



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:39 PM GMT

PDB ID : 3HM0  
Title : Crystal Structure of Probable Thioesterase from Bartonella henselae  
Authors : Seattle Structural Genomics Center for Infectious Diseases (SSGCID)  
Deposited on : 2009-05-28  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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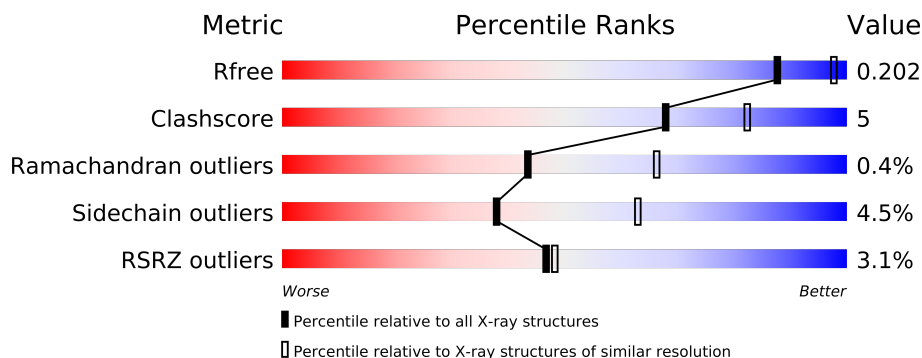
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	167	
1	B	167	
1	C	167	
1	D	167	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4045 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Probable Thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1019	651	181	184	3			
1	B	122	Total	C	N	O	S	0	0	0
			979	626	174	176	3			
1	C	124	Total	C	N	O	S	0	0	0
			987	635	174	175	3			
1	D	114	Total	C	N	O	S	0	0	0
			924	595	165	161	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q6G5R2
A	-19	ALA	-	EXPRESSION TAG	UNP Q6G5R2
A	-18	HIS	-	EXPRESSION TAG	UNP Q6G5R2
A	-17	HIS	-	EXPRESSION TAG	UNP Q6G5R2
A	-16	HIS	-	EXPRESSION TAG	UNP Q6G5R2
A	-15	HIS	-	EXPRESSION TAG	UNP Q6G5R2
A	-14	HIS	-	EXPRESSION TAG	UNP Q6G5R2
A	-13	HIS	-	EXPRESSION TAG	UNP Q6G5R2
A	-12	MET	-	EXPRESSION TAG	UNP Q6G5R2
A	-11	GLY	-	EXPRESSION TAG	UNP Q6G5R2
A	-10	THR	-	EXPRESSION TAG	UNP Q6G5R2
A	-9	LEU	-	EXPRESSION TAG	UNP Q6G5R2
A	-8	GLU	-	EXPRESSION TAG	UNP Q6G5R2
A	-7	ALA	-	EXPRESSION TAG	UNP Q6G5R2
A	-6	GLN	-	EXPRESSION TAG	UNP Q6G5R2
A	-5	THR	-	EXPRESSION TAG	UNP Q6G5R2
A	-4	GLN	-	EXPRESSION TAG	UNP Q6G5R2
A	-3	GLY	-	EXPRESSION TAG	UNP Q6G5R2
A	-2	PRO	-	EXPRESSION TAG	UNP Q6G5R2
A	-1	GLY	-	EXPRESSION TAG	UNP Q6G5R2
A	0	SER	-	EXPRESSION TAG	UNP Q6G5R2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q6G5R2
B	-19	ALA	-	EXPRESSION TAG	UNP Q6G5R2
B	-18	HIS	-	EXPRESSION TAG	UNP Q6G5R2
B	-17	HIS	-	EXPRESSION TAG	UNP Q6G5R2
B	-16	HIS	-	EXPRESSION TAG	UNP Q6G5R2
B	-15	HIS	-	EXPRESSION TAG	UNP Q6G5R2
B	-14	HIS	-	EXPRESSION TAG	UNP Q6G5R2
B	-13	HIS	-	EXPRESSION TAG	UNP Q6G5R2
B	-12	MET	-	EXPRESSION TAG	UNP Q6G5R2
B	-11	GLY	-	EXPRESSION TAG	UNP Q6G5R2
B	-10	THR	-	EXPRESSION TAG	UNP Q6G5R2
B	-9	LEU	-	EXPRESSION TAG	UNP Q6G5R2
B	-8	GLU	-	EXPRESSION TAG	UNP Q6G5R2
B	-7	ALA	-	EXPRESSION TAG	UNP Q6G5R2
B	-6	GLN	-	EXPRESSION TAG	UNP Q6G5R2
B	-5	THR	-	EXPRESSION TAG	UNP Q6G5R2
B	-4	GLN	-	EXPRESSION TAG	UNP Q6G5R2
B	-3	GLY	-	EXPRESSION TAG	UNP Q6G5R2
B	-2	PRO	-	EXPRESSION TAG	UNP Q6G5R2
B	-1	GLY	-	EXPRESSION TAG	UNP Q6G5R2
B	0	SER	-	EXPRESSION TAG	UNP Q6G5R2
C	-20	MET	-	EXPRESSION TAG	UNP Q6G5R2
C	-19	ALA	-	EXPRESSION TAG	UNP Q6G5R2
C	-18	HIS	-	EXPRESSION TAG	UNP Q6G5R2
C	-17	HIS	-	EXPRESSION TAG	UNP Q6G5R2
C	-16	HIS	-	EXPRESSION TAG	UNP Q6G5R2
C	-15	HIS	-	EXPRESSION TAG	UNP Q6G5R2
