



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:50 PM GMT

PDB ID : 1HHH  
Title : THE ANTIGENIC IDENTITY OF PEPTIDE(SLASH)MHC COMPLEXES:  
A COMPARISON OF THE CONFORMATION OF FIVE PEPTIDES PRE-  
SENTED BY HLA-A2  
Authors : Madden, D.R.; Garboczi, D.N.; Wiley, D.C.  
Deposited on : 1993-06-30  
Resolution : 3.00 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](mailto: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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

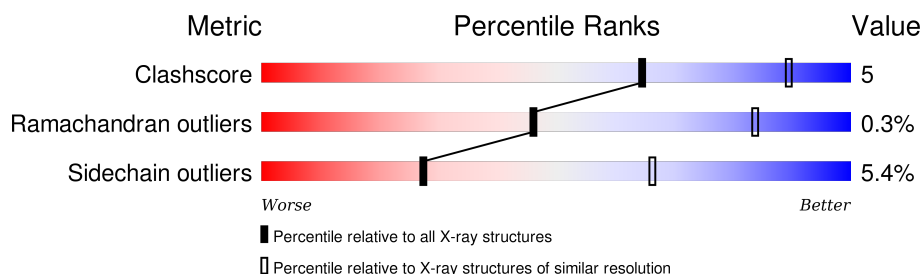
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	 80% 19% •
2	B	100	 84% 15% •
3	C	10	 60% 40%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3167 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 CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A\*0201) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	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			

- Molecule 3 is a protein called HEPATITIS B NUCLEOCAPSID PROTEIN (RESIDUES 18-27).

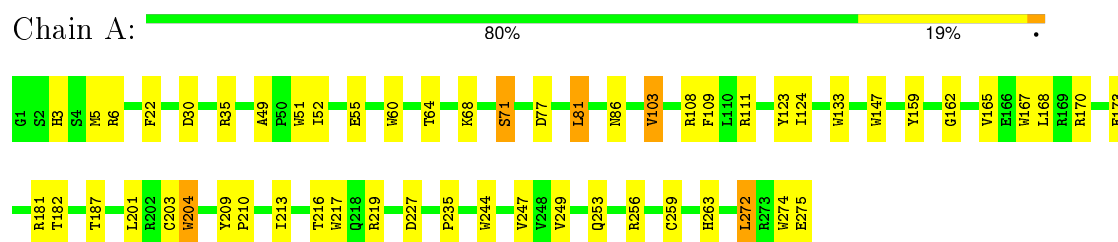
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			83	58	10	15			

### 3 Residue-property plots

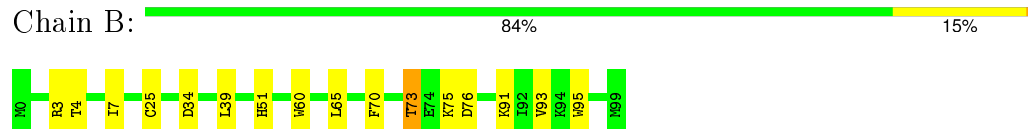
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A\*0201) (ALPHA CHAIN)



- Molecule 2: BETA 2-MICROGLOBULIN



- Molecule 3: HEPATITIS B NUCLEOCAPSID PROTEIN (RESIDUES 18-27)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.63Å 81.24Å 94.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.286 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

## 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	0.81	0/2312	1.40	33/3137 (1.1%)
2	B	0.75	0/860	1.28	8/1162 (0.7%)
3	C	0.85	0/87	1.29	0/117
All	All	0.79	0/3259	1.37	41/4416 (0.9%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	TRP	CD1-CG-CD2	9.13	113.61	106.30
1	A	204	TRP	CD1-CG-CD2	8.60	113.18	106.30
2	B	95	TRP	CD1-CG-CD2	8.38	113.00	106.30
1	A	133	TRP	CD1-CG-CD2	8.36	112.99	106.30
2	B	60	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	A	217	TRP	CE2-CD2-CG	-8.24	100.71	107.30
1	A	60	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	A	51	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	A	244	TRP	CE2-CD2-CG	-7.83	101.03	107.30
2	B	60	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	A	244	TRP	CD1-CG-CD2	7.61	112.38	106.30
1	A	274	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	A	167	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	60	TRP	CE2-CD2-CG	-7.42	101.37	107.30
2	B	95	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	133	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	A	274	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	A	204	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	108	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	A	51	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	147	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	A	6	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	244	TRP	CG-CD2-CE3	6.44	139.69	133.90
1	A	167	TRP	CE2-CD2-CG	-6.31	102.25	107.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	TRP	CB-CG-CD1	-5.99	119.21	127.00
1	A	147	TRP	CE2-CD2-CG	-5.96	102.53	107.30
1	A	170	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	217	TRP	CG-CD1-NE1	-5.72	104.38	110.10
1	A	35	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	173	GLU	CA-CB-CG	5.70	125.93	113.40
1	A	217	TRP	CG-CD2-CE3	5.69	139.02	133.90
1	A	181	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	60	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	A	55	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	204	TRP	CG-CD1-NE1	-5.38	104.72	110.10
2	B	95	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	167	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	173	GLU	OE1-CD-OE2	-5.08	117.21	123.30
2	B	60	TRP	CB-CG-CD1	-5.06	120.42	127.00
2	B	60	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	217	TRP	CB-CG-CD1	-5.01	120.49	127.00

