



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:34 PM UTC

PDB ID : 4TLF / pdb_00004tlf
Title : Crystal structure of Thiol dioxygenase from Pseudomonas aeruginosa
Authors : Fellner, M.; Tchesnokov, E.P.; Jameson, G.N.L.; Wilbanks, S.M.
Deposited on : 2014-05-29
Resolution : 2.14 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 ⓘ 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
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

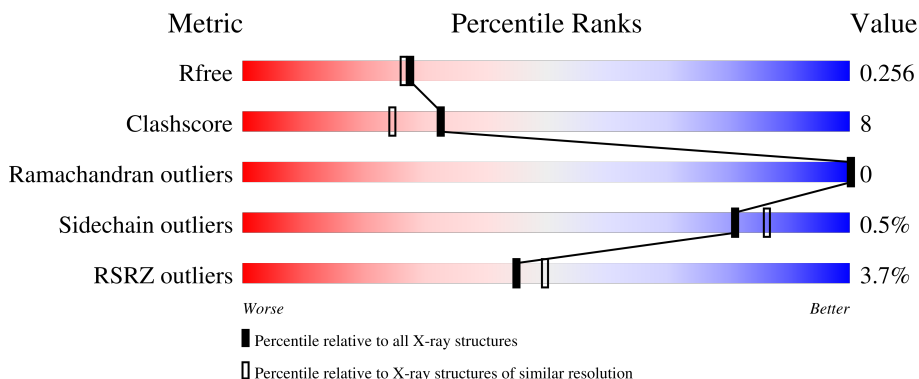
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	211	0% 81% 11% 8%
1	B	211	2% 77% 14% 9%
1	C	211	3% 75% 17% 7%
1	D	211	7% 82% 11% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6826 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 3-mercaptopropionate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1546	972	287	285	2			
1	B	193	Total	C	N	O	S	0	0	0
			1537	967	286	282	2			
1	C	196	Total	C	N	O	S	0	0	0
			1562	982	290	288	2			
1	D	198	Total	C	N	O	S	0	0	0
			1574	990	292	290	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	SER	-	expression tag	UNP Q9I0N5
A	203	ALA	-	expression tag	UNP Q9I0N5
A	204	TRP	-	expression tag	UNP Q9I0N5
A	205	SER	-	expression tag	UNP Q9I0N5
A	206	HIS	-	expression tag	UNP Q9I0N5
A	207	PRO	-	expression tag	UNP Q9I0N5
A	208	GLN	-	expression tag	UNP Q9I0N5
A	209	PHE	-	expression tag	UNP Q9I0N5
A	210	GLU	-	expression tag	UNP Q9I0N5
A	211	LYS	-	expression tag	UNP Q9I0N5
B	202	SER	-	expression tag	UNP Q9I0N5
B	203	ALA	-	expression tag	UNP Q9I0N5
B	204	TRP	-	expression tag	UNP Q9I0N5
B	205	SER	-	expression tag	UNP Q9I0N5
B	206	HIS	-	expression tag	UNP Q9I0N5
B	207	PRO	-	expression tag	UNP Q9I0N5
B	208	GLN	-	expression tag	UNP Q9I0N5
B	209	PHE	-	expression tag	UNP Q9I0N5
B	210	GLU	-	expression tag	UNP Q9I0N5
B	211	LYS	-	expression tag	UNP Q9I0N5
C	202	SER	-	expression tag	UNP Q9I0N5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	203	ALA	-	expression tag	UNP Q9I0N5
C	204	TRP	-	expression tag	UNP Q9I0N5
C	205	SER	-	expression tag	UNP Q9I0N5
C	206	HIS	-	expression tag	UNP Q9I0N5
C	207	PRO	-	expression tag	UNP Q9I0N5
C	208	GLN	-	expression tag	UNP Q9I0N5
C	209	PHE	-	expression tag	UNP Q9I0N5
C	210	GLU	-	expression tag	UNP Q9I0N5
C	211	LYS	-	expression tag	UNP Q9I0N5
D	202	SER	-	expression tag	UNP Q9I0N5
D	203	ALA	-	expression tag	UNP Q9I0N5
D	204	TRP	-	expression tag	UNP Q9I0N5
D	205	SER	-	expression tag	UNP Q9I0N5
D	206	HIS	-	expression tag	UNP Q9I0N5
D	207	PRO	-	expression tag	UNP Q9I0N5
D	208	GLN	-	expression tag	UNP Q9I0N5
D	209	PHE	-	expression tag	UNP Q9I0N5
D	210	GLU	-	expression tag	UNP Q9I0N5
D	211	LYS	-	expression tag	UNP Q9I0N5

