



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 05:22 PM UTC

PDB ID : 3USV / pdb_00003usv
Title : Structure of the precursor of a thermostable variant of papain at 3.8 Å resolution from a crystal soaked at pH 4
Authors : Roy, S.; Choudhury, D.; Biswas, S.; Dattagupta, J.K.
Deposited on : 2011-11-24
Resolution : 3.80 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

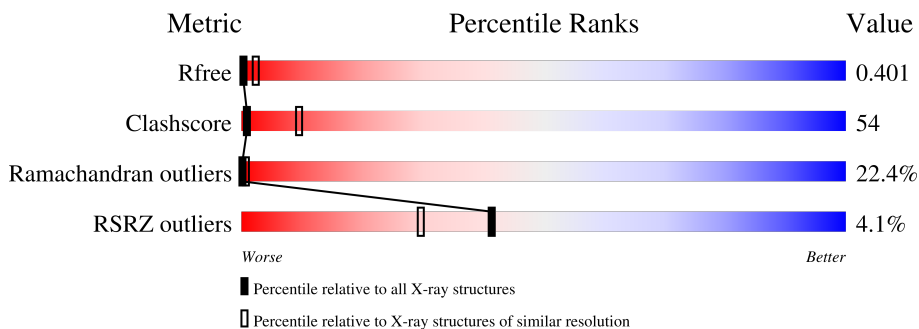
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	363	 4% 36% 35% 13% • 15%
1	C	363	 3% 36% 35% 12% • 15%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3020 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 Papain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	308	1510	893	308	309	0	0	0
1	C	308	1510	893	308	309	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	MET	-	expression tag	UNP P00784
A	-42	HIS	-	expression tag	UNP P00784
A	-41	HIS	-	expression tag	UNP P00784
A	-40	HIS	-	expression tag	UNP P00784
A	-39	HIS	-	expression tag	UNP P00784
A	-38	HIS	-	expression tag	UNP P00784
A	-37	HIS	-	expression tag	UNP P00784
A	-36	SER	-	expression tag	UNP P00784
A	-35	SER	-	expression tag	UNP P00784
A	-34	GLY	-	expression tag	UNP P00784
A	-33	LEU	-	expression tag	UNP P00784
A	-32	VAL	-	expression tag	UNP P00784
A	-31	PRO	-	expression tag	UNP P00784
A	-30	ARG	-	expression tag	UNP P00784
A	-29	GLY	-	expression tag	UNP P00784
A	-28	SER	-	expression tag	UNP P00784
A	-27	GLY	-	expression tag	UNP P00784
A	-26	MET	-	expression tag	UNP P00784
A	-25	LYS	-	expression tag	UNP P00784
A	-24	GLU	-	expression tag	UNP P00784
A	-23	THR	-	expression tag	UNP P00784
A	-22	ALA	-	expression tag	UNP P00784
A	-21	ALA	-	expression tag	UNP P00784
A	-20	ALA	-	expression tag	UNP P00784
A	-19	LYS	-	expression tag	UNP P00784

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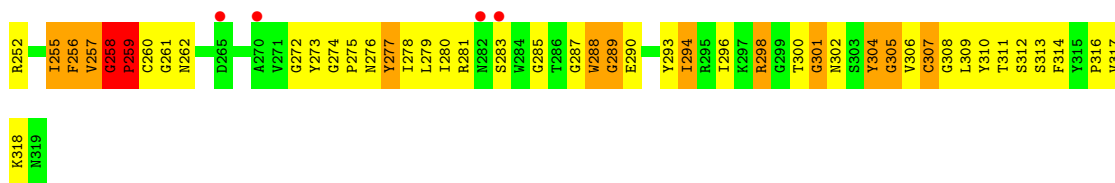
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	PHE	-	expression tag	UNP P00784
A	-17	GLU	-	expression tag	UNP P00784
A	-16	ARG	-	expression tag	UNP P00784
A	-15	GLN	-	expression tag	UNP P00784
A	-14	HIS	-	expression tag	UNP P00784
A	-13	MET	-	expression tag	UNP P00784
A	-12	ASP	-	expression tag	UNP P00784
A	-11	SER	-	expression tag	UNP P00784
A	-10	PRO	-	expression tag	UNP P00784
A	-9	ASP	-	expression tag	UNP P00784
A	-8	LEU	-	expression tag	UNP P00784
A	-7	GLY	-	expression tag	UNP P00784
A	-6	THR	-	expression tag	UNP P00784
A	-5	ASP	-	expression tag	UNP P00784
A	-4	ASP	-	expression tag	UNP P00784
A	-3	ASP	-	expression tag	UNP P00784
A	-2	ASP	-	expression tag	UNP P00784
A	-1	LYS	-	expression tag	UNP P00784
A	0	MET	-	expression tag	UNP P00784
A	132	ALA	CYS	engineered mutation	UNP P00784
A	139	SER	VAL	engineered mutation	UNP P00784
A	143	SER	GLY	engineered mutation	UNP P00784
A	281	ARG	LYS	engineered mutation	UNP P00784
C	-43	MET	-	expression tag	UNP P00784
C	-42	HIS	-	expression tag	UNP P00784
C	-41	HIS	-	expression tag	UNP P00784
C	-40	HIS	-	expression tag	UNP P00784
C	-39	HIS	-	expression tag	UNP P00784
C	-38	HIS	-	expression tag	UNP P00784
C	-37	HIS	-	expression tag	UNP P00784
C	-36	SER	-	expression tag	UNP P00784
C	-35	SER	-	expression tag	UNP P00784
C	-34	GLY	-	expression tag	UNP P00784
C	-33	LEU	-	expression tag	UNP P00784
C	-32	VAL	-	expression tag	UNP P00784
C	-31	PRO	-	expression tag	UNP P00784
C	-30	ARG	-	expression tag	UNP P00784
C	-29	GLY	-	expression tag	UNP P00784
C	-28	SER	-	expression tag	UNP P00784
C	-27	GLY	-	expression tag	UNP P00784
C	-26	MET	-	expression tag	UNP P00784
C	-25	LYS	-	expression tag	UNP P00784

