

Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 10:29 PM EST

PDB ID : 8GQI

> Title : Structure of Thiolase from Pseudomonas aeruginosa PAO1

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2022-08-30 Deposited on

2.21 Å(reported) Resolution

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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

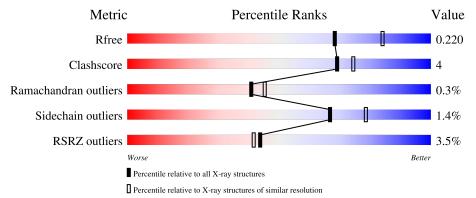
Validation Pipeline (wwPDB-VP) 2.36

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 2.21 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	A	409	91%	7%	-
1	В	409	89%	9%	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6160 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 Thiolase.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Δ	401	Total	С	N	О	S	0	0	0
1	Λ	401	2958	1838	554	554	12	U	U	0
1	D	400	Total	С	N	О	S	0	0	0
1	Ъ	400	2947	1832	550	553	12	0	U	U

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	LEU	-	expression tag	UNP Q9HY37
A	403	GLU	-	expression tag	UNP Q9HY37
A	404	HIS	-	expression tag	UNP Q9HY37
A	405	HIS	-	expression tag	UNP Q9HY37
A	406	HIS	-	expression tag	UNP Q9HY37
A	407	HIS	-	expression tag	UNP Q9HY37
A	408	HIS	-	expression tag	UNP Q9HY37
A	409	HIS	-	expression tag	UNP Q9HY37
В	402	LEU	-	expression tag	UNP Q9HY37
В	403	GLU	-	expression tag	UNP Q9HY37
В	404	HIS	-	expression tag	UNP Q9HY37
В	405	HIS	-	expression tag	UNP Q9HY37
В	406	HIS	-	expression tag	UNP Q9HY37
В	407	HIS	-	expression tag	UNP Q9HY37
В	408	HIS	-	expression tag	UNP Q9HY37
В	409	HIS	-	expression tag	UNP Q9HY37

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





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

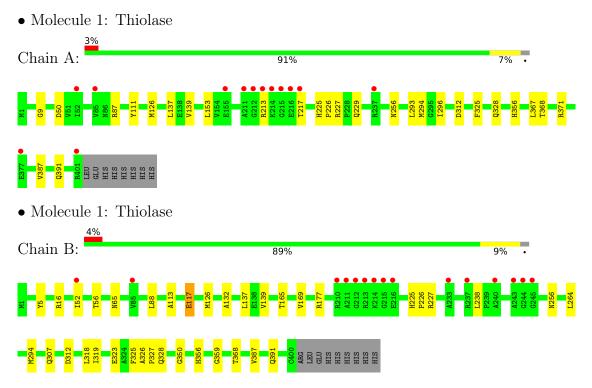
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	126	Total O 126 126	0	0
3	В	111	Total O 111 111	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants	177.37Å 177.37Å 70.59Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.39 - 2.21	Depositor
Resolution (A)	40.36 - 2.21	EDS
% Data completeness	99.2 (40.39-2.21)	Depositor
(in resolution range)	99.3 (40.36-2.21)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.214	Depositor
it, it free	0.184 , 0.220	DCC
R_{free} test set	2757 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 44.1	EDS
L-test for twinning ²	$< L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6160	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: 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	
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.78	0/2998	0.93	1/4057 (0.0%)
1	В	0.76	0/2987	0.93	1/4043 (0.0%)
All	All	0.77	0/5985	0.93	2/8100 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	В	117	GLU	CB-CA-C	-7.16	96.07	110.40
1	A	371	ARG	NE-CZ-NH1	7.04	123.82	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	2958	0	2996	18	0
1	В	2947	0	2983	26	0
2	A	6	0	8	2	0
2	В	12	0	16	1	0
3	A	126	0	0	0	0
3	В	111	0	0	3	0
All	All	6160	0	6003	44	0



