



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:09 AM GMT

PDB ID : 2FUN  
Title : alternative p35-caspase-8 complex  
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Deposited on : 2006-01-27  
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

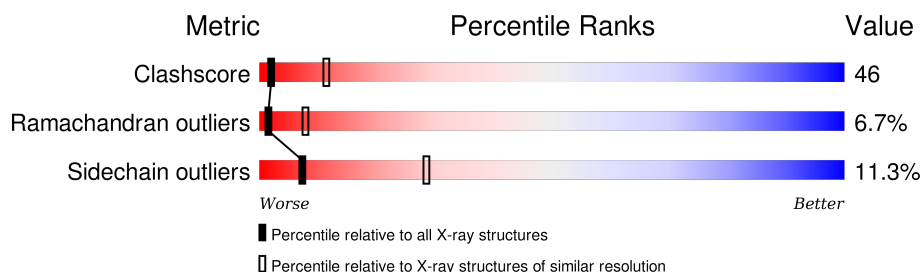
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

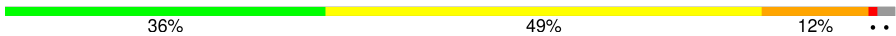
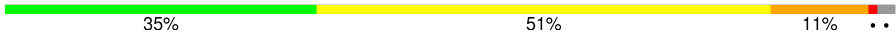
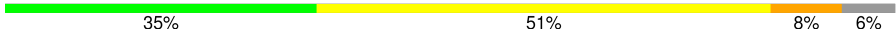

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	298	 36% 49% 12% ..
1	C	298	 35% 51% 11% ..
2	B	258	 35% 51% 8% 6%
2	D	258	 28% 51% 14% 7%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8713 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 Early 35 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2406	1541	393	461	11			
1	C	293	Total	C	N	O	S	0	0	0
			2406	1541	393	461	11			

- Molecule 2 is a protein called caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1945	1228	333	368	16			
2	D	241	Total	C	N	O	S	0	0	0
			1930	1221	331	362	16			

- Molecule 3 is water.

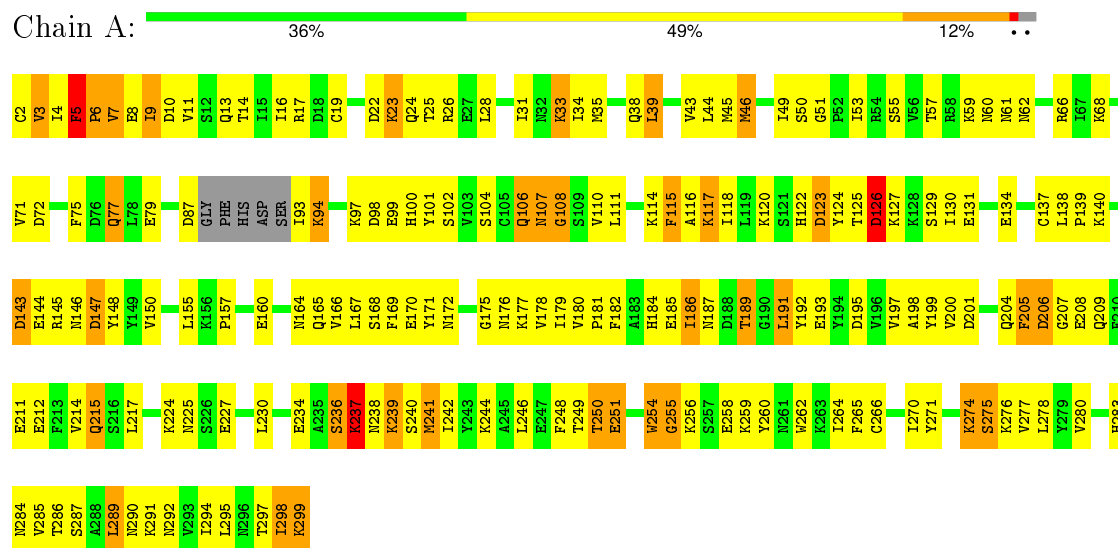
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	4	Total	O	0	0
			4	4		
3	C	9	Total	O	0	0
			9	9		
3	D	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

