wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2023 – 01:00 PM EDT

PDB ID	:	2Z2L
Title	:	Penicillin-Binding Protein 2X (PBP2X) from Streptococcus pneumoniae
Authors	:	Yamada, M.; Watanabe, T.; Takeuchi, Y.
Deposited on	:	2007-05-23
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

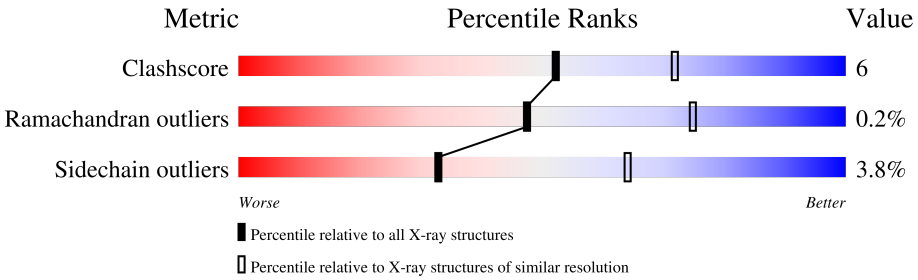
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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))
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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	A	168	79% 15% • 5%
1	D	168	71% 7% • 20%
2	B	385	80% 15% • 5%
2	E	385	80% 15% • 5%
3	C	125	83% 16% •
3	F	125	80% 18% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9852 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 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1224	766	204	250	4			
1	D	134	Total	C	N	O	S	0	0	0
			1021	634	172	212	3			

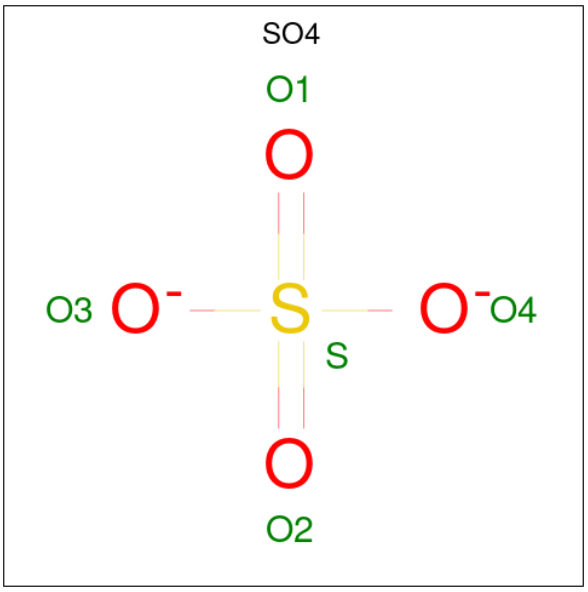
- Molecule 2 is a protein called Penicillin-binding protein 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	367	Total	C	N	O	S	0	0	0
			2814	1769	465	563	17			
2	E	367	Total	C	N	O	S	0	0	0
			2814	1769	465	563	17			

- Molecule 3 is a protein called Penicillin-binding protein 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			962	601	162	197	2			
3	F	125	Total	C	N	O	S	0	0	0
			962	601	162	197	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	13	Total O 13 13	0	0
5	C	3	Total O 3 3	0	0
5	D	6	Total O 6 6	0	0
5	E	19	Total O 19 19	0	0
5	F	5	Total O 5 5	0	0

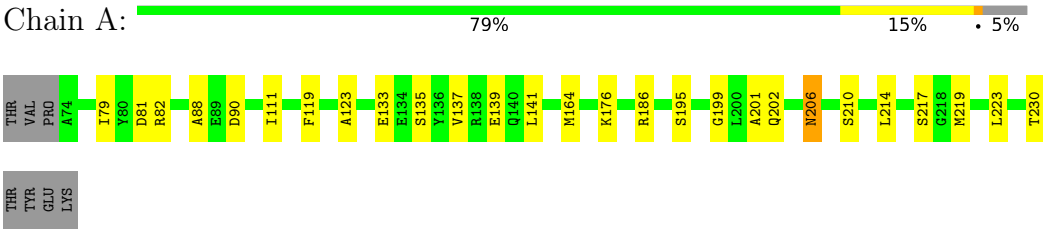
3 Residue-property plots (i)

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.

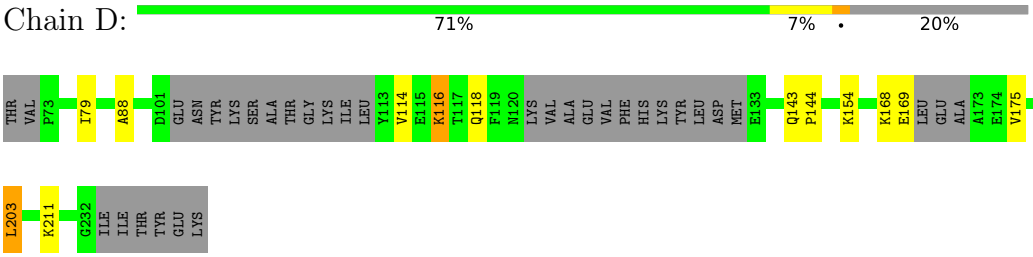
• Molecule 1: Penicillin-binding protein 2X

Chain A:



