Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 10:53 PM EDT

PDB ID	:	2PH3
Title	:	Crystal structure of 3-oxoacyl-[acyl carrier protein] reductase TTHA0415 from Thermus thermophilus
Authors	:	Swindell II, J.T.; Chen, L.; Zhu, J.; Ebihara, A.; Shinkai, A.; Kuramitsu, S.; Yokoyama, S.; Fu, Z.-Q.; Chrzas, J.; Rose, J.P.; Wang, B.C.; Southeast Collaboratory for Structural Genomics (SECSG); RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-04-10
Resolution	:	1.91 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

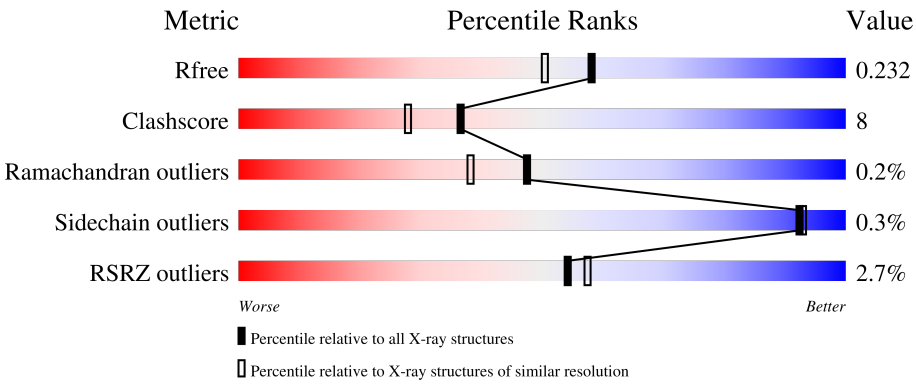
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 <=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	245	4% 87% 10% • •
1	B	245	2% 83% 13% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3809 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 3-oxoacyl-[acyl carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	1841	1155	335	345	6	0	0	0
			Total	C	N	O	S			
1	B	237	1780	1117	322	336	5	0	0	0

- Molecule 2 is water.

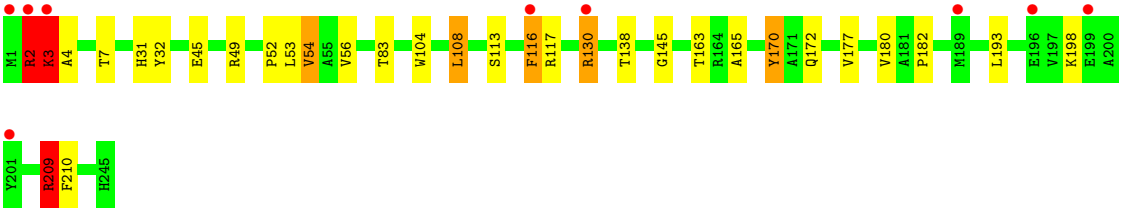
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	94	94	94	0	0
			Total	O		
2	B	94	94	94	0	0

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.

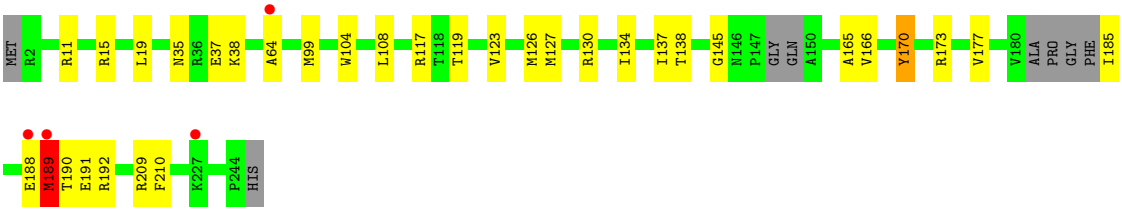
• Molecule 1: 3-oxoacyl-[acyl carrier protein] reductase

Chain A:



• Molecule 1: 3-oxoacyl-[acyl carrier protein] reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	76.53Å 76.53Å 137.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.67 – 1.91 19.67 – 1.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.67-1.91) 99.9 (19.67-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	20.81 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.229 0.199 , 0.232	Depositor DCC
R_{free} test set	1763 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.155 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3809	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.23	10/1863 (0.5%)	2.13	21/2517 (0.8%)
1	B	0.93	3/1797 (0.2%)	0.89	8/2426 (0.3%)
All	All	1.09	13/3660 (0.4%)	1.64	29/4943 (0.6%)