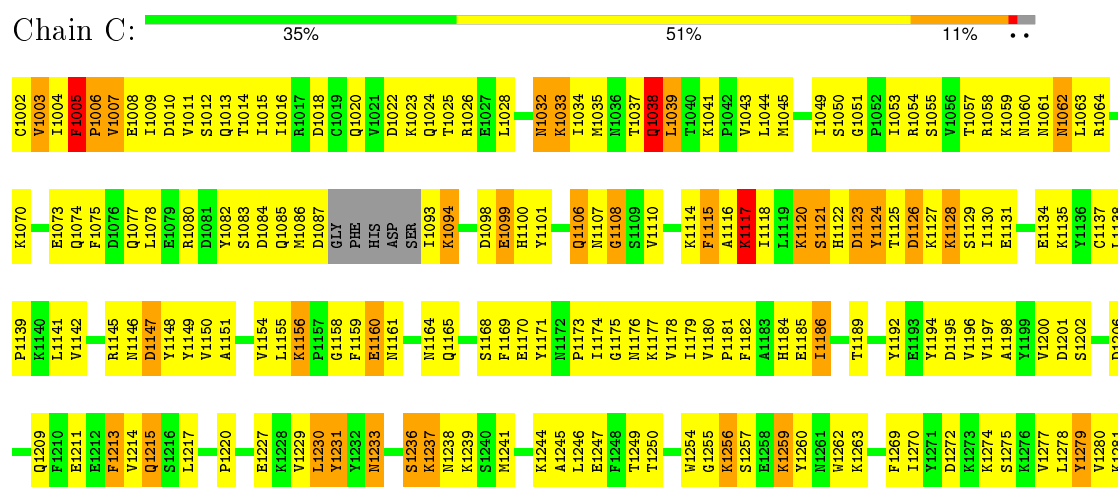
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Early 35 kDa protein



- Molecule 1: Early 35 kDa protein



L1282  
H1283  
M1284  
N1290  
K1291  
N1292  
L1295  
I1298  
K1298

• Molecule 2: caspase-8

Chain B: 35% 51% 8% 6%

L2222 D2223 R2224 V2225 V2226 Q2227 L2228 K2229 S2230 K2231 P2232 R2233 Q2234 Y2235 C2236 L2237 L2238 L2239 N2240 N2241 H2242 H2243 F2244 A2245 K2246 A2247 R2248 R2249 K2250 V2251 P2252 K2253 L2254 H2255 S2256 I2257 R2258 D2259 T2263 H2264 L2265 D2266 A2267 G2268 A2269 L2270 T2271 F2274 E2275 E2276 F2279 F2280 I2281 P2282 K2283 H2284  
H2285 T2288 V2289 R2290 Q2291 L2292 Y2293 E2294 L2295 L2296 K2297 L2298 Y2299 M2302 D2303 L2304 S2305 N2306 P2307 D2308 N2309 L2314 L2315 S2316 R2317 K2318 V2319 K2320 C2321 I2322 I2323 T2326 D2327 G2328 Q2329 E2330 A2331 P2332 P2333 Y2334 E2335 L2336 T2337 S2338 Q2339 F2340 R2344 S2347 I2357 Q2358 A2359 Q2361 Q2362 D2363 Q2366 I2369 P2370 V2371 E2372 T2373 D2374 SER L2375 GLU GLU GLN PRD TYR LEU MET ASP LEU SER SER PRD GLN T2390 R2391 P2394 A2397 D2398 P2399 L2400 L2401 G2402 N2403 A2404 V2406 P2407 L2408 C2409 V2410 S2411 Y2412 R2413 N2414 E2417 G2418 T2419 W2420 Y2421 I2422 L2425 C2426 Q2427  
S2428 L2429 R2430 E2431 R2432 C2433 P2434 D2438 L2439 L2440 T2441 L2442 E2445 E2446 N2447 Y2448 D2454 D2455 K2456 K2457 N2458 Q2460 Q2461 Q2462 N2463 P2464 Q2465 F2468 T2469 L2470 R2471 K2472 L2473 L2474 V2475 P2476 P2477 S2478 D2479

