



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:25 AM UTC

PDB ID : 1HHH / pdb_00001hhh
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

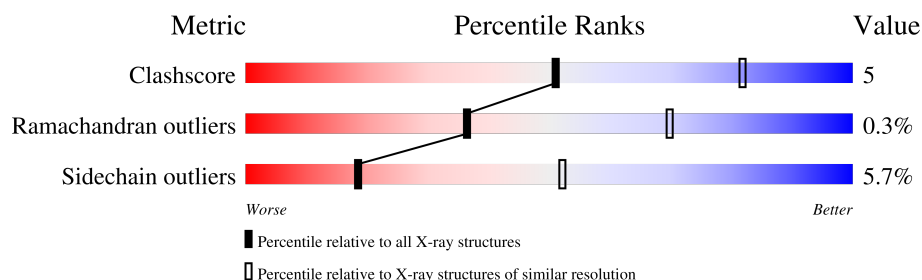
1 Overall quality at a glance

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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	 73% 24% •
2	B	100	 78% 20% ••
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).

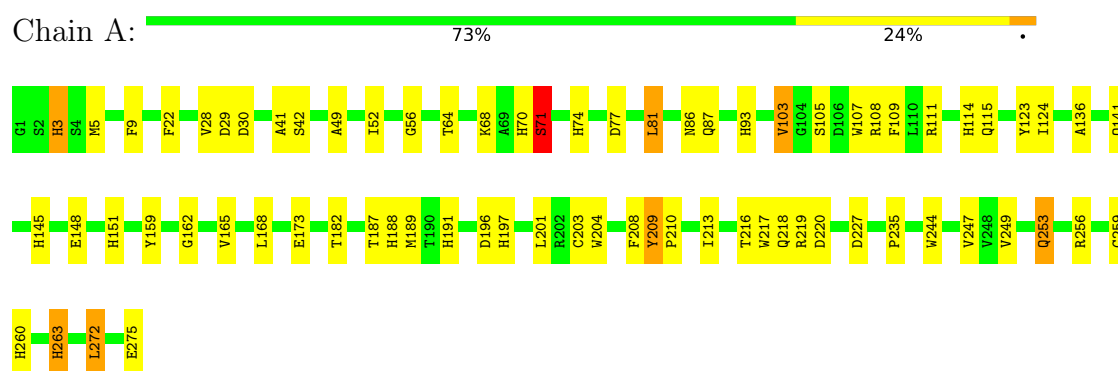
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			83	58	10	15			

3 Residue-property plots

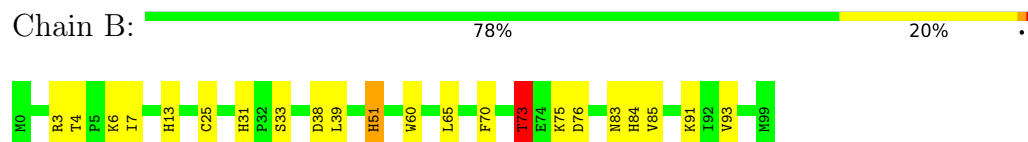
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	8.0	wwPDB-VP

