

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 4, 2021 – 10:02 AM GMT

PDB ID	:	6TTR
$\operatorname{Title}$	:	Crystal Structure of the coiled coil and GGDEF domain of DgcB from
		Caulobacter crescentus in complex with c-di-GMP
Authors	:	Holzschuh, F.; Schirmer, T.; Teixeira, R.D.
Deposited on	:	2019-12-30
Resolution	:	2.85  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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16
EDS Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	: : : : : : : : : : : : : : : : : : : :	<ul> <li>2.16</li> <li>20191225.v01 (using entries in the PDB archive December 25th 2019)</li> <li>5.8.0158</li> <li>7.0.044 (Gargrove)</li> <li>Engh &amp; Huber (2001)</li> <li>Parkinson et al. (1996)</li> <li>2.16</li> </ul>

# 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 2.85 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
$R_{free}$	130704	3168 (2.90-2.82)		
Clashscore	141614	3438 (2.90-2.82)		
Ramachandran outliers	138981	3348 (2.90-2.82)		
Sidechain outliers	138945	3351 (2.90-2.82)		
RSRZ outliers	127900	3103 (2.90-2.82)		

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	А	222	% <b>7</b> 0%	15%	•	14%
1	В	222	73%	14%	•	12%



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# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3092 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	191	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	л	191	1458	890	277	286	5	0	0	0
1	р	105	Total	С	Ν	Ο	S	0	0	0
	I D	195	1486	906	283	291	6	0		

• Molecule 1 is a protein called GGDEF diguanylate cyclase DgcB.

Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
132	MET	-	initiating methionine	UNP A0A0H3CAN8
133	GLY	-	expression tag	UNP A0A0H3CAN8
134	SER	-	expression tag	UNP A0A0H3CAN8
135	SER	-	expression tag	UNP A0A0H3CAN8
136	HIS	-	expression tag	UNP A0A0H3CAN8
137	HIS	-	expression tag	UNP A0A0H3CAN8
138	HIS	-	expression tag	UNP A0A0H3CAN8
139	HIS	-	expression tag	UNP A0A0H3CAN8
140	HIS	-	expression tag	UNP A0A0H3CAN8
141	HIS	-	expression tag	UNP A0A0H3CAN8
142	SER	-	expression tag	UNP A0A0H3CAN8
143	SER	-	expression tag	UNP A0A0H3CAN8
144	GLY	-	expression tag	UNP A0A0H3CAN8
145	LEU	-	expression tag	UNP A0A0H3CAN8
146	VAL	-	expression tag	UNP A0A0H3CAN8
147	PRO	-	expression tag	UNP A0A0H3CAN8
148	ARG	-	expression tag	UNP A0A0H3CAN8
149	GLY	-	expression tag	UNP A0A0H3CAN8
150	SER	_	expression tag	UNP A0A0H3CAN8
151	HIS	-	expression tag	UNP A0A0H3CAN8
152	MET	_	expression tag	UNP A0A0H3CAN8
261	ALA	GLU	engineered mutation	UNP A0A0H3CAN8
262	ALA	GLU	engineered mutation	UNP A0A0H3CAN8
132	MET	-	initiating methionine	UNP A0A0H3CAN8
133	GLY	-	expression tag	UNP A0A0H3CAN8
	Residue         132         133         134         135         136         137         138         139         140         141         142         143         144         145         146         147         148         149         150         151         152         261         262         132         133	Residue         Modelled           132         MET           133         GLY           134         SER           135         SER           136         HIS           137         HIS           138         HIS           139         HIS           140         HIS           142         SER           143         SER           144         GLY           145         LEU           146         VAL           147         PRO           148         ARG           149         GLY           150         SER           151         HIS           152         MET           261         ALA           262         ALA           133         GLY	Residue         Modelled         Actual           132         MET         -           133         GLY         -           134         SER         -           135         SER         -           135         SER         -           136         HIS         -           137         HIS         -           138         HIS         -           139         HIS         -           140         HIS         -           141         HIS         -           142         SER         -           143         SER         -           144         GLY         -           143         SER         -           144         GLY         -           145         LEU         -           145         LEU         -           146         VAL         -           147         PRO         -           148         ARG         -           149         GLY         -           150         SER         -           151         HIS         -           152	ResidueModelledActualComment132MET-initiating methionine133GLY-expression tag134SER-expression tag135SER-expression tag136HIS-expression tag137HIS-expression tag138HIS-expression tag139HIS-expression tag140HIS-expression tag141HIS-expression tag142SER-expression tag143SER-expression tag144GLY-expression tag145LEU-expression tag146VAL-expression tag147PRO-expression tag150SER-expression tag151HIS-expression tag152MET-expression tag152MET-expression tag153GLY-expression tag154MET-expression tag155MET-expression tag152MET-expression tag153GLY-expression tag154ALAGLUengineered mutation155MET-initiating methionine133GLY-expression tag134GLY-expression tag135HIS <t< td=""></t<>

