

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8AFG
Title	:	K352D oxalyl-CoA synthetase Pcs60p
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Deposited on	:	2022-07-17
Resolution	:	2.45 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
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.45 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	1544 (2.48-2.44)		
Clashscore	141614	1613 (2.48-2.44)		
Ramachandran outliers	138981	1598 (2.48-2.44)		
Sidechain outliers	138945	1598 (2.48-2.44)		
RSRZ outliers	127900	1523 (2.48-2.44)		

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	А	543	8%	9%	10%
1	В	543	[%] 71% 6% •	219	%



$8 \mathrm{AFG}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7369 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 Oxalate–CoA ligase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	486	Total	С	Ν	0	S	0	0	0
-	1 11	100	3826	2460	645	704	17	Ŭ		
1	В	497	Total	С	Ν	0	\mathbf{S}	0	0	0
		421	3366	2162	571	618	15	0		0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	В	1	Total 5	0 4	S 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	73	Total O 73 73	0	0
3	В	79	Total O 79 79	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: Oxalate–CoA ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	59.93Å 125.60Å 80.50Å	Deperitor
a, b, c, α , β , γ	90.00° 96.93° 90.00°	Depositor
Bosolution(A)	47.09 - 2.45	Depositor
Resolution (A)	47.05 - 2.45	EDS
% Data completeness	99.9 (47.09-2.45)	Depositor
(in resolution range)	99.9 (47.05-2.45)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.51 (at 2.45 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
B B.	0.206 , 0.247	Depositor
II, II, <i>free</i>	0.206 , 0.247	DCC
R_{free} test set	2241 reflections $(5.16%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.2	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.34, 32.6	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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).

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.57	2/3922~(0.1%)	0.99	5/5327~(0.1%)	
1	В	0.52	0/3453	0.97	10/4695~(0.2%)	
All	All	0.55	2/7375~(0.0%)	0.98	15/10022~(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	А	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	27	GLU	CD-OE1	6.46	1.32	1.25
1	А	332	GLU	CD-OE1	6.10	1.32	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	107	ASP	CB-CA-C	7.24	124.88	110.40
1	В	305	ARG	CG-CD-NE	-6.96	97.17	111.80
1	А	254	ARG	CG-CD-NE	-6.54	98.07	111.80
1	В	61	ARG	CB-CA-C	6.47	123.34	110.40
1	А	254	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	В	61	ARG	CB-CG-CD	6.00	127.20	111.60
1	В	9	ALA	CB-CA-C	5.72	118.68	110.10
1	В	305	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	А	27	GLU	N-CA-CB	5.59	120.67	110.60



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	305	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	В	61	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	А	259	VAL	CA-CB-CG2	5.46	119.09	110.90
1	В	107	ASP	CB-CA-C	5.36	121.12	110.40
1	В	387	ARG	CB-CG-CD	-5.33	97.75	111.60
1	В	254	ARG	CG-CD-NE	-5.07	101.16	111.80

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There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	461	GLU	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	А	3826	0	3809	18	0
1	В	3366	0	3345	21	0
2	А	15	0	0	1	0
2	В	10	0	0	0	0
3	А	73	0	0	0	0
3	В	79	0	0	2	0
All	All	7369	0	7154	38	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.

All (38) 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:80:LEU:HB3	1:B:84:MET:HE2	1.81	0.63
1:A:116:PRO:O	1:A:119:THR:HG23	2.01	0.60
1:A:459:ILE:HD11	1:A:493:LEU:HD11	1.86	0.57
1:A:252:THR:HG21	1:A:259:VAL:HG23	1.88	0.56



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	overlap (Å)
1:B:80:LEU:O	1:B:84:MET:HG3	2.07	0.55
1:A:259:VAL:HG13	1:A:261:VAL:CG2	2.38	0.54
1:A:221:ILE:HD13	1:A:247:GLY:HA2	1.90	0.52
1:A:271:TRP:CG	1:A:298:PRO:HD3	2.45	0.52
1:B:221:ILE:HD13	1:B:247:GLY:HA2	1.92	0.51
1:A:80:LEU:HD22	1:A:84:MET:CE	2.40	0.51
1:A:259:VAL:HG13	1:A:261:VAL:HG22	1.90	0.51
1:B:243:HIS:HA	1:B:341:HIS:CE1	2.46	0.50
1:A:243:HIS:HA	1:A:341:HIS:CE1	2.46	0.50
1:B:120:THR:HA	1:B:128:LEU:HD11	1.93	0.49
1:A:80:LEU:O	1:A:84:MET:HG3	2.12	0.49
1:A:120:THR:HA	1:A:128:LEU:HD11	1.95	0.49
1:B:116:PRO:HG3	3:B:743:HOH:O	2.15	0.47
1:B:196:HIS:HA	1:B:205:LYS:O	2.15	0.46
1:A:465:PHE:O	1:A:476:VAL:HA	2.15	0.46
1:B:61:ARG:HH11	1:B:61:ARG:HG2	1.81	0.46
1:B:238:PRO:HB3	1:B:240:PHE:CZ	2.51	0.45
1:B:252:THR:HG21	1:B:259:VAL:HG13	1.99	0.45
1:B:271:TRP:CG	1:B:298:PRO:HD3	2.51	0.45
1:B:24:ILE:HB	1:B:260:VAL:HG22	1.98	0.45
1:A:235:VAL:HG22	1:A:248:VAL:HG11	1.99	0.44
1:A:24:ILE:HB	1:A:260:VAL:HG22	1.98	0.44
1:B:235:VAL:HG22	1:B:248:VAL:HG11	2.00	0.44
1:B:266:HIS:HB2	1:B:269:LEU:HB2	2.00	0.43
1:A:80:LEU:HD22	1:A:84:MET:HE3	1.99	0.43
1:A:147:ARG:HD2	2:A:601:SO4:O1	2.18	0.43
1:B:80:LEU:HD22	1:B:84:MET:HE2	2.00	0.43
1:B:409:ARG:HG2	1:B:410:GLU:HG2	2.00	0.43
1:A:238:PRO:HB3	1:A:240:PHE:CE2	2.53	0.43
1:B:80:LEU:HB3	1:B:84:MET:CE	2.47	0.43
1:B:238:PRO:HB3	1:B:240:PHE:CE2	2.54	0.42
1:A:411:ASN:HB2	1:B:61:ARG:HD2	2.02	0.42
1:B:196:HIS:HB2	3:B:769:HOH:O	2.21	0.40
1:B:225:TYR:O	1:B:305:ARG:NH2	2.33	0.40

