



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 03:52 AM EDT

PDB ID : 5H45  
Title : Crystal structure of the C-terminal Lon protease-like domain of *Thermus thermophilus* RadA/Sms  
Authors : Inoue, M.; Fukui, K.; Fujii, Y.; Nakagawa, N.; Yano, T.; Kuramitsu, S.; Masui, R.  
Deposited on : 2016-10-30  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

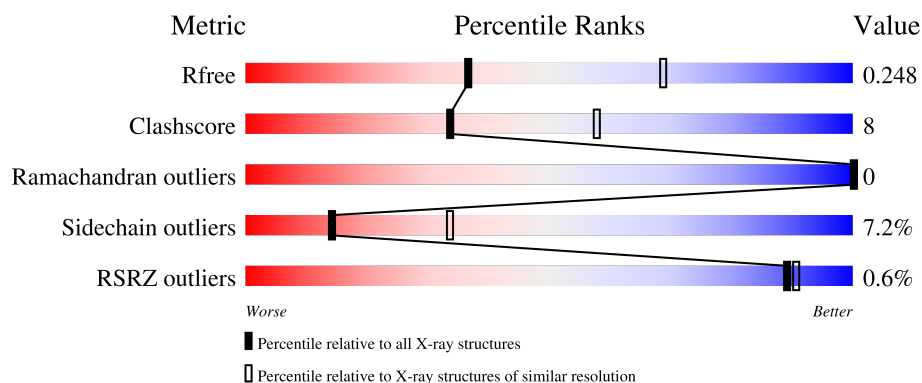
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	184	
1	B	184	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2340 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 DNA repair protein RadA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	0	0	0
			1122	713	212	197			
1	B	157	Total	C	N	O	0	0	0
			1166	741	221	204			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	initiating methionine	UNP Q5SKV2
A	241	GLY	-	expression tag	UNP Q5SKV2
A	242	SER	-	expression tag	UNP Q5SKV2
A	243	SER	-	expression tag	UNP Q5SKV2
A	244	HIS	-	expression tag	UNP Q5SKV2
A	245	HIS	-	expression tag	UNP Q5SKV2
A	246	HIS	-	expression tag	UNP Q5SKV2
A	247	HIS	-	expression tag	UNP Q5SKV2
A	248	HIS	-	expression tag	UNP Q5SKV2
A	249	HIS	-	expression tag	UNP Q5SKV2
A	250	SER	-	expression tag	UNP Q5SKV2
A	251	SER	-	expression tag	UNP Q5SKV2
A	252	GLY	-	expression tag	UNP Q5SKV2
A	253	GLU	-	expression tag	UNP Q5SKV2
A	254	ASN	-	expression tag	UNP Q5SKV2
A	255	LEU	-	expression tag	UNP Q5SKV2
A	256	TYR	-	expression tag	UNP Q5SKV2
A	257	PHE	-	expression tag	UNP Q5SKV2
A	258	GLN	-	expression tag	UNP Q5SKV2
A	259	GLY	-	expression tag	UNP Q5SKV2
A	260	HIS	-	expression tag	UNP Q5SKV2
A	261	MET	-	expression tag	UNP Q5SKV2
B	240	MET	-	initiating methionine	UNP Q5SKV2
B	241	GLY	-	expression tag	UNP Q5SKV2
B	242	SER	-	expression tag	UNP Q5SKV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	243	SER	-	expression tag	UNP Q5SKV2
B	244	HIS	-	expression tag	UNP Q5SKV2
B	245	HIS	-	expression tag	UNP Q5SKV2
B	246	HIS	-	expression tag	UNP Q5SKV2
B	247	HIS	-	expression tag	UNP Q5SKV2
B	248	HIS	-	expression tag	UNP Q5SKV2
B	249	HIS	-	expression tag	UNP Q5SKV2
B	250	SER	-	expression tag	UNP Q5SKV2
B	251	SER	-	expression tag	UNP Q5SKV2
B	252	GLY	-	expression tag	UNP Q5SKV2
B	253	GLU	-	expression tag	UNP Q5SKV2
B	254	ASN	-	expression tag	UNP Q5SKV2
B	255	LEU	-	expression tag	UNP Q5SKV2
B	256	TYR	-	expression tag	UNP Q5SKV2
B	257	PHE	-	expression tag	UNP Q5SKV2
B	258	GLN	-	expression tag	UNP Q5SKV2
B	259	GLY	-	expression tag	UNP Q5SKV2
B	260	HIS	-	expression tag	UNP Q5SKV2
B	261	MET	-	expression tag	UNP Q5SKV2

