



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7ONY / pdb_00007ony
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 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:

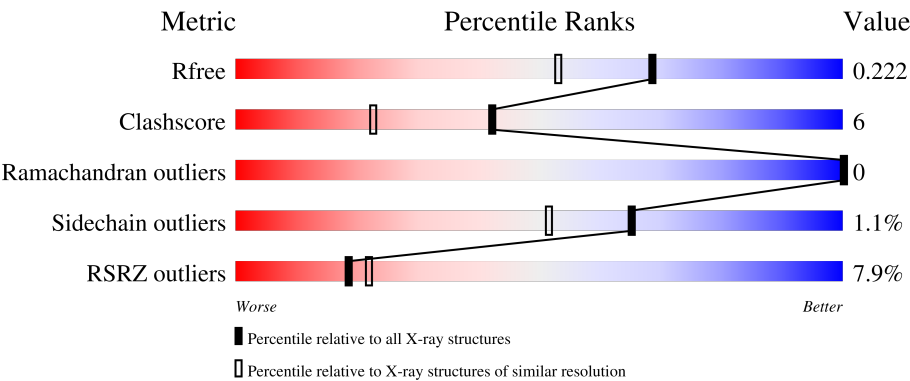
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.06Å 125.00Å 74.23Å 90.00° 122.49° 90.00°	Depositor
Resolution (Å)	39.55 – 1.77 39.55 – 1.77	Depositor EDS
% Data completeness (in resolution range)	55.5 (39.55-1.77) 55.5 (39.55-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.77Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.180 , 0.213 0.186 , 0.222	Depositor DCC
R_{free} test set	2154 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4233	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, GOL, MES

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	0.17	0/3914	0.37	0/5321

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

3.2 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	3841	0	3782	49	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	50	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.

All (50) 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: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	0.64
1:A:430:LYS:HD2	2:A:707:GOL:H32	1.81	0.62
1:A:490:LYS:HB2	1:A:504[B]:ARG:HH12	1.66	0.61
1:A:273:ARG:HH22	3:A:712[A]:MES:H71	1.65	0.60
1:A:169:ASP:HB3	1:A:171:ASP:H	1.67	0.59
1:A:288[A]:ASP:HB3	1:A:504[A]:ARG:HH12	1.71	0.55
1:A:55[B]:HIS:HE1	1:A:192:LYS:HE3	1.73	0.54
1:A:412:SER:HB2	3:A:711:MES:H32	1.90	0.54
1:A:198[A]:ASP:OD1	1:A:202:ARG:N	2.40	0.54
1:A:524:ILE:HD12	1:A:537:VAL:HG12	1.89	0.54
1:A:488:ALA:HB3	1:A:504[B]:ARG:HB2	1.90	0.54
3:A:712[A]:MES:H31	3:A:712[A]:MES:O2S	2.09	0.53
1:A:273:ARG:NH2	3:A:712[A]:MES:H71	2.24	0.53
1:A:62:ARG:HB3	1:A:76:SER:OG	2.09	0.51
1:A:55[B]:HIS:CE1	1:A:192:LYS:HG2	2.46	0.51
1:A:489[A]:ARG:HD3	1:A:502:ALA:O	2.10	0.50
1:A:324:GLN:NE2	1:A:326:GLY:O	2.42	0.50
1:A:490:LYS:HE2	1:A:504[A]:ARG:NH2	2.26	0.49
1:A:490:LYS:HE2	1:A:504[B]:ARG:HH22	1.78	0.49
1:A:169:ASP:HB2	1:A:173:ARG:H	1.78	0.49
1:A:186:LEU:O	1:A:216:GLY:HA3	2.13	0.48
1:A:488:ALA:HB3	1:A:504[A]:ARG:HB2	1.96	0.48
1:A:273:ARG:NH1	3:A:712[A]:MES:H32	2.29	0.48
1:A:155:TYR:OH	1:A:167:PHE:HA	2.15	0.46
1:A:169:ASP:CG	1:A:175:ARG:HE	2.24	0.46
1:A:262:MET:SD	1:A:286:MET:HE3	2.56	0.45
1:A:273:ARG:HB3	1:A:276:LEU:HD12	1.98	0.45
1:A:282:ARG:NH2	1:A:288[A]:ASP:OD1	2.35	0.45
1:A:298:PRO:HG3	1:A:461:LEU:HD21	1.99	0.45
1:A:420:HIS:HB2	1:A:434:LEU:HD11	1.98	0.45
1:A:286:MET:HG2	1:A:416:ILE:HG13	1.99	0.44
1:A:390[B]:ASN:OD1	5:A:801:HOH:O	2.20	0.44
1:A:441:ARG:NH1	5:A:820:HOH:O	2.51	0.44
1:A:478:GLY:N	1:A:562:THR:HB	2.20	0.44
1:A:160:VAL:HG21	1:A:229:TYR:CE1	2.53	0.43
1:A:327:ARG:NH2	5:A:812:HOH:O	2.42	0.43
1:A:503:TYR:CD1	1:A:503:TYR:C	2.97	0.42
1:A:86:PRO:O	1:A:90:MET:HG2	2.19	0.42
1:A:113:ARG:O	1:A:117:ASN:ND2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ALA:O	1:A:404:THR:HG23	2.20	0.42
1:A:115[B]:GLU:OE2	5:A:802:HOH:O	2.21	0.41
1:A:222:SER:HB2	1:A:258:GLU:HB3	2.03	0.41
1:A:108:LYS:NZ	5:A:821:HOH:O	2.52	0.41
1:A:258:GLU:CD	1:A:439:VAL:HG22	2.46	0.41
1:A:354:ILE:HD12	1:A:354:ILE:HA	1.97	0.40
1:A:322:THR:HG22	1:A:331:ARG:HG2	2.04	0.40
1:A:377:GLN:O	1:A:417:GLN:NE2	2.54	0.40

