



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 07:27 pm BST

PDB ID : 2VNE
Title : The X-ray structure of Norcoclaurine synthase from *Thalictrum flavum*
Authors : Ilari, A.; Franceschini, S.; Boffi, A.; Bonamore, A.; Pasquo, A.
Deposited on : 2008-02-04
Resolution : 2.72 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

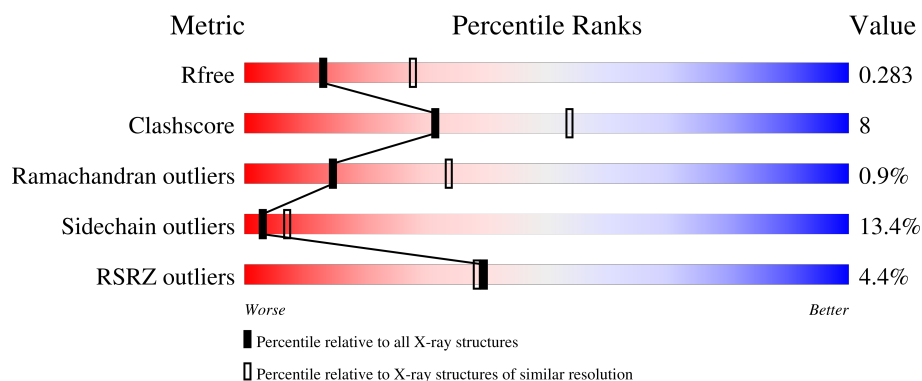
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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 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	201	<div> <div>5%</div> <div>63%</div> <div>20%</div> <div>•</div> <div>14%</div> </div>
1	B	201	<div> <div>2%</div> <div>56%</div> <div>17%</div> <div>•</div> <div>23%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2579 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 S-NORCOCLAURINE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	Se	0	0	0
			1352	876	220	251	1	4			
1	B	155	Total	C	N	O	S	Se	0	0	0
			1209	787	190	227	1	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MSE	THR	engineered mutation	UNP Q67A25
A	17	THR	ILE	engineered mutation	UNP Q67A25
A	18	GLY	ASN	engineered mutation	UNP Q67A25
A	19	SER	CYS	engineered mutation	UNP Q67A25
B	16	MSE	THR	engineered mutation	UNP Q67A25
B	17	THR	ILE	engineered mutation	UNP Q67A25
B	18	GLY	ASN	engineered mutation	UNP Q67A25
B	19	SER	CYS	engineered mutation	UNP Q67A25

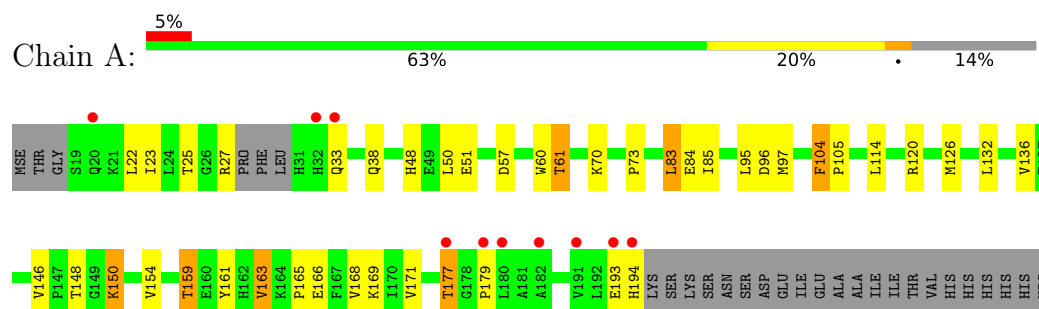
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	9	Total	O	0	0
			9	9		

