



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2018 – 02:01 am GMT

PDB ID : 1DFC
Title : CRYSTAL STRUCTURE OF HUMAN FASCIN, AN ACTIN-CROSSLINKING PROTEIN
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Deposited on : 1999-11-18
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

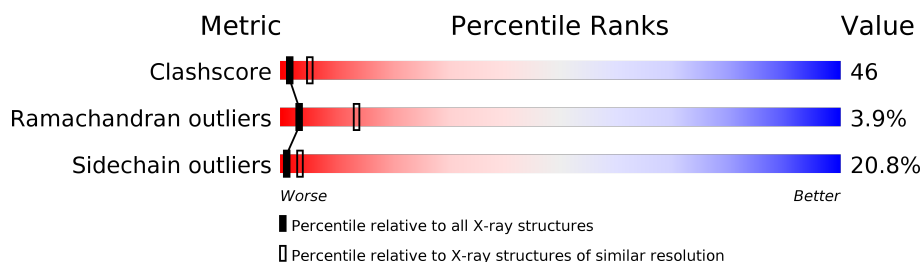
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	122078	1924 (2.90-2.90)
Ramachandran outliers	120005	1884 (2.90-2.90)
Sidechain outliers	119972	1886 (2.90-2.90)

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	493	
1	B	493	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7427 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 FASCIN.

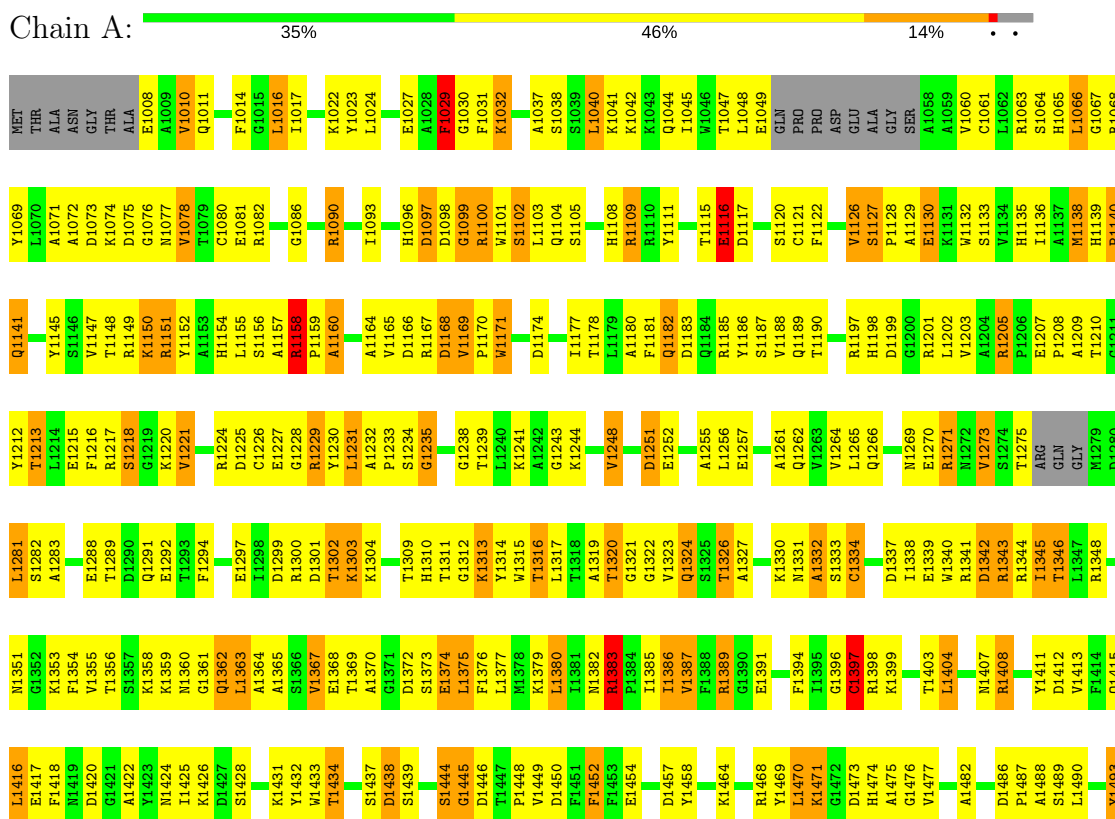
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3716	2326	663	714	13			
1	B	474	Total	C	N	O	S	0	0	0
			3711	2323	662	713	13			

3 Residue-property plots

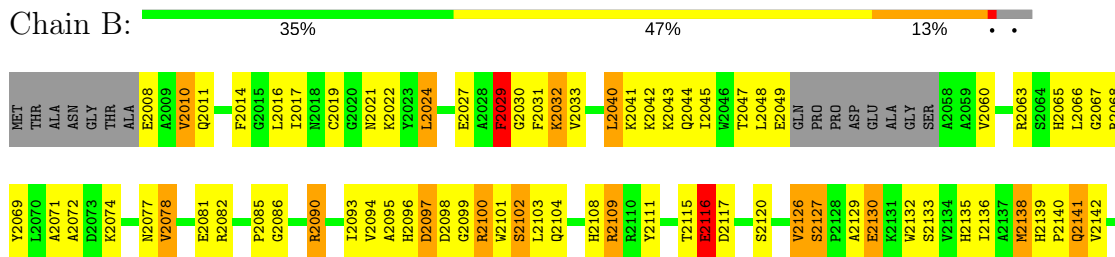
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: FASCIN



