



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 05:20 am GMT

PDB ID : 1K2D  
Title : Crystal structure of the autoimmune MHC class II I-Au complexed with myelin basic protein 1-11 at 2.2Å  
Authors : He, X.L.; Radu, C.; Ward, E.S.; Garcia, K.C.  
Deposited on : 2001-09-26  
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

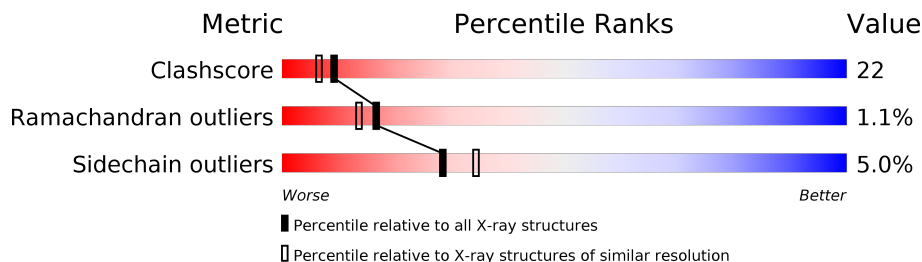
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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	189	
2	B	189	
3	P	23	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3597 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-U alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1463	946	233	281	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	CLONING ARTIFACT	UNP P14438
A	-5	SER	-	CLONING ARTIFACT	UNP P14438
A	-4	ARG	-	CLONING ARTIFACT	UNP P14438
A	-3	GLY	-	CLONING ARTIFACT	UNP P14438
A	-2	GLU	-	CLONING ARTIFACT	UNP P14438
A	-1	ASP	-	CLONING ARTIFACT	UNP P14438
A	0	ASP	-	CLONING ARTIFACT	UNP P14438
A	1	ILE	-	CLONING ARTIFACT	UNP P14438
A	2	GLU	-	CLONING ARTIFACT	UNP P14438
A	3	ALA	-	CLONING ARTIFACT	UNP P14438

- Molecule 2 is a protein called H-2 class II histocompatibility antigen, A-U beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	S	0	0	0
			1558	984	279	289	6			

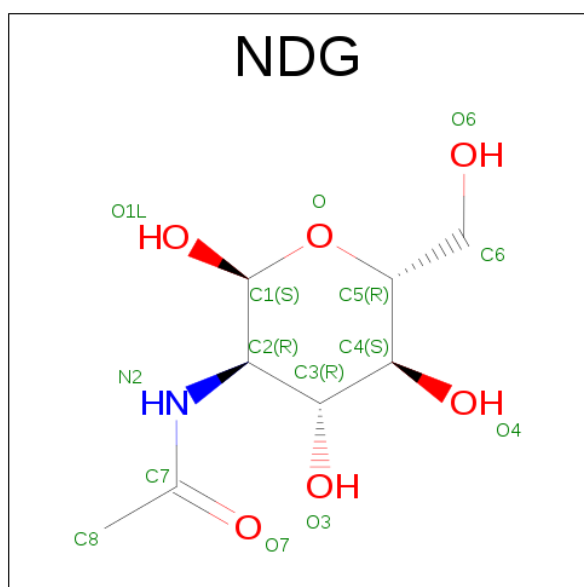
- Molecule 3 is a protein called Myelin Basic Protein peptide with 8 residue linker peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O		0	0	0
			84	49	17	18				

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	HIS	-	CLONING ARTIFACT	GB 14763906
P	-3	SER	-	CLONING ARTIFACT	GB 14763906
P	-2	ARG	-	CLONING ARTIFACT	GB 14763906
P	-1	GLY	-	CLONING ARTIFACT	GB 14763906
P	0	GLY	MET	CONFLICT	GB 14763906
P	11	GLY	-	LINKER PEPTIDE	GB 14763906
P	12	THR	-	LINKER PEPTIDE	GB 14763906
P	13	GLY	-	LINKER PEPTIDE	GB 14763906
P	14	SER	-	LINKER PEPTIDE	GB 14763906
P	15	GLY	-	LINKER PEPTIDE	GB 14763906
P	16	SER	-	LINKER PEPTIDE	GB 14763906
P	17	GLY	-	LINKER PEPTIDE	GB 14763906
P	18	SER	-	LINKER PEPTIDE	GB 14763906

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is water.

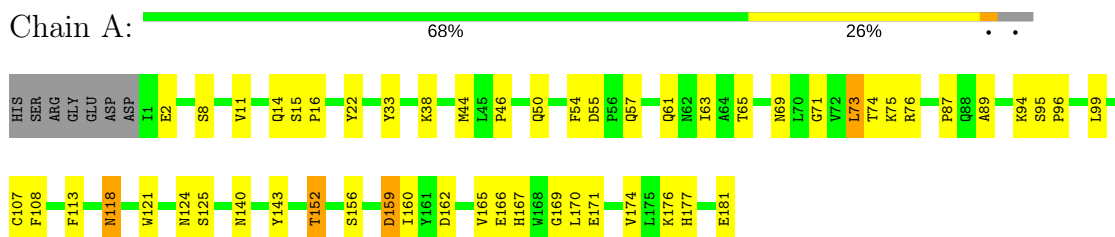
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	225	Total	O	0	0
			225	225		
6	B	207	Total	O	0	0
			207	207		
6	P	18	Total	O	0	0
			18	18		

