



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8AFG / pdb_00008afg
Title : K352D oxalyl-CoA synthetase Pcs60p
Authors : Burgi, J.; Chojnowski, G.; Wilmanns, M.
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

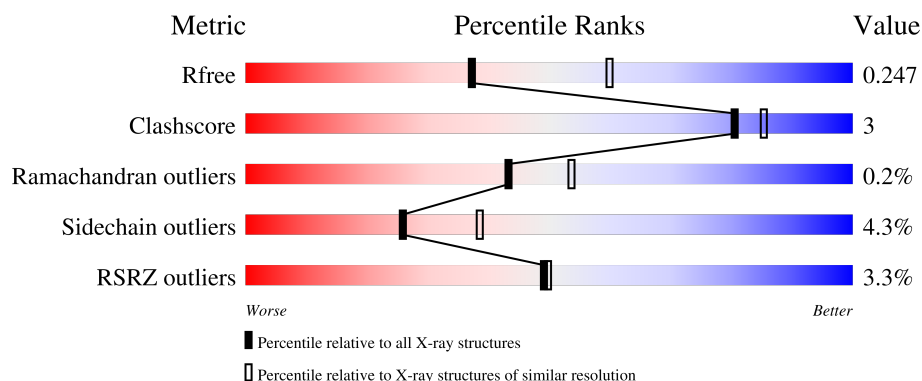
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 $\leq 5\%$. 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	543	5% 78% 11% 10%
1	B	543	% 69% 8% 21%

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	A	486	Total	C	N	O	S	0	0	0
			3826	2460	645	704	17			
1	B	427	Total	C	N	O	S	0	0	0
			3366	2162	571	618	15			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	79	Total	O	0	0
			79	79		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.93Å 125.60Å 80.50Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	47.09 – 2.45 47.09 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.09-2.45) 99.9 (47.09-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.247 0.206 , 0.247	Depositor DCC
R_{free} test set	2242 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/3922	1.36	22/5327 (0.4%)
1	B	0.73	1/3453 (0.0%)	1.35	16/4695 (0.3%)
All	All	0.74	1/7375 (0.0%)	1.36	38/10022 (0.4%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	39	HIS	CD2-NE2	5.78	1.44	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	CB-CA-C	9.00	123.34	109.84
1	A	287	THR	CB-CA-C	8.00	124.07	110.79
1	A	107	ASP	CB-CA-C	7.57	124.88	109.67
1	B	61	ARG	CB-CG-CD	6.91	127.20	111.30
1	A	27	GLU	CB-CG-CD	6.90	124.33	112.60
1	B	436	LEU	CA-C-N	6.83	129.91	121.71
1	B	436	LEU	C-N-CA	6.83	129.91	121.71
1	B	305	ARG	CG-CD-NE	-6.74	97.17	112.00
1	A	27	GLU	N-CA-CB	6.70	120.67	110.28
1	A	450	ASP	CA-CB-CG	6.69	119.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASN	CB-CA-C	6.47	120.10	111.82
1	A	203	THR	CB-CA-C	6.40	119.30	109.50
1	A	254	ARG	CG-CD-NE	-6.33	98.07	112.00
1	B	422	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	422	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	387	ARG	CB-CG-CD	-5.89	97.75	111.30
1	B	158	GLU	CB-CG-CD	5.89	122.61	112.60
1	B	107	ASP	CB-CA-C	5.70	121.12	109.67
1	A	388	GLY	CA-C-N	5.54	128.47	120.38
1	A	388	GLY	C-N-CA	5.54	128.47	120.38
1	A	158	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	325	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	504	PHE	CA-CB-CG	5.49	119.29	113.80
1	B	104	TYR	CB-CA-C	5.49	119.58	110.90
1	B	9	ALA	CB-CA-C	5.45	118.68	110.50
1	A	35	ARG	CB-CG-CD	5.42	123.76	111.30
1	B	337	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	119	THR	CB-CA-C	5.36	119.68	110.79
1	A	492	GLU	CB-CG-CD	5.35	121.70	112.60
1	A	373	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	19	ASP	CB-CA-C	5.17	119.75	110.81
1	B	408	LYS	CB-CA-C	5.13	119.30	110.79
1	A	259	VAL	CA-CB-CG2	5.11	119.09	110.40
1	A	11	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	134	PHE	CB-CA-C	5.07	119.45	109.72
1	B	388	GLY	CA-C-N	5.06	127.57	120.28
1	B	388	GLY	C-N-CA	5.06	127.57	120.28
1	A	162	LYS	CB-CA-C	5.05	119.80	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	GLU	Peptide

