



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:50 AM UTC

PDB ID : 1TLF / pdb_00001tlf
Title : UNPRECEDENTED QUATERNARY STRUCTURE OF E. COLI LAC RE-PRESSOR CORE TETRAMER: IMPLICATIONS FOR DNA LOOPING
Authors : Friedman, A.M.; Fischmann, T.O.; Steitz, T.A.
Deposited on : 1995-03-06
Resolution : 2.60 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

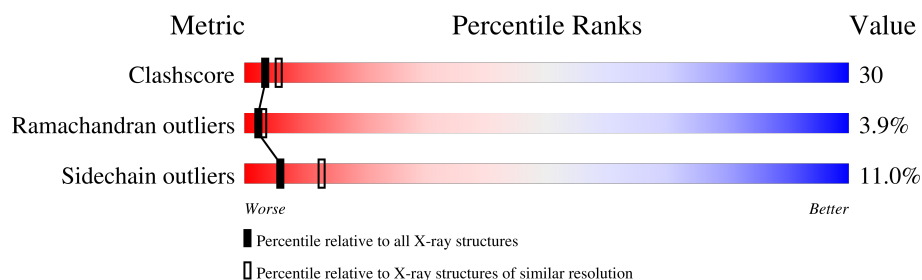
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	

2 Entry composition [i](#)

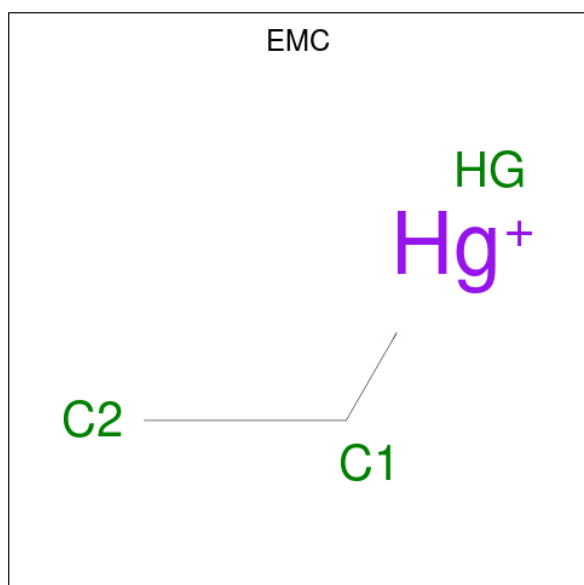
There are 3 unique types of molecules in this entry. The entry contains 10816 atoms, of which 1892 are hydrogens and 0 are deuteriums.

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 LAC REPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	B	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	C	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	D	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			

- Molecule 2 is ETHYL MERCURY ION (CCD ID: EMC) (formula: C₂H₅Hg).



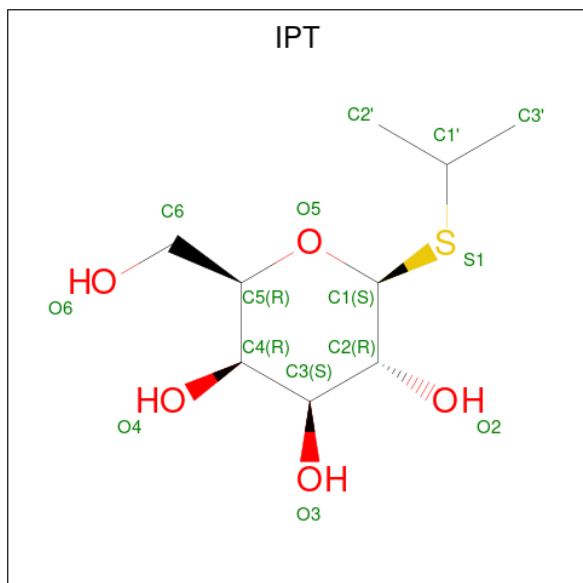
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

