



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9I5M / pdb_00009i5m
Title : Structure of cyclodipeptide synthase from *Nocardia brasiliensis* (Nbra-CDPS)
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Deposited on : 2025-01-28
Resolution : 1.73 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
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

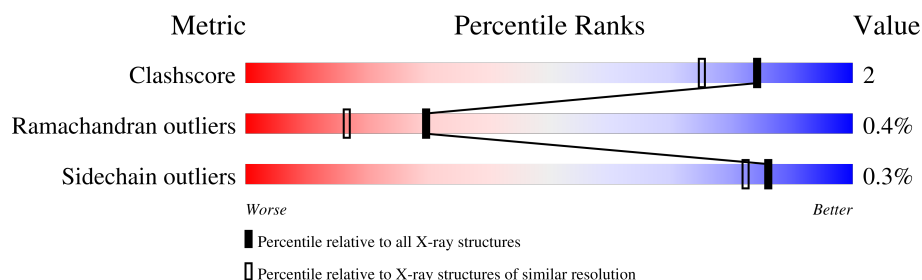
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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))
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	242	 88% 6% 6%
1	B	242	 85% 8% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4017 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 Cyclodipeptide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	3	0
			1859	1163	344	347	5			
1	B	225	Total	C	N	O	S	0	3	0
			1840	1151	341	343	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP K0F6G5
A	1	ALA	-	expression tag	UNP K0F6G5
A	240	ARG	-	expression tag	UNP K0F6G5
A	241	SER	-	expression tag	UNP K0F6G5
B	0	MET	-	initiating methionine	UNP K0F6G5
B	1	ALA	-	expression tag	UNP K0F6G5
B	240	ARG	-	expression tag	UNP K0F6G5
B	241	SER	-	expression tag	UNP K0F6G5

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	165	Total	O	0	0
			165	165		

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. 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. 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.


Note EDS was not executed.

- Molecule 1: Cyclodipeptide synthase

Chain A: 



- Molecule 1: Cyclodipeptide synthase

Chain B: 



4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.52Å 87.76Å 67.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.38 – 1.73	Depositor
% Data completeness (in resolution range)	80.9 (45.38-1.73)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: V1)	Depositor
R, R_{free}	0.212 , 0.234	Depositor
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.111	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
Total number of atoms	4017	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.70% 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: PO4

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	0/1901	0.63	0/2580
1	B	0.38	0/1882	0.66	1/2554 (0.0%)
All	All	0.38	0/3783	0.64	1/5134 (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	B	0	1

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	204	ARG	CG-CD-NE	6.07	125.35	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	ARG	Sidechain

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	1859	0	1807	9	0
1	B	1840	0	1786	10	0
2	B	5	0	0	0	0
3	A	148	0	0	0	0
3	B	165	0	0	0	0
All	All	4017	0	3593	17	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 2.

All (17) 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:39:TYR:CD1	1:B:195:PRO:HG2	2.25	0.71
1:A:139:ARG:HH11	1:A:139:ARG:HG3	1.65	0.61
1:A:138:TYR:HD1	1:A:204:ARG:HG2	1.73	0.54
1:A:39:TYR:CD1	1:A:195:PRO:HG2	2.43	0.53
1:A:106:PRO:HG2	1:B:117:SER:OG	2.11	0.50
1:A:194:TYR:O	1:A:222:PRO:HA	2.13	0.49
1:B:83:ALA:O	1:B:87:ILE:HG12	2.15	0.47
1:A:117:SER:OG	1:B:106:PRO:HG2	2.16	0.46
1:B:153:ARG:HD3	1:B:156:ARG:NH1	2.31	0.46
1:B:194:TYR:O	1:B:222:PRO:HA	2.17	0.45
1:B:30:VAL:HG11	1:B:184:TRP:CZ3	2.52	0.45
1:A:29:THR:CG2	1:A:60:VAL:HG22	2.47	0.44
1:A:204:ARG:HD2	1:A:207[B]:GLU:OE1	2.19	0.42
1:B:138:TYR:CZ	1:B:142:ILE:HD11	2.55	0.41
1:B:146:ILE:HG13	1:B:173:LEU:HD12	2.02	0.41
1:A:136:GLU:HB3	1:A:137:PRO:HD3	2.03	0.40
1:B:153:ARG:HA	1:B:153:ARG:HD2	1.76	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	229/242 (95%)	227 (99%)	1 (0%)	1 (0%)	30	16
1	B	226/242 (93%)	224 (99%)	1 (0%)	1 (0%)	30	16
All	All	455/484 (94%)	451 (99%)	2 (0%)	2 (0%)	30	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	MET
1	B	181	MET

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	196/205 (96%)	195 (100%)	1 (0%)	81	75
1	B	194/205 (95%)	194 (100%)	0	100	100
All	All	390/410 (95%)	389 (100%)	1 (0%)	86	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	130	HIS
1	A	186	HIS
1	A	214	HIS
1	B	69	GLN

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Mol	Chain	Res	Type
1	B	196	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](#)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.