wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 08:44 pm BST

PDB ID	:	1KFU
Title	:	Crystal Structure of Human m-Calpain Form II
Authors	:	Strobl, S.; Fernandez-Catalan, C.; Braun, M.; Huber, R.; Masumoto, H.; Nakagawa, K.; Irie, A.; Sorimachi, H.; Bourenkow, G.; Bartunik, H.; Suzuki, K.; Bode, W.
Deposited on	:	2001-11-23
Resolution	:	2.50 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:

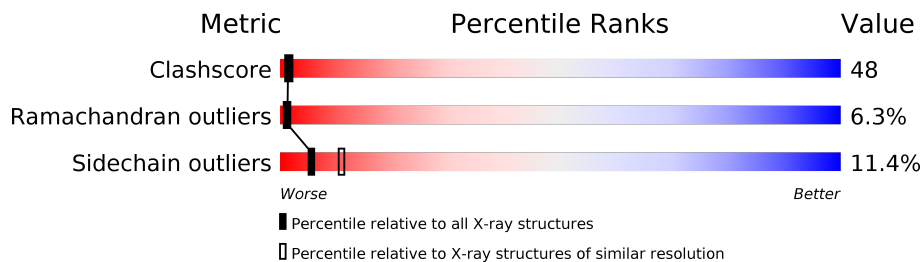|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Clashscore		48
Ramachandran outliers		6.3%
Sidechain outliers		11.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	L	699	34% 52% 12% •
2	S	184	40% 53% 7% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7530 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 M-CALPAIN LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	699	Total	C	N	O	S	0	0	0
			5628	3568	955	1079	26			

- Molecule 2 is a protein called M-CALPAIN SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	184	Total	C	N	O	S	10	0	0
			1491	935	255	290	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	287	Total	O	0	0
			287	287		
3	S	124	Total	O	0	0
			124	124		

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: M-CALPAIN LARGE SUBUNIT

• Molecule 2: M-CALPAIN SMALL SUBUNIT

Chain S:

