



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:49 am BST

PDB ID : 2UWX  
Title : Active site restructuring regulates ligand recognition in class A penicillin-binding proteins  
Authors : Macheboeuf, P.; DiGuilmi, A.M.; Job, V.; Vernet, T.; Dideberg, O.; Dessen, A.  
Deposited on : 2007-03-23  
Resolution : 2.39 Å(reported)

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](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 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	:	2.11
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)	:	2.11

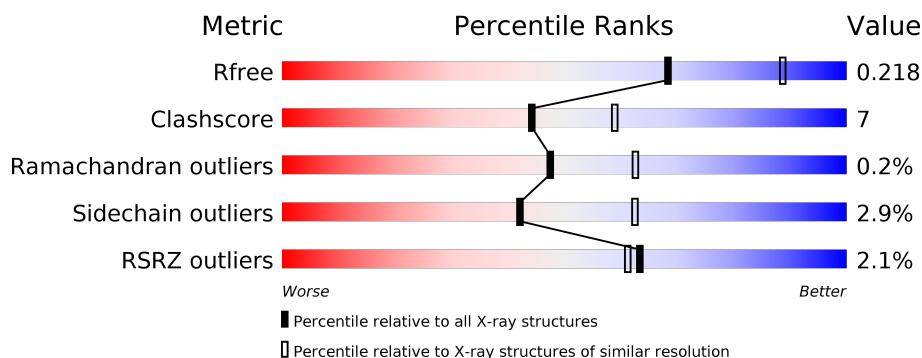
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	494	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3985 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 PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	469	3652	2285	616	734	17	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	GLN	ARG	engineered mutation	UNP Q7CRA4
A	687	GLN	ARG	engineered mutation	UNP Q7CRA4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

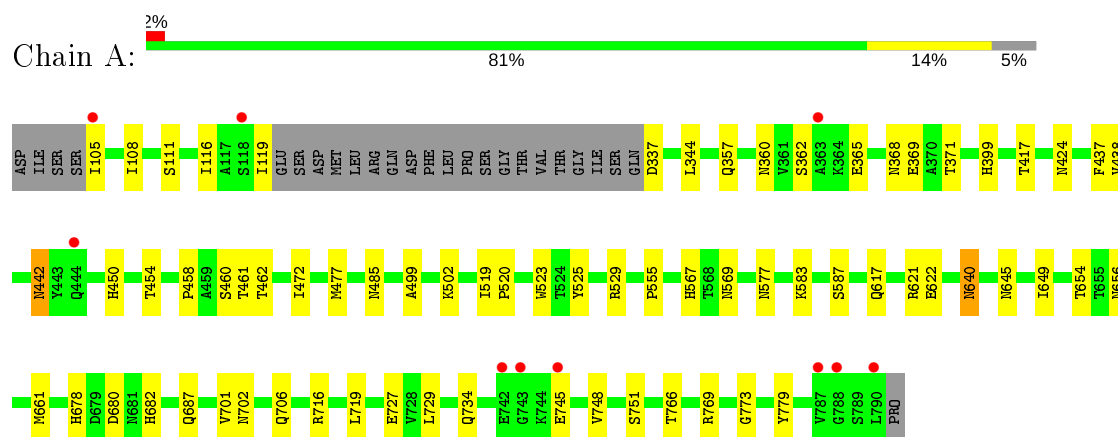
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	322	Total	O	0	0
			322	322		

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

These plots are drawn for all protein, RNA and DNA 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: PENICILLIN-BINDING PROTEIN 1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.52Å 148.65Å 98.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.39 19.96 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.65-2.39) 99.9 (19.96-2.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.162 , 0.218 0.162 , 0.218	Depositor DCC
$R_{free}$ test set	2819 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: NC1, CL, EDO, SO4

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	0.97	0/3692	0.84	2/5015 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	529	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	529	ARG	NE-CZ-NH1	7.37	123.98	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	3652	0	3479	47	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
4	A	4	0	6	1	0
5	A	322	0	0	7	0
All	All	3985	0	3485	47	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 7.

