



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:53 AM BST

PDB ID : 3CUP  
Title : Crystal structure of the MHC class II molecule I-Ag7 in complex with the peptide GAD221-235  
Authors : Corper, A.L.; Yoshida, K.; Teyton, L.; Wilson, I.A.  
Deposited on : 2008-04-16  
Resolution : 3.09 Å(reported)

This is a wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

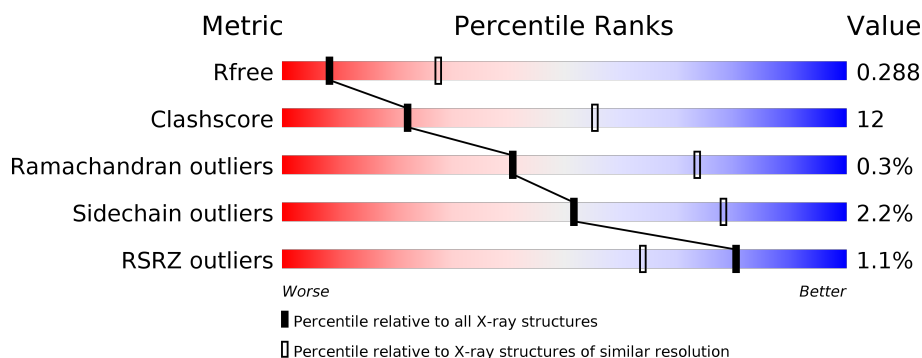
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 3.09 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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  $\leq 5\%$ . 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	190	
2	B	222	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2953 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 H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1465	948	238	277	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP P04228
A	180	SER	-	expression tag	UNP P04228
A	181	ALA	-	expression tag	UNP P04228
A	182	ASP	-	expression tag	UNP P04228
A	183	LEU	-	expression tag	UNP P04228
A	184	VAL	-	expression tag	UNP P04228
A	185	PRO	-	expression tag	UNP P04228
A	186	ARG	-	expression tag	UNP P04228

- Molecule 2 is a protein called MHC class II H2-IA-beta chain linked to GAD221-235 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1459	925	259	269	6			

There are 20 discrepancies between the modelled and reference sequences:

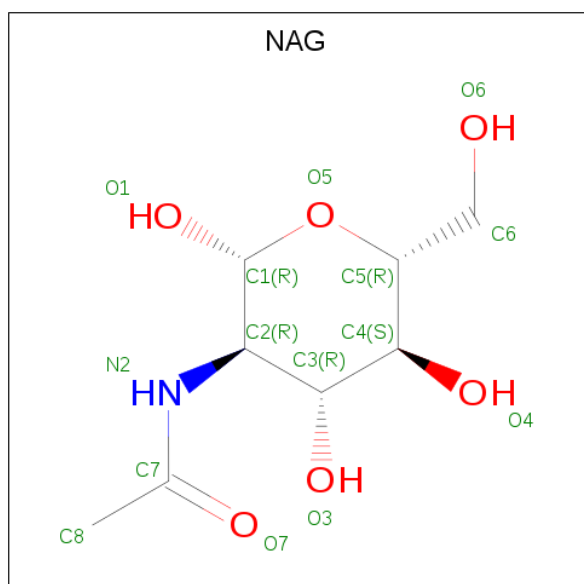
Chain	Residue	Modelled	Actual	Comment	Reference
B	215	GLY	-	expression tag	UNP Q6LDA5
B	216	SER	-	expression tag	UNP Q6LDA5
B	217	HIS	-	expression tag	UNP Q6LDA5
B	218	SER	-	expression tag	UNP Q6LDA5
B	219	ARG	-	expression tag	UNP Q6LDA5
B	220	GLY	-	expression tag	UNP Q6LDA5
B	236	GLY	-	linker	UNP Q6LDA5
B	?	SER	-	linker	UNP Q6LDA5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	GLY	-	linker	UNP Q6LDA5
B	?	SER	-	linker	UNP Q6LDA5
B	?	GLY	-	linker	UNP Q6LDA5
B	?	SER	-	linker	UNP Q6LDA5
B	429	SER	-	expression tag	UNP Q31135
B	430	SER	-	expression tag	UNP Q31135
B	431	ALA	-	expression tag	UNP Q31135
B	432	ASP	-	expression tag	UNP Q31135
B	433	LEU	-	expression tag	UNP Q31135
B	434	VAL	-	expression tag	UNP Q31135
B	435	PRO	-	expression tag	UNP Q31135
B	436	ARG	-	expression tag	UNP Q31135

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).

