



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:48 pm BST

PDB ID : 6G9T  
Title : CRYSTAL STRUCTURE OF CMY-136 class C BETA-LACTAMASE  
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Deposited on : 2018-04-11  
Resolution : 1.60 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.

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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 : 1.8.5 (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

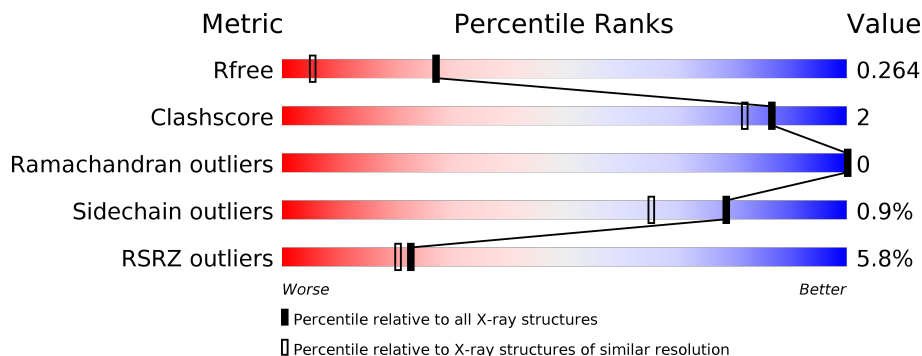
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	371	<p>2% 93% 5%</p>
1	B	371	<p>9% 91% 5%</p>

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6105 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.

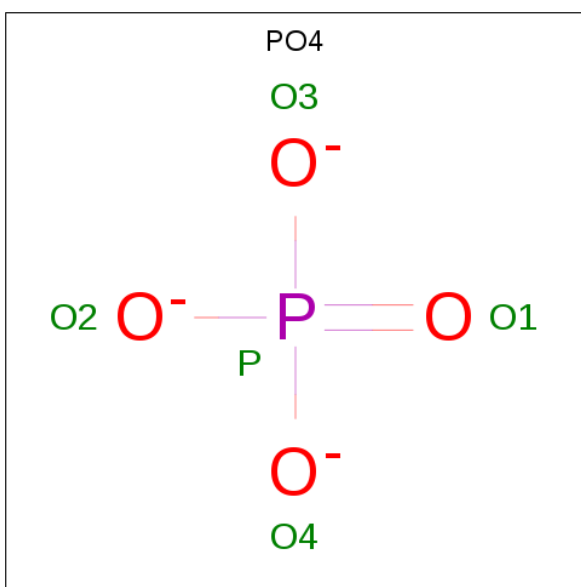
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2813	1805	489	510	9	0	2	0
1	B	359	2829	1820	489	511	9	0	5	0

There are 22 discrepancies between the modelled and reference sequences:

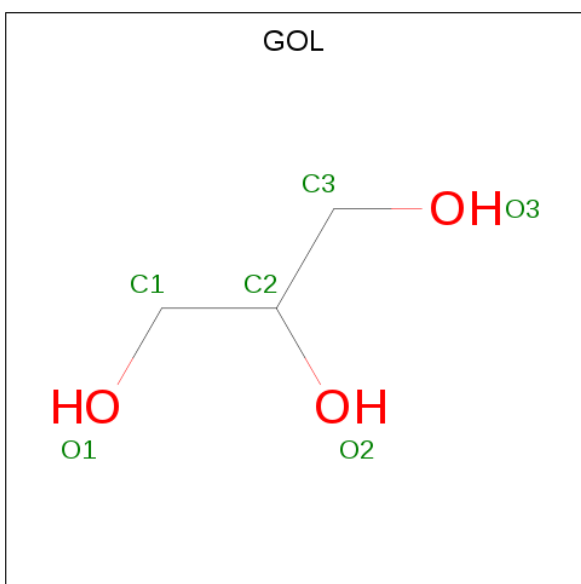
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	HIS	TYR	engineered mutation	UNP G3F7G9
A	362	PHE	-	expression tag	UNP G3F7G9
A	363	GLU	-	expression tag	UNP G3F7G9
A	364	HIS	-	expression tag	UNP G3F7G9
A	365	HIS	-	expression tag	UNP G3F7G9
A	366	HIS	-	expression tag	UNP G3F7G9
A	367	HIS	-	expression tag	UNP G3F7G9
A	368	HIS	-	expression tag	UNP G3F7G9
A	369	HIS	-	expression tag	UNP G3F7G9
A	370	HIS	-	expression tag	UNP G3F7G9
A	371	HIS	-	expression tag	UNP G3F7G9
B	221	HIS	TYR	engineered mutation	UNP G3F7G9
B	362	PHE	-	expression tag	UNP G3F7G9
B	363	GLU	-	expression tag	UNP G3F7G9
B	364	HIS	-	expression tag	UNP G3F7G9
B	365	HIS	-	expression tag	UNP G3F7G9
B	366	HIS	-	expression tag	UNP G3F7G9
B	367	HIS	-	expression tag	UNP G3F7G9
B	368	HIS	-	expression tag	UNP G3F7G9
B	369	HIS	-	expression tag	UNP G3F7G9
B	370	HIS	-	expression tag	UNP G3F7G9
B	371	HIS	-	expression tag	UNP G3F7G9

