Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 10:11 AM EDT

PDB ID	:	2Q2B
Title	:	Crystal structure of the C-terminal domain of mouse acyl-CoA thioesterase 7
Authors	:	Guncar, G.; Forwood, J.K.; Kobe, B.
Deposited on	:	2007-05-27
Resolution	:	2.50 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 (1)) were used in the production of this report:

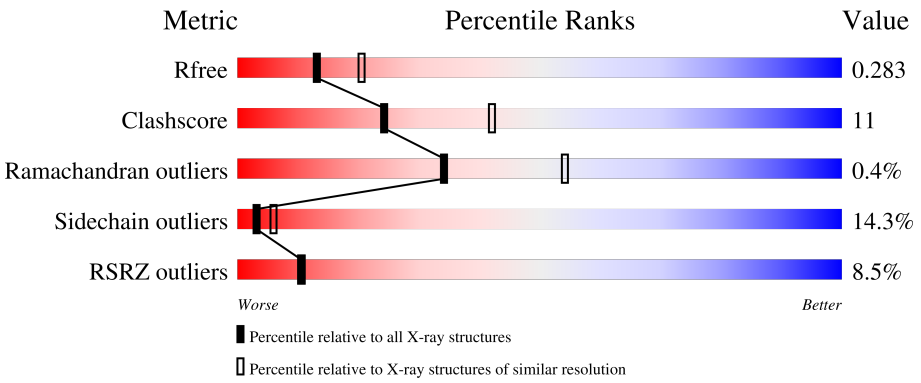
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 >=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	179	8%; 64%; 13%; •; 21%
1	B	179	6%; 53%; 21%; 5%; 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2242 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 Cytosolic acyl coenzyme A thioester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1095	689	191	207	8	0	0	0
			Total	C	N	O	S			
1	B	141	1092	688	189	207	8	38	0	0

- Molecule 2 is water.

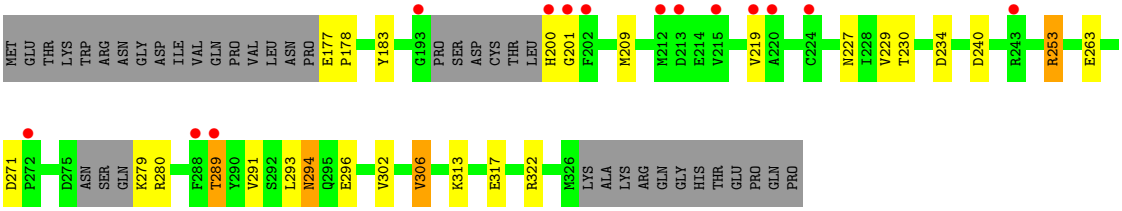
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	31	31	31	0	0
			Total	O		
2	B	24	24	24	0	0

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.

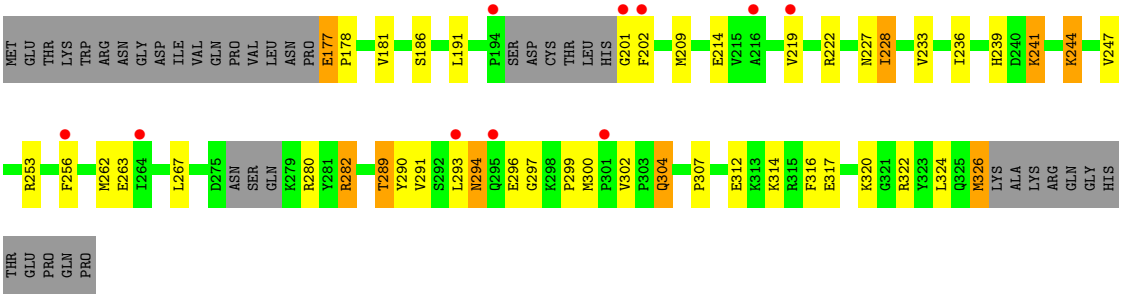
• Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

Chain A:



• Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	136.74Å 136.74Å 99.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.39 – 2.50 28.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.39-2.50) 99.9 (28.38-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.288 0.218 , 0.283	Depositor DCC
R_{free} test set	629 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2242	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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	0.51	0/1113	0.63	0/1498
1	B	0.58	0/1110	0.63	0/1495
All	All	0.55	0/2223	0.63	0/2993

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	HIS	Peptide

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	1095	0	1096	15	0
1	B	1092	0	1096	33	0
2	A	31	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	0	3	0
All	All	2242	0	2192	47	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 11.

