

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:25 PM EDT

PDB ID	:	6P52
Title	:	Crystal structure of transpeptidase domain of PBP2 from Neisseria gonor-
		rhoeae with a bound phosphate at the active site
Authors	:	Singh, A.; Davies, C.
Deposited on		
Resolution	:	1.83 Å(reported)
Deposited on	:	Singh, A.; Davies, C.

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 (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 (1)) were used in the production of this report:

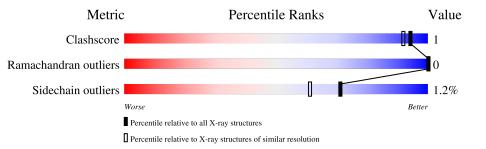
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 1.83 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	$\begin{array}{c} \textbf{Whole archive} \\ (\# \textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4964 atoms, of which 0 are hydrogens and 0 are deuteriums.

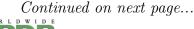
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	313	Total	С	Ν	0	S	0	6	0
	A	515	2408	1528	430	442	8	0	0	0
1	В	313	Total	С	Ν	0	S	0	1	0
	D	515	2380	1510	422	441	7	0		0

• Molecule 1 is a protein called peptidoglycan D,D-transpeptidase PenA.

Chain	Residue	Modelled	Actual	Comment	Reference
А	232	GLY	-	expression tag	UNP P08149
А	233	SER	-	expression tag	UNP P08149
А	234	GLY	-	expression tag	UNP P08149
А	235	GLY	-	expression tag	UNP P08149
А	236	ALA	-	expression tag	UNP P08149
A	297	GLY	ALA	conflict	UNP P08149
А	?	-	TYR	deletion	UNP P08149
А	?	-	ASP	deletion	UNP P08149
А	?	-	PRO	deletion	UNP P08149
А	?	-	ASN	deletion	UNP P08149
А	?	-	ARG	deletion	UNP P08149
А	?	-	PRO	deletion	UNP P08149
А	?	-	GLY	deletion	UNP P08149
А	?	-	ARG	deletion	UNP P08149
А	?	-	ALA	deletion	UNP P08149
А	?	-	ASP	deletion	UNP P08149
A	?	-	SER	deletion	UNP P08149
А	?	-	GLU	deletion	UNP P08149
А	?	-	GLN	deletion	UNP P08149
А	?	-	ARG	deletion	UNP P08149
В	232	GLY	-	expression tag	UNP P08149
В	233	SER	-	expression tag	UNP P08149
В	234	GLY	-	expression tag	UNP P08149
В	235	GLY	-	expression tag	UNP P08149
В	236	ALA	-	expression tag	UNP P08149

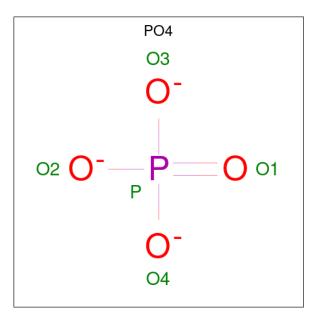
There are 40 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	297	GLY	ALA	conflict	UNP P08149
В	?	-	TYR	deletion	UNP P08149
В	?	-	ASP	deletion	UNP P08149
В	?	-	PRO	deletion	UNP P08149
В	?	-	ASN	deletion	UNP P08149
В	?	-	ARG	deletion	UNP P08149
В	?	-	PRO	deletion	UNP P08149
В	?	-	GLY	deletion	UNP P08149
В	?	-	ARG	deletion	UNP P08149
В	?	-	ALA	deletion	UNP P08149
В	?	-	ASP	deletion	UNP P08149
В	?	-	SER	deletion	UNP P08149
В	?	-	GLU	deletion	UNP P08149
В	?	-	GLN	deletion	UNP P08149
В	?	-	ARG	deletion	UNP P08149

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• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	TotalOP541	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	110	Total O 110 110	0	0
3	В	56	Total O 56 56	0	0

SEQUENCE-PLOTS INFOmissingINFO



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	41.97Å 76.87Å 86.47Å	Depositor
a, b, c, α , β , γ	90.00° 92.32° 90.00°	Depositor
Resolution (Å)	38.35 - 1.83	Depositor
% Data completeness	98.4 (38.35-1.83)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.74 (at 1.82 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.195 , 0.233	Depositor
Wilson B-factor $(Å^2)$	32.3	Xtriage
Anisotropy	0.091	Xtriage
L-test for $twinning^2$	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
Total number of atoms	4964	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	Mol Chain		lengths	Bond angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.47	0/2475	0.67	0/3351
1	В	0.40	0/2432	0.62	0/3295
All	All	0.44	0/4907	0.64	0/6646

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	А	2408	0	2462	6	0
1	В	2380	0	2417	8	0
2	А	10	0	0	0	0
3	А	110	0	0	0	0
3	В	56	0	0	0	0
All	All	4964	0	4879	13	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 1.