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



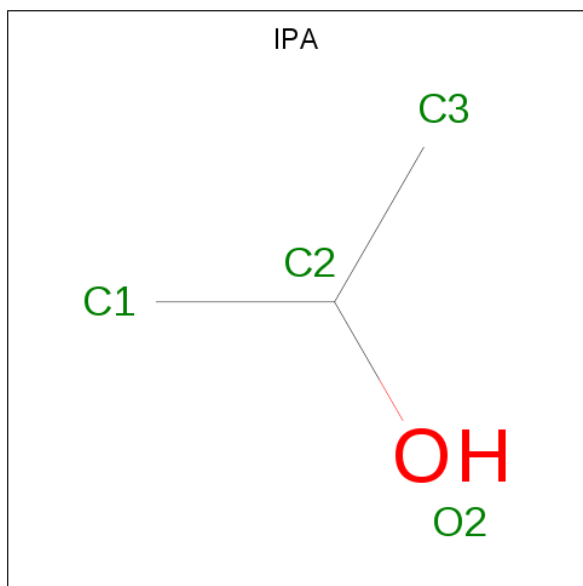
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 8 6 2	0	1
4	B	1	Total C O 4 3 1	0	0
4	B	1	Total C O 4 3 1	0	0
4	B	1	Total C O 4 3 1	0	0

- Molecule 5 is water.

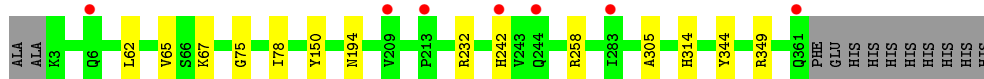
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	224	Total O 224 224	0	0
5	B	172	Total O 172 172	0	0

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

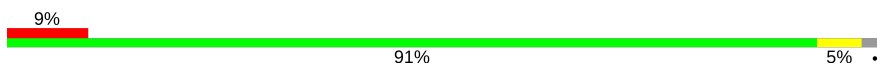
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

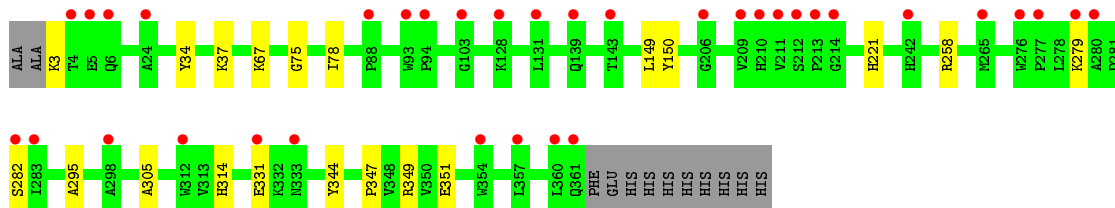
- Molecule 1: Beta-lactamase

Chain A: 