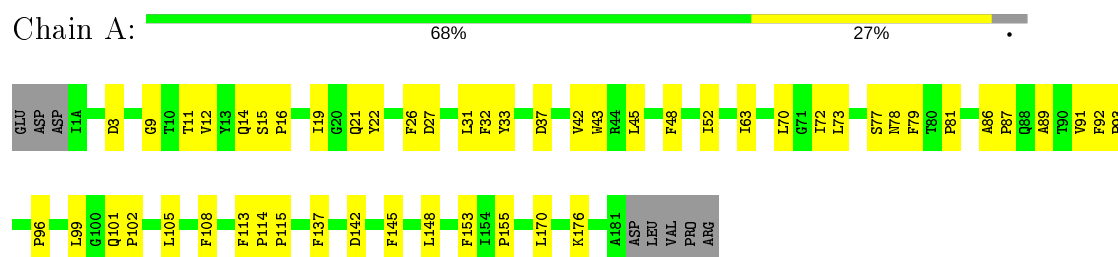


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

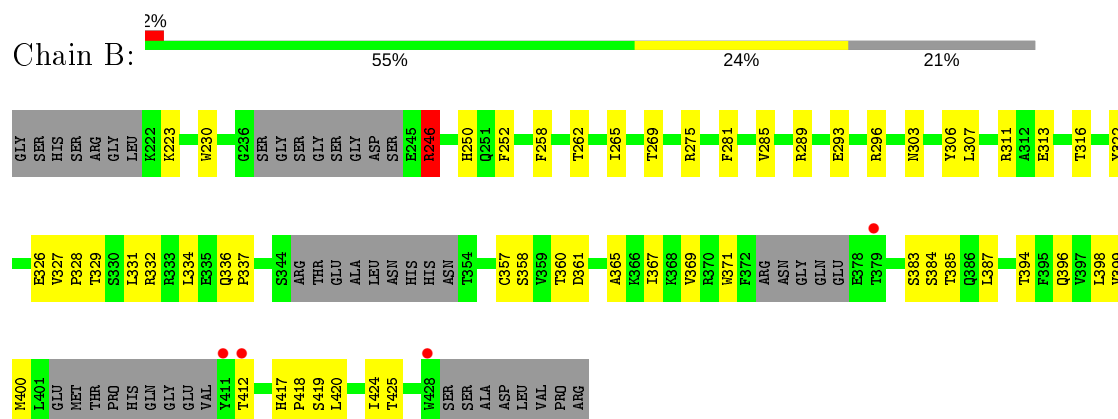
### 3 Residue-property plots

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 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: H-2 class II histocompatibility antigen, A-D alpha chain



- Molecule 2: MHC class II H2-IA-beta chain linked to GAD221-235 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.83Å 55.83Å 338.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.45 – 3.09 38.45 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.45-3.09) 98.7 (38.45-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.06Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.232 , 0.286 0.231 , 0.288	Depositor DCC
$R_{free}$ test set	563 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, NAG

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	0.25	0/1510	0.42	0/2061
2	B	0.23	0/1492	0.40	0/2015
All	All	0.24	0/3002	0.41	0/4076

There are no bond length outliers.

There are no bond angle outliers.

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	1465	0	1405	38	0
2	B	1459	0	1409	41	0
3	A	14	0	13	0	0
4	A	15	0	17	0	0
All	All	2953	0	2844	68	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 12.

The worst 5 of 68 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)
1:A:142:ASP:HB3	2:B:275:ARG:HH21	1.56	0.70
1:A:115:PRO:HG3	1:A:145:PHE:CE1	2.27	0.70
2:B:322:TYR:O	2:B:327:VAL:HG23	1.97	0.64
1:A:89:ALA:O	1:A:176:LYS:HE3	1.98	0.63
2:B:361:ASP:HA	2:B:394:THR:HB	1.81	0.62

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	180/190 (95%)	169 (94%)	11 (6%)	0	100	100
2	B	166/222 (75%)	149 (90%)	16 (10%)	1 (1%)	25	59
All	All	346/412 (84%)	318 (92%)	27 (8%)	1 (0%)	41	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	246	ARG

### 5.3.2 Protein sidechains [i](#)

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	163/171 (95%)	158 (97%)	5 (3%)	40	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	159/196 (81%)	157 (99%)	2 (1%)	69	87
All	All	322/367 (88%)	315 (98%)	7 (2%)	52	78

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
2	B	246	ARG
1	A	153	PHE
1	A	37	ASP
2	B	223	LYS

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	177	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	301	1	14,14,15	0.51	0	17,19,21	1.12	3 (17%)
4	EPE	A	302	-	15,15,15	0.79	1 (6%)	18,20,20	1.76	5 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	301	1	-	2/6/23/26	0/1/1/1
4	EPE	A	302	-	-	5/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	EPE	C10-S	2.66	1.81	1.77

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	EPE	C5-N4-C3	4.65	119.29	108.83
3	A	301	NAG	C1-O5-C5	2.91	116.13	112.19
4	A	302	EPE	C7-N4-C3	2.76	118.30	111.23
4	A	302	EPE	C7-N4-C5	2.76	118.28	111.23
4	A	302	EPE	O3S-S-C10	2.22	109.36	105.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	EPE	C8-C7-N4-C5
4	A	302	EPE	C9-C10-S-O1S
3	A	301	NAG	C8-C7-N2-C2
3	A	301	NAG	O7-C7-N2-C2
4	A	302	EPE	C9-C10-S-O3S

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	182/190 (95%)	-0.28	0 100 100	44, 59, 85, 138	0
2	B	176/222 (79%)	0.03	4 (2%) 60 39	45, 80, 133, 168	0
All	All	358/412 (86%)	-0.13	4 (1%) 80 64	44, 66, 122, 168	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	412	THR	2.8
2	B	379	THR	2.6
2	B	428	TRP	2.3
2	B	411	TYR	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 monosaccharides in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	301	14/15	0.85	0.36	94,101,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EPE	A	302	15/15	0.96	0.18	70,73,75,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.