All (13) 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:259:GLN:HE21	1:B:259:GLN:HA	1.67	0.57
1:B:428:LEU:HD13	1:B:534:THR:HG23	1.87	0.57
1:B:391:ARG:HG2	1:B:401:ALA:HB2	1.91	0.52
1:B:428:LEU:HD13	1:B:534:THR:CG2	2.41	0.51
1:A:266:VAL:HG22	1:A:278:LEU:HD12	1.94	0.49
1:A:319[A]:LYS:HD2	1:A:382:PHE:CG	2.48	0.49
1:A:391:ARG:HG3	1:A:401:ALA:HB2	1.96	0.47
1:B:278:LEU:HD21	1:B:301:ALA:HB3	1.96	0.47
1:A:264:THR:CG2	1:A:301:ALA:HB2	2.46	0.46
1:A:459:LYS:HE2	1:A:461:ILE:HD11	2.01	0.41
1:B:380:TYR:HB2	1:B:407:TRP:HB3	2.02	0.41
1:B:570:LYS:HB2	1:B:571:PRO:CD	2.51	0.41
1:A:392:MET:O	1:B:408:ARG:HD3	2.21	0.41

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	Perce	ntiles
1	А	315/329~(96%)	313~(99%)	2(1%)	0	100	100
1	В	310/329~(94%)	307~(99%)	3~(1%)	0	100	100
All	All	625/658~(95%)	620~(99%)	5(1%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	253/257~(98%)	251~(99%)	2(1%)	81 75
1	В	249/257~(97%)	245~(98%)	4 (2%)	62 49
All	All	502/514~(98%)	496 (99%)	6 (1%)	71 61

analysed, and the total number of residues.

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	385	GLU
1	А	424	LEU
1	В	259	GLN
1	В	335	GLN
1	В	512	ASN
1	В	514	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	335	GLN
1	А	360	GLN
1	А	384	HIS
1	А	425	GLN
1	А	440	HIS
1	А	452	GLN
1	В	259	GLN
1	В	335	GLN
1	В	425	GLN
1	В	472	ASN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

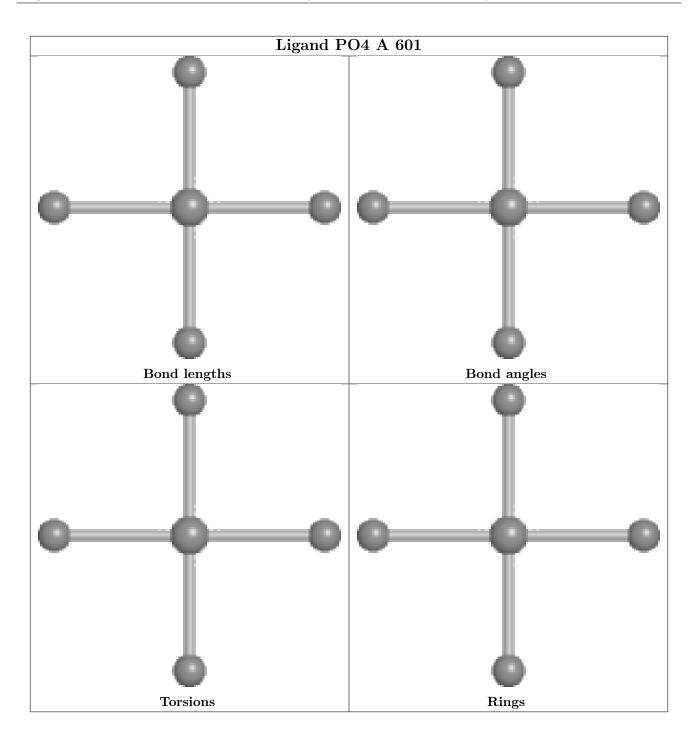
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

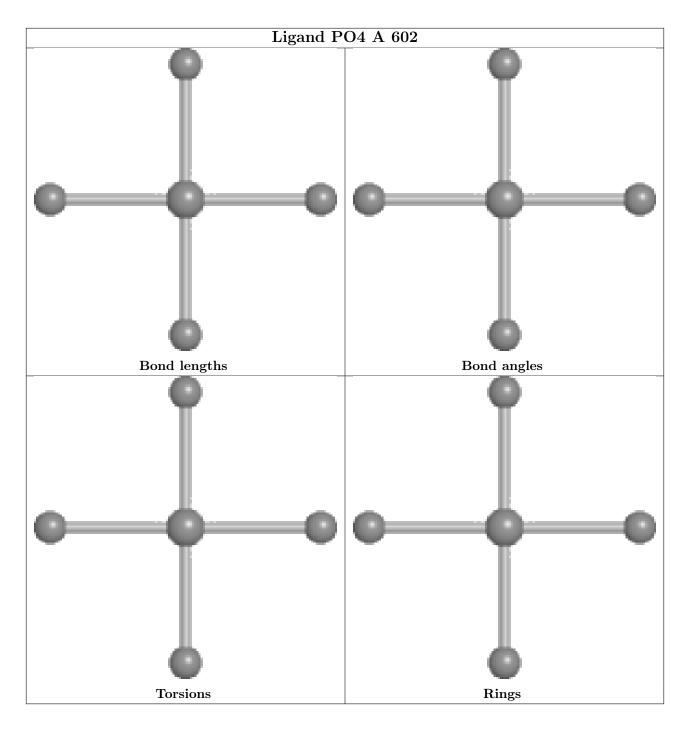












4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

