W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 12:50 AM EDT

PDB ID	:	6PD0
Title	:	Crystal structure of the bacterial cellulose synthase subunit G (BcsG) from Escherichia coli, catalytic domain
Authors	:	Anderson, A.C.; Brenner, T.; Weadge, J.T.
Deposited on	:	2019-06-18
Resolution	:	1.75 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	:	FAILED
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)	:	2.35.1

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 1.75 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6686 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 Cellulose biosynthesis protein BcsG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total 2853	C 1815	N 484	O 542	S 12	0	0	0
1	B	366	Total 2853	C 1815	N 484	O 542	S 12	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P37659
A	144	GLY	-	expression tag	UNP P37659
A	145	SER	-	expression tag	UNP P37659
A	146	SER	-	expression tag	UNP P37659
A	147	HIS	-	expression tag	UNP P37659
A	148	HIS	-	expression tag	UNP P37659
A	149	HIS	-	expression tag	UNP P37659
A	150	HIS	-	expression tag	UNP P37659
A	151	HIS	-	expression tag	UNP P37659
A	152	HIS	-	expression tag	UNP P37659
A	153	SER	-	expression tag	UNP P37659
A	154	SER	-	expression tag	UNP P37659
A	155	GLY	-	expression tag	UNP P37659
A	156	LEU	-	expression tag	UNP P37659
A	157	VAL	-	expression tag	UNP P37659
A	158	PRO	-	expression tag	UNP P37659
A	159	ARG	-	expression tag	UNP P37659
A	160	GLY	-	expression tag	UNP P37659
A	161	SER	-	expression tag	UNP P37659
A	162	HIS	-	expression tag	UNP P37659
A	163	MET	-	expression tag	UNP P37659
B	143	MET	-	initiating methionine	UNP P37659
B	144	GLY	-	expression tag	UNP P37659
B	145	SER	-	expression tag	UNP P37659
B	146	SER	-	expression tag	UNP P37659

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Chain	Residue	Modelled	Actual	Comment	Reference
B	147	HIS	-	expression tag	UNP P37659
B	148	HIS	-	expression tag	UNP P37659
B	149	HIS	-	expression tag	UNP P37659
B	150	HIS	-	expression tag	UNP P37659
B	151	HIS	-	expression tag	UNP P37659
B	152	HIS	-	expression tag	UNP P37659
B	153	SER	-	expression tag	UNP P37659
B	154	SER	-	expression tag	UNP P37659
B	155	GLY	-	expression tag	UNP P37659
B	156	LEU	-	expression tag	UNP P37659
B	157	VAL	-	expression tag	UNP P37659
B	158	PRO	-	expression tag	UNP P37659
B	159	ARG	-	expression tag	UNP P37659
B	160	GLY	-	expression tag	UNP P37659
B	161	SER	-	expression tag	UNP P37659
B	162	HIS	-	expression tag	UNP P37659
B	163	MET	-	expression tag	UNP P37659

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	533	Total 533	O 533	0	0
4	B	444	Total 444	O 444	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.51Å 76.92Å 95.92Å 90.00° 90.58° 90.00°	Depositor
Resolution (Å)	47.96 – 1.75	Depositor
% Data completeness (in resolution range)	96.7 (47.96-1.75)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.161 , 0.199	Depositor
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.181	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
Total number of atoms	6686	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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