

wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 01:36 PM BST

PDB ID : 1RK0

Title: Mhc Class I H-2Kb Heavy Chain Complexed With beta-2 Microglobulin and

Herpes Simplex Virus Glycoprotein B peptide

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Deposited on : 2003-11-20

Resolution : 2.61 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

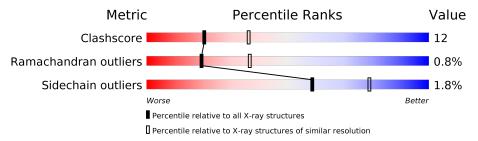
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.61 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)

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	A	274	76%	23%	•			
2	В	99	72%	27%	•			
3	Р	8	50%	50%				

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

	Mol	\mathbf{Type}	Chain	${ m Res}$	Chirality	Geometry	Clashes	Electron density
ſ	4	NAG	A	801	X	-	_	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3293 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, K-B alpha chain.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	274	Total 2232	C 1408	N 393	O 422	S 9	0	0	0

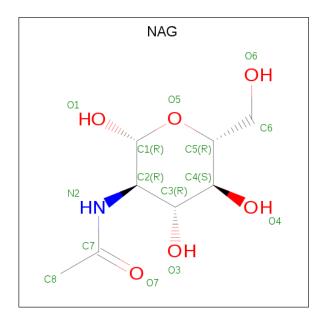
• Molecule 2 is a protein called Beta-2-microglobulin.

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 Glycoprotein B.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	Р	8	Total 65		N 11		0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	${f Atoms}$		ZeroOcc	AltConf
1	Δ	1	Total C N	О	0	0
1 1	11	1	14 8 1	5	0	

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	122	Total O 122 122	0	0
5	В	37	Total O 37 37	0	0
5	Р	2	Total O 2 2	0	0

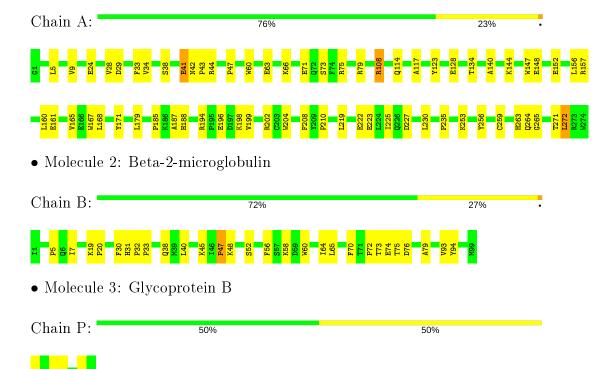


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: H-2 class I histocompatibility antigen, K-B alpha chain





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 2	Depositor	
Cell constants	134.89Å 90.22Å 45.45Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	19.98 - 2.61	Depositor	
% Data completeness	93.7 (19.98-2.61)	Depositor	
(in resolution range)	,	Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.07	Depositor	
Refinement program	CNS 1.1	Depositor	
R, R_{free}	0.199 , 0.238	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3293	wwPDB-VP	
Average B, all atoms (Å ²)	35.0	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

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		
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.37	0/2293	0.61	0/3113	
2	В	0.38	0/847	0.63	0/1148	
3	Р	0.48	0/65	0.58	0/84	
All	All	0.37	0/3205	0.62	0/4345	

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	A	2232	0	2122	55	0
2	В	821	0	796	19	0
3	Р	65	0	67	8	0
4	A	14	0	13	1	0
5	A	122	0	0	4	0
5	В	37	0	0	1	0
5	Р	2	0	0	1	0
All	All	3293	0	2998	76	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 12.



The worst 5 of 76 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:A:41:GLU:H	1:A:41:GLU:CD	1.82	0.82
1:A:253:LYS:HG3	1:A:256:TYR:HD2	1.51	0.76
1:A:144:LYS:O	1:A:148:GLU:HG3	1.89	0.73
1:A:272:LEU:N	1:A:272:LEU:HD12	2.09	0.68
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.75	0.68

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	${f Analysed}$	Favoured	${f Allowed}$	Outliers	Perce	entiles
1	A	272/274~(99%)	262 (96%)	8 (3%)	2 (1%)	22	41
2	В	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	30
3	Р	6/8 (75%)	6 (100%)	0	0	100	100
All	All	375/381 (98%)	360 (96%)	12 (3%)	3 (1%)	19	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Α	264	GLN
2	В	47	PRO
1	A	43	PRO

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 show	s the	${\bf number}$	of	residues	for	which	the	${\rm sidechain}$	conformation	was
analysed, and the total num	oer of	residues								

Mol	Chain	Analysed	Rotameric	Outliers	Perce	${f ntiles}$
1	A	$232/232 \ (100\%)$	227 (98%)	5 (2%)	52	74
2	В	94/94 (100%)	93 (99%)	1 (1%)	73	88
3	Р	7/7 (100%)	7 (100%)	0	100	100
All	All	333/333 (100%)	327 (98%)	6 (2%)	59	79

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
2	В	56	PHE
1	A	230	LEU
1	A	108	ARG
1	A	272	LEU

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

Mol	Chain	${f Res}$	Type
1	A	115	GLN
1	A	263	HIS
1	A	188	HIS
1	A	96	GLN
1	A	218	GLN

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 monosaccharides in this entry.



5.6 Ligand geometry (i)

1 ligand is 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	Pos	Link	Bo	ond leng	ths	В	ond ang	cles
MIGI	туре		main Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	801	1	14,14,15	0.76	0	17,19,21	0.55	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	NAG	A	801	1	1/1/5/7	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	801	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C3-C2-N2-C7
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

\mathbf{Mol}	Chain	${f Res}$	Type	Clashes	Symm-Clashes
4	A	801	NAG	1	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 (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.

