



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1AN4  
Title : STRUCTURE AND FUNCTION OF THE B/HLH/Z DOMAIN OF USF  
Authors : Ferre-D'Amare, A.R.; Pognonec, P.; Roeder, R.G.; Burley, S.K.  
Deposited on : 1997-03-15  
Resolution : 2.90 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

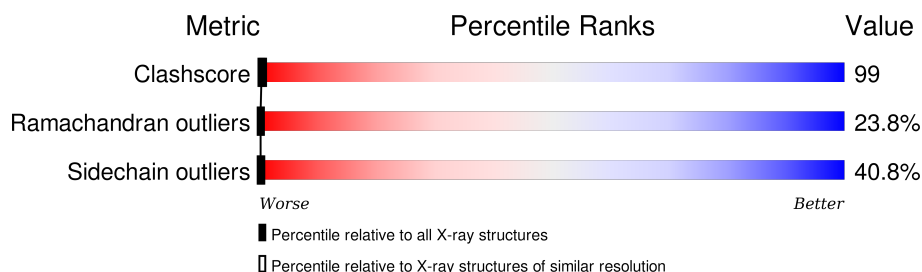
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	C	21	
2	D	21	
3	A	65	
3	B	65	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1923 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(\*CP\*AP\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*AP\*CP\*GP\*TP\*GP\*GP\*CP\*C P\*TP\*AP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	21	Total	C	N	O	P	0	0	0
			422	201	78	123	20			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*TP\*GP\*TP\*AP\*GP\*GP\*CP\*CP\*AP\*CP\*GP\*TP\*GP\*AP\*CP\*C P\*GP\*GP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	P	0	0	0
			433	205	83	125	20			

- Molecule 3 is a protein called PROTEIN (UPSTREAM STIMULATORY FACTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	65	Total	C	N	O	S	0	0	0
			534	320	109	103	2			
3	B	65	Total	C	N	O	S	0	0	0
			534	320	109	103	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	MET	ARG	CLONING ARTIFACT	UNP P22415
A	229	SER	CYS	ENGINEERED	UNP P22415
A	248	SER	CYS	ENGINEERED	UNP P22415
B	196	MET	ARG	CLONING ARTIFACT	UNP P22415
B	229	SER	CYS	ENGINEERED	UNP P22415
B	248	SER	CYS	ENGINEERED	UNP P22415

### 3 Residue-property plots

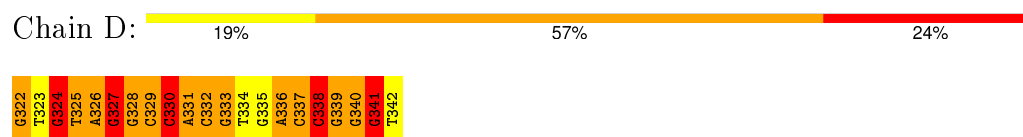
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

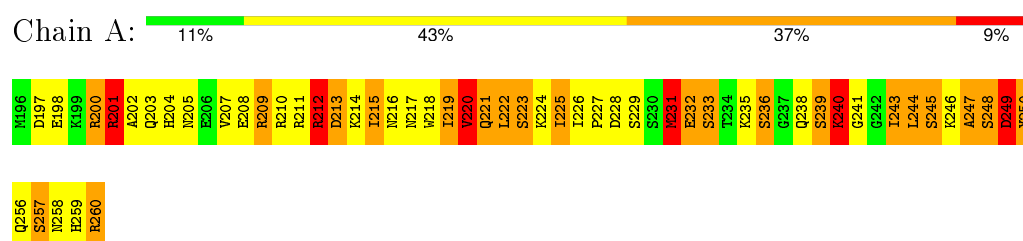
- Molecule 1: DNA (5'-D(\*CP\*AP\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*AP\*CP\*GP\*TP\*GP\*GP\*CP\*C P\*TP\*AP\*CP\*A)-3')



