



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 11:07 PM UTC

PDB ID : 9IAK / pdb_00009iak
Title : Structure of cyclodipeptide synthase from *Nocardia brasiliensis* (Nbra-CDPS)
in complex with RNA microhelices mimicking tRNA-Glu acceptor arm
Authors : Marouf, F.Z.; Charbonnier, J.B.; Fernandez Varela, P.
Deposited on : 2025-02-11
Resolution : 3.52 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 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	:	2022.3.0, CSD as543be (2022)
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

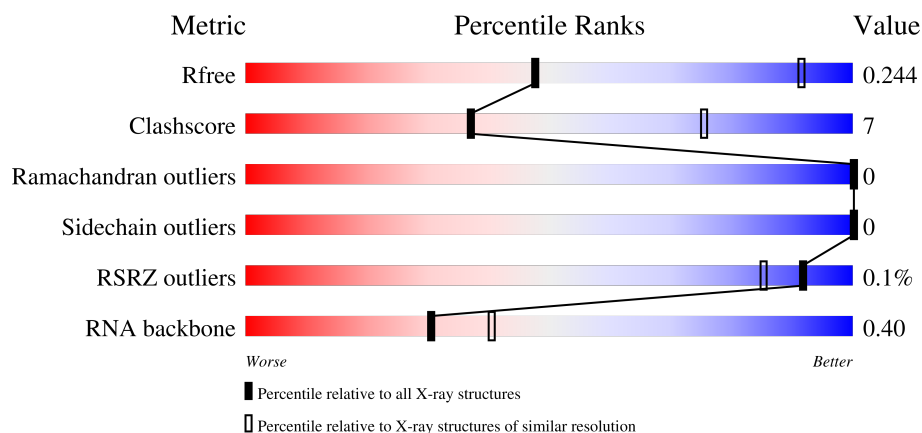
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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.








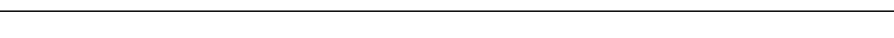
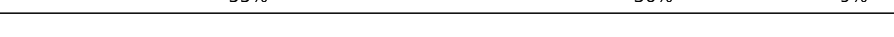
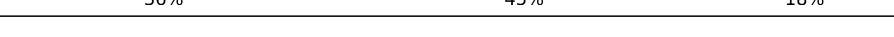
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)
RNA backbone	3983	1018 (4.00-3.04)

