



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:21 AM UTC

PDB ID : 5ILK / pdb_00005ilk
Title : Tobacco 5-epi-aristolochene synthase with partial density from MOPSO or BIS-TRIS buffer molecule in the active site
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Deposited on : 2016-03-04
Resolution : 2.35 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
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

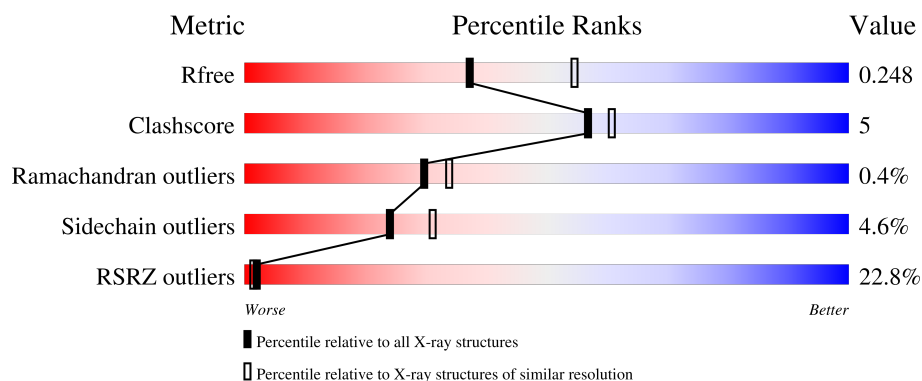
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	550	22% 83% 13% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4501 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 5-epi-aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	1	0
			4357	2791	721	826	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q40577
A	0	SER	-	expression tag	UNP Q40577

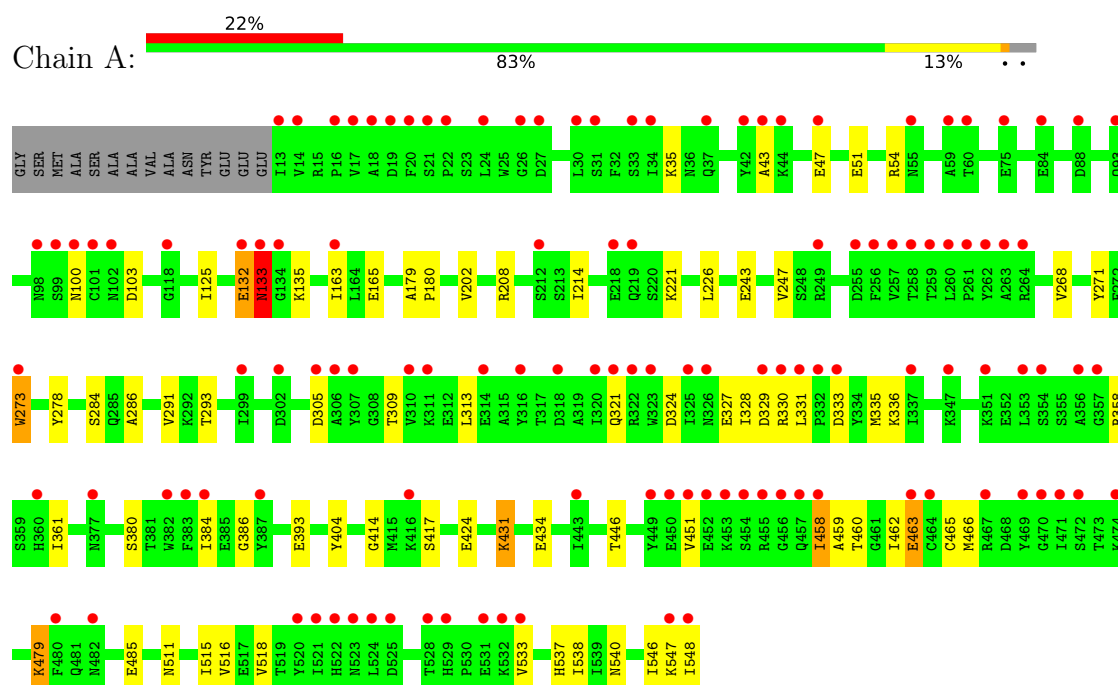
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	144	Total	O	0	0
			144	144		

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: 5-epi-aristolochene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.96Å 126.96Å 123.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.77 – 2.35 50.77 – 2.35	Depositor EDS
% Data completeness (in resolution range)	83.4 (50.77-2.35) 76.5 (50.77-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.240 0.214 , 0.248	Depositor DCC
R_{free} test set	1803 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-l,-k 0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4501	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/4456	0.77	2/6043 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	CB-CA-C	-6.01	106.60	111.71
1	A	214	ILE	N-CA-C	5.20	116.36	111.48

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	4357	0	4316	40	0
2	A	144	0	0	10	1
All	All	4501	0	4316	40	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 5.

