Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 06:18 AM EDT

PDB ID	:	3BEV
Title	:	11mer Structure of an MHC class I molecule from B21 chickens illustrate promiscuous peptide binding
Authors	:	Koch, M.; Kaufman, J.; Jones, Y.
Deposited on	:	2007-11-20
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

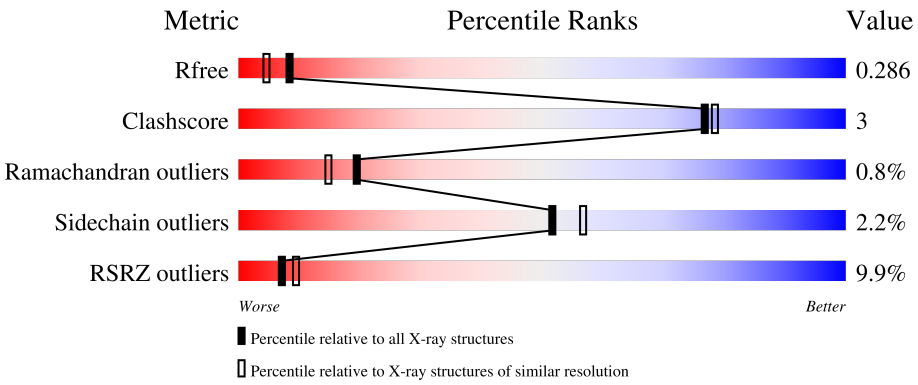
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	274	11% 86% 12% •
2	B	99	7% 90% 9% •
3	C	11	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3259 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 Major histocompatibility complex class I glycoprotein haplotype B21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2196	1375	398	415	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	ARG	-	expression tag	UNP Q95601
A	272	SER	-	expression tag	UNP Q95601
A	273	GLY	-	expression tag	UNP Q95601
A	274	GLY	-	expression tag	UNP Q95601

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	787	504	127	150	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P21611

- Molecule 3 is a protein called Hemoglobin subunit alpha-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	83	50	13	20	0	0	0

- Molecule 4 is water.

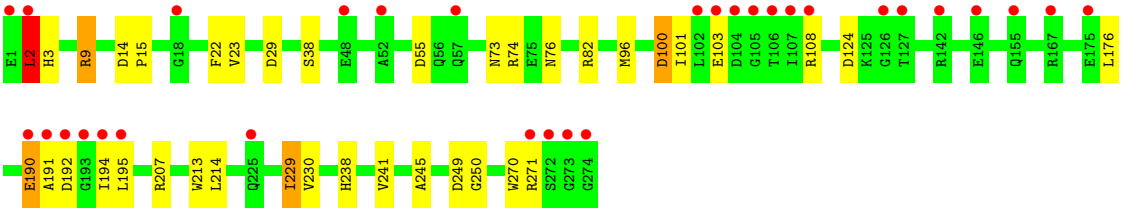
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	113	113	113	0	0
			Total	O		
4	B	69	69	69	0	0
			Total	O		
4	C	11	11	11	0	0

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 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.

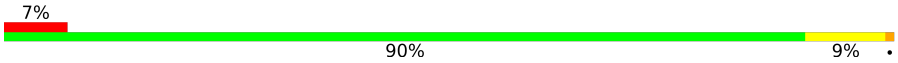
• Molecule 1: Major histocompatibility complex class I glycoprotein haplotype B21

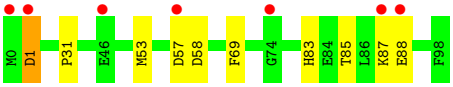
Chain A:



• Molecule 2: Beta-2-microglobulin

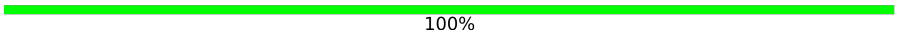
Chain B:





• Molecule 3: Hemoglobin subunit alpha-A

Chain C:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.31Å 72.20Å 72.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.10 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.10) 100.0 (19.95-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.286 0.230 , 0.286	Depositor DCC
R_{free} test set	1135 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k 0.016 for -l,-k,-h 0.016 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3259	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.60	0/2255	1.22	15/3062 (0.5%)
2	B	0.62	0/812	1.13	2/1102 (0.2%)
3	C	0.66	0/84	0.88	0/111
All	All	0.61	0/3151	1.19	17/4275 (0.4%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	LEU	CA-CB-CG	8.80	135.55	115.30
1	A	9	ARG	CA-CB-CG	6.53	127.76	113.40
1	A	15	PRO	CA-C-N	6.17	128.53	116.20
1	A	74	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	14	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	B	57	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	74	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	14	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	229	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	A	82	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	271	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	B	58	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	55	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	249	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	124	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	214	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	100	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2196	0	2080	16	0
2	B	787	0	746	3	0
3	C	83	0	70	0	0
4	A	113	0	0	1	0
4	B	69	0	0	0	0
4	C	11	0	0	0	0
All	All	3259	0	2896	18	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 3.