All (47) 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:680:ASP:OD1	1:A:682:HIS:HD2	1.53	0.92
1:A:569:ASN:HD21	1:A:583:LYS:H	1.33	0.77
1:A:337:ASP:HA	5:A:2006:HOH:O	1.86	0.76
1:A:460:NC1:H15	1:A:499:ALA:HA	1.72	0.70
1:A:460:NC1:H15	1:A:499:ALA:CA	2.22	0.69
1:A:461:THR:OG1	1:A:567:HIS:HE1	1.75	0.69
1:A:119:ILE:HD13	1:A:344:LEU:HD13	1.78	0.66
1:A:680:ASP:OD1	1:A:682:HIS:CD2	2.45	0.65
1:A:569:ASN:ND2	1:A:583:LYS:H	1.96	0.63
1:A:362:SER:OG	1:A:365:GLU:HG3	2.00	0.61
1:A:105:ILE:N	5:A:2001:HOH:O	2.34	0.59
1:A:108:ILE:HD11	1:A:119:ILE:HD11	1.84	0.58
1:A:640:ASN:HA	4:A:1794:EDO:H12	1.84	0.58
1:A:368:ASN:HD22	1:A:371:THR:H	1.51	0.57
1:A:460:NC1:H13	1:A:656:ASN:OD1	2.05	0.57
1:A:460:NC1:H15	1:A:499:ALA:N	2.20	0.56
1:A:485:ASN:HD22	1:A:520:PRO:HD3	1.69	0.56
1:A:417:THR:O	1:A:682:HIS:HE1	1.88	0.55
1:A:460:NC1:H15	1:A:499:ALA:H	1.72	0.55
1:A:702:ASN:O	1:A:706[B]:GLN:HG3	2.07	0.55
1:A:460:NC1:O34	1:A:687:GLN:HG2	2.07	0.54
1:A:577:ASN:ND2	1:A:617:GLN:HE22	2.06	0.53
1:A:645:ASN:O	1:A:716:ARG:NH2	2.43	0.51
1:A:424:ASN:HD22	1:A:438:VAL:HB	1.77	0.50
1:A:357:GLN:HG2	5:A:2023:HOH:O	2.13	0.49
1:A:108:ILE:HG22	1:A:116:ILE:HD12	1.94	0.48
1:A:621:ARG:HB2	1:A:649:ILE:HG22	1.95	0.48
1:A:450:HIS:HA	1:A:454:THR:OG1	2.13	0.48
1:A:745:GLU:HG2	5:A:2296:HOH:O	2.14	0.47
1:A:108:ILE:CD1	1:A:119:ILE:HD11	2.46	0.46
1:A:461:THR:OG1	1:A:567:HIS:CE1	2.63	0.46
1:A:577:ASN:HD22	1:A:617:GLN:HE22	1.63	0.46
1:A:485:ASN:HD22	1:A:519:ILE:HB	1.81	0.45
1:A:360:ASN:HB3	5:A:2027:HOH:O	2.16	0.45
1:A:525:TYR:HB2	1:A:555:PRO:HG3	1.99	0.44
1:A:734:GLN:NE2	1:A:766:THR:HA	2.33	0.44
1:A:734:GLN:HE21	1:A:766:THR:HA	1.82	0.43
1:A:654:THR:HG23	1:A:661:MET:SD	2.58	0.43
1:A:502:LYS:HE2	5:A:2135:HOH:O	2.16	0.43
1:A:458:PRO:HG2	1:A:462:THR:OG1	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:SER:HB2	5:A:2193:HOH:O	2.20	0.41
1:A:417:THR:OG1	1:A:678:HIS:HE1	2.03	0.41
1:A:399:HIS:HD2	1:A:437:PHE:H	1.69	0.41
1:A:472:ILE:HG13	1:A:477:MET:HG3	2.03	0.41
1:A:769:ARG:HA	1:A:779:TYR:CE1	2.56	0.41
1:A:523:TRP:CG	1:A:773:GLY:HA3	2.56	0.40
1:A:460:NC1:N33	1:A:687:GLN:HG2	2.36	0.40

