



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 01:55 PM EST

PDB ID : 2CSL  
Title : Crystal structure of TTHA0137 from *Thermus Thermophilus* HB8  
Authors : Wang, H.; Murayama, K.; Terada, T.; Chen, L.; Jin, Z.; Chrzas, J.; Liu, Z.J.; Wang, B.C.; Shirouzu, M.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-05-22  
Resolution : 2.50 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	<b>FAILED</b>
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

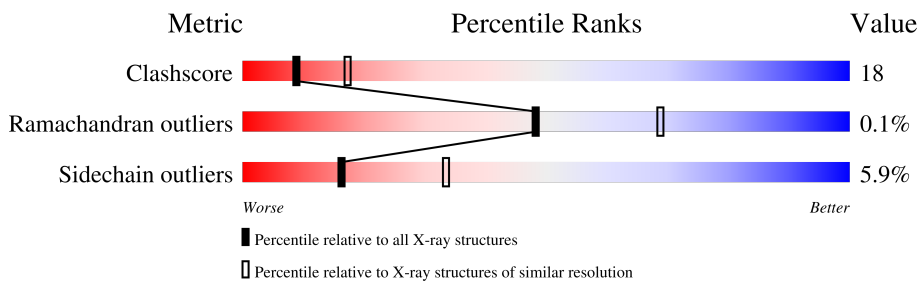
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)

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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	124	69% 28% .
1	B	124	71% 25% .
1	C	124	73% 22% 5% .
1	D	124	67% 31% .
1	E	124	74% 23% .
1	F	124	75% 23% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5703 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 protein translation initiation inhibitor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	Se	0	0	0
			924	588	158	173	2	3			
1	B	124	Total	C	N	O	S	Se	0	0	0
			924	588	158	173	2	3			
1	C	124	Total	C	N	O	S	Se	0	0	0
			924	588	158	173	2	3			
1	D	124	Total	C	N	O	S	Se	0	0	0
			924	588	158	173	2	3			
1	E	124	Total	C	N	O	S	Se	0	0	0
			924	588	158	173	2	3			
1	F	124	Total	C	N	O	S	Se	0	0	0
			924	588	158	173	2	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q5SM06
A	53	MSE	MET	modified residue	UNP Q5SM06
A	80	MSE	MET	modified residue	UNP Q5SM06
B	1	MSE	MET	modified residue	UNP Q5SM06
B	53	MSE	MET	modified residue	UNP Q5SM06
B	80	MSE	MET	modified residue	UNP Q5SM06
C	1	MSE	MET	modified residue	UNP Q5SM06
C	53	MSE	MET	modified residue	UNP Q5SM06
C	80	MSE	MET	modified residue	UNP Q5SM06
D	1	MSE	MET	modified residue	UNP Q5SM06
D	53	MSE	MET	modified residue	UNP Q5SM06
D	80	MSE	MET	modified residue	UNP Q5SM06
E	1	MSE	MET	modified residue	UNP Q5SM06
E	53	MSE	MET	modified residue	UNP Q5SM06
E	80	MSE	MET	modified residue	UNP Q5SM06
F	1	MSE	MET	modified residue	UNP Q5SM06
F	53	MSE	MET	modified residue	UNP Q5SM06

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Chain	Residue	Modelled	Actual	Comment	Reference
F	80	MSE	MET	modified residue	UNP Q5SM06

- Molecule 2 is water.

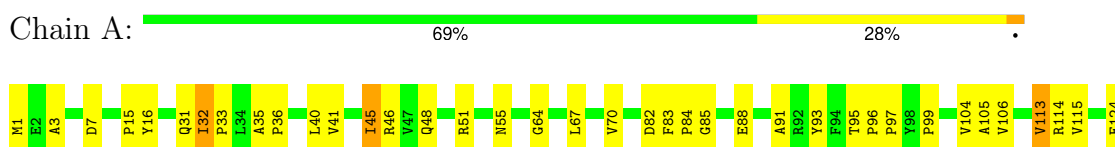
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	24	Total O 24 24	0	0
2	C	30	Total O 30 30	0	0
2	D	25	Total O 25 25	0	0
2	E	25	Total O 25 25	0	0
2	F	26	Total O 26 26	0	0

### 3 Residue-property plots

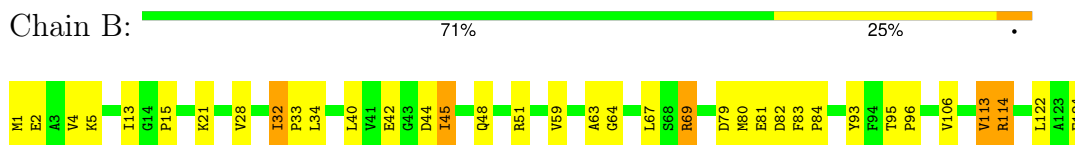
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

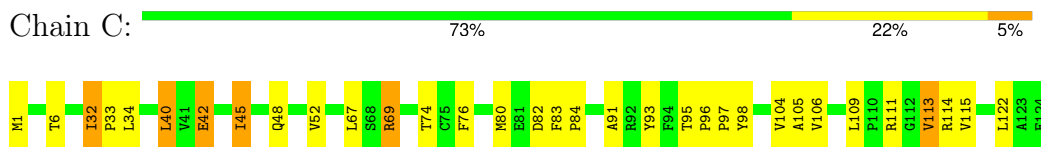
- Molecule 1: protein translation initiation inhibitor



