



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:27 PM GMT

PDB ID : 2UBP  
Title : STRUCTURE OF NATIVE UREASE FROM BACILLUS PASTEURII  
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Deposited on : 1998-11-04  
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary 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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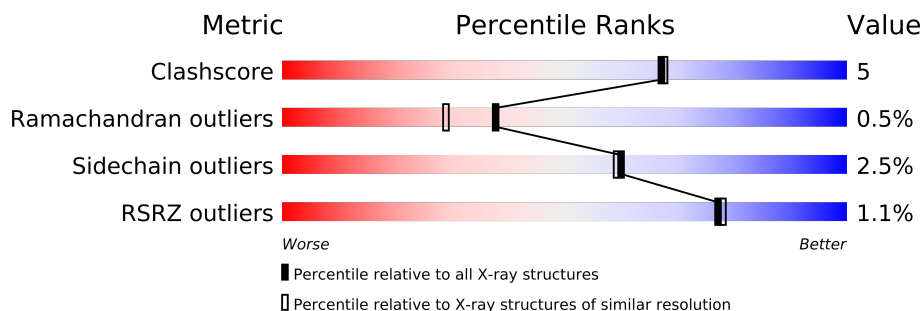
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	101	
2	B	122	
3	C	570	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	C	900	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6943 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 PROTEIN (UREASE GAMMA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	8	0	0
			781	494	133	148	6			

- Molecule 2 is a protein called PROTEIN (UREASE BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	36	0	0
			951	589	171	190	1			

- Molecule 3 is a protein called PROTEIN (UREASE ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	570	Total	C	N	O	S	44	0	0
			4323	2714	743	843	23			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	GLU	ARG	VARIANT	UNP P41020
C	28	TRP	-	INSERTION	UNP P41020
C	29	ILE	GLY	VARIANT	UNP P41020
C	36	THR	TYR	VARIANT	UNP P41020
C	37	THR	TYR	VARIANT	UNP P41020
C	38	TYR	LEU	VARIANT	UNP P41020
C	220	KCX	LYS	MODIFIED RESIDUE	UNP P41020
C	263	LEU	VAL	VARIANT	UNP P41020
C	420	ILE	MET	CONFLICT	UNP P41020

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Ni	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	124	Total	O	0	0
			124	124		
6	B	179	Total	O	0	0
			179	179		
6	C	578	Total	O	0	0
			578	578		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.36Å 131.36Å 189.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.00) 96.7 (19.88-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	7.60	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.160 , 0.200 0.163 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 63484 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: NI, SO4, ACE, KCX

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	1.16	2/790 (0.3%)	1.52	6/1065 (0.6%)
2	B	1.02	6/963 (0.6%)	1.33	7/1296 (0.5%)
3	C	0.59	0/4392	1.19	22/5955 (0.4%)
All	All	0.76	8/6145 (0.1%)	1.26	35/8316 (0.4%)

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
2	B	1	1
3	C	0	5
All	All	1	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	24.97	1.91	1.34
2	B	126	GLU	CA-CB	15.89	1.89	1.53
1	A	99	ILE	C-N	-13.81	1.02	1.34
2	B	5	ASN	N-CA	-11.16	1.24	1.46
2	B	6	TYR	N-CA	7.94	1.62	1.46

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	ACE	O-C-N	-25.11	82.53	122.70
2	B	5	ASN	N-CA-CB	20.83	148.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ILE	O-C-N	-15.02	98.66	122.70
3	C	339	ARG	NE-CZ-NH2	-11.96	114.32	120.30
3	C	5	ARG	NE-CZ-NH2	-11.83	114.38	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	5	ASN	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	ILE	Mainchain
2	B	101	ASP	Mainchain
3	C	15	THR	Mainchain
3	C	191	PRO	Mainchain
3	C	321	VAL	Mainchain

## 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	781	0	805	17	0
2	B	951	0	937	5	0
3	C	4323	0	4290	38	1
4	C	5	0	0	0	0
5	C	2	0	0	0	0
6	A	124	0	0	2	0
6	B	179	0	0	5	0
6	C	578	0	0	12	5
All	All	6943	0	6032	59	6

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 5.

