



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 3BEV / pdb_00003bev
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

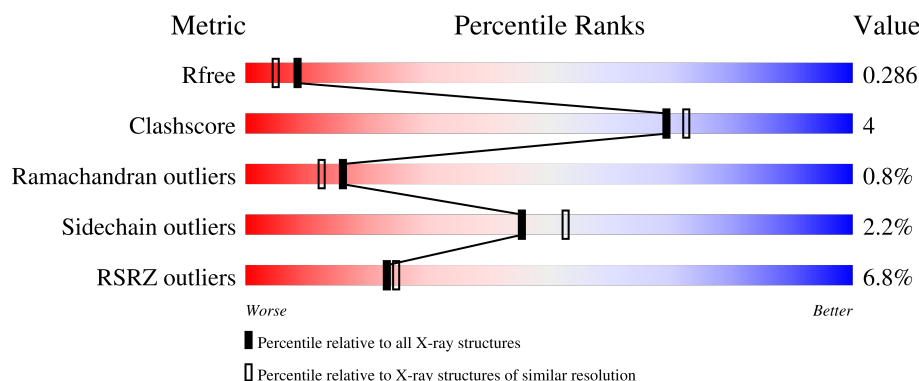
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	
2	B	99	
3	C	11	

2 Entry composition

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
1	A	274	Total	C	N	O	S	0	0	0
			2196	1375	398	415	8			

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
2	B	99	Total	C	N	O	S	0	0	0
			787	504	127	150	6			

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
3	C	11	Total	C	N	O	0	0	0
			83	50	13	20			

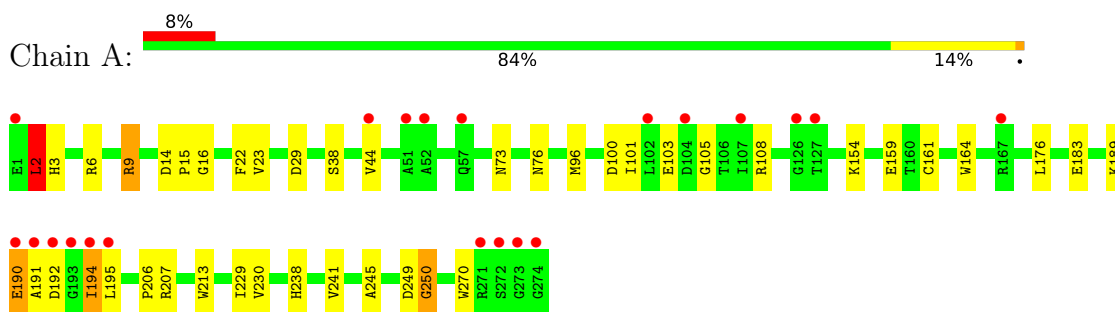
- Molecule 4 is water.

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

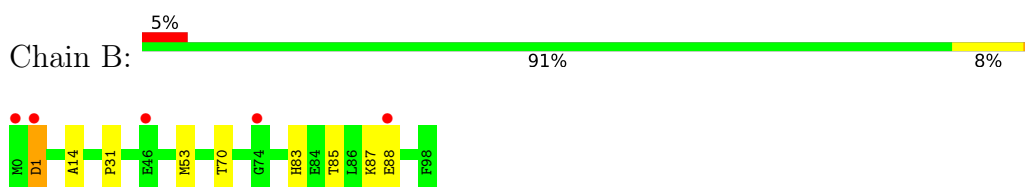
3 Residue-property plots

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.

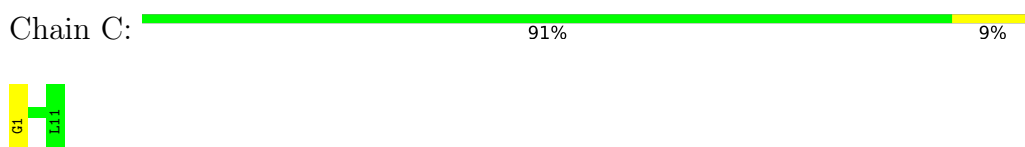
- Molecule 1: Major histocompatibility complex class I glycoprotein haplotype B21



