



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:35 AM GMT

PDB ID : 1MV5  
Title : Crystal structure of LmrA ATP-binding domain  
Authors : Yuan, Y.; Chen, H.; Patel, D.  
Deposited on : 2002-09-24  
Resolution : 3.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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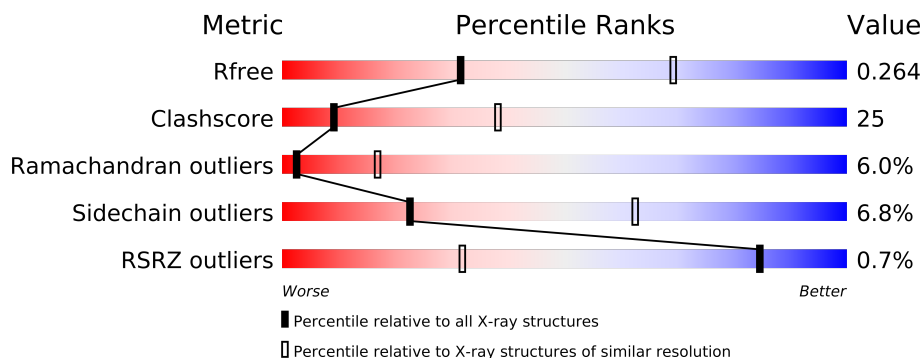
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	
1	C	243	
1	D	243	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	1601	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7671 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Multidrug resistance ABC transporter ATP-binding and per-mease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1866	1174	321	365	6			
1	B	242	Total	C	N	O	S	0	0	0
			1877	1179	320	372	6			
1	C	242	Total	C	N	O	S	0	0	0
			1862	1172	321	363	6			
1	D	241	Total	C	N	O	S	0	0	0
			1870	1175	320	369	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	MET	-	INITIATING MET	UNP Q9CHL8
B	1342	MET	-	INITIATING MET	UNP Q9CHL8
C	2342	MET	-	INITIATING MET	UNP Q9CHL8
D	3342	MET	-	INITIATING MET	UNP Q9CHL8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

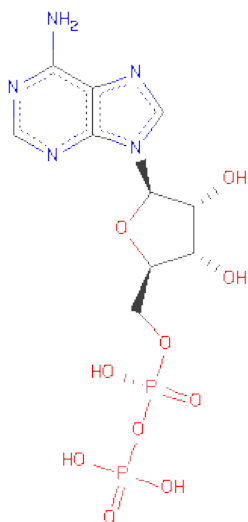
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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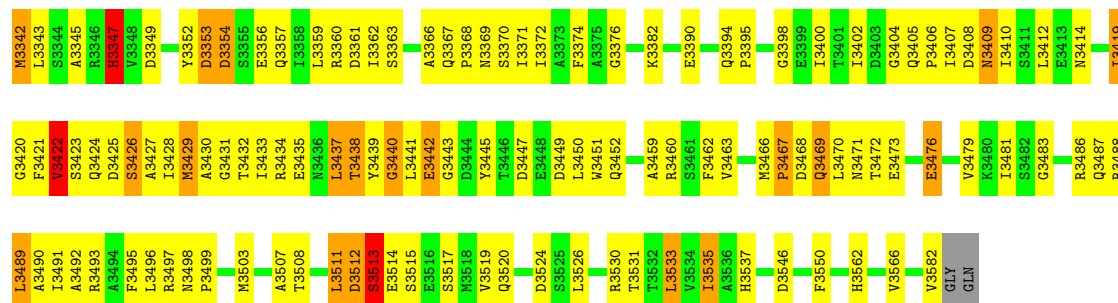
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	12	Total	O	0	0
			12	12		
5	C	24	Total	O	0	0
			24	24		
5	D	19	Total	O	0	0
			19	19		



- Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.87Å 141.87Å 120.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 28.73 – 3.11	Depositor EDS
% Data completeness (in resolution range)	84.8 (40.00-3.10) 95.5 (28.73-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.11Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.251 , 0.283 0.242 , 0.264	Depositor DCC
$R_{free}$ test set	1192 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 14.2	EDS
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 23832 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	0.99	2/1897 (0.1%)	1.11	6/2566 (0.2%)
1	B	0.98	1/1908 (0.1%)	1.18	11/2580 (0.4%)
1	C	0.93	2/1893 (0.1%)	1.12	10/2561 (0.4%)
1	D	1.00	2/1901 (0.1%)	1.14	8/2570 (0.3%)
All	All	0.97	7/7599 (0.1%)	1.14	35/10277 (0.3%)

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	C	0	1
1	D	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	ASP	CB-CG	8.63	1.69	1.51
1	B	1342	MET	SD-CE	6.14	2.12	1.77
1	C	2506	GLU	CG-CD	6.08	1.61	1.51
1	C	2445	TYR	CB-CG	5.82	1.60	1.51
1	A	518	MET	SD-CE	5.67	2.09	1.77

