



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:28 am BST

PDB ID : 5GQU
Title : Crystal structure of branching enzyme from *Cyanothece* sp. ATCC 51142
Authors : Suzuki, R.; Suzuki, E.
Deposited on : 2016-08-08
Resolution : 1.85 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 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 : 2.11
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) : 2.11

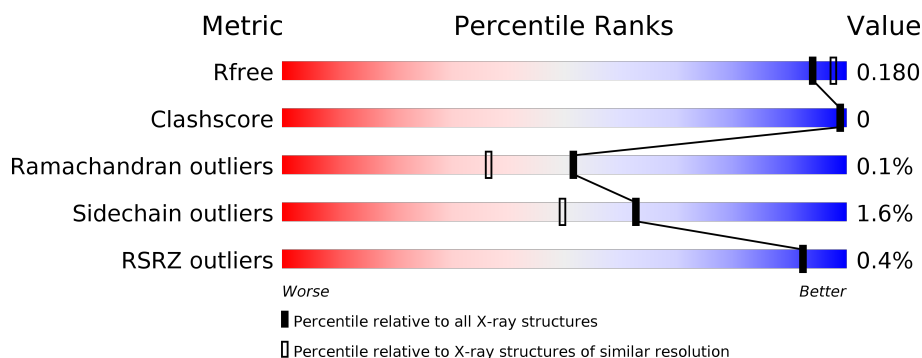
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	793	<div> <div style="width: 84%;"></div> <div style="width: 10%;"></div> <div style="width: 5%;"></div> </div> <div>84% 10% 5%</div>

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
2	GOL	A	801	-	X	-	-
2	GOL	A	807	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7177 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	755	6279	4061	1043	1151	24	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B1WPM8
A	-18	GLY	-	expression tag	UNP B1WPM8
A	-17	SER	-	expression tag	UNP B1WPM8
A	-16	SER	-	expression tag	UNP B1WPM8
A	-15	HIS	-	expression tag	UNP B1WPM8
A	-14	HIS	-	expression tag	UNP B1WPM8
A	-13	HIS	-	expression tag	UNP B1WPM8
A	-12	HIS	-	expression tag	UNP B1WPM8
A	-11	HIS	-	expression tag	UNP B1WPM8
A	-10	HIS	-	expression tag	UNP B1WPM8
A	-9	SER	-	expression tag	UNP B1WPM8
A	-8	SER	-	expression tag	UNP B1WPM8
A	-7	GLY	-	expression tag	UNP B1WPM8
A	-6	LEU	-	expression tag	UNP B1WPM8
A	-5	VAL	-	expression tag	UNP B1WPM8
A	-4	PRO	-	expression tag	UNP B1WPM8
A	-3	ARG	-	expression tag	UNP B1WPM8
A	-2	GLY	-	expression tag	UNP B1WPM8
A	-1	SER	-	expression tag	UNP B1WPM8
A	0	HIS	-	expression tag	UNP B1WPM8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	852	Total	O	0	0
			852	852		

- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Residue	Score	Category
R694	1.0	High
Y703	0.5	Low
K725	0.5	Low
V758	1.5	High
P759	1.5	High
GLU	0.5	Low
GLY	0.5	Low
THR	0.5	Low
THR	0.5	Low
ILE	0.5	Low
LYS	0.5	Low
GLU	0.5	Low
ILE	0.5	Low
ALA	0.5	Low
ALA	0.5	Low
ASP	0.5	Low
GLU	0.5	Low
GLU	0.5	Low
GLU	0.5	Low
D634	1.0	High
M439	0.5	Low
K447	0.5	Low
S466	0.5	Low
P480	0.5	Low
G481	0.5	Low
E491	0.5	Low
D517	0.5	Low
D520	0.5	Low
D525	0.5	Low
F528	0.5	Low
R529	0.5	Low
A530	0.5	Low
Y531	0.5	Low
Y542	0.5	Low
D571	0.5	Low
E572	0.5	Low
R580	0.5	Low
E600	0.5	Low
S605	0.5	Low
K610	0.5	Low
G611	0.5	Low
D612	0.5	Low
E621	0.5	Low
E640	0.5	Low
Y644	0.5	Low
D647	0.5	Low
Y650	0.5	Low
E654	0.5	Low
G658	0.5	Low
T662	1.0	High
R671	0.5	Low
D674	0.5	Low
R677	0.5	Low
V162	0.5	Low
P183	0.5	Low
E184	0.5	Low
S187	0.5	Low
Y191	0.5	Low
S206	0.5	Low
D207	0.5	Low
R216	0.5	Low
D225	0.5	Low
R241	0.5	Low
R242	0.5	Low
G243	0.5	Low
S244	0.5	Low
D245	0.5	Low
Q249	0.5	Low
M270	0.5	Low
N274	0.5	Low
K285	0.5	Low
R290	0.5	Low
E296	0.5	Low
E299	0.5	Low
M308	0.5	Low
E314	0.5	Low
R340	0.5	Low
R343	0.5	Low
P344	0.5	Low
E345	0.5	Low
R369	0.5	Low
D373	0.5	Low
S374	0.5	Low
D381	0.5	Low
Y386	0.5	Low
R412	0.5	Low
N413	0.5	Low
R432	0.5	Low
V432	0.5	Low
MET	0.5	Low
GLY	0.5	Low
SER	0.5	Low
HIS	0.5	Low
HIS	0.5	Low
HIS	0.5	Low
HIS	0.5	Low
HIS	0.5	Low
SER	0.5	Low
SER	0.5	Low
GLY	0.5	Low
LEU	0.5	Low
VAL	0.5	Low
PRO	0.5	Low
ARG	0.5	Low
GLY	0.5	Low
SER	0.5	Low
HIS	0.5	Low
HIS	0.5	Low
MET	0.5	Low
THR	0.5	Low
THR	0.5	Low
THR	0.5	Low
THR	0.5	Low
I5	0.5	Low
D8	0.5	Low
Y15	0.5	Low
N16	0.5	Low
M35	0.5	Low
R42	0.5	Low
P46	0.5	Low
K47	0.5	Low
E58	0.5	Low
V67	0.5	Low
H68	0.5	Low
Y85	0.5	Low
E91	0.5	Low
D100	0.5	Low
D111	0.5	Low
S118	0.5	Low
R124	0.5	Low
E135	0.5	Low
D164	0.5	Low
E170	0.5	Low