The worst 5 of 59 close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:0:ACE:C	1:A:1:MET:H2	1.27	1.38
1:A:0:ACE:O	1:A:0:ACE:CH3	1.66	1.32
1:A:0:ACE:O	1:A:0:ACE:H3	1.23	1.14
1:A:79:ASP:HB3	6:A:155:HOH:O	1.63	0.96
1:A:0:ACE:C	1:A:0:ACE:H1	1.28	0.89

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:1380:HOH:O	6:C:1380:HOH:O[11_555]	1.58	0.62
6:C:1389:HOH:O	6:C:1389:HOH:O[2_665]	1.64	0.56
6:C:1409:HOH:O	6:C:1409:HOH:O[12_565]	1.75	0.45
6:C:1432:HOH:O	6:C:1432:HOH:O[11_555]	2.00	0.20
3:C:327:GLN:O	3:C:327:GLN:OE1[7_556]	2.02	0.18

## 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	99/101 (98%)	99 (100%)	0	0	100	100
2	B	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	27	17
3	C	567/570 (100%)	543 (96%)	21 (4%)	3 (0%)	38	29
All	All	786/793 (99%)	756 (96%)	26 (3%)	4 (0%)	38	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ILE
3	C	396	ASN
3	C	275	HIS
3	C	367	MET

### 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	85/85 (100%)	84 (99%)	1 (1%)	82	84
2	B	101/101 (100%)	100 (99%)	1 (1%)	85	88
3	C	460/460 (100%)	446 (97%)	14 (3%)	53	50
All	All	646/646 (100%)	630 (98%)	16 (2%)	60	59

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	253	LEU
3	C	264	ARG
3	C	326	LYS
3	C	249	HIS
3	C	396	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	267	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue 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
3	KCX	C	220	3,5	11,11,12	7.17	4 (36%)	10,12,14	2.69	5 (50%)

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
3	KCX	C	220	3,5	-	0/8/10/12	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	220	KCX	O-C	17.33	1.23	1.11
3	C	220	KCX	CX-NZ	14.34	1.46	1.32
3	C	220	KCX	OQ1-CX	6.71	1.34	1.21
3	C	220	KCX	CA-C	3.38	1.54	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	220	KCX	OQ2-CX-OQ1	-4.50	116.55	122.17
3	C	220	KCX	OQ2-CX-NZ	4.20	121.55	116.33
3	C	220	KCX	C-CA-N	-3.57	110.26	113.83
3	C	220	KCX	CE-NZ-CX	-2.86	116.78	121.99
3	C	220	KCX	CD-CE-NZ	-2.65	104.22	112.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
4	SO4	C	900	-	4,4,4	3.83	1 (25%)	6,6,6	0.49	0

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
4	SO4	C	900	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	900	SO4	O4-S	-7.43	1.22	1.47

There are no bond angle outliers.

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	101/101 (100%)	-0.71	1 (0%) 79 80	12, 17, 26, 31	2 (1%)
2	B	120/122 (98%)	-0.57	0 100 100	14, 20, 27, 32	5 (4%)
3	C	570/570 (100%)	-0.64	8 (1%) 72 72	11, 16, 34, 57	17 (2%)
All	All	791/793 (99%)	-0.64	9 (1%) 77 78	11, 17, 31, 57	24 (3%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	328	ASN	4.1
1	A	100	SER	4.1
3	C	397	GLY	3.6
3	C	322	CYS	3.4
3	C	392	ALA	3.3

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

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
3	KCX	C	220	12/13	0.07	0.12	10,14,17,18	0

### 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
4	SO4	C	900	5/5	0.17	2.84	37,38,39,41	0
5	NI	C	901	1/1	0.02	-3.50	19,19,19,19	0
5	NI	C	902	1/1	0.01	-3.53	17,17,17,17	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.