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

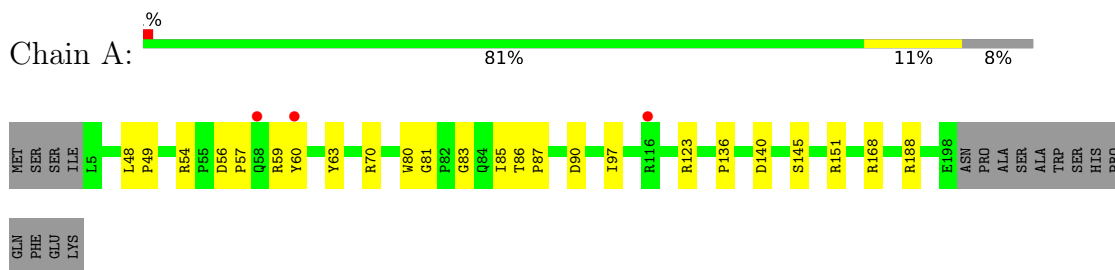
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	165	Total O 165 165	0	0
3	B	150	Total O 150 150	0	0
3	C	156	Total O 156 156	0	0
3	D	132	Total O 132 132	0	0

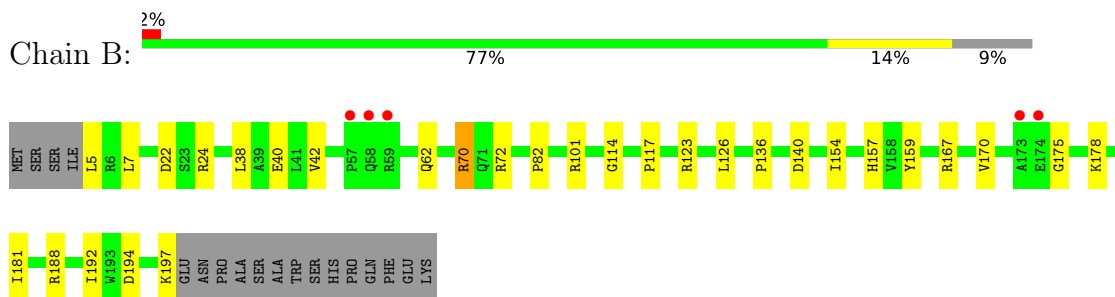
3 Residue-property plots [i](#)

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.

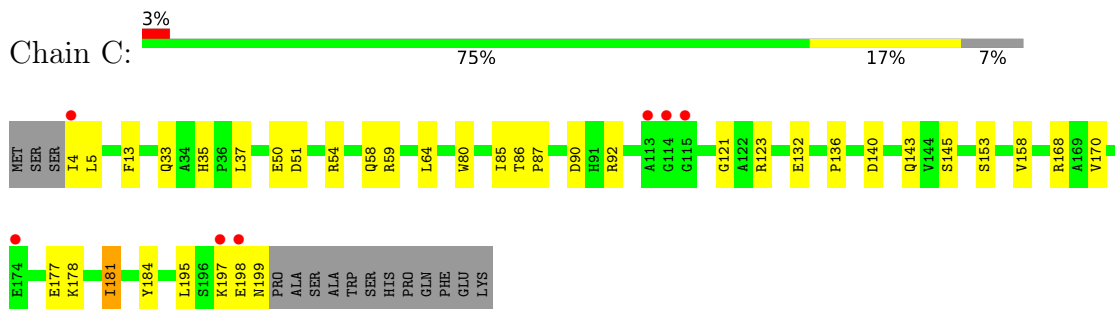
- Molecule 1: 3-mercaptopropionate dioxygenase



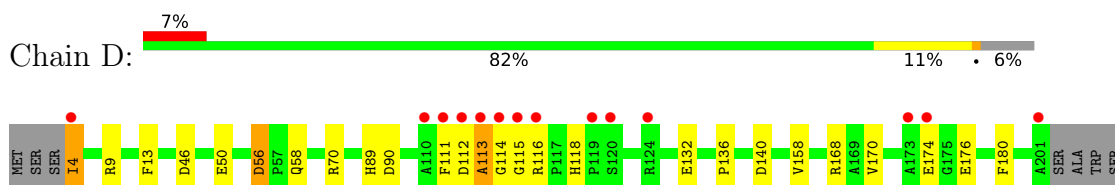
- Molecule 1: 3-mercaptopropionate dioxygenase



