



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2014 – 01:25 PM EDT

PDB ID : 4OOL  
Title : Crystal structure of PBP3 in complex with compound 14 ((2E)-2-({[(2S)-2-{[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-{{[(1,5-dihydroxy-4-oxo-1,4-dihydropyridin-2-yl)methoxy]imino}acetyl]amino}-3-oxopropyl]oxy}imino)pentanedioicacid)  
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Deposited on : 2014-02-03  
Resolution : 2.30 Å(reported)

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

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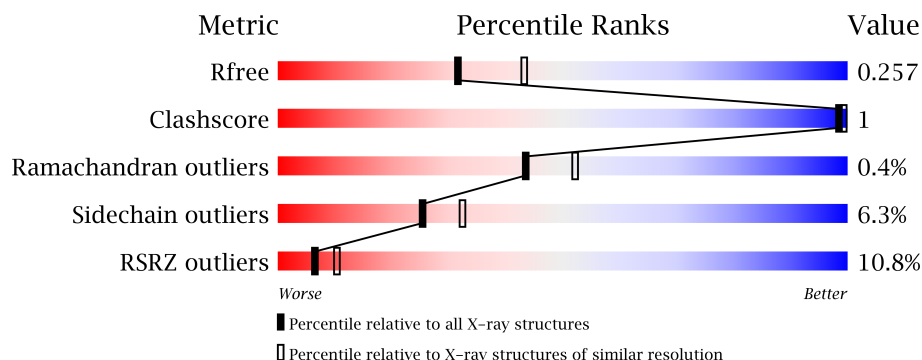
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
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) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 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 3960 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.

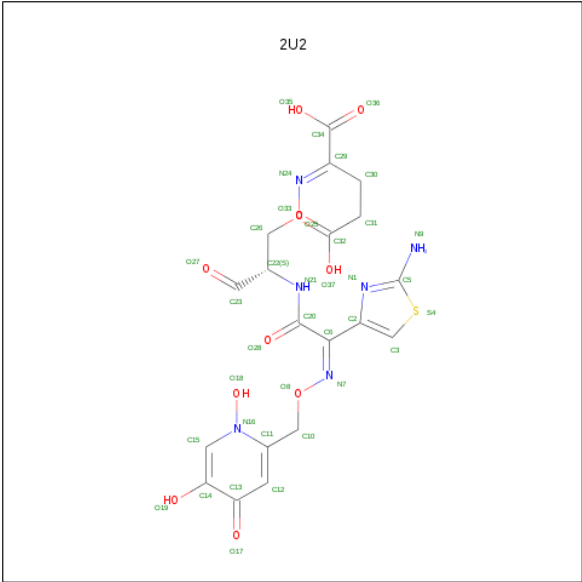
- Molecule 1 is a protein called Cell division protein FtsI [Peptidoglycan synthetase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	2	0
			3816	2411	690	703	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	INITIATING METHIONINE	UNP U6AVY0
A	43	GLY	-	EXPRESSION TAG	UNP U6AVY0
A	44	HIS	-	EXPRESSION TAG	UNP U6AVY0
A	45	HIS	-	EXPRESSION TAG	UNP U6AVY0
A	46	HIS	-	EXPRESSION TAG	UNP U6AVY0
A	47	HIS	-	EXPRESSION TAG	UNP U6AVY0
A	48	HIS	-	EXPRESSION TAG	UNP U6AVY0
A	49	HIS	-	EXPRESSION TAG	UNP U6AVY0

- Molecule 2 is (2E)-2-({[(2S)-2-{{[(2Z)-2-(2-AMINO-1,3-THIAZOL-4-YL)-2-{{[(1,5-DIHYDROXY-4-OXO-1,4-DIHYDROPYRIDIN-2-YL)METHOXY]IMINO}ACETYL]AMINO}-3-OXOPROPYL]OXY}IMINO)PENTANEDIOICACID (three-letter code: 2U2) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>6</sub>O<sub>11</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	19	6	11	1		

- Molecule 3 is water.

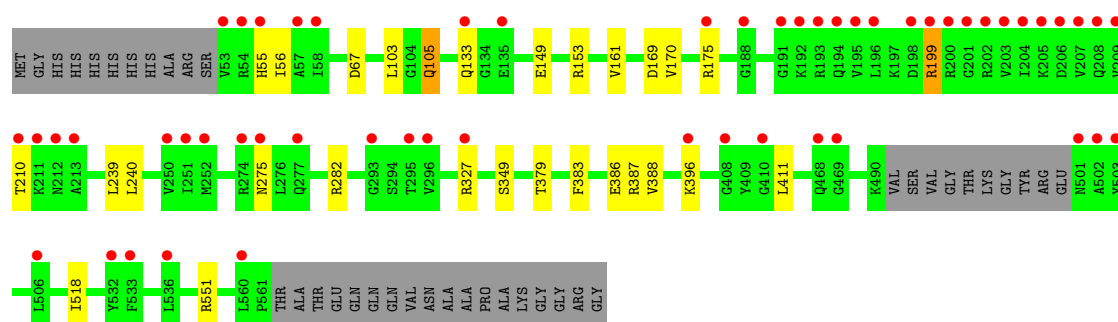
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Cell division protein FtsI [Peptidoglycan synthetase]

