wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 09:45 am BST

PDB ID	:	1EVT
Title	:	CRYSTAL STRUCTURE OF FGF1 IN COMPLEX WITH THE EXTRACELLULAR 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

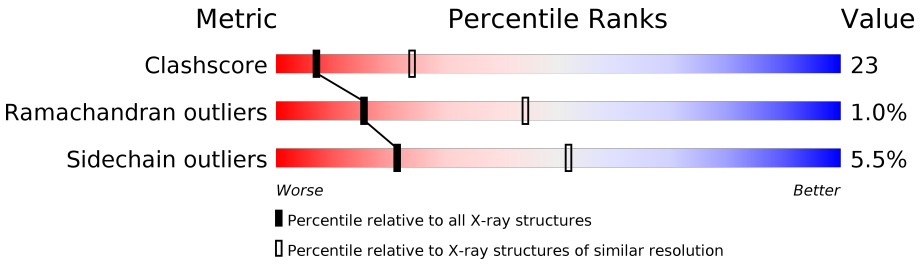
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	134	51% 46%
1	B	134	57% 37%
2	C	225	49% 33% 15%
2	D	225	51% 33% 15%

2 Entry composition

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.

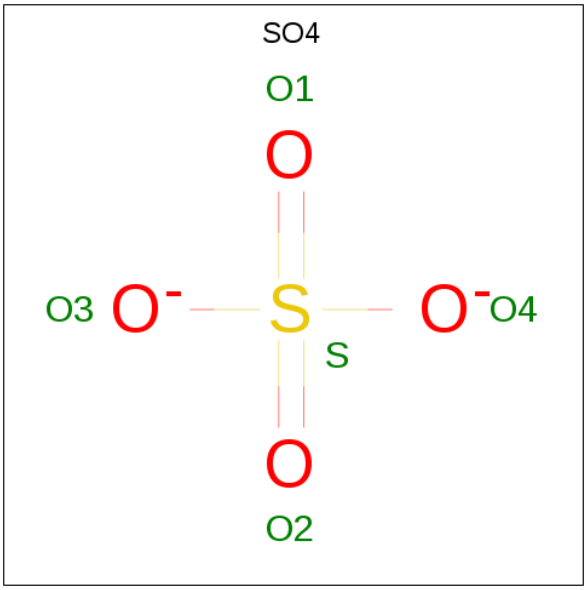
- Molecule 1 is a protein called PROTEIN (FIBROBLAST GROWTH FACTOR 1).

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

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

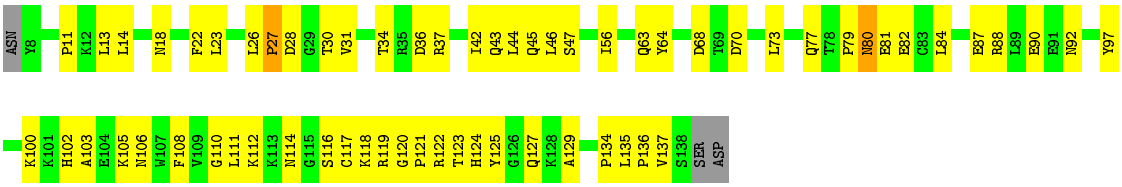
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

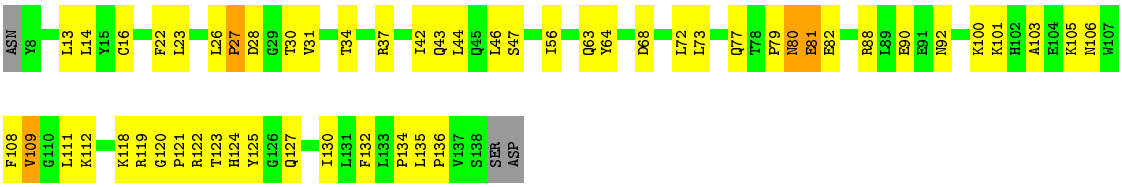
- Molecule 1: PROTEIN (FIBROBLAST GROWTH FACTOR 1)

Chain A:



