



# Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2019 – 12:15 AM EDT

PDB ID : 4C4X  
Title : Crystal structure of human bifunctional epoxide hydroxylase 2 complexed with C9  
Authors : Pilger, J.; Mazur, A.; Monecke, P.; Schreuder, H.; Elshorst, B.; Langer, T.; Schiffer, A.; Krimm, I.; Wegstroth, M.; Lee, D.; Hessler, G.; Wendt, K.-U.; Becker, S.; Griesinger, C.  
Deposited on : 2013-09-09  
Resolution : 2.17 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

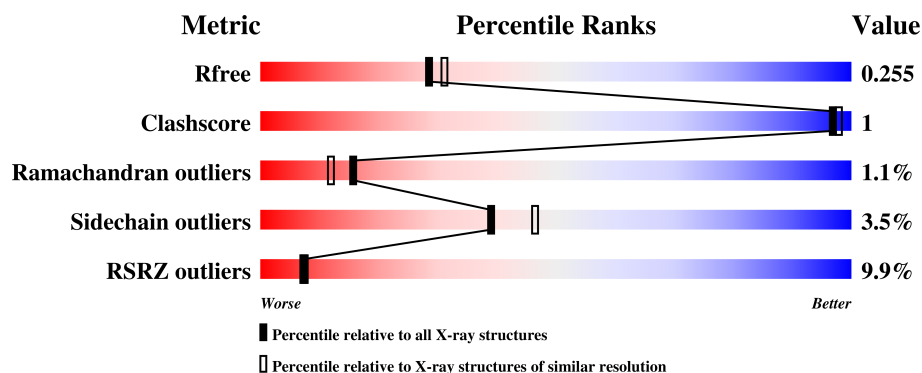
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	111664	6027 (2.20-2.16)
Clashscore	122126	6837 (2.20-2.16)
Ramachandran outliers	120053	6731 (2.20-2.16)
Sidechain outliers	120020	6731 (2.20-2.16)
RSRZ outliers	108989	5899 (2.20-2.16)

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	326	<div> <div>10%</div> <div>90%</div> <div>5% . .</div> </div>
1	B	326	<div> <div>9%</div> <div>91%</div> <div>5% .</div> </div>

## 2 Entry composition [i](#)

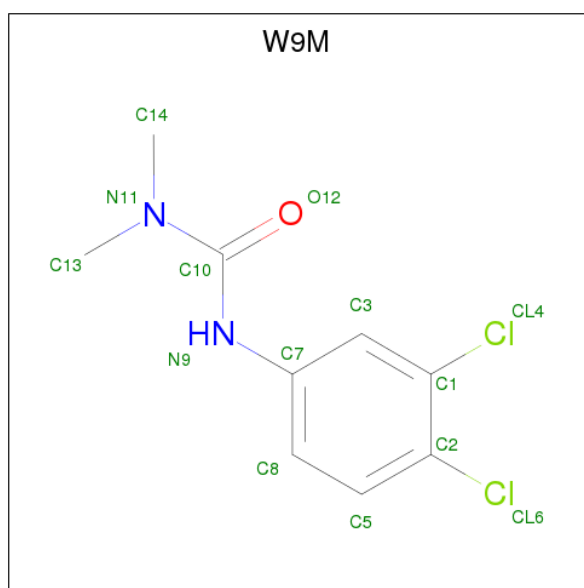
There are 3 unique types of molecules in this entry. The entry contains 5562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIFUNCTIONAL EPOXIDE HYDROLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2528	1626	425	455	22			
1	B	314	Total	C	N	O	S	0	0	0
			2533	1629	426	456	22			

- Molecule 2 is 3-(3,4-dichlorophenyl)-1,1-dimethyl-urea (three-letter code: W9M) (formula:  $C_9H_{10}Cl_2N_2O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	1
			28	18	4	4	2		
2	B	1	Total	C	Cl	N	O	0	1
			28	18	4	4	2		

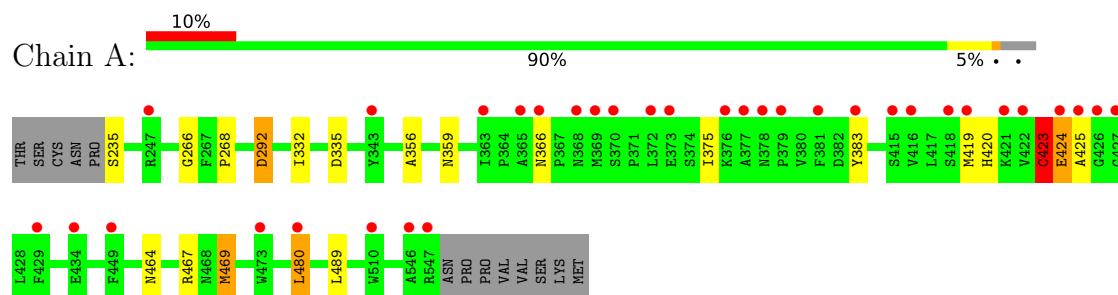
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total 232	O 232	0	0
3	B	213	Total 213	O 213	0	0

