



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:18 pm GMT

PDB ID : 1MML  
Title : MECHANISTIC IMPLICATIONS FROM THE STRUCTURE OF A CATALYTIC FRAGMENT OF MMLV REVERSE TRANSCRIPTASE  
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Deposited on : 1995-07-18  
Resolution : 1.80 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](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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

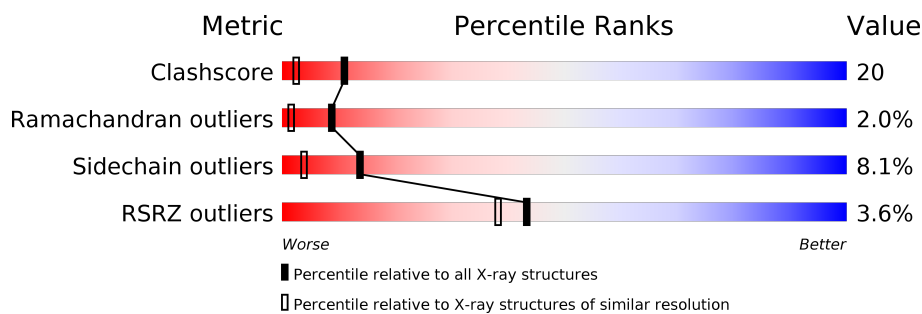
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.80 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))
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	265	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2132 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 MMLV REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2007	1293	348	359	7			

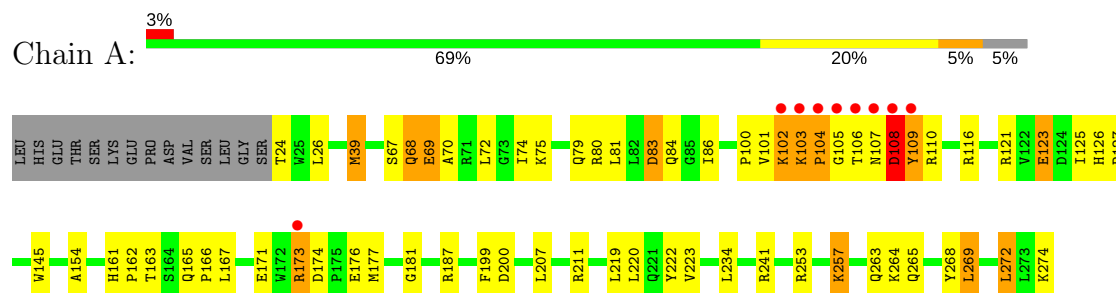
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: MMLV REVERSE TRANSCRIPTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.10Å 84.10Å 74.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.80 14.60 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 95.5 (14.60-1.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 1.81Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.198 , 0.257 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 79.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

### 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	1/2063 (0.0%)	1.55	24/2815 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	LYS	N-CA	-5.57	1.35	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	C-N-CA	19.13	169.52	121.70
1	A	187	ARG	NE-CZ-NH1	-12.85	113.88	120.30
1	A	121	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	A	241	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	110	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	A	253	ARG	NE-CZ-NH1	11.55	126.07	120.30
1	A	110	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	A	171	GLU	OE1-CD-OE2	8.96	134.05	123.30
1	A	222	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	A	211	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	222	TYR	CB-CG-CD1	7.30	125.38	121.00
1	A	173	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	83	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	A	253	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	200	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	75	LYS	CA-CB-CG	5.56	125.64	113.40
1	A	257	LYS	CA-CB-CG	5.53	125.57	113.40
1	A	110	ARG	CD-NE-CZ	5.43	131.20	123.60
1	A	167	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	109	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	24	THR	N-CA-CB	5.29	120.35	110.30
1	A	108	ASP	C-N-CA	5.26	134.85	121.70
1	A	116	ARG	NE-CZ-NH1	5.21	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	CD-NE-CZ	5.17	130.83	123.60

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	2007	0	2025	81	0
2	A	125	0	0	0	0
All	All	2132	0	2025	81	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 20.