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	A	1	7
1	B	0	1
All	All	1	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	TYR	CB-CG	-18.84	1.23	1.51
1	A	130	ARG	CZ-NH2	-18.72	1.08	1.33
1	A	130	ARG	CZ-NH1	-16.36	1.11	1.33
1	B	189	MET	CA-CB	-15.44	1.20	1.53
1	A	130	ARG	CD-NE	-13.73	1.23	1.46
1	A	54	VAL	CA-CB	-7.64	1.38	1.54
1	B	137	ILE	C-N	-7.42	1.17	1.34
1	A	209	ARG	C-N	7.01	1.50	1.34
1	A	2	ARG	C-O	5.97	1.34	1.23
1	A	3	LYS	CB-CG	-5.87	1.36	1.52
1	B	170	TYR	CA-CB	-5.64	1.41	1.53
1	A	117	ARG	CD-NE	-5.50	1.37	1.46
1	A	2	ARG	N-CA	-5.27	1.35	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	ARG	NE-CZ-NH1	66.24	153.42	120.30
1	A	130	ARG	NE-CZ-NH2	-57.89	91.35	120.30
1	A	3	LYS	CB-CA-C	16.81	144.01	110.40
1	A	2	ARG	N-CA-C	16.05	154.33	111.00
1	A	3	LYS	N-CA-CB	-14.13	85.17	110.60
1	A	2	ARG	NE-CZ-NH1	13.73	127.17	120.30
1	B	138	THR	O-C-N	-12.17	103.23	122.70
1	A	170	TYR	CA-CB-CG	11.37	135.00	113.40
1	A	209	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	A	170	TYR	CB-CA-C	9.74	129.87	110.40
1	A	2	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	117	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	B	170	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	B	209	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	A	209	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	B	138	THR	CA-C-N	8.27	135.40	117.20
1	A	2	ARG	CB-CA-C	-7.98	94.45	110.40
1	A	108	LEU	CA-CB-CG	-7.74	97.51	115.30
1	A	3	LYS	CA-CB-CG	7.61	130.15	113.40
1	A	2	ARG	C-N-CA	7.53	140.52	121.70
1	A	54	VAL	CG1-CB-CG2	-7.19	99.40	110.90
1	B	189	MET	CB-CA-C	7.18	124.76	110.40
1	B	170	TYR	CB-CG-CD2	7.12	125.28	121.00
1	A	130	ARG	CD-NE-CZ	6.97	133.36	123.60
1	B	209	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	54	VAL	CA-CB-CG2	-6.79	100.72	110.90
1	A	2	ARG	CA-C-N	-5.85	104.33	117.20
1	B	138	THR	C-N-CA	5.85	136.32	121.70
1	A	2	ARG	CD-NE-CZ	5.24	130.94	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	ARG	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	PHE	Mainchain
1	A	130	ARG	Sidechain
1	A	170	TYR	Sidechain
1	A	2	ARG	Mainchain,Peptide
1	A	209	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	3	LYS	Peptide
1	B	170	TYR	Sidechain

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	1841	0	1886	23	0
1	B	1780	0	1822	40	1
2	A	94	0	0	0	0
2	B	94	0	0	0	0
All	All	3809	0	3708	58	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 8.