All (40) 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:446:THR:OG1	2:A:601:HOH:O	2.04	0.74
1:A:202:VAL:HG23	1:A:518:VAL:HG21	1.73	0.70
1:A:103:ASP:OD1	2:A:602:HOH:O	2.11	0.68
1:A:393:GLU:OE2	2:A:603:HOH:O	2.12	0.67
1:A:51:GLU:OE1	2:A:605:HOH:O	2.15	0.64
1:A:243:GLU:OE1	1:A:271:TYR:OH	2.18	0.59
1:A:305:ASP:OD1	2:A:606:HOH:O	2.17	0.58
1:A:333:ASP:HA	1:A:336:LYS:HD2	1.84	0.58
1:A:462:ILE:O	1:A:466:MET:HG3	2.05	0.56
1:A:537:HIS:ND1	2:A:604:HOH:O	2.12	0.55
1:A:324:ASP:HB3	1:A:327:GLU:HG2	1.91	0.52
1:A:380:SER:O	1:A:384:ILE:HG12	2.10	0.51
1:A:386:GLY:HA2	1:A:458:ILE:HG12	1.93	0.50
1:A:133:ASN:ND2	2:A:608:HOH:O	2.45	0.50
1:A:135:LYS:HB2	2:A:608:HOH:O	2.10	0.49
1:A:463:GLU:HA	1:A:466:MET:HE2	1.94	0.49
1:A:404:TYR:OH	1:A:516:VAL:HG23	2.12	0.49
1:A:100:ASN:N	2:A:619:HOH:O	2.47	0.46
1:A:54:ARG:HE	1:A:54:ARG:HB2	1.47	0.46
1:A:132:GLU:OE1	1:A:132:GLU:N	2.45	0.46
1:A:358:ARG:O	1:A:361:ILE:HG12	2.16	0.46
1:A:221:LYS:HD2	1:A:226:LEU:HD22	1.99	0.44
1:A:268:VAL:HG12	1:A:538:ILE:HD13	1.99	0.44
1:A:327:GLU:HB3	1:A:330:ARG:NH1	2.33	0.44
1:A:533:VAL:HB	2:A:612:HOH:O	2.17	0.44
1:A:331:LEU:HD13	1:A:335:MET:HB3	1.99	0.44
1:A:329:ASP:HA	1:A:336:LYS:NZ	2.33	0.43
1:A:243:GLU:OE2	1:A:284:SER:OG	2.36	0.43
1:A:511:ASN:O	1:A:515:ILE:HG12	2.19	0.43
1:A:43:ALA:O	1:A:47:GLU:HG2	2.20	0.42
1:A:431:LYS:O	1:A:431:LYS:HD3	2.18	0.42
1:A:273[A]:TRP:CE2	1:A:515:ILE:HG21	2.55	0.42
1:A:465:CYS:SG	1:A:479:LYS:HE2	2.60	0.41
1:A:247:VAL:HG21	1:A:291:VAL:HG11	2.01	0.41
1:A:547:LYS:HD3	1:A:547:LYS:HA	1.87	0.41
1:A:179:ALA:HB3	1:A:180:PRO:HD3	2.02	0.41
1:A:286:ALA:HA	1:A:414:GLY:HA3	2.02	0.41
1:A:458:ILE:HD12	1:A:459:ALA:N	2.36	0.41
1:A:208:ARG:HG2	1:A:540:ASN:HB3	2.03	0.41
1:A:309:THR:O	1:A:313:LEU:HG	2.21	0.40

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:708:HOH:O	2:A:708:HOH:O[8_665]	2.05	0.15

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	535/550 (97%)	519 (97%)	14 (3%)	2 (0%)	30 34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLU
1	A	133	ASN

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	481/490 (98%)	458 (95%)	23 (5%)	23 29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	125	ILE
1	A	133	ASN
1	A	163	ILE

