



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2016 – 07:58 PM EST

PDB ID : 5LOP  
Title : Structure of the active form of /K. lactis/ Dcp1-Dcp2-Edc3 decapping complex bound to m7GDP  
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Deposited on : 2016-08-09  
Resolution : 3.50 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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-20028320

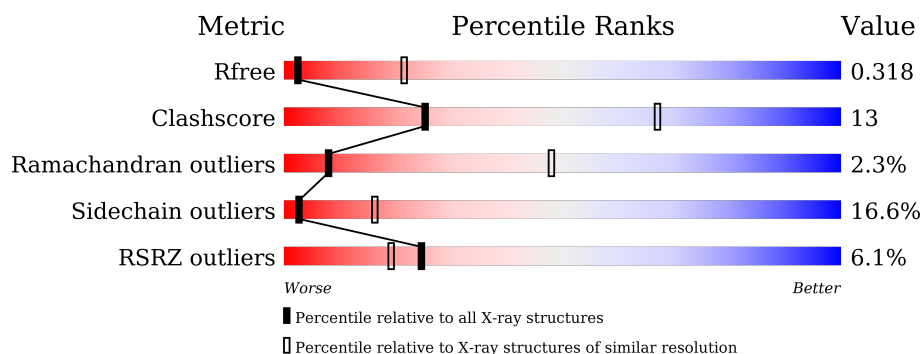
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	281	<div> <div>5%</div> <div>56%</div> <div>31%</div> <div>6%</div> <div>8%</div> </div>
2	B	188	<div> <div>7%</div> <div>53%</div> <div>35%</div> <div>5%</div> <div>8%</div> </div>
3	C	66	<div> <div>3%</div> <div>50%</div> <div>33%</div> <div>11%</div> <div>6%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4075 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 KLLA0F23980p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2121	1380	350	385	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	HIS	-	expression tag	UNP Q6CIU1
A	277	HIS	-	expression tag	UNP Q6CIU1
A	278	HIS	-	expression tag	UNP Q6CIU1
A	279	HIS	-	expression tag	UNP Q6CIU1
A	280	HIS	-	expression tag	UNP Q6CIU1
A	281	HIS	-	expression tag	UNP Q6CIU1

- Molecule 2 is a protein called KLLA0E01827p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1429	920	240	266	3			

- Molecule 3 is a protein called KLLA0A11308p.

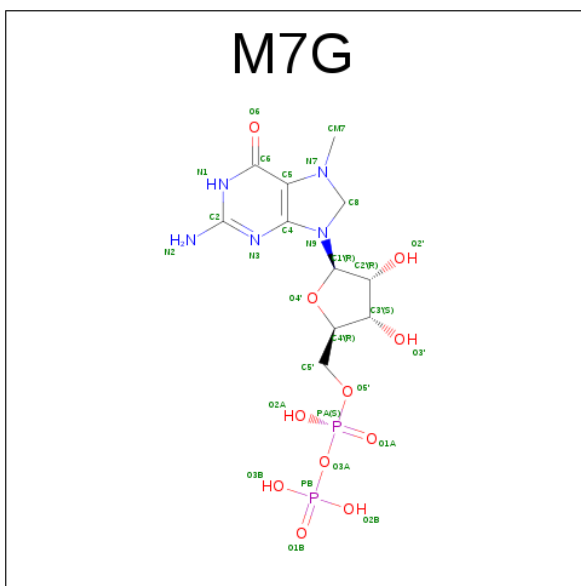
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	62	Total	C	N	O	0	0	0
			486	318	79	89			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		

- Molecule 5 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code:

M7G) (formula:  $\text{C}_{11}\text{H}_{19}\text{N}_5\text{O}_{11}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	11	5	11	2		

