



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5M41 / pdb_00005m41
Title : Crystal structure of nigrifoline
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Deposited on : 2016-10-17
Resolution : 2.10 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

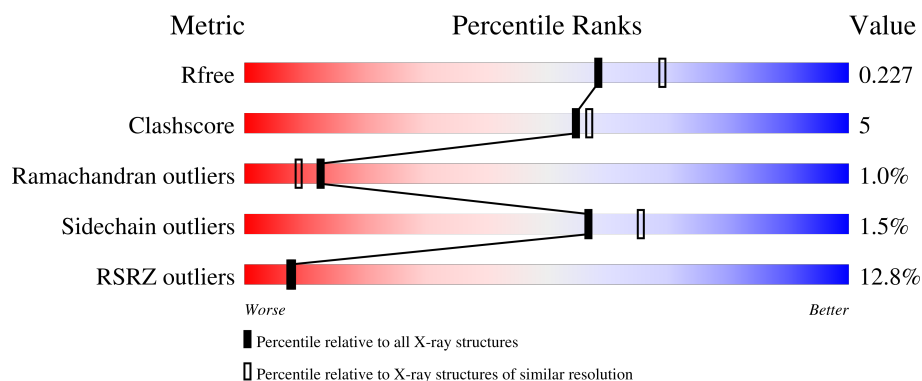
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	757	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5764 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 Nigritoxine.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	3	0
			5536	3464	976	1086	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

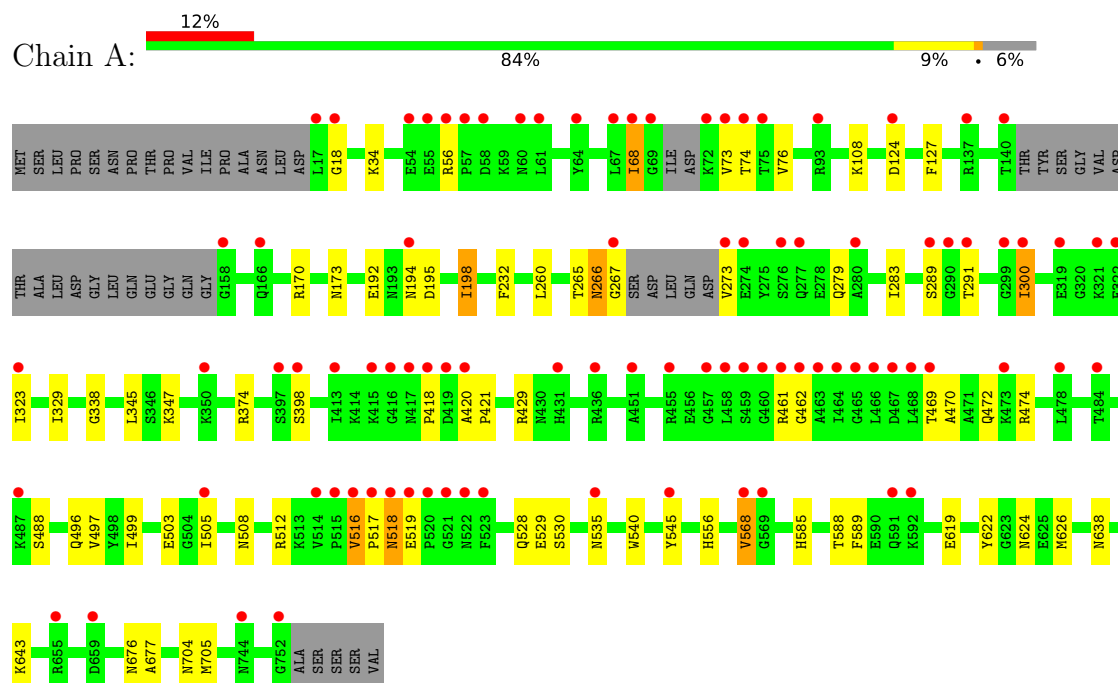
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total	O	0	0
			227	227		

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: Nigritoxine



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	185.16Å 185.16Å 185.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 2.10 58.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.00-2.10) 99.2 (58.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.193 , 0.226 0.197 , 0.227	Depositor DCC
R_{free} test set	3068 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5764	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.74	1/5643 (0.0%)	0.86	1/7628 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	ALA	CA-C	5.01	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	VAL	N-CA-C	5.35	115.55	110.42

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	5536	0	5448	53	0
2	A	1	0	0	0	0
3	A	227	0	0	9	0
All	All	5764	0	5448	53	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 5.

