



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2017 – 10:55 AM EST

PDB ID : 4O9A
Title : Crystal structure of Beta-ketothiolase (PhaA) from Ralstonia eutropha H16
Authors : Kim, E.J.; Kim, J.; Kim, S.; Kim, K.J.
Deposited on : unknown
Resolution : 1.52 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	:	rb-20030345
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)	:	rb-20030345

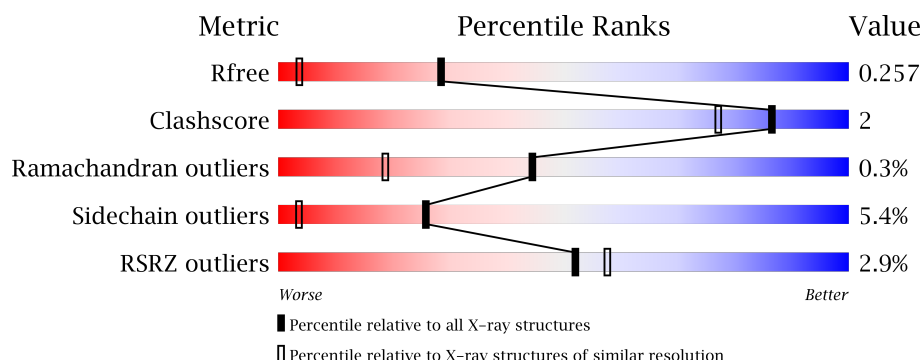
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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}	100719	2964 (1.54-1.50)
Clashscore	112137	3216 (1.54-1.50)
Ramachandran outliers	110173	3145 (1.54-1.50)
Sidechain outliers	110143	3143 (1.54-1.50)
RSRZ outliers	101464	2990 (1.54-1.50)

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 ≥ 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	398	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	398	<div> <div>3%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	C	398	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	D	398	<div> <div>4%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11616 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	538	19			
1	B	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	C	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	D	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P14611
A	-3	HIS	-	EXPRESSION TAG	UNP P14611
A	-2	HIS	-	EXPRESSION TAG	UNP P14611
A	-1	HIS	-	EXPRESSION TAG	UNP P14611
A	0	HIS	-	EXPRESSION TAG	UNP P14611
A	1	HIS	-	EXPRESSION TAG	UNP P14611
A	88	SER	CYS	ENGINEERED MUTATION	UNP P14611
B	-4	HIS	-	EXPRESSION TAG	UNP P14611
B	-3	HIS	-	EXPRESSION TAG	UNP P14611
B	-2	HIS	-	EXPRESSION TAG	UNP P14611
B	-1	HIS	-	EXPRESSION TAG	UNP P14611
B	0	HIS	-	EXPRESSION TAG	UNP P14611
B	1	HIS	-	EXPRESSION TAG	UNP P14611
B	88	SER	CYS	ENGINEERED MUTATION	UNP P14611
C	-4	HIS	-	EXPRESSION TAG	UNP P14611
C	-3	HIS	-	EXPRESSION TAG	UNP P14611
C	-2	HIS	-	EXPRESSION TAG	UNP P14611
C	-1	HIS	-	EXPRESSION TAG	UNP P14611
C	0	HIS	-	EXPRESSION TAG	UNP P14611
C	1	HIS	-	EXPRESSION TAG	UNP P14611
C	88	SER	CYS	ENGINEERED MUTATION	UNP P14611

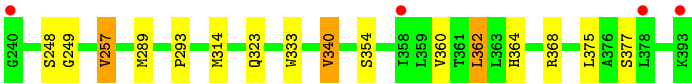
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	EXPRESSION TAG	UNP P14611
D	-3	HIS	-	EXPRESSION TAG	UNP P14611
D	-2	HIS	-	EXPRESSION TAG	UNP P14611
D	-1	HIS	-	EXPRESSION TAG	UNP P14611
D	0	HIS	-	EXPRESSION TAG	UNP P14611
D	1	HIS	-	EXPRESSION TAG	UNP P14611
D	88	SER	CYS	ENGINEERED MUTATION	UNP P14611

