



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:54 am BST

PDB ID : 2Y2H
Title : PENICILLIN-BINDING PROTEIN 1B (PBP-1B) IN COMPLEX WITH AN ALKYL BORONATE (ZA2)
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Deposited on : 2010-12-15
Resolution : 1.96 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

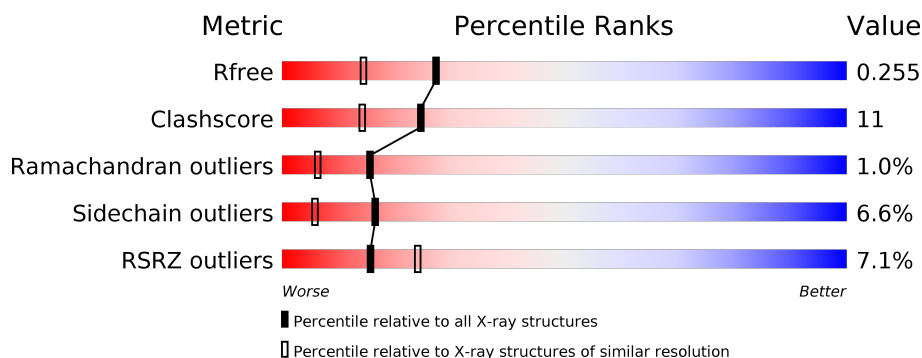
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	494	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	494	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• • •</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7669 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.

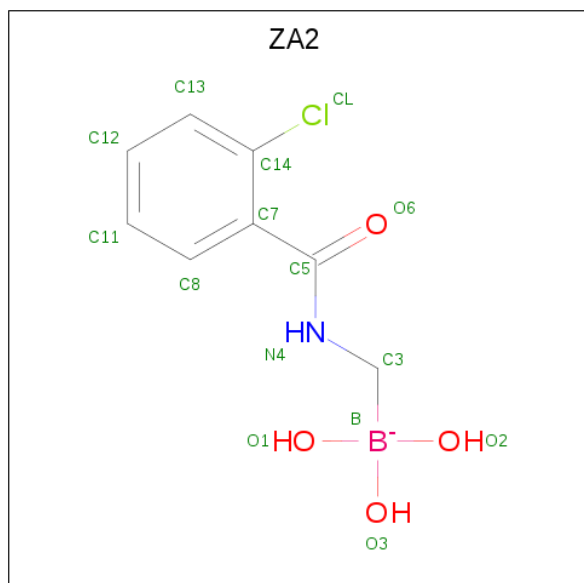
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3594	2249	609	721	15			
1	B	472	Total	C	N	O	S	0	1	0
			3639	2277	614	733	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	ASN	engineered mutation	UNP Q7CRA4
A	686	GLN	ARG	engineered mutation	UNP Q7CRA4
A	687	GLN	ARG	engineered mutation	UNP Q7CRA4
B	656	GLY	ASN	engineered mutation	UNP Q7CRA4
B	686	GLN	ARG	engineered mutation	UNP Q7CRA4
B	687	GLN	ARG	engineered mutation	UNP Q7CRA4

- Molecule 2 is [(2-CHLOROPHENYL)CARBONYLAMINO]METHYL-TRIHYDROXY-BORON (three-letter code: ZA2) (formula: C₈H₁₀BClNO₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	Cl	N	O	0	0
			14	1	8	1	1	3		
2	B	1	Total	B	C	Cl	N	O	0	0
			14	1	8	1	1	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	Cl	0	0
			8	8		
4	A	10	Total	Cl	0	0
			10	10		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total 167	O 167	0	0
6	B	211	Total 211	O 211	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.99Å 100.48Å 143.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 1.96 48.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.00-1.96) 94.8 (48.00-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.212 , 0.254 0.213 , 0.255	Depositor DCC
R_{free} test set	9459 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7669	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: NA, ZA2, SO4, CL

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	0.64	0/3667	0.66	0/4977
1	B	0.71	0/3715	0.72	2/5042 (0.0%)
All	All	0.67	0/7382	0.69	2/10019 (0.0%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	MET	CG-SD-CE	6.16	110.06	100.20
1	B	630	THR	CB-CA-C	-5.11	97.81	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	666	SER	Peptide
1	B	630	THR	Mainchain
1	B	666	SER	Peptide

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	3594	0	3459	67	0
1	B	3639	0	3502	86	0
2	A	14	0	9	1	0
2	B	14	0	9	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	10	0	0	1	0
4	B	8	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	167	0	0	6	0
6	B	211	0	0	8	0
All	All	7669	0	6979	155	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 11.