40%　　　　　　　　　　　　　　53%　　　　　　　　　7%　　·
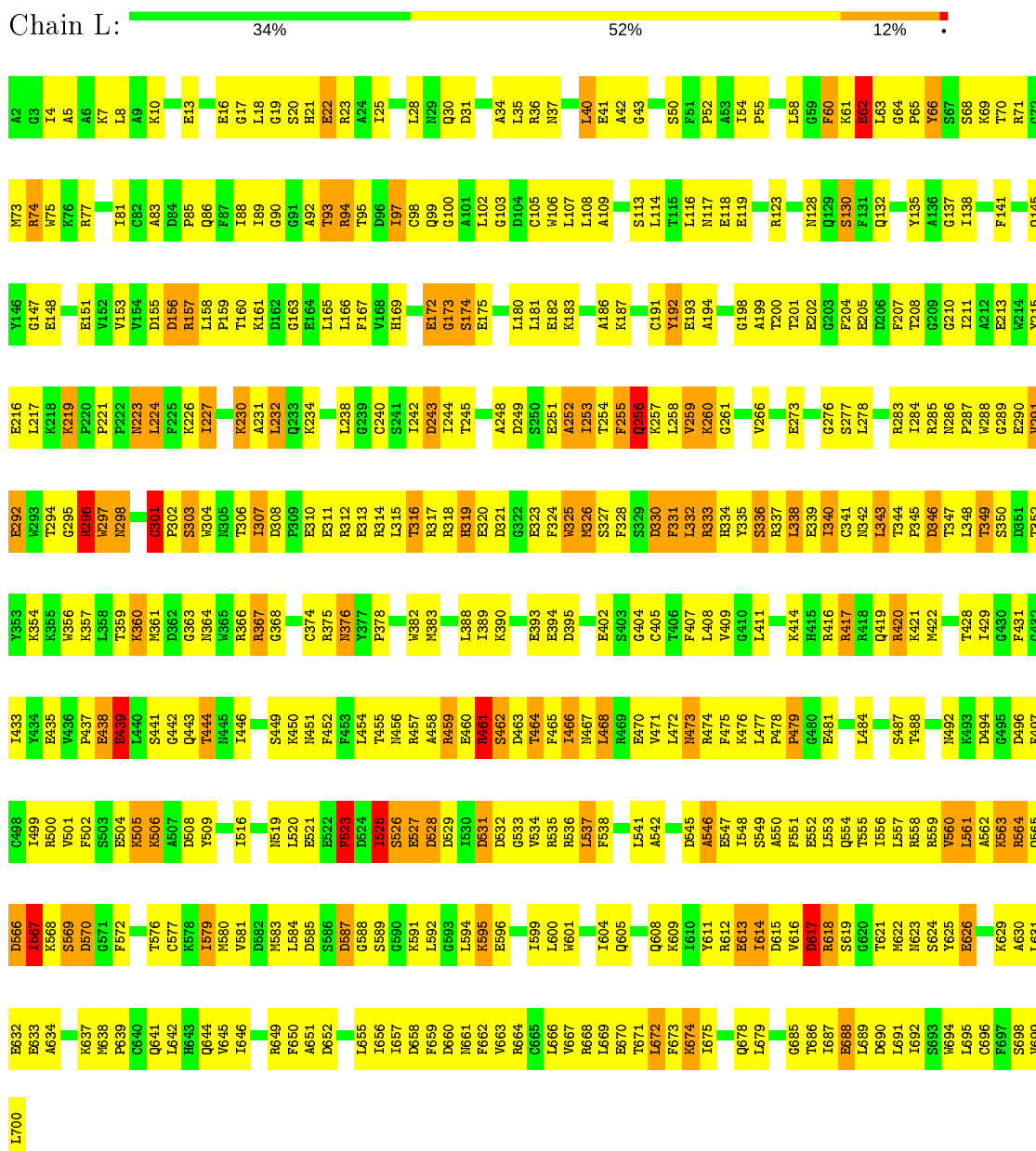
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.88Å 169.84Å 64.44Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7530	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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	L	0.64	5/5752 (0.1%)	0.83	8/7768 (0.1%)
2	S	0.58	2/1520 (0.1%)	0.73	1/2046 (0.0%)
All	All	0.63	7/7272 (0.1%)	0.81	9/9814 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	696	CYS	CB-SG	8.07	1.96	1.82
1	L	301	CYS	CB-SG	-7.64	1.69	1.82
2	S	968	SER	C-O	6.41	1.35	1.23
2	S	968	SER	C-OXT	6.00	1.34	1.23
1	L	62	GLU	C-N	-5.92	1.20	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	968	SER	CA-C-O	7.14	135.09	120.10
1	L	459	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	L	62	GLU	C-N-CA	6.71	138.47	121.70
1	L	461	ARG	NE-CZ-NH2	6.37	123.49	120.30
1	L	326	MET	CG-SD-CE	6.25	110.20	100.20

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	L	5628	0	5466	563	0
2	S	1491	0	1423	135	0
3	L	287	0	0	21	0
3	S	124	0	0	10	0
All	All	7530	0	6889	668	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 48.

The worst 5 of 668 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:L:248:ALA:O	1:L:259:VAL:HG12	1.36	1.21
1:L:525:ILE:HG22	1:L:595:LYS:HD2	1.27	1.17
1:L:61:LYS:H	1:L:64:GLY:HA3	1.05	1.11
2:S:869:ASN:HA	2:S:872:LYS:HE2	1.24	1.10
1:L:74:ARG:HD2	1:L:74:ARG:H	1.10	1.09

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	L	697/699 (100%)	546 (78%)	103 (15%)	48 (7%)	1	1
2	S	182/184 (99%)	157 (86%)	18 (10%)	7 (4%)	3	4
All	All	879/883 (100%)	703 (80%)	121 (14%)	55 (6%)	1	1

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	253	ILE

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Mol	Chain	Res	Type
1	L	256	GLN
1	L	296	ARG
1	L	298	ASN
1	L	301	CYS

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	L	602/602 (100%)	528 (88%)	74 (12%)	4	9
2	S	162/162 (100%)	149 (92%)	13 (8%)	12	23
All	All	764/764 (100%)	677 (89%)	87 (11%)	5	11

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	346	ASP
1	L	468	LEU
2	S	837	ASP
1	L	360	LYS
1	L	420	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	364	ASN
1	L	492	ASN
2	S	911	ASN
1	L	415	HIS
1	L	419	GLN

5.3.3 RNA ⓘ

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	62:GLU	C	63:LEU	N	1.20

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.