wwPDB X-ray Structure Validation Summary Report (i)

Jan 23, 2018 – 09:22 PM EST

PDB ID	:	1DF0
Title	:	Crystal structure of M-Calpain
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Deposited on	:	1999-11-16
Resolution	:	2.60 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 2.60 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.
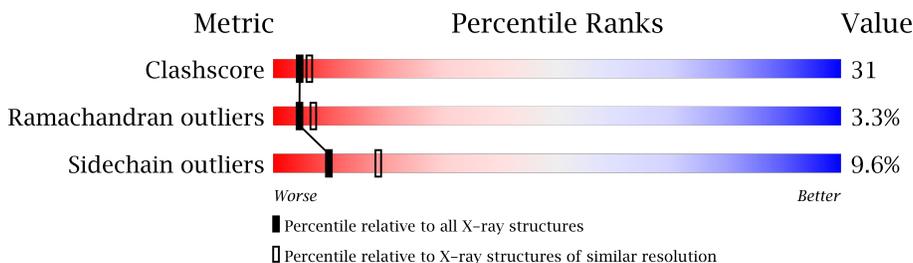
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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	A	700	44% 37% 7% 11%
2	B	184	58% 32% 5% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6749 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			4964	3169	833	939	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	ENGINEERED	UNP Q07009

- Molecule 2 is a protein called CALPAIN.

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	300	Total	O	0	0
			300	300		
3	B	58	Total	O	0	0
			58	58		

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 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
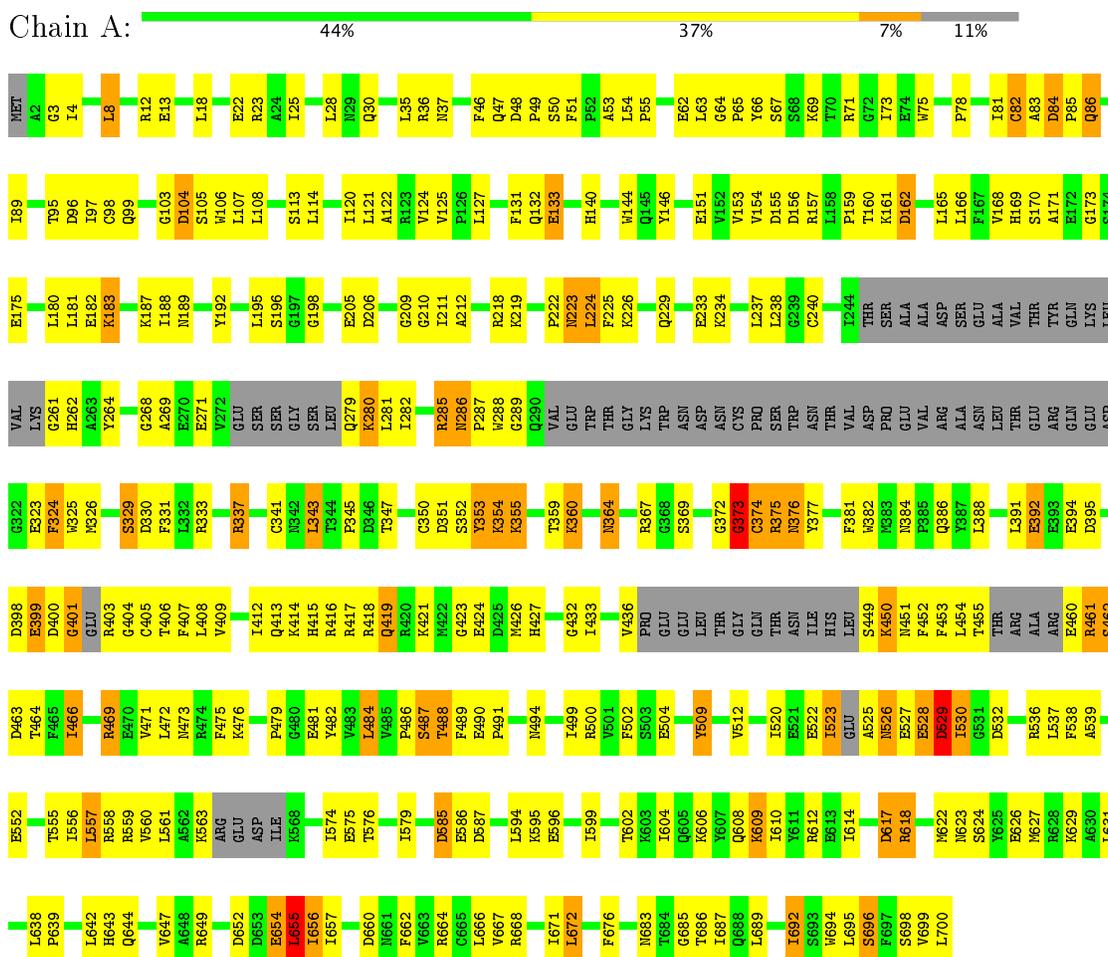
- Molecule 2: CALPAIN
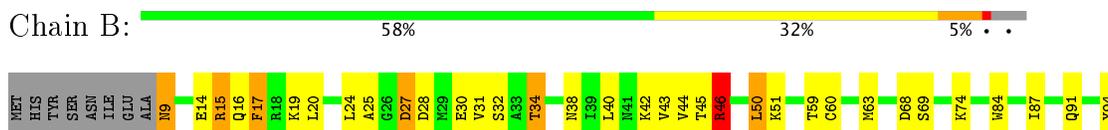
K95 R96 T99 D100 R101 S102 G103 L110 P111 E115 H120 I125 Y126 S127 M128 I129 I130 R131 R151 L152 M155 F156 F159 R160 D163 K164 N165 G166 T167 G168 Q169 I170 N173 I174 Q175 L178 Q179 L180 T181 M182 Y183 S184

