



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2017 – 11:06 AM EST

PDB ID : 5LDI  
Title : Crystal structure of E.coli LigT in apo form  
Authors : Myllykoski, M.; Kursula, P.  
Deposited on : 2016-06-27  
Resolution : 2.10 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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

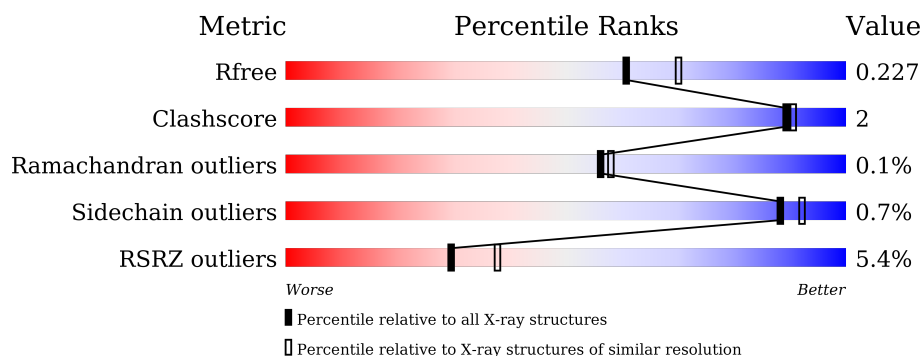
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	177	
1	B	177	
1	C	177	
1	D	177	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	201	-	-	X	-
2	CL	C	201	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11652 atoms, of which 5579 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 RNA 2',3'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	175	Total	C	H	N	O	S	0	4	0
			2850	914	1426	263	243	4			
1	B	170	Total	C	H	N	O	S	0	2	0
			2755	888	1379	252	233	3			
1	C	171	Total	C	H	N	O	S	0	0	0
			2748	879	1377	255	234	3			
1	D	172	Total	C	H	N	O	S	0	2	0
			2787	889	1397	261	238	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A140NFI1
B	0	GLY	-	expression tag	UNP A0A140NFI1
C	0	GLY	-	expression tag	UNP A0A140NFI1
D	0	GLY	-	expression tag	UNP A0A140NFI1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		

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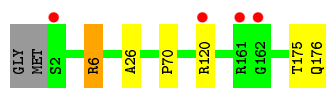
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	156	Total 156	O 156	0	0
3	C	108	Total 108	O 108	0	0
3	D	88	Total 88	O 88	0	0

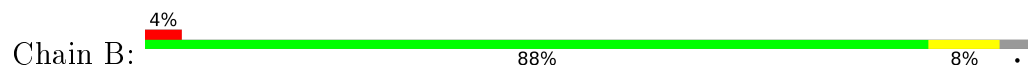
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

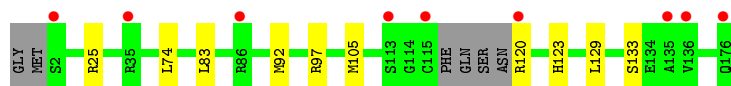
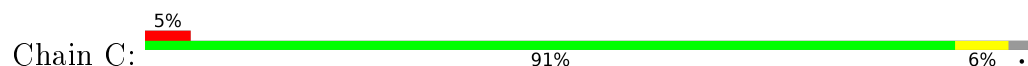
- Molecule 1: RNA 2',3'-cyclic phosphodiesterase



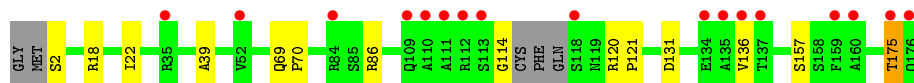
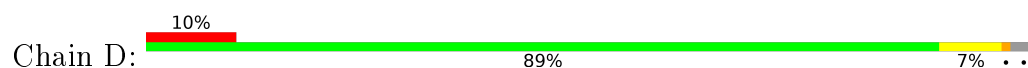
- Molecule 1: RNA 2',3'-cyclic phosphodiesterase



- Molecule 1: RNA 2',3'-cyclic phosphodiesterase



- Molecule 1: RNA 2',3'-cyclic phosphodiesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.39Å 88.32Å 73.84Å 90.00° 115.01° 90.00°	Depositor
Resolution (Å)	36.60 – 2.10 48.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.60-2.10) 99.8 (48.16-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.177 , 0.227 0.177 , 0.227	Depositor DCC
$R_{free}$ test set	2151 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.24	0/1482	0.46	0/2013
1	B	0.26	0/1422	0.48	0/1931
1	C	0.26	0/1410	0.51	0/1915
1	D	0.27	0/1438	0.55	0/1952
All	All	0.26	0/5752	0.50	0/7811

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	1424	1426	1402	5	1
1	B	1376	1379	1373	10	1
1	C	1371	1377	1377	6	0
1	D	1390	1397	1390	10	0
2	A	1	0	0	0	0
2	B	1	0	0	2	0
2	C	1	0	0	0	0
3	A	157	0	0	1	0
3	B	156	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	108	0	0	1	0
3	D	88	0	0	3	0
All	All	6073	5579	5542	27	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.