S2489	Q2415	R2348	A2283	E2215	Y2145
Y2493	L2416	N2351	N2284	F2216	S2146
	F2418		Q2285	R2217	V2147
	N2419	F2354	E2288	S2218	T2148
	D2420	V2355	T2289	G2219	R2149
	G2421	T2356	D2290	K2220	K2150
	A2422	S2357	Q2291	V2221	R2151
		K2358	E2292		Y2152
	I2425	K2359	T2293	R2224	
	K2426	N2360	F2294	D2225	S2156
	D2427	G2361	Q2295	C2226	A2157
	S2428	Q2362	L2296	E2227	R2158
	T2429	L2363		G2228	P2159
	G2430	A2364	D2299	R2229	A2160
	K2431	A2365	R2300	Y2230	D2161
	Y2432	S2366	D2301	L2231	
	V2433	V2367	T2302	A2232	A2164
	T2434	E2368	K2303	P2233	V2165
		T2369	K2304	S2234	D2166
		A2370	C2305	G2235	R2167
	D2438	G2371			D2168
	S2439	D2372	R2308	G2238	V2169
			T2309	T2239	P2170
	T2442	L2375	H2310	G2243	W2171
	S2443	F2376	T2311	K2244	G2172
	S2444	L2377	G2312		V2173
	G2445	M2378	K2313	V2248	D2174
	D2446	K2379	W2314		S2175
	T2447	L2380	W2315	D2251	
	P2448	I2381	T2316	E2252	T2178
	V2449	N2382	L2317	L2253	
	D2450	R2383	T2318	F2254	F2181
	F2451	P2384	A2319	A2255	Q2182
	F2452	I2385	T2320	L2256	D2183
	E2454	I2386	G2321	E2257	Q2184
	F2455		G2322	Q2258	R2185
	C2456	R2389	V2323	S2259	Y2186
	D2457	G2390	Q2324	C2260	S2187
	Y2458	E2391	S2325	A2261	V2188
			T2326	Q2262	Q2189
	K2464	F2394	A2327	V2263	H2193
	V2465	I2395		V2264	R2194
		G2396	K2330	L2265	
	R2468	C2397	N2331	Q2266	
	Y2469	R2398	A2332		R2197
	L2470	K2399	S2333	N2269	H2198
	K2471	V2400	C2334	E2270	D2199
	G2472	T2401		R2271	
	D2473		D2337	N2272	V2203
	H2474	L2404	I2338	V2273	A2204
	A2475	D2405	E2339	S2274	R2205
	G2476	A2406	W2340	T2275	P2206
	V2477	N2407	R2341	ARG	E2207
		R2408	D2342	GLN	P2208
	A2482		R2343	GLY	A2209
			R2344	MET	T2210
	D2486	Y2411	I2345		G2211
	P2487	D2412	T2346	D2280	Y2212
	A2488	V2413	L2347	L2281	T2213
		F2414		S2282	L2214

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.43Å 71.69Å 116.92Å 90.00° 132.17° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.6 (8.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7427	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.96	2/3793 (0.1%)	0.98	3/5126 (0.1%)
1	B	0.95	3/3788 (0.1%)	0.98	2/5119 (0.0%)
All	All	0.96	5/7581 (0.1%)	0.98	5/10245 (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
1	A	0	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2456	CYS	CB-SG	-6.68	1.70	1.82
1	A	1397	CYS	CB-SG	-6.12	1.71	1.82
1	B	2260	CYS	CB-SG	-5.68	1.72	1.81
1	A	1061	CYS	CB-SG	-5.42	1.73	1.81
1	B	2305	CYS	CB-SG	-5.34	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1383	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	B	2194	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	1387	VAL	N-CA-C	-5.67	95.70	111.00
1	A	1363	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	2404	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1452	PHE	Sidechain
1	A	1493	TYR	Sidechain
1	B	2493	TYR	Sidechain

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	3716	0	3599	343	1
1	B	3711	0	3597	336	1
All	All	7427	0	7196	679	1

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 46.

The worst 5 of 679 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:1139:HIS:CE1	1:A:1141:GLN:HG3	1.61	1.36
1:A:1416:LEU:HD12	1:A:1416:LEU:H	1.15	1.12
1:A:1158:ARG:HB2	1:A:1159:PRO:HD3	1.14	1.10
1:B:2158:ARG:HB2	1:B:2159:PRO:HD3	1.11	1.10
1:B:2158:ARG:HB2	1:B:2159:PRO:CD	1.86	1.05

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)
1:A:1075:ASP:OD1	1:B:2343:ARG:NH1[1_565]	2.15	0.05

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	469/493 (95%)	390 (83%)	61 (13%)	18 (4%)	3	14
1	B	468/493 (95%)	390 (83%)	59 (13%)	19 (4%)	3	12
All	All	937/986 (95%)	780 (83%)	120 (13%)	37 (4%)	3	13

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1029	PHE
1	A	1116	GLU
1	A	1158	ARG
1	A	1160	ALA
1	A	1227	GLU

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	391/404 (97%)	312 (80%)	79 (20%)	1	4
1	B	391/404 (97%)	307 (78%)	84 (22%)	1	3
All	All	782/808 (97%)	619 (79%)	163 (21%)	1	3

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1438	ASP

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Mol	Chain	Res	Type
1	B	2100	ARG
1	B	2404	LEU
1	A	1446	ASP
1	B	2019	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2013	GLN
1	B	2021	ASN
1	B	2182	GLN
1	B	2011	GLN
1	B	2324	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 carbohydrates in this entry.

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 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.