



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2017 – 07:26 PM EDT

PDB ID : 2PU2  
Title : AmpC beta-lactamase with bound Phthalamide inhibitor  
Authors : Babaoglu, K.; Shoichet, B.K.  
Deposited on : unknown  
Resolution : 1.86 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

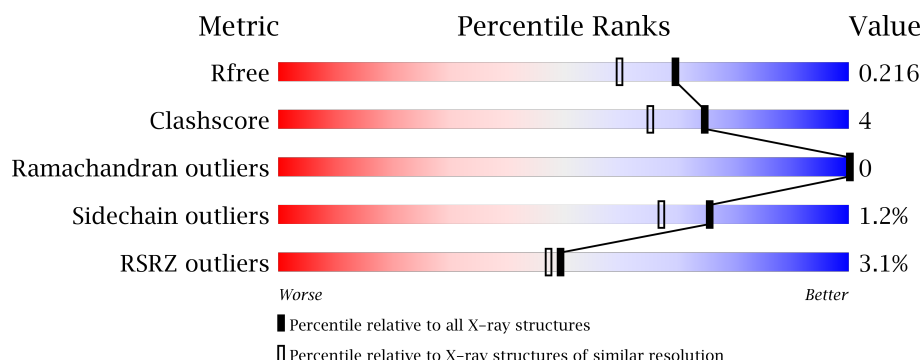
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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. 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	 3% 92% 7%
1	B	358	 4% 94% 6%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6336 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.

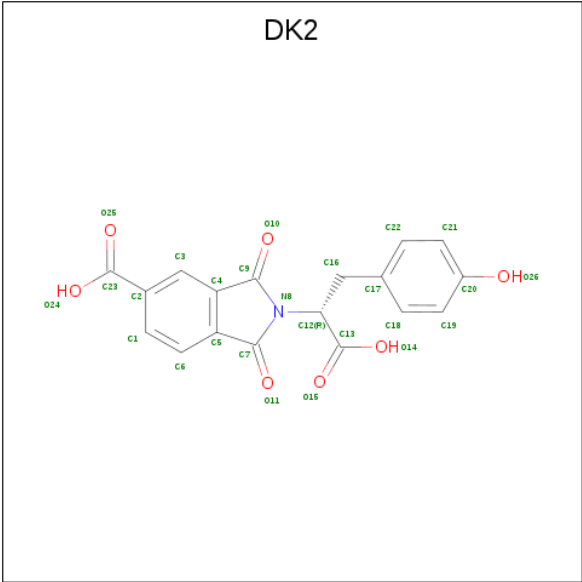
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	9	0
			2856	1842	484	524	6			
1	B	358	Total	C	N	O	S	0	9	0
			2853	1841	483	523	6			

- 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		

- Molecule 3 is 2-[(1R)-1-CARBOXY-2-(4-HYDROXYPHENYL)ETHYL]-1,3-DIOXOISOINDOLINE-5-CARBOXYLIC ACID (three-letter code: DK2) (formula: C<sub>18</sub>H<sub>13</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	B	1	Total	C	N	O	0	0
			26	18	1	7		

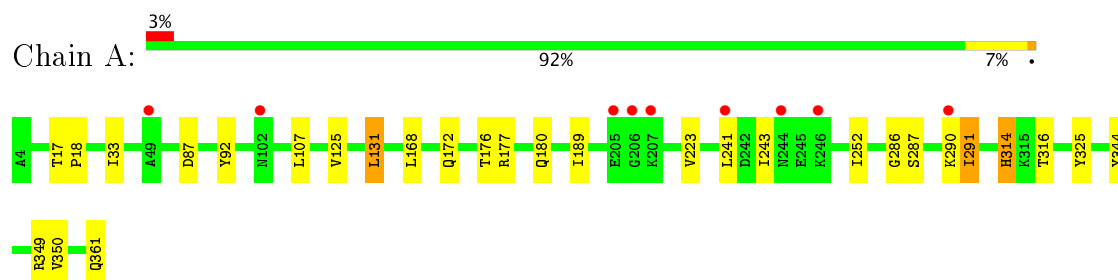
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	297	Total	O	0	0
			297	297		
4	B	273	Total	O	0	0
			273	273		

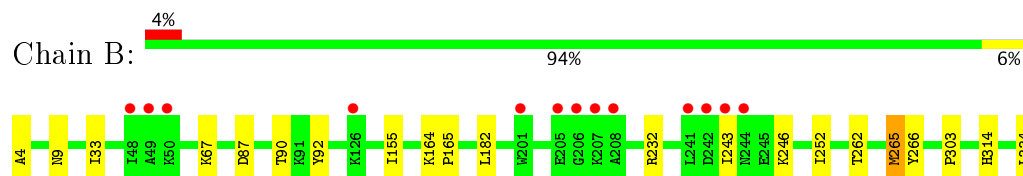
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.72Å 76.84Å 97.50Å 90.00° 115.80° 90.00°	Depositor
Resolution (Å)	30.00 – 1.86 44.80 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.86) 99.4 (44.80-1.86)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.178 , 0.212 0.182 , 0.216	Depositor DCC
$R_{free}$ test set	3326 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.97% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DK2

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	0.58	0/2957	0.65	0/4035
1	B	0.55	0/2960	0.60	0/4037
All	All	0.56	0/5917	0.63	0/8072

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	LYS	Peptide

### 5.2 Too-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 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	2856	0	2853	23	0
1	B	2853	0	2856	23	0
2	A	5	0	0	0	0
3	A	26	0	10	1	0
3	B	26	0	10	0	0
4	A	297	0	0	4	0
4	B	273	0	0	1	0
All	All	6336	0	5729	43	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.