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	248	<div><div></div><div>76%</div><div>15%</div><div>9%</div></div>
1	B	248	<div><div></div><div>73%</div><div>18%</div><div>9%</div></div>
1	C	248	<div><div></div><div>75%</div><div>16%</div><div>9%</div></div>
1	D	248	<div><div></div><div>76%</div><div>15%</div><div>9%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	248	
1	F	248	
1	G	248	
1	H	248	
1	I	248	
1	J	248	
1	K	248	
1	L	248	
1	M	248	
1	N	248	
2	O	22	
2	P	22	
2	Q	22	
2	R	22	
2	T	22	
2	U	22	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28377 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	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	B	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	C	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	D	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	E	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	F	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	G	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	H	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	I	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	J	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	K	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	L	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	M	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			
1	N	226	Total	C	N	O	S	0	0	0
			1821	1140	337	339	5			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP K0F6G5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP K0F6G5
A	240	ARG	-	expression tag	UNP K0F6G5
A	241	SER	-	expression tag	UNP K0F6G5
A	242	HIS	-	expression tag	UNP K0F6G5
A	243	HIS	-	expression tag	UNP K0F6G5
A	244	HIS	-	expression tag	UNP K0F6G5
A	245	HIS	-	expression tag	UNP K0F6G5
A	246	HIS	-	expression tag	UNP K0F6G5
A	247	HIS	-	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
B	242	HIS	-	expression tag	UNP K0F6G5
B	243	HIS	-	expression tag	UNP K0F6G5
B	244	HIS	-	expression tag	UNP K0F6G5
B	245	HIS	-	expression tag	UNP K0F6G5
B	246	HIS	-	expression tag	UNP K0F6G5
B	247	HIS	-	expression tag	UNP K0F6G5
C	0	MET	-	initiating methionine	UNP K0F6G5
C	1	ALA	-	expression tag	UNP K0F6G5
C	240	ARG	-	expression tag	UNP K0F6G5
C	241	SER	-	expression tag	UNP K0F6G5
C	242	HIS	-	expression tag	UNP K0F6G5
C	243	HIS	-	expression tag	UNP K0F6G5
C	244	HIS	-	expression tag	UNP K0F6G5
C	245	HIS	-	expression tag	UNP K0F6G5
C	246	HIS	-	expression tag	UNP K0F6G5
C	247	HIS	-	expression tag	UNP K0F6G5
D	0	MET	-	initiating methionine	UNP K0F6G5
D	1	ALA	-	expression tag	UNP K0F6G5
D	240	ARG	-	expression tag	UNP K0F6G5
D	241	SER	-	expression tag	UNP K0F6G5
D	242	HIS	-	expression tag	UNP K0F6G5
D	243	HIS	-	expression tag	UNP K0F6G5
D	244	HIS	-	expression tag	UNP K0F6G5
D	245	HIS	-	expression tag	UNP K0F6G5
D	246	HIS	-	expression tag	UNP K0F6G5
D	247	HIS	-	expression tag	UNP K0F6G5
E	0	MET	-	initiating methionine	UNP K0F6G5
E	1	ALA	-	expression tag	UNP K0F6G5
E	240	ARG	-	expression tag	UNP K0F6G5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	241	SER	-	expression tag	UNP K0F6G5
E	242	HIS	-	expression tag	UNP K0F6G5
E	243	HIS	-	expression tag	UNP K0F6G5
E	244	HIS	-	expression tag	UNP K0F6G5
E	245	HIS	-	expression tag	UNP K0F6G5
E	246	HIS	-	expression tag	UNP K0F6G5
E	247	HIS	-	expression tag	UNP K0F6G5
F	0	MET	-	initiating methionine	UNP K0F6G5
F	1	ALA	-	expression tag	UNP K0F6G5
F	240	ARG	-	expression tag	UNP K0F6G5
F	241	SER	-	expression tag	UNP K0F6G5
F	242	HIS	-	expression tag	UNP K0F6G5
F	243	HIS	-	expression tag	UNP K0F6G5
F	244	HIS	-	expression tag	UNP K0F6G5
F	245	HIS	-	expression tag	UNP K0F6G5
F	246	HIS	-	expression tag	UNP K0F6G5
F	247	HIS	-	expression tag	UNP K0F6G5
G	0	MET	-	initiating methionine	UNP K0F6G5
G	1	ALA	-	expression tag	UNP K0F6G5
G	240	ARG	-	expression tag	UNP K0F6G5
G	241	SER	-	expression tag	UNP K0F6G5
G	242	HIS	-	expression tag	UNP K0F6G5
G	243	HIS	-	expression tag	UNP K0F6G5
G	244	HIS	-	expression tag	UNP K0F6G5
G	245	HIS	-	expression tag	UNP K0F6G5
G	246	HIS	-	expression tag	UNP K0F6G5
G	247	HIS	-	expression tag	UNP K0F6G5
H	0	MET	-	initiating methionine	UNP K0F6G5
H	1	ALA	-	expression tag	UNP K0F6G5
H	240	ARG	-	expression tag	UNP K0F6G5
H	241	SER	-	expression tag	UNP K0F6G5
H	242	HIS	-	expression tag	UNP K0F6G5
H	243	HIS	-	expression tag	UNP K0F6G5
H	244	HIS	-	expression tag	UNP K0F6G5
H	245	HIS	-	expression tag	UNP K0F6G5
H	246	HIS	-	expression tag	UNP K0F6G5
H	247	HIS	-	expression tag	UNP K0F6G5
I	0	MET	-	initiating methionine	UNP K0F6G5
I	1	ALA	-	expression tag	UNP K0F6G5
I	240	ARG	-	expression tag	UNP K0F6G5
I	241	SER	-	expression tag	UNP K0F6G5
I	242	HIS	-	expression tag	UNP K0F6G5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	243	HIS	-	expression tag	UNP K0F6G5
I	244	HIS	-	expression tag	UNP K0F6G5
I	245	HIS	-	expression tag	UNP K0F6G5
I	246	HIS	-	expression tag	UNP K0F6G5
I	247	HIS	-	expression tag	UNP K0F6G5
J	0	MET	-	initiating methionine	UNP K0F6G5
J	1	ALA	-	expression tag	UNP K0F6G5
J	240	ARG	-	expression tag	UNP K0F6G5
J	241	SER	-	expression tag	UNP K0F6G5
J	242	HIS	-	expression tag	UNP K0F6G5
J	243	HIS	-	expression tag	UNP K0F6G5
J	244	HIS	-	expression tag	UNP K0F6G5
J	245	HIS	-	expression tag	UNP K0F6G5
J	246	HIS	-	expression tag	UNP K0F6G5
J	247	HIS	-	expression tag	UNP K0F6G5
K	0	MET	-	initiating methionine	UNP K0F6G5
K	1	ALA	-	expression tag	UNP K0F6G5
K	240	ARG	-	expression tag	UNP K0F6G5
K	241	SER	-	expression tag	UNP K0F6G5
K	242	HIS	-	expression tag	UNP K0F6G5
K	243	HIS	-	expression tag	UNP K0F6G5
K	244	HIS	-	expression tag	UNP K0F6G5
K	245	HIS	-	expression tag	UNP K0F6G5
K	246	HIS	-	expression tag	UNP K0F6G5
K	247	HIS	-	expression tag	UNP K0F6G5
L	0	MET	-	initiating methionine	UNP K0F6G5
L	1	ALA	-	expression tag	UNP K0F6G5
L	240	ARG	-	expression tag	UNP K0F6G5
L	241	SER	-	expression tag	UNP K0F6G5
L	242	HIS	-	expression tag	UNP K0F6G5
L	243	HIS	-	expression tag	UNP K0F6G5
L	244	HIS	-	expression tag	UNP K0F6G5
L	245	HIS	-	expression tag	UNP K0F6G5
L	246	HIS	-	expression tag	UNP K0F6G5
L	247	HIS	-	expression tag	UNP K0F6G5
M	0	MET	-	initiating methionine	UNP K0F6G5
M	1	ALA	-	expression tag	UNP K0F6G5
M	240	ARG	-	expression tag	UNP K0F6G5
M	241	SER	-	expression tag	UNP K0F6G5
M	242	HIS	-	expression tag	UNP K0F6G5
M	243	HIS	-	expression tag	UNP K0F6G5
M	244	HIS	-	expression tag	UNP K0F6G5

