

wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 07:24 PM EDT

PDB ID	:	1JQZ
Title	:	Human Acidic Fibroblast Growth Factor. 141 Amino Acid Form with Amino
		Terminal His Tag.
Authors	:	Brych, S.R.; Blaber, S.I.; Logan, T.M.; Blaber, M.
Deposited on		
Resolution	:	1.65 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 (1)) were used in the production of this report:

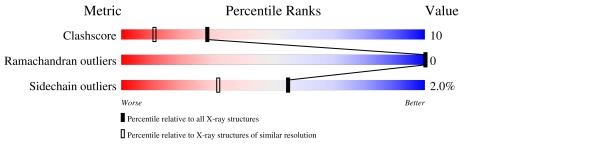
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.65 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	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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	А	146	77%	17%	•••				
1	В	146	68%	26%	•••				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2500 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	141	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			1136	720	203	209	4	0		
1	р	141	Total	С	Ν	0	S	0	1	0
			1137	720	203	209	5	0		0

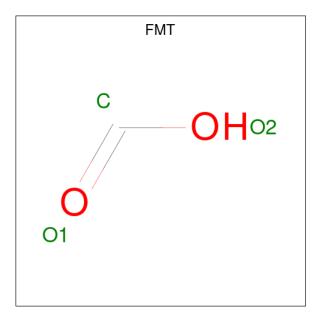
• Molecule 1 is a protein called acidic fibroblast growth factor.

Chain	Residue	Modelled	Actual	Comment	Reference
А	1A	HIS	-	expression tag	UNP P05230
А	1B	HIS	-	expression tag	UNP P05230
А	1C	HIS	-	expression tag	UNP P05230
А	1D	HIS	-	expression tag	UNP P05230
А	1E	HIS	-	expression tag	UNP P05230
А	1F	HIS	-	expression tag	UNP P05230
В	1A	HIS	-	expression tag	UNP P05230
В	1B	HIS	-	expression tag	UNP P05230
В	1C	HIS	-	expression tag	UNP P05230
В	1D	HIS	-	expression tag	UNP P05230
В	1E	HIS	-	expression tag	UNP P05230
В	1F	HIS	-	expression tag	UNP P05230

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0

• Molecule 3 is water.

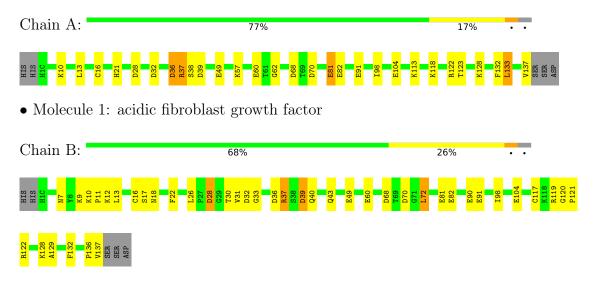
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	112	Total O 112 112	0	0
3	В	103	Total O 103 103	0	0



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	74.06Å 96.84Å 109.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.30 - 1.65	Depositor
Resolution (A)	44.25 - 1.65	EDS
% Data completeness	86.8 (44.30-1.65)	Depositor
(in resolution range)	$96.2 \ (44.25 - 1.65)$	EDS
R _{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.61 (at 1.65Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
$10, 10_{free}$	0.189 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	15.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36,63.0	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2500	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.83	6/1167~(0.5%)	1.04	12/1577~(0.8%)	
1	В	0.82	7/1173~(0.6%)	1.05	12/1585~(0.8%)	
All	All	0.83	13/2340~(0.6%)	1.05	24/3162~(0.8%)	

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	49	GLU	CD-OE2	5.92	1.32	1.25
1	А	91	GLU	CD-OE2	5.87	1.32	1.25
1	В	90	GLU	CD-OE2	5.80	1.32	1.25
1	В	60	GLU	CD-OE2	5.79	1.32	1.25
1	В	82	GLU	CD-OE2	5.78	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\mathbf{Ideal}(^{o})$
1	А	32	ASP	CB-CG-OD1	7.04	124.64	118.30
1	А	68	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	В	36	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	В	36	ASP	CB-CG-OD1	6.86	124.48	118.30
1	А	28	ASP	CB-CG-OD2	-6.67	112.30	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1136	0	1109	15	0
1	В	1137	0	1110	29	0
2	А	6	0	2	0	0
2	В	6	0	2	1	0
3	А	112	0	0	3	1
3	В	103	0	0	6	0
All	All	2500	0	2223	44	1

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.

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 10.

The worst 5 of 44 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	1.48	0.94
1:B:26:LEU:HD12	1:B:30:THR:CG2	2.17	0.73
1:B:7:ASN:HB2	3:B:1250:HOH:O	1.87	0.73
1:B:26:LEU:HB2	1:B:30:THR:CG2	2.18	0.72
1:B:39:ASP:O	1:B:43:GLN:NE2	2.30	0.64

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)
3:A:337:HOH:O	3:A:337:HOH:O[4_566]	2.19	0.01

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	Perce	ntiles
1	А	139/146~(95%)	133 (96%)	6 (4%)	0	100	100
1	В	140/146~(96%)	134 (96%)	6 (4%)	0	100	100
All	All	279/292~(96%)	267~(96%)	12~(4%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	124/129~(96%)	122~(98%)	2(2%)	62 41		
1	В	125/129~(97%)	122 (98%)	3 (2%)	49 23		
All	All	249/258~(96%)	244~(98%)	5 (2%)	55 32		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	37	ARG
1	А	133	LEU
1	В	12	LYS
1	В	37	ARG
1	В	72	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	В	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)

4 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	Turne	Chain	Dec	Link	B	ond leng	gths	B	ond ang	gles
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	FMT	В	163	-	2,2,2	0.48	0	$1,\!1,\!1$	0.28	0
2	FMT	В	162	-	2,2,2	0.22	0	$1,\!1,\!1$	0.37	0
2	FMT	А	161	-	2,2,2	0.35	0	$1,\!1,\!1$	0.28	0
2	FMT	А	160	-	2,2,2	0.52	0	$1,\!1,\!1$	0.28	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	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.