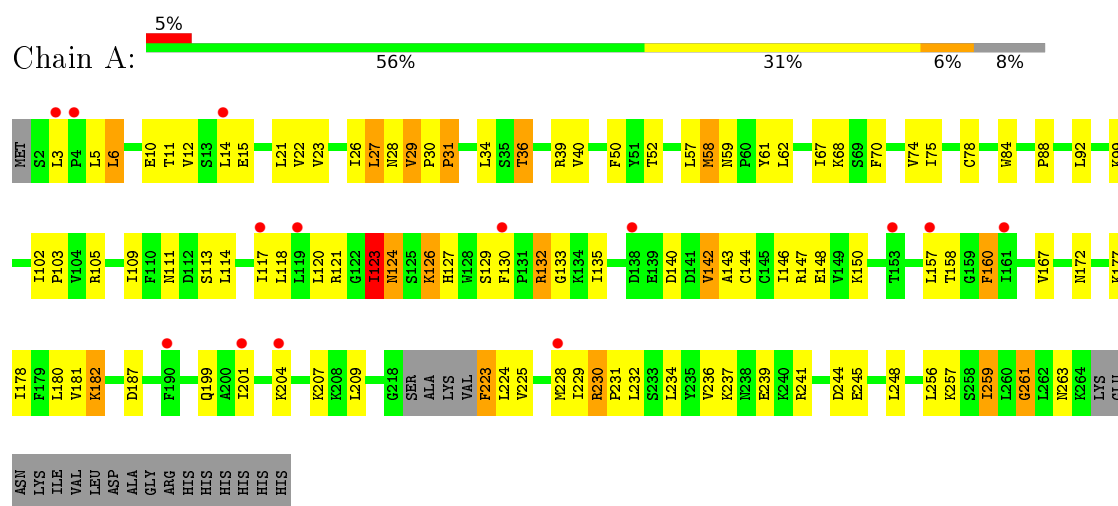
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0

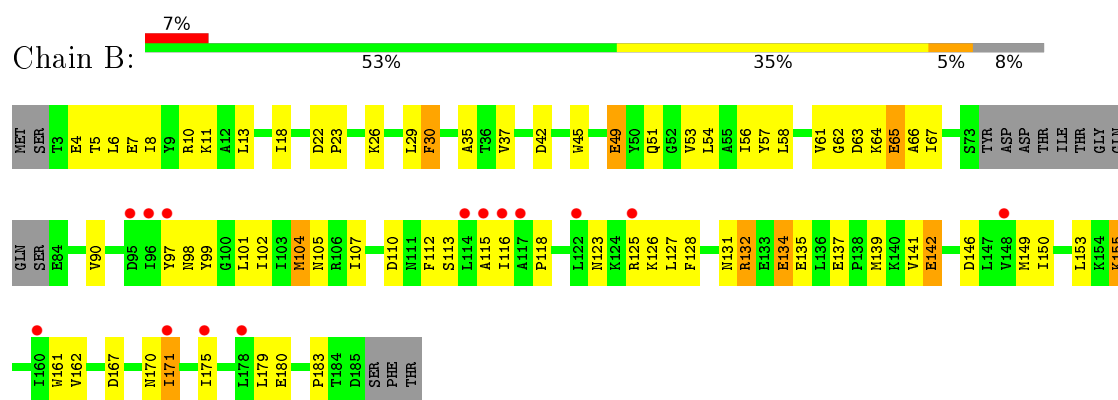
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

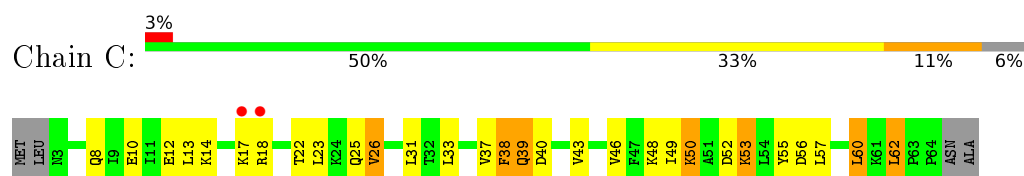
#### • Molecule 1: KLLA0F23980p



#### • Molecule 2: KLLA0E01827p



#### • Molecule 3: KLLA0A11308p



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.81Å 219.81Å 74.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.20 – 3.50 47.59 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.20-3.50) 100.0 (47.59-3.49)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.200 , 0.266 0.269 , 0.318	Depositor DCC
$R_{free}$ test set	691 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	201.6	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 243.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	229.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: MG, M7G