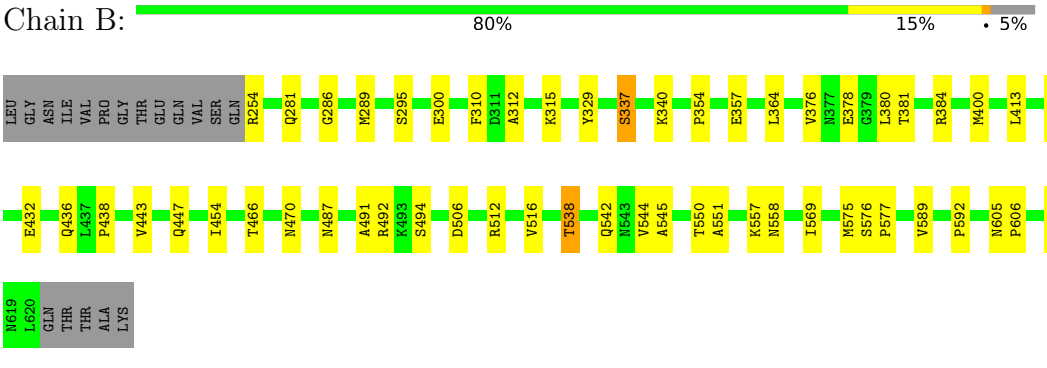
• Molecule 1: Penicillin-binding protein 2X

Chain D:



• Molecule 2: Penicillin-binding protein 2X

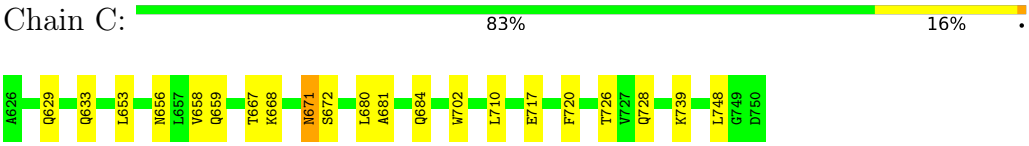
Chain B:



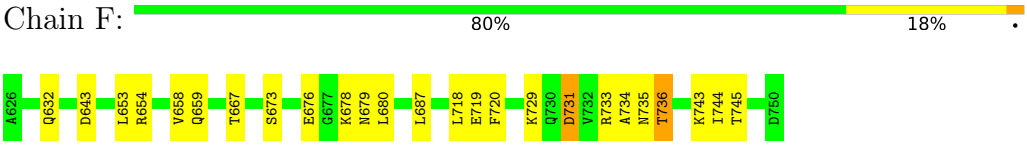
• Molecule 2: Penicillin-binding protein 2X

Chain E:

• Molecule 3: Penicillin-binding protein 2X



• Molecule 3: Penicillin-binding protein 2X



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.88Å 171.71Å 89.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85	Depositor
% Data completeness (in resolution range)	99.7 (30.00-2.85)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.224 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.39	0/1244	0.53	0/1676
1	D	0.39	0/1035	0.53	0/1391
2	B	0.40	0/2868	0.55	0/3890
2	E	0.41	0/2868	0.56	0/3890
3	C	0.35	0/975	0.51	0/1320
3	F	0.38	0/975	0.55	0/1320
All	All	0.39	0/9965	0.54	0/13487

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

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	1224	0	1191	15	0
1	D	1021	0	981	11	0
2	B	2814	0	2747	30	0
2	E	2814	0	2747	31	0
3	C	962	0	975	12	0
3	F	962	0	975	17	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	13	0	0	1	0
5	C	3	0	0	0	0
5	D	6	0	0	0	0
5	E	19	0	0	0	0
5	F	5	0	0	1	0
All	All	9852	0	9616	107	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 107 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)
2:B:340:LYS:HG2	2:B:400:MET:HG3	1.58	0.84
2:E:340:LYS:HG2	2:E:400:MET:HG3	1.70	0.74
2:E:290:THR:HG1	2:E:588:THR:HG1	1.35	0.74
2:E:337:SER:HB2	2:E:549:GLY:HA2	1.69	0.74
3:F:653:LEU:HB3	3:F:658:VAL:HB	1.71	0.72

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	
1	A	157/168 (94%)	147 (94%)	10 (6%)	0	100	100
1	D	126/168 (75%)	122 (97%)	4 (3%)	0	100	100
2	B	365/385 (95%)	347 (95%)	18 (5%)	0	100	100
2	E	365/385 (95%)	343 (94%)	20 (6%)	2 (0%)	29	57
3	C	123/125 (98%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	123/125 (98%)	116 (94%)	7 (6%)	0	100 100
All	All	1259/1356 (93%)	1195 (95%)	62 (5%)	2 (0%)	47 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	557	LYS
2	E	376	VAL

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	132/141 (94%)	127 (96%)	5 (4%)	33 64
1	D	111/141 (79%)	107 (96%)	4 (4%)	35 66
2	B	307/322 (95%)	292 (95%)	15 (5%)	25 54
2	E	307/322 (95%)	298 (97%)	9 (3%)	42 72
3	C	108/108 (100%)	104 (96%)	4 (4%)	34 65
3	F	108/108 (100%)	104 (96%)	4 (4%)	34 65
All	All	1073/1142 (94%)	1032 (96%)	41 (4%)	33 64

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	386	MET
2	E	594	HIS
2	E	427	PHE
2	E	493	LYS
3	F	643	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	377	ASN
3	F	671	ASN
3	F	728	GLN
3	F	715	ASN
2	B	542	GLN

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)

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	$\#\|Z\| > 2$
4	SO4	B	801	-	4,4,4	0.11	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.