



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:53 AM UTC

PDB ID : 5WQE / pdb_00005wqe
Title : Crystal structure of Alicyclobacillus acidoterrestris C2c1 in complex with single-guide RNA at 3.1 Angstrom resolution
Authors : Liu, L.; Wang, Y.L.
Deposited on : 2016-11-26
Resolution : 3.13 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

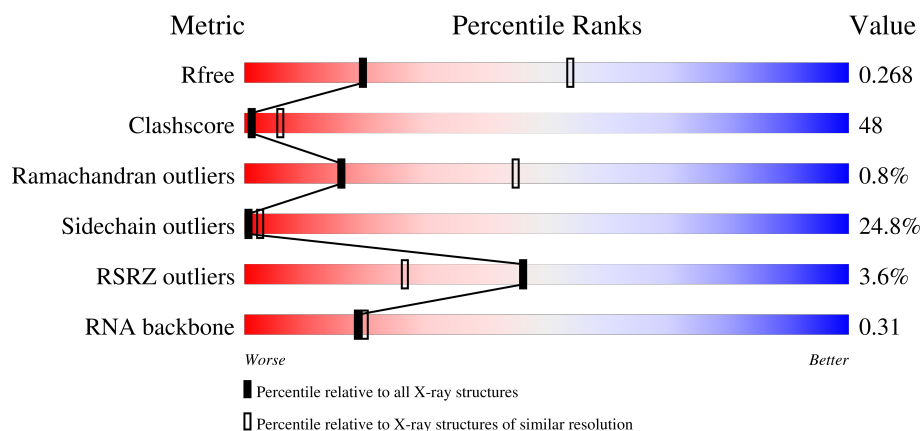
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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	1137	
2	B	112	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9308 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 CRISPR-associated endonuclease C2c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	Se	0	0	0
			7988	5033	1476	1452	8	19			

There are 8 discrepancies between the modelled and reference sequences:

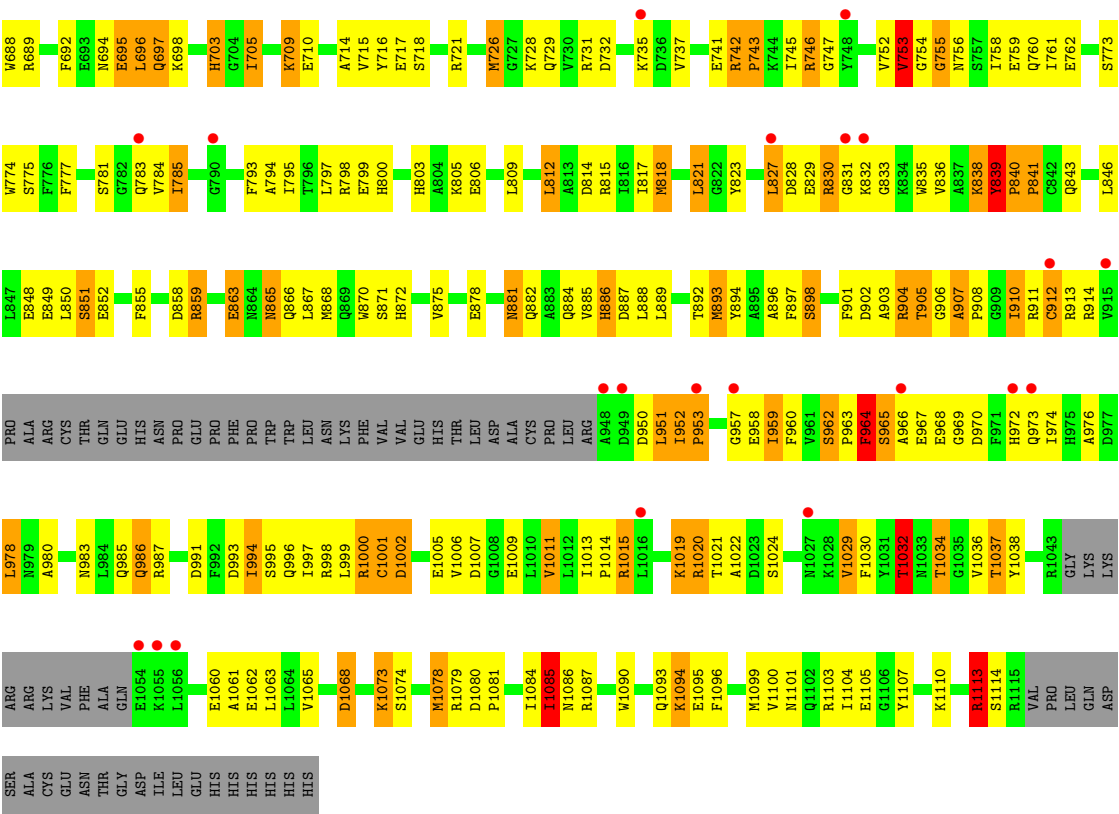
Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	LEU	-	expression tag	UNP T0D7A2
A	1131	GLU	-	expression tag	UNP T0D7A2
A	1132	HIS	-	expression tag	UNP T0D7A2
A	1133	HIS	-	expression tag	UNP T0D7A2
A	1134	HIS	-	expression tag	UNP T0D7A2
A	1135	HIS	-	expression tag	UNP T0D7A2
A	1136	HIS	-	expression tag	UNP T0D7A2
A	1137	HIS	-	expression tag	UNP T0D7A2

- Molecule 2 is a RNA chain called RNA (60-MER).

