wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 09:42 PM EDT

PDB ID	:	1JTC
Title	:	Human Acidic Fibroblast Growth Factor. 141 Amino Acid Form with Amino Terminal His Tag AND LEU 44 REPLACED BY PHE (L44F)
Authors	:	Brych, S.R.; Blaber, S.I.; Logan, T.M.; Blaber, M.
Deposited on	:	2001-08-20
Resolution	:	1.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

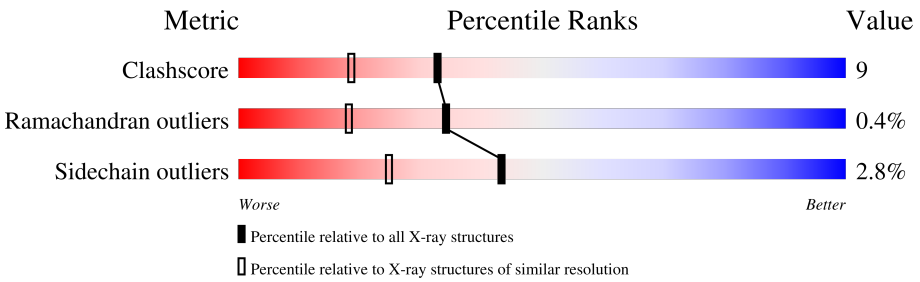
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	146	80% 14% • •
1	B	146	79% 15% • •
1	C	146	77% 17% • •
1	D	146	68% 25% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMT	D	166	-	-	X	-
2	FMT	D	167	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4996 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 acidic fibroblast growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1135	720	202	209	4	0	0	0
1	B	141	1133	720	200	209	4	0	0	0
1	C	141	1131	718	202	207	4	0	0	0
1	D	141	1139	723	203	209	4	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	HIS	-	expression tag	UNP P05230
A	1B	HIS	-	expression tag	UNP P05230
A	1C	HIS	-	expression tag	UNP P05230
A	1D	HIS	-	expression tag	UNP P05230
A	1E	HIS	-	expression tag	UNP P05230
A	1F	HIS	-	expression tag	UNP P05230
A	44	PHE	LEU	engineered mutation	UNP P05230
B	1A	HIS	-	expression tag	UNP P05230
B	1B	HIS	-	expression tag	UNP P05230
B	1C	HIS	-	expression tag	UNP P05230
B	1D	HIS	-	expression tag	UNP P05230
B	1E	HIS	-	expression tag	UNP P05230
B	1F	HIS	-	expression tag	UNP P05230
B	44	PHE	LEU	engineered mutation	UNP P05230
C	1A	HIS	-	expression tag	UNP P05230
C	1B	HIS	-	expression tag	UNP P05230
C	1C	HIS	-	expression tag	UNP P05230
C	1D	HIS	-	expression tag	UNP P05230
C	1E	HIS	-	expression tag	UNP P05230
C	1F	HIS	-	expression tag	UNP P05230
C	44	PHE	LEU	engineered mutation	UNP P05230

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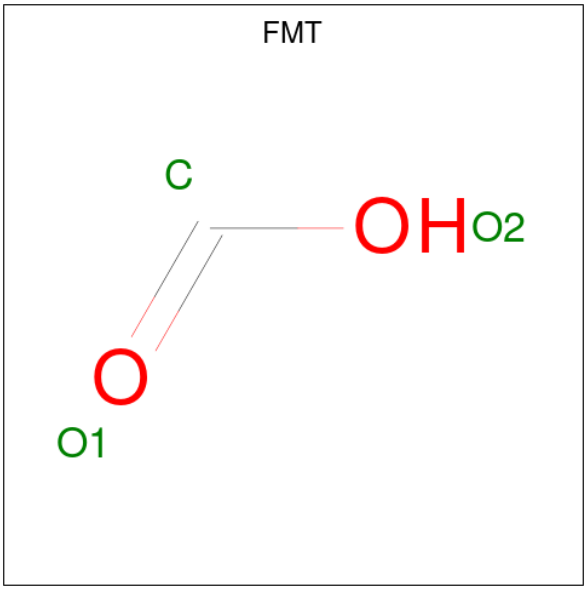
Chain	Residue	Modelled	Actual	Comment	Reference
D	1A	HIS	-	expression tag	UNP P05230
D	1B	HIS	-	expression tag	UNP P05230
D	1C	HIS	-	expression tag	UNP P05230
D	1D	HIS	-	expression tag	UNP P05230
D	1E	HIS	-	expression tag	UNP P05230
D	1F	HIS	-	expression tag	UNP P05230
D	44	PHE	LEU	engineered mutation	UNP P05230

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	3	1	2		0	0
			Total	C	O			
2	A	1	3	1	2		0	0
			Total	C	O			
2	B	1	3	1	2		0	0
			Total	C	O			
2	B	1	3	1	2		0	0
			Total	C	O			
2	C	1	3	1	2		0	0
			Total	C	O			
2	C	1	3	1	2		0	0
			Total	C	O			
2	D	1	3	1	2		0	0
			Total	C	O			
2	D	1	3	1	2		0	0

- Molecule 3 is water.

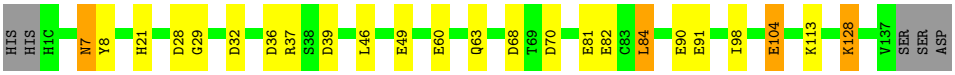
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	115	115	115	0	0
			Total	O		
3	B	101	101	101	0	0
			Total	O		
3	C	112	112	112	0	0
			Total	O		
3	D	106	106	106	0	0

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. 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.

