



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:08 PM UTC

PDB ID : 3WS4 / pdb\_00003ws4  
Title : N288Q-N321Q mutant BETA-LACTAMASE DERIVED FROM CHROMO-HALOBACTER SP.560 (Condition-2A)  
Authors : Arai, S.; Yonezawa, Y.; Okazaki, N.; Matsumoto, F.; Shimizu, R.; Yamada, M.; Adachi, M.; Tamada, T.; Tokunaga, H.; Ishibashi, M.; Tokunaga, M.; Kuroki, R.  
Deposited on : 2014-02-28  
Resolution : 1.90 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

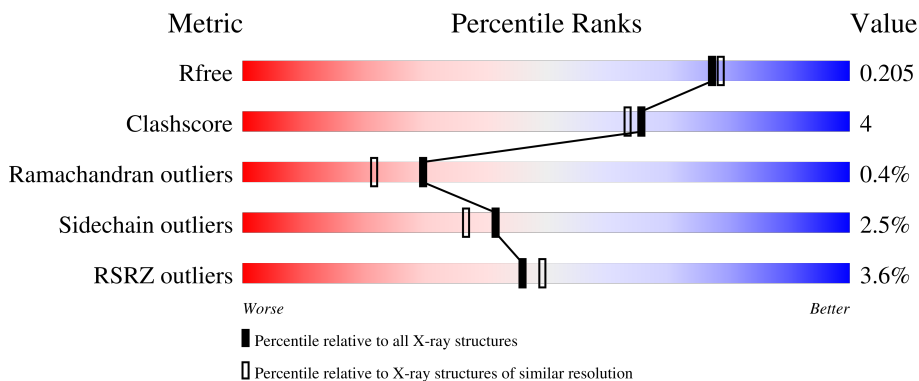
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

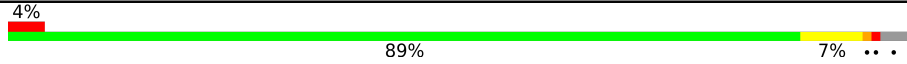
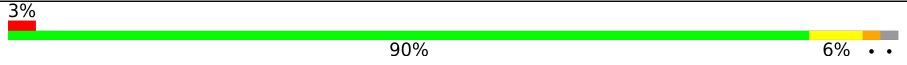

The reported resolution of this entry is 1.90 Å.

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))
$R_{free}$	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	367	
1	B	367	
1	C	367	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8710 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	357	2722	1709	457	545	11	0	3	0
1	B	359	2737	1718	459	549	11	0	3	0
1	C	358	2732	1713	460	548	11	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	GLN	ASN	engineered mutation	UNP Q76LX5
A	321	GLN	ASN	engineered mutation	UNP Q76LX5
B	288	GLN	ASN	engineered mutation	UNP Q76LX5
B	321	GLN	ASN	engineered mutation	UNP Q76LX5
C	288	GLN	ASN	engineered mutation	UNP Q76LX5
C	321	GLN	ASN	engineered mutation	UNP Q76LX5

- Molecule 2 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Sr	0	0
			3	3		
2	B	2	Total	Sr	0	0
			2	2		
2	C	3	Total	Sr	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

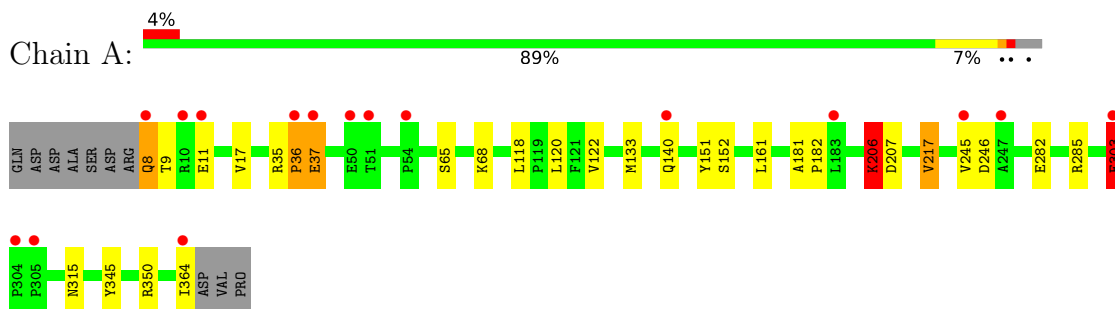
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total 159	O 159	0	0
4	B	157	Total 157	O 157	0	0
4	C	192	Total 192	O 192	0	0

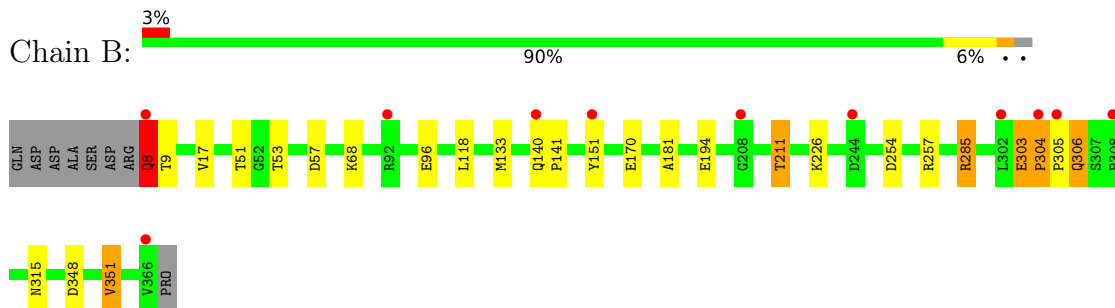
### 3 Residue-property plots [i](#)

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 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.