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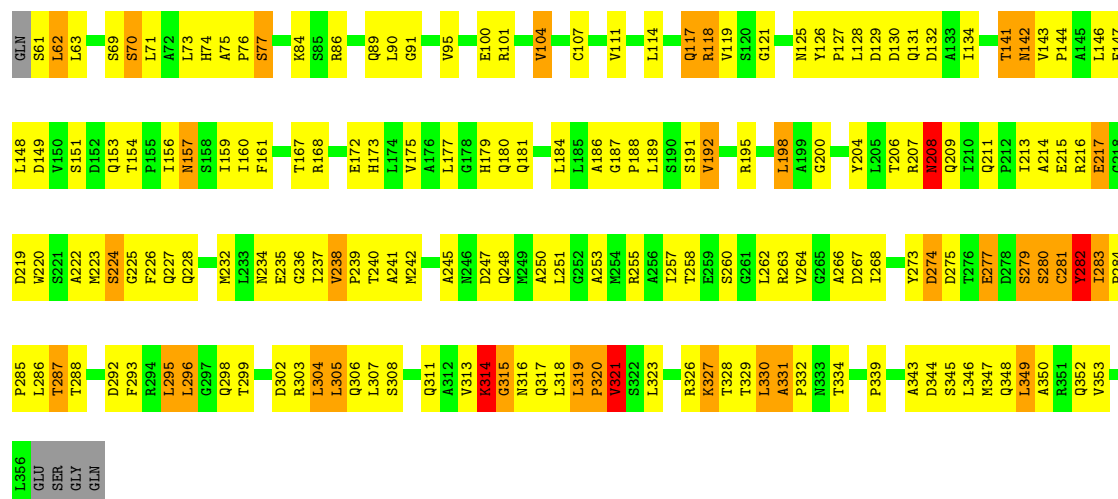
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	Hg	0	0
			3	2	1		
2	D	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 3 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: $C_9H_{18}O_5S$).

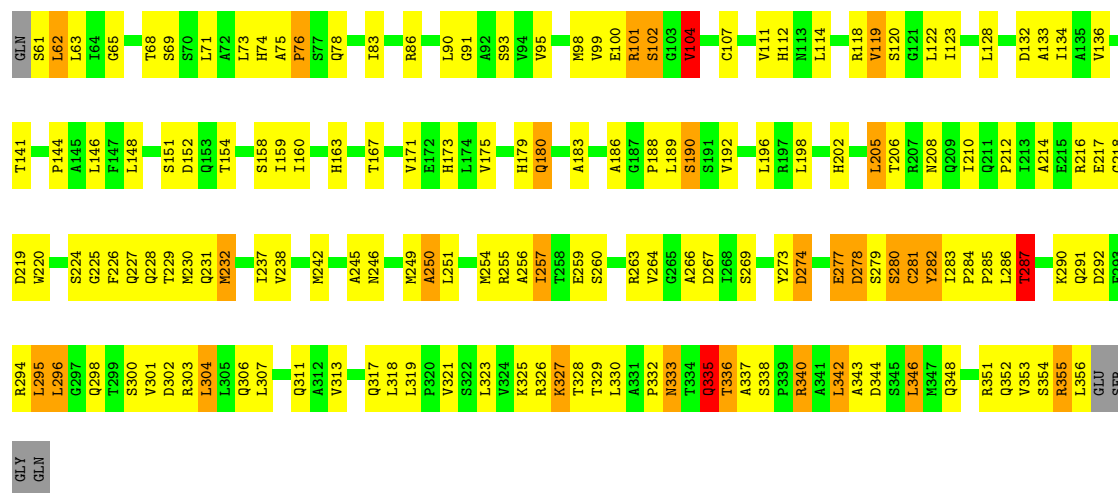


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			26	9	11	5	1		
3	B	1	Total	C	H	O	S	0	0
			26	9	11	5	1		
3	C	1	Total	C	H	O	S	0	0
			26	9	11	5	1		
3	D	1	Total	C	H	O	S	0	0
			26	9	11	5	1		



Molecule 1: LAC REPRESSOR

Chain D: 45% 44% 9% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.16Å 64.73Å 117.94Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10816	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.70	0/2242	1.19	20/3048 (0.7%)
1	B	0.71	1/2242 (0.0%)	1.23	22/3048 (0.7%)
1	C	0.76	1/2242 (0.0%)	1.28	29/3048 (1.0%)
1	D	0.75	1/2242 (0.0%)	1.22	23/3048 (0.8%)
All	All	0.73	3/8968 (0.0%)	1.23	94/12192 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	MET	SD-CE	-7.24	1.61	1.79
1	C	223	MET	SD-CE	6.25	1.95	1.79
1	B	254	MET	SD-CE	-5.03	1.67	1.79

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	74	HIS	N-CA-C	9.73	122.90	111.71
1	B	319	LEU	CA-C-N	9.43	131.63	119.84
1	B	319	LEU	C-N-CA	9.43	131.63	119.84
1	C	280	SER	N-CA-C	-9.28	101.17	111.28
1	B	282	TYR	N-CA-C	-8.95	96.65	110.17

There are no chirality outliers.

