



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2022 – 04:05 pm BST

PDB ID : 7P5R
Title : Racemic X-ray crystal structure of bacteriocin
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Deposited on : 2021-07-14
Resolution : 0.96 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	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

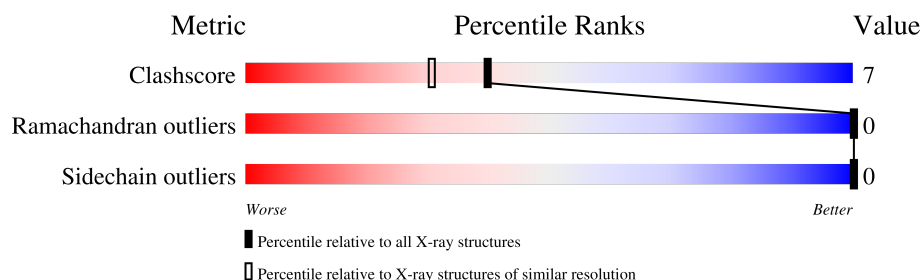
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.96 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	141614	1321 (1.06-0.86)
Ramachandran outliers	138981	1233 (1.06-0.86)
Sidechain outliers	138945	1235 (1.06-0.86)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	53	92% 8%
1	BBB	53	85% 15%
2	CCC	53	94% 6%
2	DDD	53	92% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1942 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.

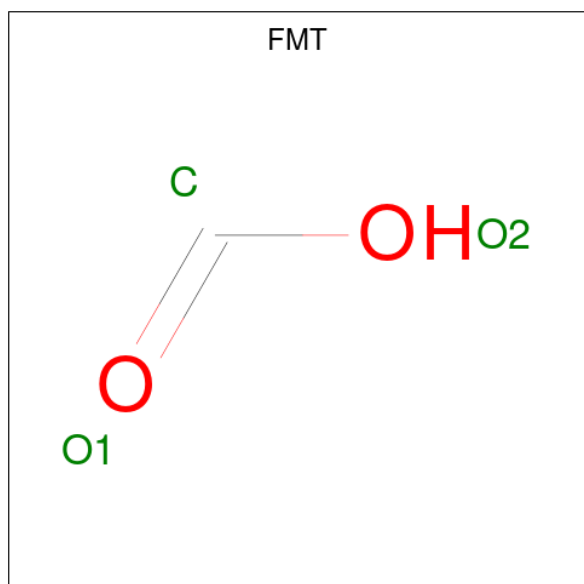
- Molecule 1 is a protein called Lactacin Q.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	53	Total	C	N	O	S	0	3	0
			434	290	73	70	1			
1	BBB	53	Total	C	N	O	S	0	3	0
			433	289	72	71	1			

- Molecule 2 is a protein called D-Lactacin Q.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DDD	53	Total	C	N	O	S	0	2	0
			426	286	71	68	1			
2	CCC	53	Total	C	N	O	S	0	4	0
			440	294	73	72	1			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 3 1 2	0	0
3	BBB	1	Total C O 3 1 2	0	0
3	BBB	1	Total C O 3 1 2	0	0
3	BBB	1	Total C O 3 1 2	0	0
3	DDD	1	Total C O 3 1 2	0	0
3	DDD	1	Total C O 3 1 2	0	0
3	CCC	1	Total C O 3 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	40	Total O 40 40	0	0
4	BBB	47	Total O 47 47	0	0
4	DDD	45	Total O 46 46	0	1
4	CCC	55	Total O 55 55	0	0

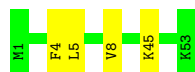
3 Residue-property plots [i](#)

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 failed to run properly.

- Molecule 1: Lacticin Q

Chain AAA:  92% 8%



- Molecule 1: Lacticin Q

Chain BBB:  85% 15%



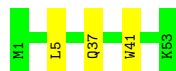
- Molecule 2: D-Lacticin Q

Chain DDD:  92% 8%



- Molecule 2: D-Lacticin Q

Chain CCC:  94% 6%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	24.21Å 27.83Å 70.45Å 95.03° 90.43° 115.41°	Depositor
Resolution (Å)	35.05 – 0.96	Depositor
% Data completeness (in resolution range)	93.0 (35.05-0.96)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 0.96Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.205	Depositor
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.274	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.62$, $\langle L^2 \rangle = 0.48$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
Total number of atoms	1942	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% 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: DTY, DLE, DAS, DGN, DTR, DSN, DPN, MED, FMT, DLY, DAL, DSG, DIL, DVA