- Molecule 1: Beta-lactamase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.58Å 58.09Å 100.08Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	16.10 – 1.60 16.10 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (16.10-1.60) 94.2 (16.10-1.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 1.60Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.234 , 0.264 0.231 , 0.264	Depositor DCC
$R_{free}$ test set	4268 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l 0.014 for k,h,-l 0.369 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.58% 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: GOL, PO4, IPA

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	0.50	0/2894	0.62	0/3945
1	B	0.51	0/2920	0.64	0/3981
All	All	0.51	0/5814	0.63	0/7926

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2813	0	2793	9	0
1	B	2829	0	2825	14	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
4	A	12	0	24	0	0
4	B	12	0	24	2	0
5	A	224	0	0	1	0
5	B	172	0	0	4	0
All	All	6105	0	5690	24	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 2.

All (24) 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:67:LYS:NZ	1:A:150:TYR:HE1	1.74	0.85
1:A:67:LYS:NZ	1:A:150:TYR:CE1	2.46	0.83
1:A:67:LYS:HZ3	1:A:150:TYR:HE1	1.26	0.78
1:B:347:PRO:O	1:B:351:GLU:HG3	1.88	0.73
1:B:67:LYS:NZ	1:B:150:TYR:HE1	1.87	0.72
1:B:67:LYS:NZ	1:B:150:TYR:CE1	2.59	0.71
1:B:67:LYS:HZ3	1:B:150:TYR:HE1	1.44	0.66
4:B:405:IPA:H13	5:B:546:HOH:O	1.99	0.63
1:B:279:LYS:HG3	1:B:282:SER:HB2	1.91	0.53
1:A:194:ASN:HB2	5:A:705:HOH:O	2.12	0.48
1:A:344:TYR:CE2	1:A:349:ARG:HG2	2.49	0.48
1:B:3:LYS:N	1:B:34:TYR:HH	2.11	0.48
1:B:344:TYR:CE2	1:B:349:ARG:HG2	2.49	0.47
1:A:232:ARG:HH22	1:B:37:LYS:HE3	1.80	0.47
1:B:75:GLY:HA2	1:B:78:ILE:HD12	1.97	0.47
1:A:62:LEU:HB3	1:A:65:VAL:HB	1.99	0.44
1:A:258:ARG:HB2	1:A:305:ALA:HB3	1.99	0.44
4:B:405:IPA:H2	5:B:582:HOH:O	2.18	0.43
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.99	0.43
1:B:258:ARG:HB2	1:B:305:ALA:HB3	2.00	0.43
1:B:67:LYS:HZ1	1:B:150:TYR:HE1	1.64	0.42
1:B:279:LYS:HE3	5:B:583:HOH:O	2.19	0.41
1:B:279:LYS:HB3	5:B:671:HOH:O	2.19	0.41
1:B:149:LEU:HD13	1:B:295:ALA:HB2	2.01	0.41

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	359/371 (97%)	354 (99%)	5 (1%)	0	100	100
1	B	361/371 (97%)	356 (99%)	5 (1%)	0	100	100
All	All	720/742 (97%)	710 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	292/301 (97%)	289 (99%)	3 (1%)	76	61
1	B	295/301 (98%)	292 (99%)	3 (1%)	76	61
All	All	587/602 (98%)	581 (99%)	6 (1%)	78	61

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242[A]	HIS
1	A	242[B]	HIS
1	A	314	HIS
1	B	221	HIS
1	B	314	HIS
1	B	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

