



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 11:09 pm GMT

PDB ID : 1EVT
Title : CRYSTAL STRUCTURE OF FGF1 IN COMPLEX WITH THE EX-
TRACELLULAR LIGAND BINDING DOMAIN OF FGF RECEPTOR 1
(FGFR1)
Authors : Plotnikov, A.N.; Hubbard, S.R.; Schlessinger, J.; Mohammadi, M.
Deposited on : 2000-04-20
Resolution : 2.80 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtrriage (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

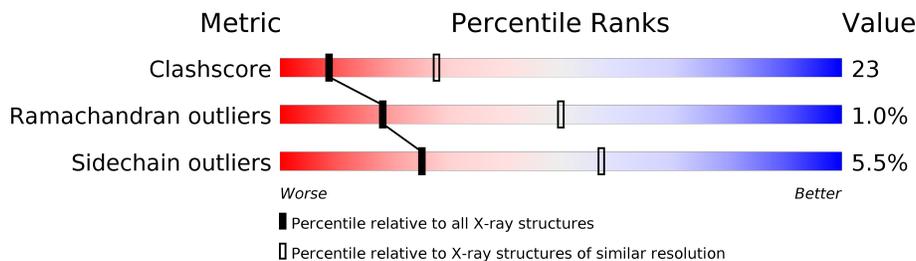
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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	134	
1	B	134	
2	C	225	
2	D	225	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4983 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.

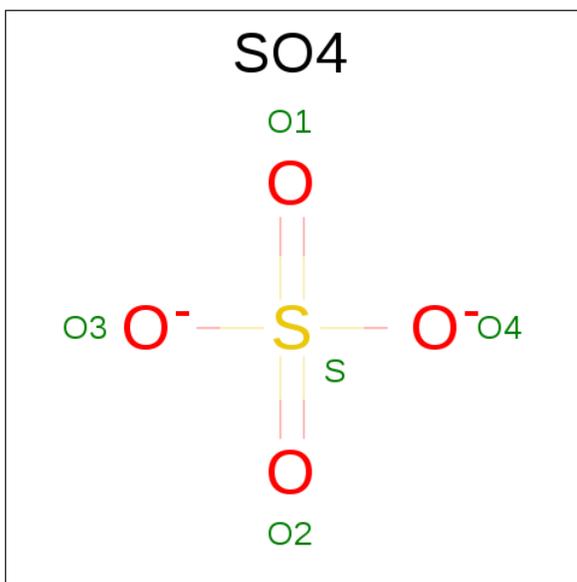
- Molecule 1 is a protein called PROTEIN (FIBROBLAST GROWTH FACTOR 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	131	1040	659	181	196	4	0	0	0
1	B	131	1040	659	181	196	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	191	1439	926	243	262	8	0	0	0
2	D	192	1444	929	244	263	8	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



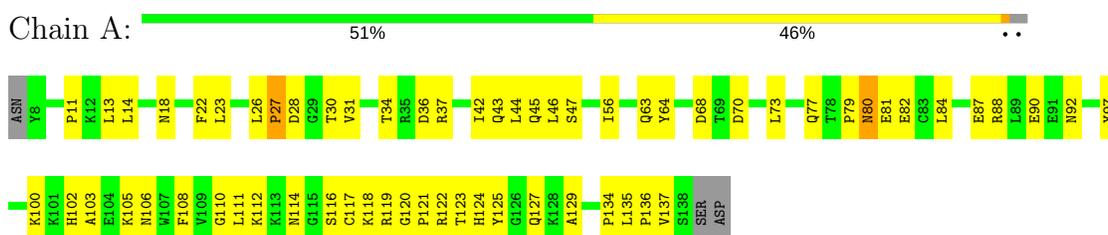
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0

3 Residue-property plots [i](#)

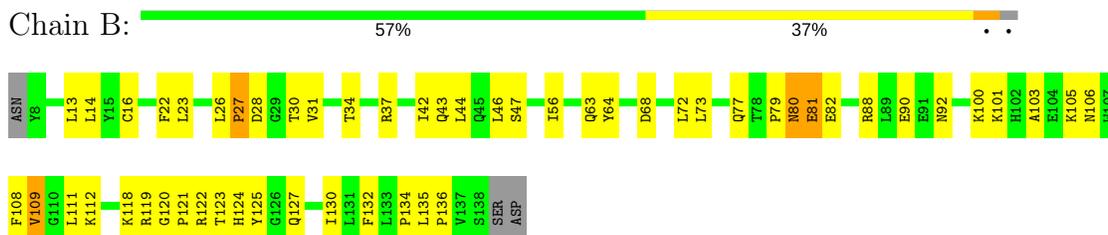
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

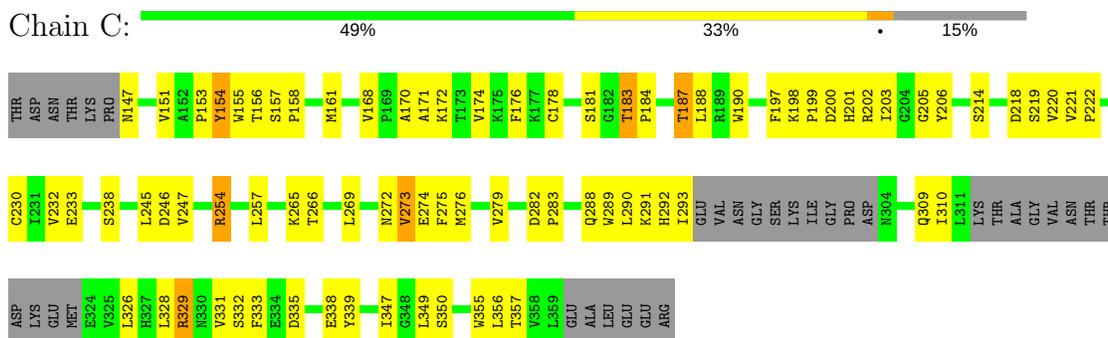
- Molecule 1: PROTEIN (FIBROBLAST GROWTH FACTOR 1)



