



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:33 PM GMT

PDB ID : 1BFB
Title : BASIC FIBROBLAST GROWTH FACTOR COMPLEXED WITH HEP-
ARIN TETRAMER FRAGMENT
Authors : Faham, S.; Rees, D.C.
Deposited on : 1995-12-12
Resolution : 1.90 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

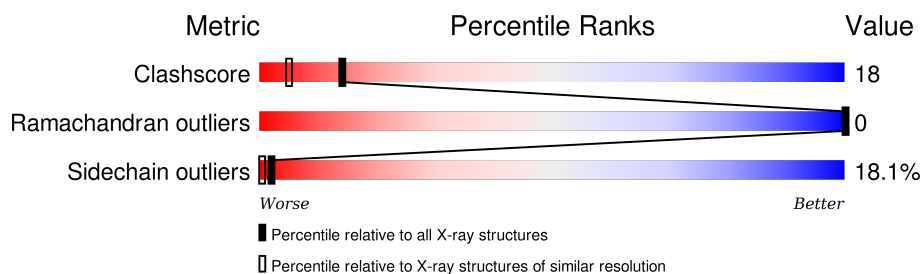
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 ≥ 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	147	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1070 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 BASIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			991	630	180	177	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	SER	CYS	ENGINEERED	UNP P09038
A	88	SER	CYS	ENGINEERED	UNP P09038

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	4	Total	C	N	O	S	0	0
			70	24	2	38	6		

- Molecule 3 is water.

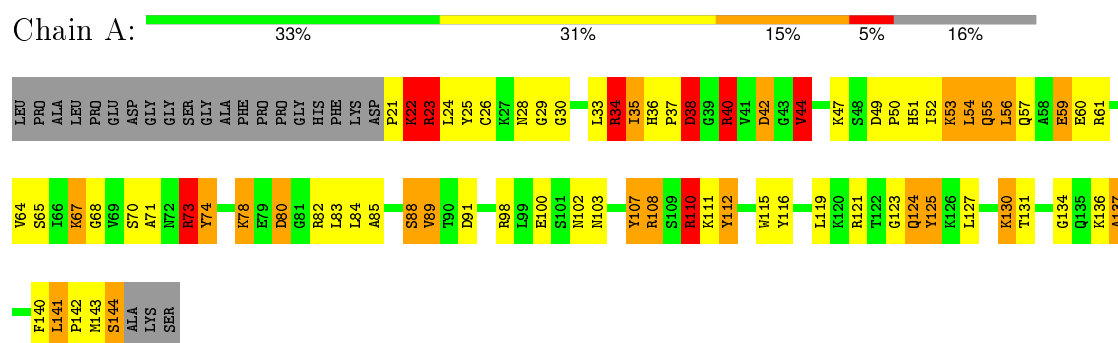
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

3 Residue-property plots [i](#)

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: BASIC FIBROBLAST GROWTH 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, α , β , γ	32.02Å 41.80Å 85.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90	Depositor
% Data completeness (in resolution range)	93.9 (5.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1070	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UAP, IDS, SGN

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	0.85	0/1012	1.96	18/1356 (1.3%)

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	51

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH1	-35.42	102.59	120.30
1	A	40	ARG	NE-CZ-NH2	-17.25	111.67	120.30
1	A	108	ARG	NE-CZ-NH2	-15.81	112.39	120.30
1	A	110	ARG	NE-CZ-NH2	-14.95	112.83	120.30
1	A	34	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	23	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	A	40	ARG	CG-CD-NE	-9.26	92.36	111.80
1	A	74	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	A	115	TRP	CD1-CG-CD2	7.21	112.06	106.30
1	A	107	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	A	38	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	25	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	A	115	TRP	CE2-CD2-CG	-6.22	102.32	107.30
1	A	116	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	121	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	40	ARG	NH1-CZ-NH2	-5.05	113.84	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	TYR	CB-CA-C	-5.03	100.34	110.40
1	A	115	TRP	CG-CD1-NE1	-5.02	105.08	110.10