C	-14	HIS	-	EXPRESSION TAG	UNP Q6G5R2
C	-13	HIS	-	EXPRESSION TAG	UNP Q6G5R2
C	-12	MET	-	EXPRESSION TAG	UNP Q6G5R2
C	-11	GLY	-	EXPRESSION TAG	UNP Q6G5R2
C	-10	THR	-	EXPRESSION TAG	UNP Q6G5R2
C	-9	LEU	-	EXPRESSION TAG	UNP Q6G5R2
C	-8	GLU	-	EXPRESSION TAG	UNP Q6G5R2
C	-7	ALA	-	EXPRESSION TAG	UNP Q6G5R2
C	-6	GLN	-	EXPRESSION TAG	UNP Q6G5R2
C	-5	THR	-	EXPRESSION TAG	UNP Q6G5R2
C	-4	GLN	-	EXPRESSION TAG	UNP Q6G5R2
C	-3	GLY	-	EXPRESSION TAG	UNP Q6G5R2
C	-2	PRO	-	EXPRESSION TAG	UNP Q6G5R2
C	-1	GLY	-	EXPRESSION TAG	UNP Q6G5R2
C	0	SER	-	EXPRESSION TAG	UNP Q6G5R2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q6G5R2
D	-19	ALA	-	EXPRESSION TAG	UNP Q6G5R2
D	-18	HIS	-	EXPRESSION TAG	UNP Q6G5R2
D	-17	HIS	-	EXPRESSION TAG	UNP Q6G5R2
D	-16	HIS	-	EXPRESSION TAG	UNP Q6G5R2
D	-15	HIS	-	EXPRESSION TAG	UNP Q6G5R2
D	-14	HIS	-	EXPRESSION TAG	UNP Q6G5R2
D	-13	HIS	-	EXPRESSION TAG	UNP Q6G5R2
D	-12	MET	-	EXPRESSION TAG	UNP Q6G5R2
D	-11	GLY	-	EXPRESSION TAG	UNP Q6G5R2
D	-10	THR	-	EXPRESSION TAG	UNP Q6G5R2
D	-9	LEU	-	EXPRESSION TAG	UNP Q6G5R2
D	-8	GLU	-	EXPRESSION TAG	UNP Q6G5R2
D	-7	ALA	-	EXPRESSION TAG	UNP Q6G5R2
D	-6	GLN	-	EXPRESSION TAG	UNP Q6G5R2
D	-5	THR	-	EXPRESSION TAG	UNP Q6G5R2
D	-4	GLN	-	EXPRESSION TAG	UNP Q6G5R2
D	-3	GLY	-	EXPRESSION TAG	UNP Q6G5R2
D	-2	PRO	-	EXPRESSION TAG	UNP Q6G5R2
D	-1	GLY	-	EXPRESSION TAG	UNP Q6G5R2
D	0	SER	-	EXPRESSION TAG	UNP Q6G5R2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	33	Total	O	0	0
			33	33		
2	C	32	Total	O	0	0
			32	32		
2	D	37	Total	O	0	0
			37	37		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.64Å 87.85Å 96.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.01 – 2.50 40.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.01-2.50) 98.4 (40.01-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.206 , 0.268 0.207 , 0.202	Depositor DCC
$R_{free}$ test set	959 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18724 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.58	0/1040	0.66	0/1401
1	B	0.64	0/999	0.77	0/1346
1	C	0.61	0/1009	0.68	0/1362
1	D	0.67	0/944	0.69	0/1271
All	All	0.62	0/3992	0.70	0/5380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1019	0	996	10	0
1	B	979	0	939	16	0
1	C	987	0	952	12	0
1	D	924	0	896	7	0
2	A	34	0	0	0	0
2	B	33	0	0	1	0
2	C	32	0	0	1	0
2	D	37	0	0	0	0
All	All	4045	0	3783	38	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:VAL:HG13	1:B:65:GLU:H	1.34	0.92
1:C:75:HIS:HD2	2:C:176:HOH:O	1.70	0.74
1:B:64:VAL:HG13	1:B:65:GLU:N	2.07	0.69
1:A:87:ASP:OD1	1:D:51:ARG:NH2	2.29	0.65
1:D:136:LEU:HB3	1:D:137:PRO:CD	2.31	0.61
1:B:51:ARG:NH2	1:C:87:ASP:OD1	2.29	0.59
1:A:23:TYR:CE2	1:D:44:ARG:HG2	2.38	0.58
1:D:136:LEU:HB3	1:D:137:PRO:HD2	1.86	0.58
1:A:127:ILE:HD12	1:A:131:GLY:HA2	1.85	0.57
