



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FQ9  
Title : CRYSTAL STRUCTURE OF A TERNARY FGF2-FGFR1-HEPARIN COMPLEX  
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Deposited on : 2000-09-04  
Resolution : 3.00 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

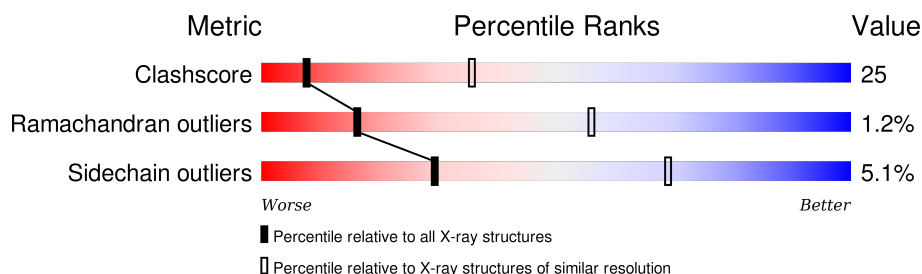
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	132	
1	B	132	
2	C	225	
2	D	225	

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
3	SGN	A	306	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5496 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 FIBROBLAST GROWTH FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			
1	B	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	ENGINEERED	UNP P09038
A	87	SER	CYS	ENGINEERED	UNP P09038
B	69	SER	CYS	ENGINEERED	UNP P09038
B	87	SER	CYS	ENGINEERED	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1638	1047	280	302	9			
2	D	196	Total	C	N	O	S	0	0	0
			1533	980	263	281	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	ENGINEERED	UNP P11362
D	185	GLN	ASN	ENGINEERED	UNP P11362

- Molecule 3 is a polymer of unknown type called SUGAR (HEPARIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	8	Total	C	N	O	S	0	0
			140	48	4	76	12		

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

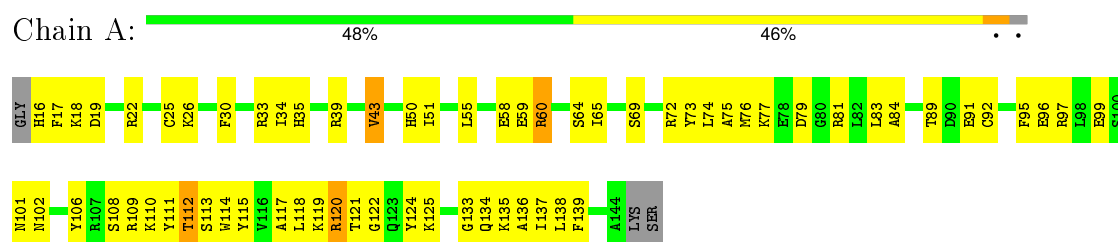
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	6	Total	C	N	O	S	0	0
			105	36	3	57	9		

### 3 Residue-property plots

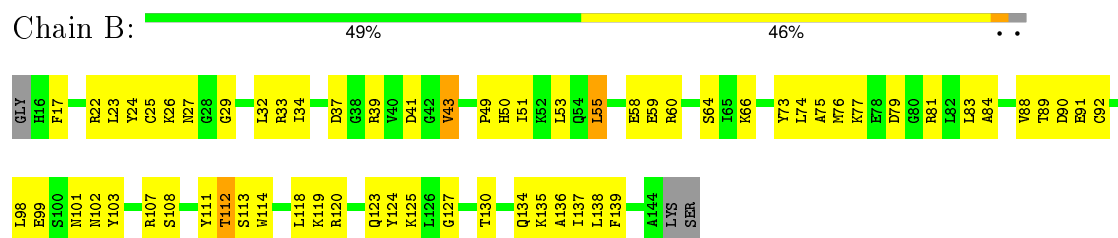
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: FIBROBLAST GROWTH FACTOR 2



#### • Molecule 1: FIBROBLAST GROWTH FACTOR 2



#### • Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1



#### • Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.89Å 98.89Å 196.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP



## 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: UAP, IDU, 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	0.44	0/1063	0.70	1/1425 (0.1%)
1	B	0.45	0/1063	0.68	1/1425 (0.1%)
2	C	0.44	0/1685	0.68	0/2299
2	D	0.42	0/1576	0.69	0/2146
All	All	0.44	0/5387	0.69	2/7295 (0.0%)

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
3	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	SER	N-CA-C	-5.30	96.68	111.00
1	B	64	SER	N-CA-C	-5.16	97.08	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	306	SGN	C1

There are no planarity outliers.

## 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	1040	0	1040	59	0
1	B	1040	0	1040	61	0
2	C	1638	0	1603	92	0
2	D	1533	0	1506	82	0
3	A	140	0	53	4	0
4	B	105	0	40	1	0
All	All	5496	0	5282	273	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 25.

