wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 08:32 AM UTC

PDB ID	:	6L73 / pdb_00006l73
Title	:	Quinolone synthase (AmQNS) from Aegle marmelos Correa
Authors	:	Mallika, V.; Abhinav, K.V.; Soniya, E.V.
Deposited on	:	2019-10-30
Resolution	:	2.00 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 (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 (i)) were used in the production of this report:

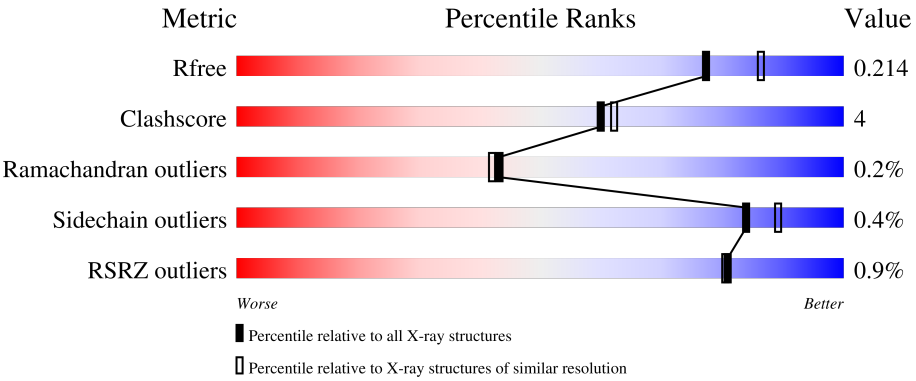
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	391	88% 8%
1	B	391	86% 10%
1	C	391	89% 7%
1	D	391	83% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12629 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			
1	B	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			
1	C	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			
1	D	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			

- Molecule 2 is water.

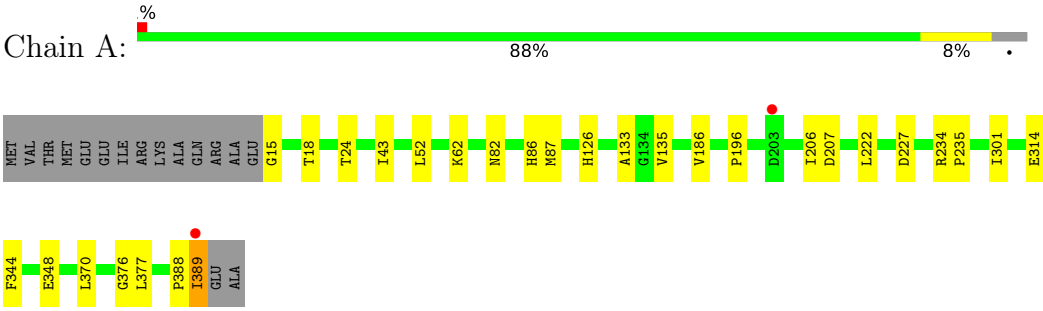
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	351	Total	O	0	0
			351	351		
2	B	278	Total	O	0	0
			278	278		
2	C	347	Total	O	0	0
			347	347		
2	D	253	Total	O	0	0
			253	253		

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.

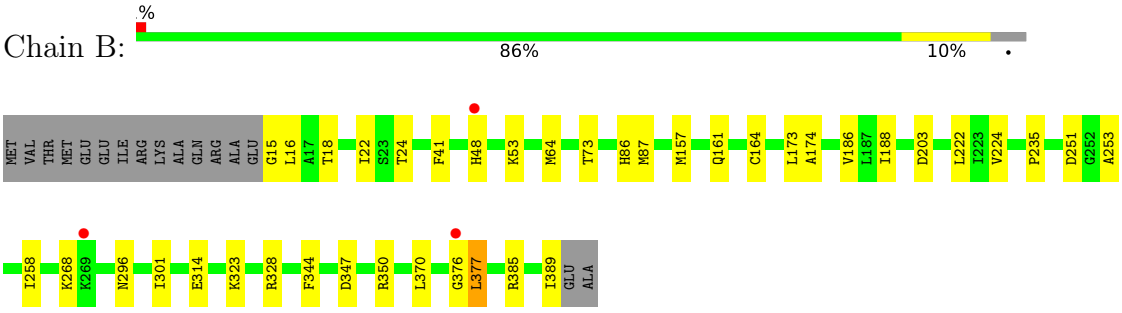
• Molecule 1: Type III polyketide synthase

Chain A:



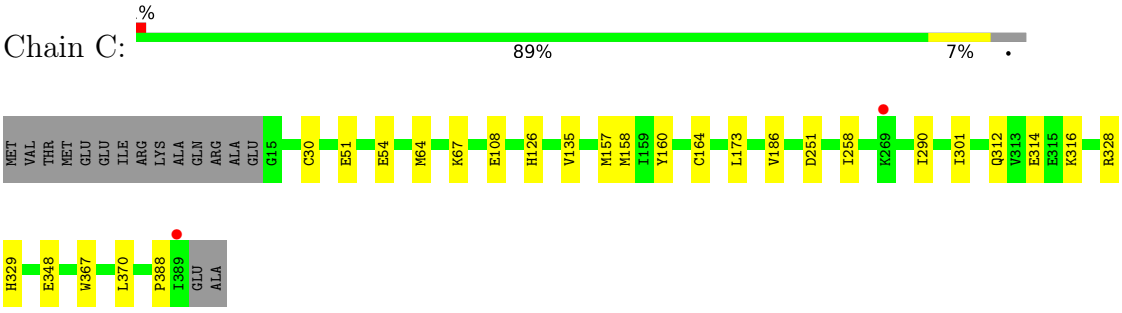
• Molecule 1: Type III polyketide synthase