• Molecule 2: caspase-8

Chain D: 28% 51% 14% 7%

L3222 D3223 K3224 V3225 V3226 Q3227 L3228 K3229 S3230 K3231 P3232 R3233 G3234 Y3235 C3236 L3237 L3238 L3239 N3240 N3241 H3242 A3245 K3246 A3247 R3248 E3249 K3250 V3251 P3252 K3253 L3254 H3255 S3256 I3257 R3260 N3261 G3262 T3263 H3264 L3265 D3266 A3267 G3268 A3269 L3270 T3271 T3272 T3273 F3274 E3275 E3276 L3277 H3278 F3279 E3280 I3281 K3282 P3283  
H3284 H3285 K3286 C3287 T3288 V3289 E3290 Q3291 L3292 E3293 L3294 L3295 R3296 K3297 L3298 Y3299 Q3300 H3304 S3305 N3306 K3307 D3308 C3309 G3313 I3314 L3315 K3316 S3317 K3320 G3321 L3322 S3323 Y3324 T3326 D3327 G3328 Q3329 L3330 A3331 P3332 I3333 E3334 E3335 G3402 L3403 T3404 L3405 K3406 K3407 C3408 S3409 V3410 S3411 R3412 R3413 N3414  
V3354 F3355 F3356 L3357 K3358 L3359 C3360 Q3361 L3362 D3363 L3364 V3365 Q3366 K3367 G3368 L3369 P3370 V3371 E3372 T3373 D3374 SER GLU GLU GLN PRD TYR LEU MET ASP LEU SER SER PRD GLN T3390 R3391 T3392 L3393 P3394 D3395 D3398 F3399 L3401 T3403 L3404 V3405 V3406 N3407 N3408 C3409 V3410 S3411 R3412 R3413 N3414  
E3417 G3418 T3419 K3420 V3421 L3422 L3425 C3426 L3429 R3430 E3431 G3432 L3433 P3434 D3438 L3439 L3442 L3443 T3444 E3445 E3446 N3447 Y3448 E3449 V3450 S3451 N3452 K3453 K3456 K3457 N3458 K3459 G3460 K3461 Q3462 N3463 P3464 Q3465 F3468 T3469 L3470 R3471 K3472 K3473 L3474 P3477 SER ASP

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.97Å 117.34Å 346.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (24.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	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	0.40	0/2454	0.65	0/3307
1	C	0.40	0/2454	0.66	0/3307
2	B	0.37	0/1987	0.60	0/2682
2	D	0.34	0/1972	0.56	0/2663
All	All	0.38	0/8867	0.62	0/11959

There are no bond length outliers.

There are no bond angle outliers.

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	2406	0	2389	219	0
1	C	2406	0	2389	210	0
2	B	1945	0	1915	168	0
2	D	1930	0	1906	211	0
3	A	10	0	0	3	0
3	B	4	0	0	2	0
3	C	9	0	0	3	0
3	D	3	0	0	1	0
All	All	8713	0	8599	796	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 46.

The worst 5 of 796 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:C:1039:LEU:HD12	1:C:1043:VAL:HG21	1.33	1.10
2:D:3273:THR:HG23	2:D:3430:ARG:HB3	1.32	1.10
2:B:2231:LYS:HB2	2:B:2232:PRO:HD3	1.34	1.08
2:D:3393:ILE:HG12	2:D:3471:ARG:HH22	1.13	1.07
1:A:104:SER:HB2	1:A:120:LYS:HD2	1.36	1.07

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	289/298 (97%)	218 (75%)	44 (15%)	27 (9%)	1	4
1	C	289/298 (97%)	221 (76%)	45 (16%)	23 (8%)	1	5
2	B	239/258 (93%)	193 (81%)	36 (15%)	10 (4%)	3	20
2	D	237/258 (92%)	181 (76%)	45 (19%)	11 (5%)	3	18
All	All	1054/1112 (95%)	813 (77%)	170 (16%)	71 (7%)	1	8

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	94	LYS
1	A	108	GLY
1	A	115	PHE
1	A	126	ASP



### 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	276/280 (99%)	252 (91%)	24 (9%)	13	43
1	C	276/280 (99%)	245 (89%)	31 (11%)	7	29
2	B	218/233 (94%)	198 (91%)	20 (9%)	11	40
2	D	216/233 (93%)	180 (83%)	36 (17%)	3	13
All	All	986/1026 (96%)	875 (89%)	111 (11%)	7	28

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1057	THR
1	C	1160	GLU
2	D	3417	GLU
1	C	1062	ASN
1	C	1120	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2407	ASN
2	B	2465	GLN
2	D	3361	GLN
2	B	2414	ASN
2	B	2447	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](#)

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.