All (43) 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:172[B]:GLN:O	1:A:176[B]:THR:HG22	1.52	1.09
1:A:286:GLY:HA2	1:A:291:ILE:HD13	1.60	0.84
1:A:87:ASP:OD2	1:A:92:TYR:OH	1.95	0.83
1:B:87:ASP:OD2	1:B:92:TYR:OH	2.05	0.74
1:A:241:LEU:HD12	1:B:246:LYS:HD3	1.75	0.68
1:B:262:THR:HG22	1:B:265:MET:HE1	1.76	0.67
1:A:176[B]:THR:HG23	1:A:177:ARG:HG3	1.76	0.66
1:B:243:ILE:CD1	1:B:252:ILE:HD12	2.25	0.66
1:B:262:THR:HG22	1:B:265:MET:CE	2.26	0.65
3:A:702:DK2:O14	4:A:999:HOH:O	2.15	0.64
1:A:243:ILE:CD1	1:A:252:ILE:HD12	2.30	0.62
1:A:125:VAL:HG11	1:A:131:LEU:HD23	1.82	0.61
1:B:243:ILE:HD12	1:B:252:ILE:HD12	1.83	0.61
1:B:262:THR:CG2	1:B:265:MET:CE	2.83	0.56
1:B:243:ILE:CD1	1:B:252:ILE:CD1	2.87	0.52
1:A:243:ILE:HD12	1:A:252:ILE:HD12	1.91	0.52
1:B:334:LEU:HG	1:B:357:LEU:HD22	1.91	0.52
1:B:262:THR:CG2	1:B:265:MET:HE2	2.41	0.51
1:B:33:ILE:HD12	1:B:33:ILE:N	2.25	0.51
1:B:262:THR:CG2	1:B:265:MET:HE1	2.41	0.50
1:A:243:ILE:CD1	1:A:252:ILE:CD1	2.90	0.50
1:B:164:LYS:HE3	4:B:893:HOH:O	2.10	0.50
1:A:344:TYR:CZ	1:A:349:ARG:HG2	2.47	0.49
1:A:33:ILE:HD12	1:A:33:ILE:N	2.28	0.49
1:A:291:ILE:HG21	4:A:916:HOH:O	2.12	0.49
1:A:241:LEU:CD1	1:B:246:LYS:HD3	2.44	0.47
1:A:241:LEU:CD1	1:B:246:LYS:CG	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HB	1:A:18:PRO:HD3	1.97	0.45
1:A:189[A]:ILE:CD1	1:A:223:VAL:HG22	2.47	0.45
1:B:4:ALA:HB3	1:B:9:ASN:OD1	2.17	0.44
1:B:182:LEU:O	1:B:232:ARG:HD3	2.18	0.43
1:A:107:LEU:HD22	1:B:303:PRO:HD3	2.00	0.42
1:A:287:SER:HB3	1:A:350:VAL:HG21	2.00	0.42
1:A:314:HIS:HE1	4:A:988:HOH:O	2.03	0.42
1:B:262:THR:HG23	1:B:265:MET:HE2	2.01	0.42
1:A:168:LEU:HD22	1:A:172[B]:GLN:HG2	2.02	0.41
1:A:316:THR:HG22	1:A:325:TYR:CD1	2.56	0.41
1:B:67[A]:LYS:HD3	1:B:155:ILE:HG21	2.01	0.41
1:A:287:SER:CB	1:A:350:VAL:HG21	2.50	0.41
1:A:180:GLN:NE2	4:A:992:HOH:O	2.53	0.41
1:B:164:LYS:HB2	1:B:165:PRO:HD3	2.03	0.41
1:B:265:MET:HG2	1:B:266:TYR:N	2.36	0.40
1:B:90:THR:O	1:B:90:THR:HG22	2.21	0.40

