



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2ERE / pdb\_00002ere  
Title : Crystal Structure of a Leu3 DNA-binding domain complexed with a 15mer DNA duplex  
Authors : Fitzgerald, M.X.; Marmorstein, R.  
Deposited on : 2005-10-24  
Resolution : 3.00 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 : 4-5-2 with Phenix2.0  
Xtrriage (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

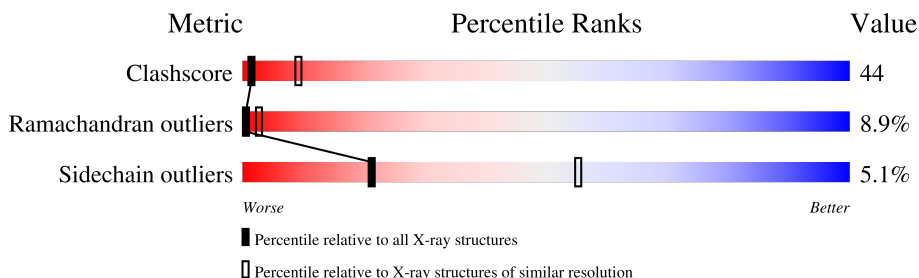
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	15	
1	D	15	
2	A	72	
2	B	72	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1506 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 5'-D(\*TP\*TP\*GP\*CP\*CP\*GP\*GP\*TP\*AP\*CP\*CP\*GP\*GP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
1	D	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			

- Molecule 2 is a protein called Regulatory protein LEU3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	60	Total	C	N	O	S	0	0	0
			435	265	86	78	6			
2	B	60	Total	C	N	O	S	0	0	0
			435	265	86	78	6			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	7	Total	O	0	0
			7	7		
4	D	11	Total	O	0	0
			11	11		
4	A	4	Total	O	0	0
			4	4		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	2	Total	O	0	0
			2	2		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 5'-D>(\*TP\*TP\*GP\*CP\*CP\*GP\*GP\*TP\*AP\*CP\*CP\*GP\*GP\*CP\*A)-3'

Chain C: 

T1  
T2 G3 C4 C5 G6 G7 T8 A9 C10 C11 G12 G13 C14 A15

- Molecule 1: 5'-D(\*TP\*TP\*GP\*CP\*CP\*GP\*GP\*TP\*AP\*CP\*CP\*GP\*GP\*CP\*A)-3'

Chain D: 

T16 T17 G18 C19 C20 G21 G22 T23 A24 C25 C26 G27 G28 C29 A30


- Molecule 2: Regulatory protein LEU3

Chain A: 

LYS ARG LYS F35 V38 E39 C40 Q43 K44 C47 D48 A49 H50 GLU ARG ALA PRO GLU P56 C57 T58 K59 C60 A61 K62 K63 M64 V65 P66 C67 I68 L69 K70 R71 D72 F73 R74 R75 K78 R79 A80 R81 N82 E83 A84 I85 E86 F89 K90 E91 L92 T93 R94 T95 L96 T97

N98 L99 THR SER ASP GLU

- Molecule 2: Regulatory protein LEU3

Chain B: 

LYS ARG LYS F35 V38 E39 C40 Q43 K44 C47 D48 A49 H50 GLU ARG ALA PRO GLU P56 C57 T58 K59 C60 A61 K62 K63 M64 V65 P66 C67 I68 L69 K70 R71 D72 F73 R74 R75 K78 R79 A80 R81 N82 E83 A84 I85 E86 F89 K90 E91 L92 T93 R94 T95 L96

T97 N98 L99 THR SER ASP GLU

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.56Å 66.56Å 122.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.12 – 3.00	Depositor
% Data completeness (in resolution range)	98.2 (32.12-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.277 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

## 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:  
ZN

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	C	0.47	0/340	0.83	0/523
1	D	0.46	0/340	0.85	0/523
2	A	0.65	0/439	0.97	1/589 (0.2%)
2	B	0.66	0/439	0.96	1/589 (0.2%)
All	All	0.58	0/1558	0.91	2/2224 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	THR	N-CA-C	-5.28	106.97	113.41
2	A	95	THR	N-CA-C	-5.13	107.15	113.41

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	C	304	0	170	21	0
1	D	304	0	170	23	0
2	A	435	0	383	38	0
2	B	435	0	383	41	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	7	0	0	1	0
4	D	11	0	0	1	0
All	All	1506	0	1106	113	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 44.

The worst 5 of 113 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:C:12:DG:H2''	1:C:13:DG:H5''	1.27	1.14
1:D:27:DG:H2''	1:D:28:DG:H5''	1.32	1.10
1:C:12:DG:C2'	1:C:13:DG:H5''	2.03	0.89
1:D:27:DG:C2'	1:D:28:DG:H5''	2.03	0.87
1:D:18:DG:H2''	1:D:19:DC:H5'	1.58	0.85

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	
2	A	56/72 (78%)	38 (68%)	13 (23%)	5 (9%)	0	3
2	B	56/72 (78%)	38 (68%)	13 (23%)	5 (9%)	0	3
All	All	112/144 (78%)	76 (68%)	26 (23%)	10 (9%)	0	3

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	71	ARG
2	A	79	ARG
2	B	71	ARG
2	B	79	ARG
2	A	62	LYS

### 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	
2	A	39/66 (59%)	37 (95%)	2 (5%)	21	55
2	B	39/66 (59%)	37 (95%)	2 (5%)	21	55
All	All	78/132 (59%)	74 (95%)	4 (5%)	21	55

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

Mol	Chain	Res	Type
2	A	35	PHE
2	A	93	THR
2	B	35	PHE
2	B	93	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	43	GLN
2	A	82	ASN
2	B	43	GLN
2	B	82	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](#)

Of 4 ligands modelled in this entry, 4 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 [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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.