wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 08:36 AM UTC

PDB ID	:	2QFC / pdb_00002qfc
Title	:	Crystal Structure of Bacillus thuringiensis PlcR complexed with PapR
Authors	:	Declerck, N.; Chaix, D.; Rugani, N.; Hoh, F.; Arold, S.T.
Deposited on	:	2007-06-27
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

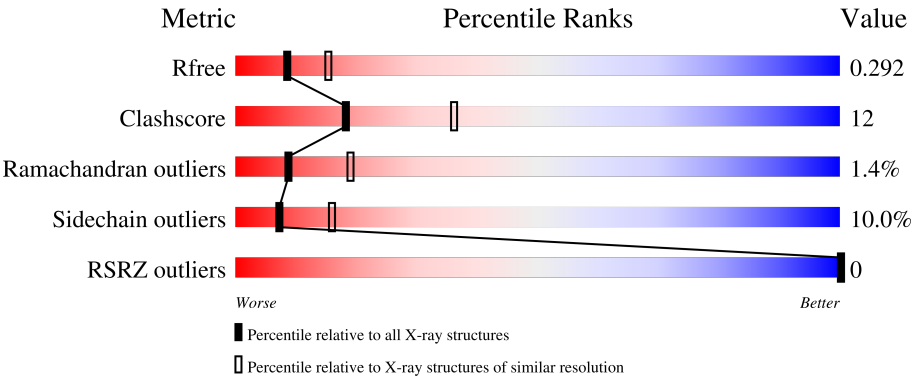
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 <=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	293	66% 25% 5%
1	B	293	70% 22%
2	C	5	40% 40% 20%
2	D	5	60% 40%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4920 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 PlcR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2384	1542	393	440	9			
1	B	284	Total	C	N	O	S	0	0	0
			2384	1542	393	440	9			

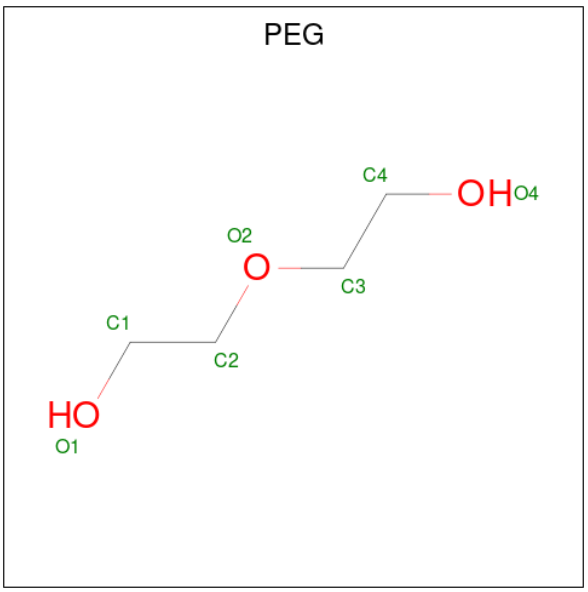
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	-	expression tag	UNP Q45782
A	287	GLU	-	expression tag	UNP Q45782
A	288	HIS	-	expression tag	UNP Q45782
A	289	HIS	-	expression tag	UNP Q45782
A	290	HIS	-	expression tag	UNP Q45782
A	291	HIS	-	expression tag	UNP Q45782
A	292	HIS	-	expression tag	UNP Q45782
A	293	HIS	-	expression tag	UNP Q45782
B	286	LEU	-	expression tag	UNP Q45782
B	287	GLU	-	expression tag	UNP Q45782
B	288	HIS	-	expression tag	UNP Q45782
B	289	HIS	-	expression tag	UNP Q45782
B	290	HIS	-	expression tag	UNP Q45782
B	291	HIS	-	expression tag	UNP Q45782
B	292	HIS	-	expression tag	UNP Q45782
B	293	HIS	-	expression tag	UNP Q45782

