



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:14 AM GMT

PDB ID : 1IEB
Title : HISTOCOMPATIBILITY ANTIGEN
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Deposited on : 1996-04-05
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

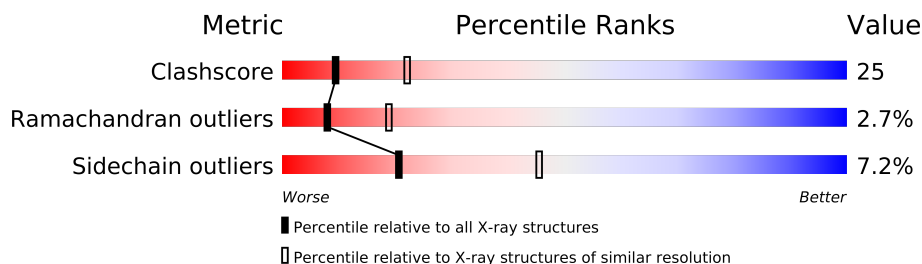
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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 ≥ 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	192	
1	C	192	
2	B	227	
2	D	227	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6672 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.

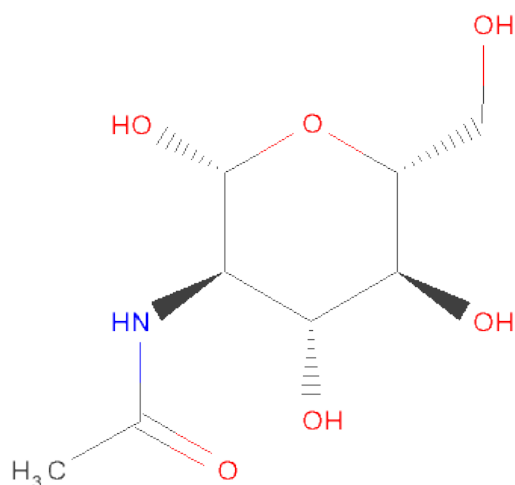
- Molecule 1 is a protein called MHC CLASS II I-EK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1488	959	243	282	4			
1	C	182	Total	C	N	O	S	0	0	0
			1488	959	243	282	4			

- Molecule 2 is a protein called MHC CLASS II I-EK.

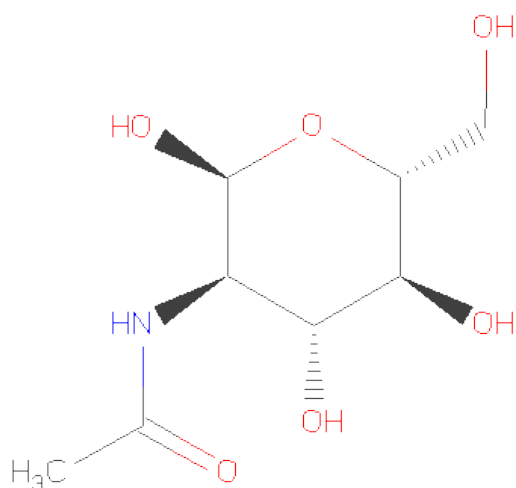
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1724	1092	302	323	7			
2	D	214	Total	C	N	O	S	0	0	0
			1724	1092	302	323	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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		
3	B	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	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	48	Total	O	0	0
			48	48		
6	C	27	Total	O	0	0
			27	27		
6	D	45	Total	O	0	0
			45	45		

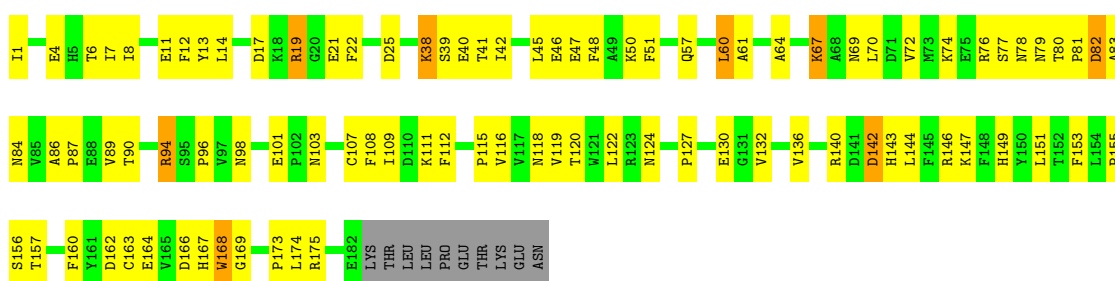
3 Residue-property plots

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.

