



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:41 PM GMT

PDB ID : 3RDT  
Title : Crystal Structure of 809.B5 TCR complexed with MHC Class II I-Ab/3k peptide  
Authors : Trenh, P.; Huseby, E.S.; Stern, L.J.  
Deposited on : 2011-04-01  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation 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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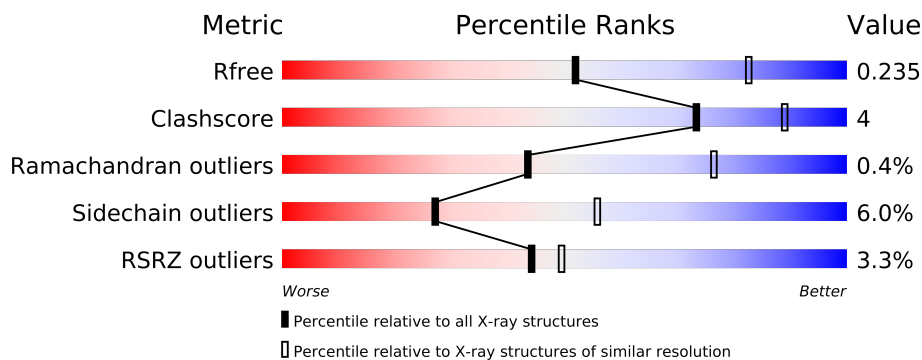
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	C	182	
2	D	217	
3	A	205	
4	B	241	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6399 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 H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	179	Total	C	N	O	S	0	0	0
			1409	913	220	273	3			

- Molecule 2 is a protein called 3K peptide, linker and MHC H-2 class II I-Ab beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	199	Total	C	N	O	S	0	0	0
			1625	1021	290	307	7			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	LINKER	UNP P14483
D	-11	GLY	-	LINKER	UNP P14483
D	-10	GLY	-	LINKER	UNP P14483
D	-9	GLY	-	LINKER	UNP P14483
D	-8	SER	-	LINKER	UNP P14483
D	-7	LEU	-	LINKER	UNP P14483
D	-6	VAL	-	LINKER	UNP P14483
D	-5	PRO	-	LINKER	UNP P14483
D	-4	ARG	-	LINKER	UNP P14483
D	-3	GLY	-	LINKER	UNP P14483
D	-2	SER	-	LINKER	UNP P14483
D	-1	GLY	-	LINKER	UNP P14483
D	0	GLY	-	LINKER	UNP P14483
D	1	GLY	-	LINKER	UNP P14483
D	2	GLY	-	LINKER	UNP P14483

- Molecule 3 is a protein called TCR 809.B5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	199	Total	C	N	O	S	0	0	0
			1512	960	240	305	7			

- Molecule 4 is a protein called TCR 809.B5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	238	Total	C	N	O	S	0	0	0
			1853	1168	324	355	6			

### 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 ( $\text{RSRZ} > 2$ ). 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.

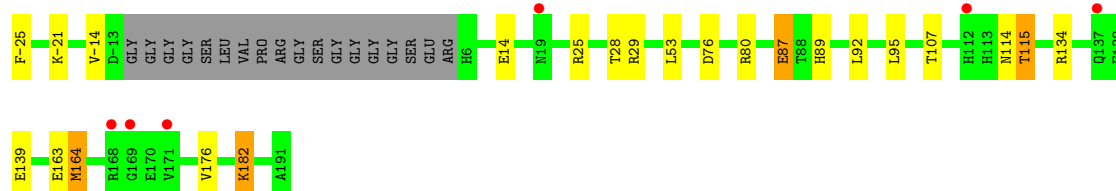
- Molecule 1: H-2 class II histocompatibility antigen, A-B alpha chain

Chain C: 



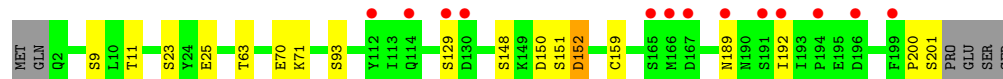
- Molecule 2: 3K peptide, linker and MHC H-2 class II I-Ab beta chain

Chain D: 



- Molecule 3: TCR 809.B5 alpha chain

Chain A: 



- Molecule 4: TCR 809.B5 beta chain

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.85Å 73.02Å 65.67Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.98 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.70) 98.3 (29.98-2.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, $R_{free}$	0.206 , 0.241 0.198 , 0.235	Depositor DCC
$R_{free}$ test set	1525 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.8	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 30635 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage'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.

## 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	C	0.46	0/1453	0.58	0/1991
2	D	0.46	0/1665	0.61	0/2262
3	A	0.40	0/1550	0.54	0/2111
4	B	0.42	0/1906	0.54	0/2603
All	All	0.43	0/6574	0.57	0/8967

There are no bond length outliers.

There are no bond angle outliers.

