



# wwPDB X-ray Structure Validation Summary Report

Feb 19, 2024 – 08:26 PM EST

PDB ID : 4KG6  
Title : Crystal Structure of AmpC beta-lactamase N152G Mutant from E. coli  
Authors : Docter, B.E.; Baggett, V.L.; Powers, R.A.; Wallar, B.J.  
Deposited on : 2013-04-28  
Resolution : 1.75 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36  
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) : 2.36

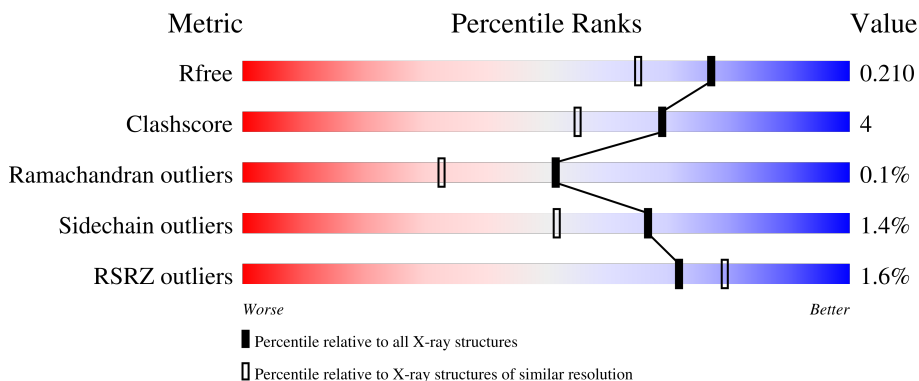
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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  $\geq 3$ , 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	358	 4% 92% 8%
1	B	358	 95% 5%
1	C	358	 93% 6%
1	D	358	 91% 9%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13019 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2848	1834	484	524	6	0	11	0
1	B	358	2863	1839	488	530	6	0	10	0
1	C	358	2842	1828	483	525	6	0	7	0
1	D	358	2838	1823	483	526	6	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	ASN	engineered mutation	UNP P00811
B	152	GLY	ASN	engineered mutation	UNP P00811
C	152	GLY	ASN	engineered mutation	UNP P00811
D	152	GLY	ASN	engineered mutation	UNP P00811

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	1
			10	8	2		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

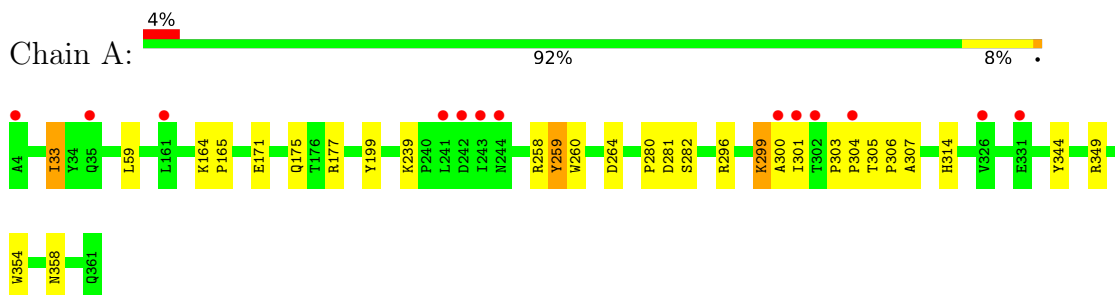
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	340	Total	O	0	7
			347	347		
3	B	442	Total	O	0	18
			460	460		
3	C	402	Total	O	0	18
			421	421		
3	D	349	Total	O	0	11
			360	360		

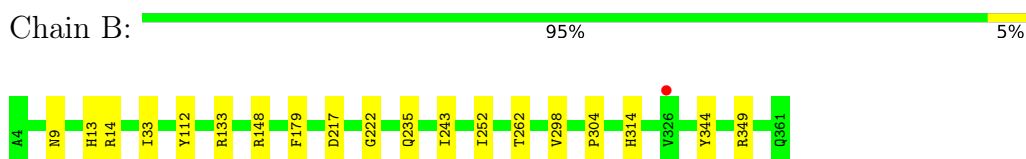
### 3 Residue-property plots [i](#)

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 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.