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	AAA	0.67	0/449	0.92	0/604
1	BBB	0.75	0/448	0.86	0/603
2	CCC	0.53	0/15	0.84	0/10
2	DDD	0.61	0/15	0.92	0/10
All	All	0.71	0/927	0.89	0/1227

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 [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	AAA	434	0	472	6	0
1	BBB	433	0	468	11	0
2	CCC	440	0	443	4	0
2	DDD	426	0	433	5	0
3	AAA	3	0	1	0	0
3	BBB	9	0	3	1	0
3	CCC	3	0	1	0	0
3	DDD	6	0	2	0	0
4	AAA	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	47	0	0	1	0
4	CCC	55	0	0	2	0
4	DDD	46	0	0	1	0
All	All	1942	0	1823	26	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 (26) 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)
2:CCC:5[B]:DLE:HD22	4:CCC:247:HOH:O	1.44	1.15
1:BBB:41:TRP:CH2	1:BBB:45:LYS:HD2	1.85	1.11
1:AAA:5:LEU:HD12	1:AAA:8[B]:VAL:CG2	1.98	0.93
2:CCC:37:DGN:OE1	2:CCC:41:DTR:CE2	2.28	0.81
1:BBB:41:TRP:CH2	1:BBB:45:LYS:CD	2.66	0.79
2:DDD:6:DLY:HG3	4:DDD:202:HOH:O	1.91	0.69
1:AAA:5:LEU:HD12	1:AAA:8[B]:VAL:HG22	1.78	0.64
1:BBB:5:LEU:HD12	1:BBB:8[A]:VAL:CG2	2.29	0.63
1:AAA:5:LEU:HA	1:AAA:8[B]:VAL:HG22	1.83	0.60
2:CCC:5[B]:DLE:CD2	4:CCC:247:HOH:O	2.23	0.59
2:DDD:4:DPN:HE1	2:DDD:23:DTR:CZ3	2.35	0.57
1:BBB:5:LEU:HD12	1:BBB:8[A]:VAL:HG22	1.86	0.56
1:BBB:6:LYS:NZ	4:BBB:402:HOH:O	2.38	0.54
1:AAA:5:LEU:HD12	1:AAA:8[B]:VAL:HG21	1.89	0.52
2:DDD:4:DPN:HE1	2:DDD:23:DTR:CH2	2.42	0.49
1:AAA:45:LYS:HD2	4:AAA:201:HOH:O	2.12	0.49
2:CCC:37:DGN:OE1	2:CCC:41:DTR:CZ2	2.62	0.47
2:DDD:6:DLY:HD3	2:DDD:39:DIL:HD13	1.96	0.46
1:BBB:4:PHE:HE2	1:BBB:23:TRP:CH2	2.34	0.46
1:BBB:41:TRP:CZ3	1:BBB:45:LYS:HD2	2.46	0.45
2:DDD:6:DLY:HG2	2:DDD:39:DIL:HG21	2.00	0.44
1:AAA:4:PHE:O	1:AAA:8[A]:VAL:HG23	2.18	0.43
1:BBB:37:GLN:HA	1:BBB:37:GLN:OE1	2.18	0.42
1:BBB:41:TRP:CZ2	1:BBB:45:LYS:HD2	2.46	0.42
1:BBB:6:LYS:HD2	3:BBB:301:FMT:H	2.01	0.40
1:BBB:4:PHE:CE2	1:BBB:23:TRP:CZ3	3.10	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	AAA	54/53 (102%)	54 (100%)	0	0	100	100
1	BBB	54/53 (102%)	54 (100%)	0	0	100	100
2	CCC	5/53 (9%)	5 (100%)	0	0	100	100
2	DDD	5/53 (9%)	5 (100%)	0	0	100	100
All	All	118/212 (56%)	118 (100%)	0	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	AAA	44/41 (107%)	44 (100%)	0	100	100
1	BBB	44/41 (107%)	44 (100%)	0	100	100
All	All	88/82 (107%)	88 (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. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

102 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	FMT	AAA	101	-	2,2,2	0.35	0	1,1,1	0.32	0
3	FMT	BBB	302	-	2,2,2	0.30	0	1,1,1	0.07	0
3	FMT	BBB	301	-	2,2,2	0.78	0	1,1,1	0.06	0
3	FMT	DDD	102	-	2,2,2	0.48	0	1,1,1	0.02	0
3	FMT	CCC	101	-	2,2,2	0.13	0	1,1,1	0.19	0
3	FMT	BBB	303	-	2,2,2	0.33	0	1,1,1	0.07	0
3	FMT	DDD	101	-	2,2,2	0.05	0	1,1,1	0.25	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	301	FMT	1	0

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](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.