



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:05 pm GMT

PDB ID : 1EMR  
Title : CRYSTAL STRUCTURE OF HUMAN LEUKEMIA INHIBITORY FACTOR (LIF)  
Authors : Robinson, R.C.; Heath, J.K.; Hawkins, N.; Samal, B.; Jones, E.Y.; Betzel, C.  
Deposited on : 2000-03-17  
Resolution : 3.50 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

<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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

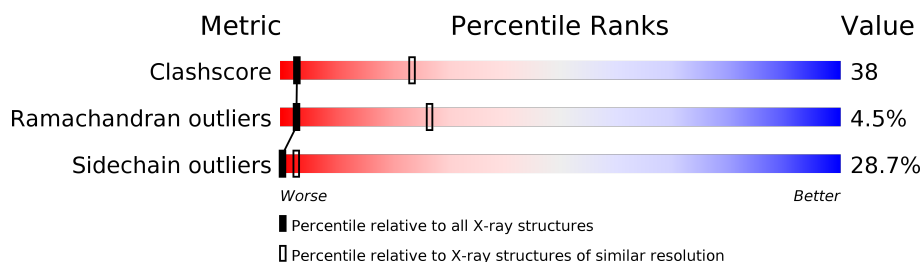
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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	A	159	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1232 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 LEUKEMIA INHIBITORY FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1232	788	214	225	5			

There are 3 discrepancies between the modelled and reference sequences:

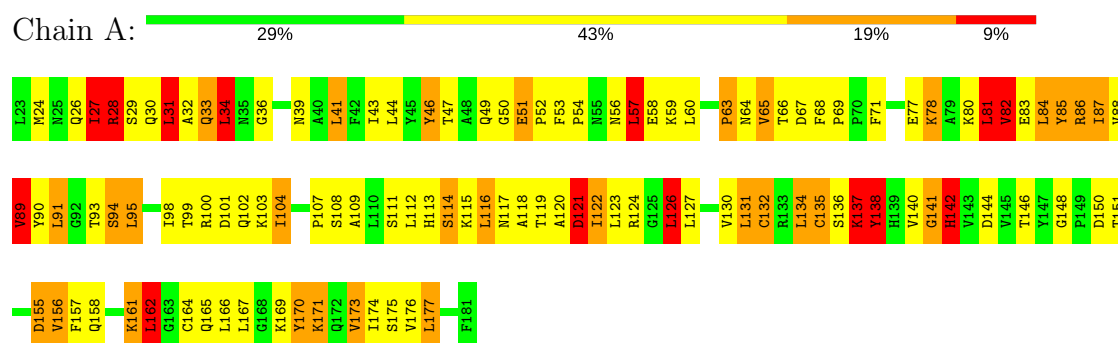
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLU	ASP	CONFLICT	UNP P15018
A	173	VAL	ILE	CONFLICT	UNP P15018
A	175	SER	ALA	CONFLICT	UNP P15018

### 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 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.

Note EDS was not executed.

#### • Molecule 1: LEUKEMIA INHIBITORY FACTOR



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.50Å 45.30Å 77.70Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.191 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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	A	0.52	0/1255	0.84	0/1698

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	A	0	48

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Mainchain
1	A	101	ASP	Mainchain
1	A	104	ILE	Mainchain
1	A	111	SER	Mainchain
1	A	113	HIS	Mainchain
1	A	117	ASN	Mainchain
1	A	119	THR	Mainchain
1	A	120	ALA	Mainchain
1	A	121	ASP	Mainchain
1	A	122	ILE	Mainchain
1	A	123	LEU	Mainchain
1	A	126	LEU	Mainchain
1	A	127	LEU	Mainchain
1	A	137	LYS	Mainchain
1	A	138	TYR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	142	HIS	Mainchain
1	A	144	ASP	Mainchain
1	A	150	ASP	Mainchain
1	A	155	ASP	Mainchain
1	A	162	LEU	Mainchain
1	A	164	CYS	Mainchain
1	A	170	TYR	Mainchain
1	A	171	LYS	Mainchain
1	A	175	SER	Mainchain
1	A	176	VAL	Mainchain
1	A	24	MET	Mainchain
1	A	27	ILE	Mainchain
1	A	28	ARG	Mainchain
1	A	31	LEU	Mainchain
1	A	33	GLN	Mainchain
1	A	34	LEU	Mainchain
1	A	36	GLY	Mainchain
1	A	46	TYR	Sidechain,Mainchain
1	A	49	GLN	Mainchain
1	A	56	ASN	Mainchain
1	A	57	LEU	Mainchain
1	A	67	ASP	Mainchain
1	A	71	PHE	Mainchain
1	A	81	LEU	Mainchain
1	A	82	VAL	Mainchain
1	A	84	LEU	Mainchain
1	A	85	TYR	Mainchain
1	A	87	ILE	Mainchain
1	A	89	VAL	Mainchain
1	A	91	LEU	Mainchain
1	A	94	SER	Mainchain
1	A	95	LEU	Mainchain

## 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	1232	0	1264	94	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1232	0	1264	94	1

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 38.