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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	507/342 (148%)	489 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

3.3.2 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	388/280 (139%)	384 (99%)	4 (1%)	68	55

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	A	209	VAL
1	A	276	LEU
1	A	503	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	372	GLN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MES	A	711	-	12,12,12	0.74	0	15,16,16	0.32	0
4	DMS	A	713	-	3,3,3	0.67	0	3,3,3	0.54	0
3	MES	A	712[B]	-	12,12,12	0.69	0	15,16,16	0.36	0
2	GOL	A	706	-	5,5,5	0.09	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	A	710[B]	-	12,12,12	0.71	0	15,16,16	0.30	0
2	GOL	A	708	-	5,5,5	0.08	0	5,5,5	0.30	0
2	GOL	A	702	-	5,5,5	0.09	0	5,5,5	0.33	0
2	GOL	A	701	-	5,5,5	0.09	0	5,5,5	0.35	0
3	MES	A	712[A]	-	12,12,12	0.74	0	15,16,16	0.32	0
2	GOL	A	703	-	5,5,5	0.08	0	5,5,5	0.40	0
2	GOL	A	707	-	5,5,5	0.09	0	5,5,5	0.35	0
2	GOL	A	705	-	5,5,5	0.09	0	5,5,5	0.29	0
2	GOL	A	709	-	5,5,5	0.09	0	5,5,5	0.34	0
2	GOL	A	704	-	5,5,5	0.09	0	5,5,5	0.31	0
3	MES	A	710[A]	-	12,12,12	0.73	0	15,16,16	0.36	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	711	-	-	3/6/14/14	0/1/1/1
3	MES	A	712[B]	-	-	2/6/14/14	0/1/1/1
2	GOL	A	706	-	-	0/4/4/4	-
3	MES	A	710[B]	-	-	1/6/14/14	0/1/1/1
2	GOL	A	708	-	-	0/4/4/4	-
2	GOL	A	702	-	-	0/4/4/4	-
2	GOL	A	701	-	-	0/4/4/4	-
3	MES	A	712[A]	-	-	2/6/14/14	0/1/1/1
2	GOL	A	703	-	-	0/4/4/4	-
2	GOL	A	707	-	-	0/4/4/4	-
2	GOL	A	705	-	-	0/4/4/4	-
2	GOL	A	709	-	-	0/4/4/4	-
2	GOL	A	704	-	-	0/4/4/4	-
3	MES	A	710[A]	-	-	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	710[A]	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
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
3	A	712[B]	MES	N4-C7-C8-S
3	A	711	MES	C8-C7-N4-C3
3	A	710[A]	MES	C7-C8-S-O2S
3	A	712[A]	MES	C7-C8-S-O2S
3	A	711	MES	C8-C7-N4-C5
3	A	712[A]	MES	C7-C8-S-O3S

There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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	330/342 (96%)	0.33	22 (6%) 24 28	16, 43, 106, 156	5 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55[A]	HIS	8.2
1	A	53	VAL	5.1
1	A	203	VAL	4.8
1	A	204	ILE	4.8
1	A	207	VAL	4.4
1	A	200	ARG	3.9
1	A	57	ALA	3.7
1	A	196	LEU	3.6
1	A	199	ARG	3.5
1	A	169	ASP	3.3
1	A	51	ARG	3.1
1	A	208	GLN	3.0
1	A	56	ILE	3.0
1	A	195	VAL	2.9
1	A	198[A]	ASP	2.8
1	A	58	ILE	2.4
1	A	336	ASN	2.4
1	A	275	ASN	2.2
1	A	197	LYS	2.2
1	A	205	LYS	2.2
1	A	78	PRO	2.1
1	A	189	VAL	2.0

4.2 Non-standard residues in protein, DNA, RNA chains

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

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.4 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($\text{\AA}^2$)	Q<0.9
2	GOL	A	709	6/6	0.65	0.19	70,77,82,82	0
3	MES	A	710[A]	12/12	0.66	0.32	51,67,77,84	12
3	MES	A	710[B]	12/12	0.66	0.32	57,69,76,80	12
3	MES	A	712[A]	12/12	0.66	0.34	39,47,54,59	12
3	MES	A	712[B]	12/12	0.66	0.34	34,46,59,59	12
2	GOL	A	705	6/6	0.83	0.15	58,62,65,82	0
2	GOL	A	701	6/6	0.83	0.14	60,65,76,85	0
2	GOL	A	708	6/6	0.84	0.14	58,61,62,73	0
3	MES	A	711	12/12	0.84	0.20	41,51,69,86	12
2	GOL	A	706	6/6	0.87	0.16	44,49,64,69	0
2	GOL	A	707	6/6	0.87	0.15	56,72,79,90	0
2	GOL	A	703	6/6	0.87	0.14	48,53,58,65	0
2	GOL	A	704	6/6	0.88	0.13	58,62,66,84	0
4	DMS	A	713	4/4	0.90	0.16	48,59,81,81	0
2	GOL	A	702	6/6	0.91	0.11	49,51,57,71	0

4.5 Other polymers [i](#)

There are no such residues in this entry.