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:126:MET:HG2	1:B:139:VAL:HG22	1.61	0.83
1:B:126:MET:CG	1:B:139:VAL:HG22	2.23	0.69
1:B:325:PHE:H	1:B:328:GLN:HE21	1.40	0.67
1:A:325:PHE:H	1:A:328:GLN:HE21	1.46	0.61
1:A:126:MET:HG2	1:A:139:VAL:HG22	1.84	0.59
1:B:132:ALA:O	3:B:601:HOH:O	2.17	0.58
1:B:323:GLU:CD	1:B:350:GLY:HA3	2.25	0.57
1:A:356:HIS:HB3	2:A:501:GOL:H11	1.87	0.56
1:B:117:GLU:HG2	1:B:359:GLY:H	1.72	0.55
1:A:387:VAL:HB	1:A:391:GLN:HB2	1.89	0.54
1:B:177:ARG:NH2	1:B:238:LEU:O	2.39	0.53
1:A:9:GLY:HA3	1:A:367:LEU:HD13	1.91	0.52
1:B:387:VAL:HB	1:B:391:GLN:HB2	1.92	0.51
1:B:117:GLU:CG	1:B:359:GLY:H	2.24	0.49
1:A:256:ASN:ND2	1:A:356:HIS:H	2.12	0.48
1:A:87:ARG:HH11	1:A:391:GLN:HE22	1.61	0.48
1:B:16:ARG:NH2	3:B:605:HOH:O	2.38	0.47
1:B:225:HIS:N	1:B:226:PRO:CD	2.78	0.47
1:B:5:TYR:O	1:B:264:LEU:HA	2.14	0.47
1:A:256:ASN:HD22	1:A:356:HIS:H	1.62	0.46
1:B:226:PRO:O	1:B:227:ARG:NH1	2.46	0.45
1:A:225:HIS:N	1:A:226:PRO:CD	2.79	0.45
1:B:165:THR:O	1:B:169:VAL:HG23	2.16	0.45
1:B:56:THR:HG22	1:B:88:LEU:HA	1.99	0.44
1:A:356:HIS:CD2	2:A:501:GOL:H12	2.53	0.44
1:A:227:ARG:HD2	1:A:229:GLN:NE2	2.32	0.44
1:B:52:ILE:O	1:B:113:ALA:HA	2.17	0.44
1:A:137:LEU:HG	1:A:139:VAL:HG23	2.00	0.43
1:B:256:ASN:HD22	1:B:356:HIS:H	1.66	0.43
1:B:326:ALA:N	1:B:327:PRO:HD2	2.34	0.43
1:A:50:ASP:HB3	1:A:111:TYR:CE2	2.54	0.42
1:A:296:ILE:C	1:A:296:ILE:HD12	2.38	0.42
1:B:126:MET:HE3	1:B:137:LEU:HD11	2.01	0.42
1:A:325:PHE:O	1:A:328:GLN:HG3	2.19	0.42
1:B:325:PHE:O	1:B:328:GLN:HG3	2.20	0.42
1:B:356:HIS:HD2	2:B:501:GOL:H11	1.85	0.42
1:B:227:ARG:HD3	1:B:227:ARG:HA	1.92	0.41

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.85	0.41
1:B:225:HIS:HE1	3:B:610:HOH:O	2.03	0.41
1:B:256:ASN:ND2	1:B:356:HIS:H	2.18	0.41
1:A:153:LEU:HD23	1:A:153:LEU:C	2.42	0.41
1:B:318:LEU:HD23	1:B:319:ILE:N	2.35	0.41
1:A:293:LEU:O	1:A:296:ILE:HG13	2.20	0.40
1:B:264:LEU:N	1:B:264:LEU:HD12	2.36	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	Perce	ntiles
1	A	399/409 (98%)	383 (96%)	15 (4%)	1 (0%)	41	45
1	В	398/409 (97%)	383 (96%)	14 (4%)	1 (0%)	41	45
All	All	797/818 (97%)	766 (96%)	29 (4%)	2 (0%)	41	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	65	ASN
1	A	213	ARG

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	291/299 (97%)	287 (99%)	4 (1%)	67 78
1	В	290/299 (97%)	286 (99%)	4 (1%)	67 78
All	All	581/598 (97%)	573 (99%)	8 (1%)	67 78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	THR
1	A	294	MET
1	A	312	ASP
1	A	368	THR
1	В	294	MET
1	В	307	GLN
1	В	312	ASP
1	В	368	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	256	ASN
1	A	307	GLN
1	A	328	GLN
1	A	348	HIS
1	A	391	GLN
1	В	58	GLN
1	В	225	HIS
1	В	256	ASN
1	В	328	GLN
1	В	348	HIS
1	В	391	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)

3 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	Type Chain Res Link		B	Bond lengths			ond ang	gles	
MIOI	Туре	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GOL	A	501	-	5,5,5	0.31	0	5,5,5	0.75	0
2	GOL	В	501	-	5,5,5	0.24	0	5,5,5	0.65	0
2	GOL	В	502	-	5,5,5	0.08	0	5,5,5	0.26	0

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	A	501	-	-	2/4/4/4	-
2	GOL	В	501	-	-	2/4/4/4	-
2	GOL	В	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	В	501	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2
2	В	502	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	В	501	GOL	O1-C1-C2-O2
2	В	502	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	2	0
2	В	501	GOL	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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	401/409 (98%)	-0.19	13 (3%) 47 45	20, 32, 55, 109	0
1	В	400/409 (97%)	-0.09	15 (3%) 40 38	20, 35, 63, 103	0
All	All	801/818 (97%)	-0.14	28 (3%) 44 41	20, 33, 60, 109	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	214	LYS	5.8
1	В	212	GLY	4.9
1	A	212	GLY	4.8
1	A	213	ARG	4.7
1	A	214	LYS	4.6
1	В	213	ARG	4.1
1	В	215	GLY	4.0
1	A	211	ALA	3.4
1	В	237	ARG	3.3
1	A	216	GLU	3.3
1	В	233	ALA	3.2
1	В	211	ALA	3.1
1	A	215	GLY	3.1
1	В	243	ALA	2.9
1	A	377	GLU	2.8
1	В	244	GLY	2.8
1	В	210	ARG	2.7
1	A	217	THR	2.7
1	В	245	GLY	2.7
1	A	237	ARG	2.6
1	A	401	ARG	2.6
1	В	240	ALA	2.6
1	В	216	GLU	2.5
1	A	155	GLU	2.4

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Mol	Chain	Res	Type	RSRZ	
1	В	85	VAL	2.4	
1	A	85	VAL	2.3	
1	В	52	ILE	2.3	
1	A	52	ILE	2.2	

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, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	GOL	A	501	6/6	0.81	0.18	37,51,54,56	0
2	GOL	В	501	6/6	0.91	0.15	44,48,49,55	0
2	GOL	В	502	6/6	0.93	0.15	54,57,58,59	0

6.5 Other polymers (i)

There are no such residues in this entry.