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	GLU	-	expression tag	UNP P00784
C	-23	THR	-	expression tag	UNP P00784
C	-22	ALA	-	expression tag	UNP P00784
C	-21	ALA	-	expression tag	UNP P00784
C	-20	ALA	-	expression tag	UNP P00784
C	-19	LYS	-	expression tag	UNP P00784
C	-18	PHE	-	expression tag	UNP P00784
C	-17	GLU	-	expression tag	UNP P00784
C	-16	ARG	-	expression tag	UNP P00784
C	-15	GLN	-	expression tag	UNP P00784
C	-14	HIS	-	expression tag	UNP P00784
C	-13	MET	-	expression tag	UNP P00784
C	-12	ASP	-	expression tag	UNP P00784
C	-11	SER	-	expression tag	UNP P00784
C	-10	PRO	-	expression tag	UNP P00784
C	-9	ASP	-	expression tag	UNP P00784
C	-8	LEU	-	expression tag	UNP P00784
C	-7	GLY	-	expression tag	UNP P00784
C	-6	THR	-	expression tag	UNP P00784
C	-5	ASP	-	expression tag	UNP P00784
C	-4	ASP	-	expression tag	UNP P00784
C	-3	ASP	-	expression tag	UNP P00784
C	-2	ASP	-	expression tag	UNP P00784
C	-1	LYS	-	expression tag	UNP P00784
C	0	MET	-	expression tag	UNP P00784
C	132	ALA	CYS	engineered mutation	UNP P00784
C	139	SER	VAL	engineered mutation	UNP P00784
C	143	SER	GLY	engineered mutation	UNP P00784
C	281	ARG	LYS	engineered mutation	UNP P00784



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.85Å 75.97Å 109.71Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	29.60 – 3.80 29.60 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.60-3.80) 70.5 (29.60-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.75Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.358 , 0.408 0.359 , 0.401	Depositor DCC
R_{free} test set	579 reflections (8.26%)	wwPDB-VP
Wilson B-factor (Å ²)	103.7	Xtrriage
Anisotropy	0.540	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.32 , 112.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.22$, $\langle L^2 \rangle = 0.09$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3020	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.83	2/1509 (0.1%)	1.73	57/2091 (2.7%)
1	C	0.85	5/1509 (0.3%)	1.74	54/2091 (2.6%)
All	All	0.84	7/3018 (0.2%)	1.73	111/4182 (2.7%)

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
1	C	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	PRO	CA-CB	6.79	1.63	1.53
1	C	257	VAL	CA-C	6.69	1.62	1.52
1	A	258	GLY	C-O	-6.30	1.15	1.24
1	C	258	GLY	N-CA	5.79	1.52	1.44
1	A	258	GLY	CA-C	-5.25	1.44	1.51

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	PRO	N-CA-C	-17.76	75.88	112.47
1	A	72	ASP	N-CA-C	-13.18	96.46	112.54
1	A	258	GLY	N-CA-C	12.72	138.30	112.34
1	A	100	VAL	N-CA-C	12.63	129.87	108.90
1	C	203	ARG	N-CA-C	-11.69	98.32	112.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	259	PRO	Mainchain

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	1510	0	687	131	0
1	C	1510	0	687	107	2
All	All	3020	0	1374	238	2

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 54.

The worst 5 of 238 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:C:217:VAL:HA	1:C:316:PRO:HA	1.05	1.05
1:A:168:TYR:O	1:A:173:GLY:HA2	1.62	0.98
1:C:217:VAL:CA	1:C:316:PRO:HA	1.96	0.96
1:C:219:GLN:HA	1:C:314:PHE:HA	1.48	0.94
1:A:170:CYS:C	1:A:172:GLY:H	1.75	0.88

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:O	1:C:192:THR:O[1_655]	2.03	0.17
1:C:103:ASP:O	1:C:192:THR:O[1_655]	2.17	0.03

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	306/363 (84%)	164 (54%)	73 (24%)	69 (22%)	0	0
1	C	306/363 (84%)	165 (54%)	73 (24%)	68 (22%)	0	1
All	All	612/726 (84%)	329 (54%)	146 (24%)	137 (22%)	0	1

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	54	ASP
1	A	70	PHE
1	A	74	SER
1	A	82	TYR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	308/363 (84%)	-0.34	13 (4%) 40 29	19, 45, 57, 59	0
1	C	308/363 (84%)	-0.42	12 (3%) 43 31	19, 45, 58, 60	0
All	All	616/726 (84%)	-0.38	25 (4%) 41 30	19, 45, 58, 60	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ASN	6.5
1	C	132	ALA	5.8
1	C	155	TYR	5.7
1	C	270	ALA	5.0
1	C	211	ALA	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.