



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:24 PM GMT

PDB ID : 1KTD  
Title : CRYSTAL STRUCTURE OF CLASS II MHC MOLECULE IEK BOUND TO  
PIGEON CYTOCHROME C PEPTIDE  
Authors : Fremont, D.H.; Dai, S.; Chiang, H.; Crawford, F.; Marrack, P.; Kappler, J.  
Deposited on : 2002-01-15  
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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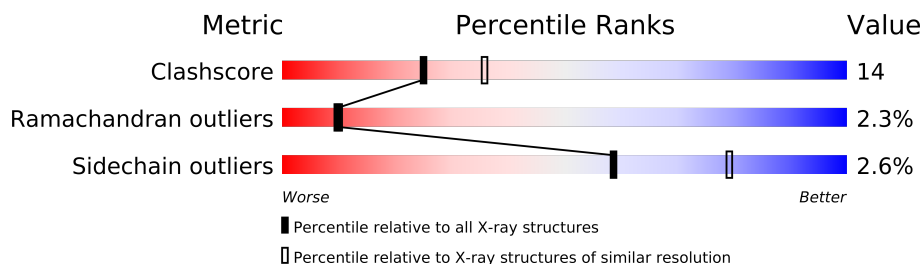
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	
1	C	182	
2	B	215	
2	D	215	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6814 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, E-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1497	963	243	287	4			
1	C	182	Total	C	N	O	S	0	0	0
			1497	963	243	287	4			

- Molecule 2 is a protein called Fusion protein consisting of cytochrome C peptide, glycine rich linker, and MHC E-beta-k.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	84	0	0
			1721	1088	298	329	6			
2	D	215	Total	C	N	O	S	69	0	0
			1721	1088	298	329	6			

There are 2 discrepancies between the modelled and reference sequences:

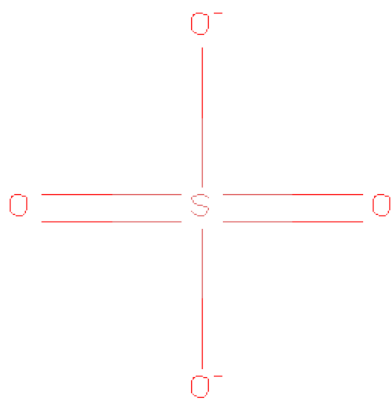
Chain	Residue	Modelled	Actual	Comment	Reference
B	12	SER	THR	ENGINEERED	UNP P00021
D	12	SER	THR	ENGINEERED	UNP P00021

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	96	Total	O		0	0
			96	96			
5	B	99	Total	O		0	0
			99	99			
5	C	71	Total	O		0	0
			71	71			
5	D	51	Total	O		0	0
			51	51			

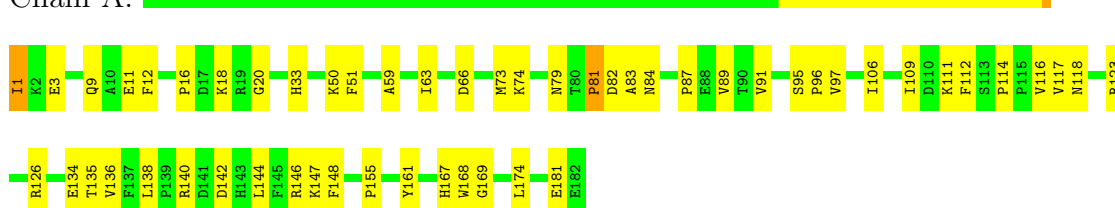
### 3 Residue-property plots

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.

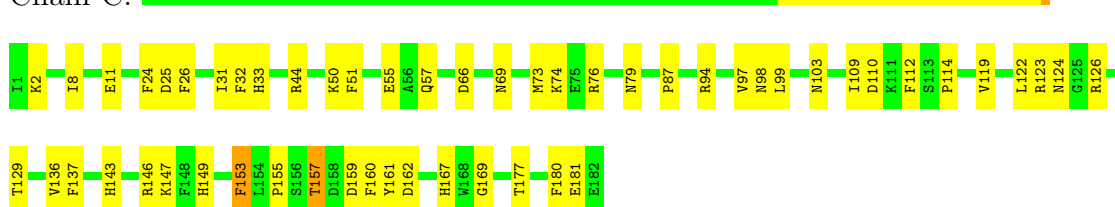
- Molecule 1: H-2 class II histocompatibility antigen, E-D alpha chain

Chain A:



