



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 19, 2023 – 02:42 AM EDT

PDB ID : 5DU7  
Title : Crystal structure of ldtMt2 at 1.79 Angstrom resolution  
Authors : Kumar, P.; Lamichhane, G.  
Deposited on : 2015-09-18  
Resolution : 1.79 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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

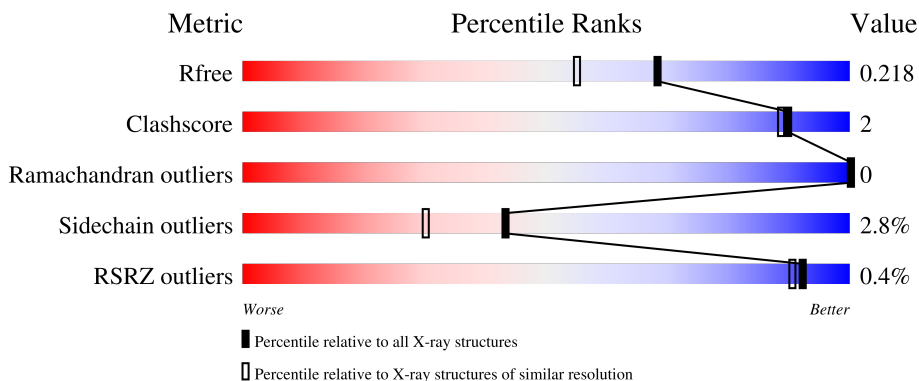
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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	370	 87% 6% •• 5%
1	B	370	 87% 5% • 6%
1	C	370	 89% 5% • 5%
1	D	370	 89% 5% • 6%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12407 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 L,D-transpeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	Total 2642	C 1657	N 463	O 514	S 8	0	0	0
1	B	349	Total 2655	C 1663	N 469	O 515	S 8	0	2	0
1	D	349	Total 2633	C 1651	N 461	O 513	S 8	0	0	0
1	C	351	Total 2650	C 1663	N 464	O 515	S 8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP O53223
A	40	HIS	-	expression tag	UNP O53223
A	41	MET	-	expression tag	UNP O53223
B	39	GLY	-	expression tag	UNP O53223
B	40	HIS	-	expression tag	UNP O53223
B	41	MET	-	expression tag	UNP O53223
D	39	GLY	-	expression tag	UNP O53223
D	40	HIS	-	expression tag	UNP O53223
D	41	MET	-	expression tag	UNP O53223
C	39	GLY	-	expression tag	UNP O53223
C	40	HIS	-	expression tag	UNP O53223
C	41	MET	-	expression tag	UNP O53223

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	463	Total 463	O 463	0	0
2	B	456	Total 456	O 456	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	D	450	Total	O	0	0
			450	450		
2	C	458	Total	O	0	0
			458	458		





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.64Å 75.53Å 94.14Å 89.04° 89.96° 92.76°	Depositor
Resolution (Å)	50.00 – 1.79 29.27 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-1.79) 83.1 (29.27-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.170 , 0.210 0.180 , 0.218	Depositor DCC
$R_{free}$ test set	7834 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.056 for h,-k,-l 0.055 for -h,k,-l 0.349 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	1.07	1/2708 (0.0%)	1.17	22/3708 (0.6%)
1	B	1.05	1/2721 (0.0%)	1.13	20/3725 (0.5%)
1	C	1.02	2/2716 (0.1%)	1.08	17/3719 (0.5%)
1	D	1.00	0/2699	1.02	10/3697 (0.3%)
All	All	1.03	4/10844 (0.0%)	1.10	69/14849 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	ASP	CB-CG	7.73	1.68	1.51
1	A	197	GLU	CD-OE1	-5.67	1.19	1.25
1	C	202	TRP	CG-CD1	-5.07	1.29	1.36
1	C	392	GLY	C-O	5.01	1.31	1.23

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	B	96	ASP	CB-CG-OD1	13.07	130.06	118.30
1	C	99	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	B	99	ARG	NE-CZ-NH1	11.87	126.23	120.30
1	A	297	ARG	NE-CZ-NH1	11.64	126.12	120.30

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	2642	0	2544	9	0
1	B	2655	0	2555	15	0
1	C	2650	0	2555	6	0
1	D	2633	0	2531	7	0
2	A	463	0	0	4	0
2	B	456	0	0	12	1
2	C	458	0	0	3	0
2	D	450	0	0	5	0
All	All	12407	0	10185	37	1

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.

The worst 5 of 37 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:B:139[B]:ARG:HD3	2:B:512:HOH:O	1.55	1.05
1:C:99:ARG:NH2	2:C:501:HOH:O	1.95	0.99
1:B:132:GLY:HA2	2:B:567:HOH:O	1.76	0.86
1:B:122:ARG:NH1	2:B:502:HOH:O	2.10	0.84
1:D:122:ARG:NH1	2:D:501:HOH:O	2.16	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:HOH:O	2:B:768:HOH:O[1_565]	1.97	0.23

## 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	348/370 (94%)	341 (98%)	7 (2%)	0	100	100
1	B	349/370 (94%)	343 (98%)	6 (2%)	0	100	100
1	C	349/370 (94%)	341 (98%)	8 (2%)	0	100	100
1	D	347/370 (94%)	339 (98%)	8 (2%)	0	100	100
All	All	1393/1480 (94%)	1364 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	281/295 (95%)	271 (96%)	10 (4%)	35	20
1	B	282/295 (96%)	274 (97%)	8 (3%)	43	30
1	C	282/295 (96%)	275 (98%)	7 (2%)	47	34
1	D	280/295 (95%)	274 (98%)	6 (2%)	53	42
All	All	1125/1180 (95%)	1094 (97%)	31 (3%)	43	30

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	126	LEU
1	C	203	LEU
1	B	393	ASP
1	C	297	ARG
1	C	94	VAL

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	127	ASN
1	A	356	ASN
1	B	127	ASN

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Mol	Chain	Res	Type
1	D	368	HIS
1	C	356	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 monosaccharides 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	350/370 (94%)	-0.57	2 (0%) 89   87	5, 13, 28, 61	0
1	B	349/370 (94%)	-0.54	0 100   100	7, 15, 27, 46	0
1	C	351/370 (94%)	-0.59	3 (0%) 84   82	7, 15, 30, 69	0
1	D	349/370 (94%)	-0.59	1 (0%) 94   92	7, 15, 28, 43	0
All	All	1399/1480 (94%)	-0.57	6 (0%) 92   90	5, 15, 28, 69	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	LEU	4.6
1	C	133	LEU	2.9
1	A	133	LEU	2.9
1	C	58	LEU	2.8
1	A	58	LEU	2.6

### 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 monosaccharides 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.