Continued on next page...

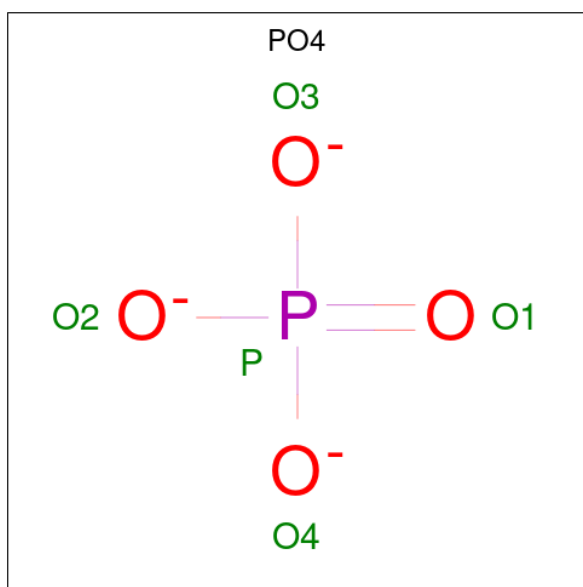
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	245	HIS	-	expression tag	UNP K0F6G5
M	246	HIS	-	expression tag	UNP K0F6G5
M	247	HIS	-	expression tag	UNP K0F6G5
N	0	MET	-	initiating methionine	UNP K0F6G5
N	1	ALA	-	expression tag	UNP K0F6G5
N	240	ARG	-	expression tag	UNP K0F6G5
N	241	SER	-	expression tag	UNP K0F6G5
N	242	HIS	-	expression tag	UNP K0F6G5
N	243	HIS	-	expression tag	UNP K0F6G5
N	244	HIS	-	expression tag	UNP K0F6G5
N	245	HIS	-	expression tag	UNP K0F6G5
N	246	HIS	-	expression tag	UNP K0F6G5
N	247	HIS	-	expression tag	UNP K0F6G5