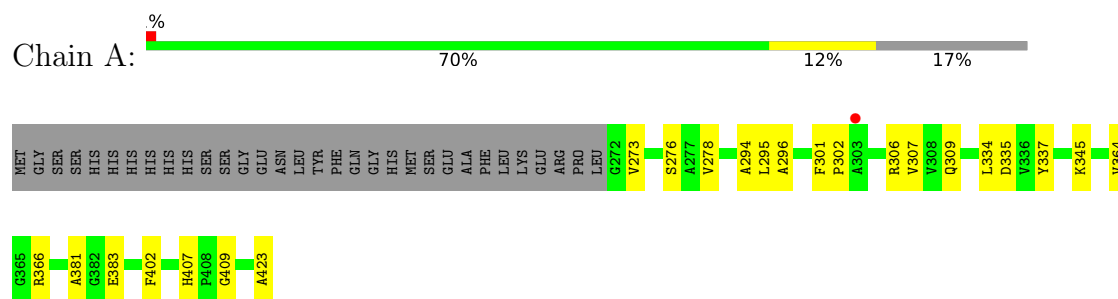
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	27	Total O 27 27	0	0

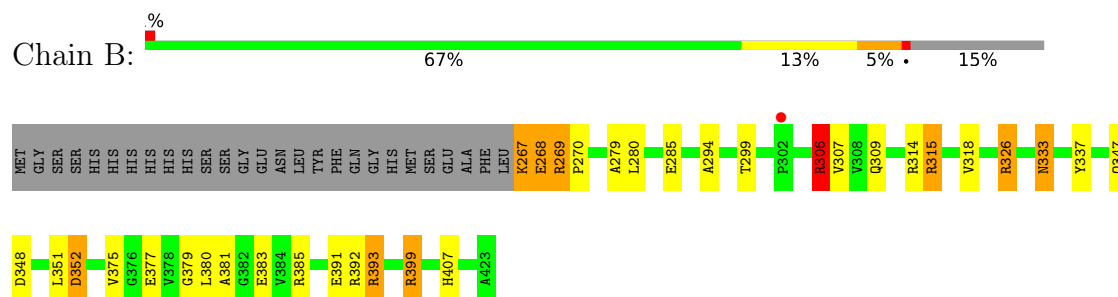
### 3 Residue-property plots [i](#)

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 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: DNA repair protein RadA



#### • Molecule 1: DNA repair protein RadA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.29Å 156.29Å 156.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 2.70 49.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-2.70) 100.0 (49.42-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.250 0.194 , 0.248	Depositor DCC
$R_{free}$ test set	948 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.65	0/1137	0.83	0/1544
1	B	0.70	0/1182	0.91	7/1604 (0.4%)
All	All	0.68	0/2319	0.87	7/3148 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	B	306	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	352	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	393	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	393	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	269	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	306	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1122	0	1186	16	0
1	B	1166	0	1236	25	0
2	A	25	0	0	0	0
2	B	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2340	0	2422	40	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 8.