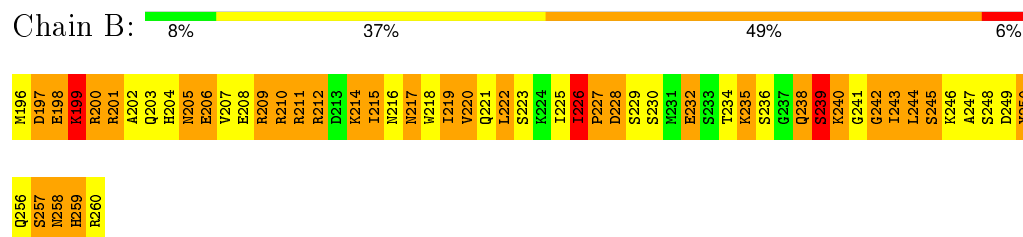
- Molecule 2: DNA (5'-D(\*GP\*TP\*GP\*TP\*AP\*GP\*GP\*CP\*CP\*AP\*CP\*GP\*TP\*GP\*AP\*CP\*C P\*GP\*GP\*GP\*T)-3')



- Molecule 3: PROTEIN (UPSTREAM STIMULATORY FACTOR)



- Molecule 3: PROTEIN (UPSTREAM STIMULATORY FACTOR)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.60 Å   54.70 Å   44.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
$R_{merge}$	7.60	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.236 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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	C	2.46	32/472 (6.8%)	3.83	88/725 (12.1%)
2	D	2.42	25/486 (5.1%)	3.47	86/750 (11.5%)
3	A	0.89	1/539 (0.2%)	1.29	3/716 (0.4%)
3	B	0.95	1/539 (0.2%)	1.48	8/716 (1.1%)
All	All	1.80	59/2036 (2.9%)	2.78	185/2907 (6.4%)

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	C	0	9
2	D	0	6
3	B	0	1
All	All	0	16

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	DT	C5-C7	10.03	1.56	1.50
2	D	342	DT	C5-C7	9.54	1.55	1.50
2	D	331	DA	P-O5'	8.80	1.68	1.59
1	C	313	DT	C5-C7	8.66	1.55	1.50
1	C	308	DT	O3'-P	8.37	1.71	1.61

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	DC	O4'-C1'-N1	25.93	126.15	108.00
1	C	309	DC	O4'-C1'-N1	25.79	126.05	108.00
1	C	310	DA	O4'-C4'-C3'	-20.02	93.99	106.00
2	D	322	DG	O4'-C1'-N9	18.81	121.17	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	327	DG	C1'-O4'-C4'	-18.54	91.56	110.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	301	DC	Sidechain
1	C	302	DA	Sidechain
1	C	306	DG	Sidechain
1	C	307	DG	Sidechain
1	C	309	DC	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	C	422	0	236	62	0
2	D	433	0	237	50	0
3	A	534	0	537	106	0
3	B	534	0	537	166	0
All	All	1923	0	1547	335	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 99.

The worst 5 of 335 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)
3:B:219:ILE:CD1	3:B:240:LYS:HE3	1.55	1.36
3:B:227:PRO:HG3	3:B:250:TYR:HE2	0.99	1.12
3:B:220:VAL:CG2	3:B:221:GLN:OE1	1.99	1.10
3:B:227:PRO:HG3	3:B:250:TYR:CE2	1.84	1.10
3:B:219:ILE:HG21	3:B:240:LYS:HG3	1.33	1.10

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	
3	A	63/65 (97%)	23 (36%)	25 (40%)	15 (24%)	0	0
3	B	63/65 (97%)	35 (56%)	13 (21%)	15 (24%)	0	0
All	All	126/130 (97%)	58 (46%)	38 (30%)	30 (24%)	0	0

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	201	ARG
3	A	231	MET
3	A	236	SER
3	A	240	LYS
3	A	247	ALA

### 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	
3	A	60/60 (100%)	34 (57%)	26 (43%)	0	0
3	B	60/60 (100%)	37 (62%)	23 (38%)	0	0
All	All	120/120 (100%)	71 (59%)	49 (41%)	0	0

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	252	GLN

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Mol	Chain	Res	Type
3	B	198	GLU
3	B	245	SER
3	A	257	SER
3	B	200	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	259	HIS
3	B	258	ASN
3	B	216	ASN
3	A	258	ASN
3	B	217	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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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