The worst 5 of 273 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)
2:D:175:LYS:HG3	2:D:216:ILE:HG12	1.42	0.99
2:D:282:ASP:HB3	2:D:283:PRO:HD3	1.44	0.98
2:C:282:ASP:HB3	2:C:283:PRO:HD3	1.45	0.96
2:D:286:HIS:HD2	2:D:314:ALA:HB3	1.37	0.90
2:C:207:LYS:HE2	2:C:209:ARG:HE	1.35	0.89

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	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	24 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	24	66
2	C	209/225 (93%)	194 (93%)	11 (5%)	4 (2%)	10	43
2	D	192/225 (85%)	176 (92%)	14 (7%)	2 (1%)	19	61
All	All	655/714 (92%)	602 (92%)	45 (7%)	8 (1%)	16	56

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	B	112	THR
2	C	271	SER
2	C	296	ASN
2	C	281	SER

### 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	110/113 (97%)	105 (96%)	5 (4%)	34	74
1	B	110/113 (97%)	106 (96%)	4 (4%)	42	79
2	C	180/198 (91%)	170 (94%)	10 (6%)	26	65
2	D	169/198 (85%)	159 (94%)	10 (6%)	24	63
All	All	569/622 (92%)	540 (95%)	29 (5%)	29	69

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	238	SER
2	C	313	THR
2	D	317	ASN
2	C	252	PRO
2	C	355	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	185	GLN
2	C	201	HIS
2	C	330	ASN
2	C	166	HIS
2	C	317	ASN

### 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 ⓘ

14 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$
3	UAP	A	301	3	12,15,16	5.04	6 (50%)	11,22,24	2.69	3 (27%)
3	SGN	A	302	3	18,20,20	1.73	3 (16%)	20,31,31	1.46	2 (10%)
3	IDS	A	303	3	12,15,17	2.61	2 (16%)	12,22,26	2.42	3 (25%)
3	SGN	A	304	3	18,20,20	1.63	2 (11%)	20,31,31	0.94	1 (5%)
3	IDS	A	305	3	12,15,17	2.43	3 (25%)	12,22,26	2.45	2 (16%)
3	SGN	A	306	3	18,20,20	1.91	3 (16%)	20,31,31	1.34	3 (15%)
3	IDU	A	307	3	12,15,17	2.39	3 (25%)	12,22,26	2.52	2 (16%)
3	SGN	A	308	3	18,20,20	2.02	2 (11%)	20,31,31	1.15	1 (5%)
4	UAP	B	301	4	12,15,16	5.22	5 (41%)	11,22,24	2.87	3 (27%)
4	SGN	B	302	4	18,20,20	1.73	2 (11%)	20,31,31	1.13	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	IDS	B	303	4	12,15,17	2.51	3 (25%)	12,22,26	2.37	3 (25%)
4	SGN	B	304	4	18,20,20	1.62	1 (5%)	20,31,31	1.03	1 (5%)
4	IDS	B	305	4	12,15,17	2.47	4 (33%)	12,22,26	3.39	4 (33%)
4	SGN	B	306	4	18,20,20	1.75	3 (16%)	20,31,31	1.05	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
3	UAP	A	301	3	-	0/5/22/25	0/1/1/1
3	SGN	A	302	3	-	0/11/31/31	0/1/1/1
3	IDS	A	303	3	-	0/5/22/29	0/1/1/1
3	SGN	A	304	3	-	0/11/31/31	0/1/1/1
3	IDS	A	305	3	-	0/5/22/29	0/1/1/1
3	SGN	A	306	3	1/1/7/8	0/11/31/31	0/1/1/1
3	IDU	A	307	3	-	0/5/22/29	0/1/1/1
3	SGN	A	308	3	-	0/11/31/31	0/1/1/1
4	UAP	B	301	4	-	0/5/22/25	0/1/1/1
4	SGN	B	302	4	-	0/11/31/31	0/1/1/1
4	IDS	B	303	4	-	0/5/22/29	0/1/1/1
4	SGN	B	304	4	-	0/11/31/31	0/1/1/1
4	IDS	B	305	4	-	0/5/22/29	0/1/1/1
4	SGN	B	306	4	-	0/11/31/31	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	IDS	O2-C2	-5.66	1.38	1.47
4	B	301	UAP	O2-C2	-5.36	1.39	1.47
4	B	303	IDS	O2-C2	-5.10	1.39	1.47
3	A	301	UAP	O2-C2	-4.93	1.39	1.47
3	A	305	IDS	O2-C2	-4.79	1.40	1.47

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	UAP	C3-C4-C5	-4.72	113.61	121.60
3	A	302	SGN	C3-C2-N	-4.67	101.35	110.64
3	A	301	UAP	C3-C4-C5	-4.51	113.98	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308	SGN	C4-C3-C2	-3.53	105.53	110.43
3	A	306	SGN	C3-C2-N	-3.20	104.29	110.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	306	SGN	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	UAP	2	0
3	A	302	SGN	1	0
3	A	305	IDS	1	0
4	B	305	IDS	1	0

## 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.