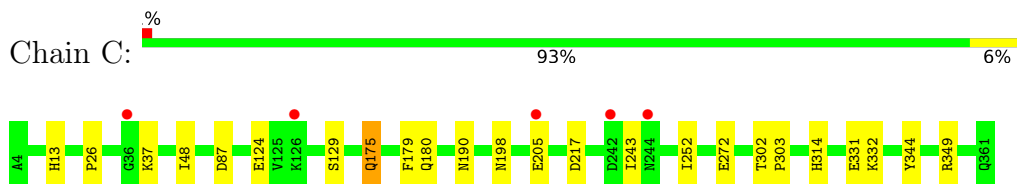
- Molecule 1: Beta-lactamase



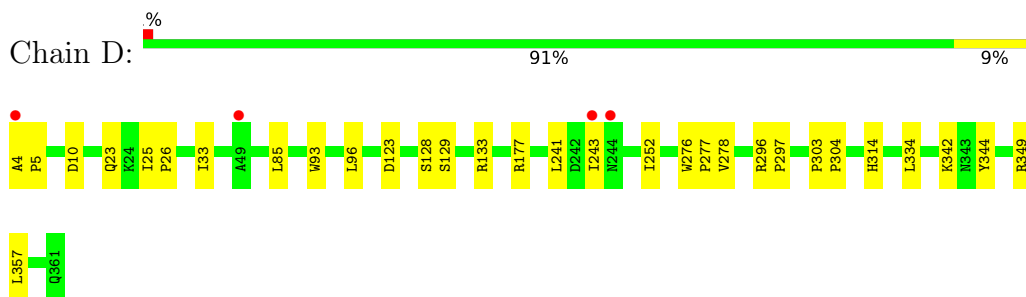
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.77Å 79.66Å 129.29Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	27.50 – 1.75 27.48 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.50-1.75) 99.8 (27.48-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.159 , 0.200 0.171 , 0.210	Depositor DCC
$R_{free}$ test set	8146 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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: 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	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.02	1/2933 (0.0%)	0.99	5/4014 (0.1%)
1	B	1.22	1/2943 (0.0%)	1.10	7/4022 (0.2%)
1	C	1.00	1/2922 (0.0%)	0.96	3/3992 (0.1%)
1	D	0.97	0/2918	0.97	6/3989 (0.2%)
All	All	1.06	3/11716 (0.0%)	1.01	21/16017 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	GLU	CD-OE1	5.57	1.31	1.25
1	A	259	TYR	CE2-CZ	-5.30	1.31	1.38
1	B	112	TYR	CE1-CZ	-5.20	1.31	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ASP	CB-CG-OD1	11.49	128.65	118.30
1	D	296	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	D	296	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	299	LYS	N-CA-C	-7.19	91.59	111.00
1	D	177	ARG	NE-CZ-NH1	6.60	123.60	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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	A	2848	0	2796	43	0
1	B	2863	0	2814	11	0
1	C	2842	0	2811	15	0
1	D	2838	0	2773	24	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	20	0	0	0	0
3	A	347	0	0	10	0
3	B	460	0	0	3	0
3	C	421	0	0	9	0
3	D	360	0	0	3	0
All	All	13019	0	11194	83	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 4.

