



Full wwPDB X-ray Structure Validation Report

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PDB ID : 3PBQ
Title : Crystal structure of PBP3 complexed with imipenem
Authors : Han, S.
Deposited on : 2010-10-20
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

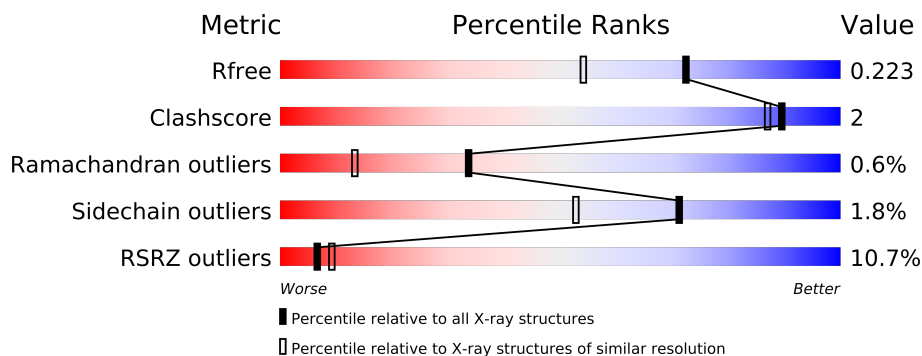
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 1.70 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}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	538	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4051 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

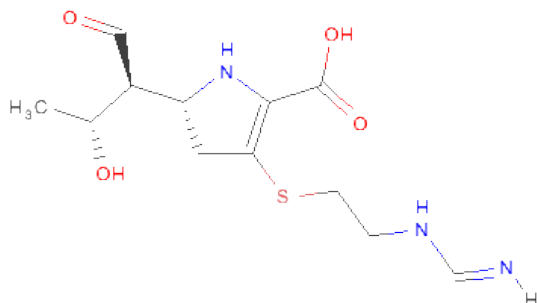
- Molecule 1 is a protein called Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	493	3759	2376	677	694	12	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	EXPRESSION TAG	UNP Q51504
A	43	GLY	-	EXPRESSION TAG	UNP Q51504
A	44	HIS	-	EXPRESSION TAG	UNP Q51504
A	45	HIS	-	EXPRESSION TAG	UNP Q51504
A	46	HIS	-	EXPRESSION TAG	UNP Q51504
A	47	HIS	-	EXPRESSION TAG	UNP Q51504
A	48	HIS	-	EXPRESSION TAG	UNP Q51504
A	49	HIS	-	EXPRESSION TAG	UNP Q51504

- Molecule 2 is (5R)-5-[(1S,2R)-1-FORMYL-2-HYDROXYPROPYL]-3-[(2-{[(E)-IMINOMETHYL]AMINO}ETHYL)SULFANYL]-4,5-DIHYDRO-1H-PYRROLE-2-CARBOXYLIC ACID (three-letter code: IM2) (formula: C₁₂H₁₉N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	20	12	3	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	272	Total	O	0	0
			272	272		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.44Å 80.18Å 87.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 1.70 29.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.62-1.70) 95.0 (29.62-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 1.70Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.185 , 0.217 0.189 , 0.223	Depositor DCC
R_{free} test set	2594 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51049 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4051	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IM2

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	0.50	0/3833	0.65	0/5202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3759	0	3808	17	0
2	A	20	0	16	0	0
3	A	272	0	0	1	0
All	All	4051	0	3824	17	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:264:ASN:HD21	1:A:285:ALA:H	1.36	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:VAL:CG1	1:A:412:SER:HB3	2.32	0.59
1:A:288:ASP:OD2	3:A:628:HOH:O	2.17	0.56
1:A:533:PHE:O	1:A:537:VAL:HG12	2.06	0.56
1:A:264:ASN:ND2	1:A:285:ALA:H	2.03	0.56
1:A:274:ARG:O	1:A:275:ASN:HB3	2.11	0.50
1:A:62:ARG:HB3	1:A:76:SER:OG	2.12	0.49
1:A:58:ILE:HD11	1:A:193:ARG:HG3	1.96	0.47
1:A:259:ILE:HD12	1:A:436:MET:HG2	1.98	0.46
1:A:178:ILE:HG21	1:A:221:LEU:HD21	1.98	0.46
1:A:242:ASN:ND2	1:A:537:VAL:HG23	2.31	0.45
1:A:400:ALA:O	1:A:404:THR:HG23	2.18	0.44
1:A:301:MET:SD	1:A:342:LEU:HD13	2.60	0.42
1:A:488:ALA:HB3	1:A:504:ARG:HB2	2.02	0.41
1:A:238:ALA:HB2	1:A:541:VAL:HG22	2.02	0.41
1:A:233:ARG:HH11	1:A:236:ARG:HH12	1.69	0.41
1:A:186:LEU:O	1:A:216:GLY:HA3	2.20	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	487/538 (90%)	474 (97%)	10 (2%)	3 (1%)	33	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	A	276	LEU
1	A	528	SER

