



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 10:06 am BST

PDB ID : 9RDE / pdb_00009rde
Title : Crystal structure of the B. licheniformis bacitacin sythetase 3 cis-E-COM-C domains
Authors : Rasche, R.; Diecker, J.; Rueschenbaum, J.; Mootz, H.D.; Kuemmel, D.
Deposited on : 2025-06-02
Resolution : 3.29 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

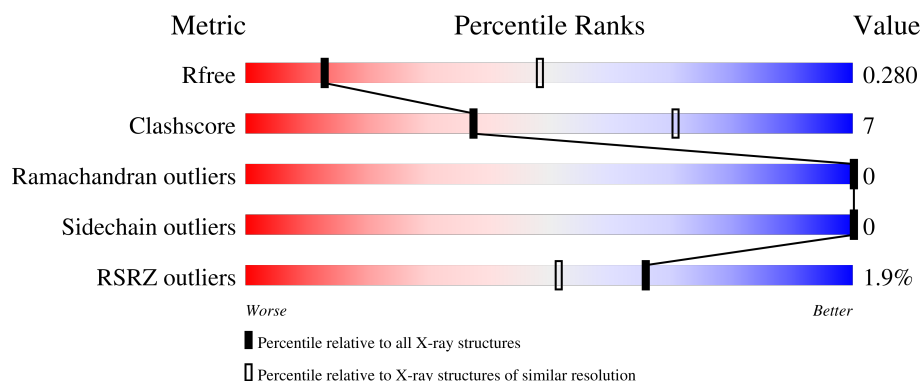
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	925	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6727 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 Bacitracin synthase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	826	Total	C	N	O	S	Se	0	0	0
			6727	4273	1168	1265	2	19			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4612	MSE	-	initiating methionine	UNP O68008
A	4613	GLY	-	expression tag	UNP O68008
A	4740	LEU	VAL	engineered mutation	UNP O68008
A	5527	GLY	-	expression tag	UNP O68008
A	5528	SER	-	expression tag	UNP O68008
A	5529	ARG	-	expression tag	UNP O68008
A	5530	SER	-	expression tag	UNP O68008
A	5531	HIS	-	expression tag	UNP O68008
A	5532	HIS	-	expression tag	UNP O68008
A	5533	HIS	-	expression tag	UNP O68008
A	5534	HIS	-	expression tag	UNP O68008
A	5535	HIS	-	expression tag	UNP O68008
A	5536	HIS	-	expression tag	UNP O68008

- Molecule 1: Bacitracin synthase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	147.75Å 147.75Å 66.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.29 49.42 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.42-3.29) 99.8 (49.42-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.237 , 0.282 0.238 , 0.280	Depositor DCC
R_{free} test set	1090 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	130.5	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6727	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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](#)

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	0.12	1/6832 (0.0%)	0.23	0/9174

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4828	MSE	SE-CE	-5.32	1.79	1.95

There are no bond angle outliers.

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	6727	0	6683	93	0
All	All	6727	0	6683	93	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.