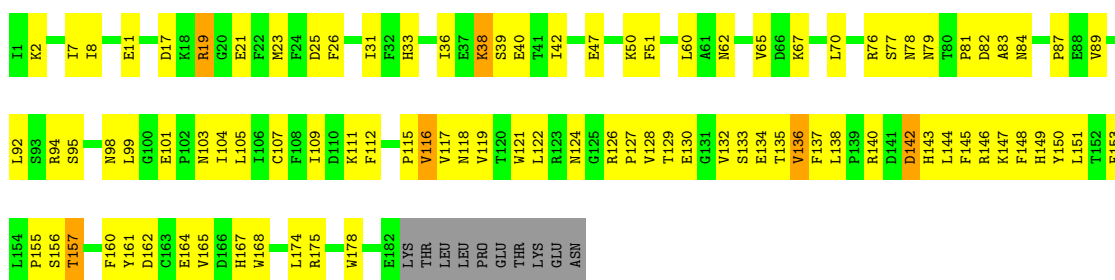
• Molecule 1: MHC CLASS II I-EK

Chain A:



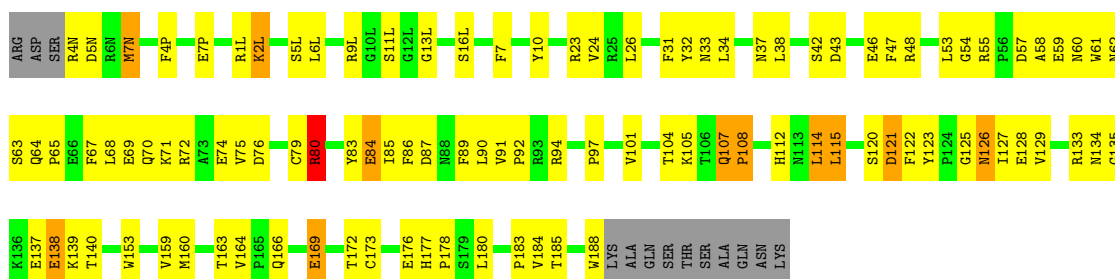
• Molecule 1: MHC CLASS II I-EK

Chain C:



• Molecule 2: MHC CLASS II I-EK

Chain B:



• Molecule 2: MHC CLASS II I-EK

V129	L53	ARG
R133	G54	ASP
N134	R55	SER
G135		R4N
K136	A58	WTN
E137	E59	
E138	N60	F4P
K139	W61	
	N62	
V148	F67	E7P
	L68	F8P
W153	E69	K6P
	Q70	R1L
Q156	K71	SSL
	R72	L6L
V159	A73	V7L
M160	E74	P6L
	V75	R9L
V164	R80	G10L
P165	H81	S11L
Q166	N82	G12L
E169	Y83	G13L
	E84	
T172	I85	S16L
C173	F86	R4
		P5
		W6
E176	F89	F7
H177	L90	L3
P178	V91	E9
S179	P92	
L180	R93	S13
	R94	E14
V184		C15
T185	P97	H16
		F17
W188	V101	Y18
LYS	Y102	N19
ALA	T103	G20
GLN	K104	T21
SER	K105	Q22
THR	T106	R23
SER	Q107	V24
ALA	P108	R25
GLN		L26
ASN	H111	L27
LYS	H112	V28
	N113	
	L114	F31
	L115	Y32
	V116	N33
	V119	L38
		R39
	F122	
		S42
	N126	
	T127	R48
	F128	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.53Å 77.53Å 319.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	83.6 (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , 0.321	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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, NDG, 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	0.60	0/1530	0.80	0/2081
1	C	0.60	0/1530	0.79	0/2081
2	B	0.54	0/1769	0.81	2/2404 (0.1%)
2	D	0.56	0/1769	0.82	1/2404 (0.0%)
All	All	0.57	0/6598	0.81	3/8970 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	PRO	N-CA-CB	5.81	110.28	103.30
2	D	108	PRO	N-CA-CB	5.56	109.97	103.30
2	B	80	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	10	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	123	TYR	Sidechain
2	B	32	TYR	Sidechain
1	C	150	TYR	Sidechain

