



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3QUK  
Title : Crystal structures of the murine class I major histocompatibility complex H-2Db in complex with LCMV-derived gp33 altered peptide ligand (Y4A)  
Authors : Allerbring, E.; Duru, A.D.; Uchtenhagen, H.; Madhurantakam, C.; Grimm, S.; Tomek, M.B.; Mazumdar, P.A.; Spetz, A.; Friemann, R.; Sandalova, T; Uhlin, M.; Nygren, P.; Achour, A.  
Deposited on : 2011-02-24  
Resolution : 2.41 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

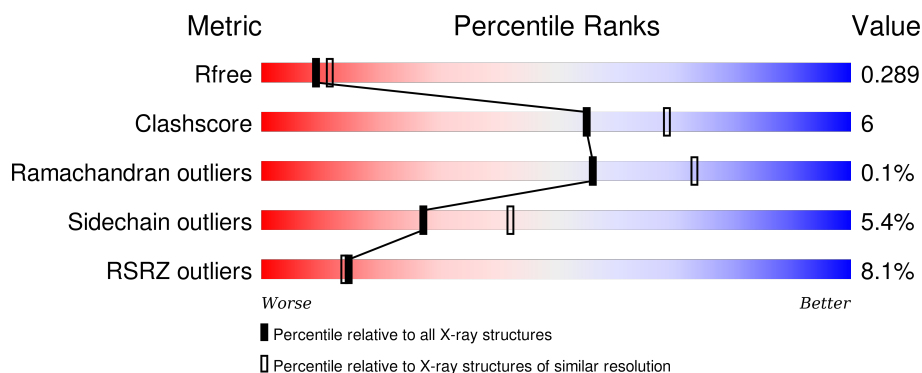
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
$R_{free}$	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	338	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>10%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	338	<div> <div>9%</div> <div> <div></div> <div>64%</div> <div>11%</div> <div>•</div> <div>23%</div> </div> </div>
2	B	99	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
2	E	99	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
3	C	9	<div> <div></div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	9	 <p>A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a red segment labeled '22%', a green segment labeled '78%', a yellow segment labeled '11%', and an orange segment labeled '11%'.</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6443 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, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	2	0
			2178	1375	385	409	9			
1	D	261	Total	C	N	O	S	0	2	0
			2173	1373	388	403	9			

- 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	1	0
			828	528	139	154	7			
2	E	99	Total	C	N	O	S	0	1	0
			832	530	142	153	7			

- Molecule 3 is a protein called Glycoprotein G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			66	42	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			66	42	11	12	1			

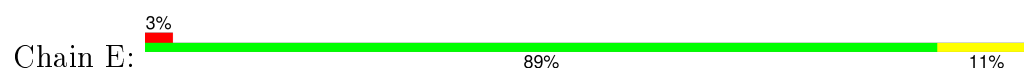
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	ALA	TYR	ENGINEERED MUTATION	UNP P07399
C	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
F	4	ALA	TYR	ENGINEERED MUTATION	UNP P07399
F	9	MET	CYS	ENGINEERED MUTATION	UNP P07399

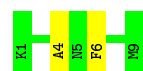
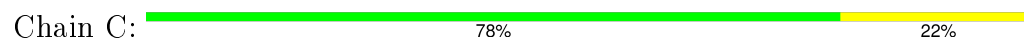
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total 110	O 110	0	0
4	B	44	Total 44	O 44	0	0
4	C	8	Total 8	O 8	0	0
4	D	87	Total 87	O 87	0	0
4	E	49	Total 49	O 49	0	0
4	F	2	Total 2	O 2	0	0

