



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 08:02 AM EST

PDB ID : 9MXA  
Title : Crystal structure of the DNA binding domain of FLI1 (wild-type) in complex with a DNA containing two contiguous GGAA sites  
Authors : Hou, C.; Tsodikov, O.V.  
Deposited on : 2025-01-17  
Resolution : 2.59 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

<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 : 4.02b-467  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

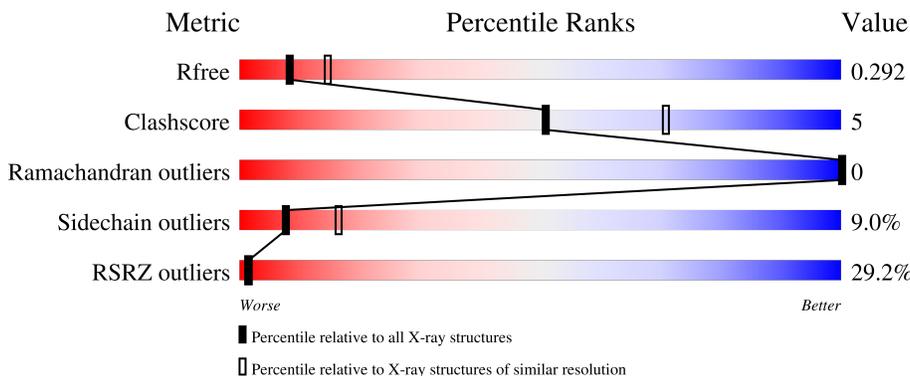
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	145	
1	D	145	
2	E	15	
3	F	15	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2144 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 Friend leukemia integration 1 transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	89	714	452	129	129	4	0	0	0
1	D	100	817	520	146	147	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	expression tag	UNP Q01543
A	256	PRO	-	expression tag	UNP Q01543
A	257	HIS	-	expression tag	UNP Q01543
A	258	MET	-	expression tag	UNP Q01543
D	255	GLY	-	expression tag	UNP Q01543
D	256	PRO	-	expression tag	UNP Q01543
D	257	HIS	-	expression tag	UNP Q01543
D	258	MET	-	expression tag	UNP Q01543

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*AP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*AP\*GP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	15	314	148	68	84	14	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*AP\*CP\*TP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*GP\*GP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	15	294	143	46	91	14	0	0	0

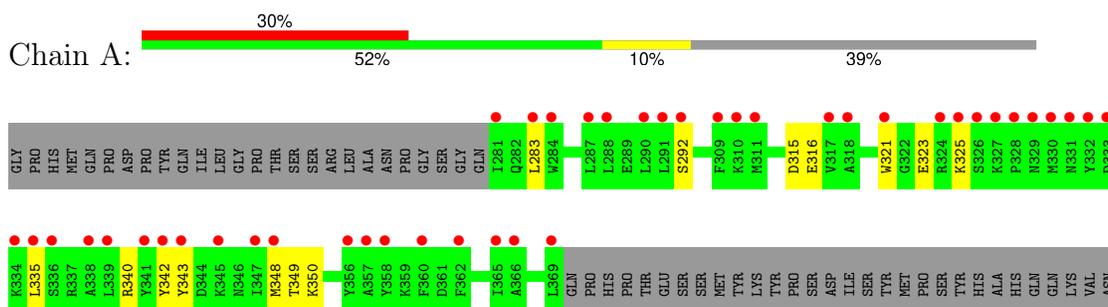
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	A	1	Total O 1 1	0	0
4	D	2	Total O 2 2	0	0
4	E	2	Total O 2 2	0	0

