



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 09:43 am GMT

PDB ID : 3N0F
Title : Crystal Structure of Isoprene Synthase from Grey Poplar Leaves (*Populus x canescens*)
Authors : Koksai, M.; Christianson, D.W.
Deposited on : 2010-05-13
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

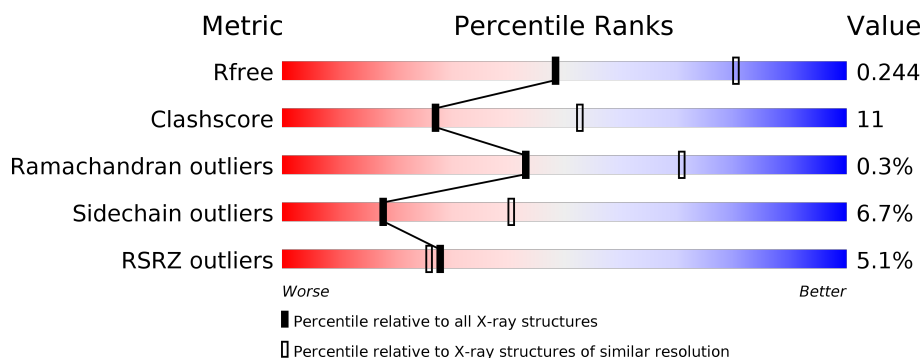
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	555	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	555	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8976 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 Isoprene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4326	2757	731	826	12			
1	B	531	Total	C	N	O	S	0	0	0
			4326	2757	731	826	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	EXPRESSION TAG	UNP Q9AR86
A	42	ARG	-	EXPRESSION TAG	UNP Q9AR86
A	43	GLY	-	EXPRESSION TAG	UNP Q9AR86
A	44	SER	-	EXPRESSION TAG	UNP Q9AR86
A	45	HIS	-	EXPRESSION TAG	UNP Q9AR86
A	46	HIS	-	EXPRESSION TAG	UNP Q9AR86
A	47	HIS	-	EXPRESSION TAG	UNP Q9AR86
A	48	HIS	-	EXPRESSION TAG	UNP Q9AR86
A	49	HIS	-	EXPRESSION TAG	UNP Q9AR86
A	50	HIS	-	EXPRESSION TAG	UNP Q9AR86
A	51	GLY	-	EXPRESSION TAG	UNP Q9AR86
A	52	SER	-	EXPRESSION TAG	UNP Q9AR86
A	59	ASP	ASN	ENGINEERED MUTATION	UNP Q9AR86
A	308	ARG	LYS	ENGINEERED MUTATION	UNP Q9AR86
A	533	TRP	CYS	ENGINEERED MUTATION	UNP Q9AR86
B	41	MET	-	EXPRESSION TAG	UNP Q9AR86
B	42	ARG	-	EXPRESSION TAG	UNP Q9AR86
B	43	GLY	-	EXPRESSION TAG	UNP Q9AR86
B	44	SER	-	EXPRESSION TAG	UNP Q9AR86
B	45	HIS	-	EXPRESSION TAG	UNP Q9AR86
B	46	HIS	-	EXPRESSION TAG	UNP Q9AR86
B	47	HIS	-	EXPRESSION TAG	UNP Q9AR86
B	48	HIS	-	EXPRESSION TAG	UNP Q9AR86
B	49	HIS	-	EXPRESSION TAG	UNP Q9AR86
B	50	HIS	-	EXPRESSION TAG	UNP Q9AR86

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Chain	Residue	Modelled	Actual	Comment	Reference
B	51	GLY	-	EXPRESSION TAG	UNP Q9AR86
B	52	SER	-	EXPRESSION TAG	UNP Q9AR86
B	59	ASP	ASN	ENGINEERED MUTATION	UNP Q9AR86
B	308	ARG	LYS	ENGINEERED MUTATION	UNP Q9AR86
B	533	TRP	CYS	ENGINEERED MUTATION	UNP Q9AR86

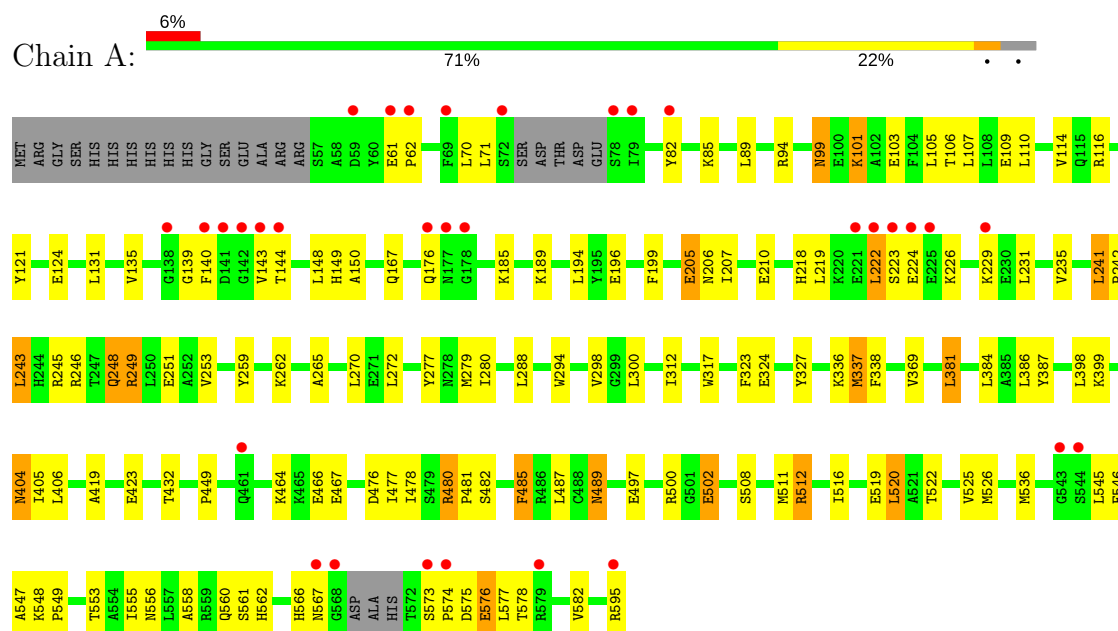
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	160	Total O 160 160	0	0
2	B	164	Total O 164 164	0	0