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3450	LEU	CB-CG-CD1	-8.51	96.54	111.00
1	C	2533	LEU	CA-CB-CG	8.09	133.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1470	LEU	CA-CB-CG	7.94	133.57	115.30
1	C	2426	SER	N-CA-C	-7.69	90.22	111.00
1	C	2445	TYR	CB-CA-C	7.50	125.39	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2572	TYR	Sidechain
1	D	3422	VAL	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1866	0	1823	77	0
1	B	1877	0	1846	74	0
1	C	1862	0	1819	103	0
1	D	1870	0	1840	132	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	2	0
3	C	31	0	12	3	0
4	B	27	0	12	2	0
4	D	27	0	12	1	0
5	A	23	0	0	1	0
5	B	12	0	0	1	0
5	C	24	0	0	5	0
5	D	19	0	0	1	0
All	All	7671	0	7376	374	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

The worst 5 of 374 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3466:MET:CE	1:D:3466:MET:SD	2.04	1.45
1:A:429:MET:SD	1:A:429:MET:CE	2.05	1.43
1:A:518:MET:SD	1:A:518:MET:CE	2.09	1.40
1:B:1342:MET:SD	1:B:1342:MET:CE	2.12	1.38
1:C:2539:LEU:HD11	5:C:4069:HOH:O	1.34	1.21

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	240/243 (99%)	198 (82%)	27 (11%)	15 (6%)	2	16
1	B	240/243 (99%)	200 (83%)	29 (12%)	11 (5%)	4	24
1	C	240/243 (99%)	202 (84%)	22 (9%)	16 (7%)	2	14
1	D	239/243 (98%)	189 (79%)	34 (14%)	16 (7%)	2	14
All	All	959/972 (99%)	789 (82%)	112 (12%)	58 (6%)	2	17

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	LEU
1	A	426	SER
1	A	444	ASP
1	A	467	PRO
1	A	476	GLU

### 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	196/204 (96%)	181 (92%)	15 (8%)	18	57
1	B	202/204 (99%)	187 (93%)	15 (7%)	20	59
1	C	195/204 (96%)	183 (94%)	12 (6%)	26	66
1	D	201/204 (98%)	189 (94%)	12 (6%)	27	67
All	All	794/816 (97%)	740 (93%)	54 (7%)	22	62

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1438	THR
1	C	2343	LEU
1	D	3467	PRO
1	B	1446	THR
1	B	1515	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2394	GLN
1	C	2409	ASN
1	D	3424	GLN
1	B	1465	ASN
1	D	3405	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ATP	A	601	-	33,33,33	2.28	13 (39%)	52,52,52	2.87	19 (36%)
4	ADP	B	1600	-	29,29,29	2.22	11 (37%)	45,45,45	2.02	5 (11%)
3	ATP	C	2601	-	33,33,33	2.40	13 (39%)	52,52,52	2.87	17 (32%)
4	ADP	D	3600	2	29,29,29	1.96	9 (31%)	45,45,45	2.17	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	601	-	-	0/22/38/38	0/1/3/3
4	ADP	B	1600	-	-	0/16/32/32	0/1/3/3
3	ATP	C	2601	-	-	0/22/38/38	0/1/3/3
4	ADP	D	3600	2	-	0/16/32/32	0/1/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2601	ATP	O5'-C5'	-4.87	1.24	1.44
3	C	2601	ATP	PA-O3A	-4.87	1.51	1.59
4	B	1600	ADP	C4-N9	-4.74	1.30	1.37
4	B	1600	ADP	PB-O3A	-4.74	1.52	1.60
3	A	601	ATP	C4-N3	4.59	1.42	1.35

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	O5'-C5'-C4'	11.43	150.90	108.94
4	D	3600	ADP	N3-C2-N1	-11.27	119.29	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1600	ADP	N3-C2-N1	-10.93	119.57	128.71
3	C	2601	ATP	O5'-C5'-C4'	10.39	147.06	108.94
3	C	2601	ATP	O3A-PB-O3B	-9.60	82.14	101.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	242/243 (99%)	-0.12	2 (0%) 83 28	20, 57, 130, 176	0
1	B	242/243 (99%)	-0.00	2 (0%) 83 28	26, 84, 144, 170	0
1	C	242/243 (99%)	-0.11	3 (1%) 75 20	17, 57, 126, 176	0
1	D	241/243 (99%)	-0.03	0 100 100	24, 86, 145, 153	0
All	All	967/972 (99%)	-0.06	7 (0%) 84 32	17, 67, 145, 176	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1583	GLY	3.5
1	C	2514	GLU	3.1
1	A	516	GLU	2.9
1	A	514	GLU	2.6
1	C	2583	GLY	2.6

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	1601	1/1	0.29	6.05	76,76,76,76	0
3	ATP	A	601	31/31	0.18	0.74	49,57,97,99	0
3	ATP	C	2601	31/31	0.17	0.34	37,52,89,95	0
4	ADP	B	1600	27/27	0.16	-0.35	19,42,53,54	0
4	ADP	D	3600	27/27	0.15	-0.64	17,37,50,52	0
2	MG	D	3601	1/1	0.14	-	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.