The worst 5 of 155 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:B:706:GLN:HG3	6:B:2182:HOH:O	1.44	1.14
1:B:495:PRO:HB2	1:B:497:MET:HE2	1.27	1.14
1:A:427:MET:HE2	1:A:568:THR:HG22	1.15	1.14
1:B:495:PRO:HB2	1:B:497:MET:CE	1.86	1.04
1:A:427:MET:CE	1:A:568:THR:HG22	1.89	1.02

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	463/494 (94%)	445 (96%)	16 (4%)	2 (0%)	34	22
1	B	469/494 (95%)	445 (95%)	17 (4%)	7 (2%)	10	3
All	All	932/988 (94%)	890 (96%)	33 (4%)	9 (1%)	15	6

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	788	GLY
1	B	743	GLY
1	B	740	SER
1	B	744	LYS
1	B	788	GLY

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	382/408 (94%)	358 (94%)	24 (6%)	18	7
1	B	388/408 (95%)	360 (93%)	28 (7%)	14	4
All	All	770/816 (94%)	718 (93%)	52 (7%)	16	5

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	780	GLN
1	B	364	LYS
1	B	751	SER
1	B	106	SER
1	B	349	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	640	ASN
1	A	692	ASN
1	B	450	HIS
1	A	606	GLN
1	B	489	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 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	ZA2	B	1000	1,5	12,14,15	1.08	1 (8%)	14,18,21	1.32	2 (14%)
3	SO4	A	1100	-	4,4,4	0.41	0	6,6,6	0.44	0
3	SO4	B	1100	-	4,4,4	0.43	0	6,6,6	0.53	0
2	ZA2	A	1000	1,5	12,14,15	0.95	0	14,18,21	1.17	1 (7%)

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	ZA2	B	1000	1,5	-	0/6/9/10	0/1/1/1
2	ZA2	A	1000	1,5	-	0/6/9/10	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	ZA2	C5-N4	2.31	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ZA2	C3-N4-C5	2.98	130.16	121.89
2	B	1000	ZA2	C3-N4-C5	2.91	129.94	121.89
2	B	1000	ZA2	C7-C14-CL	-2.49	117.31	121.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	ZA2	1	0
2	A	1000	ZA2	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](#)

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	467/494 (94%)	0.33	26 (5%) 24 33	25, 40, 76, 112	0
1	B	472/494 (95%)	0.58	41 (8%) 10 16	21, 36, 81, 121	0
All	All	939/988 (95%)	0.46	67 (7%) 16 24	21, 38, 80, 121	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	ALA	9.6
1	B	746	VAL	7.3
1	B	741	VAL	6.8
1	B	739	VAL	6.3
1	B	364	LYS	6.1

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(\AA^2)	Q<0.9
4	CL	A	1792	1/1	0.79	0.14	61,61,61,61	0
2	ZA2	B	1000	14/15	0.85	0.16	31,48,70,90	0
4	CL	B	1208	1/1	0.86	0.17	61,61,61,61	0
4	CL	A	1203	1/1	0.89	0.11	65,65,65,65	0
4	CL	B	1200	1/1	0.91	0.09	44,44,44,44	0
2	ZA2	A	1000	14/15	0.92	0.15	38,58,80,108	0
4	CL	B	1202	1/1	0.93	0.26	58,58,58,58	0
4	CL	A	1202	1/1	0.94	0.11	55,55,55,55	0
4	CL	A	1216	1/1	0.94	0.12	54,54,54,54	0
4	CL	A	1201	1/1	0.96	0.06	50,50,50,50	0
4	CL	B	1206	1/1	0.96	0.06	57,57,57,57	0
4	CL	A	1213	1/1	0.97	0.15	58,58,58,58	0
4	CL	B	1212	1/1	0.97	0.08	46,46,46,46	0
5	NA	B	1300	1/1	0.98	0.21	26,26,26,26	0
4	CL	B	1201	1/1	0.98	0.07	39,39,39,39	0
4	CL	A	1212	1/1	0.98	0.08	43,43,43,43	0
4	CL	A	1200	1/1	0.98	0.09	42,42,42,42	0
4	CL	A	1211	1/1	0.98	0.07	43,43,43,43	0
3	SO4	A	1100	5/5	0.98	0.08	38,45,46,48	0
5	NA	A	1300	1/1	0.99	0.18	30,30,30,30	0
4	CL	A	1791	1/1	0.99	0.19	31,31,31,31	0
4	CL	B	1211	1/1	0.99	0.09	33,33,33,33	0
4	CL	B	1213	1/1	0.99	0.07	46,46,46,46	0
3	SO4	B	1100	5/5	0.99	0.08	37,37,44,46	0

6.5 Other polymers

There are no such residues in this entry.