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	3826	0	3809	18	0
1	B	3366	0	3345	21	0
2	A	15	0	0	1	0
2	B	10	0	0	0	0
3	A	73	0	0	0	0
3	B	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:HD22	1:B:84:MET:HE2	1.83	0.61
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
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:B:84:MET:HE1	1:B:182:PHE:CD2	2.43	0.53
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:80:LEU:HD22	1:A:84:MET:HE3	1.98	0.44
1:A:235:VAL:HG22	1:A:248:VAL:HG11	1.99	0.44
1:B:80:LEU:HB3	1:B:84:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:ARG:HD2	2:A:601:SO4:O1	2.18	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: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

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	478/543 (88%)	462 (97%)	15 (3%)	1 (0%)	43	54
1	B	423/543 (78%)	415 (98%)	7 (2%)	1 (0%)	43	54
All	All	901/1086 (83%)	877 (97%)	22 (2%)	2 (0%)	43	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	HIS
1	B	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	A	428/476 (90%)	405 (95%)	23 (5%)	20	29
1	B	377/476 (79%)	365 (97%)	12 (3%)	34	49
All	All	805/952 (85%)	770 (96%)	35 (4%)	26	38

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

Mol	Chain	Res	Type
1	A	8	THR
1	A	27	GLU
1	A	61	ARG
1	A	99	LYS
1	A	119	THR
1	A	132	SER
1	A	181	LYS
1	A	259	VAL
1	A	268	LYS
1	A	387	ARG
1	A	397	ASN
1	A	449	LEU
1	A	450	ASP
1	A	452	ILE
1	A	454	LEU
1	A	455	SER
1	A	458	LYS
1	A	460	ASP
1	A	463	VAL
1	A	467	VAL
1	A	469	ASP
1	A	470	ASP
1	A	506	ILE
1	B	13	ASP
1	B	61	ARG
1	B	84	MET
1	B	162	LYS
1	B	205	LYS
1	B	287	THR
1	B	289	SER
1	B	324	LYS
1	B	354	LYS
1	B	397	ASN

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Mol	Chain	Res	Type
1	B	411	ASN
1	B	437	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	A	477	GLN
1	B	52	ASN
1	B	171	ASN
1	B	241	HIS
1	B	347	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 oligosaccharides 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	A	601	-	4,4,4	0.27	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	602	-	4,4,4	0.31	0	6,6,6	0.10	0
2	SO4	B	602	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	B	601	-	4,4,4	0.31	0	6,6,6	0.28	0
2	SO4	A	603	-	4,4,4	0.34	0	6,6,6	0.24	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	Type	Clashes	Symm-Clashes
2	A	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

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, 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	486/543 (89%)	-0.09	26 (5%) 32 30	25, 39, 102, 157	0
1	B	427/543 (78%)	-0.31	4 (0%) 81 82	26, 41, 64, 105	0
All	All	913/1086 (84%)	-0.20	30 (3%) 49 50	25, 40, 88, 157	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ILE	4.7
1	B	437	ILE	4.5
1	A	203	THR	3.8
1	A	478	ALA	3.6
1	A	457	PRO	3.5
1	B	199	GLY	3.4
1	A	472	TYR	3.2
1	A	475	VAL	3.1
1	B	313	ALA	2.9
1	A	471	MET	2.9
1	A	506	ILE	2.8
1	A	452	ILE	2.7
1	A	467	VAL	2.7
1	A	454	LEU	2.7
1	A	462	ALA	2.7
1	A	507	PRO	2.6
1	A	199	GLY	2.6
1	A	468	PRO	2.4
1	A	458	LYS	2.4
1	A	463	VAL	2.4
1	A	499	LYS	2.4
1	A	459	ILE	2.3
1	A	465	PHE	2.2
1	A	455	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	2.1
1	A	8	THR	2.0
1	A	494	VAL	2.0
1	A	489	THR	2.0
1	A	202	SER	2.0
1	B	303	HIS	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 oligosaccharides 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, median, 95th 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	SO4	A	603	5/5	0.77	0.18	84,102,108,109	0
2	SO4	B	602	5/5	0.88	0.10	83,84,85,98	0
2	SO4	A	601	5/5	0.89	0.12	69,73,75,76	0
2	SO4	A	602	5/5	0.92	0.08	84,86,94,96	0
2	SO4	B	601	5/5	0.97	0.06	45,47,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.