



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 10:07 AM GMT

PDB ID : 6TTS
Title : Crystal structure of the GGDEF domain of DgcB from *Caulobacter crescentus* in complex with c-di-GMP
Authors : Holzschuh, F.; Schirmer, T.; Teixeira, R.
Deposited on : 2019-12-30
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
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

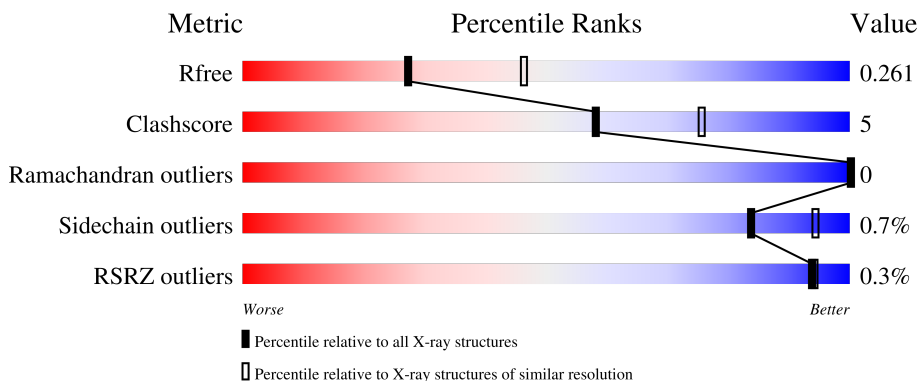
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	199	 77% 9% 14%
1	B	199	 % 78% 10% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	403	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2920 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 GGDEF diguanylate cyclase DgcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1304	797	246	256	5	0	0	0
1	B	176	1340	818	254	262	6	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

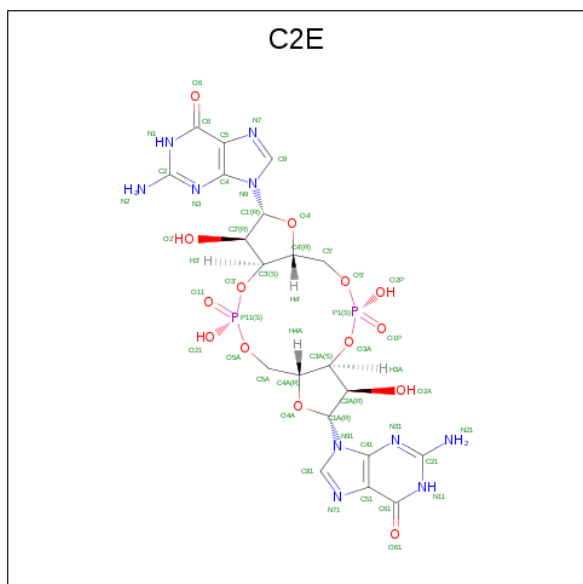
Chain	Residue	Modelled	Actual	Comment	Reference
A	155	MET	-	initiating methionine	UNP A0A0H3CAN8
A	156	GLY	-	expression tag	UNP A0A0H3CAN8
A	157	SER	-	expression tag	UNP A0A0H3CAN8
A	158	SER	-	expression tag	UNP A0A0H3CAN8
A	159	HIS	-	expression tag	UNP A0A0H3CAN8
A	160	HIS	-	expression tag	UNP A0A0H3CAN8
A	161	HIS	-	expression tag	UNP A0A0H3CAN8
A	162	HIS	-	expression tag	UNP A0A0H3CAN8
A	163	HIS	-	expression tag	UNP A0A0H3CAN8
A	164	HIS	-	expression tag	UNP A0A0H3CAN8
A	165	SER	-	expression tag	UNP A0A0H3CAN8
A	166	SER	-	expression tag	UNP A0A0H3CAN8
A	167	GLY	-	expression tag	UNP A0A0H3CAN8
A	168	LEU	-	expression tag	UNP A0A0H3CAN8
A	169	VAL	-	expression tag	UNP A0A0H3CAN8
A	170	PRO	-	expression tag	UNP A0A0H3CAN8
A	171	ARG	-	expression tag	UNP A0A0H3CAN8
A	172	GLY	-	expression tag	UNP A0A0H3CAN8
A	173	SER	-	expression tag	UNP A0A0H3CAN8
A	174	HIS	-	expression tag	UNP A0A0H3CAN8
A	175	MET	-	expression tag	UNP A0A0H3CAN8
B	155	MET	-	initiating methionine	UNP A0A0H3CAN8
B	156	GLY	-	expression tag	UNP A0A0H3CAN8
B	157	SER	-	expression tag	UNP A0A0H3CAN8
B	158	SER	-	expression tag	UNP A0A0H3CAN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	159	HIS	-	expression tag	UNP A0A0H3CAN8
B	160	HIS	-	expression tag	UNP A0A0H3CAN8
B	161	HIS	-	expression tag	UNP A0A0H3CAN8
B	162	HIS	-	expression tag	UNP A0A0H3CAN8
B	163	HIS	-	expression tag	UNP A0A0H3CAN8
B	164	HIS	-	expression tag	UNP A0A0H3CAN8
B	165	SER	-	expression tag	UNP A0A0H3CAN8
B	166	SER	-	expression tag	UNP A0A0H3CAN8
B	167	GLY	-	expression tag	UNP A0A0H3CAN8
B	168	LEU	-	expression tag	UNP A0A0H3CAN8
B	169	VAL	-	expression tag	UNP A0A0H3CAN8
B	170	PRO	-	expression tag	UNP A0A0H3CAN8
B	171	ARG	-	expression tag	UNP A0A0H3CAN8
B	172	GLY	-	expression tag	UNP A0A0H3CAN8
B	173	SER	-	expression tag	UNP A0A0H3CAN8
B	174	HIS	-	expression tag	UNP A0A0H3CAN8
B	175	MET	-	expression tag	UNP A0A0H3CAN8