There are 46 discrepancies between the modelled and reference sequences:

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6'	Γſ	ΓR
0		

Chain	Residue	Modelled	Actual	Comment	Reference
В	134	SER	-	expression tag	UNP A0A0H3CAN8
В	135	SER	-	expression tag	UNP A0A0H3CAN8
В	136	HIS	-	expression tag	UNP A0A0H3CAN8
В	137	HIS	-	expression tag	UNP A0A0H3CAN8
В	138	HIS	-	expression tag	UNP A0A0H3CAN8
В	139	HIS	-	expression tag	UNP A0A0H3CAN8
В	140	HIS	-	expression tag	UNP A0A0H3CAN8
В	141	HIS	-	expression tag	UNP A0A0H3CAN8
В	142	SER	-	expression tag	UNP A0A0H3CAN8
В	143	SER	-	expression tag	UNP A0A0H3CAN8
В	144	GLY	-	expression tag	UNP A0A0H3CAN8
В	145	LEU	-	expression tag	UNP A0A0H3CAN8
В	146	VAL	-	expression tag	UNP A0A0H3CAN8
В	147	PRO	-	expression tag	UNP A0A0H3CAN8
В	148	ARG	-	expression tag	UNP A0A0H3CAN8
В	149	GLY	-	expression tag	UNP A0A0H3CAN8
В	150	SER	-	expression tag	UNP A0A0H3CAN8
В	151	HIS	-	expression tag	UNP A0A0H3CAN8
В	152	MET	-	expression tag	UNP A0A0H3CAN8
В	261	ALA	GLU	engineered mutation	UNP A0A0H3CAN8
В	262	ALA	GLU	engineered mutation	UNP A0A0H3CAN8

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• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Ato	$\mathbf{ms}$		ZeroOcc	AltConf
2	А	1	Total 5	0 4	Р 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total         O         P           5         4         1	0	0

• Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodode cine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula:  $C_{20}H_{24}N_{10}O_{14}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	Δ	1	Total	С	Ν	Ο	Р	0	0
5	л	1	46	20	10	14	2	0	0
3	Λ	1	Total	С	Ν	Ο	Р	0	0
0	o A		46	20	10	14	2	0	0
3	В	1	Total	С	Ν	Ο	Р	0	0
		46	20	10	14	2		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: GGDEF diguanylate cyclase DgcB



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	88.08Å 148.75Å 60.40Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Bosolution} \left( \overset{\circ}{\mathbf{A}} \right)$	47.24 - 2.85	Depositor
Resolution (A)	47.24 - 2.85	EDS
% Data completeness	92.7 (47.24-2.85)	Depositor
(in resolution range)	92.7(47.24 - 2.85)	EDS
$R_{merge}$	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 2.86 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R R.	0.217 , $0.266$	Depositor
II, II, <i>free</i>	0.216 , $0.263$	DCC
$R_{free}$ test set	883 reflections $(4.98\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	59.9	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , $34.2$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3092	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: PO4,  $\rm C2E$ 

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.31	0/1477	0.50	0/1992	
1	В	0.34	0/1506	0.51	0/2030	
All	All	0.33	0/2983	0.51	0/4022	