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	0.96	16/2312 (0.7%)	1.57	31/3137 (1.0%)
2	B	0.89	4/860 (0.5%)	1.51	12/1162 (1.0%)
3	C	0.93	0/87	1.53	1/117 (0.9%)
All	All	0.94	20/3259 (0.6%)	1.55	44/4416 (1.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	HIS	CD2-NE2	-7.63	1.29	1.37
1	A	260	HIS	CD2-NE2	-7.00	1.30	1.37
2	B	84	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	114	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	74	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	263	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	188	HIS	CD2-NE2	-6.63	1.30	1.37
2	B	51	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	197	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	151	HIS	CD2-NE2	-6.46	1.30	1.37
2	B	31	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.30	1.30	1.37
2	B	13	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	145	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	3	HIS	CG-ND1	-5.78	1.31	1.38
1	A	107	TRP	NE1-CE2	-5.28	1.31	1.37
1	A	114	HIS	CG-ND1	-5.25	1.32	1.38
1	A	263	HIS	CG-ND1	-5.13	1.32	1.38
1	A	151	HIS	CG-ND1	-5.04	1.32	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	HIS	CB-CG-CD2	-6.80	122.35	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	PHE	CA-CB-CG	6.52	120.32	113.80
2	B	31	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	A	188	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	A	197	HIS	CB-CG-CD2	-6.28	123.04	131.20
2	B	84	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	A	29	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	74	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	A	136	ALA	N-CA-C	6.17	119.20	111.24
1	A	218	GLN	OE1-CD-NE2	-6.11	116.49	122.60
1	A	196	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	41	ALA	N-CA-C	6.03	117.52	111.07
1	A	28	VAL	N-CA-C	-5.99	97.76	107.28
2	B	51	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	A	173	GLU	CA-CB-CG	5.92	125.93	114.10
2	B	13	HIS	CB-CG-CD2	-5.83	123.63	131.20
1	A	244	TRP	CG-CD2-CE3	5.79	139.69	133.90
1	A	42	SER	N-CA-C	5.75	117.55	111.28
2	B	6	LYS	N-CA-C	-5.62	100.52	109.96
1	A	87	GLN	OE1-CD-NE2	-5.58	117.03	122.60
3	C	6	PHE	N-CA-C	-5.57	106.48	113.28
1	A	220	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	260	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	217	TRP	CE2-CD2-CG	-5.41	100.71	107.20
2	B	38	ASP	CA-CB-CG	5.37	117.97	112.60
2	B	83	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	191	HIS	CA-CB-CG	5.33	119.13	113.80
1	A	9	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	108	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	56	GLY	CA-C-N	5.20	125.25	119.32
1	A	56	GLY	C-N-CA	5.20	125.25	119.32
1	A	253	GLN	OE1-CD-NE2	-5.20	117.40	122.60
2	B	84	HIS	CB-CG-ND1	5.18	130.47	122.70
2	B	73	THR	N-CA-CB	-5.14	103.26	111.43
1	A	244	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	244	TRP	CB-CG-CD1	-5.13	119.21	126.90
2	B	60	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	A	217	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	A	71	SER	CA-CB-OG	5.12	121.33	111.10
1	A	141	GLN	CA-CB-CG	-5.11	103.88	114.10
1	A	208	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	197	HIS	CB-CG-ND1	5.09	130.33	122.70
2	B	85	VAL	CB-CA-C	-5.01	104.73	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	TYR	O-C-N	-5.01	116.95	122.06

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	27	0
2	B	837	0	803	6	0
3	C	83	0	77	2	0
All	All	3167	0	2976	32	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 (32) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:CZ	3:C:3:PRO:HD3	2.48	0.48
1:A:68:LYS:HB3	1:A:68:LYS:HE2	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:189:MET:HE3	1:A:189:MET:HB2	1.94	0.43
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 ⓘ

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%)	257 (94%)	15 (6%)	1 (0%)	30	65
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%)	36	70

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%)	219 (95%)	12 (5%)	21	55
2	B	95/95 (100%)	89 (94%)	6 (6%)	16	48
3	C	10/10 (100%)	9 (90%)	1 (10%)	7	29
All	All	336/336 (100%)	317 (94%)	19 (6%)	18	52

All (19) 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	105	SER
1	A	111	ARG
1	A	115	GLN
1	A	148	GLU
1	A	213	ILE
1	A	216	THR
1	A	272	LEU
1	A	275	GLU
2	B	3	ARG
2	B	4	THR
2	B	33	SER
2	B	73	THR
2	B	75	LYS
2	B	93	VAL
3	C	4	SER

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

Mol	Chain	Res	Type
1	A	218	GLN

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 oligosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.