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Sidechain
1	A	107	TYR	Sidechain
1	A	108	ARG	Sidechain
1	A	110	ARG	Sidechain
1	A	112	TYR	Mainchain
1	A	123	GLY	Mainchain
1	A	124	GLN	Mainchain
1	A	125	TYR	Sidechain,Mainchain
1	A	130	LYS	Mainchain
1	A	131	THR	Mainchain
1	A	134	GLY	Mainchain
1	A	137	ALA	Mainchain
1	A	141	LEU	Mainchain
1	A	142	PRO	Mainchain
1	A	143	MET	Mainchain
1	A	21	PRO	Mainchain
1	A	22	LYS	Mainchain
1	A	23	ARG	Sidechain,Mainchain
1	A	29	GLY	Mainchain
1	A	30	GLY	Mainchain
1	A	33	LEU	Mainchain
1	A	34	ARG	Sidechain
1	A	35	ILE	Mainchain
1	A	37	PRO	Mainchain
1	A	38	ASP	Mainchain
1	A	40	ARG	Sidechain,Mainchain
1	A	42	ASP	Mainchain
1	A	44	VAL	Mainchain
1	A	54	LEU	Mainchain
1	A	55	GLN	Mainchain
1	A	56	LEU	Mainchain
1	A	59	GLU	Mainchain
1	A	61	ARG	Mainchain
1	A	64	VAL	Mainchain
1	A	65	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	68	GLY	Mainchain
1	A	70	SER	Mainchain
1	A	71	ALA	Mainchain
1	A	73	ARG	Sidechain,Mainchain
1	A	78	LYS	Mainchain
1	A	80	ASP	Sidechain
1	A	82	ARG	Mainchain
1	A	84	LEU	Mainchain
1	A	88	SER	Mainchain
1	A	89	VAL	Mainchain
1	A	91	ASP	Sidechain
1	A	98	ARG	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	991	0	999	38	0
2	A	70	0	27	0	0
3	A	9	0	0	0	0
All	All	1070	0	1026	38	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 18.

All (38) 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:110:ARG:HG2	1:A:110:ARG:HH11	1.09	1.10
1:A:127:LEU:HD12	1:A:130:LYS:HE3	1.39	1.03
1:A:38:ASP:OD2	1:A:40:ARG:HD3	1.65	0.94
1:A:28:ASN:HA	1:A:136:LYS:HD3	1.52	0.89
1:A:38:ASP:CG	1:A:40:ARG:HD3	1.95	0.87
1:A:110:ARG:HG2	1:A:110:ARG:NH1	1.84	0.86
1:A:34:ARG:HD2	1:A:42:ASP:OD1	1.75	0.86
1:A:34:ARG:HD3	1:A:36:HIS:NE2	2.00	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HD2	1:A:52:ILE:HD12	1.67	0.75
1:A:73:ARG:HB2	1:A:85:ALA:HB1	1.68	0.75
1:A:22:LYS:HB3	1:A:22:LYS:NZ	2.06	0.71
1:A:53:LYS:HE3	1:A:53:LYS:HA	1.70	0.71
1:A:67:LYS:HE2	1:A:74:TYR:CZ	2.31	0.64
1:A:53:LYS:CE	1:A:53:LYS:HA	2.26	0.63
1:A:36:HIS:HE1	1:A:42:ASP:OD2	1.81	0.62
1:A:23:ARG:HD2	1:A:52:ILE:CD1	2.29	0.61
1:A:22:LYS:HB3	1:A:22:LYS:HZ2	1.66	0.61
1:A:34:ARG:HD3	1:A:36:HIS:CD2	2.35	0.61
1:A:111:LYS:HE2	1:A:112:TYR:CZ	2.39	0.58
1:A:102:ASN:O	1:A:103:ASN:HB2	2.04	0.56
1:A:56:LEU:HD12	1:A:56:LEU:N	2.21	0.55
1:A:110:ARG:O	1:A:110:ARG:HG3	2.07	0.54
1:A:22:LYS:CB	1:A:22:LYS:NZ	2.72	0.53
1:A:26:CYS:HB2	1:A:140:PHE:CE2	2.44	0.53
1:A:119:LEU:HD23	1:A:125:TYR:HA	1.90	0.53
1:A:34:ARG:HD3	1:A:36:HIS:CE1	2.44	0.51
1:A:28:ASN:HB2	1:A:137:ALA:HA	1.95	0.48
1:A:34:ARG:NH2	1:A:44:VAL:HG11	2.29	0.48
1:A:110:ARG:HH11	1:A:110:ARG:CG	2.01	0.47
1:A:49:ASP:O	1:A:52:ILE:HG12	2.14	0.47
1:A:24:LEU:HG	1:A:54:LEU:HD12	1.96	0.47
1:A:34:ARG:CD	1:A:36:HIS:NE2	2.75	0.46
1:A:49:ASP:OD1	1:A:50:PRO:HD2	2.17	0.44
1:A:59:GLU:O	1:A:60:GLU:HG3	2.18	0.44
1:A:35:ILE:O	1:A:51:HIS:HB3	2.19	0.43
1:A:40:ARG:HE	1:A:40:ARG:HB2	1.17	0.41
1:A:111:LYS:HE2	1:A:112:TYR:OH	2.21	0.41
1:A:22:LYS:NZ	1:A:144:SER:HA	2.36	0.41