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Hemoglobin subunit alpha-A



4 Data and refinement statistics

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) 99.8 (19.95-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.00%)	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)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.73	0/2255	1.52	24/3062 (0.8%)
2	B	0.68	0/812	1.35	2/1102 (0.2%)
3	C	0.68	0/84	1.16	0/111
All	All	0.71	0/3151	1.47	26/4275 (0.6%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	PRO	N-CA-C	6.88	123.09	113.53
1	A	9	ARG	CA-CB-CG	6.83	127.76	114.10
1	A	189	LYS	CA-C-N	6.51	133.97	121.54
1	A	189	LYS	C-N-CA	6.51	133.97	121.54
1	A	15	PRO	CA-C-N	5.98	132.46	121.70
1	A	15	PRO	C-N-CA	5.98	132.46	121.70
1	A	14	ASP	N-CA-CB	-5.78	103.93	111.09
1	A	159	GLU	N-CA-C	5.58	119.59	112.12
1	A	105	GLY	CA-C-N	5.56	129.15	120.75
1	A	105	GLY	C-N-CA	5.56	129.15	120.75
1	A	2	LEU	CA-CB-CG	5.50	135.55	116.30
1	A	154	LYS	CA-C-N	5.46	127.53	120.44
1	A	154	LYS	C-N-CA	5.46	127.53	120.44
1	A	15	PRO	O-C-N	-5.25	115.94	122.23
1	A	249	ASP	CA-C-N	5.17	125.82	120.03
1	A	249	ASP	C-N-CA	5.17	125.82	120.03
1	A	250	GLY	N-CA-C	5.15	119.12	112.83
1	A	161	CYS	CA-C-N	5.14	127.03	120.56
1	A	161	CYS	C-N-CA	5.14	127.03	120.56
2	B	14	ALA	N-CA-C	5.12	118.11	110.52
2	B	70	THR	CB-CA-C	5.12	117.00	110.34
1	A	16	GLY	CA-C-N	5.08	126.19	119.84
1	A	16	GLY	C-N-CA	5.08	126.19	119.84
1	A	206	PRO	CA-C-N	5.02	126.37	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	PRO	C-N-CA	5.02	126.37	120.09
1	A	183	GLU	N-CA-C	-5.02	101.13	109.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	18	0
2	B	787	0	746	4	0
3	C	83	0	70	1	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	21	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 4.

All (21) 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
1:A:6:ARG:CD	1:A:96:MET:HE3	2.39	0.53
2:B:31:PRO:O	2:B:83:HIS:HE1	1.93	0.51
1:A:164:TRP:CG	3:C:1:GLY:H3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:53:MET:HE3	2:B:53:MET:HA	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

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	272/274 (99%)	260 (96%)	10 (4%)	2 (1%)	18	15
2	B	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	12	9
3	C	9/11 (82%)	9 (100%)	0	0	100	100
All	All	378/384 (98%)	364 (96%)	11 (3%)	3 (1%)	16	12

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 ⓘ

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%)	219 (98%)	5 (2%)	45	53
2	B	87/87 (100%)	85 (98%)	2 (2%)	44	51
3	C	7/7 (100%)	7 (100%)	0	100	100
All	All	318/318 (100%)	311 (98%)	7 (2%)	45	53

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	44	VAL
1	A	192	ASP
1	A	194	ILE
2	B	87	LYS
2	B	88	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	56	GLN
1	A	155	GLN
1	A	202	HIS
2	B	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.62	21 (7%) 19 21	11, 25, 45, 60	2 (0%)
2	B	99/99 (100%)	0.20	5 (5%) 33 35	14, 22, 35, 51	0
3	C	11/11 (100%)	-0.10	0 100 100	17, 20, 24, 26	0
All	All	384/384 (100%)	0.49	26 (6%) 23 25	11, 24, 43, 60	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	13.1
1	A	194	ILE	6.8
1	A	273	GLY	6.3
1	A	191	ALA	5.5
1	A	272	SER	5.1
1	A	274	GLY	4.5
1	A	52	ALA	3.8
1	A	192	ASP	3.7
2	B	0	MET	3.6
1	A	195	LEU	3.6
1	A	127	THR	3.3
1	A	271	ARG	3.2
2	B	74	GLY	3.1
1	A	190	GLU	3.0
1	A	57	GLN	2.8
1	A	126	GLY	2.6
1	A	104	ASP	2.4
1	A	1	GLU	2.3
1	A	44	VAL	2.2
1	A	51	ALA	2.2
2	B	46	GLU	2.2
1	A	102	LEU	2.2
1	A	107	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	167	ARG	2.1
2	B	88	GLU	2.1
2	B	1	ASP	2.1

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 oligosaccharides 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.