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



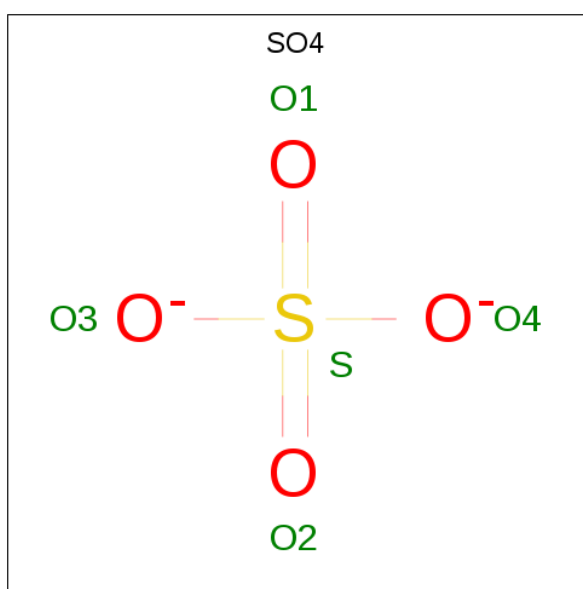
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	46	20	10	14	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		

- Molecule 4 is water.

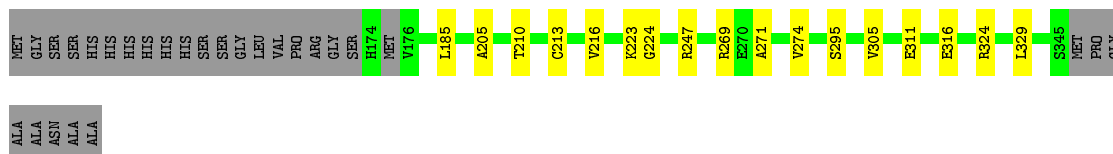
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	9	Total O 9 9	0	0

3 Residue-property plots


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

Chain A: 



- Molecule 1: GGDEF diguanylate cyclase DgcB

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	64.50Å 64.50Å 246.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.76 – 2.50 62.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.76-2.50) 99.8 (62.40-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.203 , 0.261 0.203 , 0.261	Depositor DCC
R_{free} test set	1002 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2920	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: SO4, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/1322	0.66	0/1781
1	B	0.53	0/1360	0.63	0/1832
All	All	0.52	0/2682	0.64	0/3613

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	A	1304	0	1267	13	0
1	B	1340	0	1306	16	0
2	A	184	0	88	2	0
2	B	46	0	22	0	0
3	A	15	0	0	3	0
3	B	15	0	0	0	0
4	A	7	0	0	0	0
4	B	9	0	0	0	0
All	All	2920	0	2683	27	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 5.