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	0	0
2	B	102	Total O 102 102	0	0
2	C	62	Total O 62 62	0	0
2	D	65	Total O 65 65	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.27Å 104.70Å 106.91Å 90.00° 106.12° 90.00°	Depositor
Resolution (Å)	27.86 – 1.52 27.86 – 1.52	Depositor EDS
% Data completeness (in resolution range)	91.2 (27.86-1.52) 91.2 (27.86-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.254 0.222 , 0.257	Depositor DCC
R_{free} test set	10085 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11616	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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 [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	0.95	0/2867	1.05	6/3876 (0.2%)
1	B	0.95	1/2867 (0.0%)	1.03	12/3876 (0.3%)
1	C	0.92	0/2867	1.03	13/3876 (0.3%)
1	D	0.89	0/2867	1.01	16/3876 (0.4%)
All	All	0.93	1/11468 (0.0%)	1.03	47/15504 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	ASP	CB-CG	5.42	1.63	1.51

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	340	VAL	CG1-CB-CG2	8.99	125.29	110.90
1	A	257	VAL	CG1-CB-CG2	8.82	125.02	110.90
1	B	257	VAL	CG1-CB-CG2	8.56	124.59	110.90
1	D	221	ARG	NE-CZ-NH1	8.55	124.57	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2827	0	2895	13	0
1	B	2827	0	2895	17	0
1	C	2827	0	2895	19	0
1	D	2827	0	2895	14	0
2	A	79	0	0	0	0
2	B	102	0	0	2	0
2	C	62	0	0	0	0
2	D	65	0	0	3	0
All	All	11616	0	11580	57	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 2.

The worst 5 of 57 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:44:LYS:H	1:D:47:GLN:HE21	1.35	0.72
1:D:364:HIS:HE1	2:D:445:HOH:O	1.75	0.69
1:B:364:HIS:HE1	2:B:453:HOH:O	1.79	0.65
1:B:222:GLN:HE21	1:B:222:GLN:H	1.47	0.61
1:B:392:ARG:O	1:B:393:LYS:CD	2.48	0.60

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	390/398 (98%)	379 (97%)	10 (3%)	1 (0%)	44 19
1	B	390/398 (98%)	380 (97%)	9 (2%)	1 (0%)	44 19
1	C	390/398 (98%)	379 (97%)	10 (3%)	1 (0%)	44 19
1	D	390/398 (98%)	375 (96%)	14 (4%)	1 (0%)	44 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1560/1592 (98%)	1513 (97%)	43 (3%)	4 (0%)	44 19

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 ⓘ

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	284/290 (98%)	268 (94%)	16 (6%)	25 3
1	B	284/290 (98%)	269 (95%)	15 (5%)	26 4
1	C	284/290 (98%)	269 (95%)	15 (5%)	26 4
1	D	284/290 (98%)	269 (95%)	15 (5%)	26 4
All	All	1136/1160 (98%)	1075 (95%)	61 (5%)	26 3

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	333	TRP
1	C	216	THR
1	D	323	GLN
1	B	340	VAL
1	B	393	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	364	HIS
1	D	154	GLN
1	B	154	GLN
1	D	184	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 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	392/398 (98%)	0.01	7 (1%) 69 74	10, 16, 30, 59	0
1	B	392/398 (98%)	0.02	12 (3%) 49 55	9, 17, 32, 55	0
1	C	392/398 (98%)	0.13	12 (3%) 49 55	10, 18, 34, 58	0
1	D	392/398 (98%)	0.11	15 (3%) 41 46	11, 19, 33, 66	0
All	All	1568/1592 (98%)	0.07	46 (2%) 52 58	9, 17, 33, 66	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	ARG	6.2
1	B	207	ARG	5.2
1	C	207	ARG	4.2
1	D	209	GLY	4.0
1	A	208	LYS	4.0

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 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.