There are no planarity outliers.

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	A	2213	462	2265	145	0
1	B	2213	462	2265	136	0
1	C	2213	462	2266	170	0
1	D	2213	462	2265	140	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	1	0
2	D	3	0	0	0	0
3	A	15	11	18	0	0
3	B	15	11	18	0	0
3	C	15	11	18	0	0
3	D	15	11	18	1	0
All	All	8924	1892	9133	541	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 30.

The worst 5 of 541 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:189:LEU:HD11	1:A:217:GLU:OE2	1.26	1.34
1:D:189:LEU:HD11	1:D:217:GLU:OE2	1.17	1.32
1:C:189:LEU:CD2	1:C:217:GLU:OE2	1.79	1.30
1:C:189:LEU:HD21	1:C:217:GLU:OE2	1.09	1.24
1:A:189:LEU:HG	1:A:217:GLU:OE1	1.41	1.19

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	294/301 (98%)	258 (88%)	22 (8%)	14 (5%)	2	2
1	B	294/301 (98%)	259 (88%)	26 (9%)	9 (3%)	3	5
1	C	294/301 (98%)	253 (86%)	29 (10%)	12 (4%)	2	3
1	D	294/301 (98%)	255 (87%)	28 (10%)	11 (4%)	2	3
All	All	1176/1204 (98%)	1025 (87%)	105 (9%)	46 (4%)	2	3

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	274	ASP
1	A	313	VAL
1	A	314	LYS
1	A	332	PRO

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	242/246 (98%)	216 (89%)	26 (11%)	6	14
1	B	242/246 (98%)	212 (88%)	30 (12%)	4	9
1	C	242/246 (98%)	213 (88%)	29 (12%)	5	10
1	D	242/246 (98%)	221 (91%)	21 (9%)	9	21
All	All	968/984 (98%)	862 (89%)	106 (11%)	6	13

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	LEU
1	C	224	SER
1	D	296	LEU
1	C	104	VAL
1	C	142	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	GLN
1	C	234	ASN
1	C	125	ASN
1	C	208	ASN
1	C	316	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	IPT	B	998	-	15,15,15	1.18	1 (6%)	18,21,21	0.48	0
2	EMC	D	999	-	1,2,2	0.41	0	-		
3	IPT	C	998	-	15,15,15	0.96	1 (6%)	18,21,21	0.62	0
3	IPT	D	998	-	15,15,15	1.06	1 (6%)	18,21,21	0.93	1 (5%)
2	EMC	B	999	-	1,2,2	0.79	0	-		
3	IPT	A	998	-	15,15,15	0.44	0	18,21,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EMC	C	999	-	1,2,2	0.47	0	-		
2	EMC	A	999	-	1,2,2	0.48	0	-		

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	IPT	D	998	-	-	3/6/26/26	0/1/1/1
3	IPT	C	998	-	-	1/6/26/26	0/1/1/1
3	IPT	A	998	-	-	0/6/26/26	0/1/1/1
3	IPT	B	998	-	-	1/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	998	IPT	C1-S1	-3.55	1.73	1.80
3	B	998	IPT	C1-S1	-3.37	1.73	1.80
3	C	998	IPT	C1-S1	-3.35	1.73	1.80

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	998	IPT	C6-C5-C4	2.04	118.02	113.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	998	IPT	C4-C5-C6-O6
3	D	998	IPT	C3'-C1'-S1-C1
3	C	998	IPT	C4-C5-C6-O6
3	B	998	IPT	C2'-C1'-S1-C1
3	D	998	IPT	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	998	IPT	1	0
2	C	999	EMC	1	0

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.