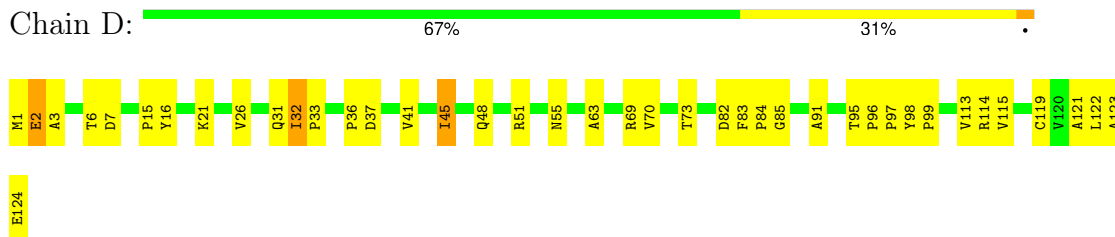
- Molecule 1: protein translation initiation inhibitor



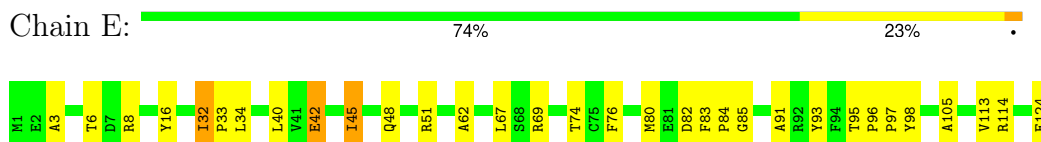
- Molecule 1: protein translation initiation inhibitor



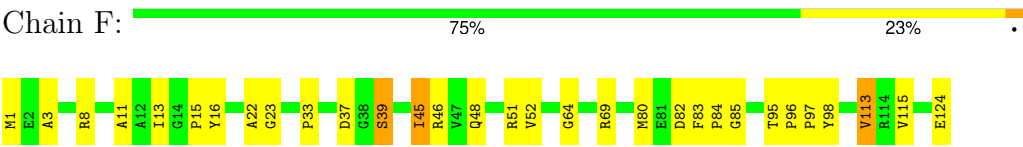
- Molecule 1: protein translation initiation inhibitor



- Molecule 1: protein translation initiation inhibitor



● Molecule 1: protein translation initiation inhibitor



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.85Å 111.99Å 111.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.67 – 2.50	Depositor
% Data completeness (in resolution range)	98.5 (45.67-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.267	Depositor
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.386	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.316 for k,h,-l 0.247 for -h,-l,-k 0.427 for l,-k,h 0.276 for k,l,h 0.276 for l,h,k	Xtriage
Total number of atoms	5703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	0.37	0/940	0.63	0/1275
1	B	0.34	0/940	0.61	0/1275
1	C	0.35	0/940	0.63	0/1275
1	D	0.34	0/940	0.61	0/1275
1	E	0.35	0/940	0.62	0/1275
1	F	0.35	0/940	0.63	0/1275
All	All	0.35	0/5640	0.62	0/7650

There are no bond length outliers.

There are no bond angle outliers.

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	924	0	932	47	0
1	B	924	0	932	43	0
1	C	924	0	932	34	0
1	D	924	0	932	48	0
1	E	924	0	932	33	0
1	F	924	0	932	31	0
2	A	29	0	0	0	0
2	B	24	0	0	0	0
2	C	30	0	0	1	0
2	D	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	25	0	0	0	0
2	F	26	0	0	1	0
All	All	5703	0	5592	204	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 18.

The worst 5 of 204 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:32:ILE:HD13	1:C:34:LEU:HG	1.37	1.06
1:E:6:THR:HG22	1:E:8:ARG:H	1.21	1.05
1:A:48:GLN:NE2	1:A:114:ARG:HG2	1.88	0.89
1:B:32:ILE:HD13	1:B:32:ILE:H	1.40	0.87
1:A:45:ILE:HD12	1:A:85:GLY:HA3	1.56	0.86

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	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
1	B	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
1	C	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
1	D	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
1	E	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
1	F	122/124 (98%)	116 (95%)	5 (4%)	1 (1%)	16	31
All	All	732/744 (98%)	691 (94%)	40 (6%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	23	GLY

### 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	94/91 (103%)	89 (95%)	5 (5%)	19	38
1	B	94/91 (103%)	87 (93%)	7 (7%)	11	23
1	C	94/91 (103%)	87 (93%)	7 (7%)	11	23
1	D	94/91 (103%)	89 (95%)	5 (5%)	19	38
1	E	94/91 (103%)	90 (96%)	4 (4%)	25	48
1	F	94/91 (103%)	89 (95%)	5 (5%)	19	38
All	All	564/546 (103%)	531 (94%)	33 (6%)	16	33

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	8	ARG
1	F	39	SER
1	F	113	VAL
1	C	6	THR
1	B	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	31	GLN
1	E	31	GLN
1	D	31	GLN
1	C	31	GLN
1	D	48	GLN

### 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

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.