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*GP*AP*CP*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	22	Total	C	N	O	P	0	0	0
			468	208	82	156	22			
2	P	22	Total	C	N	O	P	0	0	0
			468	208	82	156	22			
2	Q	22	Total	C	N	O	P	0	0	0
			468	208	82	156	22			
2	R	22	Total	C	N	O	P	0	0	0
			468	208	82	156	22			
2	T	22	Total	C	N	O	P	0	0	0
			468	208	82	156	22			
2	U	22	Total	C	N	O	P	0	0	0
			468	208	82	156	22			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

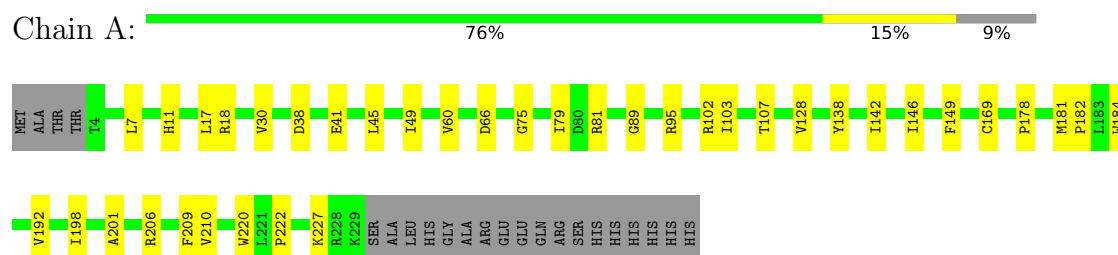
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	O	P	0	0
			5	4	1		

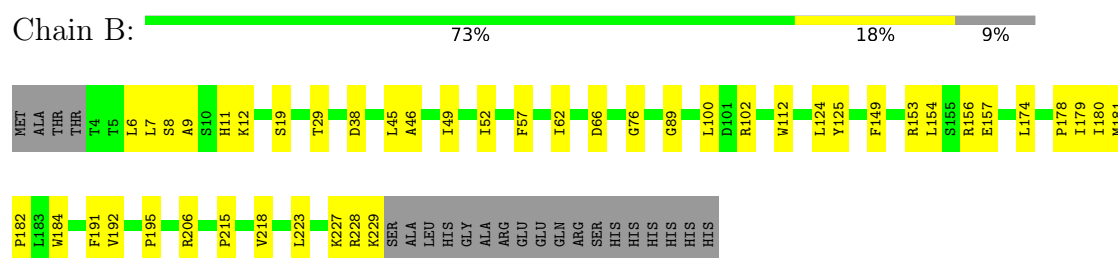
3 Residue-property plots [i](#)

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.

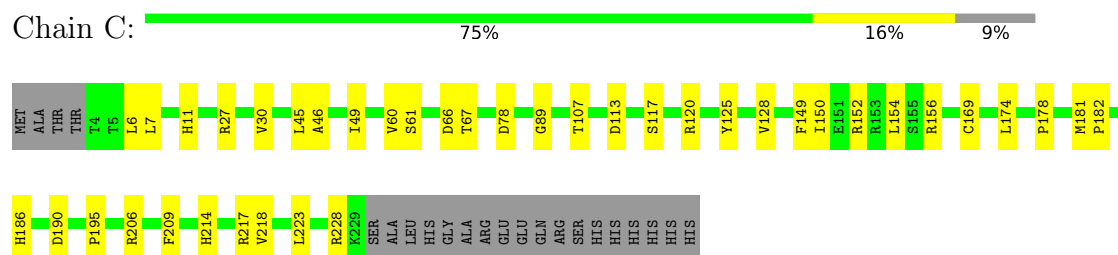
- Molecule 1: Cyclodi-peptide synthase



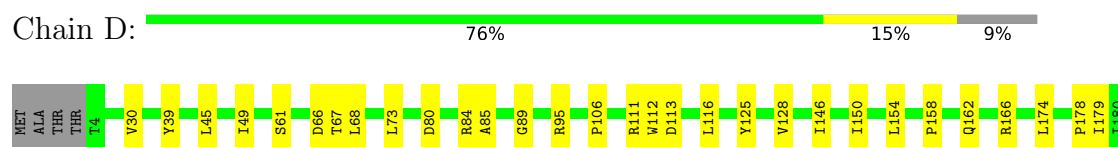
- Molecule 1: Cyclodi-peptide synthase



- Molecule 1: Cyclodi-peptide synthase



- Molecule 1: Cyclodi-peptide synthase

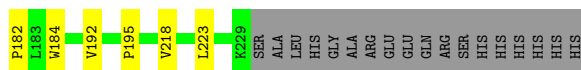
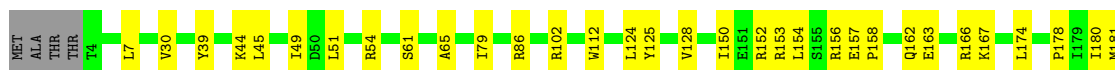






