



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:46 am GMT

PDB ID : 1PXT
Title : THE 2.8 ANGSTROMS STRUCTURE OF PEROXISOMAL 3-KETOACYL-COA THIOLASE OF SACCHAROMYCES CEREVISIAE: A FIVE LAYERED A-B-A-B-A STRUCTURE, CONSTRUCTED FROM TWO CORE DOMAINS OF IDENTICAL TOPOLOGY
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Deposited on : 1994-07-04
Resolution : 2.80 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

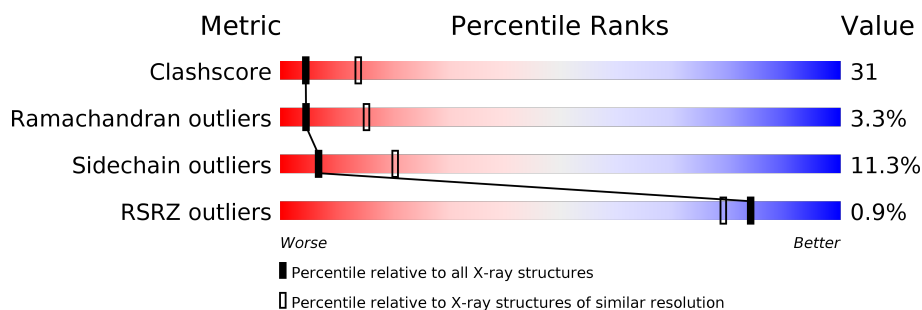
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	390	<div> <div></div> <div> <div></div> <div>43%</div> <div>39%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	390	<div> <div></div> <div> <div></div> <div>37%</div> <div>44%</div> <div>8%</div> <div>11%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5201 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.

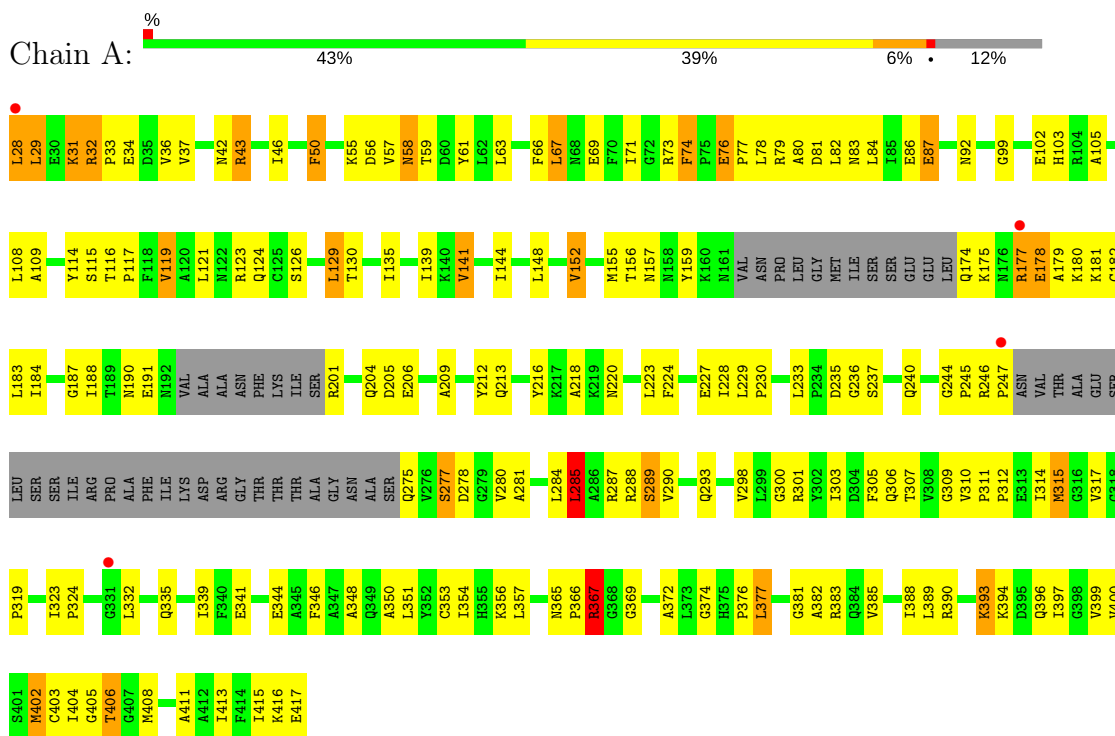
- Molecule 1 is a protein called PEROXISOMAL 3-KETOACYL-COA THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2585	1634	452	486	13			
1	B	348	Total	C	N	O	S	0	0	0
			2616	1651	457	495	13			