All (94) 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:41:LEU:HD21	1:A:167:LEU:HD22	1.35	1.07
1:A:31:LEU:HD23	1:A:126:LEU:HD11	1.61	0.83
1:A:34:LEU:HB3	1:A:174:ILE:HD11	1.61	0.81
1:A:94:SER:HB3	1:A:166:LEU:HD22	1.61	0.81
1:A:132:CYS:O	1:A:136:SER:HB2	1.84	0.77
1:A:173:VAL:O	1:A:177:LEU:HD12	1.85	0.76
1:A:81:LEU:HB3	1:A:134:LEU:HD11	1.67	0.76
1:A:78:LYS:HB2	1:A:138:TYR:CE1	2.22	0.74
1:A:69:PRO:HB2	1:A:87:ILE:HG13	1.72	0.70
1:A:81:LEU:HD13	1:A:130:VAL:HG13	1.74	0.69
1:A:68:PHE:CG	1:A:69:PRO:HD2	2.28	0.68
1:A:46:TYR:CD2	1:A:57:LEU:HD21	2.30	0.65
1:A:69:PRO:CG	1:A:87:ILE:HA	2.27	0.65
1:A:69:PRO:HG2	1:A:87:ILE:HA	1.79	0.64
1:A:94:SER:HB3	1:A:166:LEU:CD2	2.27	0.64
1:A:27:ILE:HG13	1:A:28:ARG:N	2.10	0.64
1:A:69:PRO:HB2	1:A:87:ILE:CG1	2.27	0.64
1:A:28:ARG:HD2	1:A:28:ARG:C	2.18	0.64
1:A:27:ILE:HD12	1:A:31:LEU:HG	1.80	0.64
1:A:77:GLU:HA	1:A:80:LYS:HE2	1.79	0.63
1:A:85:TYR:O	1:A:89:VAL:HG12	1.98	0.63
1:A:142:HIS:CD2	1:A:142:HIS:C	2.71	0.62
1:A:30:GLN:HB2	1:A:126:LEU:HD12	1.81	0.61
1:A:26:GLN:O	1:A:30:GLN:HG3	2.00	0.61
1:A:151:THR:O	1:A:151:THR:HG23	1.99	0.61
1:A:31:LEU:HD23	1:A:126:LEU:CD1	2.30	0.60
1:A:86:ARG:HA	1:A:89:VAL:CG1	2.32	0.60
1:A:82:VAL:HG13	1:A:86:ARG:HD3	1.83	0.59
1:A:69:PRO:HG3	1:A:90:TYR:HB3	1.86	0.58
1:A:173:VAL:HG13	1:A:177:LEU:CD1	2.34	0.57
1:A:98:ILE:HD11	1:A:166:LEU:HD23	1.86	0.57
1:A:43:ILE:HA	1:A:46:TYR:CD2	2.40	0.57
1:A:99:THR:O	1:A:103:LYS:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:O	1:A:107:PRO:HD3	2.05	0.56
1:A:174:ILE:HA	1:A:177:LEU:HD12	1.89	0.55
1:A:34:LEU:HD13	1:A:122:ILE:HG21	1.89	0.55
1:A:43:ILE:HA	1:A:46:TYR:CE2	2.42	0.54
1:A:91:LEU:HD21	1:A:170:TYR:HD1	1.72	0.54
1:A:78:LYS:HE3	1:A:140:VAL:HG22	1.90	0.53
1:A:90:TYR:CE2	1:A:148:GLY:HA3	2.45	0.52
1:A:130:VAL:O	1:A:134:LEU:HD13	2.10	0.52
1:A:65:VAL:CG1	1:A:68:PHE:HB2	2.40	0.52
1:A:78:LYS:HE3	1:A:140:VAL:CG2	2.40	0.52
1:A:82:VAL:CG1	1:A:86:ARG:HD3	2.39	0.52
1:A:29:SER:O	1:A:32:ALA:HB3	2.11	0.51
1:A:174:ILE:HA	1:A:177:LEU:CD1	2.40	0.50
1:A:30:GLN:HB2	1:A:126:LEU:CD1	2.42	0.50
1:A:162:LEU:HA	1:A:165:GLN:HG3	1.94	0.50
1:A:135:CYS:SG	1:A:141:GLY:HA2	2.52	0.49
1:A:158:GLN:O	1:A:162:LEU:HG	2.12	0.49
1:A:82:VAL:C	1:A:86:ARG:HD3	2.31	0.49
1:A:34:LEU:HB3	1:A:174:ILE:CD1	2.39	0.49
1:A:64:ASN:O	1:A:65:VAL:C	2.48	0.49
1:A:121:ASP:HA	1:A:124:ARG:HD2	1.93	0.49
1:A:82:VAL:O	1:A:86:ARG:HG2	2.13	0.48
1:A:83:GLU:HA	1:A:86:ARG:CG	2.43	0.48
1:A:115:LYS:HA	1:A:118:ALA:HB3	1.96	0.47
1:A:130:VAL:O	1:A:134:LEU:HD22	2.14	0.47
1:A:173:VAL:HG13	1:A:177:LEU:HD12	1.96	0.47
1:A:54:PRO:HA	1:A:57:LEU:HD12	1.95	0.47
1:A:95:LEU:HD12	1:A:166:LEU:HD21	1.97	0.47
1:A:112:LEU:O	1:A:116:LEU:HD22	2.15	0.47
1:A:84:LEU:HD13	1:A:177:LEU:HD22	1.96	0.46
1:A:27:ILE:CD1	1:A:31:LEU:HG	2.44	0.46
1:A:50:GLY:O	1:A:54:PRO:HD2	2.15	0.46
1:A:84:LEU:HD13	1:A:177:LEU:CD2	2.46	0.46
1:A:28:ARG:HD2	1:A:28:ARG:O	2.16	0.46
1:A:81:LEU:CB	1:A:134:LEU:HD11	2.41	0.46
1:A:98:ILE:O	1:A:102:GLN:HG2	2.16	0.45
1:A:32:ALA:O	1:A:33:GLN:C	2.55	0.44
1:A:51:GLU:HA	1:A:52:PRO:HA	1.79	0.43
1:A:173:VAL:HG13	1:A:177:LEU:HD11	1.99	0.43
1:A:53:PHE:HB2	1:A:54:PRO:HD3	2.01	0.43
1:A:131:LEU:HA	1:A:134:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HG12	1:A:46:TYR:CE2	2.54	0.43
1:A:90:TYR:C	1:A:90:TYR:CD1	2.92	0.43
1:A:114:SER:O	1:A:115:LYS:C	2.56	0.43
1:A:41:LEU:HD11	1:A:116:LEU:HD12	2.00	0.42
1:A:46:TYR:CG	1:A:57:LEU:HD21	2.55	0.42
1:A:91:LEU:O	1:A:95:LEU:HD13	2.20	0.42
1:A:65:VAL:HG12	1:A:68:PHE:HB2	2.02	0.42
1:A:78:LYS:HB2	1:A:138:TYR:CZ	2.55	0.42
1:A:161:LYS:HG2	1:A:162:LEU:N	2.35	0.41
1:A:54:PRO:HA	1:A:57:LEU:CD1	2.50	0.41
1:A:146:THR:OG1	1:A:146:THR:O	2.36	0.41
1:A:46:TYR:CE2	1:A:57:LEU:HD21	2.55	0.41
1:A:86:ARG:HG2	1:A:86:ARG:H	1.56	0.41
1:A:156:VAL:HG22	1:A:157:PHE:N	2.34	0.41
1:A:31:LEU:HD22	1:A:31:LEU:HA	1.94	0.41
1:A:68:PHE:CD1	1:A:69:PRO:HD2	2.55	0.41
1:A:77:GLU:HA	1:A:80:LYS:CE	2.50	0.41
1:A:63:PRO:HB3	1:A:169:LYS:HA	2.02	0.40
1:A:69:PRO:HD3	1:A:90:TYR:CG	2.56	0.40
1:A:69:PRO:HB2	1:A:87:ILE:HG12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:CE1	1:A:142:HIS:CE1[2_655]	1.84	0.36

