



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 06:25 PM EST

PDB ID : 6VG2  
Title : Crystal structure of the DNA binding domain of human transcription factor  
FLI1 in complex with 16-mer DNA CAGAGGATGTGGCTTC  
Authors : Hou, C.; Tsodikov, O.V.  
Deposited on : 2020-01-07  
Resolution : 3.90 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.

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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) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

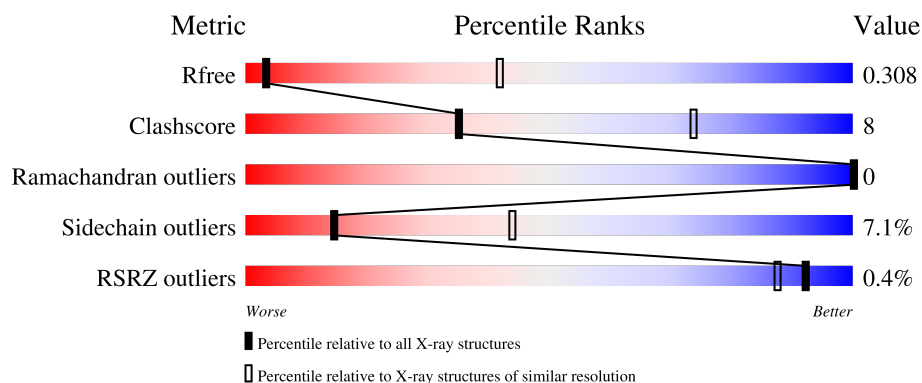
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 on 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	104	<div> <div></div> <div>69%</div> <div>19%</div> <div>11%</div> </div>
1	D	104	<div> <div>77%</div> <div>12%</div> <div>12%</div> </div>
2	B	16	<div> <div>50%</div> <div>50%</div> </div>
2	E	16	<div> <div>88%</div> <div>13%</div> </div>
3	C	16	<div> <div>75%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	16	 81% 19%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2824 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
1	A	93	Total	C	N	O	S	0	0	0
			766	489	135	138	4			
1	D	92	Total	C	N	O	S	0	0	0
			759	484	134	137	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLY	-	expression tag	UNP Q01543
A	273	PRO	-	expression tag	UNP Q01543
A	274	HIS	-	expression tag	UNP Q01543
A	275	MET	-	expression tag	UNP Q01543
D	272	GLY	-	expression tag	UNP Q01543
D	273	PRO	-	expression tag	UNP Q01543
D	274	HIS	-	expression tag	UNP Q01543
D	275	MET	-	expression tag	UNP Q01543

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	P	0	0	0
			329	157	62	95	15			
2	E	16	Total	C	N	O	P	0	0	0
			329	157	62	95	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			320	154	59	92	15			

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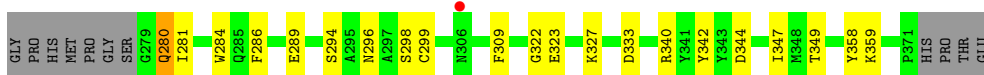
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	16	Total	C	N	O	P	0	0	0
			321	154	59	93	15			

### 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.

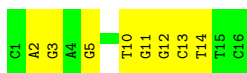
- Molecule 1: Friend leukemia integration 1 transcription factor



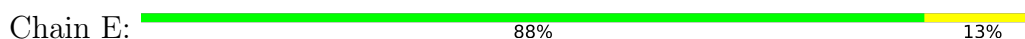
- Molecule 1: Friend leukemia integration 1 transcription factor



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




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



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



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

Chain F:   
81% 19%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.42Å 90.73Å 165.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.90 45.25 – 3.64	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.00-3.90) 95.1 (45.25-3.64)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.247 , 0.294 0.253 , 0.308	Depositor DCC
$R_{free}$ test set	319 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.5	Xtriage
Anisotropy	0.940	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 86.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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	0.64	0/786	0.74	0/1059
1	D	0.65	0/778	0.77	0/1047
2	B	0.24	0/369	0.77	0/569
2	E	0.27	0/369	0.78	0/569
3	C	0.24	0/358	0.76	0/550
3	F	0.25	0/359	0.77	0/551
All	All	0.50	0/3019	0.76	0/4345

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	766	0	737	22	0
1	D	759	0	730	6	0
2	B	329	0	182	5	0
2	E	329	0	182	3	0
3	C	320	0	178	5	0
3	F	321	0	181	2	0
All	All	2824	0	2190	39	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 8.

