wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 05:20 pm BST

PDB ID	:	4O99
Title	:	Crystal structure of Beta-ketothiolase (PhaA) from Ralstonia eutropha H16
Authors	:	Kim, E.J.; Kim, J.; Kim, S.; Kim, K.J.
Deposited on	:	2014-01-02
Resolution	:	1.96 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

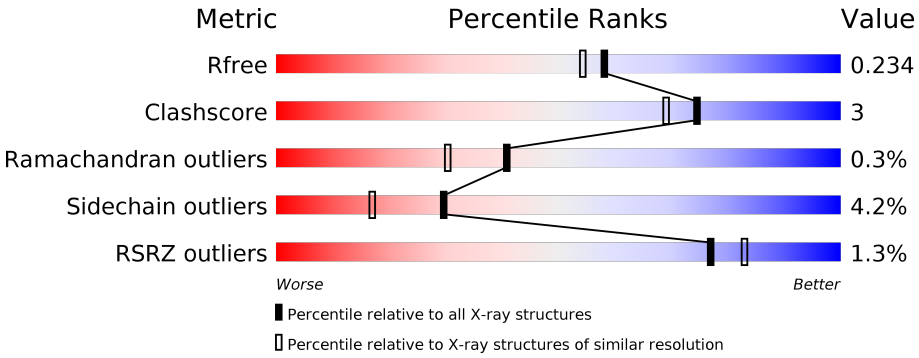
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	392	2% 92% 7%
1	B	392	% 91% 7%
1	C	392	% 90% 10%
1	D	392	% 89% 9%

2 Entry composition

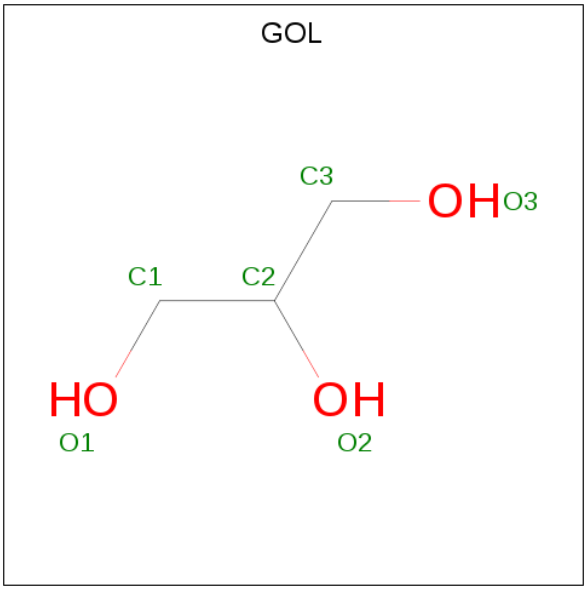
There are 3 unique types of molecules in this entry. The entry contains 12325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2827	1769	501	537	20			
1	B	392	Total	C	N	O	S	0	0	0
			2827	1769	501	537	20			
1	C	392	Total	C	N	O	S	0	0	0
			2826	1769	501	536	20			
1	D	392	Total	C	N	O	S	0	0	0
			2827	1769	501	537	20			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			6	3	3			
2	C	1	Total	C	O		0	0
			6	3	3			

- Molecule 3 is water.

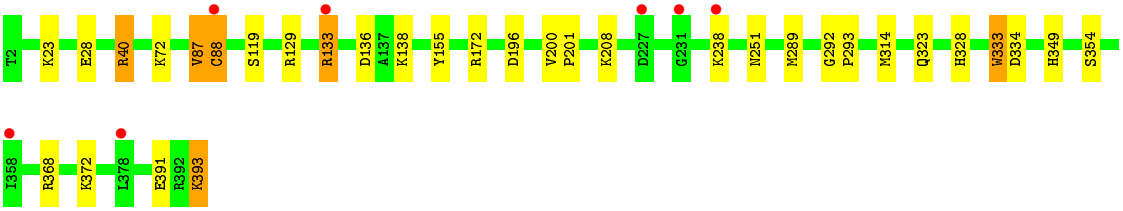
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	254	Total O 254 254	0	0
3	B	249	Total O 249 249	0	0
3	C	255	Total O 255 255	0	0
3	D	248	Total O 248 248	0	0

3 Residue-property plots (i)

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.

