

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 - 07:58 pm BST

PDB ID	:	1BII
Title	:	THE CRYSTAL STRUCTURE OF H-2DD MHC CLASS I IN COMPLEX
		WITH THE HIV-1 DERIVED PEPTIDE P18-110
Authors	:	Achour, A.; Persson, K.; Harris, R.A.; Sundback, J.; Sentman, C.L.; Lindqvist,
		Y.; Schneider, G.; Karre, K.
Deposited on	:	1998-06-11
$\operatorname{Resolution}$:	2.40 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

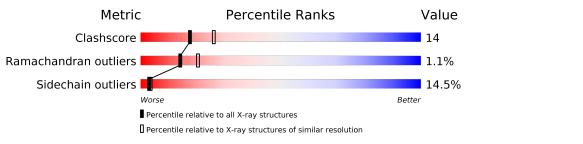
MolProbity : 4.02b-467	
Xtriage (Phenix) : NOT EXECUTED	
\mathbf{EDS} : NOT EXECUTED	
$ \begin{tabular}{lllllllllllllllllllllllllllllllllll$	25 th 2019
Ideal geometry (proteins) : Engh & Huber (2001)	
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)	
Validation Pipeline (wwPDB-VP) : 2.11	

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

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	Similar resolution
	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	4398(2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of	of chai	in		
1	А	365	45%	24%	6%	25	5%
2	В	119	53%		28%	·	17%
3	Р	10	70%			20%	10%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3210 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 MHC CLASS I H-2DD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	274	Total 2248	C 1411	N 407	0 421	S 9	0	0	0

• Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	99	Total 821	C 524	N 138	O 152	S 7	0	0	0

• Molecule 3 is a protein called DECAMERIC PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Р	10	Total 76	C 48	N 16	O 12	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	37	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 37 & 37 \end{array}$	0	0
4	В	27	Total O 27 27	0	0
4	Р	1	Total O 1 1	0	0

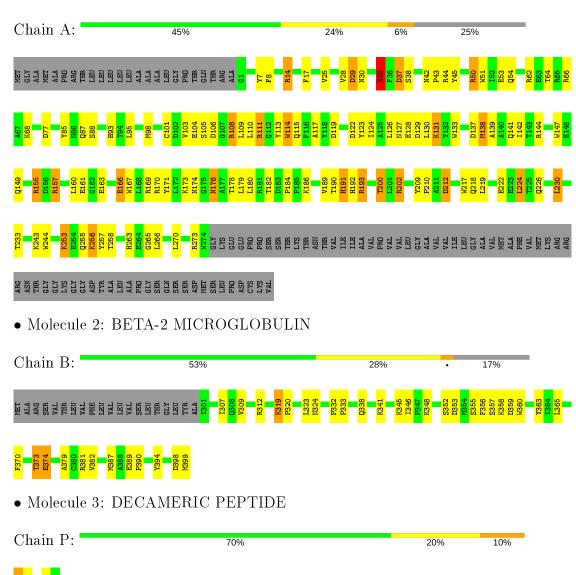




3 Residue-property plots (i)

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. 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: MHC CLASS I H-2DD



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	51.26Å 92.53Å 108.78Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 - 2.40	Depositor
% Data completeness	97.8 (6.00-2.40)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	Depositor
R_{merge}	(Not available)	Depositor
R _{sym}	0.04	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.278 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3210	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP



5 Model quality (i)

5.1 Standard geometry (i)

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/2311	1.10	9/3138~(0.3%)	
2	В	0.52	0/847	1.10	2/1148~(0.2%)	
3	Р	0.60	0/77	1.20	0/101	
All	All	0.47	0/3235	1.10	11/4387~(0.3%)	

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	202	ARG	NE-CZ-NH1	12.43	126.51	120.30
1	А	202	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	А	35	ARG	NE-CZ-NH2	-10.23	115.18	120.30
2	В	359	ASP	CB-CG-OD1	7.51	125.06	118.30
1	А	202	ARG	CD-NE-CZ	6.12	132.16	123.60

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	А	2248	0	2117	67	0
2	В	821	0	793	20	0
3	Р	76	0	79	6	0
4	А	37	0	0	1	0
4	В	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Р	1	0	0	0	0
All	All	3210	0	2989	84	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 14.

The worst 5 of 84 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:319:LYS:HD3	2:B:320:PRO:HD2	1.56	0.85
1:A:171:TYR:HH	3:P:401:ARG:N	1.86	0.72
1:A:85:TYR:HB2	1:A:87:GLN:HE21	1.55	0.72
2:B:399:MET:HB3	4:B:8:HOH:O	1.88	0.72
1:A:170:ARG:HG2	1:A:174:ASN:HD21	1.54	0.71

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	Perce	entiles
1	А	272/365~(74%)	248~(91%)	20 (7%)	4 (2%)	10	14
2	В	97/119~(82%)	90~(93%)	7 (7%)	0	100	100
3	Р	8/10 (80%)	8 (100%)	0	0	100	100
All	All	377/494 (76%)	346 (92%)	27 (7%)	4 (1%)	14	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	127	ASN
1	А	114	TRP

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Mol	Chain	\mathbf{Res}	Type
1	А	29	ASP
1	А	137	ASP

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	А	229/298~(77%)	192~(84%)	37~(16%)	2 3
2	В	94/111~(85%)	84 (89%)	10 (11%)	6 9
3	Р	7/7~(100%)	6 (86%)	1 (14%)	3 4
All	All	330/416 (79%)	282 (86%)	48 (14%)	3 3

 $5~{\rm of}~48$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	182	THR
1	А	200	THR
2	В	374	GLU
1	А	184	PRO
1	А	191	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	149	GLN
1	А	263	HIS
1	А	174	ASN
1	А	115	GLN
1	А	260	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 carbohydrates 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.



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6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

