wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:28 PM GMT

PDB ID	:	1KFX
Title	:	Crystal Structure of Human m-Calpain Form I
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Deposited on	:	2001-11-23
Resolution	:	3.15 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
http://wwpdb.org/validation/2016/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:

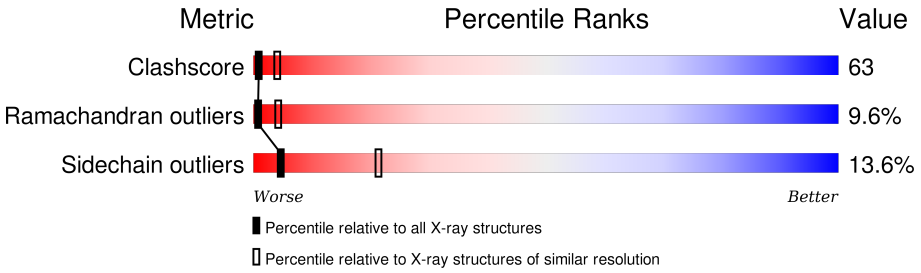
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)

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 <=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	L	699	23% 51% 16% • 8%
2	S	184	33% 52% 11% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6826 atoms, of which 1 is hydrogen 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	640	Total	C	H	N	O	S	209	0	0
			5156	3284	1	873	973	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	176	Total	C	N	O	S	47	0	0
			1426	895	244	276	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	197	Total	O	0	0
			197	197		
3	S	47	Total	O	0	0
			47	47		

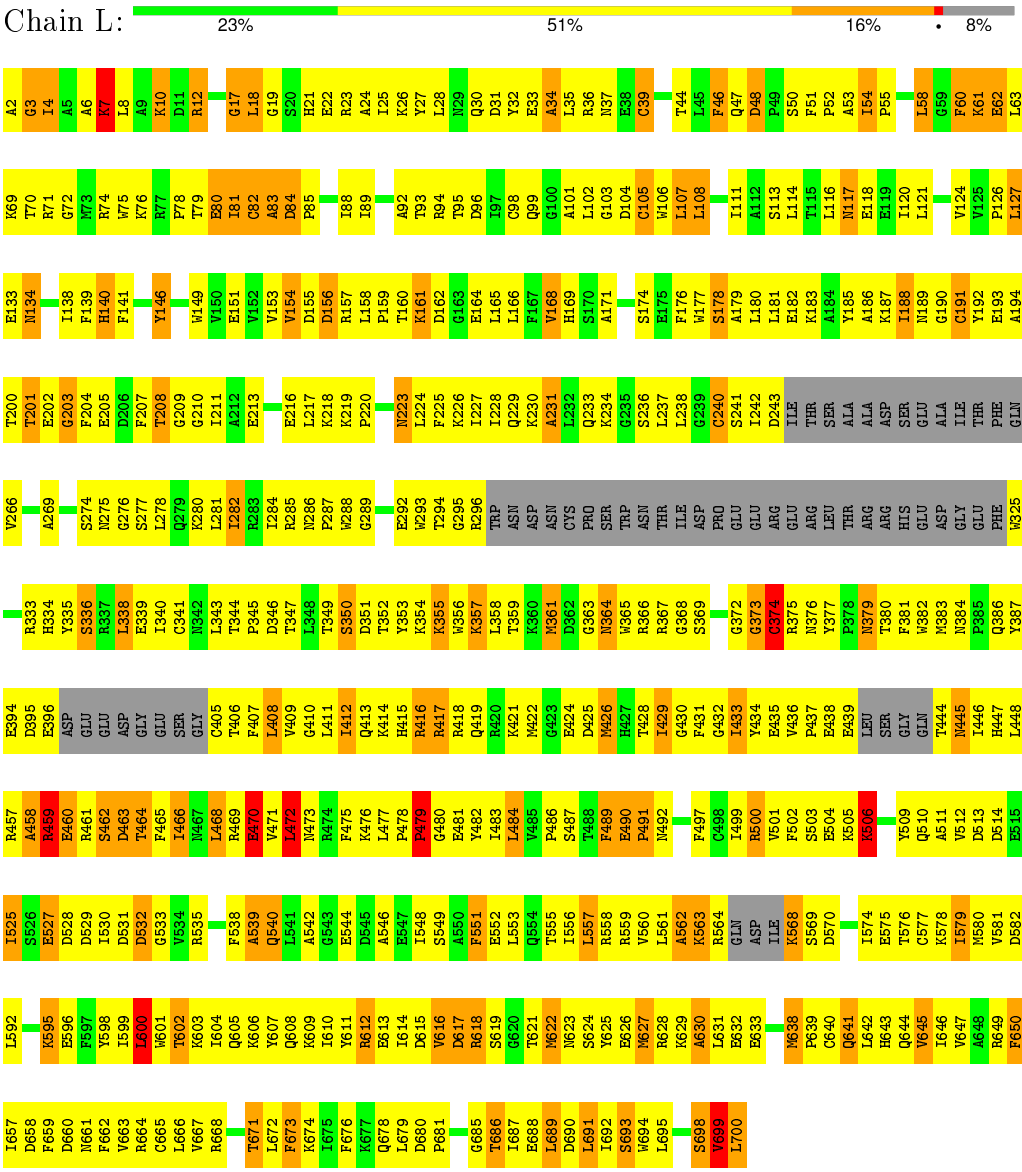
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