All (39) 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:284:TRP:HD1	1:A:342:TYR:OH	1.49	0.95
3:C:9:DG:H1'	3:C:10:DA:OP2	1.67	0.94
1:D:350:LYS:HB2	1:D:358:TYR:CE2	2.09	0.88
1:A:280:GLN:HE21	1:A:280:GLN:C	1.82	0.81
1:A:284:TRP:HD1	1:A:342:TYR:HH	0.77	0.75
1:D:350:LYS:HB2	1:D:358:TYR:CD2	2.22	0.74
1:A:284:TRP:HD1	1:A:342:TYR:CZ	2.07	0.72
1:A:342:TYR:CE1	1:A:347:ILE:HD13	2.30	0.67
3:C:10:DA:O4'	3:C:10:DA:OP2	2.20	0.60
1:A:280:GLN:HG3	1:A:280:GLN:O	2.01	0.59
2:B:14:DT:O2	3:C:11:DA:N1	2.37	0.58
1:A:333:ASP:OD2	1:A:333:ASP:C	2.43	0.57
1:A:342:TYR:CD1	1:A:347:ILE:HD12	2.42	0.55
1:A:342:TYR:CD1	1:A:347:ILE:CD1	2.91	0.54
1:D:314:PRO:HG2	1:D:356:TYR:CE2	2.43	0.53
1:A:284:TRP:CD1	1:A:342:TYR:CZ	2.93	0.53
1:A:280:GLN:O	1:A:280:GLN:CG	2.58	0.52
3:F:10:DA:C5	3:F:11:DA:C6	2.98	0.52
2:B:10:DT:H2''	2:B:11:DG:C8	2.45	0.52
3:C:9:DG:C1'	3:C:10:DA:OP2	2.51	0.51
1:A:296:ASN:O	1:A:299:CYS:N	2.41	0.51
1:D:356:TYR:OH	2:E:2:DA:OP2	2.27	0.51
1:A:342:TYR:HD1	1:A:347:ILE:HD12	1.77	0.50
2:B:12:DG:H2''	2:B:13:DC:C6	2.46	0.50
2:E:1:DC:H2''	2:E:2:DA:O5'	2.13	0.49
1:A:322:GLY:O	1:A:327:LYS:N	2.44	0.49
1:A:340:ARG:NH2	2:B:5:DG:N7	2.61	0.48
3:F:9:DG:H2''	3:F:10:DA:C8	2.49	0.48
1:A:342:TYR:CE1	1:A:347:ILE:CD1	2.96	0.47
2:E:1:DC:H1'	2:E:2:DA:OP1	2.16	0.45
1:A:349:THR:HG23	1:A:359:LYS:HB3	1.98	0.45
1:D:294:SER:O	1:D:297:ALA:HB2	2.17	0.44
1:A:286:PHE:O	1:A:289:GLU:HB3	2.17	0.43
1:A:342:TYR:OH	3:C:16:DC:OP2	2.37	0.43
1:D:335:LEU:HD23	1:D:335:LEU:O	2.20	0.42
1:A:309:PHE:CZ	1:A:358:TYR:HB2	2.55	0.41
1:A:284:TRP:HB3	1:A:342:TYR:CE2	2.56	0.41
1:A:280:GLN:CA	1:A:280:GLN:NE2	2.84	0.40
2:B:2:DA:C6	2:B:3:DG:C6	3.10	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	91/104 (88%)	79 (87%)	12 (13%)	0	100	100
1	D	90/104 (86%)	81 (90%)	9 (10%)	0	100	100
All	All	181/208 (87%)	160 (88%)	21 (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	78/89 (88%)	72 (92%)	6 (8%)	13	42
1	D	77/89 (86%)	72 (94%)	5 (6%)	17	46
All	All	155/178 (87%)	144 (93%)	11 (7%)	14	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	281	ILE
1	A	294	SER
1	A	298	SER
1	A	323	GLU

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Mol	Chain	Res	Type
1	A	344	ASP
1	D	298	SER
1	D	349	THR
1	D	351	VAL
1	D	355	ARG
1	D	362	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	D	346	ASN
1	D	363	HIS

### 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 monosaccharides 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 [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	93/104 (89%)	0.14	1 (1%) 80 73	81, 113, 148, 170	0
1	D	92/104 (88%)	0.16	0 100 100	88, 121, 150, 164	0
2	B	16/16 (100%)	-0.27	0 100 100	111, 145, 228, 232	0
2	E	16/16 (100%)	-0.46	0 100 100	104, 131, 223, 226	0
3	C	16/16 (100%)	-0.47	0 100 100	121, 156, 209, 217	0
3	F	16/16 (100%)	-0.49	0 100 100	112, 138, 212, 222	0
All	All	249/272 (91%)	0.00	1 (0%) 92 87	81, 121, 203, 232	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ASN	2.2

### 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.