	1	0
4	D	1549	0	1467	58	0
5	E	1902	0	1807	34	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
All	All	6615	0	6252	132	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.

The worst 5 of 132 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:26:TYR:HE1	4:D:28:GLY:HA3	1.16	1.07
4:D:26:TYR:HE1	4:D:28:GLY:CA	1.81	0.93
4:D:26:TYR:CE1	4:D:28:GLY:CA	2.55	0.88
4:D:26:TYR:CE1	4:D:28:GLY:HA3	2.07	0.88
1:A:274:TRP:HE3	1:A:275:GLU:H	1.24	0.85

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	273/275 (99%)	260 (95%)	9 (3%)	4 (2%)	15	28
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	197/199 (99%)	177 (90%)	14 (7%)	6 (3%)	7	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	240/242 (99%)	221 (92%)	14 (6%)	5 (2%)	11	18
All	All	816/826 (99%)	762 (93%)	39 (5%)	15 (2%)	13	23

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
4	D	126	SER
5	E	42	LEU
1	A	196	ASP
1	A	227	ASP

### 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	231/231 (100%)	216 (94%)	15 (6%)	24	43
2	B	95/95 (100%)	92 (97%)	3 (3%)	51	78
3	C	7/7 (100%)	6 (86%)	1 (14%)	5	7
4	D	176/176 (100%)	157 (89%)	19 (11%)	9	16
5	E	204/204 (100%)	184 (90%)	20 (10%)	12	20
All	All	713/713 (100%)	655 (92%)	58 (8%)	17	30

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	71	VAL
4	D	127	SER
5	E	186	ASP
4	D	72	SER
4	D	85	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	37	GLN
5	E	234	GLN
5	E	33	ASN
1	A	197	HIS
4	D	113	ASN

### 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	275/275 (100%)	0.79	41 (14%) 3 2	14, 44, 112, 129	0
2	B	100/100 (100%)	0.37	2 (2%) 62 63	15, 33, 67, 78	0
3	C	10/10 (100%)	0.18	0 100 100	13, 19, 27, 34	0
4	D	199/199 (100%)	1.44	57 (28%) 1 1	31, 72, 130, 159	0
5	E	242/242 (100%)	0.82	27 (11%) 6 5	18, 62, 109, 135	0
All	All	826/826 (100%)	0.90	127 (15%) 3 2	13, 53, 116, 159	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	126	SER	6.4
5	E	42	LEU	6.4
4	D	190	ILE	6.3
4	D	127	SER	5.8
5	E	184	LEU	5.7

### 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.