• Molecule 1: Cyclodipeptide synthase

Chain J: 76% 15% 9%



• Molecule 1: Cyclodipeptide synthase

Chain K: 76% 15% 9%



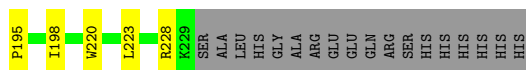
• Molecule 1: Cyclodipeptide synthase

Chain L: 75% 16% 9%



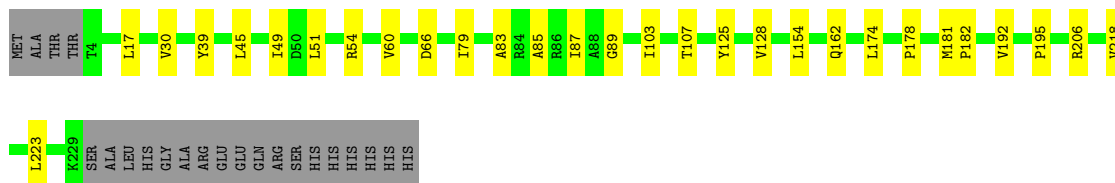
• Molecule 1: Cyclodipeptide synthase

Chain M: 77% 14% 9%

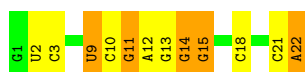


• Molecule 1: Cyclodipeptide synthase

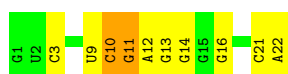
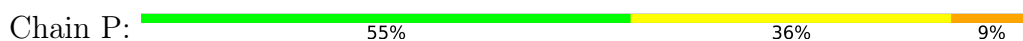
Chain N: 79% 12% 9%



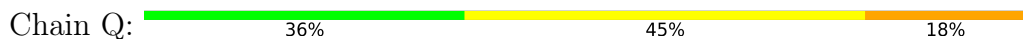
- Molecule 2: RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*G P*AP*CP*GP*CP*CP*A)-3')



- Molecule 2: RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*G P*AP*CP*GP*CP*CP*A)-3')



- Molecule 2: RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*G P*AP*CP*GP*CP*CP*A)-3')



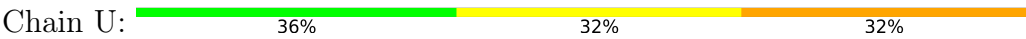
- Molecule 2: RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*G P*AP*CP*GP*CP*CP*A)-3')



- Molecule 2: RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*G P*AP*CP*GP*CP*CP*A)-3')



- Molecule 2: RNA (5'-R(P*GP*UP*CP*CP*CP*CP*UP*UP*UP*CP*GP*AP*GP*GP*GP*G P*AP*CP*GP*CP*CP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.38Å 170.50Å 323.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 3.52 48.45 – 3.52	Depositor EDS
% Data completeness (in resolution range)	75.0 (48.45-3.52) 75.1 (48.45-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.208 , 0.242 0.209 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28377	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

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	0.17	0/1862	0.41	0/2527
1	B	0.16	0/1862	0.41	0/2527
1	C	0.14	0/1862	0.37	0/2527
1	D	0.16	0/1862	0.39	0/2527
1	E	0.14	0/1862	0.38	0/2527
1	F	0.15	0/1862	0.40	0/2527
1	G	0.16	0/1862	0.40	0/2527
1	H	0.15	0/1862	0.39	0/2527
1	I	0.15	0/1862	0.36	0/2527
1	J	0.15	0/1862	0.39	0/2527
1	K	0.14	0/1862	0.38	0/2527
1	L	0.15	0/1862	0.39	0/2527
1	M	0.15	0/1862	0.38	0/2527
1	N	0.14	0/1862	0.40	0/2527
2	O	0.24	0/521	0.67	0/808
2	P	0.23	0/521	0.57	0/808
2	Q	0.23	0/521	0.65	0/808
2	R	0.23	0/521	0.62	0/808
2	T	0.24	0/521	0.63	0/808
2	U	0.22	0/521	0.64	0/808
All	All	0.16	0/29194	0.43	0/40226