1:C:103:ARG:HD2	1:C:123:GLU:OE2	2.08	0.54
1:A:15:PHE:CE1	1:A:95:ARG:HG2	2.43	0.54
1:A:107:GLU:HG2	1:A:121:LYS:HE3	1.93	0.51
1:A:19:GLN:HA	1:A:90:LEU:O	2.11	0.50
1:D:86:ILE:O	1:D:87:ASP:HB2	2.12	0.49
1:C:93:LYS:HB2	1:C:109:TYR:HB2	1.94	0.49
1:B:42:PHE:CE1	1:B:110:ILE:HG13	2.48	0.49
1:A:23:TYR:CZ	1:D:44:ARG:HG2	2.48	0.48
1:B:39:LEU:HD12	1:B:39:LEU:N	2.29	0.47
1:B:30:SER:OG	1:B:32:VAL:HG22	2.14	0.47
1:A:93:LYS:O	1:A:108:GLN:HA	2.15	0.46
1:C:63:GLY:HA2	1:C:67:GLU:O	2.16	0.45
1:C:55:PHE:HE2	1:C:64:VAL:HG11	1.81	0.45
1:A:77:GLU:HG2	1:B:77:GLU:HG2	1.98	0.44
1:B:28:ASP:C	1:B:28:ASP:OD1	2.56	0.44
1:B:128:ASN:C	1:B:128:ASN:OD1	2.56	0.43
1:A:82:ARG:HB2	1:A:117:LEU:HA	2.00	0.43
1:B:15:PHE:CE1	1:B:109:TYR:HE2	2.36	0.43
1:B:99:LEU:HD12	1:B:104:PHE:HB3	1.99	0.43
1:B:75:HIS:HD2	2:B:168:HOH:O	2.01	0.43
1:C:76:MET:HG3	1:C:122:VAL:HG13	2.01	0.42
1:D:136:LEU:CB	1:D:137:PRO:CD	2.96	0.42
1:B:87:ASP:OD1	1:C:51:ARG:NH2	2.54	0.41
1:B:16:HIS:O	1:B:93:LYS:HA	2.21	0.41
1:C:127:ILE:HG22	1:C:133:PRO:HA	2.02	0.41
1:B:51:ARG:NH2	1:C:87:ASP:CG	2.74	0.41
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.91	0.41
1:C:51:ARG:HA	1:C:55:PHE:O	2.21	0.40
1:B:15:PHE:CZ	1:B:109:TYR:HE2	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	124/167 (74%)	118 (95%)	6 (5%)	0	100	100
1	B	118/167 (71%)	109 (92%)	7 (6%)	2 (2%)	14	22
1	C	122/167 (73%)	118 (97%)	4 (3%)	0	100	100
1	D	110/167 (66%)	103 (94%)	7 (6%)	0	100	100
All	All	474/668 (71%)	448 (94%)	24 (5%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	VAL
1	B	137	PRO

### 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	106/145 (73%)	102 (96%)	4 (4%)	44	71
1	B	99/145 (68%)	94 (95%)	5 (5%)	33	57
1	C	100/145 (69%)	95 (95%)	5 (5%)	34	58
1	D	94/145 (65%)	90 (96%)	4 (4%)	40	65
All	All	399/580 (69%)	381 (96%)	18 (4%)	38	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	43	GLU
1	A	77	GLU
1	A	121	LYS
1	B	29	PHE
1	B	77	GLU
1	B	103	ARG
1	B	130	GLU
1	B	139	GLU
1	C	29	PHE
1	C	60	LEU
1	C	81	SER
1	C	114	GLU
1	C	122	VAL
1	D	29	PHE
1	D	103	ARG
1	D	106	MET
1	D	128	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	128	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	126/167 (75%)	-0.23	1 (0%) 83 84	19, 36, 55, 61	0
1	B	122/167 (73%)	-0.07	3 (2%) 54 57	19, 35, 64, 77	0
1	C	124/167 (74%)	0.01	4 (3%) 45 47	19, 36, 66, 77	0
1	D	114/167 (68%)	0.11	7 (6%) 21 20	17, 32, 75, 83	0
All	All	486/668 (72%)	-0.05	15 (3%) 47 48	17, 35, 65, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	101	GLY	3.5
1	D	102	ALA	3.0
1	D	130	GLU	2.8
1	D	69	LEU	2.7
1	B	62	SER	2.6
1	B	66	GLY	2.5
1	C	14	ALA	2.5
1	B	59	LEU	2.5
1	A	99	LEU	2.3
1	D	126	LEU	2.3
1	D	129	GLU	2.2
1	D	134	ARG	2.1
1	C	65	GLU	2.1
1	C	101	GLY	2.0
1	C	104	PHE	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.