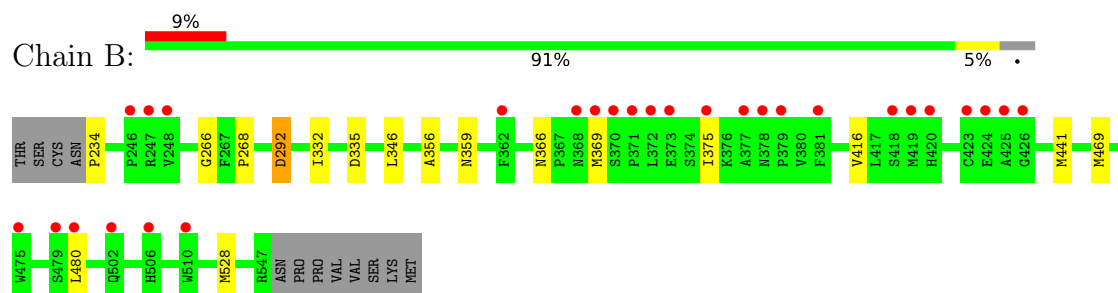
### 3 Residue-property plots [i](#)

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: BIFUNCTIONAL EPOXIDE HYDROLASE 2



#### • Molecule 1: BIFUNCTIONAL EPOXIDE HYDROLASE 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.69Å 79.87Å 88.61Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	29.63 – 2.17 44.30 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.63-2.17) 98.5 (44.30-2.17)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.211 , 0.242 0.219 , 0.255	Depositor DCC
$R_{free}$ test set	2528 reflections (7.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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: W9M

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	0.37	0/2603	0.60	2/3529 (0.1%)
1	B	0.37	0/2608	0.59	2/3536 (0.1%)
All	All	0.37	0/5211	0.60	4/7065 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	PRO	N-CA-CB	5.91	110.39	103.30
1	A	423	CYS	C-N-CA	5.75	136.07	121.70
1	B	292	ASP	N-CA-C	-5.35	96.56	111.00
1	A	292	ASP	N-CA-C	-5.32	96.64	111.00

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	2528	0	2461	7	0
1	B	2533	0	2463	3	0
2	A	28	0	20	2	0
2	B	28	0	20	1	0
3	A	232	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	213	0	0	0	0
All	All	5562	0	4964	10	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 1.

All (10) 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:B:266:GLY:HA3	1:B:335:ASP:HB3	1.75	0.68
1:A:383:TYR:HH	2:A:1548[A]:W9M:H3	1.65	0.61
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.81	0.61
1:A:332:ILE:HG12	1:A:356:ALA:HB3	1.89	0.54
1:B:332:ILE:HG12	1:B:356:ALA:HB3	1.91	0.52
1:B:335:ASP:OD1	2:B:1548[B]:W9M:H3	2.10	0.51
1:A:335:ASP:OD1	2:A:1548[B]:W9M:H3	2.19	0.43
1:A:464:ASN:HA	1:A:467:ARG:HD2	2.01	0.42
1:A:423:CYS:HA	1:A:424:GLU:O	2.20	0.42
1:A:375:ILE:HD11	1:A:469:MET:HG2	2.01	0.41

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	311/326 (95%)	293 (94%)	13 (4%)	5 (2%)	11	7
1	B	312/326 (96%)	296 (95%)	14 (4%)	2 (1%)	27	25
All	All	623/652 (96%)	589 (94%)	27 (4%)	7 (1%)	16	12

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	424	GLU
1	A	425	ALA
1	A	480	LEU
1	B	480	LEU
1	A	423	CYS
1	A	268	PRO
1	B	268	PRO

### 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	274/287 (96%)	265 (97%)	9 (3%)	41	49
1	B	274/287 (96%)	264 (96%)	10 (4%)	38	45
All	All	548/574 (96%)	529 (96%)	19 (4%)	39	46

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	SER
1	A	292	ASP
1	A	359	ASN
1	A	366	ASN
1	A	419	MET
1	A	420	HIS
1	A	469	MET
1	A	480	LEU
1	A	489	LEU
1	B	292	ASP
1	B	346	LEU
1	B	359	ASN
1	B	366	ASN
1	B	369	MET
1	B	375	ILE
1	B	416	VAL
1	B	441	MET

