



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LBG  
Title : LACTOSE OPERON REPRESSOR BOUND TO 21-BASE PAIR SYMMETRIC OPERATOR DNA, ALPHA CARBONS ONLY  
Authors : Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.  
Deposited on : 1996-01-03  
Resolution : 4.80 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

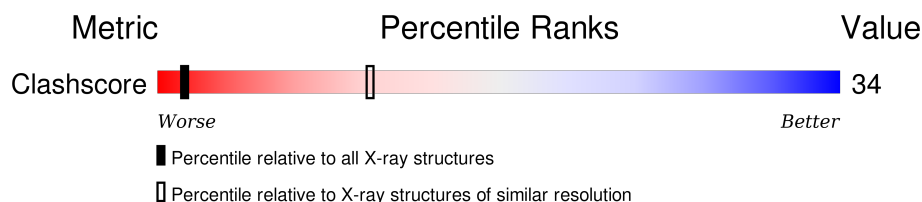
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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	102246	1017 (5.96-3.64)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	21	 14% 86%
1	F	21	 38% 62%
1	G	21	 24% 76%
1	H	21	 29% 71%
2	A	360	 99% .
2	B	360	 99% .
2	C	360	 99% .
2	D	360	 98% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3144 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 DNA chain called DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			
1	F	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			
1	G	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			
1	H	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			

- Molecule 2 is a protein called PROTEIN (LACTOSE OPERON REPRESSOR).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	A	357	Total	C	0	0	357
			357	357			
2	B	357	Total	C	0	0	357
			357	357			
2	C	357	Total	C	0	0	357
			357	357			
2	D	357	Total	C	0	0	357
			357	357			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	THR	ALA	CONFLICT	UNP P03023
B	109	THR	ALA	CONFLICT	UNP P03023
C	109	THR	ALA	CONFLICT	UNP P03023
D	109	THR	ALA	CONFLICT	UNP P03023

### 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 ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain E: 



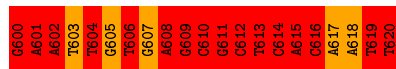
- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain F: 



- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain G: 



- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain H: 



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain A: 



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain B:  99% .



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain C:  99% .



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain D:  98% ..



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.30Å 224.40Å 112.10Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	15.00 – 4.80	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-4.80)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.260 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 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	E	3.40	68/481 (14.1%)	5.71	203/741 (27.4%)
1	F	3.02	50/481 (10.4%)	5.29	200/741 (27.0%)
1	G	3.59	49/481 (10.2%)	5.52	204/741 (27.5%)
1	H	3.18	46/481 (9.6%)	5.51	203/741 (27.4%)
All	All	3.31	213/1924 (11.1%)	5.51	810/2964 (27.3%)

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	E	3	18
1	F	1	15
1	G	3	16
1	H	3	17
All	All	10	66

The worst 5 of 213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	620	DT	P-O5'	22.13	1.81	1.59
1	G	620	DT	C5'-C4'	20.02	1.73	1.51
1	G	602	DA	P-O5'	19.05	1.78	1.59
1	H	720	DT	P-O5'	17.03	1.76	1.59
1	G	601	DA	O3'-P	16.98	1.81	1.61

The worst 5 of 810 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	420	DT	O4'-C1'-N1	41.82	137.27	108.00
1	F	520	DT	O4'-C1'-N1	32.28	130.60	108.00
1	H	702	DA	O4'-C4'-C3'	-30.45	87.73	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	600	DG	O4'-C1'-N9	29.83	128.88	108.00
1	E	401	DA	P-O3'-C3'	28.34	153.71	119.70

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	402	DA	C3'
1	E	405	DG	C1'
1	E	409	DG	C1'
1	F	520	DT	C4'
1	G	600	DG	C1'

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	400	DG	Sidechain
1	E	401	DA	Sidechain
1	E	402	DA	Sidechain
1	E	403	DT	Sidechain
1	E	404	DT	Sidechain

## 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	E	429	0	239	40	0
1	F	429	0	239	37	0
1	G	429	0	239	42	6
1	H	429	0	239	38	0
2	A	357	0	0	0	0
2	B	357	0	0	0	0
2	C	357	0	0	0	0
2	D	357	0	0	1	6
All	All	3144	0	956	139	6

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 34.



The worst 5 of 139 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:F:501:DA:H2'	1:F:502:DA:H1'	1.40	1.01
1:G:601:DA:H3'	1:G:602:DA:N7	1.94	0.82
1:H:701:DA:H3'	1:H:702:DA:C8	2.16	0.80
1:F:511:DG:N3	1:F:512:DC:H1'	1.98	0.78
1:E:405:DG:H2''	1:E:406:DT:H71	1.66	0.77

The worst 5 of 6 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:G:600:DG:N7	2:D:351:ARG:CA[1_455]	0.37	1.83
1:G:600:DG:C5	2:D:351:ARG:CA[1_455]	1.25	0.95
1:G:600:DG:O6	2:D:350:ALA:CA[1_455]	1.38	0.82
1:G:600:DG:C8	2:D:351:ARG:CA[1_455]	1.46	0.74
1:G:600:DG:C6	2:D:350:ALA:CA[1_455]	2.06	0.14

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.