All (93) 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:4865:THR:HG22	1:A:4937:LYS:HD2	1.72	0.70
1:A:4952:ILE:HG23	1:A:4956:LEU:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5279:ALA:O	1:A:5283:ASN:ND2	2.26	0.67
1:A:5141:ARG:NH2	1:A:5257:GLU:O	2.27	0.66
1:A:5116:GLU:OE1	1:A:5234:ARG:NH2	2.30	0.64
1:A:5285:LEU:HD13	1:A:5423:SER:HB2	1.81	0.61
1:A:5233:SER:HB3	1:A:5375:VAL:HG13	1.81	0.61
1:A:5162:ILE:HB	1:A:5165:ARG:HB2	1.82	0.61
1:A:4789:THR:HG22	1:A:4790:ALA:H	1.67	0.60
1:A:5310:GLU:HG2	1:A:5486:THR:HG22	1.84	0.59
1:A:4661:SER:HA	1:A:4664:LYS:HE3	1.84	0.59
1:A:4707:VAL:O	1:A:4707:VAL:HG12	2.02	0.59
1:A:5240:GLU:HG2	1:A:5256:LEU:HD21	1.84	0.59
1:A:5473:ILE:HD12	1:A:5485:LEU:HD23	1.84	0.58
1:A:5012:ALA:HB1	1:A:5019:LEU:HD11	1.84	0.58
1:A:4717:VAL:HG21	1:A:4992:LEU:HD13	1.85	0.57
1:A:4620:GLU:O	1:A:4788:LYS:NZ	2.31	0.57
1:A:4672:LYS:HA	1:A:4678:ARG:HE	1.70	0.57
1:A:4710:GLU:HG3	1:A:4712:ASP:H	1.71	0.56
1:A:5360:VAL:HG22	1:A:5381:THR:HG22	1.87	0.56
1:A:4693:ARG:HB3	1:A:4697:LYS:HD2	1.88	0.55
1:A:5506:GLN:O	1:A:5510:GLN:NE2	2.39	0.55
1:A:4739:ALA:HB3	1:A:4750:LEU:HB3	1.88	0.55
1:A:5338:LEU:HD12	1:A:5436:PHE:HE2	1.71	0.55
1:A:4651:MSE:HE2	1:A:4992:LEU:HB2	1.87	0.55
1:A:4838:GLU:HB3	1:A:5000:LYS:HB3	1.89	0.55
1:A:5314:GLU:HG2	1:A:5482:VAL:HG22	1.90	0.53
1:A:4897:ARG:HA	1:A:4906:ILE:HD11	1.89	0.53
1:A:5138:ILE:HG21	1:A:5237:ILE:HG23	1.88	0.53
1:A:5141:ARG:HD3	1:A:5244:MSE:HE1	1.91	0.53
1:A:4640:LYS:HA	1:A:4643:ARG:HH21	1.75	0.52
1:A:5096:ASN:ND2	1:A:5413:ASP:O	2.41	0.52
1:A:4668:LYS:HD3	1:A:4699:LEU:HD12	1.92	0.51
1:A:4762:SER:HB3	1:A:4910:VAL:HG13	1.92	0.51
1:A:5105:ALA:HA	1:A:5114:TYR:CZ	2.45	0.51
1:A:4975:LEU:HB2	1:A:5013:VAL:HG12	1.92	0.51
1:A:4671:ILE:HA	1:A:4677:LEU:HD12	1.93	0.51
1:A:5146:ARG:NH1	1:A:5162:ILE:O	2.44	0.50
1:A:4810:SER:O	1:A:4813:GLN:NE2	2.44	0.50
1:A:4713:GLN:HG3	1:A:4714:PRO:HD3	1.94	0.49
1:A:4923:LEU:HD22	1:A:4935:MSE:SE	2.62	0.49
1:A:5315:PHE:HB3	1:A:5319:LEU:HD23	1.94	0.49
1:A:5313:ILE:HG23	1:A:5501:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4931:ARG:NH1	1:A:5074:ASP:OD1	2.46	0.48
1:A:5116:GLU:HG2	1:A:5226:HIS:CE1	2.48	0.48
1:A:4629:THR:HG22	1:A:4799:ILE:HD11	1.95	0.48
1:A:5154:THR:OG1	1:A:5156:GLU:O	2.29	0.48
1:A:5056:ARG:HH21	1:A:5060:GLU:HG3	1.79	0.48
1:A:4855:LEU:HD21	1:A:4867:ILE:HG23	1.96	0.47
1:A:4889:ARG:NH1	1:A:4966:ALA:O	2.48	0.47
1:A:4654:ARG:NH1	1:A:4657:GLY:O	2.41	0.47
1:A:4728:ILE:HD11	1:A:4735:LEU:HD23	1.96	0.46
1:A:4798:HIS:HB2	1:A:4904:ILE:HD12	1.98	0.46
1:A:5009:GLU:HB2	1:A:5024:THR:HB	1.97	0.46
1:A:5213:THR:OG1	1:A:5217:SER:O	2.24	0.46