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	2247	0	2096	26	0
2	B	837	0	803	6	0
3	C	83	0	77	2	0
All	All	3167	0	2976	31	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 (31) 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:73:THR:HG22	2:B:76:ASP:H	1.49	0.78
1:A:219:ARG:HH11	1:A:256:ARG:HD3	1.57	0.70
1:A:253:GLN:O	1:A:256:ARG:HG2	1.98	0.63
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.82	0.61
1:A:219:ARG:NH1	1:A:256:ARG:HD3	2.18	0.57
1:A:81:LEU:HD13	3:C:10:VAL:HG21	1.87	0.56
1:A:187:THR:HB	1:A:272:LEU:HD21	1.87	0.56
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.89	0.56
1:A:49:ALA:O	1:A:52:ILE:HG22	2.05	0.55
1:A:201:LEU:HD22	1:A:249:VAL:HG21	1.89	0.54
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.92	0.51
2:B:73:THR:HG22	2:B:76:ASP:N	2.24	0.51
1:A:203:CYS:SG	1:A:272:LEU:HD11	2.52	0.49
1:A:259:CYS:HB3	1:A:272:LEU:HD12	1.94	0.49
1:A:68:LYS:HA	1:A:71:SER:HB3	1.94	0.48
1:A:210:PRO:O	1:A:263:HIS:HE1	1.96	0.48
1:A:159:TYR:CZ	3:C:3:PRO:HD3	2.48	0.48
1:A:68:LYS:HE2	1:A:68:LYS:HB3	1.73	0.46
1:A:219:ARG:NH1	1:A:256:ARG:HH11	2.13	0.45
1:A:64:THR:O	1:A:68:LYS:HG2	2.17	0.45
1:A:182:THR:HG23	1:A:210:PRO:HD2	1.99	0.44
1:A:227:ASP:O	1:A:247:VAL:HA	2.18	0.42
1:A:30:ASP:HB2	1:A:209:TYR:CE2	2.53	0.42
1:A:235:PRO:HG2	2:B:65:LEU:HD13	2.02	0.42
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.85	0.42
1:A:162:GLY:O	1:A:165:VAL:HG12	2.20	0.41
2:B:51:HIS:HA	2:B:65:LEU:O	2.20	0.41
1:A:22:PHE:CD2	1:A:71:SER:HB2	2.56	0.41
1:A:3:HIS:HB2	1:A:103:VAL:HG12	2.03	0.41
1:A:77:ASP:O	1:A:81:LEU:HB2	2.20	0.41
1:A:187:THR:HA	1:A:204:TRP:O	2.19	0.40

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	273/275 (99%)	257 (94%)	15 (6%)	1 (0%)	39	80
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
All	All	379/385 (98%)	362 (96%)	16 (4%)	1 (0%)	46	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PHE

### 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%)	222 (96%)	9 (4%)	39	77
2	B	95/95 (100%)	88 (93%)	7 (7%)	17	52
3	C	10/10 (100%)	8 (80%)	2 (20%)	1	8
All	All	336/336 (100%)	318 (95%)	18 (5%)	27	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	81	LEU
1	A	86	ASN
1	A	103	VAL
1	A	111	ARG
1	A	213	ILE
1	A	216	THR
1	A	272	LEU
1	A	275	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	3	ARG
2	B	4	THR
2	B	34	ASP
2	B	70	PHE
2	B	73	THR
2	B	75	LYS
2	B	93	VAL
3	C	4	SER
3	C	9	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	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 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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.