



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:58 PM UTC

PDB ID : 1NX0 / pdb_00001nx0
Title : Structure of Calpain Domain 6 in Complex with Calpastatin DIC
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Deposited on : 2003-02-07
Resolution : 2.30 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

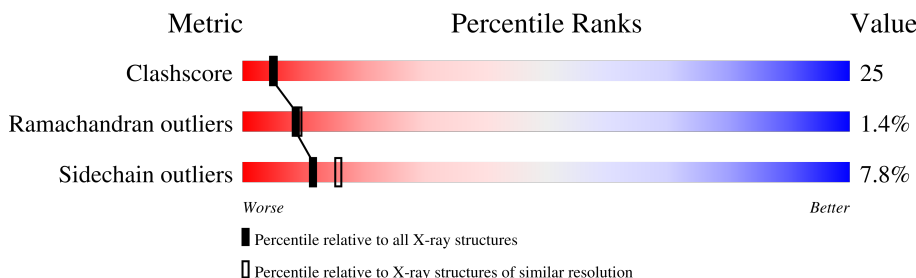
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	173	61% 34% 5%
1	B	173	52% 40% 8% .
2	C	12	50% 50%
2	D	12	33% 42% 17% 8%
3	E	5	20% 80%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3145 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 Calcium-dependent protease, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1395	881	237	267	10			
1	B	173	Total	C	N	O	S	0	0	0
			1395	881	237	267	10			

- Molecule 2 is a protein called Calpastatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			87	52	12	23			
2	D	11	Total	C	N	O	0	0	0
			80	49	11	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	612	SER	CYS	conflict	UNP P49342
D	712	SER	CYS	conflict	UNP P49342

- Molecule 3 is a protein called Small molecule inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			32	21	6	5			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		

- Molecule 5 is water.

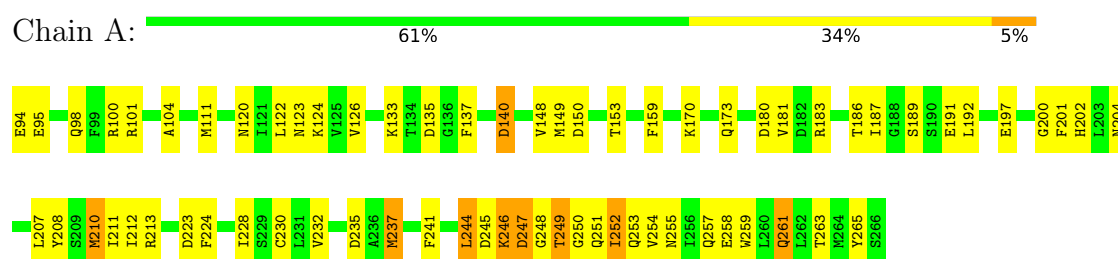
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0
5	B	47	Total 47	O 47	0	0
5	C	10	Total 10	O 10	0	0
5	D	1	Total 1	O 1	0	0
5	E	4	Total 4	O 4	0	0

3 Residue-property plots

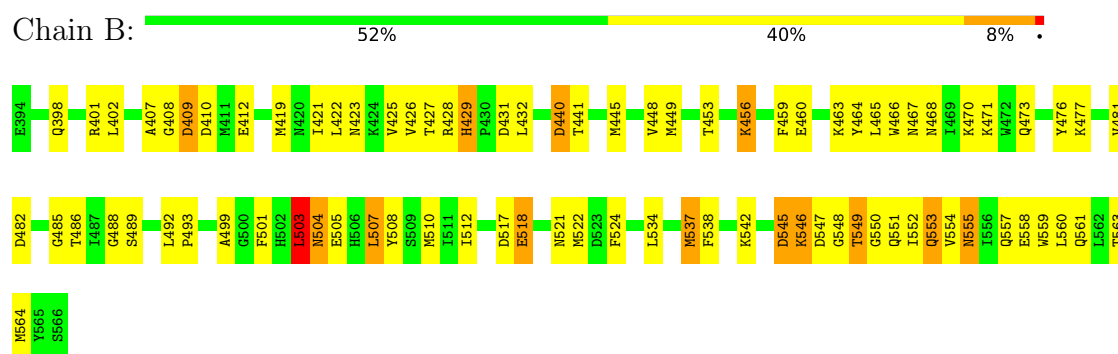
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Calcium-dependent protease, small subunit