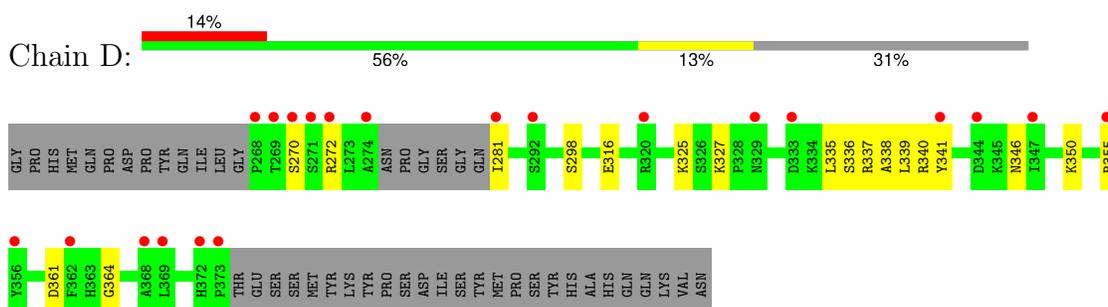
### 3 Residue-property plots [i](#)

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 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.

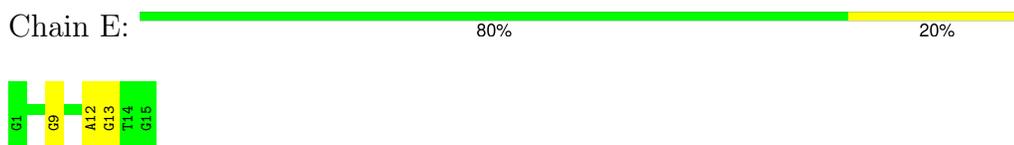
- Molecule 1: Friend leukemia integration 1 transcription factor



- Molecule 1: Friend leukemia integration 1 transcription factor



- Molecule 2: DNA (5'-D(\*GP\*AP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*AP\*GP\*TP\*G)-3')



- Molecule 3: DNA (5'-D(\*CP\*AP\*CP\*TP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*GP\*GP\*TP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.95Å 96.95Å 185.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.59 40.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.00-2.59) 98.8 (40.00-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.260 , 0.287 0.265 , 0.292	Depositor DCC
$R_{free}$ test set	678 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtrriage
Anisotropy	0.580	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 73.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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](#)

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	0.67	0/730	0.80	0/982
1	D	0.68	0/839	0.85	0/1131
2	E	0.53	0/355	0.87	0/548
3	F	0.43	0/326	0.93	0/500
All	All	0.62	0/2250	0.85	0/3161

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	714	0	683	6	0
1	D	817	0	784	9	0
2	E	314	0	168	2	0
3	F	294	0	169	4	0
4	A	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	2144	0	1804	20	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 5.

All (20) 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:283:LEU:HB3	1:A:342:TYR:OH	2.05	0.56
3:F:11:DC:H2'	3:F:12:DG:C8	2.42	0.55
3:F:3:DC:H2''	3:F:4:DT:H5'	1.91	0.53
1:A:321:TRP:O	1:A:321:TRP:CG	2.65	0.50
1:D:346:ASN:O	1:D:364:GLY:HA3	2.13	0.49
1:A:340:ARG:HD2	2:E:9:DG:N7	2.28	0.49
2:E:12:DA:H2''	2:E:13:DG:OP2	2.13	0.49
1:D:335:LEU:O	1:D:338:ALA:HB3	2.12	0.48
1:A:343:TYR:OH	1:A:350:LYS:HB2	2.14	0.48
1:D:335:LEU:C	1:D:335:LEU:HD23	2.34	0.48
1:D:316:GLU:HA	1:D:316:GLU:OE1	2.14	0.47
1:D:346:ASN:O	1:D:361:ASP:OD1	2.33	0.46
1:D:336:SER:OG	1:D:340:ARG:NH1	2.48	0.46
1:D:338:ALA:O	1:D:341:TYR:N	2.45	0.46
3:F:7:DC:H2'	3:F:8:DT:C6	2.52	0.45
1:D:338:ALA:O	1:D:339:LEU:C	2.55	0.44
3:F:11:DC:C2'	3:F:12:DG:C8	3.01	0.43
1:A:321:TRP:O	1:A:325:LYS:HB2	2.19	0.42
1:D:337:ARG:HA	1:D:340:ARG:NH2	2.34	0.42
1:A:335:LEU:C	1:A:335:LEU:HD23	2.42	0.40

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	87/145 (60%)	70 (80%)	17 (20%)	0	100	100
1	D	96/145 (66%)	91 (95%)	5 (5%)	0	100	100
All	All	183/290 (63%)	161 (88%)	22 (12%)	0	100	100

There are no Ramachandran outliers to report.