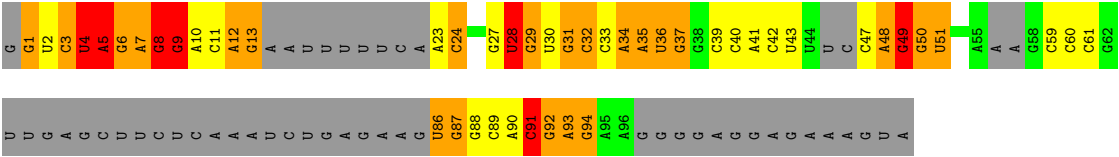
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	60	Total	C	N	O	P	0	0	0
			1278	567	241	410	60			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	3	Total	O	0	0
			3	3		



● Molecule 2: RNA (60-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.55Å 129.84Å 84.00Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	48.64 – 3.13 48.64 – 3.13	Depositor EDS
% Data completeness (in resolution range)	79.3 (48.64-3.13) 79.3 (48.64-3.13)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.238 , 0.268 0.238 , 0.268	Depositor DCC
R_{free} test set	1340 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9308	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	0.98	25/8134 (0.3%)	1.31	91/10953 (0.8%)
2	B	0.52	0/1427	1.08	12/2217 (0.5%)
All	All	0.92	25/9561 (0.3%)	1.27	103/13170 (0.8%)

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	A	0	5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	MSE	C-N	8.20	1.40	1.33
1	A	841	PRO	N-CD	-6.40	1.38	1.47
1	A	742	ARG	C-N	6.09	1.40	1.33
1	A	839	TYR	C-N	6.06	1.40	1.33
1	A	310	ALA	C-N	6.03	1.40	1.33

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	VAL	N-CA-C	32.84	144.12	110.62
1	A	295	ALA	N-CA-C	-20.10	78.36	110.32
1	A	203	GLU	CB-CA-C	-16.59	82.58	109.80
1	A	421	HIS	N-CA-C	-16.29	82.60	109.96
1	A	296	LEU	N-CA-CB	15.89	137.34	110.49

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	GLY	Peptide
1	A	531	ASP	Peptide
1	A	64	THR	Peptide
1	A	784	VAL	Peptide
1	A	912	CYS	Peptide

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	7988	0	7713	743	0
2	B	1278	0	645	126	0
3	A	39	0	0	3	0
3	B	3	0	0	0	0
All	All	9308	0	8358	841	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 48.

The worst 5 of 841 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:B:8:G:H3'	2:B:9:G:C5'	1.71	1.19
1:A:575:THR:CG2	1:A:621:LYS:HE2	1.73	1.18
1:A:758:ILE:HG23	1:A:867:LEU:HD23	1.27	1.14
1:A:1073:LYS:HA	1:A:1073:LYS:HE2	1.15	1.13
2:B:11:C:H2'	2:B:12:A:H5'	1.31	1.11

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	997/1137 (88%)	965 (97%)	24 (2%)	8 (1%)	16	45

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LEU
1	A	401	LEU
1	A	459	ILE
1	A	952	ILE
1	A	344	GLU

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	804/955 (84%)	605 (75%)	199 (25%)	1	2

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	675	GLU
1	A	830	ARG
1	A	688	TRP
1	A	753	VAL
1	A	865	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	HIS
1	A	1089	ASN
1	A	648	GLN
1	A	877	GLN

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Mol	Chain	Res	Type
1	A	618	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	55/112 (49%)	26 (47%)	9 (16%)

5 of 26 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	U
2	B	5	A
2	B	6	G
2	B	7	A
2	B	8	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	86	U
2	B	92	G
2	B	31	G
2	B	36	U
2	B	49	G

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	992/1137 (87%)	0.16	38 (3%) 44 25	11, 41, 87, 134	6 (0%)
2	B	60/112 (53%)	-0.23	0 100 100	22, 61, 124, 146	0
All	All	1052/1249 (84%)	0.14	38 (3%) 46 26	11, 43, 90, 146	6 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	TYR	7.9
1	A	953	PRO	5.2
1	A	198	GLU	5.1
1	A	790	GLY	4.9
1	A	319	ASP	4.2

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.