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.28Å 83.54Å 89.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.27 – 2.30 27.27 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.6 (27.27-2.30) 98.6 (27.27-2.29)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.186 , 0.241 0.199 , 0.257	Depositor DCC
$R_{free}$ test set	1203 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 23351 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 2U2

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	0/3897	0.70	0/5287

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	3816	0	0	2	0
2	A	37	0	0	0	0
3	A	107	0	0	0	0
All	All	3960	0	0	2	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 1.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:ASP:OD2	1:A:175:ARG:CZ	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:THR:OG1	1:A:386:GLU:OE2	2.35	0.45

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	497/538 (92%)	471 (95%)	24 (5%)	2 (0%)	43 52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	199	ARG

### 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	400/426 (94%)	375 (94%)	25 (6%)	25 32

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	56	ILE
1	A	67	ASP
1	A	103	LEU
1	A	105	GLN

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Mol	Chain	Res	Type
1	A	133	GLN
1	A	149	GLU
1	A	153	ARG
1	A	161	VAL
1	A	170	VAL
1	A	199	ARG
1	A	210	THR
1	A	239	LEU
1	A	240	LEU
1	A	275	ASN
1	A	282	ARG
1	A	327	ARG
1	A	349	SER
1	A	383	PHE
1	A	387	ARG
1	A	388	VAL
1	A	396	LYS
1	A	411	LEU
1	A	518	ILE
1	A	551	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	2U2	A	601	1	38,38,38	1.35	6 (15%)	46,51,51	2.80	11 (23%)

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	2U2	A	601	1	-	0/30/35/35	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2U2	C3-S4	3.41	1.76	1.70
2	A	601	2U2	C5-N1	-2.90	1.30	1.34
2	A	601	2U2	C12-C13	2.66	1.43	1.37
2	A	601	2U2	O18-N16	2.46	1.43	1.37
2	A	601	2U2	O35-C34	-2.45	1.22	1.30
2	A	601	2U2	O37-C32	-2.18	1.22	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	2U2	O8-N7-C6	11.41	124.80	111.30
2	A	601	2U2	O25-N24-C29	8.94	123.81	111.54
2	A	601	2U2	C26-O25-N24	6.52	116.58	108.61
2	A	601	2U2	C10-C11-N16	4.77	121.23	114.94
2	A	601	2U2	C10-O8-N7	3.55	112.03	107.97
2	A	601	2U2	C3-C2-N1	3.22	114.23	109.64
2	A	601	2U2	C2-C3-S4	-2.75	108.76	111.97
2	A	601	2U2	N9-C5-N1	2.47	126.11	122.95
2	A	601	2U2	C26-C22-N21	2.41	117.15	111.02
2	A	601	2U2	O18-N16-C11	2.34	121.09	118.29
2	A	601	2U2	C6-C20-N21	2.03	117.63	114.27

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	499/538 (92%)	0.49	54 (10%) 6 10	37, 62, 123, 166	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	GLY	9.1
1	A	195	VAL	8.9
1	A	194	GLN	8.1
1	A	207	VAL	7.5
1	A	206	ASP	7.4
1	A	202	ARG	6.9
1	A	203	VAL	6.9
1	A	209	VAL	6.5
1	A	199	ARG	6.5
1	A	204	ILE	5.8
1	A	55	HIS	5.7
1	A	205	LYS	4.9
1	A	208	GLN	4.8
1	A	196	LEU	4.8
1	A	192	LYS	4.7
1	A	198	ASP	4.7
1	A	213	ALA	4.6
1	A	57	ALA	4.5
1	A	53	VAL	4.3
1	A	54	ARG	3.8
1	A	212	ASN	3.8
1	A	277	GLN	3.6
1	A	396	LYS	3.6
1	A	58	ILE	3.5
1	A	532	TYR	3.5
1	A	536	LEU	3.4
1	A	200	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	468	GLN	3.3
1	A	193	ARG	3.3
1	A	210	THR	3.1
1	A	560	LEU	3.1
1	A	469	GLY	3.0
1	A	275	ASN	3.0
1	A	327	ARG	2.9
1	A	211	LYS	2.9
1	A	296	VAL	2.9
1	A	408	GLY	2.8
1	A	175	ARG	2.8
1	A	295	THR	2.7
1	A	502	ALA	2.7
1	A	191	GLY	2.6
1	A	188	GLY	2.6
1	A	410	GLY	2.6
1	A	274	ARG	2.5
1	A	135	GLU	2.5
1	A	293	GLY	2.4
1	A	506	LEU	2.4
1	A	250	VAL	2.3
1	A	251	ILE	2.3
1	A	503	TYR	2.3
1	A	501	ASN	2.3
1	A	252	MET	2.2
1	A	133	GLN	2.1
1	A	533	PHE	2.1

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	2U2	A	601	37/37	0.27	1.25	54,88,120,120	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.