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Mol	Chain	Res	Type
1	A	165	GLU
1	A	273[A]	TRP
1	A	273[B]	TRP
1	A	278	TYR
1	A	293	THR
1	A	321	GLN
1	A	328	ILE
1	A	417	SER
1	A	424	GLU
1	A	431	LYS
1	A	434	GLU
1	A	451	VAL
1	A	458	ILE
1	A	460	THR
1	A	463	GLU
1	A	479	LYS
1	A	485	GLU
1	A	546	ILE
1	A	548	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	529	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, 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	536/550 (97%)	1.35	122 (22%) 2 1	22, 48, 85, 114	1 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ILE	10.2
1	A	548	ILE	6.4
1	A	101	CYS	5.8
1	A	100	ASN	5.6
1	A	99	SER	5.3
1	A	19	ASP	5.0
1	A	14	VAL	4.7
1	A	451	VAL	4.6
1	A	311	LYS	4.4
1	A	219	GLN	4.4
1	A	330	ARG	4.3
1	A	456	GLY	4.1
1	A	258	THR	4.1
1	A	416	LYS	4.1
1	A	325	ILE	4.0
1	A	457	GLN	3.9
1	A	306	ALA	3.9
1	A	24	LEU	3.9
1	A	37	GLN	3.9
1	A	450	GLU	3.8
1	A	452	GLU	3.8
1	A	18	ALA	3.8
1	A	455	ARG	3.7
1	A	356	ALA	3.6
1	A	16	PRO	3.6
1	A	326	ASN	3.6
1	A	133	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	453	LYS	3.6
1	A	458	ILE	3.5
1	A	26	GLY	3.5
1	A	259	THR	3.5
1	A	262	TYR	3.4
1	A	329	ASP	3.4
1	A	257	VAL	3.4
1	A	524	LEU	3.4
1	A	522	HIS	3.4
1	A	17	VAL	3.3
1	A	84	GLU	3.3
1	A	273[A]	TRP	3.3
1	A	467	ARG	3.2
1	A	31	SER	3.2
1	A	307	TYR	3.2
1	A	98	ASN	3.2
1	A	523	ASN	3.2
1	A	383	PHE	3.1
1	A	454	SER	3.1
1	A	357	GLY	3.1
1	A	320	ILE	3.0
1	A	333	ASP	3.0
1	A	337	ILE	3.0
1	A	525	ASP	3.0
1	A	331	LEU	3.0
1	A	463	GLU	3.0
1	A	471	ILE	2.9
1	A	310	VAL	2.9
1	A	93	GLN	2.9
1	A	323	TRP	2.9
1	A	132	GLU	2.9
1	A	449	TYR	2.8
1	A	218	GLU	2.8
1	A	520	TYR	2.8
1	A	163	ILE	2.7
1	A	547	LYS	2.7
1	A	353	LEU	2.7
1	A	384	ILE	2.7
1	A	531	GLU	2.7
1	A	318	ASP	2.7
1	A	34	ILE	2.7
1	A	305	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	472	SER	2.6
1	A	43	ALA	2.6
1	A	134	GLY	2.6
1	A	299	ILE	2.6
1	A	354	SER	2.6
1	A	47	GLU	2.5
1	A	260	LEU	2.5
1	A	360	HIS	2.5
1	A	469	TYR	2.5
1	A	256	PHE	2.5
1	A	321	GLN	2.5
1	A	75	GLU	2.5
1	A	533	VAL	2.5
1	A	118	GLY	2.5
1	A	20	PHE	2.4
1	A	263	ALA	2.4
1	A	322	ARG	2.4
1	A	33	SER	2.4
1	A	42	TYR	2.4
1	A	102	ASN	2.4
1	A	482	ASN	2.3
1	A	22	PRO	2.3
1	A	474	LYS	2.3
1	A	44	LYS	2.3
1	A	347	LYS	2.3
1	A	464	CYS	2.2
1	A	316	TYR	2.2
1	A	387	TYR	2.2
1	A	532	LYS	2.2
1	A	255	ASP	2.2
1	A	21	SER	2.2
1	A	314	GLU	2.2
1	A	377	ASN	2.2
1	A	261	PRO	2.2
1	A	351	LYS	2.2
1	A	59	ALA	2.2
1	A	521	ILE	2.1
1	A	27	ASP	2.1
1	A	302	ASP	2.1
1	A	470	GLY	2.1
1	A	264	ARG	2.1
1	A	30	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	443	ILE	2.1
1	A	480	PHE	2.1
1	A	212	SER	2.0
1	A	528	THR	2.0
1	A	529	HIS	2.0
1	A	55	ASN	2.0
1	A	332	PRO	2.0
1	A	249	ARG	2.0
1	A	382	TRP	2.0
1	A	60	THR	2.0
1	A	88	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.