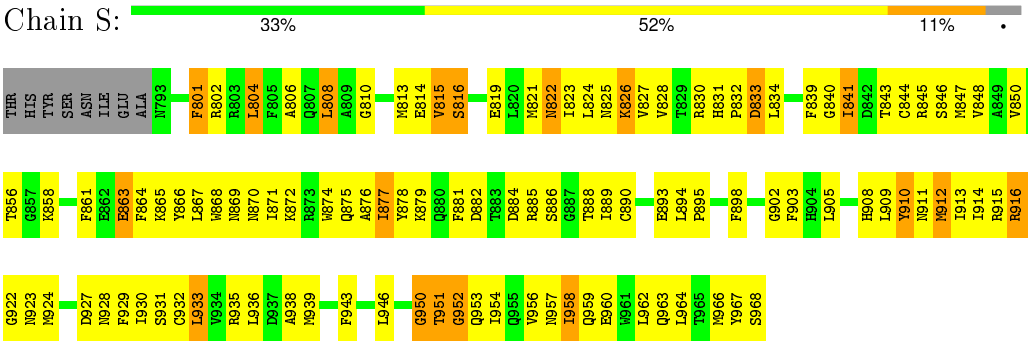
- Molecule 1: M-CALPAIN LARGE SUBUNIT

Chain L:



- Molecule 2: M-CALPAIN SMALL SUBUNIT

Chain S:


33%
52%
11%
THR HIS TYR SER ASN ILE GLU ALA N793 F801 R802 R803 L804 F805 A806 Q807 L808 A809 G810 M813 E814 V815 S816 E819 L820 M821 N822 I823 L824 N825 K826 V827 V828 T829 R830 H831 P832 D833 L834 F839 G840 I841 D842 T843 C844 R845 S846 M847 V848 A849 V850 M851 D852 S853 D854 T855 T856 G857 K858 F861 E862 E863 F864 K865 Y866 L867 W868 N869 N870 I871 K872 R873 W874 Q875 A876 I877 Y878 K879 Q880 F881 D882 T883 D884 R885 S886 G887 T888 I889 C890 E893 L894 P895 F898 G902 F903 H904 L905 H908 L909 Y910 N911 M912 I913 I914 R915 R916 Y917 S918 D919 E920 S921 G922 N923 M924 D927 N928 F929 I930 S931 C932 L933 Y934 R935 L936 D937 A938 M939 F943 L946 G950 T951 G952 Q953 I954 Q955 V956 N957 I958 Q959 E960 W961 L962 Q963 L964 T965 M966 Y967 S968

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.78Å 133.25Å 77.53Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-3.15)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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	L	0.55	1/5265 (0.0%)	0.79	5/7099 (0.1%)
2	S	0.51	0/1453	0.72	0/1954
All	All	0.54	1/6718 (0.0%)	0.77	5/9053 (0.1%)

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
2	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	700	LEU	C-O	-6.97	1.10	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	612	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	L	472	LEU	CA-CB-CG	6.17	129.48	115.30
1	L	107	LEU	CA-CB-CG	5.36	127.63	115.30
1	L	650	PHE	N-CA-C	5.09	124.75	111.00
1	L	60	PHE	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	917	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	L	5155	1	5044	659	0
2	S	1426	0	1367	143	0
3	L	197	0	0	3	0
3	S	47	0	0	1	0
All	All	6825	1	6411	783	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 63.

The worst 5 of 783 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:638:MET:HG3	1:L:643:HIS:NE2	1.66	1.09
1:L:99:GLN:OE1	1:L:103:GLY:HA3	1.56	1.05
1:L:361:MET:HB2	1:L:509:TYR:CE1	1.93	1.04
1:L:4:ILE:HD13	1:L:4:ILE:H	1.23	1.00
2:S:877:ILE:H	2:S:877:ILE:HD12	1.29	0.98

There are no symmetry-related clashes.

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	L	628/699 (90%)	416 (66%)	149 (24%)	63 (10%)	1 4
2	S	174/184 (95%)	132 (76%)	28 (16%)	14 (8%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	802/883 (91%)	548 (68%)	177 (22%)	77 (10%)	1 4

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	34	ALA
1	L	61	LYS
1	L	62	GLU
1	L	82	CYS
1	L	83	ALA

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	L	550/602 (91%)	467 (85%)	83 (15%)	3 17
2	S	155/162 (96%)	142 (92%)	13 (8%)	14 47
All	All	705/764 (92%)	609 (86%)	96 (14%)	5 21

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	426	MET
1	L	479	PRO
2	S	822	ASN
1	L	429	ILE
1	L	466	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	379	ASN
1	L	519	ASN
2	S	955	GLN

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Mol	Chain	Res	Type
1	L	384	ASN
1	L	492	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.