All (40) 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:B:306:ARG:HH11	1:B:306:ARG:HG3	1.26	1.00
1:B:269:ARG:HB2	1:B:270:PRO:HD2	1.46	0.97
1:B:267:LYS:O	1:B:267:LYS:HD2	1.65	0.96
1:A:307:VAL:CG2	1:A:337:TYR:HD1	1.82	0.92
1:B:306:ARG:HG3	1:B:306:ARG:NH1	1.95	0.78
1:A:366:ARG:HH11	1:A:423:ALA:HB3	1.48	0.78
1:B:379:GLY:HA3	1:B:383:GLU:OE2	1.84	0.75
1:B:285:GLU:O	1:B:392:ARG:NH2	2.19	0.75
1:A:407:HIS:HD2	1:A:409:GLY:H	1.39	0.70
1:A:307:VAL:CG2	1:A:337:TYR:CD1	2.73	0.69
1:A:307:VAL:HG22	1:A:337:TYR:HD1	1.58	0.68
1:A:307:VAL:HG22	1:A:337:TYR:CD1	2.32	0.65
1:B:269:ARG:HB2	1:B:270:PRO:CD	2.24	0.65
1:B:269:ARG:CB	1:B:270:PRO:HD2	2.29	0.58
1:B:333:ASN:H	1:B:333:ASN:HD22	1.51	0.58
1:B:307:VAL:HB	1:B:337:TYR:CD1	2.41	0.55
1:B:280:LEU:HB2	1:B:375:VAL:CG2	2.38	0.54
1:B:399:ARG:HH11	1:B:399:ARG:HB3	1.73	0.53
1:B:348:ASP:OD2	1:B:393:ARG:NH1	2.38	0.52
1:B:268:GLU:HA	1:B:268:GLU:OE1	2.10	0.51
1:A:306:ARG:NH2	1:A:334:LEU:O	2.44	0.50
1:A:366:ARG:NH1	1:A:423:ALA:HB3	2.23	0.50
1:A:407:HIS:HD2	1:A:409:GLY:N	2.09	0.50
1:B:375:VAL:O	1:B:407:HIS:HA	2.11	0.50
1:B:318:VAL:HG13	1:B:380:LEU:HD13	1.94	0.49
1:A:407:HIS:CD2	1:A:409:GLY:H	2.27	0.49
1:B:377:GLU:HB3	1:B:385:ARG:HB2	1.97	0.47
1:B:279:ALA:CB	1:B:351:LEU:HD23	2.47	0.45
1:B:326:ARG:HE	1:B:381:ALA:HA	1.82	0.44
1:B:299:THR:HG22	1:B:333:ASN:O	2.18	0.43
1:B:380:LEU:HD12	1:B:380:LEU:HA	1.87	0.43
1:A:294:ALA:HA	1:A:337:TYR:O	2.18	0.43
1:A:301:PHE:HB3	1:A:302:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:CB	1:B:270:PRO:CD	2.93	0.42
1:A:381:ALA:HB3	1:A:383:GLU:OE1	2.20	0.42
1:B:315:ARG:NH1	1:B:352:ASP:OD2	2.53	0.42
1:A:296:ALA:HA	1:A:335:ASP:O	2.20	0.42
1:B:294:ALA:HA	1:B:337:TYR:O	2.21	0.41
1:A:295:LEU:HB2	1:B:380:LEU:HG	2.03	0.40
1:A:278:VAL:HG11	1:A:402:PHE:CZ	2.56	0.40

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	150/184 (82%)	147 (98%)	3 (2%)	0	100	100
1	B	155/184 (84%)	151 (97%)	4 (3%)	0	100	100
All	All	305/368 (83%)	298 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	109/137 (80%)	104 (95%)	5 (5%)	27	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	114/137 (83%)	103 (90%)	11 (10%)	8	19
All	All	223/274 (81%)	207 (93%)	16 (7%)	14	34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	VAL
1	A	276	SER
1	A	309	GLN
1	A	345	LYS
1	A	364	VAL
1	B	267	LYS
1	B	268	GLU
1	B	306	ARG
1	B	309	GLN
1	B	314	ARG
1	B	315	ARG
1	B	326	ARG
1	B	333	ASN
1	B	347	GLN
1	B	391	GLU
1	B	399	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	B	333	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 [i](#)

There are no monosaccharides 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	152/184 (82%)	-0.15	1 (0%) 87 89	34, 49, 79, 104	0
1	B	157/184 (85%)	-0.15	1 (0%) 89 91	33, 46, 82, 123	0
All	All	309/368 (83%)	-0.15	2 (0%) 89 91	33, 48, 82, 123	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	ALA	3.2
1	B	302	PRO	2.6

### 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 monosaccharides 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.