



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 01:49 AM UTC

PDB ID : 1U5I / pdb_00001u5i
Title : Crystal Structure analysis of rat m-calpain mutant Lys10 Thr
Authors : Hosfield, C.M.; Pal, G.P.; Elce, J.S.; Jia, Z.
Deposited on : 2004-07-27
Resolution : 2.86 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 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
Xtriage (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

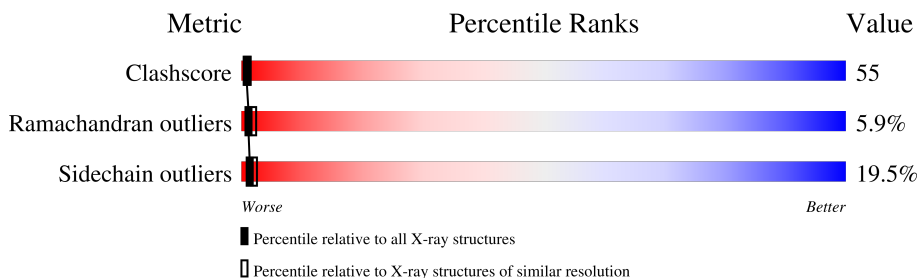
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

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	700	
2	B	184	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6706 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 Calpain 2, large [catalytic] subunit precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4980	3176	836	945	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	THR	LYS	engineered mutation	UNP Q07009
A	105	SER	CYS	engineered mutation	UNP Q07009

- Molecule 2 is a protein called Calpain small subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1427	897	246	274	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q64537

- Molecule 3 is water.

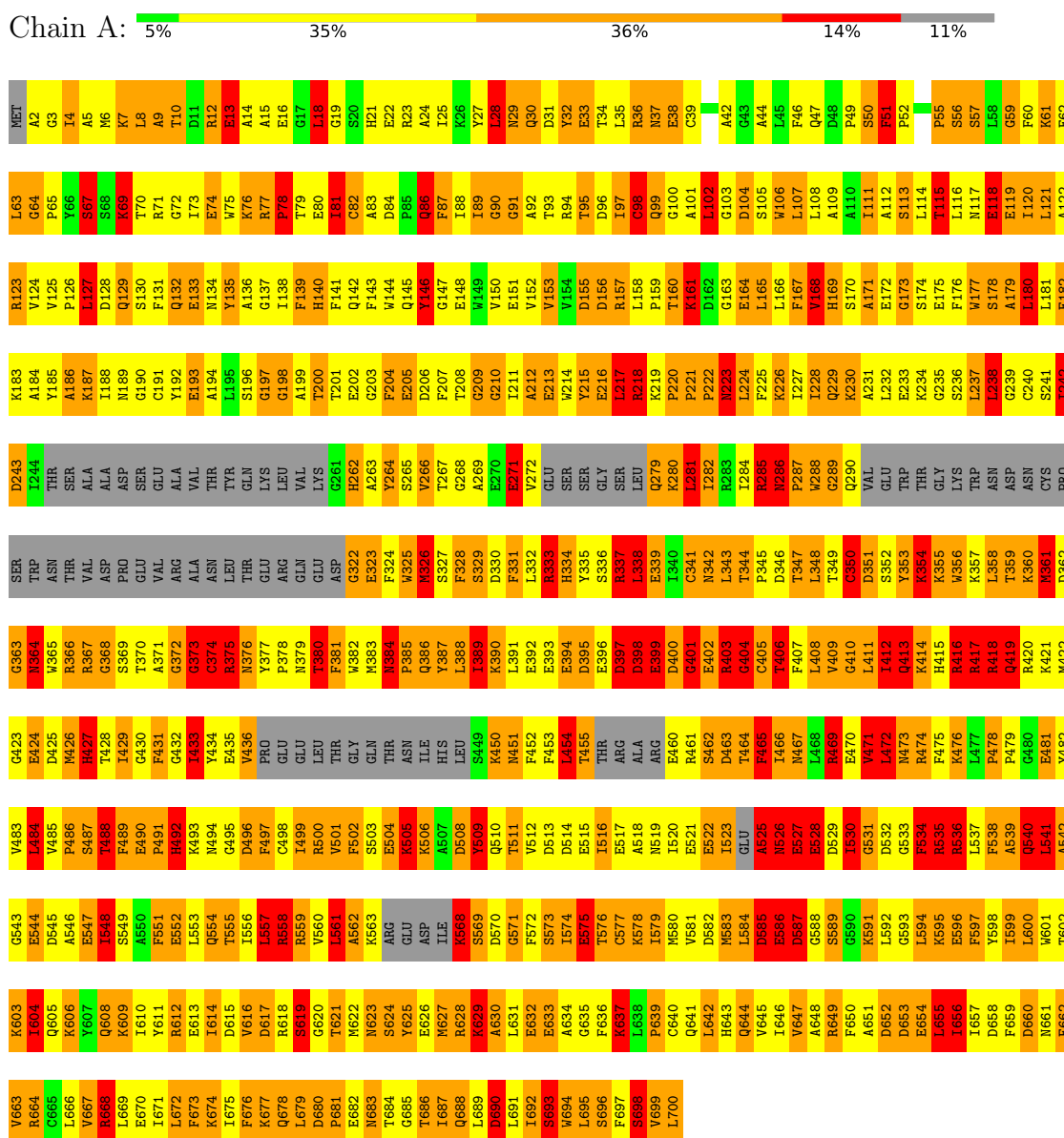
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	52	Total	O	0	0
			52	52		

