



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9UUZ / pdb\_00009uuz  
Title : Crystal structure of Thoeris protein ThsA  
Authors : Wang, H.; Feng, Y.; Li, D.  
Deposited on : 2025-05-08  
Resolution : 2.59 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](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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (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

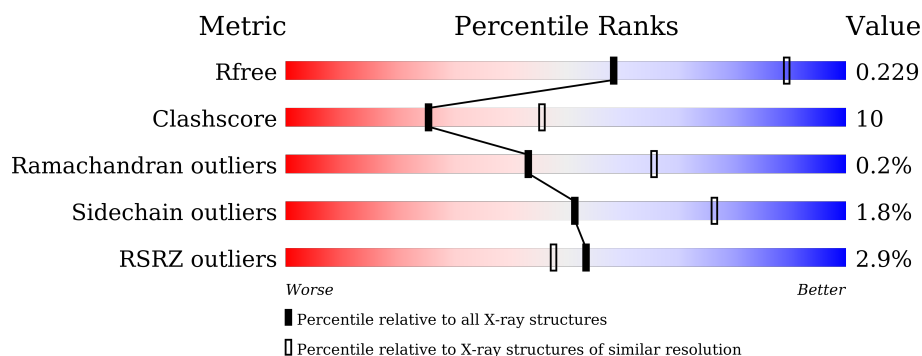
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	221	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	221	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	221	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	D	221	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7396 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 Thoeris protein ThsA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	Se	0	0	0
			1794	1153	303	333	1	4			
1	B	216	Total	C	N	O	S	Se	0	0	0
			1788	1150	302	331	1	4			
1	C	218	Total	C	N	O	S	Se	0	0	0
			1797	1156	303	333	1	4			
1	D	215	Total	C	N	O	S	Se	0	0	0
			1780	1144	301	330	1	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP I2C645
A	78	PRO	-	expression tag	UNP I2C645
A	79	LEU	-	expression tag	UNP I2C645
A	80	GLY	-	expression tag	UNP I2C645
A	81	SER	-	expression tag	UNP I2C645
B	77	GLY	-	expression tag	UNP I2C645
B	78	PRO	-	expression tag	UNP I2C645
B	79	LEU	-	expression tag	UNP I2C645
B	80	GLY	-	expression tag	UNP I2C645
B	81	SER	-	expression tag	UNP I2C645
C	77	GLY	-	expression tag	UNP I2C645
C	78	PRO	-	expression tag	UNP I2C645
C	79	LEU	-	expression tag	UNP I2C645
C	80	GLY	-	expression tag	UNP I2C645
C	81	SER	-	expression tag	UNP I2C645
D	77	GLY	-	expression tag	UNP I2C645
D	78	PRO	-	expression tag	UNP I2C645
D	79	LEU	-	expression tag	UNP I2C645
D	80	GLY	-	expression tag	UNP I2C645
D	81	SER	-	expression tag	UNP I2C645

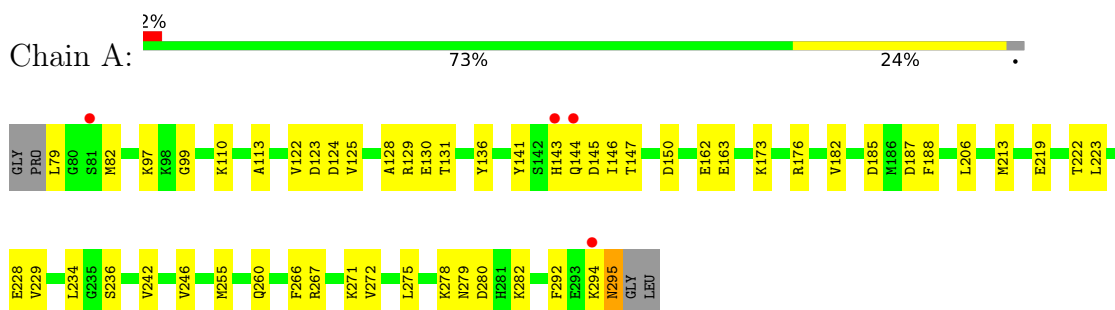
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total 85	O 85	0	0
2	B	52	Total 52	O 52	0	0
2	C	58	Total 58	O 58	0	0
2	D	42	Total 42	O 42	0	0

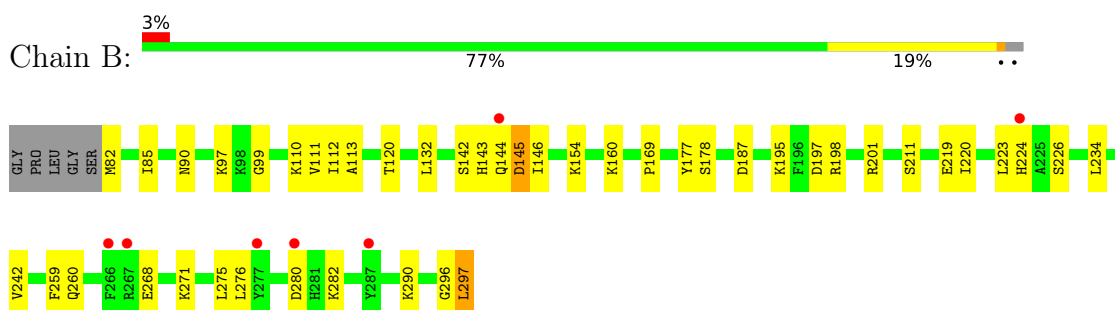
### 3 Residue-property plots [i](#)

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.