All (58) 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:185:ILE:HG22	1:B:210:PHE:CD1	2.12	0.85
1:B:104:TRP:CZ2	1:B:108:LEU:HD11	2.12	0.85
1:B:185:ILE:HG21	1:B:210:PHE:CE1	2.14	0.82
1:B:127:MET:O	1:B:130:ARG:NH1	2.12	0.81
1:A:172:GLN:CB	1:A:172:GLN:CD	2.50	0.81
1:B:185:ILE:CG2	1:B:210:PHE:CD1	2.64	0.80
1:B:123:VAL:HA	1:B:126:MET:HE2	1.65	0.78
1:B:104:TRP:CE2	1:B:108:LEU:CD1	2.69	0.75
1:B:104:TRP:CE2	1:B:108:LEU:HD12	2.22	0.74
1:A:2:ARG:HH22	1:A:52:PRO:HG2	1.52	0.73
1:B:11:ARG:HH21	1:B:38:LYS:NZ	1.87	0.72
1:B:188:GLU:HG3	1:B:190:THR:H	1.58	0.69
1:B:104:TRP:CZ2	1:B:108:LEU:CD1	2.76	0.69
1:B:119:THR:HG23	1:B:134:ILE:HD13	1.77	0.67
1:A:116:PHE:CD1	1:B:104:TRP:CE3	2.85	0.65
1:B:126:MET:CE	1:B:134:ILE:HD11	2.28	0.64
1:B:185:ILE:HG21	1:B:210:PHE:CD1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:MET:HE3	1:B:134:ILE:HD11	1.82	0.62
1:A:113:SER:O	1:A:116:PHE:HB3	2.01	0.61
1:B:185:ILE:HG22	1:B:210:PHE:HD1	1.63	0.61
1:A:172:GLN:CB	1:A:172:GLN:NE2	2.65	0.60
1:B:189:MET:CB	1:B:189:MET:SD	2.91	0.58
1:B:11:ARG:HH21	1:B:38:LYS:HZ3	1.52	0.56
1:B:104:TRP:NE1	1:B:108:LEU:HD12	2.19	0.56
1:A:116:PHE:CE1	1:B:99:MET:SD	2.99	0.56
1:B:185:ILE:CG2	1:B:210:PHE:CE1	2.85	0.55
1:B:185:ILE:HG21	1:B:210:PHE:HE1	1.69	0.53
1:B:123:VAL:CA	1:B:126:MET:HE2	2.36	0.53
1:A:172:GLN:CB	1:A:172:GLN:HE21	2.21	0.53
1:B:189:MET:O	1:B:192:ARG:HB2	2.10	0.51
1:A:104:TRP:CE2	1:A:108:LEU:HD13	2.46	0.51
1:A:116:PHE:HE1	1:B:99:MET:SD	2.34	0.51
1:B:166:VAL:HG12	1:B:177:VAL:HG21	1.91	0.51
1:A:4:ALA:HB2	1:A:83:THR:HB	1.94	0.49
1:A:2:ARG:HG3	1:A:3:LYS:HG3	1.95	0.49
1:B:35:ASN:OD1	1:B:37:GLU:HG3	2.13	0.48
1:A:138:THR:O	1:A:182:PRO:HD2	2.13	0.48
1:A:193:LEU:O	1:A:198:LYS:HE3	2.13	0.48
1:B:185:ILE:CG2	1:B:210:PHE:HD1	2.17	0.47
1:A:7:THR:HA	1:A:31:HIS:HB3	1.97	0.47
1:A:2:ARG:NH2	1:A:52:PRO:HG2	2.27	0.47
1:A:209:ARG:HG2	1:A:210:PHE:O	2.15	0.47
1:B:37:GLU:HG3	1:B:38:LYS:N	2.29	0.46
1:B:126:MET:HE1	1:B:134:ILE:HD11	1.96	0.46
1:A:45:GLU:O	1:A:49:ARG:HG3	2.17	0.45
1:A:180:VAL:O	1:A:182:PRO:HD3	2.16	0.45
1:A:163:THR:HG23	1:A:177:VAL:HG12	1.98	0.44
1:A:145:GLY:O	1:B:165:ALA:HA	2.17	0.44
1:B:11:ARG:NH2	1:B:38:LYS:NZ	2.62	0.44
1:A:165:ALA:HA	1:B:145:GLY:O	2.18	0.43
1:B:35:ASN:OD1	1:B:37:GLU:CG	2.66	0.43
1:B:104:TRP:NE1	1:B:108:LEU:CD1	2.79	0.43
1:B:37:GLU:HG3	1:B:38:LYS:H	1.84	0.43
1:A:32:TYR:HE2	1:A:56:VAL:HG12	1.84	0.42
1:B:64:ALA:HA	1:B:117:ARG:NH2	2.36	0.41
1:B:11:ARG:HH21	1:B:38:LYS:HZ1	1.64	0.41
1:B:15:ARG:NH1	1:B:19:LEU:HD11	2.36	0.41
1:A:53:LEU:C	1:A:54:VAL:HG23	2.42	0.41

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:B:173:ARG:NH1	1:B:191:GLU:OE2[3_775]	1.79	0.41

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	243/245 (99%)	234 (96%)	9 (4%)	0	100	100
1	B	231/245 (94%)	220 (95%)	10 (4%)	1 (0%)	34	24
All	All	474/490 (97%)	454 (96%)	19 (4%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	MET

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	182/183 (100%)	181 (100%)	1 (0%)	88	89
1	B	176/183 (96%)	176 (100%)	0	100	100
All	All	358/366 (98%)	357 (100%)	1 (0%)	92	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	234	GLN
1	A	245	HIS
1	B	86	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 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	137:ILE	C	138:THR	N	1.17

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	245/245 (100%)	-0.03	9 (3%)	41	44	8, 14, 29, 34	0
1	B	237/245 (96%)	-0.06	4 (1%)	70	72	7, 15, 28, 37	0
All	All	482/490 (98%)	-0.05	13 (2%)	54	57	7, 15, 29, 37	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	MET	5.8
1	A	1	MET	4.9
1	B	64	ALA	3.7
1	B	188	GLU	3.3
1	A	196	GLU	3.0
1	A	2	ARG	2.9
1	A	189	MET	2.8
1	A	201	TYR	2.4
1	A	116	PHE	2.3
1	B	227	LYS	2.2
1	A	199	GLU	2.1
1	A	130	ARG	2.1
1	A	3	LYS	2.1

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 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.