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Mol	Chain	Res	Type
1	B	469	MET
1	B	528	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	ASN
1	A	518	HIS
1	B	366	ASN
1	B	505	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	W9M	A	1548[A]	-	14,14,14	1.79	1 (7%)	19,19,19	1.04	2 (10%)
2	W9M	A	1548[B]	-	14,14,14	1.79	1 (7%)	19,19,19	1.36	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	W9M	B	1548[A]	-	14,14,14	1.81	1 (7%)	19,19,19	1.03	2 (10%)
2	W9M	B	1548[B]	-	14,14,14	1.82	1 (7%)	19,19,19	1.22	2 (10%)

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	W9M	A	1548[A]	-	-	0/8/8/8	0/1/1/1
2	W9M	A	1548[B]	-	-	0/8/8/8	0/1/1/1
2	W9M	B	1548[A]	-	-	0/8/8/8	0/1/1/1
2	W9M	B	1548[B]	-	-	0/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1548[A]	W9M	C10-N11	6.67	1.46	1.35
2	A	1548[B]	W9M	C10-N11	6.68	1.46	1.35
2	B	1548[A]	W9M	C10-N11	6.76	1.46	1.35
2	B	1548[B]	W9M	C10-N11	6.78	1.46	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1548[B]	W9M	O12-C10-N11	-3.19	117.09	122.19
2	B	1548[B]	W9M	O12-C10-N11	-2.98	117.42	122.19
2	A	1548[A]	W9M	O12-C10-N11	-2.78	117.75	122.19
2	B	1548[A]	W9M	O12-C10-N11	-2.76	117.78	122.19
2	B	1548[A]	W9M	N9-C10-N11	3.29	117.94	115.66
2	A	1548[A]	W9M	N9-C10-N11	3.36	117.99	115.66
2	B	1548[B]	W9M	N9-C10-N11	4.26	118.61	115.66
2	A	1548[B]	W9M	N9-C10-N11	4.86	119.03	115.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1548[A]	W9M	1	0
2	A	1548[B]	W9M	1	0
2	B	1548[B]	W9M	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	313/326 (96%)	0.51	34 (10%) 5 5	20, 33, 71, 88	0
1	B	314/326 (96%)	0.47	28 (8%) 9 10	19, 33, 70, 87	0
All	All	627/652 (96%)	0.49	62 (9%) 7 7	19, 33, 71, 88	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	MET	8.4
1	B	418	SER	5.5
1	B	368	ASN	5.3
1	A	372	LEU	5.2
1	B	370	SER	5.1
1	B	377	ALA	5.0
1	A	510	TRP	4.9
1	B	426	GLY	4.9
1	A	418	SER	4.7
1	B	369	MET	4.7
1	A	426	GLY	4.6
1	A	424	GLU	4.4
1	A	416	VAL	4.2
1	A	247	ARG	4.2
1	B	379	PRO	4.0
1	A	425	ALA	3.8
1	B	419	MET	3.7
1	B	372	LEU	3.6
1	B	480	LEU	3.6
1	A	373	GLU	3.5
1	B	510	TRP	3.5
1	B	373	GLU	3.3
1	B	378	ASN	3.3
1	A	383	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	246	PRO	3.2
1	B	424	GLU	3.2
1	A	376	LYS	3.2
1	B	425	ALA	3.1
1	A	379	PRO	3.0
1	A	343	TYR	2.9
1	B	375	ILE	2.9
1	B	502	GLN	2.9
1	A	480	LEU	2.8
1	A	381	PHE	2.8
1	B	506	HIS	2.8
1	A	429	PHE	2.8
1	A	365	ALA	2.7
1	B	420	HIS	2.6
1	A	378	ASN	2.6
1	A	377	ALA	2.6
1	A	546	ALA	2.5
1	A	415	SER	2.5
1	A	370	SER	2.4
1	A	421	LYS	2.4
1	B	423	CYS	2.4
1	A	422	VAL	2.4
1	B	248	VAL	2.4
1	A	369	MET	2.4
1	A	434	GLU	2.4
1	A	473	TRP	2.4
1	B	371	PRO	2.3
1	B	381	PHE	2.3
1	B	362	PHE	2.2
1	A	363	ILE	2.2
1	A	449	PHE	2.2
1	B	475	TRP	2.1
1	A	368	ASN	2.1
1	B	479	SER	2.1
1	A	366	ASN	2.1
1	B	247	ARG	2.1
1	A	427	GLY	2.1
1	A	547	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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( $\text{\AA}^2$ )	Q<0.9
2	W9M	A	1548[B]	14/14	0.81	0.24	72,73,73,73	14
2	W9M	A	1548[A]	14/14	0.81	0.24	62,62,63,63	14
2	W9M	B	1548[B]	14/14	0.84	0.28	76,76,76,76	14
2	W9M	B	1548[A]	14/14	0.84	0.28	69,70,70,71	14

### 6.5 Other polymers [i](#)

There are no such residues in this entry.