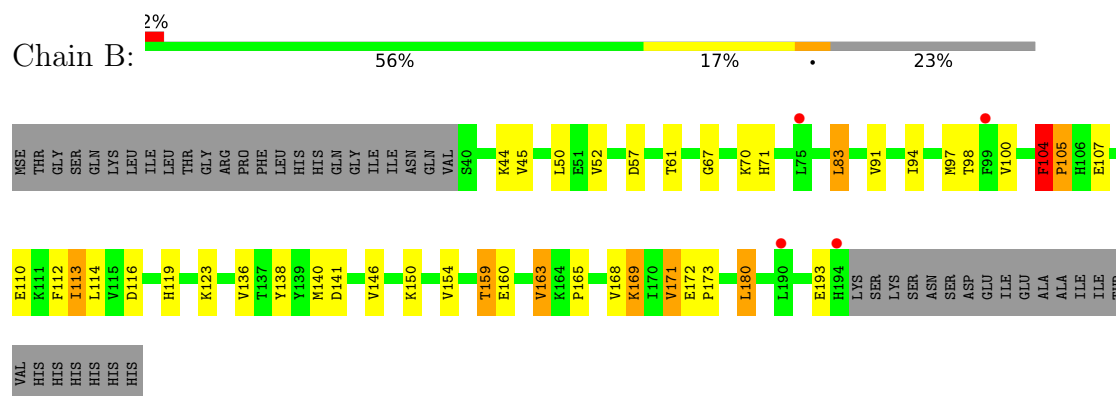
3 Residue-property plots

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: S-NORCOCLAURINE SYNTHASE



• Molecule 1: S-NORCOCLAURINE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.31Å 86.31Å 118.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.74 – 2.72 74.74 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.6 (74.74-2.72) 90.7 (74.74-2.72)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.239 , 0.285 0.238 , 0.283	Depositor DCC
R_{free} test set	624 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2579	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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	0.44	0/1380	0.64	0/1868
1	B	0.43	0/1236	0.63	1/1676 (0.1%)
All	All	0.44	0/2616	0.64	1/3544 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	50	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	PHE	Peptide
1	B	104	PHE	Peptide

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	1352	0	1364	19	0
1	B	1209	0	1213	22	0
2	A	9	0	0	1	0
2	B	9	0	0	0	0
All	All	2579	0	2577	41	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 8.