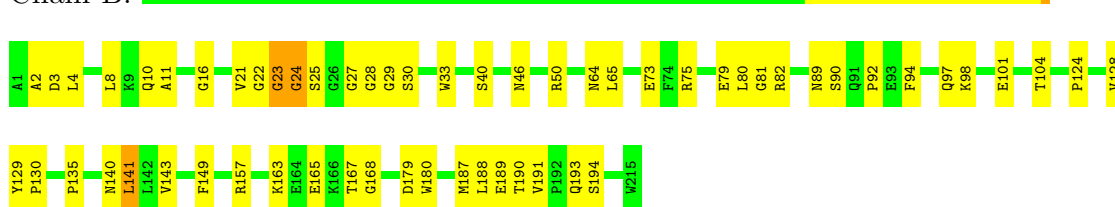
- Molecule 1: H-2 class II histocompatibility antigen, E-D alpha chain

Chain C:



- Molecule 2: Fusion protein consisting of cytochrome C peptide, glycine rich linker, and MHC E-beta-k

Chain B:



- Molecule 2: Fusion protein consisting of cytochrome C peptide, glycine rich linker, and MHC E-beta-k

Chain D:



P119	R120	R121	V122	E123	P124
V128	Y129	P130	T131	K132	
P135	L136	E137			
N140	L141	L142	V143	C144	
F149	V150	P151			
V156	R157	W158	F159	R160	
K163	V186				
S194	Y198				
H204	P205	S206	L207		
V211					
W215					

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.52Å 57.30Å 116.57Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.3 (10.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.43	0/1539	0.65	0/2091
1	C	0.39	0/1539	0.61	0/2091
2	B	0.39	0/1766	0.63	0/2400
2	D	0.36	0/1766	0.61	0/2400
All	All	0.39	0/6610	0.63	0/8982

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	A	1497	0	1420	42	0
1	C	1497	0	1422	42	0
2	B	1721	0	1637	47	0
2	D	1721	0	1638	56	0
3	A	28	0	26	3	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	96	0	0	1	0
5	B	99	0	0	2	0
5	C	71	0	0	0	0
5	D	51	0	0	1	0
All	All	6814	0	6169	171	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 14.

The worst 5 of 171 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:160:ARG:HB3	2:D:160:ARG:HH11	1.30	0.96
2:B:73:GLU:HG3	2:B:75:ARG:HH12	1.41	0.86
1:A:51:PHE:O	2:B:2:ALA:HA	1.76	0.86
1:C:123:ARG:HE	1:C:161:TYR:HE2	1.26	0.83
2:D:140:ASN:HD22	2:D:141:LEU:N	1.88	0.72

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	180/182 (99%)	173 (96%)	5 (3%)	2 (1%)	21	29
1	C	180/182 (99%)	169 (94%)	10 (6%)	1 (1%)	33	47
2	B	213/215 (99%)	188 (88%)	19 (9%)	6 (3%)	8	6
2	D	213/215 (99%)	186 (87%)	18 (8%)	9 (4%)	4	3
All	All	786/794 (99%)	716 (91%)	52 (7%)	18 (2%)	10	10

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	ALA

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Mol	Chain	Res	Type
2	D	46	ASN
2	D	135	PRO
2	D	136	LEU
2	D	194	SER

### 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	165/165 (100%)	161 (98%)	4 (2%)	61	81
1	C	165/165 (100%)	161 (98%)	4 (2%)	61	81
2	B	187/187 (100%)	182 (97%)	5 (3%)	57	78
2	D	187/187 (100%)	182 (97%)	5 (3%)	57	78
All	All	704/704 (100%)	686 (97%)	18 (3%)	59	79

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	141	LEU
1	C	24	PHE
2	D	137	GLU
2	B	50	ARG
2	B	140	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	143	HIS
1	C	149	HIS
2	D	10	GLN
1	C	98	ASN
1	C	167	HIS

### 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 ⓘ

5 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	602	1	12,14,15	0.47	0	15,19,21	0.75	0
3	NAG	A	604	1	12,14,15	0.45	0	15,19,21	0.75	0
3	NAG	B	601	2	12,14,15	0.48	0	15,19,21	0.64	0
4	SO4	B	800	-	4,4,4	0.11	0	6,6,6	0.10	0
3	NAG	C	603	1	12,14,15	0.37	0	15,19,21	0.82	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
3	NAG	A	602	1	-	1/6/23/26	0/1/1/1
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	2	-	0/6/23/26	0/1/1/1
4	SO4	B	800	-	-	0/0/0/0	0/0/0/0
3	NAG	C	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAG	O7-C7-N2-C2

There are no ring outliers.

## 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 ⓘ

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.