There are no symmetry-related clashes.

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	122/147 (83%)	115 (94%)	7 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	105/123 (85%)	86 (82%)	19 (18%)	2	0

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	34	ARG
1	A	40	ARG
1	A	44	VAL
1	A	47	LYS
1	A	53	LYS
1	A	55	GLN
1	A	57	GLN
1	A	67	LYS
1	A	73	ARG
1	A	78	LYS
1	A	80	ASP
1	A	83	LEU
1	A	88	SER
1	A	89	VAL
1	A	110	ARG
1	A	124	GLN
1	A	141	LEU
1	A	144	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	135	GLN

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 ⓘ

4 carbohydrates 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	UAP	A	301	2	12,15,16	2.71	3 (25%)	11,22,24	1.15	1 (9%)
2	SGN	A	302	2	18,20,20	1.90	3 (16%)	20,31,31	1.18	3 (15%)
2	IDS	A	303	2	12,15,17	2.23	2 (16%)	12,22,26	1.36	1 (8%)
2	SGN	A	304	2	18,20,20	1.70	1 (5%)	20,31,31	1.07	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UAP	A	301	2	-	0/5/22/25	0/1/1/1
2	SGN	A	302	2	-	0/11/31/31	0/1/1/1
2	IDS	A	303	2	-	0/5/22/29	0/1/1/1
2	SGN	A	304	2	-	0/11/31/31	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	UAP	C3-C4	-5.71	1.43	1.50
2	A	303	IDS	O2-C2	-5.47	1.39	1.47
2	A	301	UAP	O2-C2	-4.54	1.40	1.47
2	A	302	SGN	C2-N	-2.52	1.43	1.47
2	A	302	SGN	O1S-S1	3.45	1.45	1.42
2	A	303	IDS	O2-S	4.67	1.72	1.57
2	A	301	UAP	O2-S	5.30	1.74	1.57
2	A	302	SGN	O6-S2	5.83	1.75	1.57
2	A	304	SGN	O6-S2	6.34	1.77	1.57

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	UAP	O5-C1-C2	-2.77	108.13	111.26
2	A	304	SGN	C3-C4-C5	-2.72	105.46	110.20
2	A	302	SGN	O4-C4-C3	-2.39	104.96	110.34
2	A	302	SGN	O5-C5-C4	-2.06	105.82	109.68
2	A	302	SGN	C4-C3-C2	-2.02	107.63	110.43
2	A	303	IDS	C1-C2-C3	3.77	115.04	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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