All (41) 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:B:113:ILE:HG21	1:B:140:MSE:HE1	1.76	0.68
1:A:95:LEU:HD23	1:A:97:MSE:HE3	1.76	0.67
1:A:57:ASP:O	1:A:61:THR:HG22	1.96	0.66
1:B:165:PRO:O	1:B:168:VAL:HG22	1.97	0.65
1:B:136:VAL:HG22	1:B:163:VAL:HG13	1.78	0.65
1:B:104:PHE:CD2	1:B:105:PRO:HD3	2.35	0.62
1:B:116:ASP:OD2	1:B:119:HIS:HD2	1.82	0.62
1:A:150:LYS:HE3	1:A:150:LYS:HA	1.81	0.62
1:B:44:LYS:HA	1:B:44:LYS:HE2	1.83	0.59
1:B:67:GLY:O	1:B:71:HIS:HD2	1.86	0.59
1:B:172:GLU:HG3	1:B:173:PRO:HD3	1.87	0.56
1:A:51:GLU:OE2	1:A:148:THR:HG21	2.04	0.56
1:B:163:VAL:HG11	1:B:171:VAL:HG11	1.90	0.54
1:B:141:ASP:OD1	1:B:159:THR:HB	2.10	0.52
1:B:159:THR:HG22	1:B:180:LEU:HD22	1.92	0.52
1:B:97:MSE:O	1:B:107:GLU:HA	2.10	0.52
1:A:179:PRO:HD3	2:A:2009:HOH:O	2.10	0.51
1:B:168:VAL:HG23	1:B:169:LYS:HD2	1.92	0.51
1:B:104:PHE:O	1:B:105:PRO:O	2.29	0.51
1:A:141:ASP:OD1	1:A:159:THR:HB	2.11	0.49
1:A:104:PHE:CD2	1:A:104:PHE:C	2.85	0.49
1:B:94:ILE:HA	1:B:110:GLU:O	2.13	0.48
1:B:83:LEU:HD23	1:B:97:MSE:HG2	1.96	0.47
1:A:60:TRP:CG	1:A:120:ARG:HG2	2.50	0.47
1:B:45:VAL:HG22	1:B:160:GLU:HG3	1.95	0.47
1:A:73:PRO:HD3	1:A:83:LEU:HD12	1.97	0.46
1:B:57:ASP:O	1:B:61:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TYR:OH	1:B:140:MSE:HG3	2.16	0.46
1:A:136:VAL:HG22	1:A:163:VAL:HG13	1.97	0.45
1:A:140:MSE:O	1:A:159:THR:HA	2.18	0.44
1:A:138:TYR:O	1:A:161:TYR:HA	2.18	0.44
1:B:104:PHE:O	1:B:105:PRO:C	2.55	0.44
1:A:126:MSE:HB2	1:A:139:TYR:HB3	2.01	0.43
1:A:48:HIS:HB2	1:A:177:THR:OG1	2.19	0.42
1:A:33:GLN:NE2	1:A:38:GLN:HB3	2.34	0.42
1:B:114:LEU:HD22	1:B:123:LYS:HG3	2.00	0.42
1:A:165:PRO:HA	1:A:168:VAL:HG13	2.02	0.41
1:A:126:MSE:HE3	1:A:132:LEU:HG	2.03	0.41
1:A:148:THR:O	1:A:148:THR:CG2	2.69	0.41
1:B:172:GLU:N	1:B:173:PRO:CD	2.84	0.41
1:A:84:GLU:HB3	1:A:96:ASP:HB3	2.03	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	Percentiles	
1	A	169/201 (84%)	161 (95%)	7 (4%)	1 (1%)	22	43
1	B	153/201 (76%)	144 (94%)	7 (5%)	2 (1%)	10	24
All	All	322/402 (80%)	305 (95%)	14 (4%)	3 (1%)	14	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	PHE
1	B	105	PRO
1	A	105	PRO

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	150/170 (88%)	129 (86%)	21 (14%)	3	6
1	B	134/170 (79%)	117 (87%)	17 (13%)	3	8
All	All	284/340 (84%)	246 (87%)	38 (13%)	3	7

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	23	ILE
1	A	25	THR
1	A	27	ARG
1	A	50	LEU
1	A	61	THR
1	A	70	LYS
1	A	83	LEU
1	A	85	ILE
1	A	114	LEU
1	A	146	VAL
1	A	150	LYS
1	A	154	VAL
1	A	159	THR
1	A	163	VAL
1	A	166	GLU
1	A	169	LYS
1	A	171	VAL
1	A	177	THR
1	A	193	GLU
1	A	194	HIS
1	B	52	VAL
1	B	70	LYS
1	B	83	LEU
1	B	91	VAL
1	B	98	THR
1	B	100	VAL

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Mol	Chain	Res	Type
1	B	112	PHE
1	B	113	ILE
1	B	146	VAL
1	B	150	LYS
1	B	154	VAL
1	B	159	THR
1	B	163	VAL
1	B	169	LYS
1	B	171	VAL
1	B	180	LEU
1	B	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	162	HIS
1	B	71	HIS
1	B	119	HIS
1	B	125	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	169/201 (84%)	0.41	10 (5%) 29 28	45, 56, 75, 97	0
1	B	151/201 (75%)	0.18	4 (2%) 57 56	47, 57, 71, 90	0
All	All	320/402 (79%)	0.30	14 (4%) 39 38	45, 57, 75, 97	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	HIS	3.1
1	A	193	GLU	2.8
1	A	180	LEU	2.8
1	B	194	HIS	2.8
1	A	179	PRO	2.7
1	A	20	GLN	2.7
1	B	190	LEU	2.6
1	A	32	HIS	2.3
1	B	99	PHE	2.3
1	A	182	ALA	2.2
1	A	177	THR	2.2
1	A	191	VAL	2.1
1	B	75	LEU	2.1
1	A	33	GLN	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.