### 3 Residue-property plots [i](#)

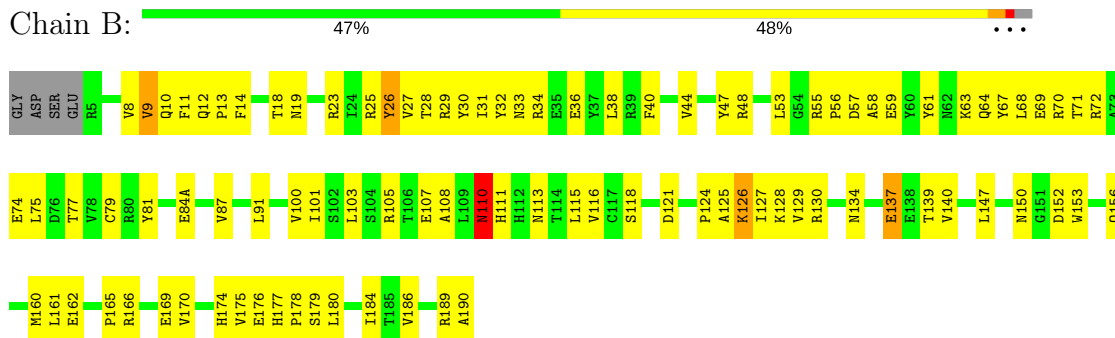
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

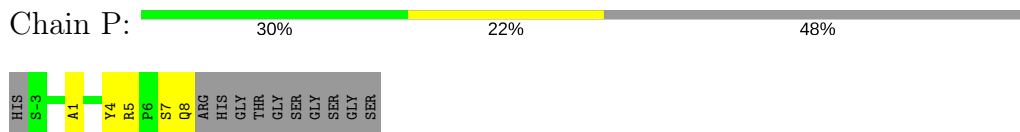
- Molecule 1: H-2 class II histocompatibility antigen, A-U alpha chain



- Molecule 2: H-2 class II histocompatibility antigen, A-U beta chain



- Molecule 3: Myelin Basic Protein peptide with 8 residue linker peptide



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.15Å 110.59Å 94.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.3 (50.00-2.20)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.248 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/1508	0.68	0/2059
2	B	0.42	0/1597	0.67	0/2170
3	P	0.78	0/85	1.25	2/113 (1.8%)
All	All	0.45	0/3190	0.70	2/4342 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	5	ARG	NE-CZ-NH1	-7.60	116.50	120.30
3	P	5	ARG	CG-CD-NE	-5.28	100.70	111.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1463	0	1389	50	0
2	B	1558	0	1499	95	0
3	P	84	0	75	7	0
4	A	14	0	13	0	0
5	A	14	0	13	1	0
5	B	14	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	225	0	0	10	0
6	B	207	0	0	9	0
6	P	18	0	0	1	0
All	All	3597	0	3002	136	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 22.

The worst 5 of 136 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:72:ARG:HA	6:B:576:HOH:O	1.69	0.93
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.54	0.87
2:B:126:LYS:HE2	2:B:126:LYS:C	1.98	0.82
5:A:502:NAG:H62	6:A:589:HOH:O	1.82	0.80
1:A:160:ILE:HG23	1:A:177:HIS:CE1	2.17	0.79

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	180/189 (95%)	171 (95%)	9 (5%)	0	100	100
2	B	183/189 (97%)	159 (87%)	20 (11%)	4 (2%)	8	4
3	P	10/23 (44%)	8 (80%)	2 (20%)	0	100	100
All	All	373/401 (93%)	338 (91%)	31 (8%)	4 (1%)	17	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	58	ALA
2	B	79	CYS
2	B	110	ASN
2	B	140	VAL

### 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	163/169 (96%)	156 (96%)	7 (4%)	33	41
2	B	172/175 (98%)	162 (94%)	10 (6%)	23	27
3	P	8/16 (50%)	8 (100%)	0	100	100
All	All	343/360 (95%)	326 (95%)	17 (5%)	28	34

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	VAL
2	B	26	TYR
2	B	110	ASN
1	A	159	ASP
2	B	126	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
2	B	177	HIS
2	B	111	HIS
1	A	101	GLN
2	B	150	ASN

### 5.3.3 RNA

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](#)

3 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	$\# Z  > 2$
4	NDG	A	501	1	14,14,15	0.68	0	15,19,21	0.68	0
5	NAG	A	502	1	14,14,15	0.59	0	15,19,21	0.76	0
5	NAG	B	503	2	14,14,15	0.51	0	15,19,21	0.76	0

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
4	NDG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	502	1	-	1/6/23/26	0/1/1/1
5	NAG	B	503	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	NAG	O7-C7-N2-C2
5	A	502	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	NAG	1	0
5	B	503	NAG	3	0

## 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.