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	1821	0	1782	27	0
1	B	1821	0	1782	33	0
1	C	1821	0	1782	31	0
1	D	1821	0	1782	23	0
1	E	1821	0	1782	29	0
1	F	1821	0	1782	24	0
1	G	1821	0	1782	28	0
1	H	1821	0	1782	34	0
1	I	1821	0	1782	25	0
1	J	1821	0	1782	27	0
1	K	1821	0	1782	25	0
1	L	1821	0	1782	28	0
1	M	1821	0	1782	22	0
1	N	1821	0	1782	19	0
2	O	468	0	239	8	0
2	P	468	0	239	4	0
2	Q	468	0	239	12	0
2	R	468	0	239	6	0
2	T	468	0	239	8	0
2	U	468	0	239	13	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
All	All	28377	0	26382	387	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 7.

The worst 5 of 387 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:I:6:LEU:HD22	1:I:228:ARG:HH12	1.16	1.07
1:E:214:HIS:HB3	1:E:217:ARG:HD3	1.60	0.81
1:E:154:LEU:HD13	1:E:162:GLN:HE22	1.46	0.81
2:Q:9:U:H2'	2:Q:11:G:H1	1.46	0.81
1:N:195:PRO:HA	1:N:223:LEU:HB2	1.65	0.78

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	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
1	B	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
1	C	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
1	D	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
1	E	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
1	F	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
1	G	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
1	H	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
1	I	224/248 (90%)	217 (97%)	7 (3%)	0	100	100
1	J	224/248 (90%)	217 (97%)	7 (3%)	0	100	100
1	K	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
1	L	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
1	M	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
1	N	224/248 (90%)	214 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3136/3472 (90%)	3016 (96%)	120 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	193/211 (92%)	193 (100%)	0	100	100
1	B	193/211 (92%)	193 (100%)	0	100	100
1	C	193/211 (92%)	193 (100%)	0	100	100
1	D	193/211 (92%)	193 (100%)	0	100	100
1	E	193/211 (92%)	193 (100%)	0	100	100
1	F	193/211 (92%)	193 (100%)	0	100	100
1	G	193/211 (92%)	193 (100%)	0	100	100
1	H	193/211 (92%)	193 (100%)	0	100	100
1	I	193/211 (92%)	193 (100%)	0	100	100
1	J	193/211 (92%)	193 (100%)	0	100	100
1	K	193/211 (92%)	193 (100%)	0	100	100
1	L	193/211 (92%)	193 (100%)	0	100	100
1	M	193/211 (92%)	193 (100%)	0	100	100
1	N	193/211 (92%)	193 (100%)	0	100	100
All	All	2702/2954 (92%)	2702 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	108	ASN
1	N	71	HIS
1	J	130	HIS
1	L	96	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	O	21/22 (95%)	10 (47%)	0
2	P	21/22 (95%)	8 (38%)	1 (4%)
2	Q	21/22 (95%)	9 (42%)	0
2	R	21/22 (95%)	6 (28%)	0
2	T	21/22 (95%)	9 (42%)	0
2	U	21/22 (95%)	10 (47%)	1 (4%)
All	All	126/132 (95%)	52 (41%)	2 (1%)

5 of 52 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	O	2	U
2	O	3	C
2	O	9	U
2	O	10	C
2	O	11	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	P	9	U
2	U	7	U