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	1488	0	1412	91	0
1	C	1488	0	1412	84	0
2	B	1724	0	1622	89	0
2	D	1724	0	1622	79	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
3	C	14	0	13	2	0
3	D	14	0	13	0	0
4	A	14	0	13	1	0
4	C	14	0	13	1	0
5	D	5	0	0	0	0
6	A	39	0	0	6	0
6	B	48	0	0	3	0
6	C	27	0	0	3	0
6	D	45	0	0	2	0
All	All	6672	0	6146	311	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 25.

The worst 5 of 311 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:LYS:HE3	1:A:149:HIS:HE1	1.12	1.11
1:C:147:LYS:HE3	1:C:149:HIS:HE1	1.12	1.10
1:C:147:LYS:HE3	1:C:149:HIS:CE1	2.03	0.93
1:A:147:LYS:HE3	1:A:149:HIS:CE1	2.03	0.93
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.53	0.89

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	180/192 (94%)	162 (90%)	14 (8%)	4 (2%)	10	25
1	C	180/192 (94%)	164 (91%)	12 (7%)	4 (2%)	10	25
2	B	212/227 (93%)	178 (84%)	27 (13%)	7 (3%)	6	13
2	D	212/227 (93%)	182 (86%)	24 (11%)	6 (3%)	8	18
All	All	784/838 (94%)	686 (88%)	77 (10%)	21 (3%)	8	19

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	107	GLN
2	B	108	PRO
2	D	107	GLN
2	D	108	PRO
1	A	17	ASP

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	163/175 (93%)	151 (93%)	12 (7%)	20	43
1	C	163/175 (93%)	150 (92%)	13 (8%)	17	37
2	B	186/205 (91%)	174 (94%)	12 (6%)	24	51
2	D	186/205 (91%)	173 (93%)	13 (7%)	21	47
All	All	698/760 (92%)	648 (93%)	50 (7%)	21	45

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	169	GLU
1	C	67	LYS
2	D	169	GLU
2	B	172	THR
1	C	19	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	GLN
1	C	143	HIS
2	D	126	ASN
2	B	126	ASN
2	D	64	GLN

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 ⓘ

7 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	193	1	12,14,15	0.50	0	15,19,21	0.50	0
4	NDG	A	194	1	12,14,15	0.71	0	15,19,21	0.77	0
3	NAG	B	199	2	12,14,15	0.70	0	15,19,21	0.49	0
3	NAG	C	193	1	12,14,15	0.42	0	15,19,21	0.76	0
4	NDG	C	194	1	12,14,15	0.50	0	15,19,21	0.73	0
3	NAG	D	199	2	12,14,15	0.34	0	15,19,21	0.61	0
5	SO4	D	200	-	4,4,4	0.92	0	6,6,6	0.39	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	193	1	-	0/6/23/26	0/1/1/1
4	NDG	A	194	1	-	0/6/23/26	0/1/1/1
3	NAG	B	199	2	-	0/6/23/26	1/1/1/1
3	NAG	C	193	1	-	0/6/23/26	0/1/1/1
4	NDG	C	194	1	-	0/6/23/26	0/1/1/1
3	NAG	D	199	2	-	0/6/23/26	1/1/1/1
5	SO4	D	200	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	199	NAG	C1-C2-C3-C4-C5-O5
3	B	199	NAG	C1-C2-C3-C4-C5-O5

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.