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	365/358 (102%)	357 (98%)	8 (2%)	0	100	100
1	B	365/358 (102%)	359 (98%)	6 (2%)	0	100	100
All	All	730/716 (102%)	716 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	301/292 (103%)	297 (99%)	4 (1%)	73	63
1	B	301/292 (103%)	298 (99%)	3 (1%)	80	74
All	All	602/584 (103%)	595 (99%)	7 (1%)	75	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	291	ILE
1	A	314	HIS
1	A	361	GLN
1	B	265	MET
1	B	314	HIS
1	B	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	13	HIS
1	A	23	GLN
1	A	35	GLN
1	A	102	ASN
1	A	137	ASN
1	A	180	GLN
1	A	358	ASN
1	A	361	GLN
1	B	22	GLN
1	B	23	GLN
1	B	52	GLN
1	B	137	ASN
1	B	175	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	A	601	-	4,4,4	0.82	0	6,6,6	0.63	0
3	DK2	A	702	-	21,28,28	1.41	4 (19%)	33,41,41	3.14	15 (45%)
3	DK2	B	701	-	21,28,28	1.37	4 (19%)	33,41,41	3.07	13 (39%)

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	PO4	A	601	-	-	0/0/0/0	0/0/0/0
3	DK2	A	702	-	-	0/8/32/32	0/3/3/3
3	DK2	B	701	-	-	0/8/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	DK2	C7-N8	-2.86	1.35	1.40
3	B	701	DK2	C7-N8	-2.85	1.35	1.40
3	B	701	DK2	C9-N8	-2.68	1.35	1.40
3	A	702	DK2	C9-N8	-2.01	1.36	1.40
3	B	701	DK2	O10-C9	2.91	1.28	1.22
3	B	701	DK2	O11-C7	3.20	1.29	1.22
3	A	702	DK2	O10-C9	3.24	1.29	1.22
3	A	702	DK2	O11-C7	3.64	1.30	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	DK2	C9-N8-C7	-7.77	103.73	111.60
3	B	701	DK2	C9-N8-C7	-7.64	103.85	111.60
3	A	702	DK2	C5-C4-C9	-5.63	103.49	108.27
3	B	701	DK2	C5-C4-C9	-4.77	104.22	108.27
3	B	701	DK2	C4-C5-C7	-4.34	104.58	108.27
3	A	702	DK2	C4-C5-C7	-3.38	105.40	108.27
3	A	702	DK2	O10-C9-C4	-3.34	122.12	128.68
3	B	701	DK2	O10-C9-C4	-3.12	122.55	128.68
3	A	702	DK2	C17-C16-C12	-3.11	108.21	113.95
3	A	702	DK2	O11-C7-C5	-3.04	122.70	128.68
3	B	701	DK2	O11-C7-C5	-3.03	122.72	128.68
3	A	702	DK2	C16-C12-N8	-2.81	108.47	112.50
3	B	701	DK2	C17-C16-C12	-2.75	108.89	113.95
3	B	701	DK2	C16-C12-N8	-2.38	109.09	112.50
3	A	702	DK2	C1-C2-C23	-2.23	117.45	120.45
3	A	702	DK2	C4-C3-C2	-2.14	117.75	121.38
3	B	701	DK2	C4-C3-C2	-2.03	117.94	121.38
3	A	702	DK2	C1-C6-C5	-2.02	117.80	121.01
3	B	701	DK2	C12-N8-C9	2.13	129.65	123.90
3	A	702	DK2	C6-C5-C7	2.24	133.12	129.65
3	A	702	DK2	C12-N8-C9	2.31	130.13	123.90
3	B	701	DK2	C6-C5-C7	2.53	133.58	129.65
3	B	701	DK2	C3-C4-C9	3.33	134.73	129.29
3	A	702	DK2	C3-C4-C9	3.66	135.28	129.29
3	A	702	DK2	C4-C9-N8	8.13	113.64	105.89
3	B	701	DK2	C4-C9-N8	8.14	113.65	105.89
3	B	701	DK2	C5-C7-N8	8.20	113.70	105.89
3	A	702	DK2	C5-C7-N8	8.24	113.74	105.89

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
3	A	702	DK2	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 ⓘ

### 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	358/358 (100%)	-0.21	9 (2%) 58 56	15, 25, 36, 44	8 (2%)
1	B	358/358 (100%)	-0.09	13 (3%) 43 41	18, 27, 40, 48	2 (0%)
All	All	716/716 (100%)	-0.15	22 (3%) 49 47	15, 26, 38, 48	10 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	LEU	5.0
1	A	206	GLY	4.3
1	B	206	GLY	4.2
1	B	205	GLU	4.1
1	B	207	LYS	4.1
1	A	205[A]	GLU	3.2
1	B	49	ALA	3.1
1	B	126	LYS	3.1
1	B	50	LYS	3.0
1	B	48	ILE	2.9
1	B	208	ALA	2.9
1	B	244	ASN	2.8
1	A	244	ASN	2.7
1	A	207[A]	LYS	2.6
1	A	241	LEU	2.5
1	B	242	ASP	2.3
1	B	201	TRP	2.3
1	A	246	LYS	2.2
1	B	243	ILE	2.2
1	A	49	ALA	2.1
1	A	290	LYS	2.1
1	A	102	ASN	2.0

## 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 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DK2	A	702	26/26	0.80	0.15	1.34	35,40,45,46	0
3	DK2	B	701	26/26	0.90	0.11	0.24	30,36,40,40	0
2	PO4	A	601	5/5	0.79	0.35	-	32,34,35,36	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.