All (81) 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:69:GLU:HB3	1:A:106:THR:N	1.81	0.95
1:A:126:HIS:HB3	1:A:127:PRO:CD	1.99	0.91
1:A:104:PRO:O	1:A:109:TYR:OH	1.90	0.89
1:A:103:LYS:HE2	1:A:109:TYR:HA	1.56	0.88
1:A:69:GLU:HB3	1:A:105:GLY:C	1.98	0.83
1:A:107:ASN:O	1:A:109:TYR:CD1	2.35	0.80
1:A:69:GLU:HB3	1:A:105:GLY:CA	2.13	0.79
1:A:174:ASP:OD1	1:A:176:GLU:HG2	1.84	0.77
1:A:126:HIS:HB3	1:A:127:PRO:HD2	1.65	0.77
1:A:103:LYS:HG3	1:A:108:ASP:C	2.06	0.76
1:A:103:LYS:HB3	1:A:104:PRO:HD2	1.67	0.76
1:A:265:GLN:OE1	1:A:274:LYS:HE3	1.85	0.75
1:A:161:HIS:HD2	1:A:163:THR:H	1.34	0.75
1:A:173:ARG:NH2	1:A:181:GLY:HA2	2.01	0.75
1:A:103:LYS:HG3	1:A:108:ASP:O	1.88	0.73
1:A:272:LEU:HD11	1:A:274:LYS:HB3	1.73	0.71
1:A:104:PRO:HD2	1:A:107:ASN:ND2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:HE1	1:A:84:GLN:HE22	1.56	0.70
1:A:103:LYS:CD	1:A:108:ASP:O	2.42	0.68
1:A:126:HIS:CB	1:A:127:PRO:CD	2.66	0.67
1:A:265:GLN:CG	1:A:274:LYS:HB2	2.25	0.67
1:A:103:LYS:HB3	1:A:104:PRO:CD	2.24	0.67
1:A:161:HIS:CD2	1:A:163:THR:H	2.12	0.65
1:A:272:LEU:HD13	1:A:272:LEU:C	2.16	0.65
1:A:126:HIS:CB	1:A:127:PRO:HD3	2.26	0.64
1:A:173:ARG:CZ	1:A:181:GLY:HA2	2.28	0.63
1:A:69:GLU:HB3	1:A:106:THR:H	1.62	0.62
1:A:173:ARG:NH1	1:A:181:GLY:O	2.32	0.62
1:A:103:LYS:CB	1:A:104:PRO:CD	2.80	0.60
1:A:105:GLY:C	1:A:107:ASN:H	2.03	0.59
1:A:272:LEU:CD1	1:A:274:LYS:HB3	2.32	0.58
1:A:126:HIS:HB3	1:A:127:PRO:HD3	1.85	0.58
1:A:103:LYS:CG	1:A:108:ASP:O	2.51	0.58
1:A:265:GLN:HG2	1:A:274:LYS:CB	2.33	0.58
1:A:173:ARG:NH1	1:A:173:ARG:HG2	2.20	0.57
1:A:265:GLN:OE1	1:A:274:LYS:CE	2.52	0.56
1:A:174:ASP:HB3	1:A:177:MET:HB2	1.88	0.56
1:A:74:ILE:HD11	1:A:100:PRO:HA	1.88	0.56
1:A:165:GLN:N	1:A:166:PRO:CD	2.70	0.55
1:A:69:GLU:CB	1:A:106:THR:H	2.20	0.54
1:A:69:GLU:CB	1:A:105:GLY:CA	2.83	0.54
1:A:69:GLU:CB	1:A:106:THR:N	2.62	0.54
1:A:103:LYS:HD2	1:A:108:ASP:O	2.08	0.53
1:A:39:MET:HE1	1:A:84:GLN:NE2	2.23	0.53
1:A:173:ARG:CZ	1:A:181:GLY:CA	2.87	0.53
1:A:145:TRP:CE2	1:A:264:LYS:HE3	2.46	0.51
1:A:70:ALA:HB1	1:A:100:PRO:HB3	1.91	0.51
1:A:103:LYS:HG2	1:A:109:TYR:HA	1.92	0.51
1:A:173:ARG:NH1	1:A:181:GLY:N	2.58	0.51
1:A:39:MET:CE	1:A:84:GLN:HE22	2.23	0.50
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.12	0.50
1:A:103:LYS:CE	1:A:109:TYR:HA	2.34	0.49
1:A:265:GLN:CG	1:A:274:LYS:CB	2.91	0.48