All (53) 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:420:ALA:HB1	1:A:421:PRO:HD2	1.57	0.86
1:A:265:THR:O	1:A:266:ASN:HB2	1.79	0.81
1:A:545:TYR:HD1	3:A:966:HOH:O	1.64	0.80
1:A:568:VAL:O	1:A:589:PHE:O	2.06	0.74
1:A:279:GLN:O	1:A:283:ILE:HG12	1.91	0.70
1:A:398:SER:HB2	1:A:624:ASN:HD21	1.62	0.63
1:A:18:GLY:HA3	1:A:374:ARG:HH11	1.65	0.62
1:A:420:ALA:HB1	1:A:421:PRO:CD	2.28	0.62
1:A:338:GLY:HA2	1:A:626:MET:CE	2.32	0.60
1:A:18:GLY:HA3	1:A:374:ARG:NH1	2.18	0.58
1:A:516:VAL:O	1:A:518:ASN:N	2.37	0.58
1:A:323:ILE:HD13	1:A:347:LYS:HE2	1.88	0.56
1:A:469:THR:HG23	1:A:472:GLN:H	1.71	0.55
1:A:124[B]:ASP:OD1	1:A:127:PHE:HD2	1.90	0.55
1:A:192:GLU:HG3	1:A:198:ILE:HD12	1.87	0.54
1:A:638:ASN:O	1:A:643:LYS:HE3	2.06	0.54
1:A:676:ASN:HB2	3:A:1039:HOH:O	2.06	0.54
1:A:68:ILE:HG22	1:A:68:ILE:O	2.07	0.53
1:A:503:GLU:HB3	1:A:505:ILE:HD12	1.91	0.53
1:A:429:ARG:NH2	3:A:902:HOH:O	2.27	0.52
1:A:512:ARG:NH1	1:A:528:GLN:OE1	2.37	0.52
1:A:265:THR:O	1:A:266:ASN:CB	2.56	0.51
1:A:461:ARG:HB3	1:A:499:ILE:HD11	1.93	0.51
1:A:461:ARG:HD2	1:A:497:VAL:HB	1.93	0.51
1:A:34:LYS:HD3	3:A:954:HOH:O	2.10	0.50
1:A:124[B]:ASP:OD1	1:A:127:PHE:CD2	2.64	0.50
1:A:474:ARG:HG2	1:A:704:ASN:O	2.12	0.49
1:A:588:THR:HG22	3:A:1098:HOH:O	2.13	0.48
1:A:535:ASN:ND2	3:A:904:HOH:O	2.40	0.48
1:A:496:GLN:HG3	1:A:556:HIS:CE1	2.49	0.47
1:A:338:GLY:HA2	1:A:626:MET:HE2	1.97	0.47
1:A:338:GLY:CA	1:A:626:MET:HE1	2.45	0.47
1:A:619:GLU:CG	3:A:1006:HOH:O	2.63	0.47
1:A:76:VAL:H	1:A:173:ASN:HD21	1.64	0.46
1:A:338:GLY:HA2	1:A:626:MET:HE1	1.97	0.46
1:A:374:ARG:NH2	3:A:906:HOH:O	2.48	0.46
1:A:338:GLY:C	1:A:626:MET:HE1	2.41	0.46
1:A:470:ALA:O	1:A:474:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HH11	1:A:56:ARG:HB3	1.81	0.44
1:A:300:ILE:H	1:A:300:ILE:HG13	1.63	0.44
1:A:585:HIS:CG	1:A:705:MET:HB3	2.52	0.44
1:A:508:ASN:O	1:A:529:GLU:HA	2.18	0.43
1:A:374:ARG:NE	3:A:906:HOH:O	2.50	0.43
1:A:329:ILE:HD12	1:A:345:LEU:HD22	2.02	0.42
1:A:530:SER:HB3	1:A:540:TRP:CZ3	2.54	0.42
1:A:619:GLU:O	1:A:622:TYR:O	2.37	0.41
1:A:232:PHE:HB2	1:A:260:LEU:HD13	2.02	0.41
1:A:530:SER:HB3	1:A:540:TRP:CH2	2.56	0.41
1:A:194:ASN:O	1:A:195:ASP:C	2.64	0.41
1:A:289:SER:OG	1:A:291:THR:HG22	2.21	0.41
1:A:266:ASN:HA	1:A:267:GLY:HA3	1.65	0.40
1:A:76:VAL:H	1:A:173:ASN:ND2	2.19	0.40
1:A:512:ARG:HD2	1:A:540:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	707/757 (93%)	678 (96%)	22 (3%)	7 (1%)	12 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	418	PRO
1	A	518	ASN
1	A	68	ILE
1	A	517	PRO
1	A	516	VAL