- Molecule 2 is a protein called C-terminus pentapeptide from PapR protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			47	34	5	8			
2	D	5	Total	C	N	O	0	0	0
			47	34	5	8			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	B	13	Total O 13 13	0	0
4	D	1	Total O 1 1	0	0

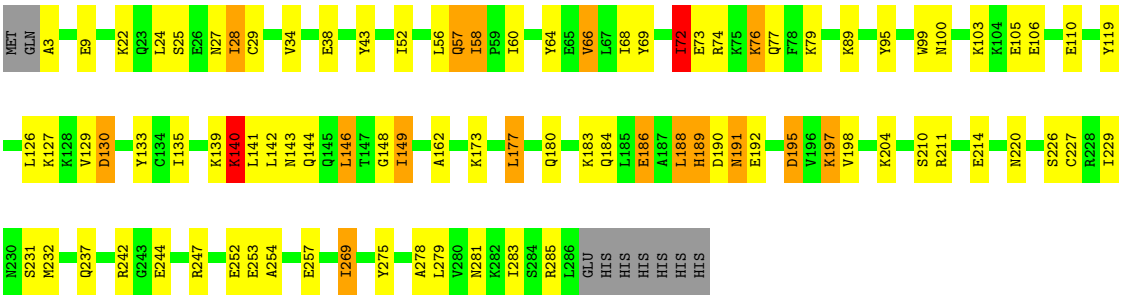
3 Residue-property plots (i)

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 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: PlcR protein

Chain A:

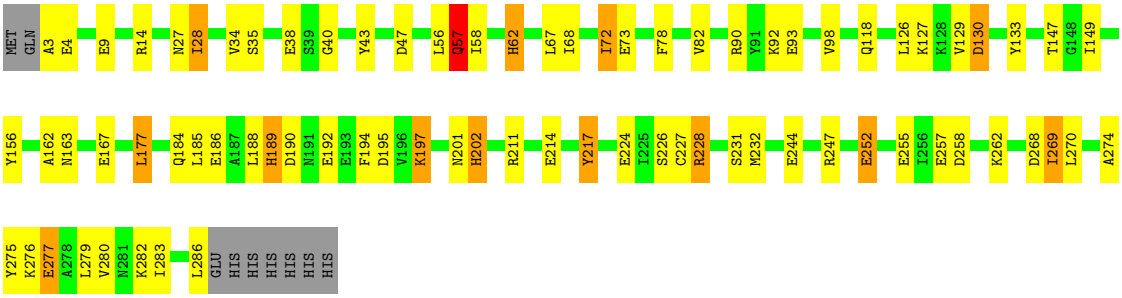




• Molecule 1: PlcR protein

Chain B:





• Molecule 2: C-terminus pentapeptide from PapR protein

Chain C:





• Molecule 2: C-terminus pentapeptide from PapR protein

Chain D:




L44
F48

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	85.68Å 85.68Å 189.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.12 – 2.60 74.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.12-2.60) 99.9 (74.12-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.304 0.213 , 0.292	Depositor DCC
R_{free} test set	1234 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG

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	0.95	3/2429 (0.1%)	1.07	5/3265 (0.2%)
1	B	1.28	3/2429 (0.1%)	1.15	11/3265 (0.3%)
2	C	0.93	0/49	0.91	0/64
2	D	0.77	0/49	0.88	0/64
All	All	1.13	6/4956 (0.1%)	1.11	16/6658 (0.2%)

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	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	HIS	CE1-NE2	35.18	1.67	1.32
1	B	62	HIS	CG-ND1	19.57	1.59	1.38
1	B	62	HIS	CG-CD2	15.80	1.53	1.35
1	A	285	ARG	CZ-NH1	9.36	1.45	1.32
1	A	285	ARG	CD-NE	6.64	1.55	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	HIS	ND1-CG-CD2	9.43	115.53	106.10
1	B	62	HIS	CG-CD2-NE2	-8.07	99.13	107.20
1	A	140	LYS	N-CA-C	-6.03	104.82	111.82
1	B	231	SER	N-CA-C	5.92	118.59	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	ASP	CB-CA-C	-5.62	98.01	109.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	LEU	Peptide

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	2384	0	2404	68	0
1	B	2384	0	2404	57	0
2	C	47	0	41	4	0
2	D	47	0	41	3	0
3	A	21	0	30	7	0
3	B	7	0	10	2	0
4	A	16	0	0	1	0
4	B	13	0	0	1	0
4	D	1	0	0	0	0
All	All	4920	0	4930	119	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 12.