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

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	D	303	-	4,4,4	1.59	1 (25%)	6,6,6	0.63	0
3	PO4	C	301	-	4,4,4	1.54	1 (25%)	6,6,6	0.66	0
3	PO4	I	301	-	4,4,4	1.55	1 (25%)	6,6,6	0.57	0
3	PO4	L	301	-	4,4,4	1.55	1 (25%)	6,6,6	0.62	0
3	PO4	M	301	-	4,4,4	1.60	1 (25%)	6,6,6	0.46	0
3	PO4	B	301	-	4,4,4	1.58	1 (25%)	6,6,6	0.47	0
3	PO4	G	301	-	4,4,4	1.55	1 (25%)	6,6,6	0.55	0
3	PO4	D	302	-	4,4,4	1.57	1 (25%)	6,6,6	0.47	0
3	PO4	E	301	-	4,4,4	1.61	1 (25%)	6,6,6	0.45	0
3	PO4	F	301	-	4,4,4	1.56	1 (25%)	6,6,6	0.74	0
3	PO4	K	301	-	4,4,4	1.58	1 (25%)	6,6,6	0.53	0
3	PO4	A	301	-	4,4,4	1.59	1 (25%)	6,6,6	0.40	0
3	PO4	D	301	-	4,4,4	1.55	1 (25%)	6,6,6	0.58	0
3	PO4	J	301	-	4,4,4	1.59	1 (25%)	6,6,6	0.54	0
3	PO4	H	301	-	4,4,4	1.52	1 (25%)	6,6,6	0.72	0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	PO4	P-O1	2.85	1.57	1.50
3	M	301	PO4	P-O1	2.81	1.57	1.50
3	J	301	PO4	P-O1	2.80	1.57	1.50
3	A	301	PO4	P-O1	2.79	1.57	1.50
3	B	301	PO4	P-O1	2.76	1.57	1.50

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

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	226/248 (91%)	-0.42	0	100	100	40, 74, 122, 161	0
1	B	226/248 (91%)	-0.47	0	100	100	44, 71, 125, 167	0
1	C	226/248 (91%)	-0.19	0	100	100	55, 104, 163, 191	0
1	D	226/248 (91%)	-0.40	0	100	100	37, 78, 140, 169	0
1	E	226/248 (91%)	-0.30	0	100	100	56, 96, 179, 213	0
1	F	226/248 (91%)	-0.32	0	100	100	50, 89, 152, 192	0
1	G	226/248 (91%)	-0.44	0	100	100	56, 85, 140, 181	0
1	H	226/248 (91%)	-0.19	0	100	100	71, 111, 159, 170	0
1	I	226/248 (91%)	-0.27	0	100	100	68, 107, 168, 195	0
1	J	226/248 (91%)	-0.27	0	100	100	62, 105, 160, 197	0
1	K	226/248 (91%)	-0.20	1 (0%)	88	70	79, 119, 168, 198	0
1	L	226/248 (91%)	-0.30	1 (0%)	88	70	63, 93, 128, 184	0
1	M	226/248 (91%)	-0.32	0	100	100	70, 109, 162, 186	0
1	N	226/248 (91%)	-0.26	0	100	100	71, 116, 168, 191	0
2	O	22/22 (100%)	0.18	0	100	100	142, 173, 183, 194	0
2	P	22/22 (100%)	-0.34	0	100	100	129, 160, 179, 187	0
2	Q	22/22 (100%)	-0.00	0	100	100	154, 270, 354, 384	0
2	R	22/22 (100%)	-0.30	0	100	100	124, 146, 153, 163	0
2	T	22/22 (100%)	0.10	0	100	100	178, 253, 306, 335	0
2	U	22/22 (100%)	0.07	0	100	100	159, 279, 333, 335	0
All	All	3296/3604 (91%)	-0.30	2 (0%)	92	85	37, 99, 169, 384	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	149	PHE	2.6
1	L	21	GLY	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 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
3	PO4	L	301	5/5	0.69	0.16	114,116,138,140	0
3	PO4	D	302	5/5	0.78	0.14	135,140,171,175	0
3	PO4	I	301	5/5	0.81	0.10	91,107,122,132	0
3	PO4	M	301	5/5	0.81	0.09	109,117,145,146	0
3	PO4	C	301	5/5	0.83	0.12	71,87,117,122	0
3	PO4	D	303	5/5	0.84	0.10	96,100,114,141	0
3	PO4	E	301	5/5	0.84	0.10	82,104,112,123	0
3	PO4	H	301	5/5	0.84	0.12	108,111,132,144	0
3	PO4	D	301	5/5	0.87	0.25	141,147,168,183	0
3	PO4	G	301	5/5	0.88	0.08	107,125,133,144	0
3	PO4	K	301	5/5	0.88	0.08	110,120,139,148	0
3	PO4	J	301	5/5	0.89	0.08	78,92,122,136	0
3	PO4	B	301	5/5	0.89	0.13	98,101,128,129	0
3	PO4	F	301	5/5	0.93	0.07	75,81,113,114	0
3	PO4	A	301	5/5	0.94	0.08	90,96,115,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.