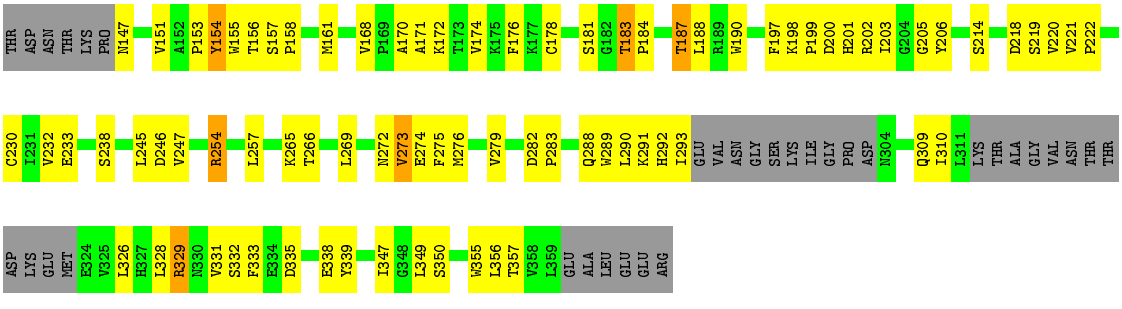
- Molecule 1: PROTEIN (FIBROBLAST GROWTH FACTOR 1)

Chain B:



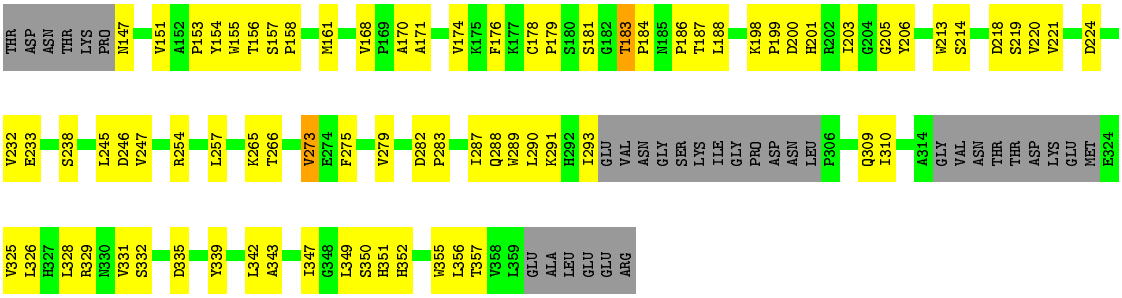
- Molecule 2: PROTEIN (FIBROBLAST GROWTH FACTOR RECEPTOR 1)

Chain C:



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

Chain D:


THR ASP ASN THR LYS PRO N147 V151 A152 P153 Y154 W155 T156 S157 P158 M161 V168 P169 A170 A171 V174 K175 F176 K177 C178 P179 S180 S181 G182 T183 P184 N185 P186 T187 L188 K198 P199 D200 H201 R202 I203 G204 G205 Y206 W213 S214 D218 S219 V220 V221 D224
V232 E233 S238 L245 D246 V247 R254 L257 K265 T266 V273 E274 F275 V279 D282 P283 I287 Q288 W289 L290 K291 H292 I293 GLU VAL ASN GLY SER LYS ILE GLY PRO ASP ASN LEU P306 Q309 I310 A314 GLY VAL ASN THR THR ASP LYS GLU MET E324
V325 L326 H327 L328 R329 N330 V331 S332 D335 Y339 L342 A343 I347 G348 L349 S350 H351 H352 W355 L356 T357 V358 L359 GLU ALA LEU GLU GLU ARG

4 Data and refinement statistics (i)

Xtriage (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.	Xtriage
Total number of atoms	4983	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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: 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(^{o})	Ideal(^{o})
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

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%)	19	49
1	B	129/134 (96%)	120 (93%)	8 (6%)	1 (1%)	19	49
2	C	185/225 (82%)	172 (93%)	11 (6%)	2 (1%)	14	41
2	D	186/225 (83%)	170 (91%)	14 (8%)	2 (1%)	14	41
All	All	629/718 (88%)	582 (92%)	41 (6%)	6 (1%)	15	44

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%)	22	53
1	B	112/118 (95%)	107 (96%)	5 (4%)	27	60
2	C	150/198 (76%)	140 (93%)	10 (7%)	16	43
2	D	150/198 (76%)	142 (95%)	8 (5%)	22	54
All	All	524/632 (83%)	495 (94%)	29 (6%)	21	52

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

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	4003	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	B	4000	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	A	4002	-	4,4,4	0.26	0	6,6,6	0.22	0
3	SO4	B	4001	-	4,4,4	0.25	0	6,6,6	0.20	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.