14 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	402	-	4,4,4	1.81	0	6,6,6	0.75	0
4	IPA	B	405	-	3,3,3	0.80	0	3,3,3	0.31	0
4	IPA	A	405	-	3,3,3	0.66	0	3,3,3	0.51	0
2	PO4	A	401	-	4,4,4	1.80	1 (25%)	6,6,6	0.87	0
2	PO4	B	401	-	4,4,4	2.62	2 (50%)	6,6,6	0.75	0
4	IPA	A	406[B]	-	3,3,3	0.66	0	3,3,3	0.48	0
3	GOL	A	404	-	5,5,5	0.13	0	5,5,5	0.42	0
2	PO4	A	403	-	4,4,4	2.49	1 (25%)	6,6,6	0.77	0
2	PO4	B	402	-	4,4,4	1.89	0	6,6,6	0.40	0
3	GOL	B	404	-	5,5,5	0.09	0	5,5,5	0.35	0
4	IPA	B	407	-	3,3,3	0.72	0	3,3,3	0.57	0
4	IPA	A	406[A]	-	3,3,3	0.59	0	3,3,3	0.50	0
3	GOL	B	403	-	5,5,5	0.10	0	5,5,5	0.54	0
4	IPA	B	406	-	3,3,3	0.56	0	3,3,3	0.59	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
3	GOL	B	403	-	-	1/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PO4	P-O1	4.19	1.60	1.50
2	A	403	PO4	P-O1	4.16	1.60	1.50
2	A	401	PO4	P-O4	2.10	1.60	1.54
2	B	401	PO4	P-O2	2.06	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-C3
3	B	404	GOL	O2-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	405	IPA	2	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	359/371 (96%)	0.29	7 (1%) 66 65	8, 15, 34, 65	0
1	B	359/371 (96%)	0.87	35 (9%) 7 6	11, 18, 35, 75	0
All	All	718/742 (96%)	0.58	42 (5%) 23 20	8, 17, 35, 75	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242[A]	HIS	5.7
1	B	211	VAL	5.6
1	B	354	TRP	5.1
1	B	242	HIS	4.7
1	B	209	VAL	4.7
1	B	276[A]	TRP	4.5
1	B	280	ALA	4.4
1	B	139	GLN	3.7
1	B	277	PRO	3.4
1	B	282	SER	3.2
1	B	361	GLN	3.1
1	B	5	GLU	3.0
1	B	128	LYS	3.0
1	B	312	TRP	3.0
1	B	212	SER	2.9
1	B	6	GLN	2.8
1	B	131	LEU	2.8
1	A	6	GLN	2.7
1	B	360	LEU	2.6
1	A	244	GLN	2.5
1	B	279	LYS	2.5
1	B	93	TRP	2.5
1	B	24	ALA	2.4
1	B	103	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	209	VAL	2.3
1	B	283	ILE	2.3
1	B	331	GLU	2.3
1	A	283	ILE	2.3
1	B	94	PRO	2.2
1	B	4	THR	2.2
1	A	361	GLN	2.2
1	B	213	PRO	2.1
1	B	333	ASN	2.1
1	B	214	GLY	2.1
1	B	265	MET	2.1
1	B	88	PRO	2.1
1	B	357	LEU	2.1
1	B	210	HIS	2.1
1	B	298	ALA	2.1
1	B	206	GLY	2.0
1	B	143	THR	2.0
1	A	213	PRO	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. 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
2	PO4	A	402	5/5	0.57	0.19	40,42,43,44	0
4	IPA	A	405	4/4	0.74	0.18	35,35,35,35	0
4	IPA	B	405	4/4	0.78	0.19	21,22,24,25	0
4	IPA	A	406[B]	4/4	0.79	0.23	24,24,25,25	4
4	IPA	A	406[A]	4/4	0.79	0.23	20,20,20,20	4

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Atoms</b>	<b>RSCC</b>	<b>RSR</b>	<b>B-factors(Å<sup>2</sup>)</b>	<b>Q&lt;0.9</b>
3	GOL	B	403	6/6	0.83	0.15	15,17,21,23	0
2	PO4	B	402	5/5	0.84	0.23	54,56,56,57	0
4	IPA	B	406	4/4	0.84	0.18	31,31,32,33	0
4	IPA	B	407	4/4	0.87	0.15	20,21,23,29	0
3	GOL	B	404	6/6	0.87	0.13	26,30,32,33	0
2	PO4	A	403	5/5	0.89	0.12	39,39,40,41	0
3	GOL	A	404	6/6	0.91	0.14	14,18,19,23	0
2	PO4	B	401	5/5	0.93	0.11	18,24,26,29	0
2	PO4	A	401	5/5	0.95	0.09	14,20,23,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.