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	А	1458	0	1429	23	0
1	В	1486	0	1453	19	0
2	А	5	0	0	0	0
2	В	5	0	0	1	0
3	А	92	0	44	1	0
3	В	46	0	22	2	0
All	All	3092	0	2948	41	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 (41) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:316:GLU:OE2	1:B:324:ARG:HD3	2.01	0.59
1:B:212:ILE:HG13	1:B:268:PRO:HA	1.86	0.58
1:B:290:MET:HE1	1:B:301:GLY:N	2.18	0.57
1:A:189:ALA:HB3	1:A:256:ALA:HB2	1.86	0.57
1:A:316:GLU:HG2	1:A:320:SER:HB3	1.89	0.54
1:B:183:ASP:OD2	1:B:257:ARG:HD3	2.07	0.54
1:B:257:ARG:NH1	1:B:260:GLY:O	2.41	0.54
1:A:280:GLU:OE2	1:A:283:ARG:NH2	2.28	0.53
1:B:235:ASP:OD1	3:B:401:C2E:N1	2.31	0.52
1:A:266:ILE:HG22	1:A:268:PRO:HD3	1.91	0.52
1:A:309:PHE:CE1	1:A:342:ALA:HB2	2.45	0.52
1:B:214:LEU:HD21	1:B:322:MET:SD	2.50	0.52
1:A:296:THR:OG1	1:A:298:GLU:OE2	2.21	0.51
1:B:181:THR:HB	1:B:193:ALA:HB2	1.93	0.49
1:B:225:PHE:CE2	1:B:237:VAL:HG21	2.49	0.48
1:A:200:ARG:HH11	1:A:200:ARG:HG2	1.79	0.47
1:A:239:ARG:HB3	3:A:402:C2E:H4'	1.97	0.47
1:B:206:GLU:OE1	1:B:312:ARG:NH2	2.48	0.46
1:A:216:VAL:HG12	1:A:329:LEU:HD22	1.97	0.46
1:A:244:VAL:HG13	1:A:285:GLU:HG2	1.97	0.46
1:B:158:ARG:O	1:B:162:SER:HB2	2.16	0.46
1:A:169:LEU:HD13	1:B:170:ARG:HG3	1.98	0.46
1:A:214:LEU:HD21	1:A:322:MET:CE	2.46	0.46
1:A:212:ILE:HG22	1:A:268:PRO:HA	1.98	0.45
1:A:166:VAL:CG1	1:A:170:ARG:HH11	2.30	0.45
1:A:166:VAL:HG13	1:A:170:ARG:HD3	1.99	0.44
1:A:216:VAL:CG1	1:A:329:LEU:HD22	2.47	0.44
1:A:185:LEU:HD11	1:A:235:ASP:HB3	1.99	0.44
1:B:309:PHE:CE1	1:B:342:ALA:HB2	2.53	0.44
1:B:333:LYS:HE2	2:B:402:PO4:O3	2.18	0.43
1:A:238:ILE:HD13	1:A:257:ARG:NH1	2.33	0.43
1:A:322:MET:HE2	1:A:322:MET:HB2	1.76	0.43
1:A:210:THR:OG1	1:A:269:ARG:HG2	2.19	0.42
1:A:334:ARG:HD3	1:A:334:ARG:HA	1.85	0.42
1:B:189:ALA:HB1	1:B:193:ALA:HB3	2.02	0.42
1:A:273:SER:O	1:A:277:THR:HG23	2.20	0.41
1:B:150:SER:O	1:B:154:SER:N	2.47	0.41
1:B:226:ASN:ND2	3:B:401:C2E:H1'	2.36	0.40
1:A:229:TRP:HE3	1:A:293:ARG:HH21	1.70	0.40
1:B:292:LYS:HD2	1:B:297:ASN:OD1	2.21	0.40
1:B:317:SER:O	1:B:321:VAL:HG23	2.22	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	Perce	ntiles
1	А	189/222~(85%)	186~(98%)	3(2%)	0	100	100
1	В	193/222~(87%)	189 (98%)	3 (2%)	1 (0%)	29	57
All	All	382/444 (86%)	375(98%)	6 (2%)	1 (0%)	41	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	150	SER

#### 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	Rotameric Outliers	
1	А	147/170~(86%)	145~(99%)	2(1%)	67 86
1	В	150/170~(88%)	146 (97%)	4 (3%)	44 74
All	All	297/340~(87%)	291~(98%)	6(2%)	55 80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	298	GLU
1	А	334	ARG

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Mol	Chain	Res	Type
1	В	162	SER
1	В	211	THR
1	В	212	ILE
1	В	334	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	232	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

5 ligands 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.

### 5.7 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,  $95^{th}$  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	$ $ $<$ $\mathbf{RSRZ}>$	#RSRZ $>2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	191/222 (86%)	0.13	2 (1%) 82 81	38, 54, 111, 119	0
1	В	195/222 (87%)	0.21	5 (2%) 56 52	39, 58, 109, 124	0
All	All	386/444 (86%)	0.17	7 (1%) 68 66	38, 55, 110, 124	0

All (7) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	171	GLU	3.6
1	А	168	ARG	3.1
1	В	166	VAL	2.6
1	В	167	GLU	2.3
1	А	155	LEU	2.2
1	В	170	ARG	2.1
1	В	168	ARG	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 monosaccharides 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,  $95^{th}$  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	${f B}$ -factors(Å <sup>2</sup> )	Q<0.9
2	PO4	В	402	5/5	0.94	0.15	$59,\!66,\!75,\!80$	0
3	C2E	В	401	46/46	0.97	0.16	$41,\!52,\!56,\!57$	0
3	C2E	А	402	46/46	0.97	0.17	$33,\!45,\!51,\!54$	0
2	PO4	А	401	5/5	0.98	0.15	$52,\!56,\!58,\!64$	0
3	C2E	А	403	46/46	0.98	0.16	$38,\!47,\!51,\!53$	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