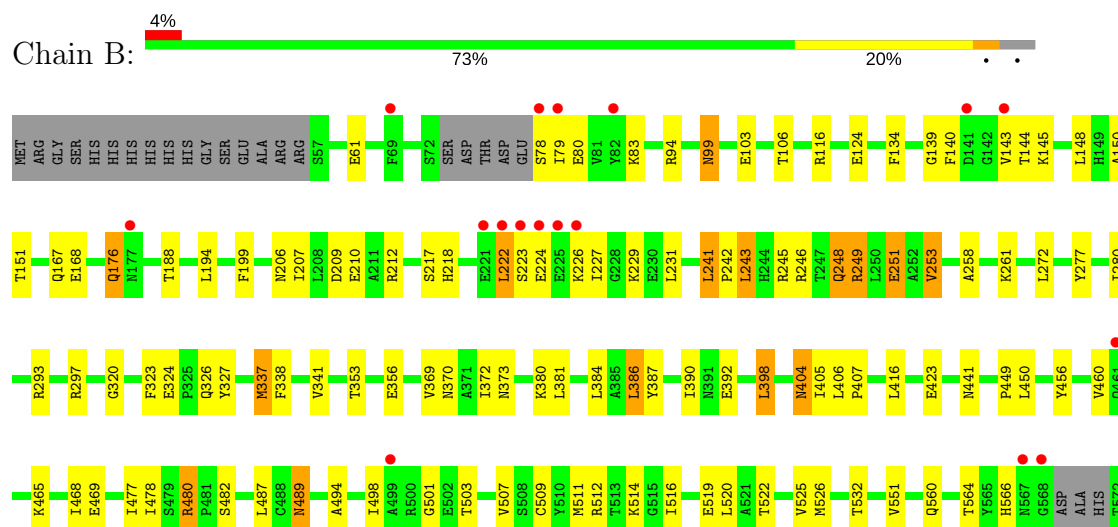
3 Residue-property plots

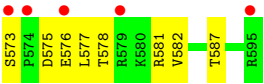
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Isoprene synthase



• Molecule 1: Isoprene synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.42Å 155.42Å 142.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.10 – 2.70 39.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.10-2.70) 95.1 (39.13-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.245 0.198 , 0.244	Depositor DCC
R_{free} test set	4863 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

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	0.38	0/4415	0.54	0/5966
1	B	0.38	0/4415	0.54	0/5966
All	All	0.38	0/8830	0.54	0/11932

There are no bond length outliers.

There are no bond angle outliers.

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	4326	0	4241	97	0
1	B	4326	0	4241	90	0
2	A	160	0	0	1	0
2	B	164	0	0	7	0
All	All	8976	0	8482	187	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 11.

The worst 5 of 187 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:337:MET:HA	1:A:337:MET:HE3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLN:HE22	1:A:249:ARG:HH21	1.17	0.91
1:B:560:GLN:HE21	1:B:564:THR:HG23	1.39	0.86
1:A:248:GLN:NE2	1:A:249:ARG:HH21	1.75	0.85
1:B:337:MET:HE2	1:B:337:MET:HA	1.58	0.83

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	525/555 (95%)	506 (96%)	18 (3%)	1 (0%)	49	77
1	B	525/555 (95%)	504 (96%)	19 (4%)	2 (0%)	36	64
All	All	1050/1110 (95%)	1010 (96%)	37 (4%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLU
1	B	79	ILE
1	B	222	LEU

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	466/486 (96%)	434 (93%)	32 (7%)	17	39
1	B	466/486 (96%)	436 (94%)	30 (6%)	19	43
All	All	932/972 (96%)	870 (93%)	62 (7%)	18	40

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	LEU
1	B	99	ASN
1	B	469	GLU
1	A	595	ARG
1	B	124	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	489	ASN
1	A	527	ASN
1	B	404	ASN
1	A	483	HIS
1	B	248	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	531/555 (95%)	0.03	32 (6%)	22 20	13, 31, 69, 83	5 (0%)
1	B	531/555 (95%)	-0.09	22 (4%)	37 35	9, 29, 66, 82	5 (0%)
All	All	1062/1110 (95%)	-0.03	54 (5%)	28 26	9, 30, 68, 83	10 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ILE	5.2
1	B	223	SER	4.3
1	A	176	GLN	4.3
1	A	222	LEU	4.2
1	B	573	SER	4.2

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 carbohydrates 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.