



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 02:20 AM GMT

PDB ID : 3BOW
Title : Structure of M-calpain in complex with Calpastatin
Authors : Hanna, R.A.; Campbell, R.L.; Davies, P.L.
Deposited on : 2007-12-17
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

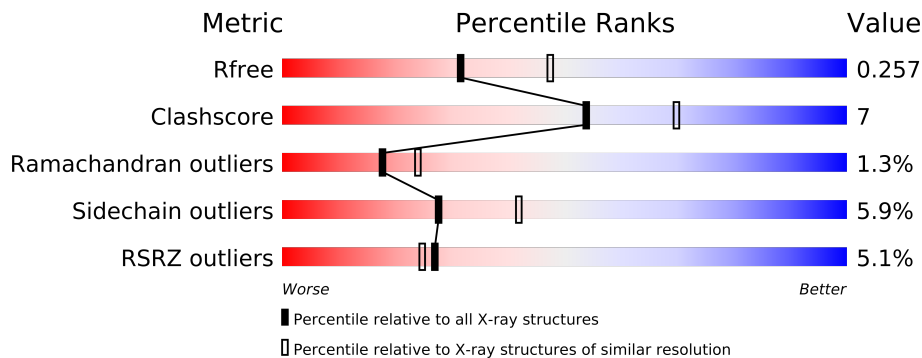
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	714	
2	B	184	
3	C	95	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7587 atoms, of which 0 are hydrogen and 0 are deuterium.

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 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	1	0
			5470	3482	919	1045	24			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	ENGINEERED	UNP Q07009
A	701	GLY	-	EXPRESSION TAG	UNP Q07009
A	702	LYS	-	EXPRESSION TAG	UNP Q07009
A	703	LEU	-	EXPRESSION TAG	UNP Q07009
A	704	ALA	-	EXPRESSION TAG	UNP Q07009
A	705	ALA	-	EXPRESSION TAG	UNP Q07009
A	706	ALA	-	EXPRESSION TAG	UNP Q07009
A	707	LEU	-	EXPRESSION TAG	UNP Q07009
A	708	GLU	-	EXPRESSION TAG	UNP Q07009
A	709	HIS	-	EXPRESSION TAG	UNP Q07009
A	710	HIS	-	EXPRESSION TAG	UNP Q07009
A	711	HIS	-	EXPRESSION TAG	UNP Q07009
A	712	HIS	-	EXPRESSION TAG	UNP Q07009
A	713	HIS	-	EXPRESSION TAG	UNP Q07009
A	714	HIS	-	EXPRESSION TAG	UNP Q07009

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1410	888	243	269	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	MET	-	EXPRESSION TAG	UNP Q64537

- Molecule 3 is a protein called Calpastatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	0	0	0
			521	317	87	117			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	570	MET	-	EXPRESSION TAG	UNP P27321
C	646	PRO	LEU	SEE REMARK 999	UNP P27321

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Ca	0	0
			4	4		
4	A	6	Total	Ca	0	0
			6	6		

- Molecule 5 is water.

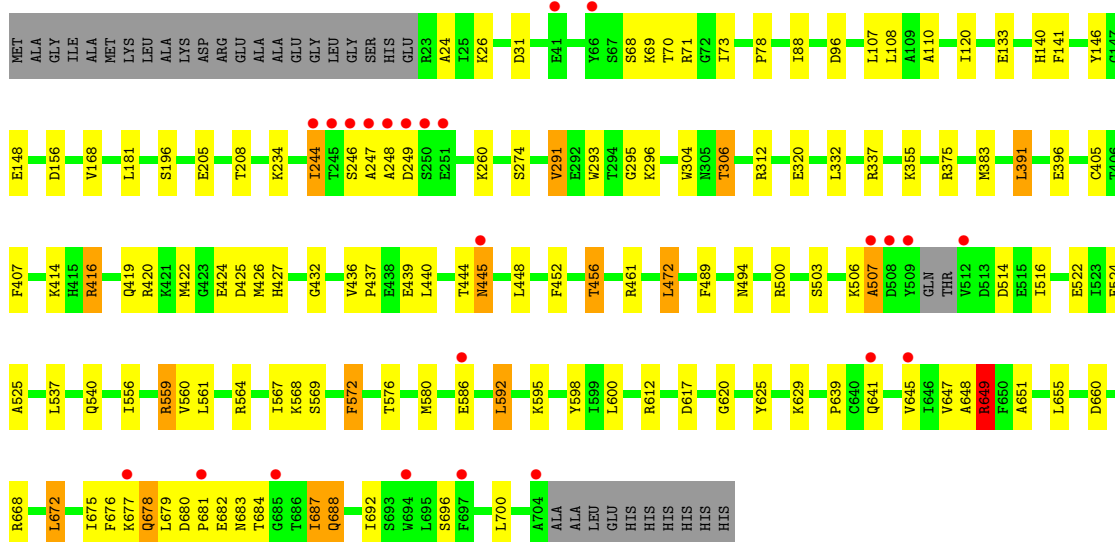
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	15	Total	O	0	0
			15	15		
5	C	9	Total	O	0	0
			9	9		

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.