1:A:5371:ILE:HD13	1:A:5374:MSE:SE	2.66	0.46
1:A:5115:PHE:CE1	1:A:5197:GLY:HA2	2.51	0.45
1:A:4929:MSE:HA	1:A:4932:THR:HB	1.97	0.45
1:A:5336:THR:HG23	1:A:5401:VAL:HG13	1.99	0.45
1:A:5222:TRP:HH2	1:A:5229:LEU:HD21	1.82	0.45
1:A:5170:ASP:OD2	1:A:5189:TYR:OH	2.24	0.45
1:A:5145:LEU:HD11	1:A:5375:VAL:HG11	1.99	0.45
1:A:4809:LEU:HG	1:A:4812:LYS:HE3	1.97	0.45
1:A:5211:MSE:HG3	1:A:5219:THR:OG1	2.18	0.44
1:A:4893:GLU:HG3	1:A:4971:LEU:HD11	1.99	0.44
1:A:4890:ILE:HG22	1:A:4970:ILE:HG23	2.00	0.44
1:A:4669:GLU:HG3	1:A:4783:VAL:HG21	1.99	0.44
1:A:4889:ARG:HB2	1:A:4920:PHE:HD1	1.83	0.43
1:A:4931:ARG:O	1:A:4935:MSE:HG2	2.18	0.43
1:A:5322:ARG:NH1	1:A:5512:VAL:HG21	2.33	0.43
1:A:5172:HIS:CD2	1:A:5211:MSE:HB3	2.54	0.43
1:A:4629:THR:H	1:A:4632:GLN:NE2	2.17	0.43
1:A:4657:GLY:HA2	1:A:4747:ASP:HB2	2.01	0.43
1:A:5401:VAL:HG23	1:A:5404:GLN:NE2	2.34	0.43
1:A:4807:LYS:O	1:A:4810:SER:OG	2.35	0.42
1:A:4977:GLN:HA	1:A:5014:VAL:HG23	2.01	0.42
1:A:5319:LEU:HD13	1:A:5322:ARG:HH22	1.83	0.42
1:A:4826:LEU:HB2	1:A:5030:TYR:CE1	2.55	0.42
1:A:5148:SER:HB2	1:A:5165:ARG:HH12	1.84	0.42
1:A:4662:ILE:HG23	1:A:4777:LEU:HD23	2.00	0.42
1:A:5284:TYR:HE2	1:A:5404:GLN:HG3	1.85	0.41
1:A:5118:MSE:HE3	1:A:5234:ARG:HD2	2.02	0.41
1:A:5210:LEU:HD11	1:A:5218:TYR:HD2	1.86	0.41
1:A:5247:MSE:HG3	1:A:5254:HIS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4675:ASP:OD2	1:A:4678:ARG:NH2	2.48	0.41
1:A:4626:VAL:HG23	1:A:4793:GLN:HA	2.03	0.41
1:A:5316:PRO:HD2	1:A:5319:LEU:HD23	2.02	0.41
1:A:5145:LEU:HD21	1:A:5237:ILE:HD13	2.03	0.41
1:A:4750:LEU:HD21	1:A:4752:ILE:HD11	2.02	0.41
1:A:5406:LEU:O	1:A:5409:ARG:HB3	2.20	0.40
1:A:4835:PHE:CE2	1:A:5007:PRO:HG3	2.56	0.40
1:A:4745:ASN:O	1:A:4745:ASN:ND2	2.52	0.40
1:A:5256:LEU:HD12	1:A:5256:LEU:HA	1.89	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	810/925 (88%)	794 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	720/785 (92%)	720 (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. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4632	GLN
1	A	4645	HIS
1	A	4690	GLN
1	A	4713	GLN
1	A	4719	GLN
1	A	4939	HIS
1	A	5168	ASN
1	A	5177	GLN
1	A	5404	GLN
1	A	5513	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	807/925 (87%)	-0.15	15 (1%)	66 51	72, 146, 226, 308	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4638	LEU	6.5
1	A	5475	ALA	4.2
1	A	5342	TRP	3.2
1	A	4637	SER	3.0
1	A	4723	GLU	3.0
1	A	5474	VAL	2.8
1	A	4635	TYR	2.8
1	A	5436	PHE	2.5
1	A	5274	LYS	2.4
1	A	4955	TYR	2.4
1	A	5469	TYR	2.3
1	A	5323	ILE	2.1
1	A	5360	VAL	2.1
1	A	4951	GLY	2.0
1	A	5425	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.