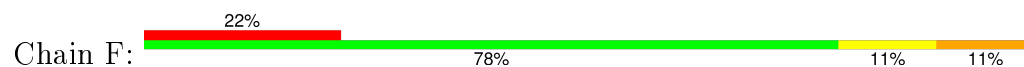




- Molecule 3: Glycoprotein G1



- Molecule 3: Glycoprotein G1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.51Å 126.21Å 96.47Å 90.00° 124.54° 90.00°	Depositor
Resolution (Å)	33.90 – 2.41 33.89 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.90-2.41) 99.0 (33.89-2.41)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.242 , 0.285 0.248 , 0.289	Depositor DCC
$R_{free}$ test set	2252 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 44585 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/2240	0.59	0/3035
1	D	0.47	0/2238	0.61	0/3030
2	B	0.53	0/854	0.63	1/1158 (0.1%)
2	E	0.49	0/858	0.60	0/1162
3	C	0.68	0/66	0.65	0/86
3	F	0.77	0/66	0.72	0/86
All	All	0.49	0/6322	0.61	1/8557 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	41	LYS	CB-CA-C	-5.43	99.53	110.40

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	2178	0	2034	27	0
1	D	2173	0	2042	35	0
2	B	828	0	802	13	0
2	E	832	0	808	5	0
3	C	66	0	70	2	0
3	F	66	0	70	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	110	0	0	3	0
4	B	44	0	0	2	0
4	C	8	0	0	0	0
4	D	87	0	0	0	0
4	E	49	0	0	0	0
4	F	2	0	0	0	0
All	All	6443	0	5826	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 6.

The worst 5 of 76 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:D:19:GLU:CG	1:D:75[B]:ARG:HH21	1.31	1.42
1:D:19:GLU:CG	1:D:75[B]:ARG:NH2	2.00	1.23
1:D:19:GLU:HG3	1:D:75[B]:ARG:NH2	1.65	1.08
1:D:19:GLU:HG2	1:D:75[B]:ARG:HH21	0.93	1.07
1:D:19:GLU:HG2	1:D:75[B]:ARG:NH2	1.66	1.02

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	254/338 (75%)	244 (96%)	9 (4%)	1 (0%)	39	54
1	D	253/338 (75%)	245 (97%)	8 (3%)	0	100	100
2	B	98/99 (99%)	94 (96%)	4 (4%)	0	100	100
2	E	98/99 (99%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	717/892 (80%)	690 (96%)	26 (4%)	1 (0%)	56	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LEU

### 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	224/280 (80%)	212 (95%)	12 (5%)	27	42
1	D	223/280 (80%)	210 (94%)	13 (6%)	25	38
2	B	95/94 (101%)	89 (94%)	6 (6%)	22	34
2	E	95/94 (101%)	92 (97%)	3 (3%)	46	67
3	C	6/6 (100%)	6 (100%)	0	100	100
3	F	6/6 (100%)	5 (83%)	1 (17%)	3	3
All	All	649/760 (85%)	614 (95%)	35 (5%)	27	42

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	73	THR
1	D	39	ASP
2	E	85	ASP
2	B	75	THR
2	B	93	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
2	B	31	HIS
1	D	192	HIS
1	A	192	HIS
1	D	97	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 carbohydrates 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	262/338 (77%)	0.46	20 (7%) 17 16	24, 52, 84, 117	0
1	D	261/338 (77%)	0.61	30 (11%) 6 6	20, 56, 82, 105	0
2	B	99/99 (100%)	0.35	5 (5%) 32 31	38, 54, 66, 68	0
2	E	99/99 (100%)	0.28	3 (3%) 54 52	40, 54, 65, 69	0
3	C	9/9 (100%)	0.74	0 100 100	42, 47, 49, 49	0
3	F	9/9 (100%)	1.28	2 (22%) 1 1	45, 49, 55, 58	0
All	All	739/892 (82%)	0.49	60 (8%) 15 14	20, 54, 81, 117	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	GLY	5.3
1	A	17	LEU	4.6
1	A	251	LEU	4.3
1	A	181	ARG	4.2
1	A	274	TRP	4.1

### 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 carbohydrates 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.