- Molecule 1: 3-mercaptopropionate dioxygenase



- Molecule 1: 3-mercaptopropionate dioxygenase



HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.94Å 66.94Å 377.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.30 – 2.14 44.30 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.30-2.14) 99.7 (44.30-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.251 0.211 , 0.256	Depositor DCC
R_{free} test set	2487 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: FE2

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	0.56	0/1588	0.90	0/2159
1	B	0.54	0/1579	0.90	2/2147 (0.1%)
1	C	0.58	0/1604	0.91	2/2181 (0.1%)
1	D	0.56	1/1617 (0.1%)	0.86	3/2200 (0.1%)
All	All	0.56	1/6388 (0.0%)	0.89	7/8687 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	115	GLY	C-O	-6.18	1.18	1.24

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	HIS	CA-C-N	-6.46	113.03	119.56
1	C	35	HIS	C-N-CA	-6.46	113.03	119.56
1	D	113	ALA	N-CA-C	-5.59	104.57	111.33
1	B	114	GLY	CA-C-N	-5.53	116.86	123.44
1	B	114	GLY	C-N-CA	-5.53	116.86	123.44

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	1546	0	1494	24	0
1	B	1537	0	1488	25	0
1	C	1562	0	1511	28	0
1	D	1574	0	1523	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	165	0	0	8	1
3	B	150	0	0	12	3
3	C	156	0	0	10	2
3	D	132	0	0	6	0
All	All	6826	0	6016	97	3

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 8.

The worst 5 of 97 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:174:GLU:OE1	1:D:176:GLU:HG2	1.56	1.04
1:D:112:ASP:O	1:D:114:GLY:O	1.97	0.81
1:B:40:GLU:OE2	3:B:401:HOH:O	2.03	0.77
1:D:56:ASP:OD2	3:D:401:HOH:O	2.03	0.77
1:B:123:ARG:NH1	3:B:405:HOH:O	2.22	0.72

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:481:HOH:O	3:B:527:HOH:O[7_645]	2.15	0.05
3:B:541:HOH:O	3:C:517:HOH:O[7_555]	2.15	0.05
3:B:442:HOH:O	3:C:533:HOH:O[7_555]	2.19	0.01

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	192/211 (91%)	186 (97%)	6 (3%)	0	100	100
1	B	191/211 (90%)	184 (96%)	7 (4%)	0	100	100
1	C	194/211 (92%)	186 (96%)	8 (4%)	0	100	100
1	D	196/211 (93%)	190 (97%)	6 (3%)	0	100	100
All	All	773/844 (92%)	746 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	164/179 (92%)	164 (100%)	0	100	100
1	B	163/179 (91%)	162 (99%)	1 (1%)	78	84
1	C	166/179 (93%)	165 (99%)	1 (1%)	78	84
1	D	167/179 (93%)	166 (99%)	1 (1%)	78	84
All	All	660/716 (92%)	657 (100%)	3 (0%)	81	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	ARG
1	C	181	ILE
1	D	4	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	43	HIS
1	D	61	GLN
1	D	142	HIS

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	194/211 (91%)	-0.07	3 (1%) 72 76	12, 22, 40, 55	0
1	B	193/211 (91%)	-0.02	5 (2%) 57 61	12, 23, 40, 59	0
1	C	196/211 (92%)	0.10	7 (3%) 46 51	13, 22, 47, 74	0
1	D	198/211 (93%)	0.20	14 (7%) 22 25	13, 24, 52, 80	0
All	All	781/844 (92%)	0.05	29 (3%) 45 50	12, 23, 45, 80	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	115	GLY	6.4
1	D	201	ALA	4.9
1	B	57	PRO	4.2
1	C	114	GLY	4.0
1	A	58	GLN	3.4

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($\text{\AA}^2$)	Q<0.9
2	FE2	D	301	1/1	0.98	0.05	30,30,30,30	0
2	FE2	C	301	1/1	0.99	0.02	22,22,22,22	0
2	FE2	A	301	1/1	1.00	0.01	26,26,26,26	0
2	FE2	B	301	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.