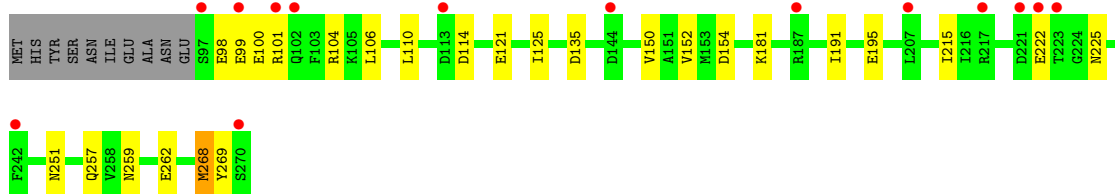
• Molecule 1: Calpain-2 catalytic subunit

Chain A: 



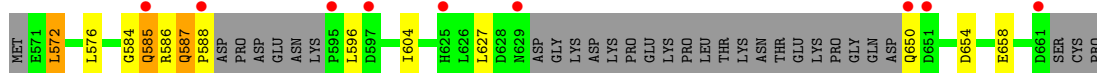
• Molecule 2: Calpain small subunit 1

Chain B: 



• Molecule 3: Calpastatin

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.48Å 66.98Å 108.66Å 90.00° 100.76° 90.00°	Depositor
Resolution (Å)	66.23 – 2.40 66.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (66.23-2.40) 96.5 (66.29-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.258 0.199 , 0.257	Depositor DCC
R_{free} test set	1819 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 22.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36195 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7587	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.49	0/5595	0.63	2/7562 (0.0%)
2	B	0.45	0/1437	0.61	0/1932
3	C	0.36	0/526	0.61	0/707
All	All	0.47	0/7558	0.63	2/10201 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	472	LEU	CA-CB-CG	5.42	127.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5470	0	5312	86	0
2	B	1410	0	1361	17	0
3	C	521	0	490	10	0
4	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
5	A	152	0	0	6	0
5	B	15	0	0	0	0
5	C	9	0	0	0	0
All	All	7587	0	7163	100	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 100 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:587:GLN:HB3	3:C:588:PRO:HA	1.09	1.07
1:A:524:GLU:O	1:A:524:GLU:HG3	1.48	1.05
3:C:587:GLN:HB3	3:C:588:PRO:CA	1.92	0.99
1:A:678:GLN:O	1:A:679:LEU:HB2	1.70	0.91
3:C:587:GLN:CB	3:C:588:PRO:HA	2.01	0.87

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	A	677/714 (95%)	642 (95%)	25 (4%)	10 (2%)	15	20
2	B	172/184 (94%)	164 (95%)	8 (5%)	0	100	100
3	C	59/95 (62%)	55 (93%)	2 (3%)	2 (3%)	6	4
All	All	908/993 (91%)	861 (95%)	35 (4%)	12 (1%)	18	24

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	SER
1	A	678	GLN

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Mol	Chain	Res	Type
1	A	683	ASN
3	C	587	GLN
1	A	248	ALA

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	A	585/613 (95%)	550 (94%)	35 (6%)	27	41
2	B	153/162 (94%)	146 (95%)	7 (5%)	37	55
3	C	60/88 (68%)	55 (92%)	5 (8%)	16	24
All	All	798/863 (92%)	751 (94%)	47 (6%)	28	42

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	540	GLN
1	A	592	LEU
3	C	585	GLN
1	A	561	LEU
1	A	612	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	HIS
1	A	445	ASN
2	B	109	GLN
1	A	415	HIS
1	A	688	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	680/714 (95%)	0.25	24 (3%) 42 40	2, 8, 28, 57	0
2	B	174/184 (94%)	0.63	14 (8%) 12 11	7, 15, 21, 29	0
3	C	65/95 (68%)	0.78	9 (13%) 4 3	2, 7, 16, 17	0
All	All	919/993 (92%)	0.36	47 (5%) 27 25	2, 10, 27, 57	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ALA	6.3
1	A	704	ALA	5.7
1	A	247	ALA	5.5
1	A	507	ALA	5.2
1	A	694	TRP	4.9

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	A	719	1/1	0.13	-0.55	11,11,11,11	0
4	CA	A	716	1/1	0.12	-1.45	6,6,6,6	0
4	CA	A	718	1/1	0.07	-1.51	19,19,19,19	0
4	CA	B	403	1/1	0.06	-1.79	20,20,20,20	0
4	CA	A	720	1/1	0.06	-2.00	33,33,33,33	0
4	CA	B	401	1/1	0.06	-2.07	17,17,17,17	0
4	CA	B	404	1/1	0.10	-2.24	17,17,17,17	0
4	CA	A	715	1/1	0.08	-2.52	8,8,8,8	0
4	CA	B	402	1/1	0.08	-2.66	15,15,15,15	0
4	CA	A	717	1/1	0.09	-2.77	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.