

wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2021 – 02:06 PM BST

PDB ID : 7ONY

Title : Crystal structure of PBP3 from P. aeruginosa Authors : Freischem, S.; Grimm, I.; Weiergraeber, O.H.

Deposited on : 2021-05-26

Resolution : 1.77 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 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) : NOT EXECUTED EDS : NOT EXECUTED

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)

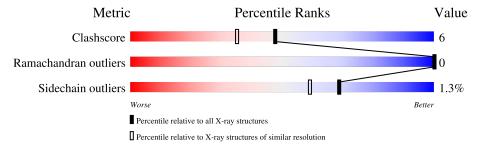
Validation Pipeline (wwPDB-VP) : 2.23.1

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 1.77 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	10184 (1.80-1.76)		
Ramachandran outliers	138981	10051 (1.80-1.76)		
Sidechain outliers	138945	10050 (1.80-1.76)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	Α.	E 91							
1	Α	531	83%	12%	5%				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4233 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.

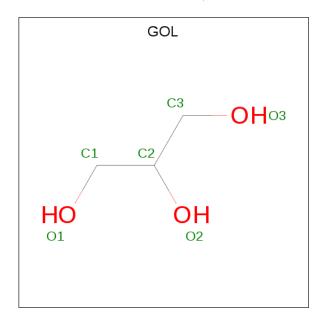
• Molecule 1 is a protein called Peptidoglycan D,D-transpeptidase FtsI.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	505	Total	С	N	О	S	0	0	0
1	A	303	3841	2418	692	719	12	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	MET	=	initiating methionine	UNP G3XD46
A	564	LYS	-	expression tag	UNP G3XD46
A	565	LEU	-	expression tag	UNP G3XD46
A	566	VAL	-	expression tag	UNP G3XD46
A	567	PRO	-	expression tag	UNP G3XD46
A	568	ARG	-	expression tag	UNP G3XD46
A	569	GLY	=	expression tag	UNP G3XD46

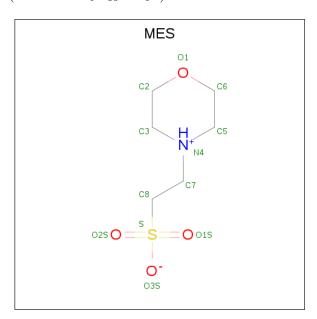
• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





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

• Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
3	Δ	1	Total	С	N	О	S	0	1	
)	Λ	1	24	12	2	8	2	0		
2	Λ	1	Total	С	N	О	S	0	0	
3	A	1	12	6	1	4	1		0	

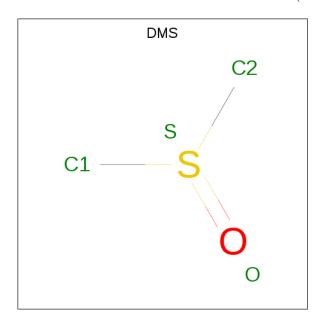
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Mol	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$			ZeroOcc	AltConf
2	Λ	1	Total	С	N	Ο	S	0	1
) J	A	1	24	12	2	8	2	0	1

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Λ	1	Total	С	О	S	0	0
4	А	1	4	2	1	1	0	U

• Molecule 5 is water.

\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	274	Total O 274 274	0	1

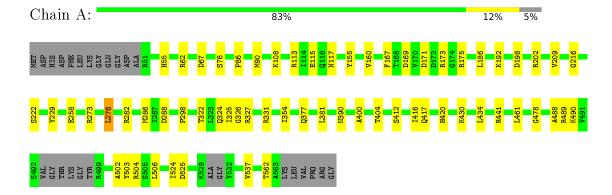


3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: Peptidoglycan D,D-transpeptidase FtsI





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	104.06Å 125.00Å 74.23Å	Depositor	
a, b, c, α , β , γ	90.00° 122.49° 90.00°	Depositor	
Resolution (Å)	39.55 - 1.77	Depositor	
% Data completeness	55.5 (39.55-1.77)	Depositor	
(in resolution range)	,	Беровног	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	PHENIX 1.19.1	Depositor	
R, R_{free}	0.180 , 0.213	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4233	wwPDB-VP	
Average B, all atoms (Å ²)	49.0	wwPDB-VP	



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, MES, DMS

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	Α	0.27	0/3914	0.55	0/5321	

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	3841	0	3782	47	0
2	A	54	0	72	2	0
3	A	60	0	65	5	0
4	A	4	0	6	0	0
5	A	274	0	0	6	0
All	All	4233	0	3925	48	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 6.

