

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 09:25 pm BST

PDB ID	:	3BUY
Title	:	MHC-I in complex with peptide
Authors	:	Rossjohn, J.; La Gruta, N.L.; Purcell, A.W.; Turner, S.J.; Dunstone, M.A.
Deposited on	:	2008-01-03
Resolution	:	2.60 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:

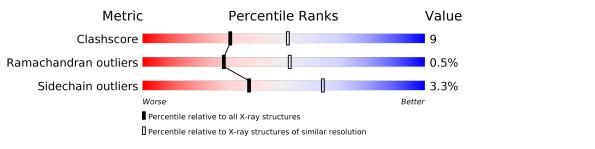
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25 th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455(2.60-2.60)
Sidechain outliers	138945	3455(2.60-2.60)

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 chain		
1	А	275	77%	23%	•
2	В	99	79%	21%	
3	С	9	78%	22%	_



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3229 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 I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	275	Total 2257	C 1426	N 399	O 423	S o	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 epitope of PB1-F2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	С	9	Total 72	C I 47 1	N 13	0 12	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	55	Total O 55 55	0	0
4	В	24	TotalO2424	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 colorcoded 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: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:	77%	23% •
P2 H3 S4 V11 V12 P15 P15 P15 P15 P15 P15 P29	F33 538 538 538 538 538 744 744 744 744 744 744 759 863 863 766 863 766 863 766 72 72 72 72 72 72 72 72 72 72 72 72 72	R75 L81 L81 S92 D106 W107 W107 W107 W113 Y113 Y113 Y113 Y113
D129 L130 Q141 B144 B144 Q146 Q149 Q149 Q149 D156 L168 L168	A177 1178 1178 1178 1180 8184 8184 8184 8186 8186 8186 8186 8186	1233 1233 1233 1234 1234 1255 1265 1265 1266 1266 1266 1266 1275 1275
• Molecule 2: Beta-2-	microglobulin	
Chain B:	79%	21%
11 88 81 81 81 915 915 813 813 813 813 813 813 813 813 813 813	Q38 140 140 153 168 168 168 168 168 168 168 168 168 168	
• Molecule 3: epitope	of PB1-F2	
Chain C:	78%	22%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	55.76Å 55.76 Å 278.60 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.60	Depositor
% Data completeness	93.2 (30.00-2.60)	Depositor
(in resolution range)	35.2 (50.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	REFMAC $5.2.0005$	Depositor
R, R_{free}	0.243 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3229	wwPDB-VP
Average B, all atoms $(Å^2)$	2.0	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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/2324	0.53	0/3155	
2	В	0.40	0/847	0.54	0/1148	
3	С	0.36	0/72	0.61	0/96	
All	All	0.38	0/3243	0.53	0/4399	

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 (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	2257	0	2127	42	0
2	В	821	0	796	15	0
3	С	72	0	86	3	0
4	А	55	0	0	4	0
4	В	24	0	0	0	0
All	All	3229	0	3009	56	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 9.

The worst 5 of 56 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:202:ARG:CG	1:A:202:ARG:HH11	2.02	0.72
1:A:177:ALA:O	1:A:181:ARG:HG3	1.90	0.72
1:A:144:ARG:O	1:A:148:GLU:HG3	1.96	0.66
4:A:303:HOH:O	2:B:53:ASP:HB3	1.95	0.66
1:A:194:ARG:HG2	4:A:302:HOH:O	1.95	0.66

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	А	273/275~(99%)	257 (94%)	15~(6%)	1 (0%)	34 57
2	В	97/99~(98%)	92~(95%)	4 (4%)	1 (1%)	15 32
3	С	7/9~(78%)	6 (86%)	1 (14%)	0	100 100
All	All	377/383~(98%)	355 (94%)	20~(5%)	2(0%)	29 52

All (2) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	107	TRP
2	В	85	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	Percentil	es
1	А	233/234~(100%)	223~(96%)	10 (4%)	29 54	
2	В	94/94~(100%)	93~(99%)	1 (1%)	73 88	
3	С	9/9~(100%)	9~(100%)	0	100 100)
All	All	336/337~(100%)	325~(97%)	11 (3%)	38 64	

5 of 11 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	179	LEU
1	А	202	ARG
1	А	255	GLN
1	А	154	GLU
1	А	226	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	256	ASN
1	А	263	HIS
2	В	31	HIS
1	А	188	HIS
2	В	17	ASN

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.



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.

