



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1DFC / pdb_00001dfc
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

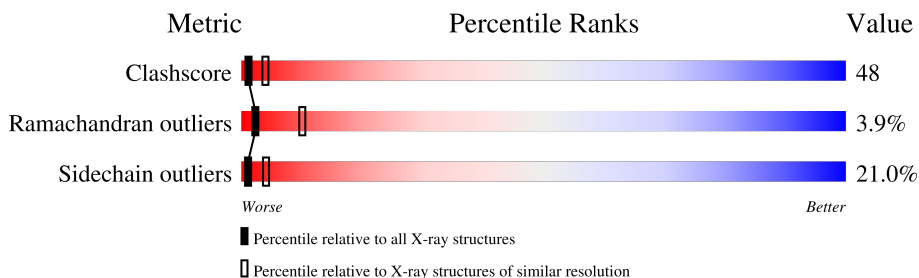
1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	493	 33% 45% 17% . .
1	B	493	 31% 46% 17% . .

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
			Total	C	N	O	S			
1	A	475	Total 3716	C 2326	N 663	O 714	S 13	0	0	0
1	B	474	Total 3711	C 2323	N 662	O 713	S 13	0	0	0

3 Residue-property plots

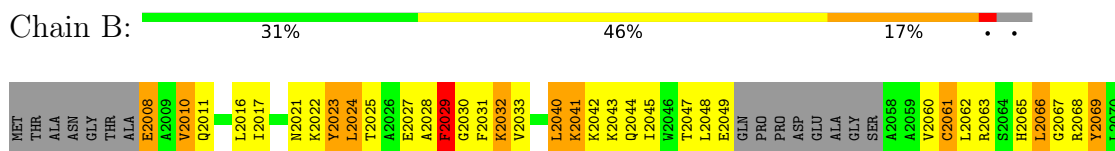
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: FASCIN



A2071	V2147	L2214	MET	T2345	Y2411	A2475
A2072	T2148	E2215	D2280	T2346	D2412	G2476
K2073	R2149	F2216	L2281	L2347	V2413	V2477
K2150	R2150	R2217	S2282	R2348	F2414	A2482
R2151	R2151	S2218	A2283	N2351	G2415	D2486
V2077	Y2152	G2219	N2284	K2351	L2416	P2487
V2078	S2156	K2220	Q2285	F2354	E2417	A2488
E2081	A2157	V2221	E2288	V2355	N2418	S2489
R2082	R2158	R2224	T2289	T2356	N2419	Y2493
P2085	P2159	D2225	D2290	S2357	D2420	
G2086	A2160	C2226	Q2291	K2358	G2421	
R2090	E2161	G2227	E2292	K2359	A2422	
L2093	E2162	G2228	F2293	N2360		
V2094	L2163	R2229	F2294	G2361	I2425	
A2095	A2164	Y2230	L2296	Q2362	K2426	
H2096	D2166	L2231	L2296	L2363	D2427	
D2097	R2167	A2232		A2364	S2428	
D2098	D2168	P2233	D2299	A2365	T2429	
G2099	D2169	S2234	R2300	S2366	G2430	
R2100	V2169	G2235	D2301	V2367	K2431	
V2101	P2170	G2236	T2302	E2368	W2432	
S2102	W2171	S2237	K2303	T2369	W2433	
L2103	G2172	G2238	K2304	A2370	T2434	
Q2104	V2173	T2239		G2371	V2435	
H2108	D2174	L2240	R2308	D2372	G2436	
R2109	S2175	G2243	T2309	S2373	S2437	
R2110	T2178	K2244	H2310	E2374	D2438	
Y2111	Q2182	V2248	T2311	L2375	S2439	
T2115	D2183	D2251	Q2312	F2376	T2442	
D2116	R2185	E2252	K2313	L2377	S2443	
D2117	R2186	L2253	W2314	W2378	S2444	
S2120	S2187	F2254	T2315	K2379	G2445	
V2126	V2188	A2255	L2316	L2380	G2446	
S2127	Q2189	L2256	T2317	T2381	D2447	
P2128	T2190	E2257	T2318	N2382	T2447	
A2129	A2191	Q2258	A2319	R2383	P2448	
E2130	D2192	S2259	T2320	P2384	V2449	
K2131	H2193	C2260	G2321	T2385	D2450	
W2132	R2197	A2261	G2322	L2386	F2451	
S2133	H2198	Q2262	D2326	V2387	F2452	
V2134	D2199	V2264	K2330	F2388	F2453	
H2135	L2202	L2265	N2331	R2389	E2454	
T2136	L2202	A2267	A2332	G2390	F2455	
A2137	V2203	R2268	S2333	E2391	C2456	
R2205	A2204	E2270	C2334	F2394	D2457	
P2206	R2206	R2271	D2337	I2395	Y2458	
E2207	E2207	N2272	I2338	L2396	N2459	
P2208	P2208	V2273	E2339	G2396		
Q2141	A2209	S2274	W2340	C2397	A2462	
V2142	T2210	T2275	R2341	R2398	I2463	
Y2145	G2211	ARG	D2342	K2399	K2464	
S2146	Y2212	GLN	R2343	V2400	V2465	
		GLY	R2344	T2401	V2469	
				L2404	Y2470	
				D2405	K2471	
				A2406	G2472	
				N2407	D2473	
				R2408	H2474	

4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	7427	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.18	7/3793 (0.2%)	1.37	33/5126 (0.6%)
1	B	1.18	6/3788 (0.2%)	1.36	39/5119 (0.8%)
All	All	1.18	13/7581 (0.2%)	1.36	72/10245 (0.7%)

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

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1386	ILE	CA-CB	6.74	1.64	1.54
1	A	1060	VAL	CA-CB	6.36	1.63	1.54
1	B	2386	ILE	CA-CB	6.24	1.64	1.54
1	A	1139	HIS	C-N	-6.11	1.28	1.34
1	A	1183	ASP	CA-C	-5.94	1.46	1.53

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1387	VAL	N-CA-C	-9.18	95.70	108.27
1	A	1486	ASP	N-CA-C	-8.48	100.52	108.07
1	B	2263	VAL	N-CA-C	7.98	120.45	108.80
1	B	2028	ALA	N-CA-C	-7.73	103.73	113.01
1	A	1028	ALA	N-CA-C	-7.68	103.80	113.01

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 [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	3716	0	3599	352	1
1	B	3711	0	3597	357	1
All	All	7427	0	7196	709	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 48.

The worst 5 of 709 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 [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	469/493 (95%)	390 (83%)	61 (13%)	18 (4%)	2	10
1	B	468/493 (95%)	390 (83%)	59 (13%)	19 (4%)	2	9
All	All	937/986 (95%)	780 (83%)	120 (13%)	37 (4%)	2	10

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 [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	391/404 (97%)	311 (80%)	80 (20%)	1	4
1	B	391/404 (97%)	307 (78%)	84 (22%)	1	3
All	All	782/808 (97%)	618 (79%)	164 (21%)	1	4

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2205	ARG

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Mol	Chain	Res	Type
1	B	2375	LEU
1	B	2240	LEU
1	B	2303	LYS
1	B	2404	LEU

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

Mol	Chain	Res	Type
1	B	2189	GLN
1	B	2324	GLN
1	B	2424	ASN
1	B	2415	GLN
1	A	1392	HIS

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 oligosaccharides 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 [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.