Chain B:



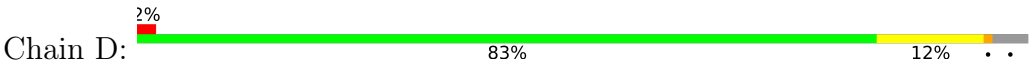
• Molecule 1: Type III polyketide synthase

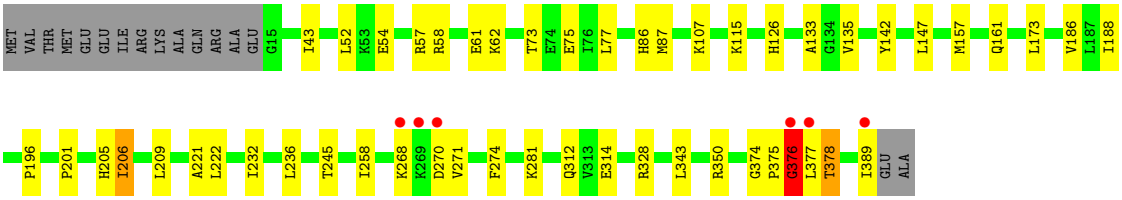
Chain C:



• Molecule 1: Type III polyketide synthase

Chain D:




MET VAL THR MET GLU GLU ILE ARG LYS ALA GLN ARG ALA GLU G15 I43 L52 K53 E54 R57 R58 E61 K62 T73 E74 E75 I76 L77 H86 M87 K107 K115 H126 A133 G134 V135 Y142 L147 M157 Q161 L173 V186 L187 I188
P196 P201 H205 I206 L209 A221 L222 I232 L236 T245 I258 K268 K269 D270 V271 F274 K281 Q312 V313 E314 R328 L343 R350 G374 P375 G376 L377 T378 I389 GLU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.32Å 59.76Å 104.51Å 90.04° 96.86° 92.55°	Depositor
Resolution (Å)	39.25 – 2.00 39.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.25-2.00) 97.5 (39.25-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.159 , 0.214 0.159 , 0.214	Depositor DCC
R_{free} test set	4296 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12629	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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	0.33	0/2906	0.54	0/3942
1	B	0.30	0/2906	0.51	0/3942
1	C	0.32	0/2906	0.53	2/3942 (0.1%)
1	D	0.30	0/2906	0.56	3/3942 (0.1%)
All	All	0.32	0/11624	0.54	5/15768 (0.0%)

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	2
1	B	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	376	GLY	CA-C-N	-8.22	108.15	122.79
1	D	376	GLY	C-N-CA	-8.22	108.15	122.79
1	D	376	GLY	N-CA-C	-6.88	99.63	111.47
1	C	388	PRO	CA-C-N	5.79	132.12	121.70
1	C	388	PRO	C-N-CA	5.79	132.12	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	GLY	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	B	376	GLY	Peptide
1	D	375	PRO	Peptide
1	D	376	GLY	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	A	2850	0	2855	20	0
1	B	2850	0	2855	27	0
1	C	2850	0	2855	20	0
1	D	2850	0	2855	38	0
2	A	351	0	0	4	1
2	B	278	0	0	6	0
2	C	347	0	0	5	0
2	D	253	0	0	6	0
All	All	12629	0	11420	99	1

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 4.

The worst 5 of 99 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:A:135:VAL:HG11	1:B:161:GLN:HG3	1.65	0.77
1:C:164:CYS:SG	2:C:641:HOH:O	2.44	0.75
1:A:126:HIS:HB2	1:A:186:VAL:HG22	1.68	0.74
1:D:126:HIS:HB2	1:D:186:VAL:HG22	1.68	0.73
1:D:376:GLY:O	2:D:401:HOH:O	2.06	0.72

All (1) 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)
2:A:563:HOH:O	2:A:566:HOH:O[1_565]	2.17	0.03

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	373/391 (95%)	362 (97%)	10 (3%)	1 (0%)	36	35
1	B	373/391 (95%)	362 (97%)	10 (3%)	1 (0%)	36	35
1	C	373/391 (95%)	361 (97%)	12 (3%)	0	100	100
1	D	373/391 (95%)	363 (97%)	9 (2%)	1 (0%)	36	35
All	All	1492/1564 (95%)	1448 (97%)	41 (3%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	B	377	LEU
1	D	378	THR

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	309/327 (94%)	307 (99%)	2 (1%)	78	85
1	B	309/327 (94%)	309 (100%)	0	100	100
1	C	309/327 (94%)	309 (100%)	0	100	100
1	D	309/327 (94%)	306 (99%)	3 (1%)	68	75
All	All	1236/1308 (94%)	1231 (100%)	5 (0%)	84	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	389	ILE
1	D	206	ILE
1	D	232	ILE
1	D	389	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	HIS
1	B	143	GLN
1	C	180	ASN
1	D	48	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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			OWAB(Å^2)	Q<0.9
1	A	375/391 (95%)	-0.65	2 (0%)	87	87	6, 12, 23, 46	0
1	B	375/391 (95%)	-0.40	3 (0%)	82	82	7, 17, 33, 57	0
1	C	375/391 (95%)	-0.62	2 (0%)	87	87	7, 13, 25, 44	0
1	D	375/391 (95%)	-0.30	6 (1%)	70	70	8, 18, 37, 55	0
All	All	1500/1564 (95%)	-0.49	13 (0%)	81	80	6, 15, 32, 57	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	376	GLY	6.3
1	D	269	LYS	3.7
1	B	269	LYS	3.5
1	A	389	ILE	2.8
1	D	389	ILE	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.