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: Calpain 2, large [catalytic] subunit precursor



- Molecule 2: Calpain small subunit 1

T181	L121	R61
M182	N122	S62
Y183	Q123	M63
S184	H124	V64
	I125	A65
	Y126	V66
	S127	M67
	M128	S69
	I130	D70
	R131	T71
	R132	T72
	Y133	G73
	S134	K74
	D135	L75
	E136	G76
	T137	F77
	G138	E78
	M139	E79
	M140	F80
	D141	K81
	F142	X82
	D143	L83
	M144	B84
	F145	N85
	I146	M86
	S147	I87
	G148	K88
	L149	K89
	V150	W90
	R151	Q91
	L152	G92
	D153	I93
	A154	Y94
	M155	K95
	F156	B96
	R157	F97
	A158	N98
	F159	T99
	R160	D100
	S161	I101
	L162	S102
	D163	G103
	K164	T104
	N165	I105
	G166	G106
	T167	S107
	G168	I108
	Q169	E109
	T170	L110
	Q171	P111
	V172	G112
	N173	A113
	T174	F114
	Q175	E115
	E176	A116
	T177	A117
	L178	G118
	Q179	F119
	T180	H120

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.66Å 156.52Å 64.23Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	25.00 – 2.86	Depositor
% Data completeness (in resolution range)	90.1 (25.00-2.86)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6706	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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	3.80	789/5083 (15.5%)	2.62	381/6854 (5.6%)
2	B	3.42	189/1454 (13.0%)	2.42	90/1955 (4.6%)
All	All	3.72	978/6537 (15.0%)	2.57	471/8809 (5.3%)

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	19
2	B	0	2
All	All	0	21

The worst 5 of 978 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ASP	C-N	38.72	1.90	1.33
1	A	402	GLU	C-N	38.24	1.87	1.33
1	A	521	GLU	C-N	24.21	1.64	1.33
1	A	527	GLU	C-N	-22.08	1.02	1.33
1	A	522	GLU	C-N	21.55	1.58	1.33

The worst 5 of 471 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ILE	CA-C-O	26.97	152.56	120.74
1	A	400	ASP	CA-C-N	-24.90	72.61	121.41
1	A	400	ASP	C-N-CA	-24.90	72.61	121.41
1	A	400	ASP	O-C-N	19.55	147.06	122.43
1	A	399	GLU	CA-C-N	18.92	156.13	122.64

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	18	LEU	Mainchain
1	A	197	GLY	Peptide
1	A	9	ALA	Mainchain
1	A	98	CYS	Mainchain

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	4980	0	4809	539	10
2	B	1427	0	1375	167	9
3	A	247	0	0	67	0
3	B	52	0	0	23	0
All	All	6706	0	6184	697	10

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 55.

The worst 5 of 697 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:218:ARG:CG	1:A:218:ARG:CB	1.74	1.66
1:A:409:VAL:CB	1:A:409:VAL:CG1	1.76	1.64
1:A:628:ARG:CD	1:A:628:ARG:CG	1.76	1.63
1:A:699:VAL:CB	1:A:699:VAL:CG1	1.77	1.62
1:A:455:THR:CB	1:A:455:THR:CG2	1.80	1.60

The worst 5 of 10 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:527:GLU:OE1	2:B:19:LYS:CE[1_554]	0.67	1.53
1:A:527:GLU:CD	2:B:19:LYS:CE[1_554]	0.84	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLU:CD	2:B:19:LYS:NZ[1_554]	1.15	1.05
1:A:527:GLU:OE1	2:B:19:LYS:CD[1_554]	1.29	0.91
1:A:527:GLU:OE2	2:B:19:LYS:NZ[1_554]	1.33	0.87

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	609/700 (87%)	506 (83%)	70 (12%)	33 (5%)	1	2
2	B	174/184 (95%)	130 (75%)	31 (18%)	13 (8%)	1	1
All	All	783/884 (89%)	636 (81%)	101 (13%)	46 (6%)	1	2

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	351	ASP
1	A	354	LYS
1	A	373	GLY
1	A	399	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	522/603 (87%)	417 (80%)	105 (20%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	155/162 (96%)	128 (83%)	27 (17%)	2	3
All	All	677/765 (88%)	545 (80%)	132 (20%)	1	2

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	36	LEU
2	B	91	GLN
2	B	148	CYS
1	A	388	LEU
1	A	380	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
2	B	139	ASN
1	A	451	ASN
2	B	23	GLN
1	A	419	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	400:ASP	C	401:GLY	N	1.90
1	A	402:GLU	C	403:ARG	N	1.87
1	A	521:GLU	C	522:GLU	N	1.64
1	A	401:GLY	C	402:GLU	N	1.15
1	A	527:GLU	C	528:GLU	N	1.02

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.