1:A:39:MET:SD	1:A:86:ILE:HD11	2.53	0.48
1:A:103:LYS:CG	1:A:109:TYR:HA	2.44	0.48
1:A:107:ASN:O	1:A:109:TYR:HD1	1.95	0.47
1:A:268:TYR:O	1:A:269:LEU:HB2	2.13	0.47
1:A:103:LYS:CE	1:A:108:ASP:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:CB	1:A:104:PRO:HD2	2.40	0.46
1:A:274:LYS:HE3	1:A:274:LYS:HB2	1.79	0.46
1:A:207:LEU:HD13	1:A:219:LEU:HD21	1.99	0.44
1:A:154:ALA:HB1	1:A:199:PHE:CZ	2.52	0.44
1:A:145:TRP:NE1	1:A:264:LYS:HE3	2.32	0.44
1:A:39:MET:HB2	1:A:39:MET:HE2	1.82	0.44
1:A:103:LYS:HB3	1:A:107:ASN:HD22	1.83	0.44
1:A:69:GLU:CA	1:A:106:THR:H	2.30	0.44
1:A:104:PRO:HD2	1:A:107:ASN:HD22	1.81	0.44
1:A:69:GLU:C	1:A:106:THR:H	2.21	0.43
1:A:173:ARG:HH11	1:A:173:ARG:HG2	1.83	0.43
1:A:272:LEU:C	1:A:272:LEU:CD1	2.84	0.43
1:A:67:SER:HB2	1:A:69:GLU:OE2	2.18	0.43
1:A:173:ARG:NH1	1:A:181:GLY:CA	2.82	0.43
1:A:265:GLN:OE1	1:A:274:LYS:NZ	2.50	0.42
1:A:104:PRO:O	1:A:109:TYR:CZ	2.71	0.42
1:A:68:GLN:HB2	1:A:68:GLN:HE21	1.62	0.42
1:A:80:ARG:O	1:A:84:GLN:HG3	2.19	0.42
1:A:103:LYS:HE3	1:A:108:ASP:O	2.20	0.41
1:A:107:ASN:O	1:A:109:TYR:CE1	2.72	0.41
1:A:173:ARG:CG	1:A:173:ARG:HH11	2.33	0.41
1:A:161:HIS:CD2	1:A:163:THR:HG23	2.55	0.40
1:A:105:GLY:HA2	1:A:109:TYR:OH	2.20	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	249/265 (94%)	239 (96%)	5 (2%)	5 (2%)	<b>9</b> <b>1</b>

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	103	LYS
1	A	104	PRO
1	A	108	ASP
1	A	223	VAL

### 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	221/234 (94%)	203 (92%)	18 (8%)	14 4

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	39	MET
1	A	68	GLN
1	A	69	GLU
1	A	72	LEU
1	A	79	GLN
1	A	81	LEU
1	A	83	ASP
1	A	108	ASP
1	A	123	GLU
1	A	125	ILE
1	A	162	PRO
1	A	220	LEU
1	A	234	LEU
1	A	257	LYS
1	A	263	GLN
1	A	269	LEU
1	A	272	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	77	HIS
1	A	84	GLN
1	A	107	ASN
1	A	161	HIS
1	A	214	HIS
1	A	249	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 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	251/265 (94%)	-0.33	9 (3%) 43 38	8, 18, 43, 82	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	PRO	10.4
1	A	106	THR	8.2
1	A	108	ASP	6.9
1	A	107	ASN	5.9
1	A	105	GLY	5.6
1	A	103	LYS	4.1
1	A	102	LYS	3.1
1	A	173	ARG	2.7
1	A	109	TYR	2.3

### 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.