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.75Å 133.75Å 185.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.85 38.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.29-1.85) 100.0 (38.50-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.72 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.147 , 0.170 0.160 , 0.180	Depositor DCC
R_{free} test set	7187 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7177	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: GOL, MG

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	1.44	43/6502 (0.7%)	1.29	47/8848 (0.5%)

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	2

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ARG	CZ-NH1	9.75	1.45	1.33
1	A	58	GLU	CD-OE2	9.40	1.35	1.25
1	A	285	TRP	CB-CG	-8.90	1.34	1.50
1	A	299	GLU	CD-OE2	8.57	1.35	1.25
1	A	658	CYS	CB-SG	-8.21	1.68	1.82

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ARG	NE-CZ-NH2	-24.49	108.05	120.30
1	A	412	ARG	NE-CZ-NH1	17.23	128.92	120.30
1	A	242	ARG	NE-CZ-NH2	-16.65	111.98	120.30
1	A	412	ARG	CD-NE-CZ	12.67	141.33	123.60
1	A	612	ASP	CB-CG-OD1	-9.27	109.96	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLU	Mainchain
1	A	412	ARG	Sidechain

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	6279	0	5865	4	0
2	A	42	0	56	2	0
3	A	4	0	0	0	0
4	A	852	0	0	1	0
All	All	7177	0	5921	5	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 0.

All (5) 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:46:PRO:O	1:A:47:LYS:HB2	2.05	0.56
2:A:801:GOL:H2	4:A:967:HOH:O	2.16	0.45
1:A:182:VAL:HA	1:A:183:PRO:HD2	1.94	0.42
1:A:244:SER:HB3	1:A:249:GLN:NE2	2.36	0.40
1:A:528:PHE:CD2	2:A:802:GOL:H2	2.57	0.40

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	754/793 (95%)	734 (97%)	19 (2%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	HIS

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	669/700 (96%)	658 (98%)	11 (2%)	62 49

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	ASP
1	A	413	ASN
1	A	491	GLU
1	A	369	HIS
1	A	447	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	16	ASN
1	A	634	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
2	GOL	A	804	-	5,5,5	1.09	0	5,5,5	1.34	1 (20%)
2	GOL	A	801	-	5,5,5	1.71	2 (40%)	5,5,5	2.75	3 (60%)
2	GOL	A	805	-	5,5,5	0.34	0	5,5,5	1.24	1 (20%)
2	GOL	A	802	-	5,5,5	2.68	3 (60%)	5,5,5	2.11	1 (20%)
2	GOL	A	806	-	5,5,5	0.82	0	5,5,5	1.88	1 (20%)
2	GOL	A	803	-	5,5,5	0.95	0	5,5,5	0.50	0
2	GOL	A	807	-	5,5,5	2.04	2 (40%)	5,5,5	2.14	2 (40%)

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
2	GOL	A	804	-	-	2/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	A	805	-	-	4/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	A	806	-	-	0/4/4/4	-
2	GOL	A	803	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	807	-	-	3/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	GOL	O3-C3	4.18	1.60	1.42
2	A	807	GOL	O3-C3	3.78	1.58	1.42
2	A	802	GOL	C3-C2	2.78	1.63	1.51
2	A	801	GOL	O2-C2	2.75	1.51	1.43
2	A	802	GOL	O2-C2	2.64	1.51	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GOL	O2-C2-C3	4.49	128.91	109.12
2	A	802	GOL	O3-C3-C2	3.84	128.63	110.20
2	A	806	GOL	C3-C2-C1	3.35	124.71	111.70
2	A	801	GOL	O1-C1-C2	3.28	125.93	110.20
2	A	807	GOL	O1-C1-C2	3.15	125.31	110.20

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	804	GOL	C1-C2-C3-O3
2	A	804	GOL	O2-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	A	805	GOL	O1-C1-C2-C3
2	A	805	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0
2	A	802	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	755/793 (95%)	-0.44	3 (0%) 92 92	14, 21, 42, 77	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	VAL	3.7
1	A	35	ASN	3.5
1	A	759	PRO	2.5

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 carbohydrates 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
2	GOL	A	801	6/6	0.75	0.28	33,41,43,51	0
2	GOL	A	804	6/6	0.83	0.32	37,54,58,58	0
2	GOL	A	802	6/6	0.85	0.16	27,43,55,55	0
2	GOL	A	805	6/6	0.87	0.30	45,53,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	811	1/1	0.89	0.26	44,44,44,44	0
2	GOL	A	806	6/6	0.91	0.21	33,53,59,60	0
2	GOL	A	807	6/6	0.92	0.14	27,41,44,45	0
2	GOL	A	803	6/6	0.94	0.12	33,34,35,35	0
3	MG	A	809	1/1	0.98	0.04	22,22,22,22	0
3	MG	A	810	1/1	0.98	0.07	23,23,23,23	0
3	MG	A	808	1/1	0.98	0.13	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.