All (18) 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:23:VAL:HG21	2:B:53:MET:HB3	1.72	0.70
1:A:194:ILE:HG21	1:A:250:GLY:N	2.10	0.67
1:A:194:ILE:HD13	1:A:250:GLY:H	1.59	0.67
1:A:190:GLU:HB3	1:A:195:LEU:HB2	1.88	0.55
2:B:31:PRO:O	2:B:83:HIS:HE1	1.93	0.51
1:A:100:ASP:HB2	1:A:108:ARG:HB2	1.91	0.51
1:A:195:LEU:HD21	4:A:353:HOH:O	2.11	0.49
1:A:194:ILE:HG12	1:A:270:TRP:HZ3	1.79	0.48
1:A:195:LEU:HD23	1:A:245:ALA:O	2.15	0.46
1:A:2:LEU:HD22	1:A:103:GLU:HB3	1.98	0.46
1:A:3:HIS:HD2	1:A:101:ILE:HD11	1.81	0.45
1:A:29:ASP:HB2	1:A:176:LEU:HD22	1.98	0.45
1:A:213:TRP:HE1	1:A:241:VAL:HG12	1.82	0.44
1:A:207:ARG:HG3	1:A:229:ILE:HG21	1.99	0.44
1:A:22:PHE:HB3	1:A:38:SER:HB3	2.01	0.43
2:B:1:ASP:HB3	2:B:85:THR:HG22	2.02	0.42
1:A:230:VAL:HG23	1:A:238:HIS:HB3	2.01	0.42
1:A:73:ASN:HA	1:A:76:ASN:HB2	2.04	0.40

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	A	272/274 (99%)	260 (96%)	10 (4%)	2 (1%)	22	18
2	B	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	15	11
3	C	9/11 (82%)	9 (100%)	0	0	100	100
All	All	378/384 (98%)	364 (96%)	11 (3%)	3 (1%)	19	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	GLU
2	B	1	ASP
1	A	191	ALA

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	A	224/224 (100%)	220 (98%)	4 (2%)	59	65
2	B	87/87 (100%)	84 (97%)	3 (3%)	37	39
3	C	7/7 (100%)	7 (100%)	0	100	100
All	All	318/318 (100%)	311 (98%)	7 (2%)	52	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	9	ARG
1	A	96	MET
1	A	192	ASP
2	B	69	PHE
2	B	87	LYS
2	B	88	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
2	B	83	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 monosaccharides 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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	274/274 (100%)	1.03	31 (11%) 5 6	12, 25, 45, 60	2 (0%)
2	B	99/99 (100%)	0.49	7 (7%) 16 20	14, 22, 35, 51	0
3	C	11/11 (100%)	0.36	0 100 100	17, 20, 24, 26	0
All	All	384/384 (100%)	0.87	38 (9%) 7 9	12, 24, 43, 60	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	24.0
1	A	273	GLY	15.6
1	A	272	SER	12.6
1	A	191	ALA	11.6
1	A	192	ASP	9.6
1	A	194	ILE	8.3
1	A	271	ARG	7.5
1	A	274	GLY	6.9
1	A	52	ALA	5.6
2	B	0	MET	5.6
1	A	1	GLU	5.2
1	A	2	LEU	3.7
1	A	57	GLN	3.7
1	A	105	GLY	3.6
1	A	104	ASP	3.3
2	B	46	GLU	3.1
1	A	102	LEU	2.9
1	A	103	GLU	2.9
2	B	74	GLY	2.8
2	B	87	LYS	2.8
1	A	106	THR	2.8
1	A	195	LEU	2.7
1	A	127	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	88	GLU	2.6
2	B	57	ASP	2.6
1	A	167	ARG	2.5
1	A	18	GLY	2.4
2	B	1	ASP	2.4
1	A	48	GLU	2.3
1	A	108	ARG	2.3
1	A	126	GLY	2.2
1	A	175	GLU	2.1
1	A	225	GLN	2.1
1	A	146	GLU	2.1
1	A	142	ARG	2.1
1	A	107	ILE	2.1
1	A	155	GLN	2.1
1	A	190	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.