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Mol	Chain	Res	Type
1	A	462	GLY

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	600/637 (94%)	591 (98%)	9 (2%)	57 65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	A	74	THR
1	A	108	LYS
1	A	170	ARG
1	A	198	ILE
1	A	273	VAL
1	A	300	ILE
1	A	488	SER
1	A	519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	39	ASN
1	A	42	GLN
1	A	51	GLN
1	A	112	ASN
1	A	173	ASN
1	A	442	GLN
1	A	561	ASN
1	A	584	HIS
1	A	591	GLN
1	A	735	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	712/757 (94%)	0.65	91 (12%) 7 8	26, 52, 97, 149	3 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	LEU	9.7
1	A	69	GLY	8.8
1	A	464	ILE	8.8
1	A	68	ILE	8.0
1	A	73	VAL	7.5
1	A	418	PRO	7.4
1	A	463	ALA	6.8
1	A	300	ILE	5.7
1	A	140	THR	5.7
1	A	466	LEU	5.3
1	A	752	GLY	5.3
1	A	158	GLY	5.0
1	A	517	PRO	4.8
1	A	419	ASP	4.8
1	A	64	TYR	4.6
1	A	520	PRO	4.5
1	A	267	GLY	4.4
1	A	74	THR	4.3
1	A	461	ARG	4.3
1	A	462	GLY	4.2
1	A	273	VAL	4.0
1	A	415	LYS	4.0
1	A	460	GLY	3.9
1	A	137	ARG	3.9
1	A	61	LEU	3.8
1	A	484	THR	3.8
1	A	431	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	416	GLY	3.8
1	A	458	LEU	3.6
1	A	417	ASN	3.6
1	A	57	PRO	3.6
1	A	569	GLY	3.5
1	A	516	VAL	3.5
1	A	55	GLU	3.5
1	A	455	ARG	3.5
1	A	72	LYS	3.5
1	A	545	TYR	3.4
1	A	505	ILE	3.4
1	A	56	ARG	3.3
1	A	518	ASN	3.3
1	A	290	GLY	3.2
1	A	280	ALA	3.2
1	A	523	PHE	3.2
1	A	465	GLY	3.1
1	A	93	ARG	3.1
1	A	289	SER	3.1
1	A	277	GLN	3.0
1	A	350	LYS	3.0
1	A	568	VAL	3.0
1	A	467	ASP	2.9
1	A	274	GLU	2.8
1	A	60	ASN	2.8
1	A	398	SER	2.8
1	A	436[A]	ARG	2.8
1	A	478	LEU	2.8
1	A	744	ASN	2.8
1	A	591	GLN	2.8
1	A	659	ASP	2.8
1	A	487	LYS	2.8
1	A	18	GLY	2.7
1	A	323	ILE	2.7
1	A	420	ALA	2.7
1	A	54	GLU	2.6
1	A	67	LEU	2.6
1	A	459	SER	2.6
1	A	291	THR	2.6
1	A	473	LYS	2.5
1	A	75	THR	2.5
1	A	194	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	413	ILE	2.5
1	A	321	LYS	2.5
1	A	592	LYS	2.5
1	A	515	PRO	2.4
1	A	519	GLU	2.4
1	A	166	GLN	2.4
1	A	521	GLY	2.4
1	A	535	ASN	2.3
1	A	58	ASP	2.2
1	A	319	GLU	2.2
1	A	469	THR	2.2
1	A	514	VAL	2.2
1	A	322	GLU	2.2
1	A	468	LEU	2.2
1	A	124[A]	ASP	2.2
1	A	457	GLY	2.2
1	A	451	ALA	2.2
1	A	276	SER	2.2
1	A	655	ARG	2.1
1	A	299	GLY	2.1
1	A	397	SER	2.1
1	A	522	ASN	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](#)

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, 95th 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	B-factors(Å ²)	Q<0.9
2	MG	A	801	1/1	0.98	0.14	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.