### 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	71/127 (56%)	65 (92%)	6 (8%)	8	18
1	D	84/127 (66%)	76 (90%)	8 (10%)	7	14
All	All	155/254 (61%)	141 (91%)	14 (9%)	8	16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	SER
1	A	315	ASP
1	A	316	GLU
1	A	323	GLU
1	A	348	MET
1	A	349	THR
1	D	270	SER
1	D	272	ARG
1	D	281	ILE
1	D	298	SER
1	D	325	LYS
1	D	327	LYS
1	D	350	LYS
1	D	355	ARG

Sometimes 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 oligosaccharides 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

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	89/145 (61%)	2.03	43 (48%) <b>0</b> <b>0</b>	99, 132, 174, 188	0
1	D	100/145 (68%)	1.15	21 (21%) <b>3</b> <b>2</b>	64, 81, 145, 158	0
2	E	15/15 (100%)	0.32	0 <b>100</b> <b>100</b>	74, 89, 140, 170	0
3	F	15/15 (100%)	0.23	0 <b>100</b> <b>100</b>	72, 86, 126, 130	0
All	All	219/320 (68%)	1.39	64 (29%) <b>1</b> <b>1</b>	64, 106, 164, 188	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	TYR	5.1
1	D	270	SER	4.9
1	A	356	TYR	4.6
1	D	268	PRO	4.5
1	A	317	VAL	4.5
1	A	369	LEU	4.5
1	D	271	SER	4.4
1	A	325	LYS	4.3
1	A	281	ILE	4.1
1	A	333	ASP	4.1
1	A	329	ASN	4.0
1	A	328	PRO	4.0
1	A	332	TYR	3.7
1	A	341	TYR	3.7
1	A	331	ASN	3.6
1	A	362	PHE	3.4
1	D	274	ALA	3.4
1	A	321	TRP	3.3
1	D	344	ASP	3.2
1	A	327	LYS	3.2
1	A	287	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	372	HIS	3.1
1	A	284	TRP	3.1
1	A	330	MET	2.9
1	A	345	LYS	2.9
1	A	283	LEU	2.8
1	A	347	ILE	2.8
1	D	269	THR	2.7
1	A	334	LYS	2.7
1	A	360	PHE	2.7
1	A	339	LEU	2.7
1	D	373	PRO	2.7
1	D	362	PHE	2.7
1	A	343	TYR	2.6
1	A	365	ILE	2.6
1	D	369	LEU	2.5
1	A	326	SER	2.5
1	A	292	SER	2.5
1	D	320	ARG	2.5
1	D	356	TYR	2.5
1	A	366	ALA	2.4
1	A	290	LEU	2.4
1	D	292	SER	2.4
1	D	355	ARG	2.4
1	D	281	ILE	2.4
1	D	347	ILE	2.3
1	D	368	ALA	2.3
1	A	288	LEU	2.2
1	D	333	ASP	2.2
1	A	357	ALA	2.2
1	A	309	PHE	2.2
1	D	341	TYR	2.2
1	A	336	SER	2.2
1	D	272	ARG	2.2
1	D	329	ASN	2.2
1	A	291	LEU	2.2
1	A	348	MET	2.1
1	A	311	MET	2.1
1	A	318	ALA	2.1
1	A	338	ALA	2.1
1	A	342	TYR	2.1
1	A	335	LEU	2.0
1	A	310	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	324	ARG	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.