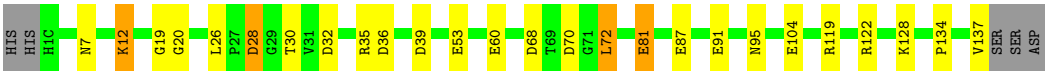
- Molecule 1: acidic fibroblast growth factor

Chain A:



- Molecule 1: acidic fibroblast growth factor

Chain B:

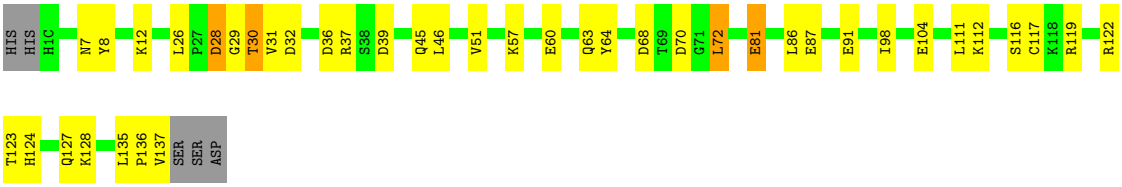


- Molecule 1: acidic fibroblast growth factor

Chain C:

- Molecule 1: acidic fibroblast growth factor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.92Å 73.78Å 109.13Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	36.90 – 1.70 48.46 – 1.70	Depositor EDS
% Data completeness (in resolution range)	76.4 (36.90-1.70) 85.3 (48.46-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available) 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT

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	0.81	7/1167 (0.6%)	1.11	13/1578 (0.8%)
1	B	0.82	6/1165 (0.5%)	1.06	12/1575 (0.8%)
1	C	0.80	6/1163 (0.5%)	1.09	10/1573 (0.6%)
1	D	0.84	5/1171 (0.4%)	1.08	10/1582 (0.6%)
All	All	0.82	24/4666 (0.5%)	1.08	45/6308 (0.7%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	GLU	CD-OE2	6.71	1.33	1.25
1	D	104	GLU	CD-OE2	6.70	1.33	1.25
1	C	104	GLU	CD-OE2	5.81	1.32	1.25
1	A	49	GLU	CD-OE2	5.75	1.31	1.25
1	A	91	GLU	CD-OE2	5.61	1.31	1.25

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	28	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	D	32	ASP	CB-CG-OD1	7.16	124.74	118.30
1	C	68	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	68	ASP	CB-CG-OD1	7.08	124.67	118.30

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	1135	0	1096	13	0
1	B	1133	0	1096	17	0
1	C	1131	0	1092	14	0
1	D	1139	0	1107	34	0
2	A	6	0	2	1	0
2	B	6	0	2	1	0
2	C	6	0	2	1	0
2	D	6	0	2	4	0
3	A	115	0	0	2	0
3	B	101	0	0	2	0
3	C	112	0	0	1	0
3	D	106	0	0	5	0
All	All	4996	0	4399	78	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 9.

The worst 5 of 78 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:B:26:LEU:HB2	1:B:30:THR:HG22	1.37	1.03
1:D:26:LEU:HB2	1:D:30:THR:HG22	1.41	1.02
1:C:7:ASN:ND2	1:C:7:ASN:H	1.70	0.88
1:A:7:ASN:ND2	1:A:7:ASN:H	1.71	0.87
1:A:7:ASN:H	1:A:7:ASN:HD22	1.29	0.80

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	139/146 (95%)	131 (94%)	8 (6%)	0	100	100
1	B	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
1	C	139/146 (95%)	130 (94%)	7 (5%)	2 (1%)	11	2
1	D	139/146 (95%)	130 (94%)	9 (6%)	0	100	100
All	All	556/584 (95%)	523 (94%)	31 (6%)	2 (0%)	34	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	5	PRO
1	C	6	GLY

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	123/129 (95%)	120 (98%)	3 (2%)	49	31
1	B	123/129 (95%)	119 (97%)	4 (3%)	38	19
1	C	122/129 (95%)	118 (97%)	4 (3%)	38	19
1	D	124/129 (96%)	121 (98%)	3 (2%)	49	31
All	All	492/516 (95%)	478 (97%)	14 (3%)	43	25

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	ASN
1	C	10	LYS
1	D	137	VAL
1	D	30	THR
1	D	72	LEU

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

Mol	Chain	Res	Type
1	A	7	ASN
1	C	7	ASN
1	D	45	GLN
1	D	77	GLN

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMT	A	161	-	2,2,2	0.36	0	1,1,1	0.26	0
2	FMT	B	162	-	2,2,2	0.33	0	1,1,1	0.26	0
2	FMT	D	166	-	2,2,2	0.29	0	1,1,1	0.32	0
2	FMT	A	160	-	2,2,2	0.34	0	1,1,1	0.32	0
2	FMT	D	167	-	2,2,2	0.29	0	1,1,1	0.31	0
2	FMT	C	164	-	2,2,2	0.38	0	1,1,1	0.27	0
2	FMT	C	165	-	2,2,2	0.35	0	1,1,1	0.26	0
2	FMT	B	163	-	2,2,2	0.36	0	1,1,1	0.29	0

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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	161	FMT	1	0
2	D	166	FMT	2	0
2	D	167	FMT	2	0
2	C	165	FMT	1	0
2	B	163	FMT	1	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.