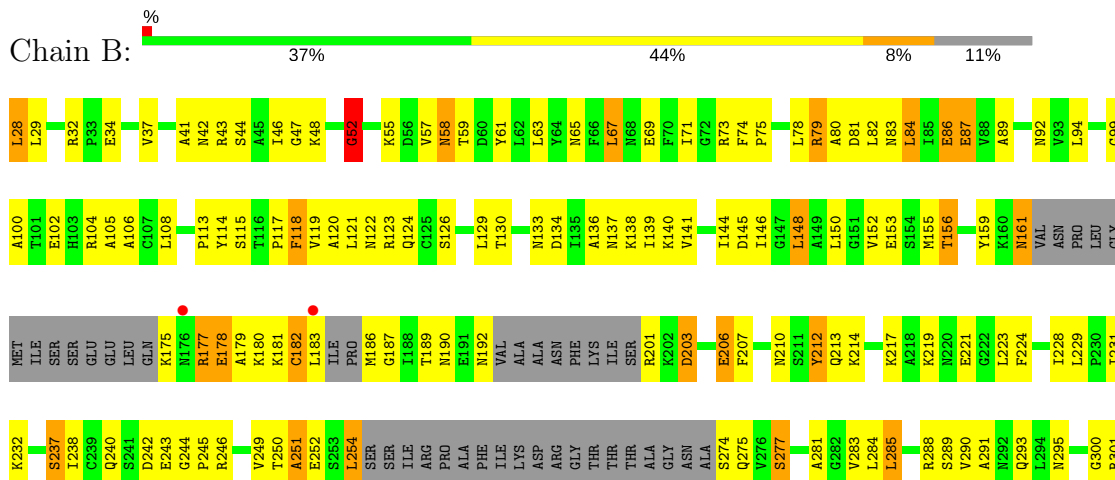
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: PEROXISOMAL 3-KETOACYL-COA THIOLASE



• Molecule 1: PEROXISOMAL 3-KETOACYL-COA THIOLASE



Y302	L377
I303	G378
D304	C379
F305	
Q306	R383
T307	
V308	I388
G309	L389
V310	R390
P311	E391
P312	L392
E313	K393
I314	K394
H315	D395
	Q396
P319	
A320	V399
Y321	V400
A322	S401
I323	M402
	C403
V326	I404
L327	G405
E328	T406
	G407
Q335	M408
D336	G409
I337	A410
D338	A411
I339	A412
F340	I413
E341	E414
I342	I415
N343	K416
E344	E417
A345	
F346	
A347	
A348	
Q349	
C353	
I354	
H355	
K356	
I359	
D360	
L361	
N362	
K363	
V364	
N365	
P366	
A370	
I371	
	G374

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.78Å 93.72Å 120.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 23.89 – 2.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 90.1 (23.89-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.75Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , 0.334 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 104.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.62	0/2622	0.87	4/3543 (0.1%)
1	B	0.64	0/2651	0.90	2/3581 (0.1%)
All	All	0.63	0/5273	0.89	6/7124 (0.1%)

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	B	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	VAL	CB-CA-C	-5.65	100.67	111.40
1	B	121	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	285	LEU	CA-CB-CG	5.35	127.59	115.30
1	B	52	GLY	N-CA-C	5.33	126.41	113.10
1	A	119	VAL	CB-CA-C	-5.21	101.49	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	321	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	2585	0	2628	157	0
1	B	2616	0	2655	183	0
All	All	5201	0	5283	327	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 31.

The worst 5 of 327 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:28:LEU:HD21	1:A:332:LEU:HD21	1.27	1.06
1:A:50:PHE:H	1:A:156:THR:HG22	1.20	1.00
1:A:28:LEU:HD11	1:A:332:LEU:HD11	1.47	0.94
1:B:81:ASP:HB3	1:B:84:LEU:HD12	1.45	0.94
1:B:63:LEU:HD11	1:B:150:LEU:HD13	1.50	0.92

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	335/390 (86%)	279 (83%)	46 (14%)	10 (3%)	5	17
1	B	338/390 (87%)	302 (89%)	24 (7%)	12 (4%)	4	13
All	All	673/780 (86%)	581 (86%)	70 (10%)	22 (3%)	4	15

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	B	177	ARG
1	B	178	GLU
1	B	182	CYS
1	B	251	ALA

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	273/311 (88%)	248 (91%)	25 (9%)	11	30
1	B	277/311 (89%)	240 (87%)	37 (13%)	4	13
All	All	550/622 (88%)	488 (89%)	62 (11%)	7	20

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	ASN
1	B	118	PHE
1	B	366	PRO
1	B	84	LEU
1	B	141	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN
1	B	58	ASN
1	B	192	ASN
1	A	335	GLN
1	B	213	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 carbohydrates 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, 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	343/390 (87%)	-0.45	4 (1%) 79 72	3, 25, 49, 70	0
1	B	348/390 (89%)	-0.55	2 (0%) 89 86	3, 20, 43, 65	0
All	All	691/780 (88%)	-0.50	6 (0%) 84 79	3, 23, 46, 70	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	LEU	2.7
1	A	247	PRO	2.4
1	A	331	GLY	2.3
1	A	28	LEU	2.3
1	B	176	ASN	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 carbohydrates 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.