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	393/426 (92%)	386 (98%)	7 (2%)	71 53

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	GLU
1	A	153	ARG
1	A	175	ARG
1	A	199	ARG
1	A	275	ASN
1	A	349	SER
1	A	529	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	237	ASN
1	A	264	ASN
1	A	265	GLN
1	A	275	ASN
1	A	283	ASN
1	A	324	GLN
1	A	420	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
2	IM2	A	999	1	20,20,20	39.33	12 (60%)	26,26,26	4.06	11 (42%)

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	IM2	A	999	1	-	4/18/32/32	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	IM2	C25-N26	174.87	1.40	1.20
2	A	999	IM2	C1-C5	10.03	1.64	1.52
2	A	999	IM2	C6-C5	-9.02	1.46	1.55
2	A	999	IM2	C3-C31	-5.61	1.41	1.48
2	A	999	IM2	O62-C61	5.51	1.54	1.43
2	A	999	IM2	C1-C2	5.41	1.63	1.50
2	A	999	IM2	C25-N24	4.63	1.47	1.37
2	A	999	IM2	C5-N4	-4.12	1.39	1.46
2	A	999	IM2	C22-S21	3.84	1.99	1.81
2	A	999	IM2	C3-N4	-3.24	1.32	1.38
2	A	999	IM2	C23-N24	2.86	1.55	1.47
2	A	999	IM2	C22-C23	2.36	1.60	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	IM2	N24-C25-N26	10.43	130.94	122.01
2	A	999	IM2	C5-C1-C2	-9.33	94.00	102.89
2	A	999	IM2	C61-C6-C5	7.14	120.04	112.14
2	A	999	IM2	C5-C6-C7	-6.94	101.25	112.28
2	A	999	IM2	C22-S21-C2	6.34	116.30	104.19
2	A	999	IM2	C6-C5-N4	6.10	123.96	113.22
2	A	999	IM2	C2-C3-C31	3.87	135.98	128.25
2	A	999	IM2	O62-C61-C6	-2.92	101.49	108.64
2	A	999	IM2	C23-N24-C25	2.75	126.98	122.14
2	A	999	IM2	C3-C2-S21	-2.38	120.84	123.83
2	A	999	IM2	O62-C61-C62	2.17	116.07	109.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	IM2	O31-C31-C3-N4
2	A	999	IM2	O31-C31-C3-C2
2	A	999	IM2	O32-C31-C3-N4
2	A	999	IM2	O32-C31-C3-C2

There are no ring outliers.

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 ⓘ

6.1 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	493/538 (91%)	0.60	53 (10%) 6 9	10, 21, 55, 91	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	VAL	17.9
1	A	530	ALA	11.8
1	A	529	LYS	9.8
1	A	562	THR	9.6
1	A	561	PRO	8.8
1	A	210	THR	8.7
1	A	528	SER	7.8
1	A	275	ASN	7.8
1	A	195	VAL	7.6
1	A	211	LYS	7.5
1	A	56	ILE	6.9
1	A	560	LEU	5.8
1	A	189	VAL	5.7
1	A	196	LEU	5.0
1	A	274	ARG	4.9
1	A	212	ASN	4.9
1	A	527	PRO	4.6
1	A	328	TYR	4.6
1	A	276	LEU	4.6
1	A	327	ARG	4.5
1	A	207	VAL	4.5
1	A	208	GLN	4.2
1	A	194	GLN	4.0
1	A	501	ASN	4.0
1	A	131	PRO	4.0
1	A	55	HIS	3.9
1	A	209	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	192	LYS	3.6
1	A	135	GLU	3.5
1	A	116	GLN	3.3
1	A	503	TYR	3.3
1	A	188	GLY	3.2
1	A	54	ARG	3.2
1	A	193	ARG	3.1
1	A	109	LEU	3.1
1	A	139	ALA	3.0
1	A	214	LYS	3.0
1	A	213	ALA	2.9
1	A	278	PRO	2.9
1	A	502	ALA	2.8
1	A	170	VAL	2.8
1	A	118	ALA	2.8
1	A	199	ARG	2.5
1	A	531	GLY	2.5
1	A	514	THR	2.3
1	A	468	GLN	2.3
1	A	117	ASN	2.3
1	A	132	GLU	2.2
1	A	418	LEU	2.2
1	A	133	GLN	2.1
1	A	490	LYS	2.1
1	A	130	THR	2.1
1	A	140	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	IM2	A	999	20/20	0.10	0.13	14,24,53,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.