All (47) 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:201:GLY:O	1:B:202:PHE:HD1	1.52	0.91
1:B:201:GLY:O	1:B:202:PHE:CD1	2.30	0.84
1:B:201:GLY:HA3	1:B:244:LYS:HD2	1.66	0.76
1:B:177:GLU:N	2:B:40:HOH:O	2.22	0.72
1:A:294:ASN:C	1:A:294:ASN:HD22	1.95	0.70
1:B:256:PHE:HD2	1:B:316:PHE:CE1	2.13	0.67
1:A:253:ARG:HG2	2:A:11:HOH:O	1.98	0.63
1:B:263:GLU:OE1	1:B:322:ARG:NH1	2.35	0.60
1:B:294:ASN:HD22	1:B:296:GLU:H	1.49	0.59
1:B:201:GLY:N	1:B:244:LYS:HZ3	2.00	0.59
1:B:201:GLY:HA3	1:B:244:LYS:CD	2.33	0.56
1:A:289:THR:HG22	2:A:4:HOH:O	2.04	0.55
1:B:256:PHE:CD2	1:B:316:PHE:CE1	2.94	0.55
1:B:177:GLU:N	1:B:178:PRO:CD	2.69	0.55
1:A:279:LYS:CD	1:A:280:ARG:H	2.21	0.54
1:B:201:GLY:C	1:B:202:PHE:CD1	2.82	0.53
1:A:279:LYS:HD3	1:A:280:ARG:H	1.72	0.53
1:B:289:THR:HG22	2:B:3:HOH:O	2.08	0.52
1:A:227:ASN:ND2	1:A:293:LEU:O	2.35	0.51
1:B:324:LEU:O	1:B:326:MET:HG3	2.12	0.50
1:B:228:ILE:HD12	1:B:290:TYR:HD2	1.78	0.49
1:B:241:LYS:HD3	1:B:241:LYS:H	1.77	0.49
1:A:177:GLU:N	1:A:178:PRO:CD	2.76	0.49
1:B:291:VAL:HG13	1:B:299:PRO:HB3	1.94	0.49
1:A:294:ASN:ND2	1:A:296:GLU:H	2.12	0.48
1:B:293:LEU:HD22	1:B:297:GLY:O	2.14	0.47
1:B:304:GLN:OE1	1:B:304:GLN:HA	2.15	0.47
1:B:267:LEU:HD13	1:B:282:ARG:NH1	2.31	0.46
1:B:262:MET:O	1:B:289:THR:HA	2.17	0.45
1:A:263:GLU:OE1	1:A:322:ARG:NH1	2.49	0.45
1:B:181:VAL:HG21	1:B:312:GLU:HG2	1.98	0.45
1:B:186:SER:OG	1:B:222:ARG:NH1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:HD22	1:A:296:GLU:H	1.65	0.44
1:A:294:ASN:C	1:A:294:ASN:ND2	2.68	0.44
1:B:263:GLU:CD	1:B:322:ARG:NH1	2.71	0.44
1:B:326:MET:SD	2:B:7:HOH:O	2.61	0.44
1:B:307:PRO:HB3	1:B:312:GLU:HB3	2.00	0.44
1:B:241:LYS:H	1:B:241:LYS:CD	2.31	0.43
1:A:306:VAL:O	1:A:306:VAL:CG1	2.67	0.43
1:B:233:VAL:HG11	1:B:236:ILE:HD11	2.01	0.43
1:B:201:GLY:N	1:B:244:LYS:NZ	2.68	0.42
1:A:200:HIS:HB3	2:A:23:HOH:O	2.19	0.41
1:B:177:GLU:N	1:B:178:PRO:HD3	2.35	0.41
1:A:177:GLU:O	1:A:183:TYR:HB2	2.21	0.41
1:B:228:ILE:HD13	1:B:291:VAL:O	2.21	0.41
1:A:209:MET:HE2	1:B:209:MET:HB3	2.03	0.40
1:B:267:LEU:HD22	1:B:282:ARG:HH11	1.86	0.40

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	135/179 (75%)	132 (98%)	2 (2%)	1 (1%)	22 39
1	B	135/179 (75%)	127 (94%)	8 (6%)	0	100 100
All	All	270/358 (75%)	259 (96%)	10 (4%)	1 (0%)	34 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	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	122/157 (78%)	108 (88%)	14 (12%)	5 11
1	B	122/157 (78%)	101 (83%)	21 (17%)	2 3
All	All	244/314 (78%)	209 (86%)	35 (14%)	3 6

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	VAL
1	A	229	VAL
1	A	230	THR
1	A	234	ASP
1	A	240	ASP
1	A	253	ARG
1	A	271	ASP
1	A	289	THR
1	A	291	VAL
1	A	294	ASN
1	A	302	VAL
1	A	306	VAL
1	A	313	LYS
1	A	317	GLU
1	B	177	GLU
1	B	191	LEU
1	B	214	GLU
1	B	219	VAL
1	B	227	ASN
1	B	228	ILE
1	B	241	LYS
1	B	244	LYS
1	B	247	VAL
1	B	253	ARG
1	B	280	ARG
1	B	282	ARG
1	B	289	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	294	ASN
1	B	300	MET
1	B	302	VAL
1	B	304	GLN
1	B	314	LYS
1	B	317	GLU
1	B	320	LYS
1	B	326	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	294	ASN
1	A	304	GLN
1	B	239	HIS
1	B	294	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)

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	141/179 (78%)	0.41	14 (9%)	7	7	29, 38, 43, 47	1 (0%)
1	B	141/179 (78%)	0.52	10 (7%)	16	16	32, 38, 43, 48	9 (6%)
All	All	282/358 (78%)	0.47	24 (8%)	10	10	29, 38, 43, 48	10 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	PRO	5.7
1	A	243	ARG	4.8
1	A	200	HIS	3.7
1	B	295	GLN	3.2
1	A	202	PHE	3.1
1	B	201	GLY	3.0
1	A	219	VAL	2.8
1	A	224	CYS	2.6
1	B	293	LEU	2.5
1	A	272	PRO	2.4
1	B	264	ILE	2.4
1	A	288	PHE	2.4
1	A	212	MET	2.3
1	A	220	ALA	2.3
1	A	215	VAL	2.3
1	B	202	PHE	2.2
1	B	301	PRO	2.2
1	A	289	THR	2.2
1	B	216	ALA	2.2
1	A	201	GLY	2.2
1	B	256	PHE	2.2
1	A	193	GLY	2.1
1	A	213	ASP	2.1
1	B	219	VAL	2.0

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.