The worst 5 of 119 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:62:HIS:CE1	1:B:62:HIS:NE2	1.67	1.49
1:A:57:GLN:HB2	1:A:58:ILE:HA	1.29	1.08
1:A:99:TRP:CZ3	3:A:1004:PEG:H21	2.05	0.91
1:A:188:LEU:O	1:A:189:HIS:HB2	1.71	0.90
1:A:140:LYS:HE2	3:A:1003:PEG:O2	1.74	0.87

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	282/293 (96%)	262 (93%)	16 (6%)	4 (1%)	9 19
1	B	282/293 (96%)	255 (90%)	23 (8%)	4 (1%)	9 19
2	C	3/5 (60%)	3 (100%)	0	0	100 100
2	D	3/5 (60%)	3 (100%)	0	0	100 100
All	All	570/596 (96%)	523 (92%)	39 (7%)	8 (1%)	9 19

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	28	ILE
1	B	28	ILE
1	B	57	GLN
1	B	189	HIS

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	256/265 (97%)	227 (89%)	29 (11%)	5 12
1	B	256/265 (97%)	234 (91%)	22 (9%)	10 22
2	C	5/5 (100%)	4 (80%)	1 (20%)	1 2
2	D	5/5 (100%)	5 (100%)	0	100 100
All	All	522/540 (97%)	470 (90%)	52 (10%)	7 16

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ILE
1	B	98	VAL
1	B	269	ILE
1	B	27	ASN
1	B	47	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	GLN
1	B	88	GLN
1	B	281	ASN
1	B	112	GLN
1	A	281	ASN

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)

4 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	PEG	A	1003	-	6,6,6	1.00	0	5,5,5	0.64	0
3	PEG	B	1002	-	6,6,6	0.85	0	5,5,5	0.35	0
3	PEG	A	1004	-	6,6,6	0.87	0	5,5,5	0.92	0
3	PEG	A	1001	-	6,6,6	0.88	0	5,5,5	1.07	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	1003	-	-	0/4/4/4	-
3	PEG	B	1002	-	-	1/4/4/4	-
3	PEG	A	1004	-	-	2/4/4/4	-
3	PEG	A	1001	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	PEG	C3-O2-C2	-2.02	104.42	113.26

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	PEG	O2-C3-C4-O4
3	A	1001	PEG	O1-C1-C2-O2
3	A	1001	PEG	C4-C3-O2-C2
3	A	1004	PEG	C1-C2-O2-C3
3	A	1001	PEG	O2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	PEG	2	0
3	B	1002	PEG	2	0
3	A	1004	PEG	3	0
3	A	1001	PEG	2	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

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, 95^{th} 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	284/293 (96%)	-1.17	0	100	100	12, 30, 91, 96	0
1	B	284/293 (96%)	-1.19	0	100	100	13, 29, 94, 96	0
2	C	5/5 (100%)	-0.88	0	100	100	66, 67, 70, 71	0
2	D	5/5 (100%)	-0.68	0	100	100	70, 72, 75, 76	0
All	All	578/596 (96%)	-1.17	0	100	100	12, 30, 94, 96	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	PEG	A	1001	7/7	0.97	0.07	53,59,63,63	0
3	PEG	A	1003	7/7	0.98	0.08	62,68,72,72	0
3	PEG	A	1004	7/7	0.99	0.07	60,66,73,75	0
3	PEG	B	1002	7/7	0.99	0.06	55,59,64,66	0

6.5 Other polymers (i)

There are no such residues in this entry.