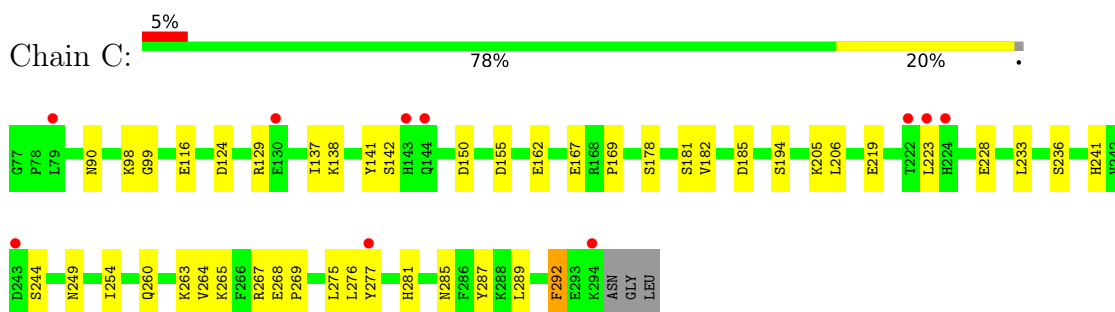
#### • Molecule 1: Thoeris protein ThsA



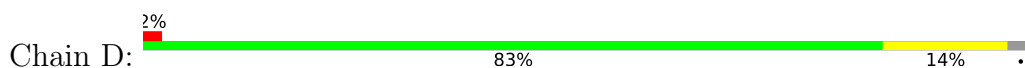
#### • Molecule 1: Thoeris protein ThsA

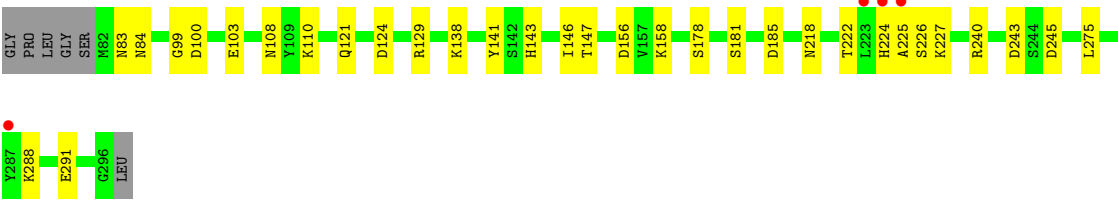


#### • Molecule 1: Thoeris protein ThsA



#### • Molecule 1: Thoeris protein ThsA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.74Å 89.23Å 87.63Å 90.00° 93.01° 90.00°	Depositor
Resolution (Å)	39.29 – 2.59 39.29 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.29-2.59) 98.5 (39.29-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.42 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.181 , 0.231 0.182 , 0.229	Depositor DCC
$R_{free}$ test set	1979 reflections (6.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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	0.24	0/1825	0.48	0/2449
1	B	0.20	0/1820	0.42	0/2444
1	C	0.20	0/1829	0.37	0/2455
1	D	0.19	0/1812	0.40	1/2433 (0.0%)
All	All	0.21	0/7286	0.42	1/9781 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	ASN	N-CA-C	-5.79	107.20	114.56

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	1794	0	1801	47	0
1	B	1788	0	1796	39	0
1	C	1797	0	1805	32	1
1	D	1780	0	1785	20	0
2	A	85	0	0	24	0
2	B	52	0	0	13	0
2	C	58	0	0	12	0
2	D	42	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7396	0	7187	137	1

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 10.

The worst 5 of 137 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:222:THR:HG23	2:A:305:HOH:O	1.43	1.14
1:B:144:GLN:N	2:B:301:HOH:O	1.80	1.12
1:B:143:HIS:CB	2:B:301:HOH:O	2.01	1.08
1:A:144:GLN:C	2:A:304:HOH:O	1.95	1.06
1:B:143:HIS:CA	2:B:301:HOH:O	2.04	1.04

All (1) 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:155:ASP:OD1	1:C:287:TYR:OH[2_556]	2.14	0.06

## 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	215/221 (97%)	207 (96%)	8 (4%)	0	100	100
1	B	214/221 (97%)	205 (96%)	8 (4%)	1 (0%)	24	46
1	C	216/221 (98%)	208 (96%)	8 (4%)	0	100	100
1	D	213/221 (96%)	200 (94%)	12 (6%)	1 (0%)	24	46
All	All	858/884 (97%)	820 (96%)	36 (4%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	SER
1	B	242	VAL

### 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	200/198 (101%)	197 (98%)	3 (2%)	57	80
1	B	199/198 (100%)	195 (98%)	4 (2%)	48	74
1	C	200/198 (101%)	195 (98%)	5 (2%)	42	69
1	D	198/198 (100%)	196 (99%)	2 (1%)	68	86
All	All	797/792 (101%)	783 (98%)	14 (2%)	51	76

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	142	SER
1	C	162	GLU
1	D	224	HIS
1	C	292	PHE
1	D	84	ASN

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

Mol	Chain	Res	Type
1	D	84	ASN
1	D	90	ASN
1	D	279	ASN
1	D	218	ASN
1	C	133	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](#)

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	213/221 (96%)	-0.20	4 (1%) 66 61	13, 24, 50, 73	0
1	B	212/221 (95%)	-0.01	7 (3%) 49 43	16, 29, 55, 77	0
1	C	214/221 (96%)	-0.13	10 (4%) 36 30	13, 24, 53, 82	0
1	D	211/221 (95%)	-0.06	4 (1%) 66 61	14, 30, 51, 73	0
All	All	850/884 (96%)	-0.10	25 (2%) 53 48	13, 27, 53, 82	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	TYR	4.9
1	B	287	TYR	3.8
1	C	224	HIS	3.2
1	A	144	GLN	3.1
1	C	294	LYS	3.1

### 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.