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	Depositor
Cell constants a, b, c, α, β, γ	57.70Å 80.18Å 80.72Å 60.37° 70.85° 79.49°	Depositor
Resolution (Å)	25.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.6 (25.00-2.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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	0.48	0/5070	0.72	3/6841 (0.0%)
2	B	0.54	0/1454	0.73	2/1955 (0.1%)
All	All	0.49	0/6524	0.72	5/8796 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	ASP	N-CA-C	-6.43	93.64	111.00
1	A	373	GLY	N-CA-C	6.43	129.16	113.10
2	B	156	PHE	CB-CG-CD1	-5.46	116.98	120.80
2	B	152	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	289	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	156	PHE	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	4964	0	4807	337	0
2	B	1427	0	1375	77	0
3	A	300	0	0	20	0
3	B	58	0	0	6	0
All	All	6749	0	6182	390	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 31.

The worst 5 of 390 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:281:LEU:HD21	1:A:326:MET:H	1.16	1.08
1:A:281:LEU:HD22	1:A:325:TRP:HE3	1.12	1.06
1:A:523:ILE:H	1:A:523:ILE:HD12	1.23	1.01
1:A:692:ILE:HD12	1:A:692:ILE:H	1.27	0.97
1:A:281:LEU:HD22	1:A:325:TRP:CE3	1.99	0.95

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	612/700 (87%)	528 (86%)	61 (10%)	23 (4%)	4	5
2	B	174/184 (95%)	162 (93%)	9 (5%)	3 (2%)	11	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	786/884 (89%)	690 (88%)	70 (9%)	26 (3%)	4 7

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	133	GLU
1	A	223	ASN
1	A	352	SER
1	A	354	LYS

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	520/603 (86%)	470 (90%)	50 (10%)	10 18
2	B	155/162 (96%)	140 (90%)	15 (10%)	9 18
All	All	675/765 (88%)	610 (90%)	65 (10%)	10 18

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	LYS
1	A	523	ILE
2	B	115	GLU
1	A	466	ILE
1	A	487	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	419	GLN
2	B	91	GLN

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Mol	Chain	Res	Type
1	A	413	GLN
1	A	427	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 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 (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.