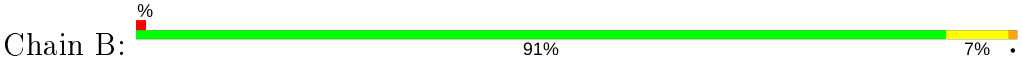
- Molecule 1: Acetyl-CoA acetyltransferase

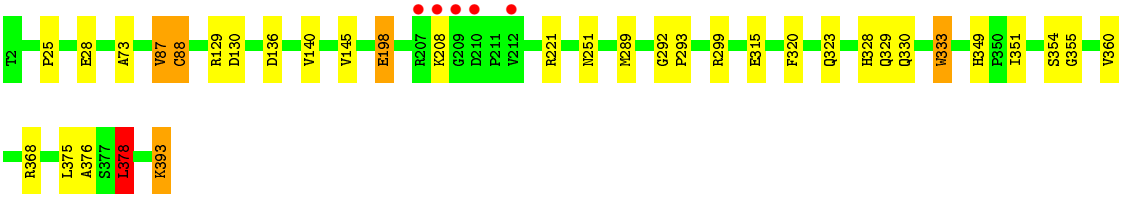
Chain A:



- Molecule 1: Acetyl-CoA acetyltransferase

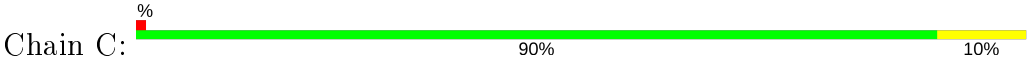
Chain B:

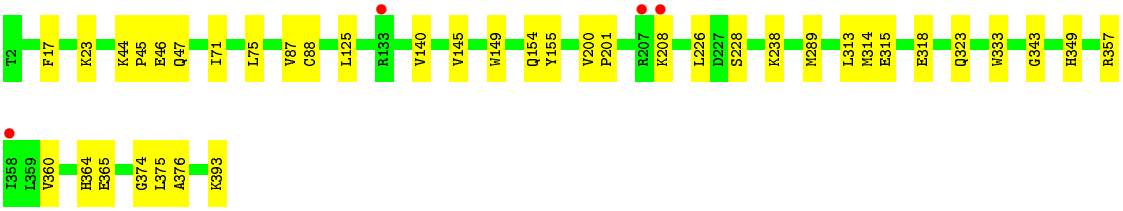




- Molecule 1: Acetyl-CoA acetyltransferase

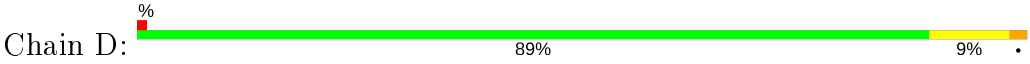
Chain C:

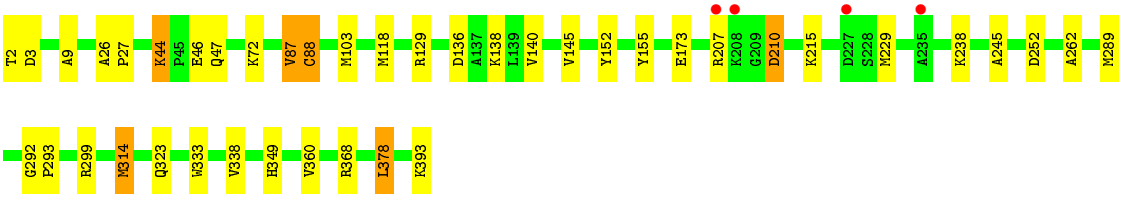




- Molecule 1: Acetyl-CoA acetyltransferase

Chain D:




T2
D3
A9
A26
P27
K44
P45
E46
Q47
K72
V87
C88
M103
M118
R129
D136
A137
K138
L139
V140
V145
Y152
Y155
E173
R207
K208
G209
D210
K215
D227
S228
M229
A235
K238
A245
D252
A262
M289