The worst 5 of 48 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:478:GLY:H	1:A:562:THR:HB	1.40	0.86
1:A:488:ALA:HB2	1:A:506:LEU:HD11	1.77	0.65
1:A:325:ILE:HG22	2:A:701:GOL:H11	1.78	0.65
1:A:490:LYS:NZ	5:A:806:HOH:O	2.27	0.65
1:A:430:LYS:HD2	2:A:707:GOL:H32	1.81	0.62

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	5
1	A	507/531 (96%)	489 (96%)	18 (4%)	0	100 100	П

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	388/423 (92%)	383 (99%)	5 (1%)	69 59		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	209	VAL

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	503	TYR
1	A	525	ASP

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)

15 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	Tune	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	A	712[A]	-	12,12,12	0.76	0	14,16,16	0.30	0
2	GOL	A	706	_	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	A	709	_	5,5,5	0.10	0	5,5,5	0.34	0
2	GOL	A	707	_	5,5,5	0.10	0	5,5,5	0.35	0
3	MES	A	712[B]	_	12,12,12	0.70	0	14,16,16	0.44	0
2	GOL	A	704	_	5,5,5	0.10	0	5,5,5	0.32	0
3	MES	A	711	_	12,12,12	0.75	0	14,16,16	0.38	0
2	GOL	A	708	_	5,5,5	0.08	0	5,5,5	0.31	0



Mol	Trino	Chain	Res	Link	Во	ond leng	gths	В	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	A	710[A]	-	12,12,12	0.74	0	14,16,16	0.38	0
2	GOL	A	702	-	5,5,5	0.09	0	5,5,5	0.34	0
3	MES	A	710[B]	-	12,12,12	0.72	0	14,16,16	0.37	0
4	DMS	A	713	-	3,3,3	0.66	0	3,3,3	0.53	0
2	GOL	A	705	_	5,5,5	0.09	0	5,5,5	0.29	0
2	GOL	A	701	-	5,5,5	0.09	0	5,5,5	0.35	0
2	GOL	A	703	-	5,5,5	0.08	0	5,5,5	0.40	0

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	MES	A	712[A]	-	-	2/6/14/14	0/1/1/1
2	GOL	A	706	-	-	0/4/4/4	-
2	GOL	A	709	-	-	0/4/4/4	-
2	GOL	A	707	-	ı	0/4/4/4	-
3	MES	A	712[B]	_	1	2/6/14/14	0/1/1/1
2	GOL	A	704	-	-	0/4/4/4	-
3	MES	A	711	_	-	3/6/14/14	0/1/1/1
2	GOL	A	708	-	=	0/4/4/4	-
3	MES	A	710[A]	_	-	3/6/14/14	0/1/1/1
2	GOL	A	702	-	-	0/4/4/4	-
3	MES	A	710[B]	-	-	1/6/14/14	0/1/1/1
2	GOL	A	705	-		0/4/4/4	-
2	GOL	A	701	_	-	0/4/4/4	_
2	GOL	A	703	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	710[A]	MES	C7-C8-S-O1S
3	A	710[B]	MES	C8-C7-N4-C5
3	A	712[B]	MES	C8-C7-N4-C5
3	A	710[A]	MES	C7-C8-S-O3S
3	A	711	MES	N4-C7-C8-S



There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	712[A]	MES	4	0
2	A	707	GOL	1	0
3	A	711	MES	1	0
2	A	701	GOL	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