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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	Percen	tiles
1	А	478/543~(88%)	462 (97%)	15 (3%)	1 (0%)	47	57
1	В	423/543 (78%)	415 (98%)	7 (2%)	1 (0%)	47	57
All	All	901/1086 (83%)	877 (97%)	22 (2%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	341	HIS
1	В	341	HIS

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	А	428/476~(90%)	406 (95%)	22~(5%)	24 31
1	В	377/476~(79%)	368~(98%)	9 (2%)	49 61
All	All	805/952~(85%)	774 (96%)	31 (4%)	32 42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	8	THR
1	А	27	GLU
1	А	35	ARG
1	А	61	ARG



	J	1	1 5
Mol	Chain	Res	Type
1	А	132	SER
1	А	167	ARG
1	А	259	VAL
1	А	268	LYS
1	А	387	ARG
1	А	397	ASN
1	А	450	ASP
1	A	452	ILE
1	А	454	LEU
1	А	455	SER
1	А	458	LYS
1	А	460	ASP
1	А	463	VAL
1	А	469	ASP
1	А	470	ASP
1	А	471	MET
1	А	491	GLU
1	А	506	ILE
1	В	13	ASP
1	В	61	ARG
1	В	132	SER
1	В	162	LYS
1	В	289	SER
1	В	397	ASN
1	В	409	ARG
1	В	411	ASN
1	В	437	ILE

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	474	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	SO4	В	602	-	4,4,4	0.35	0	$6,\!6,\!6$	0.18	0
2	SO4	А	603	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	А	602	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	В	601	-	4,4,4	0.38	0	6,6,6	0.29	0
2	SO4	А	601	-	4,4,4	0.37	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain Res Ty		Type	Clashes	Symm-Clashes	
2	А	601	SO4	1	0	

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, 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	486/543~(89%)	0.23	45 (9%) 8 5	25, 39, 102, 157	0
1	В	427/543~(78%)	-0.11	7 (1%) 72 69	26, 41, 64, 105	0
All	All	913/1086~(84%)	0.07	52 (5%) 23 20	25, 40, 88, 157	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	472	TYR	9.5
1	А	475	VAL	7.8
1	А	493	LEU	7.5
1	А	471	MET	7.2
1	В	436	LEU	6.3
1	А	459	ILE	6.1
1	А	490	TYR	6.0
1	А	440	GLY	5.8
1	А	473	GLY	5.5
1	А	438	ASN	5.5
1	А	491	GLU	5.4
1	А	203	THR	5.0
1	А	489	THR	4.2
1	А	460	ASP	4.1
1	А	444	ILE	4.1
1	А	506	ILE	3.9
1	А	463	VAL	3.6
1	В	437	ILE	3.5
1	А	447	ILE	3.3
1	А	439	ARG	3.3
1	A	455	SER	3.3
1	А	452	ILE	3.2
1	A	437	ILE	3.2
1	A	470	ASP	3.2



Mol	Chain	\mathbf{Res}	Type	RSRZ	
1	А	465	PHE	3.2	
1	А	504	PHE	3.1	
1	А	453	MET	3.1	
1	В	203	THR	3.1	
1	А	505	LYS	3.1	
1	А	457	PRO	3.1	
1	А	478	ALA	3.0	
1	А	503	SER	3.0	
1	А	454	LEU	3.0	
1	А	495	ASN	2.8	
1	А	492	GLU	2.8	
1	А	496	PHE	2.8	
1	А	443	LYS	2.8	
1	В	9	ALA	2.8	
1	А	461	GLU	2.7	
1	А	476	VAL	2.6	
1	А	462	ALA	2.5	
1	А	469	ASP	2.5	
1	А	468	PRO	2.5	
1	А	494	VAL	2.4	
1	В	350	PRO	2.3	
1	А	202	SER	2.3	
1	А	467	VAL	2.3	
1	В	438	ASN	2.2	
1	А	498	LYS	2.2	
1	А	456	HIS	2.2	
1	В	311	SER	2.1	
1	А	507	PRO	2.1	

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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)

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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	SO4	А	603	5/5	0.82	0.30	84,102,108,109	0
2	SO4	А	602	5/5	0.93	0.10	84,86,94,96	0
2	SO4	А	601	5/5	0.94	0.14	69,73,75,76	0
2	SO4	В	602	5/5	0.96	0.17	83,84,85,98	0
2	SO4	В	601	5/5	0.98	0.12	45,47,47,49	0

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.

6.5 Other polymers (i)

There are no such residues in this entry.