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	0.54	0/2169	0.78	0/2926
2	B	0.52	0/1461	0.81	1/1983 (0.1%)
3	C	0.48	0/494	0.80	0/664
All	All	0.53	0/4124	0.79	1/5573 (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	146	ASP	CB-CG-OD2	5.21	122.99	118.30

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	2121	0	2151	52	0
2	B	1429	0	1423	42	0
3	C	486	0	522	15	0
4	A	3	0	0	0	0
5	A	29	0	16	0	0
6	A	7	0	0	0	0
All	All	4075	0	4112	103	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 13.

The worst 5 of 103 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:29:VAL:HG22	1:A:30:PRO:HD2	1.63	0.81
2:B:30:PHE:HE1	2:B:56:ILE:HD12	1.51	0.76
2:B:141:VAL:HG11	2:B:175:ILE:HG21	1.69	0.74
3:C:12:GLU:HB2	3:C:56:ASP:HB2	1.68	0.74
1:A:230:ARG:HG3	1:A:231:PRO:HD3	1.68	0.74

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	253/281 (90%)	224 (88%)	23 (9%)	6 (2%)	7	47
2	B	167/188 (89%)	141 (84%)	22 (13%)	4 (2%)	7	47
3	C	60/66 (91%)	54 (90%)	5 (8%)	1 (2%)	11	54
All	All	480/535 (90%)	419 (87%)	50 (10%)	11 (2%)	8	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	158	THR
2	B	49	GLU
2	B	97	TYR
2	B	104	MET



### 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	238 / 257 (93%)	197 (83%)	41 (17%)	2	15
2	B	158 / 172 (92%)	136 (86%)	22 (14%)	4	25
3	C	55 / 58 (95%)	43 (78%)	12 (22%)	1	7
All	All	451 / 487 (93%)	376 (83%)	75 (17%)	3	16

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
2	B	4	GLU
3	C	49	ILE
1	A	225	VAL
1	A	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
2	B	105	ASN
2	B	31	HIS
1	A	124	ASN
2	B	51	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z  > 2$
5	M7G	A	303	4	27,31,31	1.00	2 (7%)	30,49,49	2.33	3 (10%)

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
5	M7G	A	303	4	-	0/16/44/44	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	M7G	C6-C5	2.50	1.45	1.41
5	A	303	M7G	C6-N1	2.97	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	303	M7G	C5-C6-N1	-8.14	111.27	123.39
5	A	303	M7G	C5-C4-N9	2.58	110.41	106.25
5	A	303	M7G	C6-N1-C2	8.31	125.62	115.88

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	59:ARG	C	60:ASP	N	2.97
1	A	13:SER	C	14:LEU	N	2.78

## 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	259/281 (92%)	0.11	14 (5%)	29 23	163, 213, 264, 286	0
2	B	173/188 (92%)	0.18	14 (8%)	15 12	128, 248, 282, 297	0
3	C	62/66 (93%)	-0.17	2 (3%)	51 42	221, 246, 269, 280	0
All	All	494/535 (92%)	0.10	30 (6%)	25 19	128, 231, 279, 297	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	PHE	4.6
1	A	138	ASP	3.9
2	B	171	ILE	3.8
2	B	175	ILE	3.8
2	B	97	TYR	3.7

### 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( $\text{\AA}^2$ )	Q<0.9
4	MG	A	302	1/1	0.98	0.34	1.24	130,130,130,130	0
5	M7G	A	303	29/29	0.94	0.31	0.43	191,206,223,227	0
4	MG	A	304	1/1	0.97	0.64	-	131,131,131,131	0
4	MG	A	301	1/1	0.94	0.33	-	139,139,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.