



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2025 – 02:05 PM EDT

PDB ID : 9PKF / pdb\_00009pkf  
Title : Mur35 Fab with HBV c18I pMHC  
Authors : Mortenson, D.E.  
Deposited on : 2025-07-14  
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](mailto: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>.

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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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

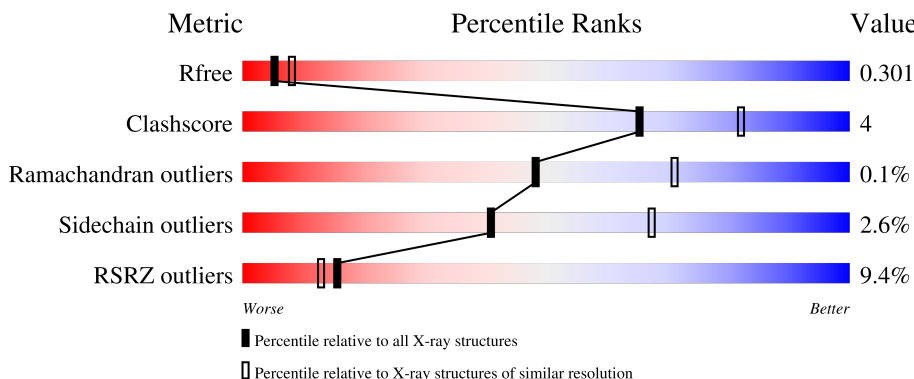
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	301	<div> <div>3%</div> <div>83%</div> <div>13%</div> </div>
2	H	237	<div> <div>17%</div> <div>72%</div> <div>14%</div> <div>14%</div> </div>
3	L	215	<div> <div>10%</div> <div>76%</div> <div>16%</div> <div>7%</div> </div>
4	P	10	<div> <div>100%</div> </div>
5	B	100	<div> <div>%</div> <div>90%</div> <div>8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6045 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	261	Total	C	N	O	S	0	0	0
			2086	1312	380	385	9			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8WLS4
A	277	GLY	-	expression tag	UNP Q8WLS4
A	278	SER	-	expression tag	UNP Q8WLS4
A	279	GLY	-	expression tag	UNP Q8WLS4
A	280	GLY	-	expression tag	UNP Q8WLS4
A	281	SER	-	expression tag	UNP Q8WLS4
A	282	GLY	-	expression tag	UNP Q8WLS4
A	283	GLY	-	expression tag	UNP Q8WLS4
A	284	SER	-	expression tag	UNP Q8WLS4
A	285	ALA	-	expression tag	UNP Q8WLS4
A	286	GLY	-	expression tag	UNP Q8WLS4
A	287	GLY	-	expression tag	UNP Q8WLS4
A	288	GLY	-	expression tag	UNP Q8WLS4
A	289	LEU	-	expression tag	UNP Q8WLS4
A	290	ASN	-	expression tag	UNP Q8WLS4
A	291	ASP	-	expression tag	UNP Q8WLS4
A	292	ILE	-	expression tag	UNP Q8WLS4
A	293	PHE	-	expression tag	UNP Q8WLS4
A	294	GLU	-	expression tag	UNP Q8WLS4
A	295	ALA	-	expression tag	UNP Q8WLS4
A	296	GLN	-	expression tag	UNP Q8WLS4
A	297	LYS	-	expression tag	UNP Q8WLS4
A	298	ILE	-	expression tag	UNP Q8WLS4
A	299	GLU	-	expression tag	UNP Q8WLS4
A	300	TRP	-	expression tag	UNP Q8WLS4

- Molecule 2 is a protein called Mur35 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	205	Total	C	N	O	S	0	3	0
			1518	954	253	305	6			

- Molecule 3 is a protein called Mur35 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	199	Total	C	N	O	S	0	1	0
			1432	890	240	297	5			

- Molecule 4 is a protein called c18I peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	10	Total	C	N	O	0	0	0
			84	59	10	15			

- Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	98	Total	C	N	O	S	0	2	0
			792	505	132	152	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

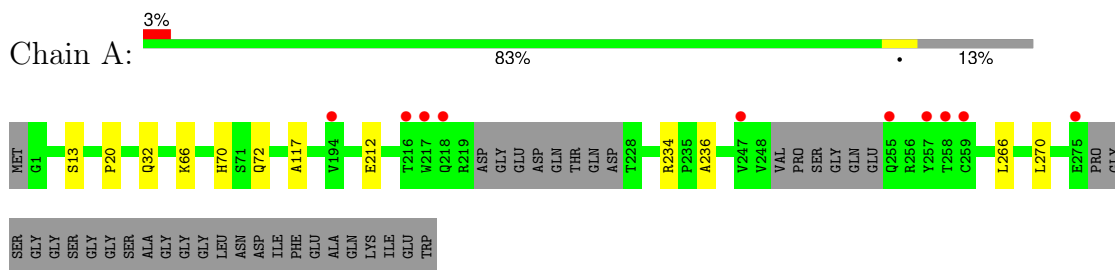
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		
6	H	36	Total	O	0	0
			36	36		
6	L	19	Total	O	0	0
			19	19		
6	P	4	Total	O	0	0
			4	4		
6	B	16	Total	O	0	0
			16	16		