The worst 5 of 83 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:A:259:TYR:O	1:A:301[B]:ILE:HG22	1.64	0.95
1:C:175:GLN:HG3	3:C:786:HOH:O	1.68	0.93
1:A:301[B]:ILE:HD11	1:A:305:THR:OG1	1.75	0.87
2:A:402:PO4:O3	3:A:831:HOH:O	1.95	0.85
1:A:301[B]:ILE:HG12	1:A:303[B]:PRO:O	1.82	0.80

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	367/358 (102%)	359 (98%)	8 (2%)	0	100	100
1	B	366/358 (102%)	360 (98%)	6 (2%)	0	100	100
1	C	363/358 (101%)	357 (98%)	6 (2%)	0	100	100
1	D	364/358 (102%)	358 (98%)	5 (1%)	1 (0%)	41	22
All	All	1460/1432 (102%)	1434 (98%)	25 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5	PRO

### 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	295/291 (101%)	291 (99%)	4 (1%)	67	52
1	B	298/291 (102%)	296 (99%)	2 (1%)	84	75
1	C	297/291 (102%)	291 (98%)	6 (2%)	55	34
1	D	293/291 (101%)	289 (99%)	4 (1%)	67	52
All	All	1183/1164 (102%)	1167 (99%)	16 (1%)	67	52

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

Mol	Chain	Res	Type
1	D	297	PRO
1	D	278	VAL
1	C	205	GLU
1	D	128	SER
1	C	175	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	ASN
1	C	13	HIS
1	C	198	ASN
1	C	175	GLN
1	B	13	HIS

### 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](#)

8 ligands are 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	PO4	C	401[A]	-	4,4,4	1.09	0	6,6,6	0.88	0
2	PO4	C	402	-	4,4,4	0.70	0	6,6,6	1.21	0
2	PO4	A	402	-	4,4,4	1.33	1 (25%)	6,6,6	1.65	1 (16%)
2	PO4	B	401	-	4,4,4	0.82	0	6,6,6	0.85	0
2	PO4	C	401[B]	-	4,4,4	0.79	0	6,6,6	0.57	0
2	PO4	C	403	-	4,4,4	1.25	1 (25%)	6,6,6	0.27	0
2	PO4	A	401	-	4,4,4	1.04	0	6,6,6	0.77	0
2	PO4	B	402	-	4,4,4	1.65	1 (25%)	6,6,6	1.80	2 (33%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	PO4	P-O2	-2.95	1.45	1.54
2	A	402	PO4	P-O2	-2.30	1.47	1.54
2	C	403	PO4	P-O1	2.12	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	PO4	O4-P-O2	3.35	118.73	107.97
2	B	402	PO4	O2-P-O1	2.60	120.41	110.89
2	B	402	PO4	O3-P-O1	-2.33	102.37	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	PO4	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, 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	358/358 (100%)	0.03	13 (3%) 42 49	18, 26, 43, 60	0
1	B	358/358 (100%)	-0.27	1 (0%) 94 95	11, 20, 38, 51	0
1	C	358/358 (100%)	-0.24	5 (1%) 75 82	14, 21, 38, 52	0
1	D	358/358 (100%)	-0.19	4 (1%) 80 86	16, 24, 40, 62	0
All	All	1432/1432 (100%)	-0.17	23 (1%) 72 79	11, 23, 41, 62	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	ALA	5.1
1	A	302[A]	THR	4.0
1	A	4	ALA	3.6
1	A	244	ASN	3.4
1	A	300	ALA	3.2

### 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 monosaccharides 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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	C	403	5/5	0.60	0.33	62,76,86,91	0
2	PO4	A	401	5/5	0.86	0.23	45,45,48,51	5
2	PO4	C	401[B]	5/5	0.88	0.17	28,38,39,41	5
2	PO4	C	401[A]	5/5	0.88	0.17	46,46,52,55	5
2	PO4	A	402	5/5	0.89	0.21	21,26,34,35	5
2	PO4	B	402	5/5	0.94	0.12	18,22,25,26	5
2	PO4	C	402	5/5	0.95	0.17	51,53,62,64	0
2	PO4	B	401	5/5	0.97	0.21	40,50,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.