G292
P293
R299
M314
Q323
W333
V338
H349
V360
R368
L378
K393

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.38Å 105.47Å 106.91Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	30.62 – 1.96 30.62 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.62-1.96) 94.4 (30.62-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	15.71 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.171 , 0.230 0.183 , 0.234	Depositor DCC
R_{free} test set	4901 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	1.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.89	1/2867 (0.0%)	0.94	10/3876 (0.3%)
1	B	0.92	2/2867 (0.1%)	0.91	5/3876 (0.1%)
1	C	0.87	0/2866	0.90	3/3876 (0.1%)
1	D	0.88	1/2867 (0.0%)	0.90	5/3876 (0.1%)
All	All	0.89	4/11467 (0.0%)	0.91	23/15504 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	88	CYS	CB-SG	-6.71	1.70	1.82
1	A	88	CYS	CB-SG	-5.97	1.72	1.81
1	B	198	GLU	CB-CG	-5.27	1.42	1.52
1	B	88	CYS	CB-SG	-5.09	1.73	1.81

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	368	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	D	136	ASP	CB-CG-OD1	8.00	125.50	118.30
1	C	375	LEU	CA-CB-CG	7.67	132.93	115.30
1	A	334	ASP	CB-CG-OD1	6.93	124.54	118.30
1	C	357	ARG	NE-CZ-NH1	6.85	123.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2827	0	2895	17	0
1	B	2827	0	2895	22	0
1	C	2826	0	2895	18	0
1	D	2827	0	2895	21	0
2	A	6	0	8	0	0
2	C	6	0	8	0	0
3	A	254	0	0	1	0
3	B	249	0	0	2	0
3	C	255	0	0	1	0
3	D	248	0	0	2	0
All	All	12325	0	11596	74	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 3.

The worst 5 of 74 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:D:103:MET:HG2	3:D:572:HOH:O	1.35	1.22
1:D:140:VAL:HG11	1:D:145:VAL:HG21	1.68	0.75
1:B:328:HIS:HD2	1:B:333:TRP:HE1	1.35	0.73
1:D:140:VAL:CG1	1:D:145:VAL:HG21	2.21	0.70
1:C:45:PRO:HB3	1:C:75:LEU:HD23	1.77	0.66

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	390/392 (100%)	378 (97%)	11 (3%)	1 (0%)	41	30
1	B	390/392 (100%)	379 (97%)	10 (3%)	1 (0%)	41	30
1	C	390/392 (100%)	382 (98%)	7 (2%)	1 (0%)	41	30
1	D	390/392 (100%)	381 (98%)	8 (2%)	1 (0%)	41	30
All	All	1560/1568 (100%)	1520 (97%)	36 (2%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	B	87	VAL
1	C	87	VAL
1	D	87	VAL

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	284/284 (100%)	272 (96%)	12 (4%)	30	17
1	B	284/284 (100%)	277 (98%)	7 (2%)	47	38
1	C	284/284 (100%)	271 (95%)	13 (5%)	27	14
1	D	284/284 (100%)	268 (94%)	16 (6%)	21	9
All	All	1136/1136 (100%)	1088 (96%)	48 (4%)	30	17

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	125	LEU
1	C	238	LYS
1	D	323	GLN
1	C	155	TYR
1	C	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	323	GLN
1	B	349	HIS
1	D	184	ASN
1	B	328	HIS
1	B	329	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	C	401	-	5,5,5	0.56	0	5,5,5	0.56	0
2	GOL	A	401	-	5,5,5	0.44	0	5,5,5	1.45	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	GOL	O3-C3-C2	-2.70	97.26	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	392/392 (100%)	-0.18	7 (1%)	68	76	12, 20, 37, 60	0
1	B	392/392 (100%)	-0.31	5 (1%)	77	83	12, 19, 34, 63	0
1	C	392/392 (100%)	-0.27	4 (1%)	82	87	12, 19, 34, 75	0
1	D	392/392 (100%)	-0.23	4 (1%)	82	87	12, 20, 37, 60	0
All	All	1568/1568 (100%)	-0.25	20 (1%)	77	83	12, 20, 36, 75	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	ARG	4.1
1	C	207	ARG	4.1
1	C	208	LYS	3.8
1	D	207	ARG	3.2
1	D	208	LYS	3.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	401	6/6	0.87	0.12	22,32,34,35	0
2	GOL	C	401	6/6	0.96	0.09	24,26,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.