All (27) 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)
2:B:201:CL:CL	3:B:397:HOH:O	2.30	0.86
1:B:6:ARG:NH2	1:C:83:LEU:O	2.21	0.73
1:A:120:ARG:NH2	1:B:40:ASP:OD1	2.26	0.69
1:B:6:ARG:NH1	1:C:133:SER:O	2.28	0.67
1:B:112:ARG:NH2	2:B:201:CL:CL	2.71	0.61
1:D:69:GLN:O	1:D:175:THR:N	2.35	0.59
1:A:120:ARG:NH2	3:A:302:HOH:O	2.38	0.55
1:C:97:ARG:NH2	3:C:306:HOH:O	2.40	0.54
1:D:114:GLY:O	3:D:201:HOH:O	2.19	0.54
1:B:101:GLN:NE2	3:B:304:HOH:O	2.42	0.53
1:B:13:LEU:O	1:B:18:ARG:NH1	2.44	0.50
1:B:69:GLN:NE2	1:B:98:GLY:O	2.38	0.49
1:D:120:ARG:HB3	1:D:121:PRO:HD2	1.96	0.48
1:A:6:ARG:NH1	1:D:22:ILE:HD11	2.29	0.47
1:D:86:ARG:CD	1:D:131:ASP:HA	2.46	0.46
1:B:35:ARG:NH2	1:B:162:GLY:O	2.49	0.45
1:D:2:SER:N	3:D:208:HOH:O	2.49	0.45
1:B:83:LEU:HD21	1:B:135:ALA:HB2	1.98	0.44
1:C:25:ARG:HD2	1:C:129:LEU:CD1	2.48	0.44
1:C:74:LEU:HD22	1:C:92:MET:SD	2.58	0.43
1:C:120:ARG:NH1	1:C:123:HIS:H	2.17	0.43
1:A:6:ARG:HH12	1:D:22:ILE:HD11	1.85	0.42
1:D:157:SER:OG	3:D:202:HOH:O	2.21	0.42
1:D:18[B]:ARG:NH1	1:D:39:ALA:O	2.40	0.42
1:A:70:PRO:HA	1:A:175:THR:O	2.20	0.41
1:B:13:LEU:HD21	1:B:126:ILE:HD13	2.02	0.41
1:D:70:PRO:HA	1:D:175:THR:HA	2.02	0.41

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)
1:A:26:ALA:O	1:B:66:ARG:HH12[2_745]	1.58	0.02

## 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	177/177 (100%)	176 (99%)	1 (1%)	0	100	100
1	B	168/177 (95%)	167 (99%)	1 (1%)	0	100	100
1	C	167/177 (94%)	166 (99%)	1 (1%)	0	100	100
1	D	170/177 (96%)	168 (99%)	1 (1%)	1 (1%)	30	24
All	All	682/708 (96%)	677 (99%)	4 (1%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	175	THR

### 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	149/146 (102%)	147 (99%)	2 (1%)	76	82
1	B	141/146 (97%)	141 (100%)	0	100	100
1	C	141/146 (97%)	140 (99%)	1 (1%)	88	92
1	D	144/146 (99%)	143 (99%)	1 (1%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	575/584 (98%)	571 (99%)	4 (1%)	88	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	176	GLN
1	C	105	MET
1	D	136	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	175/177 (98%)	0.08	4 (2%) 64 70	27, 43, 82, 131	0
1	B	170/177 (96%)	0.06	7 (4%) 41 50	25, 44, 91, 122	0
1	C	171/177 (96%)	0.17	9 (5%) 30 39	27, 51, 101, 140	0
1	D	172/177 (97%)	0.48	17 (9%) 9 13	29, 58, 117, 146	0
All	All	688/708 (97%)	0.20	37 (5%) 29 38	25, 49, 100, 146	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	GLN	6.7
1	A	161	ARG	6.6
1	D	136	VAL	5.6
1	D	111	ALA	5.5
1	D	137	THR	5.2
1	D	112	ARG	5.1
1	D	176	GLN	5.0
1	D	159	PHE	4.6
1	D	134	GLU	4.2
1	A	120	ARG	4.0
1	D	52	VAL	3.8
1	B	116	PHE	3.6
1	B	32	GLU	3.5
1	C	2	SER	3.4
1	C	115	CYS	3.4
1	A	162	GLY	3.3
1	D	135	ALA	3.2
1	D	113	SER	3.0
1	C	113	SER	2.9
1	C	120	ARG	2.9
1	D	35	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	159[A]	PHE	2.8
1	A	2	SER	2.7
1	D	110	ALA	2.7
1	B	161	ARG	2.6
1	D	160	ALA	2.5
1	C	35	ARG	2.4
1	D	175	THR	2.4
1	C	136	VAL	2.4
1	D	109	GLN	2.4
1	D	118	SER	2.3
1	B	160[A]	ALA	2.3
1	C	86	ARG	2.2
1	B	35	ARG	2.2
1	C	135	ALA	2.1
1	D	84	ARG	2.1
1	B	135	ALA	2.1

## 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](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	C	201	1/1	0.91	0.30	6.74	77,77,77,77	0
2	CL	B	201	1/1	0.99	0.10	-3.10	51,51,51,51	0
2	CL	A	201	1/1	0.92	0.07	-	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.