All (27) 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:295:SER:HB3	3:A:403:SO4:O3	1.86	0.76
1:A:205:ALA:HA	1:A:210:THR:HG22	1.78	0.66
1:A:271:ALA:HB3	1:A:274:VAL:HG23	1.83	0.61
1:B:248:VAL:HG12	1:B:253:ARG:NH1	2.16	0.60
1:B:293:ARG:HG2	1:B:300:LEU:HD21	1.85	0.58
1:A:223:LYS:HD2	2:A:401:C2E:H4'	1.85	0.57
1:A:210:THR:OG1	1:A:269:ARG:HG2	2.06	0.56
1:B:248:VAL:HG12	1:B:253:ARG:HH12	1.72	0.55
1:B:317:SER:O	1:B:321:VAL:HG23	2.06	0.55
1:B:344:GLU:N	1:B:344:GLU:OE2	2.41	0.52
1:A:224:GLY:N	3:A:402:SO4:O2	2.37	0.52
1:A:316:GLU:OE2	1:A:324:ARG:HD3	2.11	0.50
1:B:214:LEU:HD12	1:B:265:MET:O	2.12	0.50
1:A:205:ALA:HB1	1:A:210:THR:O	2.11	0.50
1:A:295:SER:CB	3:A:403:SO4:O3	2.58	0.49
1:A:213:CYS:SG	1:A:311:GLU:HG2	2.56	0.46
1:A:247:ARG:HD2	1:B:170:PRO:O	2.17	0.44
1:B:214:LEU:HD21	1:B:322:MET:HE2	2.00	0.43
1:B:194:PHE:HZ	1:B:214:LEU:HD11	1.82	0.43
1:B:213:CYS:SG	1:B:311:GLU:HG3	2.59	0.43
1:A:216:VAL:HG12	1:A:329:LEU:HD22	2.01	0.42
1:B:312:ARG:NH1	1:B:316:GLU:O	2.51	0.42
1:B:316:GLU:OE1	1:B:324:ARG:HD3	2.20	0.42
1:B:316:GLU:HG2	1:B:320:SER:OG	2.20	0.41
1:B:214:LEU:HD21	1:B:322:MET:SD	2.60	0.41
2:A:407:C2E:N7	1:B:289:ARG:NH2	2.67	0.40
1:A:185:LEU:HD13	1:B:185:LEU:HD13	2.02	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	168/199 (84%)	165 (98%)	3 (2%)	0	100	100
1	B	174/199 (87%)	170 (98%)	4 (2%)	0	100	100
All	All	342/398 (86%)	335 (98%)	7 (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	132/152 (87%)	131 (99%)	1 (1%)	81	93
1	B	136/152 (90%)	135 (99%)	1 (1%)	84	94
All	All	268/304 (88%)	266 (99%)	2 (1%)	84	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	VAL
1	B	248	VAL

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](#)

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](#)

11 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, 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	171/199 (85%)	0.06	0 100 100	15, 28, 45, 67	0
1	B	176/199 (88%)	-0.04	1 (0%) 89 90	16, 27, 46, 80	0
All	All	347/398 (87%)	0.01	1 (0%) 94 94	15, 27, 46, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	TYR	2.4

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, 95th 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	SO4	A	404	5/5	0.93	0.16	60,64,78,80	0
3	SO4	A	403	5/5	0.95	0.16	49,50,55,61	0
3	SO4	B	403	5/5	0.95	0.15	44,50,67,69	0
2	C2E	B	404	46/46	0.96	0.14	19,25,33,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C2E	A	406	46/46	0.97	0.14	17,25,33,47	0
3	SO4	B	401	5/5	0.97	0.15	31,36,39,46	0
2	C2E	A	407	46/46	0.98	0.15	16,22,27,29	0
2	C2E	A	401	46/46	0.98	0.16	14,20,28,29	0
2	C2E	A	405	46/46	0.98	0.15	16,21,25,30	0
3	SO4	A	402	5/5	0.99	0.18	23,24,24,25	5
3	SO4	B	402	5/5	0.99	0.18	22,22,23,25	5

6.5 Other polymers [i](#)

There are no such residues in this entry.