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	467/494 (94%)	453 (97%)	13 (3%)	1 (0%)	47 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	ASN

### 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	382/408 (94%)	371 (97%)	11 (3%)	42 62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	SER
1	A	369	GLU
1	A	442	ASN
1	A	622	GLU
1	A	640	ASN
1	A	701	VAL
1	A	719	LEU
1	A	727	GLU
1	A	729	LEU
1	A	748	VAL
1	A	751	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	372	GLN
1	A	399	HIS
1	A	403	GLN
1	A	424	ASN
1	A	442	ASN
1	A	447	GLN
1	A	485	ASN
1	A	494	ASN
1	A	514	ASN
1	A	567	HIS
1	A	569	ASN
1	A	572	GLN
1	A	577	ASN
1	A	606	GLN
1	A	635	ASN
1	A	640	ASN
1	A	678	HIS
1	A	682	HIS
1	A	734	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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
1	NC1	A	460	1	35,43,44	2.55	7 (20%)	32,59,61	2.81	14 (43%)

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
1	NC1	A	460	1	-	6/24/53/55	0/2/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	NC1	O32-N30	10.44	1.40	1.22
1	A	460	NC1	C24-C25	5.91	1.50	1.41
1	A	460	NC1	OG-C7	5.86	1.45	1.33
1	A	460	NC1	C25-N30	-2.62	1.40	1.45
1	A	460	NC1	C19-C4	-2.61	1.48	1.52
1	A	460	NC1	C22-C5	2.39	1.50	1.42
1	A	460	NC1	O8-C7	2.05	1.26	1.21

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	NC1	C6-S1-C2	7.08	108.36	94.47
1	A	460	NC1	C17-C16-S15	-6.74	107.51	112.98
1	A	460	NC1	C14-C13-C11	-5.68	102.10	113.39
1	A	460	NC1	C2-N3-C4	4.46	128.81	118.32
1	A	460	NC1	C6-C5-C22	-4.08	116.53	120.47
1	A	460	NC1	C25-C24-C23	-3.96	119.90	124.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	NC1	C26-C25-C24	-3.74	119.15	123.12
1	A	460	NC1	C13-C11-N10	3.36	121.29	115.88
1	A	460	NC1	C2-C9-N10	2.87	116.31	110.02
1	A	460	NC1	O12-C11-N10	-2.63	118.51	122.95
1	A	460	NC1	OG-C7-C9	2.28	114.99	111.32
1	A	460	NC1	C28-C27-N33	-2.19	117.73	119.38
1	A	460	NC1	C23-C22-C5	-2.17	121.90	126.33
1	A	460	NC1	C28-C27-C26	2.04	122.68	120.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	460	NC1	C24-C25-N30-O32
1	A	460	NC1	C26-C25-N30-O32
1	A	460	NC1	O8-C7-OG-CB
1	A	460	NC1	C9-C7-OG-CB
1	A	460	NC1	C26-C27-N33-O35
1	A	460	NC1	C28-C27-N33-O35

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	460	NC1	7	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
2	SO4	A	1791	-	4,4,4	0.56	0	6,6,6	0.41	0
4	EDO	A	1794	-	3,3,3	0.27	0	2,2,2	1.52	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	EDO	A	1794	-	-	0/1/1/1	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1794	EDO	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	468/494 (94%)	-0.31	10 (2%) 63 61	18, 30, 59, 86	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	788	GLY	3.1
1	A	743	GLY	2.9
1	A	363	ALA	2.8
1	A	787	VAL	2.6
1	A	118	SER	2.4
1	A	444	GLN	2.4
1	A	742	GLU	2.4
1	A	105	ILE	2.3
1	A	745	GLU	2.2
1	A	790	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	NC1	A	460	41/42	0.94	0.15	21,37,46,49	18

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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
4	EDO	A	1794	4/4	0.97	0.18	36,43,44,46	0
3	CL	A	1792	1/1	0.98	0.09	41,41,41,41	0
3	CL	A	1793	1/1	0.99	0.15	32,32,32,32	1
2	SO4	A	1791	5/5	0.99	0.07	23,25,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.