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	157/159 (99%)	125 (80%)	25 (16%)	7 (4%)	3	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	109	ALA
1	A	138	TYR
1	A	65	VAL
1	A	137	LYS
1	A	141	GLY
1	A	63	PRO

### 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	136/136 (100%)	97 (71%)	39 (29%)	<b>0</b> <b>3</b>

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	28	ARG
1	A	31	LEU
1	A	34	LEU
1	A	39	ASN
1	A	41	LEU
1	A	44	LEU
1	A	47	THR
1	A	51	GLU
1	A	57	LEU
1	A	58	GLU
1	A	59	LYS
1	A	60	LEU
1	A	78	LYS
1	A	81	LEU
1	A	82	VAL
1	A	86	ARG
1	A	88	VAL

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Mol	Chain	Res	Type
1	A	89	VAL
1	A	93	THR
1	A	108	SER
1	A	114	SER
1	A	116	LEU
1	A	121	ASP
1	A	126	LEU
1	A	131	LEU
1	A	132	CYS
1	A	134	LEU
1	A	135	CYS
1	A	137	LYS
1	A	138	TYR
1	A	142	HIS
1	A	155	ASP
1	A	156	VAL
1	A	161	LYS
1	A	162	LEU
1	A	171	LYS
1	A	173	VAL
1	A	177	LEU

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	35	ASN
1	A	106	ASN
1	A	142	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.