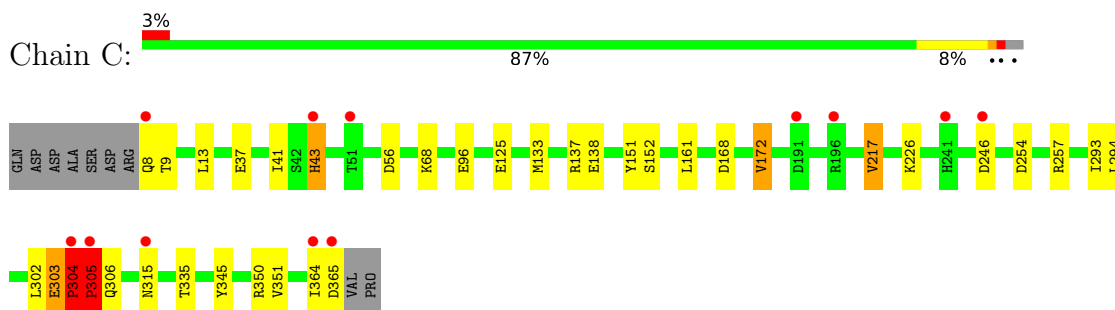
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.02Å 115.02Å 67.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.02 – 1.90 28.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.02-1.90) 99.8 (28.02-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.20 (at 1.91Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.182 , 0.216 0.177 , 0.205	Depositor DCC
$R_{free}$ test set	4015 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CL, SR

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	0.96	0/2787	0.98	6/3800 (0.2%)
1	B	0.98	1/2802 (0.0%)	1.04	10/3822 (0.3%)
1	C	1.01	0/2788	1.01	9/3801 (0.2%)
All	All	0.98	1/8377 (0.0%)	1.01	25/11423 (0.2%)

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
1	B	0	1
1	C	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	ALA	C-O	-5.38	1.19	1.24

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	GLU	CA-C-N	-16.68	103.20	120.38
1	B	303	GLU	C-N-CA	-16.68	103.20	120.38
1	A	303	GLU	CA-C-N	-9.10	111.00	120.38
1	A	303	GLU	C-N-CA	-9.10	111.00	120.38
1	C	303	GLU	CA-C-N	-7.53	112.62	120.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLU	Peptide
1	B	303	GLU	Peptide
1	C	304	PRO	Peptide
1	C	305	PRO	Peptide

## 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	2722	0	2657	17	0
1	B	2737	0	2670	17	0
1	C	2732	0	2658	28	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	159	0	0	1	0
4	B	157	0	0	2	0
4	C	192	0	0	3	0
All	All	8710	0	7985	62	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 62 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:C:37:GLU:HG2	4:C:542:HOH:O	1.42	1.14
1:A:282:GLU:OE1	1:A:285[A]:ARG:NH2	1.91	1.03
1:C:137[B]:ARG:NH1	1:C:138[B]:GLU:OE2	2.04	0.89
1:C:305:PRO:HB2	1:C:306:GLN:HA	1.56	0.86
1:C:304:PRO:N	1:C:305:PRO:HD3	1.92	0.85

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	358/367 (98%)	348 (97%)	8 (2%)	2 (1%)	21	13
1	B	360/367 (98%)	350 (97%)	9 (2%)	1 (0%)	36	29
1	C	358/367 (98%)	349 (98%)	8 (2%)	1 (0%)	36	29
All	All	1076/1101 (98%)	1047 (97%)	25 (2%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	305	PRO
1	A	37	GLU
1	B	306	GLN
1	A	303	GLU

### 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	286/292 (98%)	279 (98%)	7 (2%)	43	38
1	B	288/292 (99%)	283 (98%)	5 (2%)	53	52
1	C	286/292 (98%)	277 (97%)	9 (3%)	35	29
All	All	860/876 (98%)	839 (98%)	21 (2%)	42	38

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	96	GLU
1	C	217	VAL
1	C	351	VAL
1	C	246	ASP
1	C	172	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	HIS
1	C	113	HIS
1	C	315	ASN
1	C	251	GLN
1	B	8	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

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 [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	357/367 (97%)	0.36	16 (4%) 38 40	14, 31, 55, 94	3 (0%)
1	B	359/367 (97%)	0.33	11 (3%) 51 55	19, 29, 48, 95	3 (0%)
1	C	358/367 (97%)	0.24	12 (3%) 48 51	17, 28, 49, 81	2 (0%)
All	All	1074/1101 (97%)	0.31	39 (3%) 46 49	14, 29, 51, 95	8 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	PRO	7.2
1	B	304	PRO	6.1
1	C	365	ASP	4.7
1	B	366	VAL	4.6
1	A	304	PRO	4.5

### 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 oligosaccharides 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	SR	C	401	1/1	0.95	0.12	48,48,48,48	0
3	CL	B	403	1/1	0.95	0.18	39,39,39,39	0
3	CL	A	404	1/1	0.98	0.08	39,39,39,39	0
2	SR	A	401	1/1	0.98	0.09	35,35,35,35	0
3	CL	C	404	1/1	0.98	0.10	32,32,32,32	0
2	SR	B	402	1/1	0.99	0.08	22,22,22,22	0
2	SR	A	402	1/1	0.99	0.05	28,28,28,28	0
2	SR	C	402	1/1	0.99	0.08	31,31,31,31	0
2	SR	B	401	1/1	1.00	0.07	30,30,30,30	0
2	SR	A	403	1/1	1.00	0.05	21,21,21,21	0
2	SR	C	403	1/1	1.00	0.06	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.