- Molecule 1: PROTEIN (FIBROBLAST GROWTH FACTOR 1)



- Molecule 2: PROTEIN (FIBROBLAST GROWTH FACTOR RECEPTOR 1)



- Molecule 2: PROTEIN (FIBROBLAST GROWTH FACTOR RECEPTOR 1)



THR	V232	V325	THR	V174	V355
ASP	E233	L326	ASN	K175	L356
ASN	S238	R327	GLY	F176	T357
THR	L245	L328	ASN	K177	V358
LYS	D246	R329	GLY	C178	GLU
PRO	V247	N330	GLY	L290	ALA
M147	R254	V331	GLY	P179	LEU
V151	L257	S332	GLY	S180	GLU
A152	K266	D335	GLY	S181	GLU
P153	T266	Y339	GLY	G182	GLU
Y154	V273	L342	GLY	T183	ARG
H155	F275	A343	GLY	P184	
T156	V279	L347	GLY	P185	
S157	D282	G348	GLY	P186	
P158	P283	L349	GLY	T187	
M161	L287	S350	GLY	L188	
V168	Q288	H351	GLY	K198	
P169	W289	H352	GLY	P199	
A170	L290	V355	GLY	D200	
A171	K291	L356	GLY	H201	
V174	H292	T357	GLY	LEU	
K175	L293	V358	GLY	P306	
F176	GLU	L359	GLY	Q309	
K177	VAL	GLU	GLY	I310	
C178	ASN	ALA	GLY	A314	
P179	ASN	LEU	GLY	GLY	
S180	ASN	GLU	GLY	VAL	
S181	GLY	GLU	GLY	ASN	
G182	ASN	GLU	GLY	THR	
T183	GLY	GLU	GLY	THR	
P184	ASN	GLU	GLY	ASP	
P185	GLY	GLU	GLY	LYS	
P186	GLY	GLU	GLY	GLU	
T187	PRO	GLU	GLY	MET	
L188	ASP	GLU	GLY	E324	
K198	ASN	GLU	GLY		
P199	ASN	GLU	GLY		
D200	LEU	GLU	GLY		
H201	P306	GLU	GLY		
LEU	Q309	GLU	GLY		
P306	I310	GLU	GLY		
Q309	A314	GLU	GLY		
I310	GLY	GLU	GLY		
A314	VAL	GLU	GLY		
GLY	ASN	GLU	GLY		
VAL	THR	GLU	GLY		
ASN	THR	GLU	GLY		
THR	THR	GLU	GLY		
S219	ASP	GLU	GLY		
V220	LYS	GLU	GLY		
V221	GLU	GLU	GLY		
D224	MET	GLU	GLY		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.55Å 64.06Å 64.14Å 93.40° 111.17° 97.18°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	95.7 (25.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4983	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: SO4

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	0.46	0/1064	0.69	0/1437
1	B	0.43	0/1064	0.69	1/1437 (0.1%)
2	C	0.47	0/1483	0.69	0/2038
2	D	0.46	0/1488	0.68	0/2043
All	All	0.46	0/5099	0.68	1/6955 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	VAL	N-CA-C	-5.15	97.09	111.00

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	1040	0	1014	52	0
1	B	1040	0	1014	43	0
2	C	1439	0	1337	69	0
2	D	1444	0	1346	62	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4983	0	4711	220	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 23.

The worst 5 of 220 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:293:ILE:HD11	2:D:309:GLN:HB2	1.40	1.00
2:D:273:VAL:HG13	2:D:328:LEU:HB2	1.44	0.97
1:B:80:ASN:HD22	1:B:82:GLU:H	1.08	0.94
2:C:293:ILE:HD11	2:C:309:GLN:HB2	1.50	0.93
1:A:27:PRO:HA	1:A:63:GLN:HE22	1.40	0.85

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	129/134 (96%)	120 (93%)	8 (6%)	1 (1%)	22	55
1	B	129/134 (96%)	120 (93%)	8 (6%)	1 (1%)	22	55
2	C	185/225 (82%)	172 (93%)	11 (6%)	2 (1%)	17	47
2	D	186/225 (83%)	170 (91%)	14 (8%)	2 (1%)	17	47
All	All	629/718 (88%)	582 (92%)	41 (6%)	6 (1%)	18	50

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	329	ARG
2	D	329	ARG

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Mol	Chain	Res	Type
2	D	219	SER
2	C	219	SER
1	A	27	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	112/118 (95%)	106 (95%)	6 (5%)	26	58
1	B	112/118 (95%)	107 (96%)	5 (4%)	32	66
2	C	150/198 (76%)	140 (93%)	10 (7%)	19	48
2	D	150/198 (76%)	142 (95%)	8 (5%)	26	59
All	All	524/632 (83%)	495 (94%)	29 (6%)	25	57

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

Mol	Chain	Res	Type
2	C	183	THR
2	C	200	ASP
2	D	273	VAL
2	C	187	THR
2	C	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	241	HIS
2	C	284	GLN
2	D	286	HIS
1	B	80	ASN
1	B	106	ASN

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 carbohydrates 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	4002	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	A	4003	-	4,4,4	0.27	0	6,6,6	0.14	0
3	SO4	B	4000	-	4,4,4	0.32	0	6,6,6	0.13	0
3	SO4	B	4001	-	4,4,4	0.32	0	6,6,6	0.20	0

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	SO4	A	4002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4003	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4000	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4001	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.