



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:47 PM UTC

PDB ID : 8EC5 / pdb_00008ec5
Title : Structures of HLA-B8E76C loaded with long peptides reveal novel features at the N-terminus of the groove
Authors : Li, L.; Bouvier, M.
Deposited on : 2022-09-01
Resolution : 1.22 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

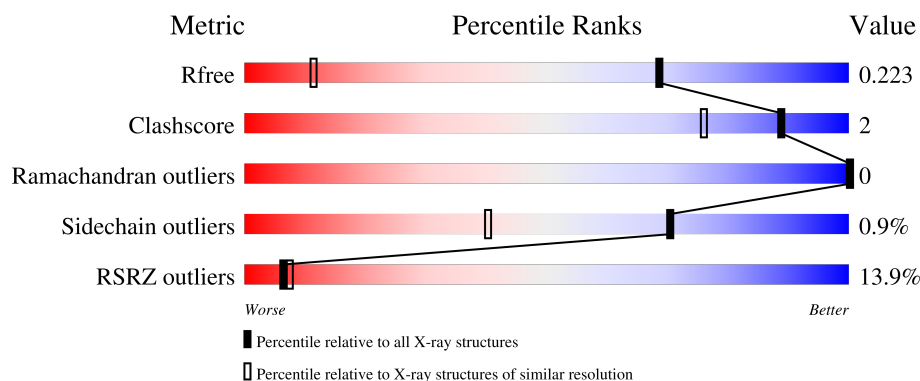
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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	276	10% 86% 7% 7%
2	B	99	19% 94% 5%
3	C	20	20% 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3356 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 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2088	1292	384	404	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	CYS	GLU	engineered mutation	UNP R4ZGR5

- 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
			829	528	140	158	3			

- Molecule 3 is a protein called peptide RARARARARARAFVKKKYCL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			82	56	13	12	1			

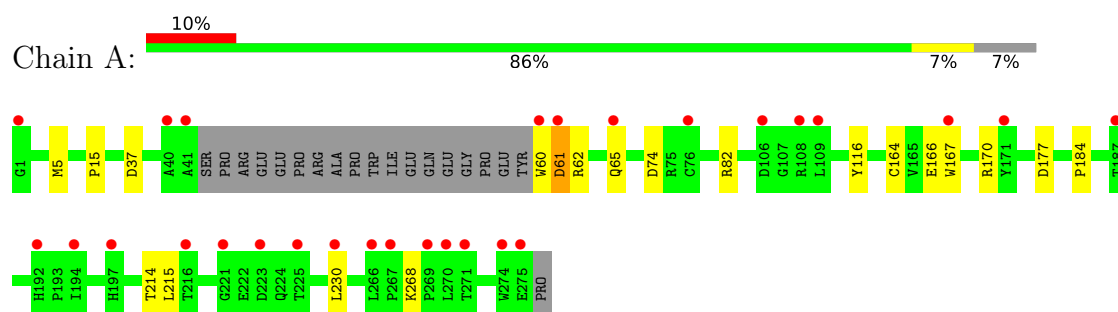
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		
4	B	100	Total	O	0	0
			100	100		
4	C	8	Total	O	0	0
			8	8		

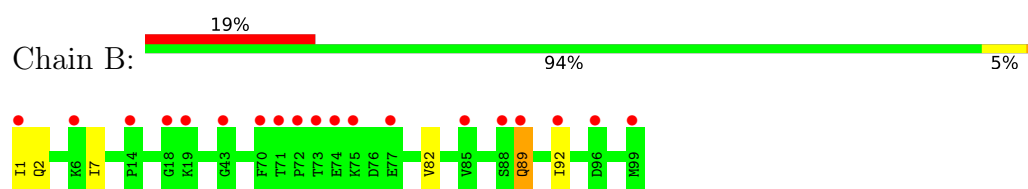
3 Residue-property plots [i](#)

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.

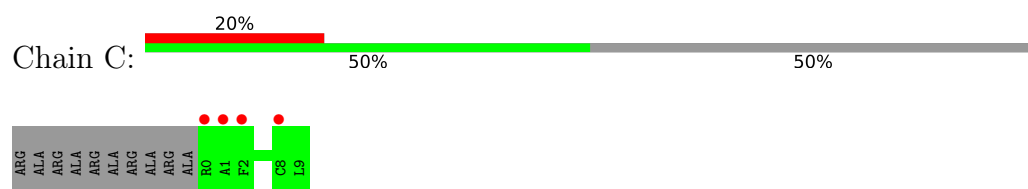
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin



- Molecule 3: peptide RARARARARARAFVKKKYCL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.76Å 81.15Å 110.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 1.22 24.00 – 1.22	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.00-1.22) 98.1 (24.00-1.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 1.22Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.199 , 0.212 0.208 , 0.223	Depositor DCC
R_{free} test set	6556 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3356	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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	1.25	3/2141 (0.1%)	1.19	6/2907 (0.2%)
2	B	1.17	2/852 (0.2%)	1.16	0/1152
3	C	1.03	0/83	1.20	0/107
All	All	1.22	5/3076 (0.2%)	1.18	6/4166 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	VAL	C-O	7.24	1.31	1.24
1	A	15	PRO	C-O	-6.69	1.14	1.23
1	A	37	ASP	C-O	6.19	1.30	1.24
1	A	184	PRO	C-O	-5.54	1.18	1.24
2	B	7	ILE	C-O	5.12	1.29	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LEU	CA-C-O	-5.53	114.59	120.40
1	A	61	ASP	CA-C-O	-5.49	114.77	120.92
1	A	74	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	215	LEU	N-CA-CB	-5.04	102.86	110.77
1	A	60	TRP	CA-C-N	5.01	128.34	120.82
1	A	60	TRP	C-N-CA	5.01	128.34	120.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	TYR	Sidechain

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	2088	0	1948	7	0
2	B	829	0	794	3	0
3	C	82	0	90	0	0
4	A	249	0	0	4	0
4	B	100	0	0	1	0
4	C	8	0	0	0	0
All	All	3356	0	2832	10	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 2.

All (10) 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:1:ILE:HG23	2:B:2:GLN:H	1.65	0.60
1:A:82:ARG:NH2	4:A:302:HOH:O	2.45	0.49
2:B:89:GLN:O	2:B:89:GLN:OE1	2.30	0.49
1:A:177:ASP:OD2	4:A:301:HOH:O	2.20	0.45
1:A:5:MET:HE2	1:A:164:CYS:SG	2.58	0.44
1:A:214:THR:HG22	4:A:449:HOH:O	2.18	0.43
1:A:61:ASP:OD1	1:A:65:GLN:NE2	2.51	0.43
1:A:167:TRP:CZ3	1:A:170:ARG:HD2	2.55	0.41
2:B:92:ILE:HD11	4:B:194:HOH:O	2.21	0.41
1:A:166:GLU:HG3	4:A:524:HOH:O	2.21	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	253/276 (92%)	248 (98%)	5 (2%)	0	100	100
2	B	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	C	8/20 (40%)	8 (100%)	0	0	100	100
All	All	358/395 (91%)	352 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	218/235 (93%)	216 (99%)	2 (1%)	70	40
2	B	94/94 (100%)	93 (99%)	1 (1%)	65	32
3	C	8/14 (57%)	8 (100%)	0	100	100
All	All	320/343 (93%)	317 (99%)	3 (1%)	70	40

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	268	LYS
2	B	89	GLN

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	72	GLN
1	A	141	GLN
1	A	192	HIS
1	A	224	GLN
1	A	226	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 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	257/276 (93%)	0.85	28 (10%)	10 12	11, 16, 32, 60	0
2	B	99/99 (100%)	1.13	19 (19%)	3 4	12, 20, 37, 51	0
3	C	10/20 (50%)	1.45	4 (40%)	1 0	15, 19, 28, 43	0
All	All	366/395 (92%)	0.94	51 (13%)	6 7	11, 17, 34, 60	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	TRP	10.4
2	B	1	ILE	7.6
3	C	0	ARG	4.8
1	A	171	TYR	3.5
1	A	197	HIS	3.3
1	A	267	PRO	3.3
3	C	1	ALA	3.3
1	A	221	GLY	3.3
2	B	89	GLN	3.2
1	A	40	ALA	3.2
1	A	230	LEU	3.1
1	A	194	ILE	3.0
2	B	73	THR	2.8
1	A	274	TRP	2.8
2	B	75	LYS	2.8
1	A	41	ALA	2.8
2	B	71	THR	2.7
2	B	70	PHE	2.7
2	B	88	SER	2.7
1	A	275	GLU	2.7
1	A	266	LEU	2.7
1	A	1	GLY	2.6
2	B	92	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLN	2.5
1	A	108	ARG	2.4
1	A	61	ASP	2.4
3	C	8	CYS	2.4
1	A	187	THR	2.4
2	B	99	MET	2.4
1	A	216	THR	2.3
1	A	269	PRO	2.3
1	A	270	LEU	2.3
2	B	18	GLY	2.3
2	B	72	PRO	2.2
1	A	76	CYS	2.2
1	A	223	ASP	2.2
1	A	167	TRP	2.2
1	A	109	LEU	2.2
2	B	74	GLU	2.2
1	A	192	HIS	2.1
3	C	2	PHE	2.1
2	B	77	GLU	2.1
2	B	43	GLY	2.1
1	A	225	THR	2.1
1	A	271	THR	2.1
2	B	19	LYS	2.1
1	A	106	ASP	2.1
2	B	96	ASP	2.1
2	B	14	PRO	2.1
2	B	6	LYS	2.0
2	B	85	VAL	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 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.