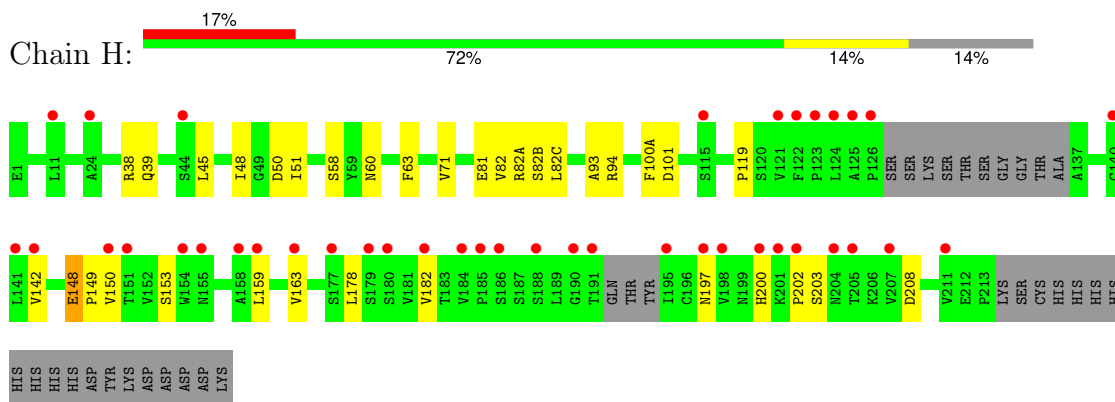
### 3 Residue-property plots

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.

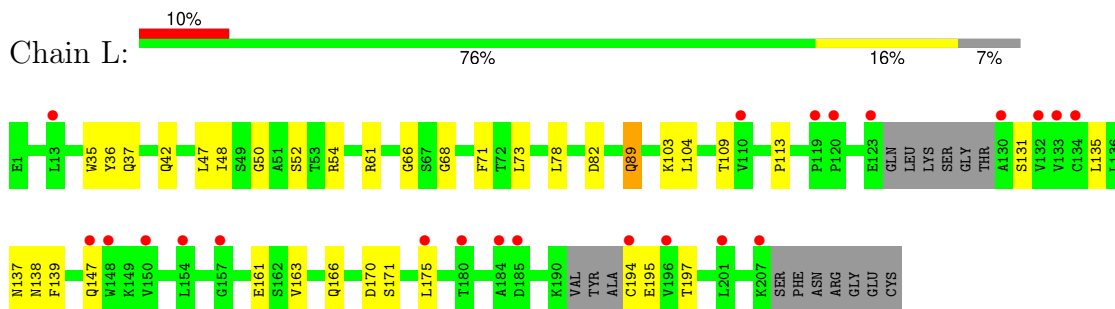
- Molecule 1: MHC class I antigen



- Molecule 2: Mur35 Heavy Chain



- Molecule 3: Mur35 Light Chain




- Molecule 4: c18I peptide



There are no outlier residues recorded for this chain.

● Molecule 5: Beta-2-microglobulin

Chain B:  % 90% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.17Å 73.02Å 72.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.42 – 2.60 45.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.42-2.60) 95.1 (45.42-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.247 , 0.303 0.253 , 0.301	Depositor DCC
$R_{free}$ test set	1387 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	0.07	0/2146	0.23	0/2917
2	H	0.08	0/1565	0.24	0/2133
3	L	0.08	0/1465	0.25	0/2005
4	P	0.08	0/88	0.24	0/118
5	B	0.06	0/821	0.23	0/1118
All	All	0.07	0/6085	0.23	0/8291

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	2086	0	1928	7	0
2	H	1518	0	1409	17	0
3	L	1432	0	1291	16	0
4	P	84	0	79	0	0
5	B	792	0	720	6	0
6	A	58	0	0	0	0
6	B	16	0	0	0	0
6	H	36	0	0	0	0
6	L	19	0	0	0	0
6	P	4	0	0	0	0
All	All	6045	0	5427	42	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.

The worst 5 of 42 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)
3:L:36:TYR:HE2	3:L:89:GLN:HG2	1.60	0.66
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.81	0.61
3:L:61:ARG:NE	3:L:82:ASP:OD2	2.36	0.59
5:B:5:PRO:HB3	5:B:30:PHE:HB3	1.87	0.56
2:H:50:ASP:OD1	2:H:58:SER:OG	2.20	0.54

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	255/301 (85%)	244 (96%)	11 (4%)	0	100	100
2	H	202/237 (85%)	187 (93%)	15 (7%)	0	100	100
3	L	194/215 (90%)	177 (91%)	16 (8%)	1 (0%)	25	47
4	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
5	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
All	All	757/863 (88%)	710 (94%)	46 (6%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	68	GLY

### 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	207/247 (84%)	205 (99%)	2 (1%)	73	88
2	H	165/205 (80%)	159 (96%)	6 (4%)	30	56
3	L	149/186 (80%)	141 (95%)	8 (5%)	18	39
4	P	10/10 (100%)	10 (100%)	0	100	100
5	B	86/95 (90%)	86 (100%)	0	100	100
All	All	617/743 (83%)	601 (97%)	16 (3%)	41	67

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	194	CYS
3	L	170	ASP
3	L	42	GLN
3	L	135	LEU
2	H	148	GLU

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

Mol	Chain	Res	Type
3	L	93	ASN
3	L	158	ASN
3	L	199	GLN
3	L	42	GLN
1	A	86	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 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/301 (86%)	0.40	10 (3%) 44 38	40, 55, 114, 166	0
2	H	205/237 (86%)	1.01	40 (19%) 4 3	45, 70, 145, 167	3 (1%)
3	L	199/215 (92%)	0.83	22 (11%) 12 9	46, 77, 130, 171	1 (0%)
4	P	10/10 (100%)	0.54	0 100 100	40, 51, 60, 62	0
5	B	98/100 (98%)	0.46	1 (1%) 79 75	37, 67, 105, 115	2 (2%)
All	All	773/863 (89%)	0.68	73 (9%) 15 13	37, 67, 130, 171	6 (0%)

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	179	SER	5.0
2	H	198	VAL	4.5
3	L	120	PRO	4.1
1	A	255	GLN	3.8
3	L	119[A]	PRO	3.5

### 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.