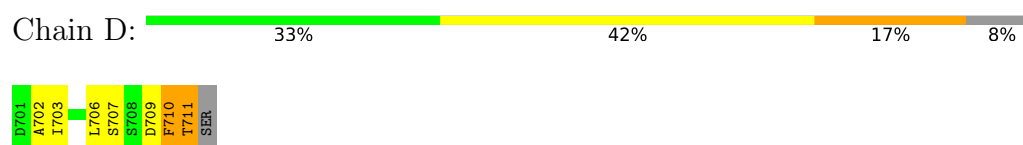
- Molecule 1: Calcium-dependent protease, small subunit



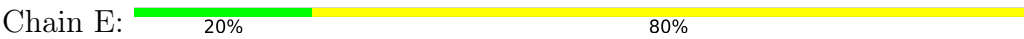
- Molecule 2: Calpastatin



- Molecule 2: Calpastatin



- Molecule 3: Small molecule inhibitor



A801
A802
A803
A804
A805

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.78Å 83.30Å 92.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.218 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3145	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.46	1/1422 (0.1%)	0.94	5/1911 (0.3%)
1	B	0.41	1/1422 (0.1%)	0.90	5/1911 (0.3%)
2	C	0.45	0/87	0.87	1/116 (0.9%)
2	D	0.39	0/80	1.15	1/108 (0.9%)
3	E	0.51	0/31	1.84	1/40 (2.5%)
All	All	0.43	2/3042 (0.1%)	0.94	13/4086 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	MET	SD-CE	-7.03	1.61	1.79
1	B	537	MET	SD-CE	-6.13	1.64	1.79

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PHE	N-CA-C	7.85	119.47	111.07
1	B	524	PHE	N-CA-C	7.05	118.66	110.97
3	E	803	ALA	N-CA-C	7.03	125.77	110.80
1	A	135	ASP	N-CA-C	-6.28	105.38	113.16
2	D	702	ALA	N-CA-C	-5.55	106.00	112.89

There are no chirality outliers.

There are no planarity outliers.

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	A	1395	0	1345	68	0
1	B	1395	0	1346	95	0
2	C	87	0	74	5	0
2	D	80	0	69	11	0
3	E	32	0	38	4	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	88	0	0	0	0
5	B	47	0	0	3	0
5	C	10	0	0	0	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
All	All	3145	0	2872	146	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 25.

The worst 5 of 146 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:237:MET:HE2	1:B:563:THR:HG21	1.46	0.98
1:A:254:VAL:HG23	1:A:258:GLU:HB2	1.55	0.88
1:A:210:MET:HE1	1:B:453:THR:HB	1.58	0.83
1:B:431:ASP:OD2	1:B:477:LYS:HE2	1.83	0.79
1:B:555:ASN:ND2	1:B:558:GLU:H	1.81	0.78

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	171/173 (99%)	162 (95%)	6 (4%)	3 (2%)	6	6
1	B	171/173 (99%)	157 (92%)	12 (7%)	2 (1%)	10	12
2	C	10/12 (83%)	10 (100%)	0	0	100	100
2	D	9/12 (75%)	9 (100%)	0	0	100	100
3	E	3/5 (60%)	0	3 (100%)	0	100	100
All	All	364/375 (97%)	338 (93%)	21 (6%)	5 (1%)	9	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	LYS
1	A	249	THR
1	B	409	ASP
1	A	245	ASP
1	B	546	LYS

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	150/150 (100%)	141 (94%)	9 (6%)	17	25
1	B	150/150 (100%)	136 (91%)	14 (9%)	8	11
2	C	10/10 (100%)	10 (100%)	0	100	100
2	D	9/10 (90%)	7 (78%)	2 (22%)	1	1
3	E	2/2 (100%)	2 (100%)	0	100	100
All	All	321/322 (100%)	296 (92%)	25 (8%)	11	16

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	460	GLU
1	B	507	LEU
2	D	711	THR

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Mol	Chain	Res	Type
1	B	504	ASN
1	B	518	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	468	ASN
1	B	473	GLN
1	B	557	GLN
1	B	553	GLN
1	B	555	ASN

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](#)

Of 6 ligands modelled in this entry, 6 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.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.