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	C	1409	0	24	9	0
2	D	1625	0	0	10	0
3	A	1512	0	0	6	0
4	B	1853	0	15	4	0
All	All	6399	0	39	27	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 4.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1:GLU:H	1:C:1:GLU:CD	1.89	0.76
2:D:-25:PHE:CZ	2:D:89:HIS:CD2	2.88	0.62
2:D:-25:PHE:CE2	2:D:89:HIS:CD2	2.91	0.59
1:C:175:LEU:N	1:C:175:LEU:CD1	2.67	0.58
1:C:0:ILE:HD12	1:C:0:ILE:N	2.21	0.56
4:B:221:GLN:CG	4:B:222:ASP:N	2.68	0.56
1:C:75:LYS:O	1:C:78:ASN:N	2.43	0.52
2:D:76:ASP:OD1	2:D:80:ARG:NE	2.44	0.51
2:D:115:THR:CB	2:D:163:GLU:OE1	2.60	0.49
2:D:87:GLU:CA	2:D:87:GLU:OE1	2.61	0.49
3:A:151:SER:O	3:A:152:ASP:CB	2.60	0.48
1:C:0:ILE:O	1:C:0:ILE:HG22	2.15	0.47
2:D:134:ARG:NH1	2:D:139:GLU:OE2	2.49	0.46
3:A:159:CYS:CB	4:B:189:ARG:NH2	2.81	0.44
4:B:31:TYR:CD1	4:B:31:TYR:N	2.85	0.43
1:C:1:GLU:CD	1:C:1:GLU:N	2.66	0.43
1:C:26:PHE:CD1	2:D:87:GLU:OE2	2.71	0.43
2:D:114:ASN:CB	2:D:164:MET:CE	2.96	0.43
1:C:171:GLU:N	1:C:171:GLU:OE1	2.52	0.42
2:D:14:GLU:OE1	2:D:29:ARG:NH1	2.53	0.42
1:C:103:ASN:OD1	1:C:104:THR:N	2.53	0.42
3:A:148:SER:OG	3:A:150:ASP:O	2.38	0.42
3:A:25:GLU:O	3:A:71:LYS:NZ	2.53	0.42
3:A:200:PRO:O	3:A:201:SER:CB	2.68	0.41
2:D:182:LYS:CD	2:D:182:LYS:N	2.84	0.41
4:B:36:ASP:OD1	4:B:85:SER:OG	2.38	0.41
3:A:70:GLU:O	3:A:71:LYS:C	2.60	0.41

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	C	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
2	D	195/217 (90%)	189 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	197/205 (96%)	184 (93%)	11 (6%)	2 (1%)	22	51
4	B	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	43	76
All	All	805/845 (95%)	772 (96%)	30 (4%)	3 (0%)	43	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	129	SER
3	A	152	ASP
4	B	113	LEU

### 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	C	154/163 (94%)	144 (94%)	10 (6%)	24	51
2	D	175/189 (93%)	162 (93%)	13 (7%)	20	43
3	A	163/183 (89%)	156 (96%)	7 (4%)	40	72
4	B	196/206 (95%)	185 (94%)	11 (6%)	30	59
All	All	688/741 (93%)	647 (94%)	41 (6%)	27	56

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	GLU
1	C	15	SER
1	C	18	ASP
1	C	36	LEU
1	C	45	LEU
1	C	66	VAL
1	C	98	LEU
1	C	135	THR
1	C	171	GLU
1	C	175	LEU
2	D	-21	LYS

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Mol	Chain	Res	Type
2	D	-14	VAL
2	D	25	ARG
2	D	28	THR
2	D	53	LEU
2	D	87	GLU
2	D	92	LEU
2	D	95	LEU
2	D	107	THR
2	D	115	THR
2	D	164	MET
2	D	176	VAL
2	D	182	LYS
3	A	9	SER
3	A	11	THR
3	A	23	SER
3	A	63	THR
3	A	93	SER
3	A	189	ASN
3	A	192	ILE
4	B	18	THR
4	B	23	GLN
4	B	24	THR
4	B	26	ASN
4	B	37	THR
4	B	77	GLU
4	B	108	SER
4	B	167	CYS
4	B	180	ASN
4	B	189	ARG
4	B	195	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	C	179/182 (98%)	-0.16	0 100 100	23, 43, 77, 107	0
2	D	199/217 (91%)	-0.01	6 (3%) 48 54	23, 45, 79, 103	0
3	A	199/205 (97%)	0.11	13 (6%) 18 21	25, 54, 106, 163	0
4	B	238/241 (98%)	-0.03	8 (3%) 43 48	25, 48, 88, 129	0
All	All	815/845 (96%)	-0.02	27 (3%) 44 49	23, 48, 91, 163	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	178	ALA	4.7
4	B	179	LEU	4.1
2	D	168	ARG	3.9
3	A	129	SER	3.8
3	A	114	GLN	3.8
4	B	180	ASN	3.8
3	A	192	ILE	3.4
3	A	130	ASP	3.4
3	A	191	SER	3.1
3	A	166	MET	2.9
2	D	169	GLY	2.8
2	D	19	ASN	2.8
3	A	194	PRO	2.6
3	A	112	TYR	2.5
3	A	189	ASN	2.5
4	B	177	PRO	2.5
3	A	199	PHE	2.5
2	D	171	VAL	2.4
3	A	165	SER	2.4
4	B	216	ASN	2.2
4	B	214	SER	2.2

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Mol	Chain	Res	Type	RSRZ
4	B	77	GLU	2.2
4	B	78	LEU	2.2
3	A	196	ASP	2.2
2	D	112	HIS	2.1
2	D	137	GLN	2.1
3	A	167	ASP	2.1

## 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.